



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 12:51 PM JST

PDB ID : 9VPC / pdb_00009vpc
EMDB ID : EMD-65238
Title : Cryo-EM structure of the IF1 bound bovine ATP synthase tetramer
Authors : Nakano, A.; Jiko, C.; Yamashita, E.; Yokoyama, K.; Gerle, C.
Deposited on : 2025-07-03
Resolution : 7.20 Å(reported)
Based on initial model : 7AJD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

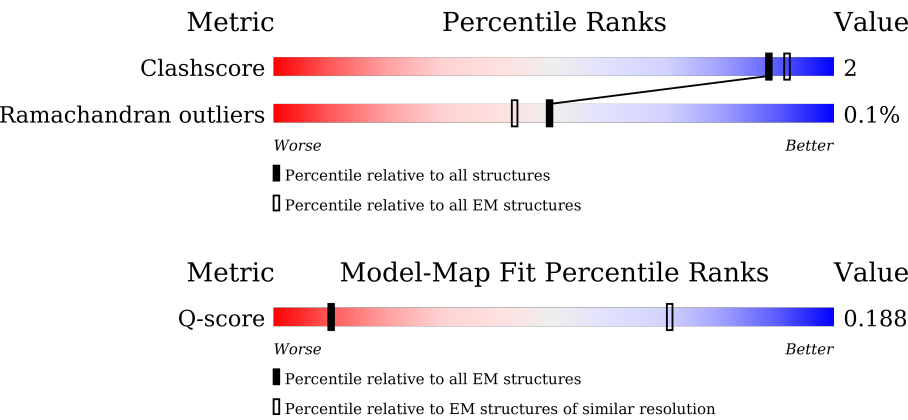
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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.



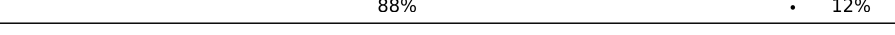
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	444 (6.70 - 7.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	18	66	62% 38%
1	28	66	62% 38%
1	38	66	62% 38%
1	48	66	62% 38%
2	1A	553	90% 8%
2	1B	553	83% 14%

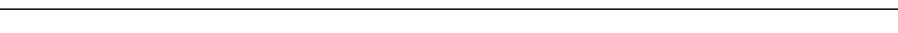
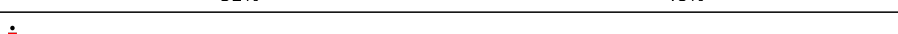
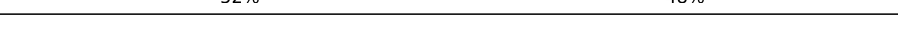
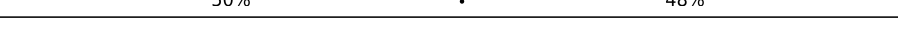
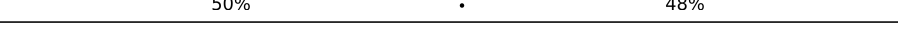
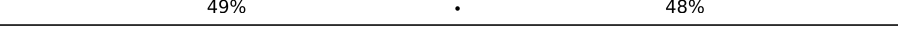
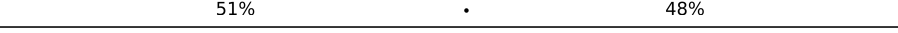
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Mol	Chain	Length	Quality of chain
2	1C	553	 88% 10%
2	2A	553	 91% 8%
2	2B	553	 86% 14%
2	2C	553	 90% 10%
2	3A	553	 90% 8%
2	3B	553	 83% 14%
2	3C	553	 88% 10%
2	4A	553	 91% 8%
2	4B	553	 85% 14%
2	4C	553	 89% 10%
3	1D	528	 88% 11%
3	1E	528	 88% 12%
3	1F	528	 88% 12%
3	2D	528	 88% 11%
3	2E	528	 87% 12%
3	2F	528	 88% 12%
3	3D	528	 88% 11%
3	3E	528	 88% 12%
3	3F	528	 88% 12%
3	4D	528	 88% 11%
3	4E	528	 87% 12%
3	4F	528	 88% 12%
4	1G	298	 91% 9%
4	2G	298	 91% 9%
4	3G	298	 91% 9%

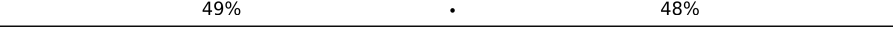
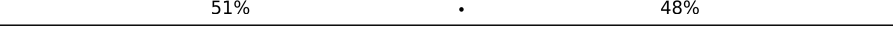
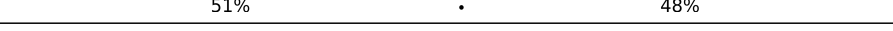
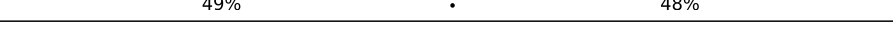
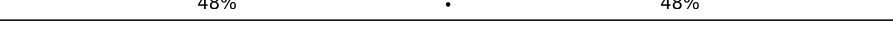
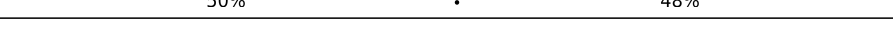
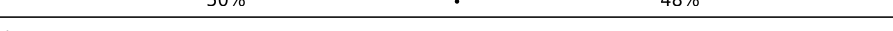
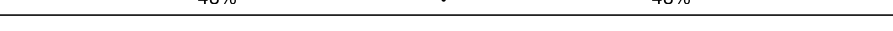
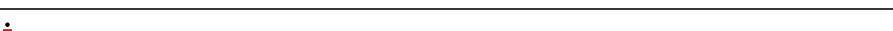
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Mol	Chain	Length	Quality of chain
4	4G	298	
5	1H	168	
5	2H	168	
5	3H	168	
5	4H	168	
6	1I	51	
6	2I	51	
6	3I	51	
6	4I	51	
7	1J	109	
7	2J	109	
7	3J	109	
7	4J	109	
8	1K	143	
8	1L	143	
8	1M	143	
8	1N	143	
8	1O	143	
8	1P	143	
8	1Q	143	
8	1R	143	
8	2K	143	
8	2L	143	
8	2M	143	
8	2N	143	

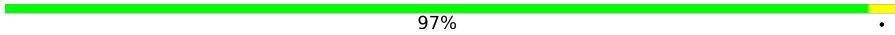
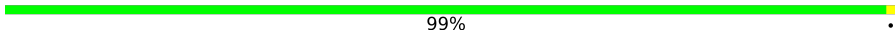
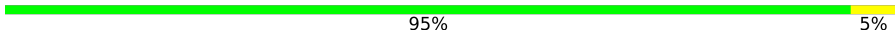
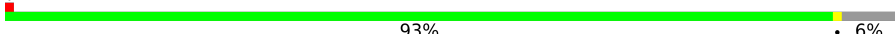
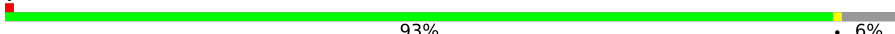
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Mol	Chain	Length	Quality of chain
8	2O	143	
8	2P	143	
8	2Q	143	
8	2R	143	
8	3K	143	
8	3L	143	
8	3M	143	
8	3N	143	
8	3O	143	
8	3P	143	
8	3Q	143	
8	3R	143	
8	4K	143	
8	4L	143	
8	4M	143	
8	4N	143	
8	4O	143	
8	4P	143	
8	4Q	143	
8	4R	143	
9	1S	213	
9	2S	213	
9	3S	213	
9	4S	213	
10	1a	226	

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Mol	Chain	Length	Quality of chain
10	2a	226	 97% .
10	3a	226	 99% .
10	4a	226	 95% 5%
11	1b	256	 79% . 18%
11	2b	256	 80% . 18%
11	3b	256	 78% . 18%
11	4b	256	 80% . 18%
12	1d	161	 91% 5% .
12	2d	161	 15% 81% 15% .
12	3d	161	 91% 6% .
12	4d	161	 16% 81% 16% .
13	1e	71	 77% . 21%
13	2e	71	 75% . 21%
13	3e	71	 77% . 21%
13	4e	71	 75% . 21%
14	1f	88	 90% 5% 6%
14	2f	88	 93% . 6%
14	3f	88	 90% 5% 6%
14	4f	88	 93% . 6%
15	1g	103	 72% 5% 23%
15	2g	103	 72% 5% 23%
15	3g	103	 72% 5% 23%
15	4g	103	 72% 5% 23%
16	1h	108	 39% . 59%
16	2h	108	 44% 56%

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Mol	Chain	Length	Quality of chain
16	3h	108	
16	4h	108	
17	1j	60	
17	2j	60	
17	3j	60	
17	4j	60	
18	1k	58	
18	2k	58	
18	3k	58	
18	4k	58	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 101921 atoms, of which 594 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP synthase F(0) complex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	18	41	Total	C	N	O	0	0
			205	123	41	41		
1	28	41	Total	C	N	O	0	0
			205	123	41	41		
1	38	41	Total	C	N	O	0	0
			205	123	41	41		
1	48	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1A	508	Total	C	N	O	0	0
			2491	1475	508	508		
2	1B	477	Total	C	N	O	0	0
			2339	1385	477	477		
2	1C	498	Total	C	N	O	0	0
			2443	1447	498	498		
2	2A	508	Total	C	N	O	0	0
			2491	1475	508	508		
2	2B	477	Total	C	N	O	0	0
			2339	1385	477	477		
2	2C	498	Total	C	N	O	0	0
			2443	1447	498	498		
2	3A	508	Total	C	N	O	0	0
			2491	1475	508	508		
2	3B	477	Total	C	N	O	0	0
			2339	1385	477	477		
2	3C	498	Total	C	N	O	0	0
			2443	1447	498	498		
2	4A	508	Total	C	N	O	0	0
			2491	1475	508	508		
2	4B	477	Total	C	N	O	0	0
			2339	1385	477	477		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	4C	498	Total	C	N	O	0	0
			2443	1447	498	498		

- Molecule 3 is a protein called ATP synthase F(1) complex catalytic subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1D	469	Total	C	N	O	0	0
			2300	1362	469	469		
3	1E	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	1F	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	2D	469	Total	C	N	O	0	0
			2300	1362	469	469		
3	2E	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	2F	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	3D	469	Total	C	N	O	0	0
			2300	1362	469	469		
3	3E	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	3F	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	4D	469	Total	C	N	O	0	0
			2300	1362	469	469		
3	4E	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	4F	467	Total	C	N	O	0	0
			2290	1356	467	467		

- Molecule 4 is a protein called ATP synthase F(1) complex subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1G	272	Total	C	N	O	0	0
			1347	803	272	272		
4	2G	272	Total	C	N	O	0	0
			1347	803	272	272		
4	3G	272	Total	C	N	O	0	0
			1347	803	272	272		
4	4G	272	Total	C	N	O	0	0
			1347	803	272	272		

- Molecule 5 is a protein called ATP synthase F(1) complex subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1H	132	Total	C	N	O	0	0
			653	389	132	132		
5	2H	132	Total	C	N	O	0	0
			653	389	132	132		
5	3H	132	Total	C	N	O	0	0
			653	389	132	132		
5	4H	132	Total	C	N	O	0	0
			653	389	132	132		

- Molecule 6 is a protein called ATP synthase F(1) complex subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1I	47	Total	C	N	O	0	0
			233	139	47	47		
6	2I	47	Total	C	N	O	0	0
			233	139	47	47		
6	3I	47	Total	C	N	O	0	0
			233	139	47	47		
6	4I	47	Total	C	N	O	0	0
			233	139	47	47		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	1J	56	Total	C	N	O	0	0
			278	166	56	56		
7	2J	53	Total	C	N	O	0	0
			264	158	53	53		
7	3J	56	Total	C	N	O	0	0
			279	167	56	56		
7	4J	53	Total	C	N	O	0	0
			264	158	53	53		

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1K	74	Total	C	N	O	0	0
			359	211	74	74		
8	1L	74	Total	C	N	O	0	0
			359	211	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	1M	75	Total 364	C 214	N 75	O 75	0	0
8	1N	75	Total 364	C 214	N 75	O 75	0	0
8	1O	75	Total 364	C 214	N 75	O 75	0	0
8	1P	74	Total 359	C 211	N 74	O 74	0	0
8	1Q	75	Total 364	C 214	N 75	O 75	0	0
8	1R	75	Total 364	C 214	N 75	O 75	0	0
8	2K	74	Total 359	C 211	N 74	O 74	0	0
8	2L	74	Total 359	C 211	N 74	O 74	0	0
8	2M	75	Total 364	C 214	N 75	O 75	0	0
8	2N	75	Total 364	C 214	N 75	O 75	0	0
8	2O	75	Total 364	C 214	N 75	O 75	0	0
8	2P	74	Total 359	C 211	N 74	O 74	0	0
8	2Q	75	Total 364	C 214	N 75	O 75	0	0
8	2R	75	Total 364	C 214	N 75	O 75	0	0
8	3K	74	Total 359	C 211	N 74	O 74	0	0
8	3L	74	Total 359	C 211	N 74	O 74	0	0
8	3M	75	Total 364	C 214	N 75	O 75	0	0
8	3N	75	Total 364	C 214	N 75	O 75	0	0
8	3O	75	Total 364	C 214	N 75	O 75	0	0
8	3P	74	Total 359	C 211	N 74	O 74	0	0
8	3Q	75	Total 364	C 214	N 75	O 75	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	3R	75	Total	C	N	O	0	0
			364	214	75	75		
8	4K	74	Total	C	N	O	0	0
			359	211	74	74		
8	4L	74	Total	C	N	O	0	0
			359	211	74	74		
8	4M	75	Total	C	N	O	0	0
			364	214	75	75		
8	4N	75	Total	C	N	O	0	0
			364	214	75	75		
8	4O	75	Total	C	N	O	0	0
			364	214	75	75		
8	4P	74	Total	C	N	O	0	0
			359	211	74	74		
8	4Q	75	Total	C	N	O	0	0
			364	214	75	75		
8	4R	75	Total	C	N	O	0	0
			364	214	75	75		

- Molecule 9 is a protein called ATP synthase peripheral stalk subunit OSCP, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	1S	188	Total	C	N	O	0	0
			931	555	188	188		
9	2S	188	Total	C	N	O	0	0
			931	555	188	188		
9	3S	188	Total	C	N	O	0	0
			931	555	188	188		
9	4S	188	Total	C	N	O	0	0
			931	555	188	188		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1a	226	Total	C	N	O	0	0
			1119	667	226	226		
10	2a	226	Total	C	N	O	0	0
			1119	667	226	226		
10	3a	226	Total	C	N	O	0	0
			1119	667	226	226		
10	4a	226	Total	C	N	O	0	0
			1119	667	226	226		

- Molecule 11 is a protein called ATP synthase peripheral stalk subunit b, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	1b	209	Total	C	N	O	0	0
			1035	617	209	209		
11	2b	209	Total	C	N	O	0	0
			1035	617	209	209		
11	3b	209	Total	C	N	O	0	0
			1035	617	209	209		
11	4b	209	Total	C	N	O	0	0
			1035	617	209	209		

- Molecule 12 is a protein called ATP synthase peripheral stalk subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1d	155	Total	C	H	N	O	0	0
			1070	463	297	155	155		
12	2d	155	Total	C	N	O		0	0
			773	463	155	155			
12	3d	155	Total	C	H	N	O	0	0
			1070	463	297	155	155		
12	4d	155	Total	C	N	O		0	0
			773	463	155	155			

- Molecule 13 is a protein called ATP synthase F(0) complex subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	1e	56	Total	C	N	O	0	0
			277	165	56	56		
13	2e	56	Total	C	N	O	0	0
			277	165	56	56		
13	3e	56	Total	C	N	O	0	0
			277	165	56	56		
13	4e	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 14 is a protein called ATP synthase F(0) complex subunit f, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1f	83	Total	C	N	O	0	0
			409	243	83	83		
14	2f	83	Total	C	N	O	0	0
			409	243	83	83		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	3f	83	Total	C	N	O	0	0
			409	243	83	83		
14	4f	83	Total	C	N	O	0	0
			409	243	83	83		

- Molecule 15 is a protein called ATP synthase F(0) complex subunit g, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	1g	79	Total	C	N	O	0	0
			390	232	79	79		
15	2g	79	Total	C	N	O	0	0
			390	232	79	79		
15	3g	79	Total	C	N	O	0	0
			390	232	79	79		
15	4g	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 16 is a protein called ATP synthase peripheral stalk subunit F6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1h	44	Total	C	N	O	0	0
			216	128	44	44		
16	2h	47	Total	C	N	O	0	0
			231	137	47	47		
16	3h	44	Total	C	N	O	0	0
			216	128	44	44		
16	4h	47	Total	C	N	O	0	0
			231	137	47	47		

- Molecule 17 is a protein called ATP synthase F(0) complex subunit j, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1j	48	Total	C	N	O	0	0
			238	142	48	48		
17	2j	48	Total	C	N	O	0	0
			238	142	48	48		
17	3j	48	Total	C	N	O	0	0
			238	142	48	48		
17	4j	48	Total	C	N	O	0	0
			238	142	48	48		

- Molecule 18 is a protein called ATP synthase F(0) complex subunit k, mitochondrial.

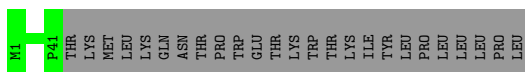
Mol	Chain	Residues	Atoms				AltConf	Trace
18	1k	36	Total 177	C 105	N 36	O 36	0	0
18	2k	36	Total 177	C 105	N 36	O 36	0	0
18	3k	36	Total 177	C 105	N 36	O 36	0	0
18	4k	36	Total 177	C 105	N 36	O 36	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

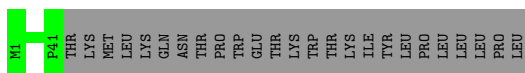
- Molecule 1: ATP synthase F(0) complex subunit 8

Chain 18:  62% 38%



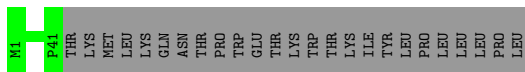
- Molecule 1: ATP synthase F(0) complex subunit 8

Chain 28:  62% 38%



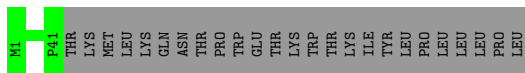
- Molecule 1: ATP synthase F(0) complex subunit 8

Chain 38:  62% 38%

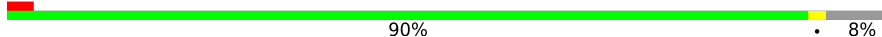


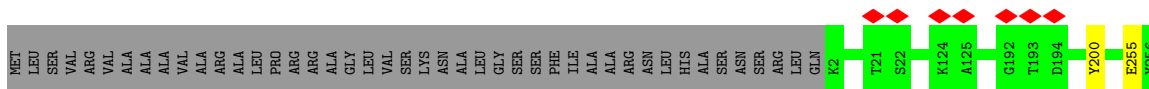
- Molecule 1: ATP synthase F(0) complex subunit 8

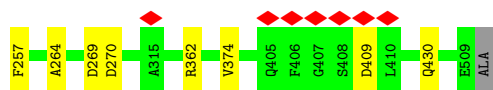
Chain 48:  62% 38%



- Molecule 2: ATP synthase subunit alpha

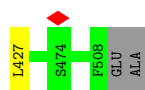
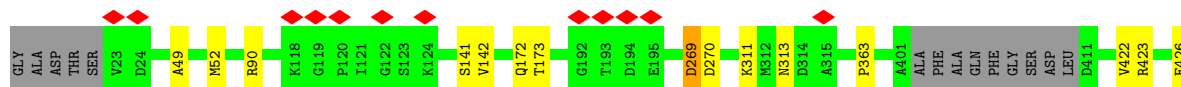
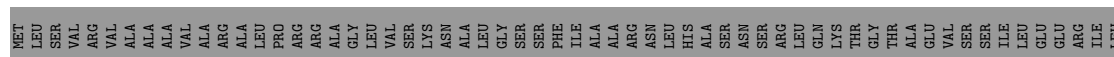
Chain 1A:  90% 8%





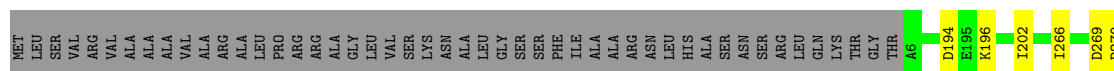
- Molecule 2: ATP synthase subunit alpha

Chain 1B: 83% 14%



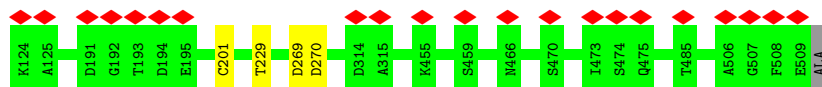
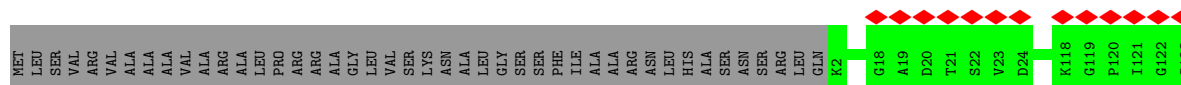
- Molecule 2: ATP synthase subunit alpha

Chain 1C: 88% 10%



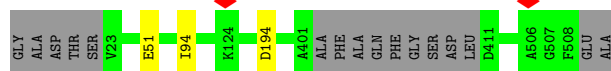
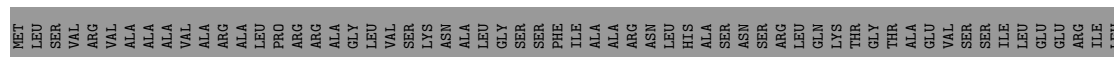
- Molecule 2: ATP synthase subunit alpha

Chain 2A: 6% 91% 8%



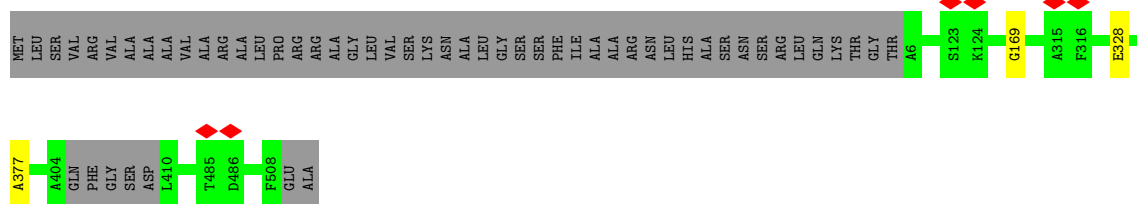
- Molecule 2: ATP synthase subunit alpha

Chain 2B: 86% 14%



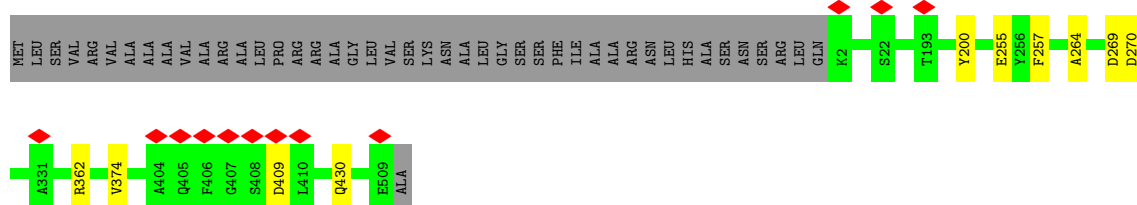
- Molecule 2: ATP synthase subunit alpha

Chain 2C:  90% 10%



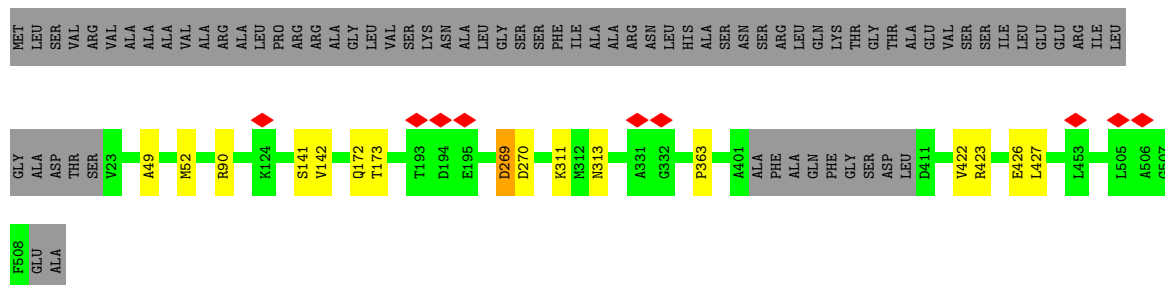
- Molecule 2: ATP synthase subunit alpha

Chain 3A:  90% 8%



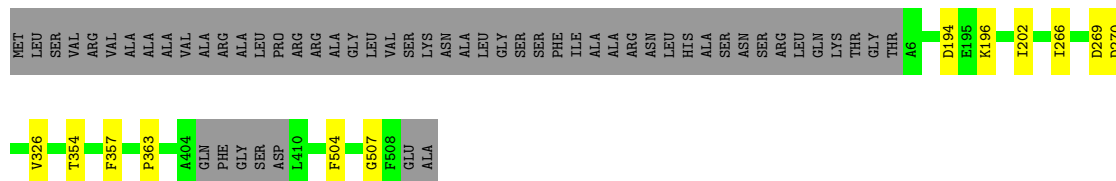
- Molecule 2: ATP synthase subunit alpha

Chain 3B:  83% 14%



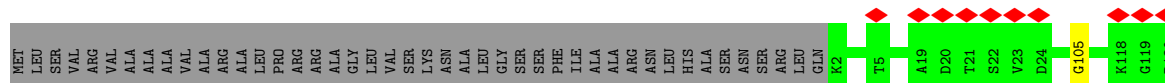
- Molecule 2: ATP synthase subunit alpha

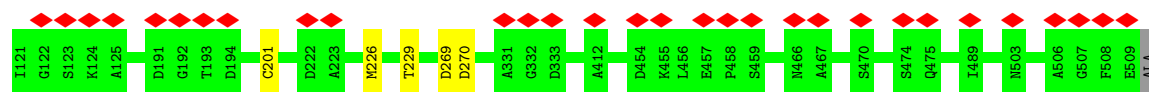
Chain 3C:  88% 10%



- Molecule 2: ATP synthase subunit alpha

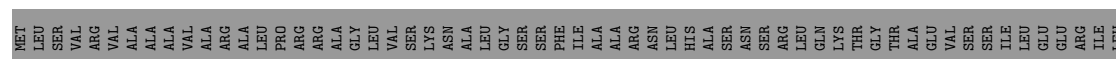
Chain 4A:  91% 8% 7%





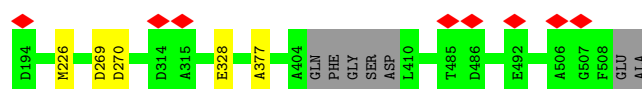
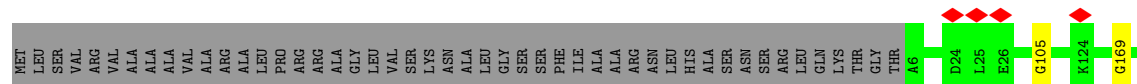
- Molecule 2: ATP synthase subunit alpha

Chain 4B: 85% 14%



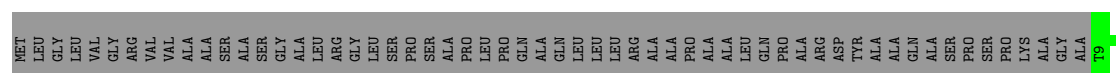
- Molecule 2: ATP synthase subunit alpha

Chain 4C: 89% 10%



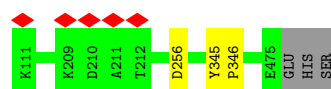
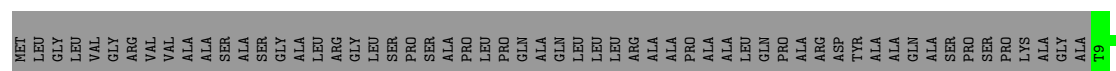
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 1D: 88% 11%



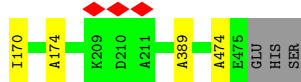
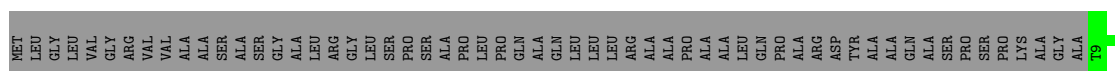
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 1E: 88% 12%

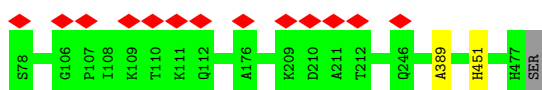
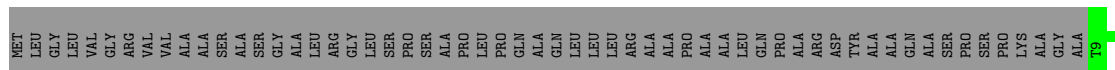


- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

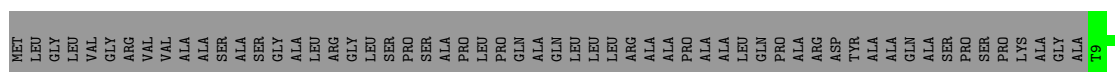
Chain 1F: 88% 12%



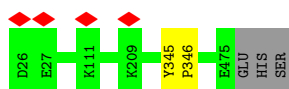
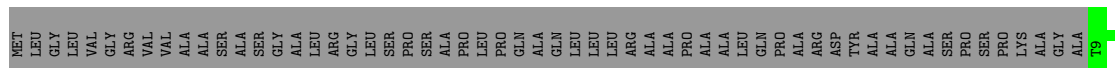
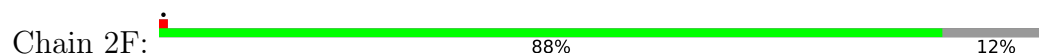
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial



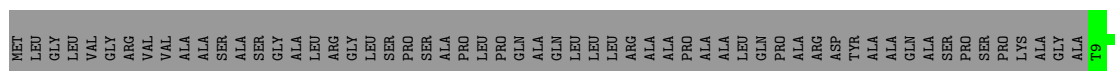
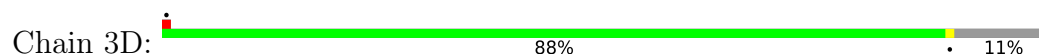
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial



- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

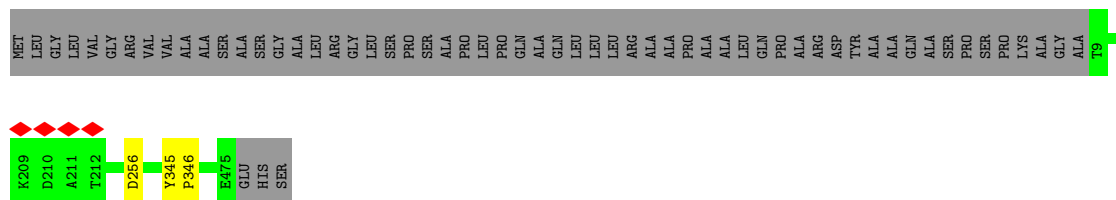


- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial



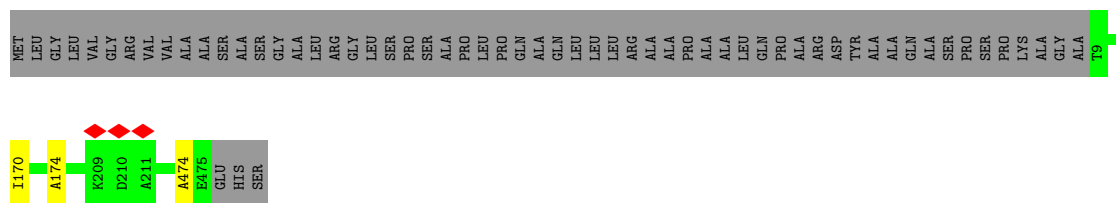
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 3E:  88% 12%



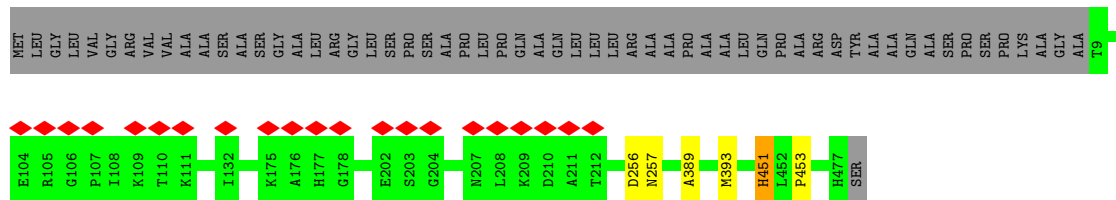
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 3F:  88% 12%



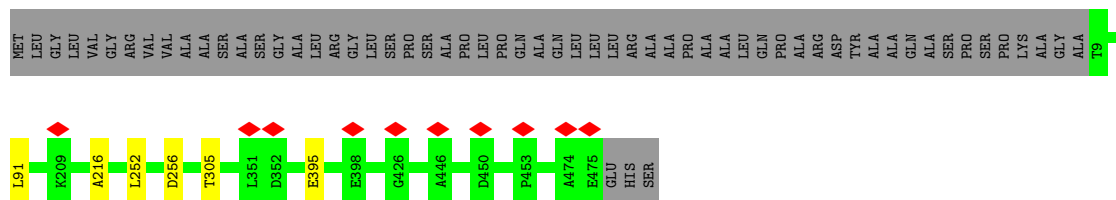
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 4D:  88% 11%



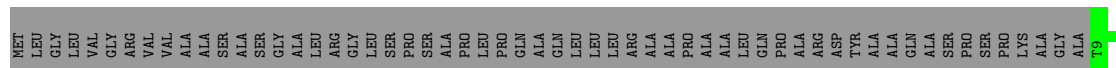
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

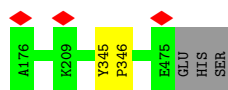
Chain 4E:  87% 12%



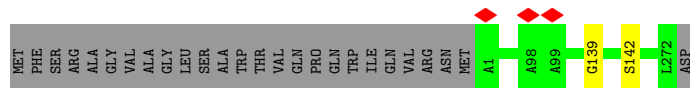
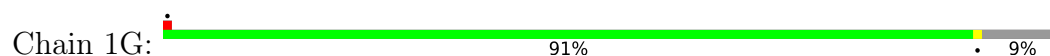
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain 4F:  88% 12%

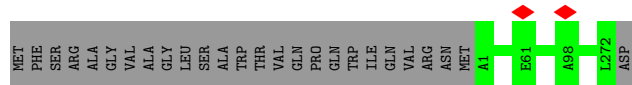
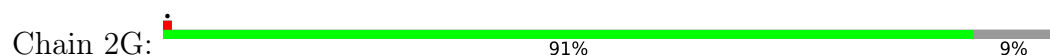




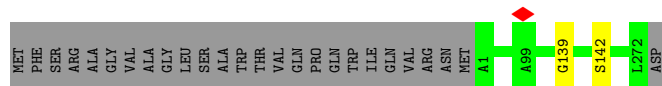
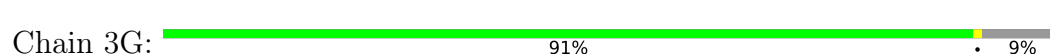
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial



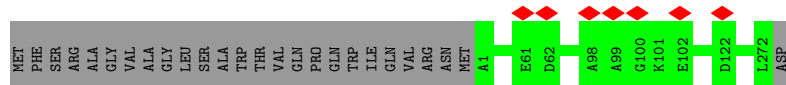
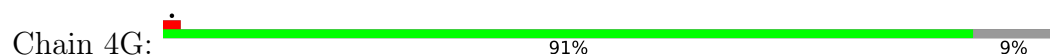
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial



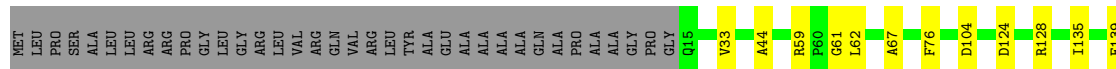
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial



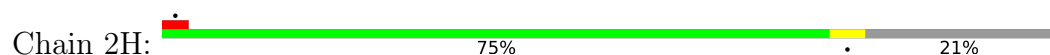
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial

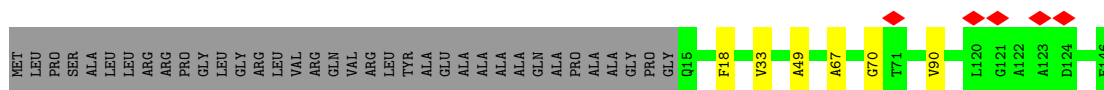


- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

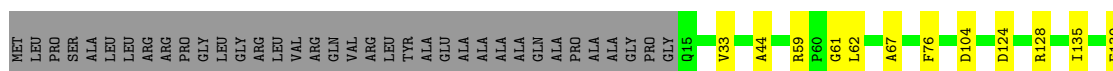
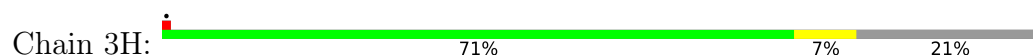


- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

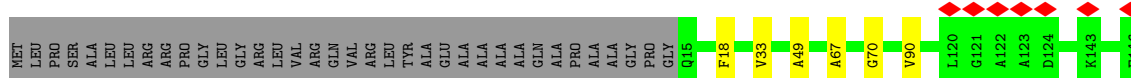
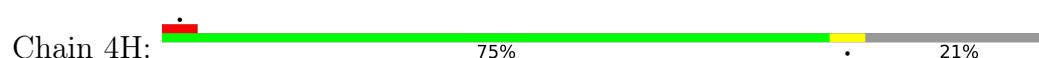




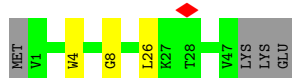
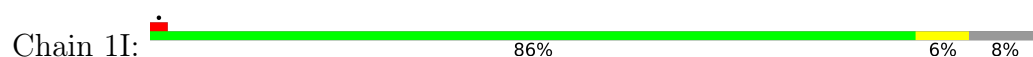
- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial



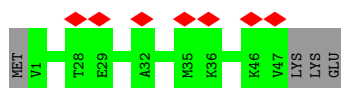
- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial



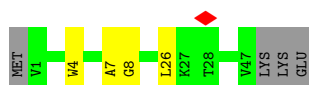
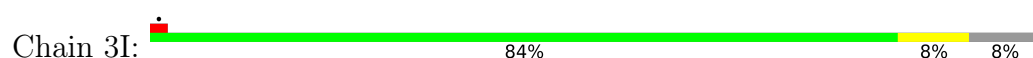
- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial



- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial

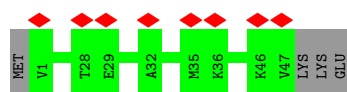


- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial



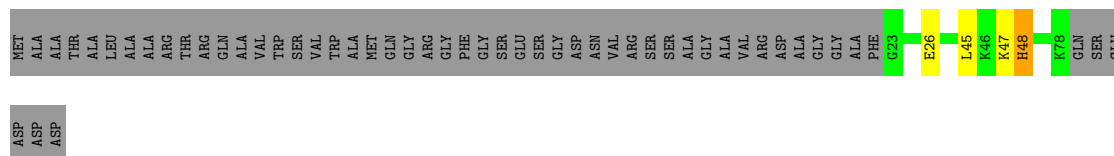
- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial





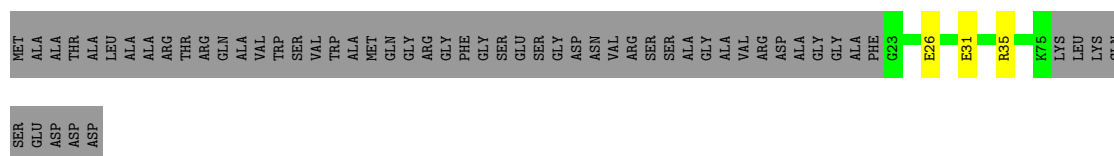
- Molecule 7: ATPase inhibitor, mitochondrial

Chain 1J: 48% 49%



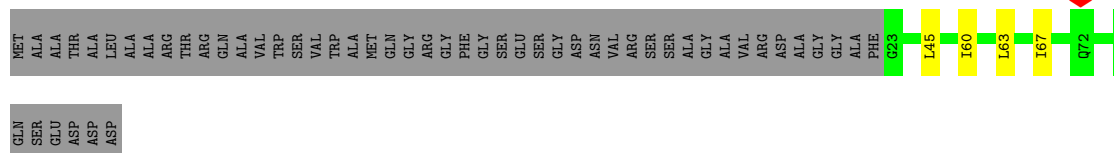
- Molecule 7: ATPase inhibitor, mitochondrial

Chain 2J: 46% 51%



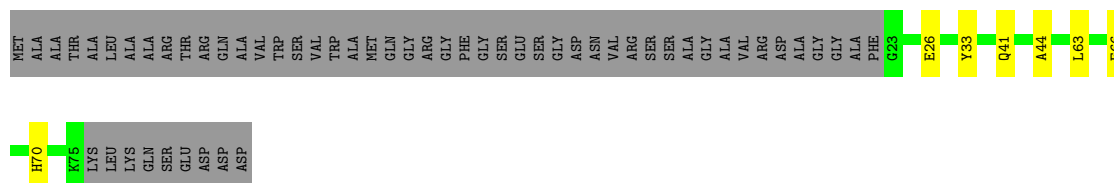
- Molecule 7: ATPase inhibitor, mitochondrial

Chain 3J: 48% 49%



- Molecule 7: ATPase inhibitor, mitochondrial

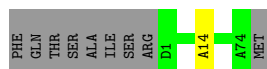
Chain 4J: 42% 6% 51%



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

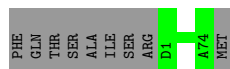
Chain 1K: 51% 48%





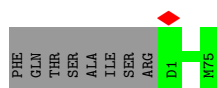
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 1L: 52% 48%



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 1M: 52% 48%



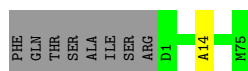
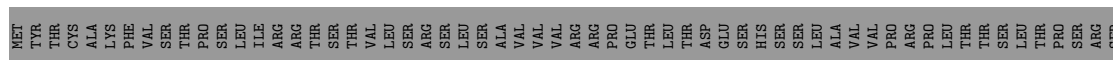
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 1N: 50% 48%



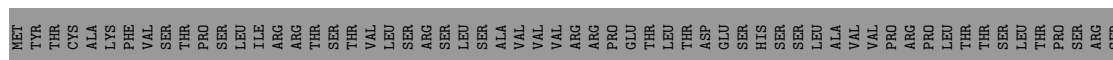
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 1O: 52% 48%



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 1P: 50% 48%



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 2N:  50% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR SER THR PRO SER ARG SER

PHE GLN THR SER ALA ILE SER ARG D1 G35 R38 A74 M75

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 2O:  50% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR SER THR PRO SER ARG SER

PHE GLN THR SER ALA ILE SER ARG D1 G12 A13 A14 A68 M75

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 2P:  48% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR SER THR PRO SER ARG SER

PHE GLN THR SER ALA ILE SER ARG D1 A14 G35 Y36 A37 R38 L65 A68 A74 MET

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 2Q:  50% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR SER THR PRO SER ARG SER

PHE GLN THR SER ALA ILE SER ARG D1 G12 A13 A14 I15 V16 A68 M75

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

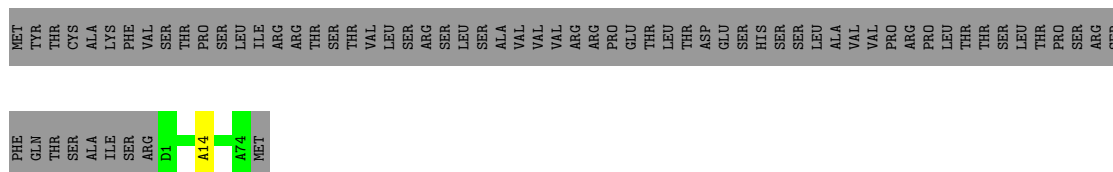
Chain 2R:  50% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR SER THR PRO SER ARG SER

PHE GLN THR SER ALA ILE SER ARG D1 A14 G17 N39 P40 S41 M75

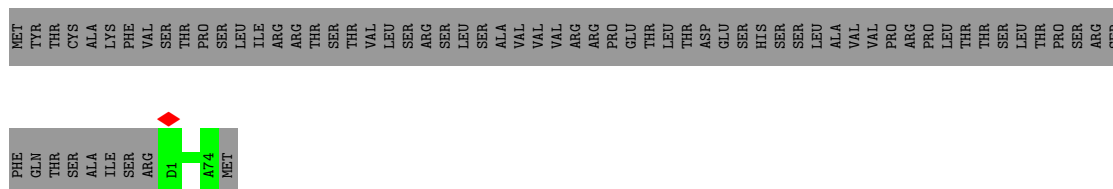
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3K: 



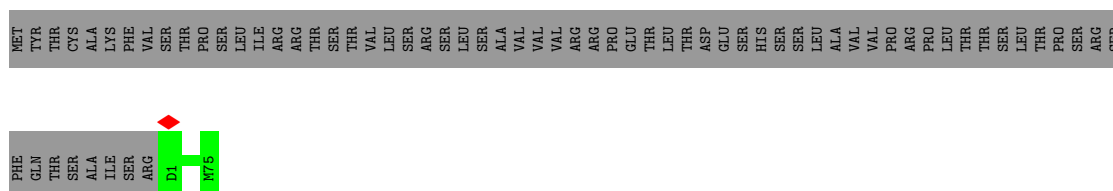
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3L: 



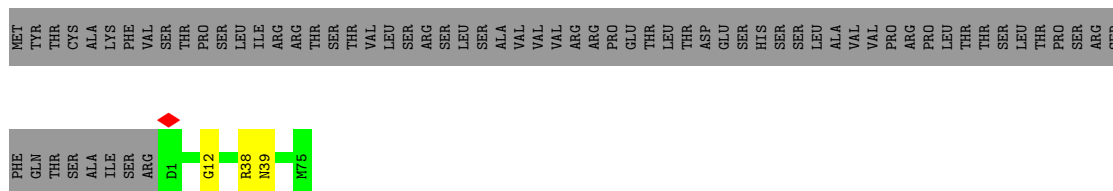
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3M: 



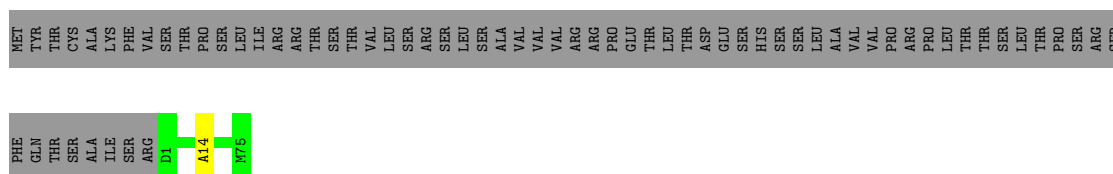
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3N: 



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3O: 



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3P:  50% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU SER HIS SER SER LEU ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

PHE GLN THR SER CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3Q:  49% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU SER HIS SER SER LEU ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

PHE GLN THR SER CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 3R:  51% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU SER HIS SER SER LEU ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

PHE GLN THR SER CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 4K:  51% 48%

MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU SER HIS SER SER LEU ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

PHE GLN THR SER CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 4L:  49% 48%

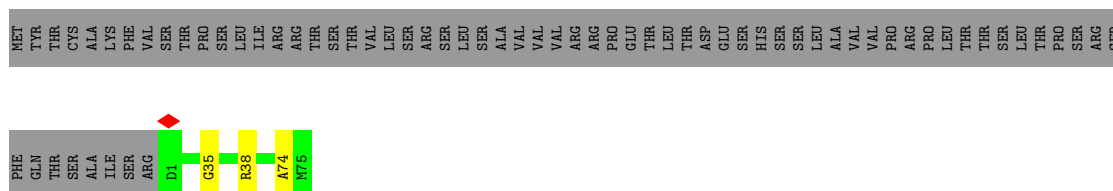
MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG ARG PRO GLU THR THR ASP GLU SER HIS SER SER LEU ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

PHE GLN THR SER CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG ARG THR THR VAL LEU SER ARG SER LEU SER ALA VAL VAL VAL ARG PRO THR THR THR THR PRO SER ARG SER

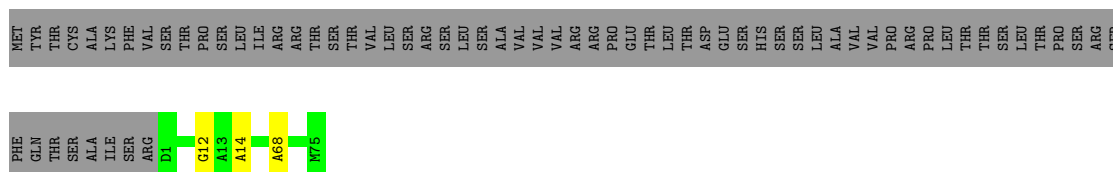
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

Chain 4M:  48% 48%

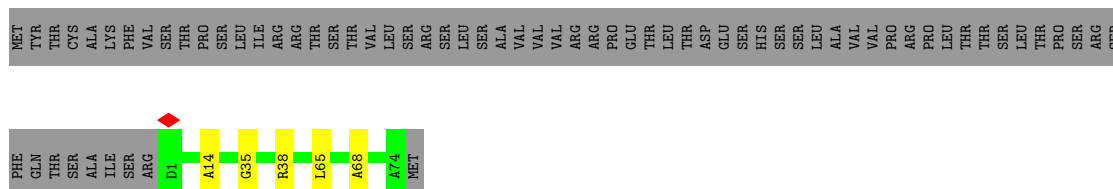
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



MET TYR THR CYS ALA LYS PHE VAL SER THR PRO SER LEU ILE ARG THR THR VAL SER ARG SER LEU VAL ALA VAL ARG ARG PRO GLU THR LEU THR ASP GLU SER HIS SER SER LEU ALA VAL VAL PRO ARG PRO LEU THR THR LEU THR PRO SER ARG SER

PHE GLN THR SER ALA ILE ARG D1 A14 G17 N39 P40 S41 M75

- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain 1S:  5% 86% 12%

MET ALA ALA LEU VAL SER GLY LEU SER GLN GLN VAL ARG CYS PHE SER THR SER VAL VAL ARG PRO F1 P49 K50 K67 D71 A74 K75 E76 K77 P117 V120 A125 E128 A129 T163 G167 E188 ILE LEU

- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain 2S:  13% 87% 12%

MET ALA ALA LEU VAL SER GLY LEU SER GLN GLN VAL ARG CYS PHE SER THR SER VAL VAL ARG PRO F1 A2 K3 K28 Q29 N30 P49 K50 M51 A52 A53 K67 S68 L69 S70 D71 M72 T73 A74 K75 E76 K77 T121 A125 L126 D127 E128 A129 T132 E133 T136 K144 G145 K153 E188 ILE LEU

- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain 3S:  85% 12%

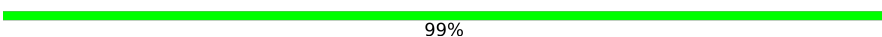
MET ALA ALA LEU VAL SER GLY LEU SER GLN GLN VAL ARG CYS PHE SER THR SER VAL VAL ARG PRO F1 K75 P117 V120 D127 E128 A129 T130 L131 I163 G167 E188 ILE LEU

- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain 4S:  8% 87% 12%

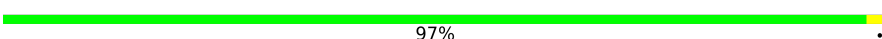
MET ALA ALA LEU VAL SER GLY LEU SER GLN GLN VAL ARG CYS PHE SER THR SER VAL VAL ARG PRO F1 K28 Q29 P49 K50 M51 A52 A53 L56 K67 D71 A74 K75 E76 K77 T121 E128 A129 T132 K144 K153 E188 ILE LEU

- Molecule 10: ATP synthase F(0) complex subunit a

Chain 1a:  99%

M1 M182 A189 T226

- Molecule 10: ATP synthase F(0) complex subunit a

Chain 2a:  97%



- Molecule 10: ATP synthase F(0) complex subunit a

Chain 3a: 99%



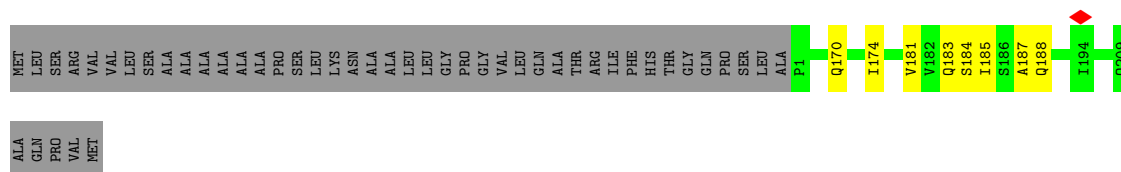
- Molecule 10: ATP synthase F(0) complex subunit a

Chain 4a: 95%



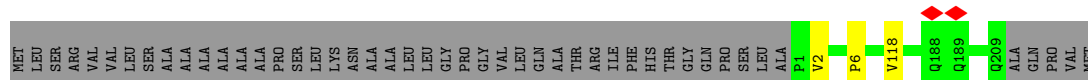
- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

Chain 1b: 79%



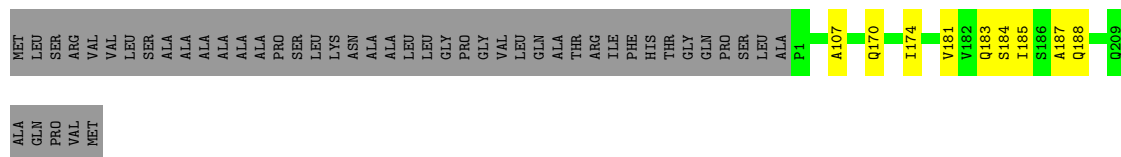
- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

Chain 2b: 80%



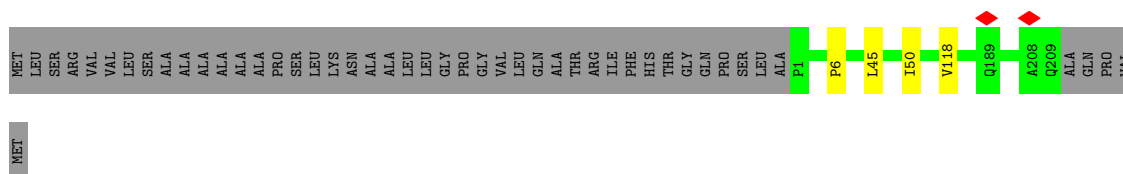
- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

Chain 3b: 78%



- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

Chain 4b: 80%



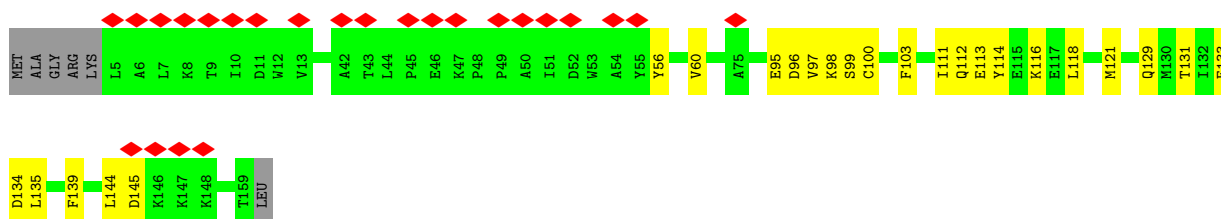
- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

Chain 1d: 91% 5% .



- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

Chain 2d: 15% 81% 15% .



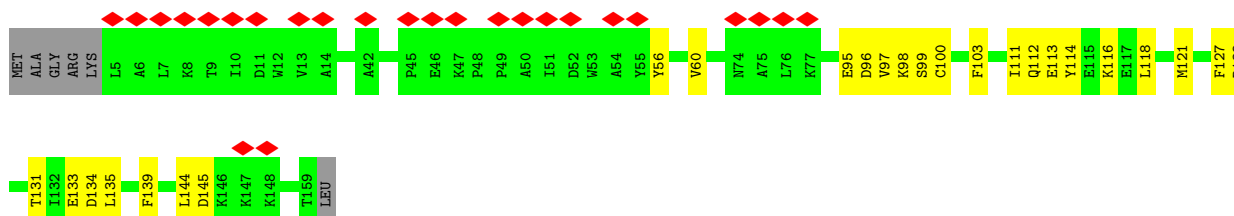
- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

Chain 3d: 91% 6% .



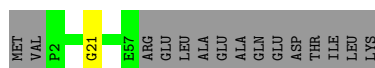
- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

Chain 4d: 16% 81% 16% .



- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain 1e: 77% 21% .



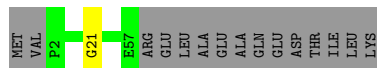
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain 2e:  75% 21%



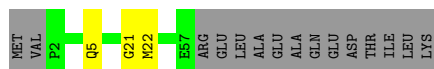
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain 3e:  77% 21%



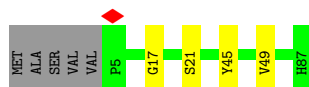
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain 4e:  75% 21%

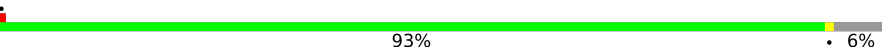


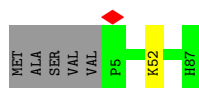
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

Chain 1f:  90% 5% 6%



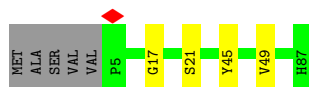
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

Chain 2f:  93% 6%

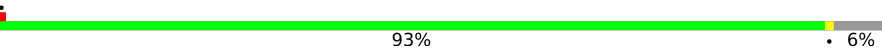


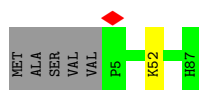
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

Chain 3f:  90% 5% 6%



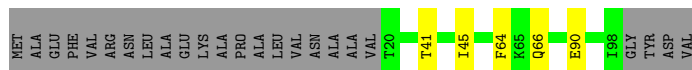
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

Chain 4f:  93% 6%



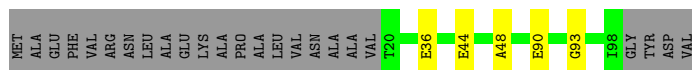
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial

Chain 1g: 72% 5% 23%



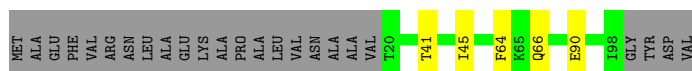
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial

Chain 2g: 72% 5% 23%



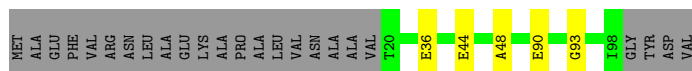
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial

Chain 3g: 72% 5% 23%



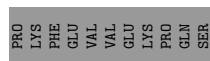
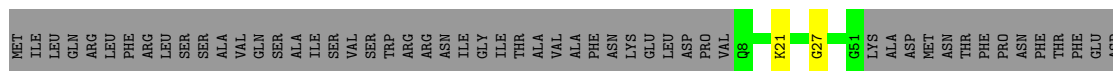
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial

Chain 4g: 72% 5% 23%



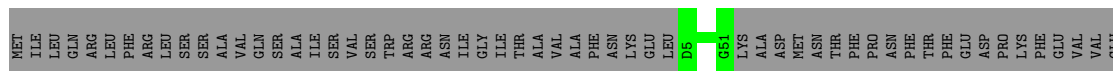
- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain 1h: 39% 0% 59%



- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain 2h: 44% 0% 56%



LYS
PRO
GLN
SER

- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain 3h:  39% 59%

MET ILE LEU GLN ARG LEU PHE ARG LEU SER SER SER ALA VAL GLN SER ALA ILE ILE VAL TRP ARG ARG ASN ILE GLY ILE THR VAL VAL PHE ASN LYS LEU LEU ASP PRO VAL Q8 K21 G27 G51 LYS ALA ASP MET ASN THR PHE PRO ASN PHE THR PHE GLU ASP

PRO
LYS
PHE
GLU
VAL
VAL
GLU
LYS
PRO
GLN
SER

- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain 4h:  44% 56%

MET ILE LEU GLN ARG LEU PHE ARG LEU SER SER SER ALA VAL GLN SER ALA ILE ILE VAL TRP ARG ARG ASN ILE GLY ILE THR VAL VAL PHE ASN LYS LEU LEU D5 M49 Y50 G51 LYS ALA ASP MET ASN THR PHE PRO ASN PHE THR PHE GLU ASP PRO LYS PHE GLU VAL

VAL
GLU
LYS
PRO
GLN
SER

- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial

Chain 1j:  73% 7% 20%

MET L2 Y21 W25 K43 A47 L48 K49 ALA SER SER SER ALA ALA ALA PRO HIS HIS HIS HIS

- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial

Chain 2j:  80% 20%

MET L2 K49 ALA SER SER ALA ALA PRO HIS GLY HIS HIS

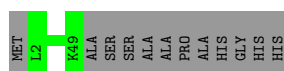
- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial

Chain 3j:  5% 73% 7% 20%

MET L2 Y21 W25 K43 K46 A47 L48 K49 ALA SER SER SER ALA ALA ALA PRO HIS GLY HIS HIS

- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial

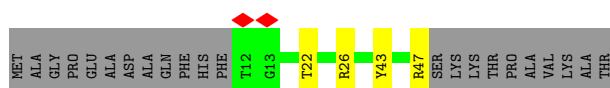
Chain 4j:  80% 20%



- Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



- Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



- Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



- Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00519	Depositor
Map size (Å)	547.308, 547.308, 547.308	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5202999, 1.5202999, 1.5202999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	18	0.22	0/204	0.46	0/284
1	28	0.24	0/204	0.61	0/284
1	38	0.22	0/204	0.45	0/284
1	48	0.24	0/204	0.61	0/284
2	1A	0.34	0/2490	0.56	0/3455
2	1B	0.34	0/2337	0.67	5/3241 (0.2%)
2	1C	0.34	0/2441	0.56	0/3386
2	2A	0.23	0/2490	0.51	0/3455
2	2B	0.23	0/2337	0.51	0/3241
2	2C	0.23	0/2441	0.51	0/3386
2	3A	0.34	0/2490	0.56	0/3455
2	3B	0.34	0/2337	0.67	5/3241 (0.2%)
2	3C	0.35	0/2441	0.57	0/3386
2	4A	0.23	0/2490	0.51	0/3455
2	4B	0.23	0/2337	0.51	0/3241
2	4C	0.23	0/2441	0.52	0/3386
3	1D	0.33	0/2299	0.62	3/3190 (0.1%)
3	1E	0.35	0/2289	0.60	0/3176
3	1F	0.33	0/2289	0.59	0/3176
3	2D	0.23	0/2299	0.54	0/3190
3	2E	0.23	0/2289	0.51	2/3176 (0.1%)
3	2F	0.23	0/2289	0.49	0/3176
3	3D	0.33	0/2299	0.62	3/3190 (0.1%)
3	3E	0.35	0/2289	0.61	0/3176
3	3F	0.33	0/2289	0.59	0/3176
3	4D	0.23	0/2299	0.54	0/3190
3	4E	0.23	0/2289	0.51	2/3176 (0.1%)
3	4F	0.23	0/2289	0.49	0/3176
4	1G	0.27	0/1346	0.55	0/1875
4	2G	0.21	0/1346	0.40	0/1875
4	3G	0.27	0/1346	0.55	0/1875
4	4G	0.21	0/1346	0.40	0/1875
5	1H	0.25	0/652	0.52	0/907
5	2H	0.19	0/652	0.45	0/907

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	3H	0.25	0/652	0.52	0/907
5	4H	0.19	0/652	0.45	0/907
6	1I	0.25	0/232	0.39	0/322
6	2I	0.18	0/232	0.39	0/322
6	3I	0.25	0/232	0.39	0/322
6	4I	0.19	0/232	0.39	0/322
7	1J	1.12	0/277	1.55	0/385
7	2J	1.13	0/263	1.54	0/366
7	3J	1.08	0/278	1.48	0/387
7	4J	1.13	0/263	1.54	0/366
8	1K	0.23	0/358	0.35	0/493
8	1L	0.22	0/358	0.40	0/493
8	1M	0.21	0/363	0.46	0/500
8	1N	0.24	0/363	0.49	0/500
8	1O	0.22	0/363	0.41	0/500
8	1P	0.23	0/358	0.41	0/493
8	1Q	0.24	0/363	0.39	0/500
8	1R	0.23	0/363	0.38	0/500
8	2K	0.24	0/358	0.46	0/493
8	2L	0.22	0/358	0.46	0/493
8	2M	0.24	0/363	0.43	0/500
8	2N	0.28	0/363	0.58	1/500 (0.2%)
8	2O	0.27	0/363	0.49	0/500
8	2P	0.23	0/358	0.48	0/493
8	2Q	0.27	0/363	0.50	0/500
8	2R	0.25	0/363	0.54	0/500
8	3K	0.24	0/358	0.35	0/493
8	3L	0.22	0/358	0.40	0/493
8	3M	0.21	0/363	0.45	0/500
8	3N	0.25	0/363	0.49	0/500
8	3O	0.22	0/363	0.41	0/500
8	3P	0.23	0/358	0.41	0/493
8	3Q	0.25	0/363	0.39	0/500
8	3R	0.23	0/363	0.38	0/500
8	4K	0.24	0/358	0.46	0/493
8	4L	0.23	0/358	0.45	0/493
8	4M	0.24	0/363	0.43	0/500
8	4N	0.28	0/363	0.58	1/500 (0.2%)
8	4O	0.27	0/363	0.48	0/500
8	4P	0.23	0/358	0.48	0/493
8	4Q	0.27	0/363	0.50	0/500
8	4R	0.26	0/363	0.55	0/500
9	1S	0.26	0/930	0.48	0/1295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	2S	0.17	0/930	0.38	0/1295
9	3S	0.26	0/930	0.48	0/1295
9	4S	0.17	0/930	0.38	0/1295
10	1a	0.23	0/1118	0.43	0/1557
10	2a	0.23	0/1118	0.44	0/1557
10	3a	0.23	0/1118	0.43	0/1557
10	4a	0.23	0/1118	0.44	0/1557
11	1b	0.68	0/1034	0.81	0/1440
11	2b	0.49	0/1034	0.65	0/1440
11	3b	0.62	0/1034	0.74	0/1440
11	4b	0.42	0/1034	0.59	0/1440
12	1d	0.21	0/772	0.42	0/1078
12	2d	0.22	0/772	0.50	0/1078
12	3d	0.21	0/772	0.42	0/1078
12	4d	0.22	0/772	0.49	0/1078
13	1e	0.18	0/276	0.34	0/383
13	2e	0.22	0/276	0.34	0/383
13	3e	0.19	0/276	0.34	0/383
13	4e	0.22	0/276	0.34	0/383
14	1f	0.19	0/408	0.35	0/566
14	2f	0.23	0/408	0.54	0/566
14	3f	0.19	0/408	0.35	0/566
14	4f	0.23	0/408	0.54	0/566
15	1g	0.19	0/389	0.34	0/540
15	2g	0.21	0/389	0.56	0/540
15	3g	0.18	0/389	0.34	0/540
15	4g	0.21	0/389	0.56	0/540
16	1h	0.18	0/215	0.36	0/297
16	2h	0.15	0/230	0.37	0/318
16	3h	0.18	0/215	0.36	0/297
16	4h	0.15	0/230	0.37	0/318
17	1j	0.21	0/237	0.46	0/329
17	2j	0.17	0/237	0.36	0/329
17	3j	0.22	0/237	0.46	0/329
17	4j	0.18	0/237	0.36	0/329
18	1k	0.20	0/176	0.33	0/243
18	2k	0.18	0/176	0.36	0/243
18	3k	0.20	0/176	0.33	0/243
18	4k	0.18	0/176	0.36	0/243
All	All	0.31	0/101203	0.55	22/140422 (0.0%)

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
2	1A	0	1
2	1B	0	1
2	1C	0	1
2	3A	0	1
2	3B	0	1
2	3C	0	1
3	1E	0	1
3	3E	0	1
All	All	0	8

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3B	141	SER	N-CA-C	7.64	118.77	108.23
2	1B	141	SER	N-CA-C	7.60	118.72	108.23
3	3D	389	ALA	N-CA-C	-6.29	107.45	114.62
3	1D	389	ALA	N-CA-C	-6.26	107.48	114.62
8	4N	74	ALA	N-CA-C	-5.34	106.52	114.64
8	2N	74	ALA	N-CA-C	-5.33	106.53	114.64
3	3D	311	TYR	CA-C-N	-5.33	118.97	122.60
3	3D	311	TYR	C-N-CA	-5.33	118.97	122.60
3	1D	311	TYR	CA-C-N	-5.28	119.01	122.60
3	1D	311	TYR	C-N-CA	-5.28	119.01	122.60
2	3B	49	ALA	CA-C-N	5.07	131.23	121.54
2	3B	49	ALA	C-N-CA	5.07	131.23	121.54
2	1B	141	SER	CA-C-N	5.07	131.09	121.97
2	1B	141	SER	C-N-CA	5.07	131.09	121.97
2	3B	141	SER	CA-C-N	5.06	131.08	121.97
2	3B	141	SER	C-N-CA	5.06	131.08	121.97
2	1B	49	ALA	CA-C-N	5.06	131.20	121.54
2	1B	49	ALA	C-N-CA	5.06	131.20	121.54
3	4E	256	ASP	CA-C-N	5.01	130.71	121.70
3	4E	256	ASP	C-N-CA	5.01	130.71	121.70
3	2E	256	ASP	CA-C-N	5.00	130.70	121.70
3	2E	256	ASP	C-N-CA	5.00	130.70	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1A	374	VAL	Peptide
2	1B	269	ASP	Peptide
2	1C	269	ASP	Peptide
3	1E	256	ASP	Peptide
2	3A	374	VAL	Peptide
2	3B	269	ASP	Peptide
2	3C	269	ASP	Peptide
3	3E	256	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	18	205	0	81	0	0
1	28	205	0	81	0	0
1	38	205	0	81	0	0
1	48	205	0	81	0	0
2	1A	2491	0	1191	4	0
2	1B	2339	0	1113	6	0
2	1C	2443	0	1168	7	0
2	2A	2491	0	1191	2	0
2	2B	2339	0	1113	1	0
2	2C	2443	0	1168	1	0
2	3A	2491	0	1191	4	0
2	3B	2339	0	1113	6	0
2	3C	2443	0	1168	7	0
2	4A	2491	0	1191	3	0
2	4B	2339	0	1113	2	0
2	4C	2443	0	1168	3	0
3	1D	2300	0	1094	1	0
3	1E	2290	0	1090	1	0
3	1F	2290	0	1090	10	0
3	2D	2300	0	1094	1	0
3	2E	2290	0	1090	3	0
3	2F	2290	0	1090	1	0
3	3D	2300	0	1094	1	0
3	3E	2290	0	1090	1	0
3	3F	2290	0	1090	11	0
3	4D	2300	0	1094	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4E	2290	0	1090	2	0
3	4F	2290	0	1090	1	0
4	1G	1347	0	641	1	0
4	2G	1347	0	641	0	0
4	3G	1347	0	641	1	0
4	4G	1347	0	641	0	0
5	1H	653	0	326	9	0
5	2H	653	0	326	6	0
5	3H	653	0	326	9	0
5	4H	653	0	326	6	0
6	1I	233	0	119	2	0
6	2I	233	0	119	0	0
6	3I	233	0	119	3	0
6	4I	233	0	119	0	0
7	1J	278	0	129	10	0
7	2J	264	0	124	2	0
7	3J	279	0	130	13	0
7	4J	264	0	124	13	0
8	1K	359	0	199	1	0
8	1L	359	0	199	0	0
8	1M	364	0	201	0	0
8	1N	364	0	201	4	0
8	1O	364	0	201	1	0
8	1P	359	0	199	4	0
8	1Q	364	0	201	5	0
8	1R	364	0	201	2	0
8	2K	359	0	199	3	0
8	2L	359	0	199	3	0
8	2M	364	0	201	4	0
8	2N	364	0	201	1	0
8	2O	364	0	201	2	0
8	2P	359	0	199	4	0
8	2Q	364	0	201	3	0
8	2R	364	0	201	3	0
8	3K	359	0	199	2	0
8	3L	359	0	199	0	0
8	3M	364	0	201	0	0
8	3N	364	0	201	4	0
8	3O	364	0	201	1	0
8	3P	359	0	199	4	0
8	3Q	364	0	201	5	0
8	3R	364	0	201	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	4K	359	0	199	3	0
8	4L	359	0	199	3	0
8	4M	364	0	201	4	0
8	4N	364	0	201	1	0
8	4O	364	0	201	2	0
8	4P	359	0	199	3	0
8	4Q	364	0	201	3	0
8	4R	364	0	201	3	0
9	1S	931	0	427	2	0
9	2S	931	0	427	1	0
9	3S	931	0	427	3	0
9	4S	931	0	427	1	0
10	1a	1119	0	498	1	0
10	2a	1119	0	498	3	0
10	3a	1119	0	498	1	0
10	4a	1119	0	498	13	0
11	1b	1035	0	459	5	0
11	2b	1035	0	459	7	0
11	3b	1035	0	459	6	0
11	4b	1035	0	459	4	0
12	1d	773	297	342	4	0
12	2d	773	0	342	20	0
12	3d	773	297	342	5	0
12	4d	773	0	342	24	0
13	1e	277	0	129	1	0
13	2e	277	0	129	3	0
13	3e	277	0	129	1	0
13	4e	277	0	129	3	0
14	1f	409	0	184	2	0
14	2f	409	0	184	1	0
14	3f	409	0	184	2	0
14	4f	409	0	184	1	0
15	1g	390	0	178	3	0
15	2g	390	0	178	4	0
15	3g	390	0	178	3	0
15	4g	390	0	178	4	0
16	1h	216	0	92	1	0
16	2h	231	0	97	0	0
16	3h	216	0	92	1	0
16	4h	231	0	97	0	0
17	1j	238	0	107	2	0
17	2j	238	0	107	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	3j	238	0	107	2	0
17	4j	238	0	107	0	0
18	1k	177	0	80	1	0
18	2k	177	0	80	2	0
18	3k	177	0	80	1	0
18	4k	177	0	80	2	0
All	All	101327	594	48561	286	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 2.

All (286) 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)
5:1H:44:ALA:HB3	8:1N:38:ARG:O	1.10	1.26
5:3H:44:ALA:HB3	8:3N:38:ARG:O	1.10	1.23
11:2b:118:VAL:CB	12:2d:99:SER:CB	2.18	1.21
3:4D:451:HIS:O	7:4J:44:ALA:HB3	1.35	1.20
11:4b:118:VAL:CB	12:4d:99:SER:CB	2.21	1.19
5:1H:44:ALA:CB	8:1N:38:ARG:O	1.92	1.17
5:3H:44:ALA:CB	8:3N:38:ARG:O	1.92	1.15
3:1F:474:ALA:CB	7:1J:45:LEU:CB	2.25	1.14
3:4D:453:PRO:HA	7:4J:41:GLN:CB	1.79	1.13
5:4H:49:ALA:HB3	8:4K:41:SER:CB	1.83	1.08
5:2H:49:ALA:HB3	8:2K:41:SER:CB	1.83	1.08
10:4a:38:VAL:N	12:4d:128:ASP:HA	1.67	1.07
10:4a:38:VAL:H	12:4d:128:ASP:HA	0.91	1.07
10:4a:38:VAL:CB	12:4d:128:ASP:CB	2.34	1.05
10:4a:36:ARG:CB	12:4d:128:ASP:O	2.08	1.02
3:3F:474:ALA:HA	7:3J:45:LEU:CB	1.91	1.01
3:3F:474:ALA:HB1	7:3J:45:LEU:O	1.61	0.99
10:4a:37:LEU:CB	12:4d:127:PHE:O	2.11	0.98
3:4D:393:MET:CB	7:4J:33:TYR:CB	2.44	0.96
3:1F:474:ALA:HB1	7:1J:45:LEU:CB	1.96	0.93
7:3J:60:ILE:CB	7:4J:70:HIS:CB	2.49	0.90
5:4H:49:ALA:CB	8:4K:41:SER:CB	2.51	0.89
5:2H:49:ALA:CB	8:2K:41:SER:CB	2.51	0.88
11:2b:2:VAL:CB	12:2d:129:GLN:HA	2.05	0.86
7:3J:63:LEU:CB	7:4J:66:GLU:CB	2.54	0.85
17:1j:21:TYR:O	17:1j:25:TRP:N	2.10	0.85
17:3j:21:TYR:O	17:3j:25:TRP:N	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1F:474:ALA:HB2	7:1J:45:LEU:CB	2.07	0.82
12:2d:96:ASP:O	12:2d:100:CYS:N	2.13	0.81
3:1F:474:ALA:HA	7:1J:45:LEU:CB	2.11	0.81
3:3F:474:ALA:HB1	7:3J:45:LEU:C	2.06	0.80
12:4d:96:ASP:O	12:4d:100:CYS:N	2.13	0.80
3:1F:474:ALA:CA	7:1J:45:LEU:CB	2.60	0.79
3:3F:474:ALA:HB1	7:3J:45:LEU:CA	2.15	0.76
3:3F:474:ALA:CB	7:3J:45:LEU:HA	2.16	0.74
3:1F:389:ALA:HA	7:1J:26:GLU:CB	2.18	0.73
5:3H:135:ILE:O	5:3H:139:GLU:N	2.22	0.72
3:1F:474:ALA:HB1	7:1J:45:LEU:CA	2.19	0.72
14:1f:17:GLY:O	14:1f:21:SER:N	2.23	0.72
3:3F:474:ALA:CA	7:3J:45:LEU:CB	2.68	0.72
3:2D:389:ALA:HA	7:2J:26:GLU:CB	2.20	0.72
3:3F:474:ALA:CB	7:3J:45:LEU:CA	2.68	0.72
5:1H:135:ILE:O	5:1H:139:GLU:N	2.22	0.71
14:3f:17:GLY:O	14:3f:21:SER:N	2.23	0.71
18:4k:22:THR:O	18:4k:26:ARG:N	2.20	0.70
11:2b:2:VAL:CB	12:2d:129:GLN:CA	2.69	0.70
5:3H:62:LEU:HA	5:3H:76:PHE:HA	1.73	0.70
5:1H:62:LEU:HA	5:1H:76:PHE:HA	1.73	0.70
3:4D:451:HIS:O	7:4J:44:ALA:CB	2.28	0.70
8:3N:12:GLY:HA2	8:3O:14:ALA:HB2	1.75	0.69
3:3F:474:ALA:HB2	7:3J:45:LEU:HA	1.75	0.68
8:3P:19:ALA:HB1	8:3Q:20:GLY:HA3	1.76	0.67
8:1N:12:GLY:HA2	8:1O:14:ALA:HB2	1.75	0.67
18:2k:43:TYR:O	18:2k:47:ARG:N	2.23	0.67
18:2k:22:THR:O	18:2k:26:ARG:N	2.20	0.67
8:1P:19:ALA:HB1	8:1Q:20:GLY:HA3	1.76	0.66
8:2M:70:LEU:HA	8:2M:74:ALA:HB3	1.78	0.66
8:4P:35:GLY:O	8:4P:38:ARG:N	2.29	0.66
18:4k:43:TYR:O	18:4k:47:ARG:N	2.23	0.66
8:2P:35:GLY:O	8:2P:38:ARG:N	2.29	0.65
14:1f:45:TYR:O	14:1f:49:VAL:N	2.30	0.65
8:2Q:14:ALA:HB3	8:2Q:68:ALA:HB2	1.79	0.65
3:4D:451:HIS:CB	7:4J:44:ALA:HB1	2.27	0.65
14:3f:45:TYR:O	14:3f:49:VAL:N	2.30	0.64
8:4M:70:LEU:HA	8:4M:74:ALA:HB3	1.78	0.64
3:4D:451:HIS:C	7:4J:44:ALA:HB3	2.20	0.64
15:3g:41:THR:O	15:3g:45:ILE:N	2.30	0.64
11:1b:181:VAL:O	11:1b:185:ILE:N	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4Q:14:ALA:HB3	8:4Q:68:ALA:HB2	1.79	0.63
12:2d:98:LYS:O	12:2d:103:PHE:N	2.32	0.63
2:1B:422:VAL:O	2:1B:426:GLU:CB	2.47	0.63
2:1B:423:ARG:O	2:1B:427:LEU:N	2.31	0.63
8:4L:5:ALA:HB1	8:4M:6:ALA:HB3	1.81	0.63
5:1H:124:ASP:O	5:1H:128:ARG:N	2.28	0.63
2:3B:422:VAL:O	2:3B:426:GLU:CB	2.47	0.63
5:2H:49:ALA:H	8:2K:41:SER:CB	2.12	0.63
2:3B:423:ARG:O	2:3B:427:LEU:N	2.31	0.62
12:4d:98:LYS:O	12:4d:103:PHE:N	2.32	0.62
3:1F:474:ALA:HB1	7:1J:45:LEU:C	2.24	0.62
3:4D:389:ALA:HA	7:4J:26:GLU:CB	2.29	0.62
5:4H:49:ALA:H	8:4K:41:SER:CB	2.12	0.62
3:4D:453:PRO:CA	7:4J:41:GLN:CB	2.69	0.61
8:2L:5:ALA:HB1	8:2M:6:ALA:HB3	1.81	0.61
15:1g:41:THR:O	15:1g:45:ILE:N	2.30	0.61
11:3b:181:VAL:O	11:3b:185:ILE:N	2.24	0.61
3:4D:451:HIS:O	7:4J:41:GLN:O	2.19	0.60
12:3d:56:TYR:O	12:3d:60:VAL:N	2.27	0.60
11:1b:184:SER:HA	11:1b:187:ALA:HB3	1.84	0.59
8:2O:12:GLY:HA2	8:2P:14:ALA:HB2	1.83	0.59
11:3b:184:SER:HA	11:3b:187:ALA:HB3	1.84	0.59
8:4O:12:GLY:HA2	8:4P:14:ALA:HB2	1.83	0.59
12:1d:56:TYR:O	12:1d:60:VAL:N	2.27	0.58
5:3H:124:ASP:O	5:3H:128:ARG:N	2.28	0.58
2:4B:51:GLU:HA	2:4B:94:ILE:HA	1.86	0.58
2:2B:51:GLU:HA	2:2B:94:ILE:HA	1.86	0.58
8:4R:39:ASN:O	8:4R:41:SER:N	2.36	0.57
8:2R:39:ASN:O	8:2R:41:SER:N	2.36	0.57
11:3b:183:GLN:O	11:3b:187:ALA:N	2.35	0.57
17:3j:43:LYS:O	17:3j:47:ALA:N	2.37	0.56
2:1B:311:LYS:O	2:1B:313:ASN:N	2.38	0.56
3:3F:474:ALA:CB	7:3J:45:LEU:CB	2.84	0.56
8:3Q:12:GLY:HA2	8:3R:14:ALA:HB2	1.87	0.56
11:3b:184:SER:O	11:3b:188:GLN:N	2.28	0.56
8:1Q:12:GLY:HA2	8:1R:14:ALA:HB2	1.87	0.56
17:1j:43:LYS:O	17:1j:47:ALA:N	2.37	0.56
2:3B:311:LYS:O	2:3B:313:ASN:N	2.38	0.56
12:4d:111:ILE:O	12:4d:114:TYR:N	2.39	0.56
12:4d:135:LEU:O	12:4d:139:PHE:N	2.34	0.56
12:2d:56:TYR:O	12:2d:60:VAL:N	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2d:111:ILE:O	12:2d:114:TYR:N	2.39	0.55
11:2b:2:VAL:O	12:2d:129:GLN:CB	2.53	0.55
5:1H:44:ALA:HB2	8:1N:39:ASN:HA	1.89	0.55
11:3b:107:ALA:HB1	12:3d:114:TYR:CB	2.37	0.55
5:2H:18:PHE:HA	5:2H:90:VAL:O	2.07	0.54
12:2d:135:LEU:O	12:2d:139:PHE:N	2.34	0.54
5:1H:104:ASP:H	6:1I:26:LEU:HA	1.73	0.54
2:1C:354:THR:O	2:1C:357:PHE:N	2.40	0.54
7:1J:47:LYS:O	7:1J:48:HIS:C	2.50	0.54
5:4H:18:PHE:HA	5:4H:90:VAL:O	2.08	0.54
5:3H:104:ASP:H	6:3I:26:LEU:HA	1.73	0.54
12:2d:118:LEU:O	12:2d:121:MET:N	2.35	0.54
2:3C:354:THR:O	2:3C:357:PHE:N	2.40	0.54
11:1b:183:GLN:O	11:1b:187:ALA:N	2.35	0.54
5:2H:33:VAL:HA	5:2H:67:ALA:HA	1.90	0.53
5:3H:44:ALA:HB2	8:3N:39:ASN:HA	1.89	0.53
6:3I:4:TRP:O	6:3I:8:GLY:N	2.23	0.53
7:3J:67:ILE:CB	7:4J:63:LEU:CB	2.87	0.53
8:4Q:12:GLY:HA2	8:4R:14:ALA:HB2	1.91	0.53
8:2Q:12:GLY:HA2	8:2R:14:ALA:HB2	1.91	0.53
5:4H:33:VAL:HA	5:4H:67:ALA:HA	1.90	0.52
11:1b:184:SER:O	11:1b:188:GLN:N	2.28	0.52
12:3d:95:GLU:O	12:3d:99:SER:N	2.39	0.51
13:4e:5:GLN:HA	15:4g:36:GLU:HA	1.93	0.51
8:4P:65:LEU:HA	8:4P:68:ALA:HB3	1.93	0.51
12:4d:56:TYR:O	12:4d:60:VAL:N	2.30	0.51
11:2b:118:VAL:CB	12:2d:99:SER:CA	2.87	0.51
3:1F:170:ILE:O	3:1F:174:ALA:HB3	2.10	0.50
3:3F:170:ILE:O	3:3F:174:ALA:HB3	2.10	0.50
13:2e:5:GLN:HA	15:2g:36:GLU:HA	1.93	0.50
12:4d:111:ILE:O	12:4d:112:GLN:C	2.55	0.50
2:3B:52:MET:HA	2:3B:90:ARG:HA	1.93	0.50
8:3P:5:ALA:HA	8:3Q:6:ALA:HB1	1.94	0.49
3:1F:474:ALA:CB	7:1J:45:LEU:CA	2.83	0.49
2:1C:354:THR:C	2:1C:357:PHE:H	2.21	0.49
9:1S:117:PRO:O	9:1S:167:GLY:N	2.42	0.49
2:1B:52:MET:HA	2:1B:90:ARG:HA	1.93	0.49
12:2d:111:ILE:O	12:2d:112:GLN:C	2.55	0.49
3:3D:345:TYR:HA	3:3D:346:PRO:C	2.38	0.49
3:1D:345:TYR:HA	3:1D:346:PRO:C	2.38	0.49
8:1P:5:ALA:HA	8:1Q:6:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2P:65:LEU:HA	8:2P:68:ALA:HB3	1.93	0.48
2:3C:354:THR:C	2:3C:357:PHE:H	2.21	0.48
11:4b:118:VAL:CB	12:4d:99:SER:CA	2.90	0.48
12:4d:97:VAL:O	12:4d:98:LYS:C	2.57	0.48
5:2H:67:ALA:HB3	5:2H:70:GLY:O	2.13	0.48
2:3C:270:ASP:HA	2:3C:326:VAL:O	2.14	0.48
5:4H:67:ALA:HB3	5:4H:70:GLY:O	2.13	0.48
8:2Q:16:VAL:HA	8:2R:17:GLY:HA2	1.96	0.47
6:1I:4:TRP:O	6:1I:8:GLY:N	2.23	0.47
9:2S:121:THR:HA	9:2S:153:LYS:O	2.14	0.47
2:1C:270:ASP:HA	2:1C:326:VAL:O	2.14	0.47
9:4S:121:THR:HA	9:4S:153:LYS:O	2.14	0.47
12:1d:111:ILE:O	12:1d:112:GLN:C	2.58	0.47
11:1b:170:GLN:O	11:1b:174:ILE:N	2.46	0.47
8:2L:5:ALA:HB2	8:2M:3:ASP:HA	1.97	0.47
8:4L:5:ALA:HB2	8:4M:3:ASP:HA	1.97	0.47
8:4Q:16:VAL:HA	8:4R:17:GLY:HA2	1.96	0.47
12:1d:121:MET:O	12:1d:124:ILE:N	2.43	0.47
8:2N:35:GLY:O	8:2N:38:ARG:N	2.47	0.47
9:3S:117:PRO:O	9:3S:167:GLY:N	2.42	0.46
12:2d:97:VAL:O	12:2d:98:LYS:C	2.57	0.46
8:4N:35:GLY:O	8:4N:38:ARG:N	2.47	0.46
11:2b:2:VAL:CB	12:2d:129:GLN:CB	2.94	0.46
12:3d:111:ILE:O	12:3d:112:GLN:C	2.58	0.46
2:1A:362:ARG:O	2:1A:430:GLN:N	2.49	0.46
10:4a:58:MET:O	10:4a:61:HIS:N	2.49	0.45
12:4d:118:LEU:O	12:4d:121:MET:N	2.35	0.45
10:2a:58:MET:O	10:2a:61:HIS:N	2.49	0.45
5:3H:59:ARG:O	5:3H:61:GLY:N	2.50	0.45
15:4g:44:GLU:O	15:4g:48:ALA:N	2.30	0.45
2:3A:362:ARG:O	2:3A:430:GLN:N	2.49	0.45
10:4a:38:VAL:CB	12:4d:128:ASP:CA	2.93	0.45
5:1H:59:ARG:O	5:1H:61:GLY:N	2.50	0.45
2:4B:269:ASP:HA	2:4B:270:ASP:HA	1.75	0.45
12:1d:95:GLU:O	12:1d:99:SER:N	2.39	0.45
8:2O:14:ALA:HB3	8:2O:68:ALA:HB2	1.98	0.45
12:4d:113:GLU:O	12:4d:116:LYS:N	2.50	0.45
10:4a:37:LEU:CA	12:4d:127:PHE:O	2.63	0.45
8:4O:14:ALA:HB3	8:4O:68:ALA:HB2	1.98	0.45
12:2d:113:GLU:O	12:2d:116:LYS:N	2.50	0.44
7:2J:31:GLU:O	7:2J:35:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1A:255:GLU:C	2:1A:257:PHE:H	2.25	0.44
2:2A:201:CYS:O	2:2A:229:THR:HA	2.18	0.44
9:3S:127:ASP:O	9:3S:131:LEU:N	2.47	0.44
2:3C:194:ASP:O	2:3C:196:LYS:N	2.51	0.44
2:1C:194:ASP:O	2:1C:196:LYS:N	2.51	0.44
10:1a:182:MET:HA	10:1a:189:ALA:HB2	1.99	0.44
2:3A:255:GLU:C	2:3A:257:PHE:H	2.25	0.44
2:1A:269:ASP:HA	2:1A:270:ASP:HA	1.79	0.44
11:3b:170:GLN:O	11:3b:174:ILE:N	2.46	0.44
2:4A:201:CYS:O	2:4A:229:THR:HA	2.18	0.44
12:3d:121:MET:O	12:3d:124:ILE:N	2.43	0.44
2:4A:269:ASP:HA	2:4A:270:ASP:HA	1.77	0.44
3:4F:345:TYR:HA	3:4F:346:PRO:C	2.43	0.44
10:2a:120:LYS:O	10:2a:123:ALA:N	2.51	0.43
3:4D:256:ASP:HA	3:4D:257:ASN:HA	1.79	0.43
10:4a:120:LYS:O	10:4a:123:ALA:N	2.51	0.43
15:1g:64:PHE:C	15:1g:66:GLN:H	2.26	0.43
2:3C:202:ILE:O	2:3C:266:ILE:HA	2.18	0.43
2:3C:504:PHE:O	2:3C:507:GLY:N	2.50	0.43
12:2d:95:GLU:O	12:2d:96:ASP:C	2.61	0.43
3:3F:474:ALA:HB1	7:3J:45:LEU:HA	1.86	0.43
8:4L:1:ASP:O	8:4L:4:THR:N	2.52	0.43
3:2F:345:TYR:HA	3:2F:346:PRO:C	2.43	0.43
8:2L:1:ASP:O	8:2L:4:THR:N	2.52	0.43
12:2d:96:ASP:O	12:2d:97:VAL:C	2.62	0.43
10:3a:182:MET:HA	10:3a:189:ALA:HB2	2.00	0.43
2:1C:202:ILE:O	2:1C:266:ILE:HA	2.18	0.43
4:1G:139:GLY:O	4:1G:142:SER:N	2.51	0.43
12:4d:133:GLU:O	12:4d:134:ASP:C	2.61	0.43
2:1C:504:PHE:O	2:1C:507:GLY:N	2.50	0.43
10:2a:105:ALA:HB2	10:2a:157:ALA:HB2	2.01	0.43
8:1P:8:PHE:CB	8:1Q:10:GLY:HA3	2.49	0.43
3:2E:252:LEU:HA	3:2E:305:THR:O	2.19	0.43
9:3S:120:VAL:HA	9:3S:163:ILE:O	2.19	0.43
10:4a:105:ALA:HB2	10:4a:157:ALA:HB2	2.01	0.43
2:3A:200:TYR:O	2:3A:264:ALA:HA	2.19	0.42
8:3P:8:PHE:CB	8:3Q:10:GLY:HA3	2.48	0.42
13:3e:21:GLY:O	15:3g:90:GLU:HA	2.19	0.42
15:3g:64:PHE:C	15:3g:66:GLN:H	2.26	0.42
9:1S:120:VAL:HA	9:1S:163:ILE:O	2.19	0.42
2:3B:172:GLN:O	2:3B:173:THR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3P:19:ALA:HB2	8:3Q:17:GLY:O	2.20	0.42
12:2d:144:LEU:O	12:2d:145:ASP:C	2.63	0.42
4:3G:139:GLY:O	4:3G:142:SER:N	2.51	0.42
2:4C:269:ASP:HA	2:4C:270:ASP:HA	1.80	0.42
12:4d:131:THR:O	12:4d:134:ASP:N	2.52	0.42
12:4d:144:LEU:O	12:4d:145:ASP:C	2.63	0.42
13:1e:21:GLY:O	15:1g:90:GLU:HA	2.19	0.42
2:2A:269:ASP:HA	2:2A:270:ASP:HA	1.76	0.42
12:2d:131:THR:O	12:2d:134:ASP:N	2.52	0.42
12:2d:133:GLU:O	12:2d:134:ASP:C	2.61	0.42
13:2e:22:MET:O	15:2g:93:GLY:HA3	2.20	0.42
18:3k:43:TYR:O	18:3k:46:LEU:N	2.49	0.42
11:4b:6:PRO:O	14:4f:52:LYS:N	2.53	0.42
11:4b:45:LEU:O	11:4b:50:ILE:N	2.45	0.42
8:1P:19:ALA:HB2	8:1Q:17:GLY:O	2.20	0.42
11:2b:6:PRO:O	14:2f:52:LYS:N	2.53	0.42
3:4E:91:LEU:HA	3:4E:216:ALA:HB2	2.02	0.42
5:3H:33:VAL:CB	5:3H:67:ALA:HA	2.50	0.42
5:1H:33:VAL:CB	5:1H:67:ALA:HA	2.50	0.42
8:1K:14:ALA:HB2	8:1R:12:GLY:CA	2.49	0.42
13:2e:21:GLY:O	15:2g:90:GLU:HA	2.20	0.42
2:4C:169:GLY:O	2:4C:328:GLU:HA	2.20	0.42
3:4E:252:LEU:HA	3:4E:305:THR:O	2.19	0.42
13:4e:21:GLY:O	15:4g:90:GLU:HA	2.20	0.42
2:1C:354:THR:HA	2:1C:357:PHE:CB	2.50	0.41
8:3K:14:ALA:HB2	8:3R:12:GLY:CA	2.49	0.41
16:3h:21:LYS:O	16:3h:27:GLY:HA2	2.21	0.41
12:4d:95:GLU:O	12:4d:96:ASP:C	2.61	0.41
3:4D:451:HIS:C	7:4J:44:ALA:CB	2.89	0.41
13:4e:22:MET:O	15:4g:93:GLY:HA3	2.20	0.41
10:4a:37:LEU:N	12:4d:127:PHE:O	2.53	0.41
16:1h:21:LYS:O	16:1h:27:GLY:HA2	2.21	0.41
8:2M:15:THR:C	8:2M:17:GLY:H	2.29	0.41
2:4C:105:GLY:HA2	2:4C:226:MET:O	2.20	0.41
8:4M:15:THR:C	8:4M:17:GLY:H	2.29	0.41
2:1A:200:TYR:O	2:1A:264:ALA:HA	2.19	0.41
2:1B:172:GLN:O	2:1B:173:THR:C	2.62	0.41
3:2E:256:ASP:HA	3:2E:257:ASN:HA	1.82	0.41
2:1B:269:ASP:O	2:1B:270:ASP:C	2.63	0.41
2:2C:169:GLY:O	2:2C:328:GLU:HA	2.20	0.41
15:2g:44:GLU:O	15:2g:48:ALA:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3C:354:THR:HA	2:3C:357:PHE:CB	2.50	0.41
8:3K:14:ALA:HB2	8:3R:12:GLY:HA2	2.03	0.41
10:4a:182:MET:HA	10:4a:185:SER:O	2.21	0.41
2:3B:269:ASP:O	2:3B:270:ASP:C	2.63	0.41
3:3E:345:TYR:HA	3:3E:346:PRO:C	2.46	0.41
18:1k:43:TYR:O	18:1k:46:LEU:N	2.50	0.41
2:3A:269:ASP:HA	2:3A:270:ASP:HA	1.79	0.41
3:2E:91:LEU:HA	3:2E:216:ALA:HB2	2.02	0.40
3:1E:345:TYR:HA	3:1E:346:PRO:C	2.46	0.40
8:2P:35:GLY:C	8:2P:37:ALA:N	2.79	0.40
10:4a:38:VAL:N	12:4d:128:ASP:CA	2.60	0.40
6:3I:4:TRP:HA	6:3I:7:ALA:HB3	2.03	0.40
2:4A:105:GLY:HA2	2:4A:226:MET:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	18	39/66 (59%)	39 (100%)	0	0	100	100
1	28	39/66 (59%)	37 (95%)	2 (5%)	0	100	100
1	38	39/66 (59%)	39 (100%)	0	0	100	100
1	48	39/66 (59%)	37 (95%)	2 (5%)	0	100	100
2	1A	506/553 (92%)	457 (90%)	48 (10%)	1 (0%)	43	78
2	1B	473/553 (86%)	430 (91%)	41 (9%)	2 (0%)	30	67
2	1C	494/553 (89%)	457 (92%)	36 (7%)	1 (0%)	43	78
2	2A	506/553 (92%)	472 (93%)	34 (7%)	0	100	100
2	2B	473/553 (86%)	449 (95%)	23 (5%)	1 (0%)	43	78
2	2C	494/553 (89%)	462 (94%)	31 (6%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3A	506/553 (92%)	457 (90%)	48 (10%)	1 (0%)	43	78
2	3B	473/553 (86%)	430 (91%)	41 (9%)	2 (0%)	30	67
2	3C	494/553 (89%)	457 (92%)	36 (7%)	1 (0%)	43	78
2	4A	506/553 (92%)	472 (93%)	34 (7%)	0	100	100
2	4B	473/553 (86%)	449 (95%)	23 (5%)	1 (0%)	43	78
2	4C	494/553 (89%)	463 (94%)	30 (6%)	1 (0%)	43	78
3	1D	467/528 (88%)	420 (90%)	47 (10%)	0	100	100
3	1E	465/528 (88%)	428 (92%)	37 (8%)	0	100	100
3	1F	465/528 (88%)	428 (92%)	37 (8%)	0	100	100
3	2D	467/528 (88%)	441 (94%)	25 (5%)	1 (0%)	43	78
3	2E	465/528 (88%)	440 (95%)	24 (5%)	1 (0%)	43	78
3	2F	465/528 (88%)	445 (96%)	20 (4%)	0	100	100
3	3D	467/528 (88%)	420 (90%)	47 (10%)	0	100	100
3	3E	465/528 (88%)	428 (92%)	37 (8%)	0	100	100
3	3F	465/528 (88%)	429 (92%)	36 (8%)	0	100	100
3	4D	467/528 (88%)	441 (94%)	25 (5%)	1 (0%)	43	78
3	4E	465/528 (88%)	440 (95%)	24 (5%)	1 (0%)	43	78
3	4F	465/528 (88%)	445 (96%)	20 (4%)	0	100	100
4	1G	270/298 (91%)	254 (94%)	16 (6%)	0	100	100
4	2G	270/298 (91%)	257 (95%)	13 (5%)	0	100	100
4	3G	270/298 (91%)	254 (94%)	16 (6%)	0	100	100
4	4G	270/298 (91%)	257 (95%)	13 (5%)	0	100	100
5	1H	130/168 (77%)	114 (88%)	16 (12%)	0	100	100
5	2H	130/168 (77%)	123 (95%)	7 (5%)	0	100	100
5	3H	130/168 (77%)	114 (88%)	16 (12%)	0	100	100
5	4H	130/168 (77%)	123 (95%)	7 (5%)	0	100	100
6	1I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
6	2I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
6	3I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
6	4I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
7	1J	54/109 (50%)	53 (98%)	0	1 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2J	51/109 (47%)	51 (100%)	0	0	100	100
7	3J	54/109 (50%)	54 (100%)	0	0	100	100
7	4J	51/109 (47%)	51 (100%)	0	0	100	100
8	1K	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
8	1L	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	1M	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	1N	73/143 (51%)	68 (93%)	5 (7%)	0	100	100
8	1O	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	1P	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	1Q	73/143 (51%)	72 (99%)	1 (1%)	0	100	100
8	1R	73/143 (51%)	72 (99%)	1 (1%)	0	100	100
8	2K	72/143 (50%)	67 (93%)	5 (7%)	0	100	100
8	2L	72/143 (50%)	70 (97%)	1 (1%)	1 (1%)	9	40
8	2M	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	2N	73/143 (51%)	65 (89%)	8 (11%)	0	100	100
8	2O	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	2P	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
8	2Q	73/143 (51%)	67 (92%)	6 (8%)	0	100	100
8	2R	73/143 (51%)	66 (90%)	7 (10%)	0	100	100
8	3K	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
8	3L	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	3M	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	3N	73/143 (51%)	68 (93%)	5 (7%)	0	100	100
8	3O	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	3P	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	3Q	73/143 (51%)	72 (99%)	1 (1%)	0	100	100
8	3R	73/143 (51%)	72 (99%)	1 (1%)	0	100	100
8	4K	72/143 (50%)	67 (93%)	5 (7%)	0	100	100
8	4L	72/143 (50%)	70 (97%)	1 (1%)	1 (1%)	9	40
8	4M	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	4N	73/143 (51%)	65 (89%)	8 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	4O	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	4P	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
8	4Q	73/143 (51%)	67 (92%)	6 (8%)	0	100	100
8	4R	73/143 (51%)	66 (90%)	7 (10%)	0	100	100
9	1S	186/213 (87%)	176 (95%)	10 (5%)	0	100	100
9	2S	186/213 (87%)	181 (97%)	5 (3%)	0	100	100
9	3S	186/213 (87%)	176 (95%)	10 (5%)	0	100	100
9	4S	186/213 (87%)	181 (97%)	5 (3%)	0	100	100
10	1a	224/226 (99%)	216 (96%)	8 (4%)	0	100	100
10	2a	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	30	67
10	3a	224/226 (99%)	216 (96%)	8 (4%)	0	100	100
10	4a	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	30	67
11	1b	207/256 (81%)	201 (97%)	6 (3%)	0	100	100
11	2b	207/256 (81%)	200 (97%)	7 (3%)	0	100	100
11	3b	207/256 (81%)	201 (97%)	6 (3%)	0	100	100
11	4b	207/256 (81%)	200 (97%)	7 (3%)	0	100	100
12	1d	153/161 (95%)	134 (88%)	19 (12%)	0	100	100
12	2d	153/161 (95%)	129 (84%)	24 (16%)	0	100	100
12	3d	153/161 (95%)	134 (88%)	19 (12%)	0	100	100
12	4d	153/161 (95%)	129 (84%)	24 (16%)	0	100	100
13	1e	54/71 (76%)	54 (100%)	0	0	100	100
13	2e	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
13	3e	54/71 (76%)	54 (100%)	0	0	100	100
13	4e	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
14	1f	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
14	2f	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
14	3f	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
14	4f	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
15	1g	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
15	2g	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
15	3g	77/103 (75%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	4g	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
16	1h	42/108 (39%)	40 (95%)	2 (5%)	0	100	100
16	2h	45/108 (42%)	44 (98%)	1 (2%)	0	100	100
16	3h	42/108 (39%)	40 (95%)	2 (5%)	0	100	100
16	4h	45/108 (42%)	44 (98%)	1 (2%)	0	100	100
17	1j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
17	2j	46/60 (77%)	45 (98%)	1 (2%)	0	100	100
17	3j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
17	4j	46/60 (77%)	45 (98%)	1 (2%)	0	100	100
18	1k	34/58 (59%)	32 (94%)	2 (6%)	0	100	100
18	2k	34/58 (59%)	33 (97%)	1 (3%)	0	100	100
18	3k	34/58 (59%)	32 (94%)	2 (6%)	0	100	100
18	4k	34/58 (59%)	33 (97%)	1 (3%)	0	100	100
All	All	20372/25692 (79%)	19076 (94%)	1275 (6%)	21 (0%)	49	83

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1A	409	ASP
2	1B	142	VAL
2	1B	363	PRO
2	1C	363	PRO
2	2B	194	ASP
2	2C	377	ALA
3	2D	451	HIS
3	2E	395	GLU
2	3A	409	ASP
2	3B	142	VAL
2	3B	363	PRO
2	3C	363	PRO
2	4B	194	ASP
2	4C	377	ALA
3	4D	451	HIS
3	4E	395	GLU
8	2L	44	GLN
8	4L	44	GLN
7	1J	48	HIS

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Mol	Chain	Res	Type
10	2a	17	LEU
10	4a	17	LEU

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

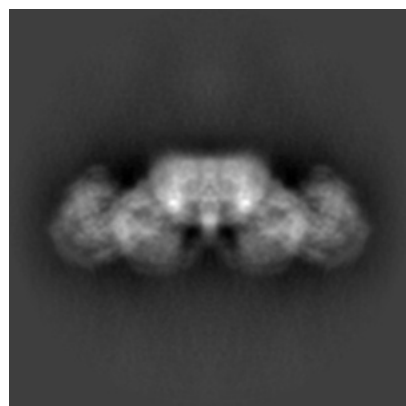
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65238. These allow visual inspection of the internal detail of the map and identification of artifacts.

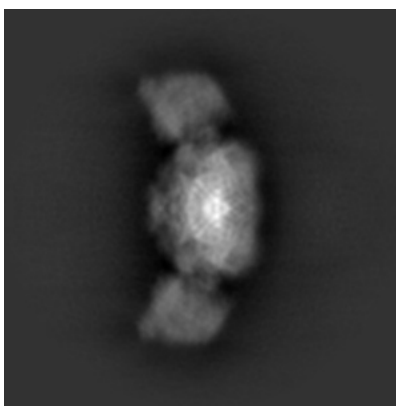
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

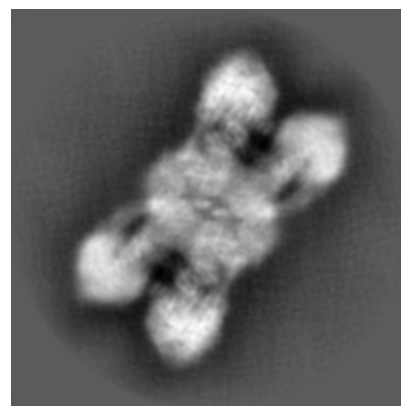
6.1.1 Primary map



X

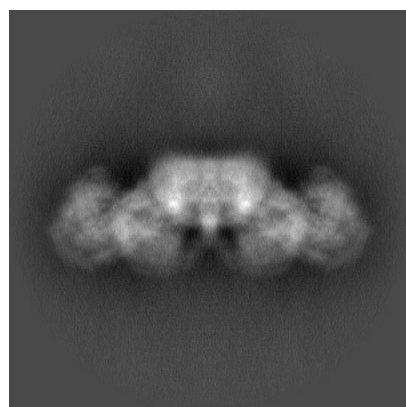


Y

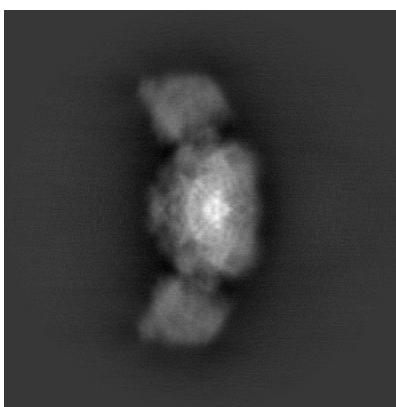


Z

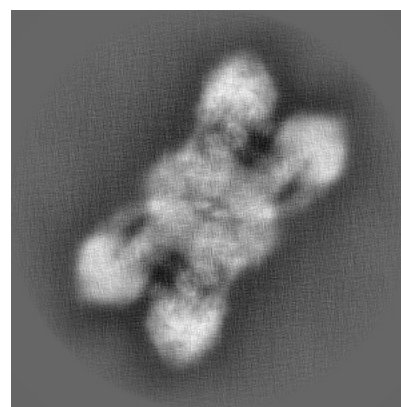
6.1.2 Raw map



X



Y

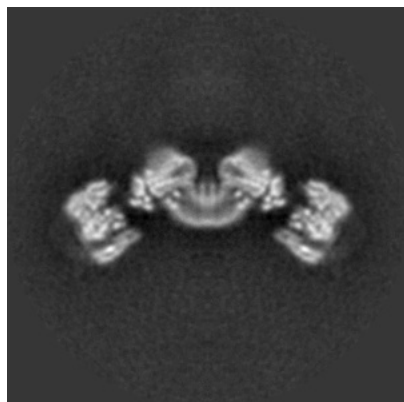


Z

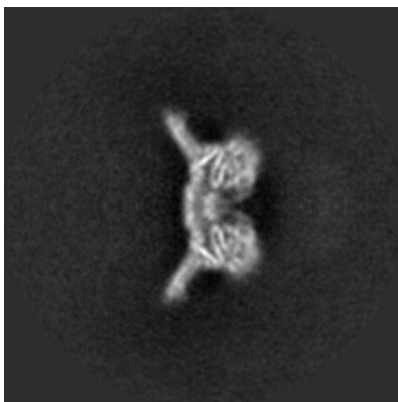
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

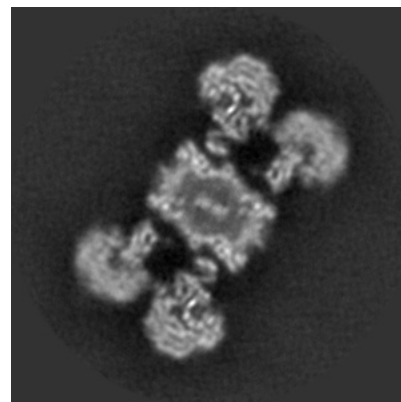
6.2.1 Primary map



X Index: 180

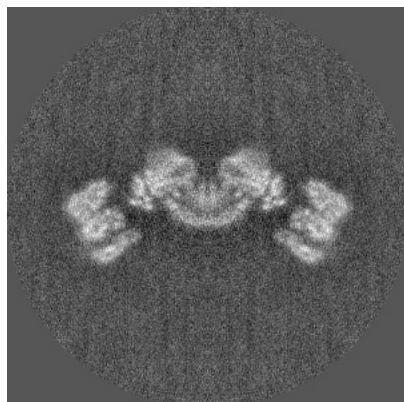


Y Index: 180

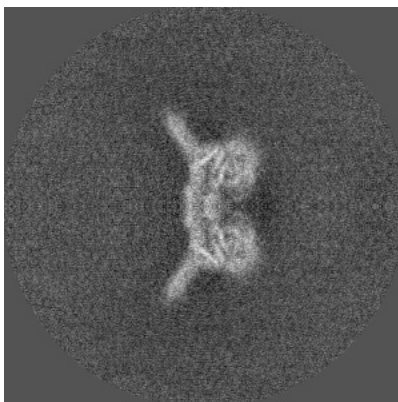


Z Index: 180

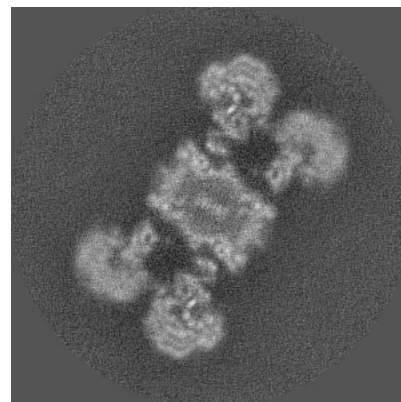
6.2.2 Raw map



X Index: 180



Y Index: 180

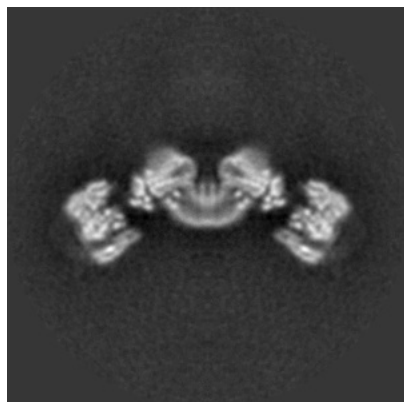


Z Index: 180

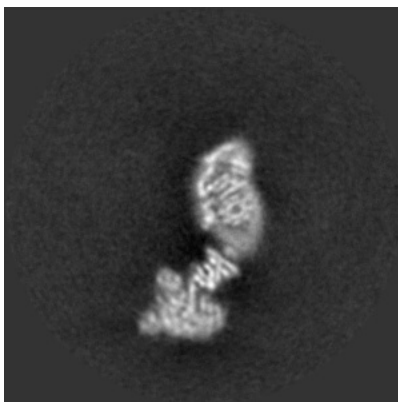
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

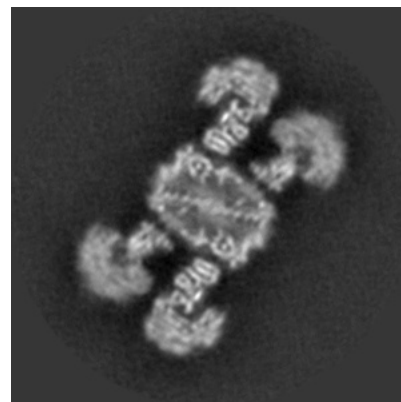
6.3.1 Primary map



X Index: 180

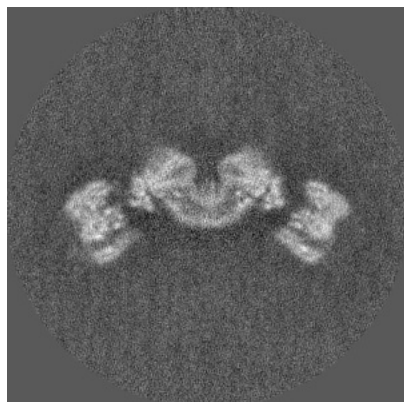


Y Index: 148

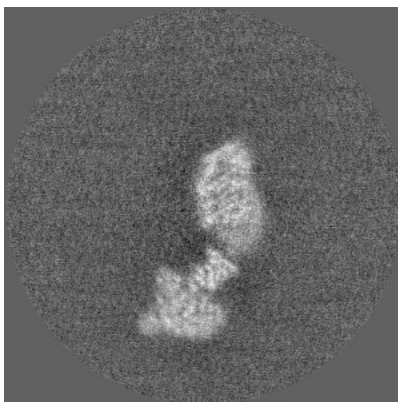


Z Index: 185

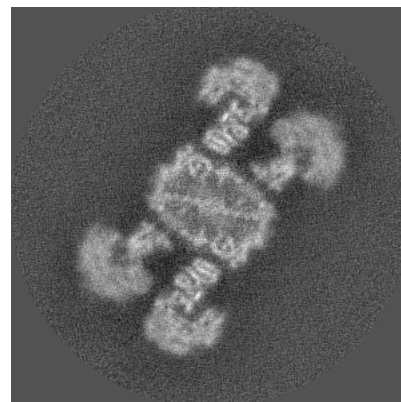
6.3.2 Raw map



X Index: 179



Y Index: 147



Z Index: 185

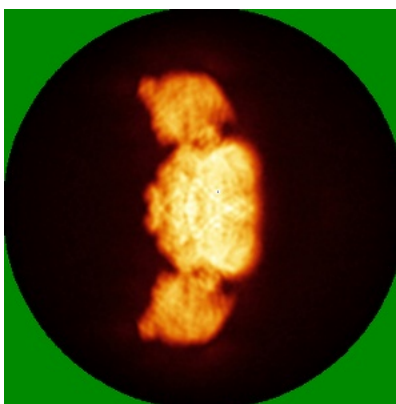
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

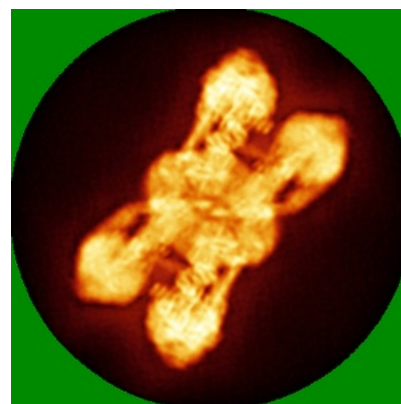
6.4.1 Primary map



X

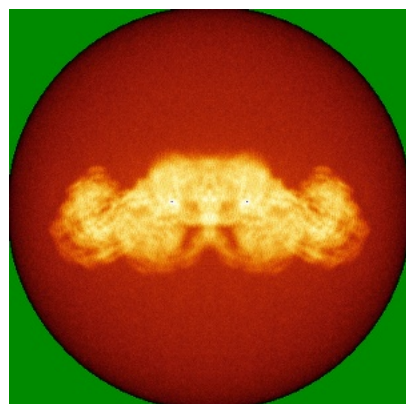


Y

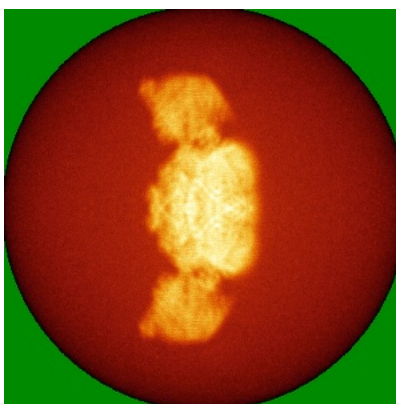


Z

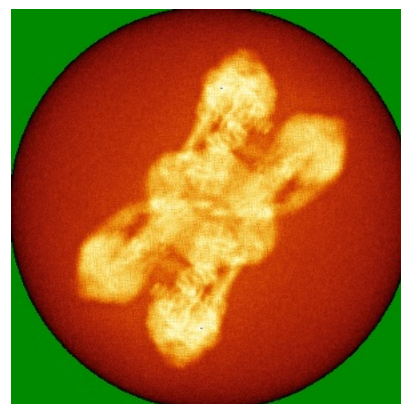
6.4.2 Raw map



X



Y

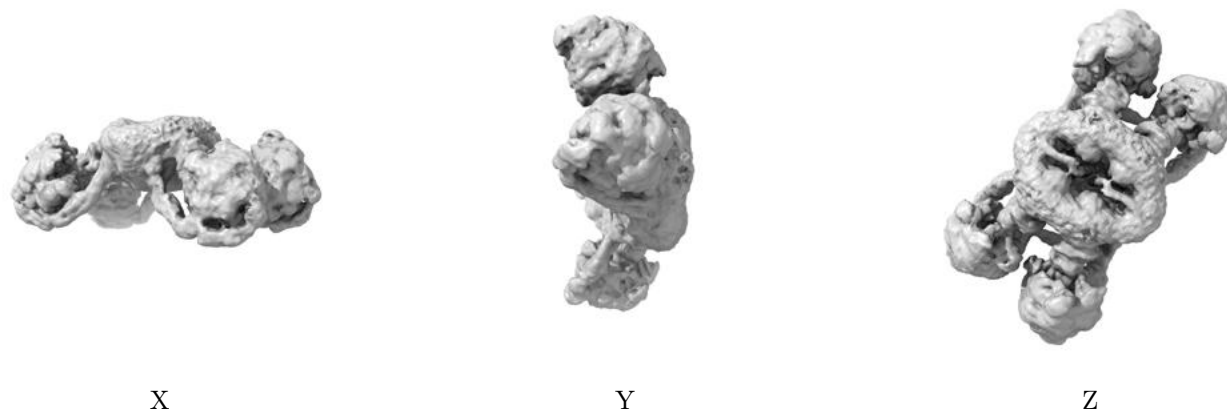


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

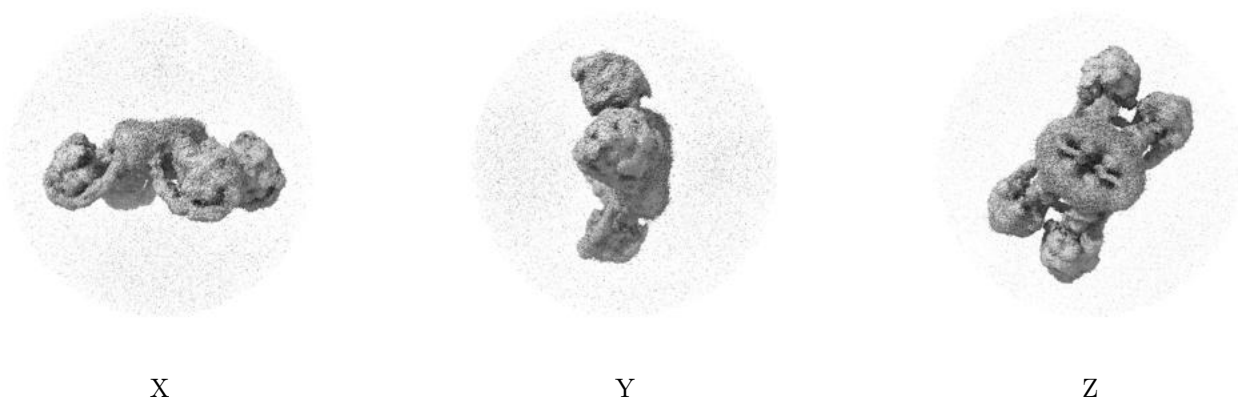
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00519. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

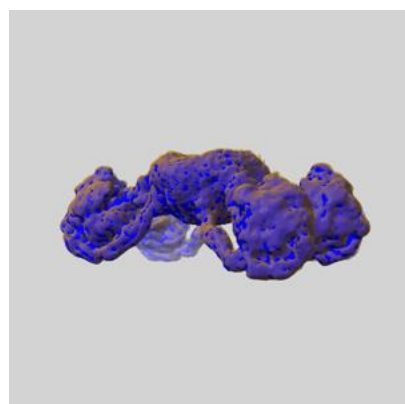
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

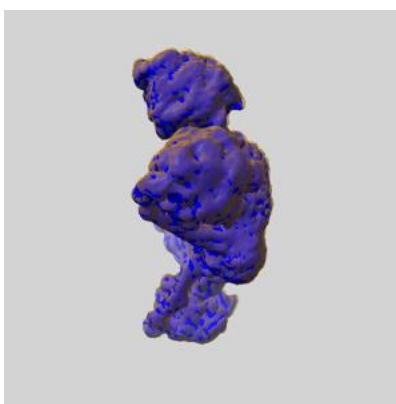
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

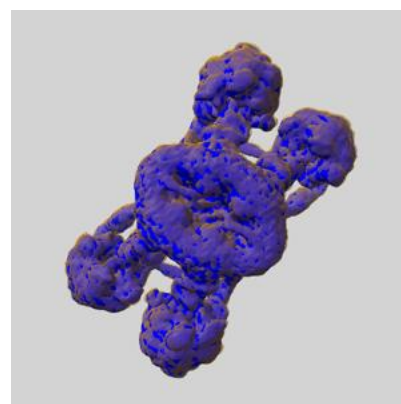
6.6.1 emd_65238_msk_1.map [i](#)



X



Y

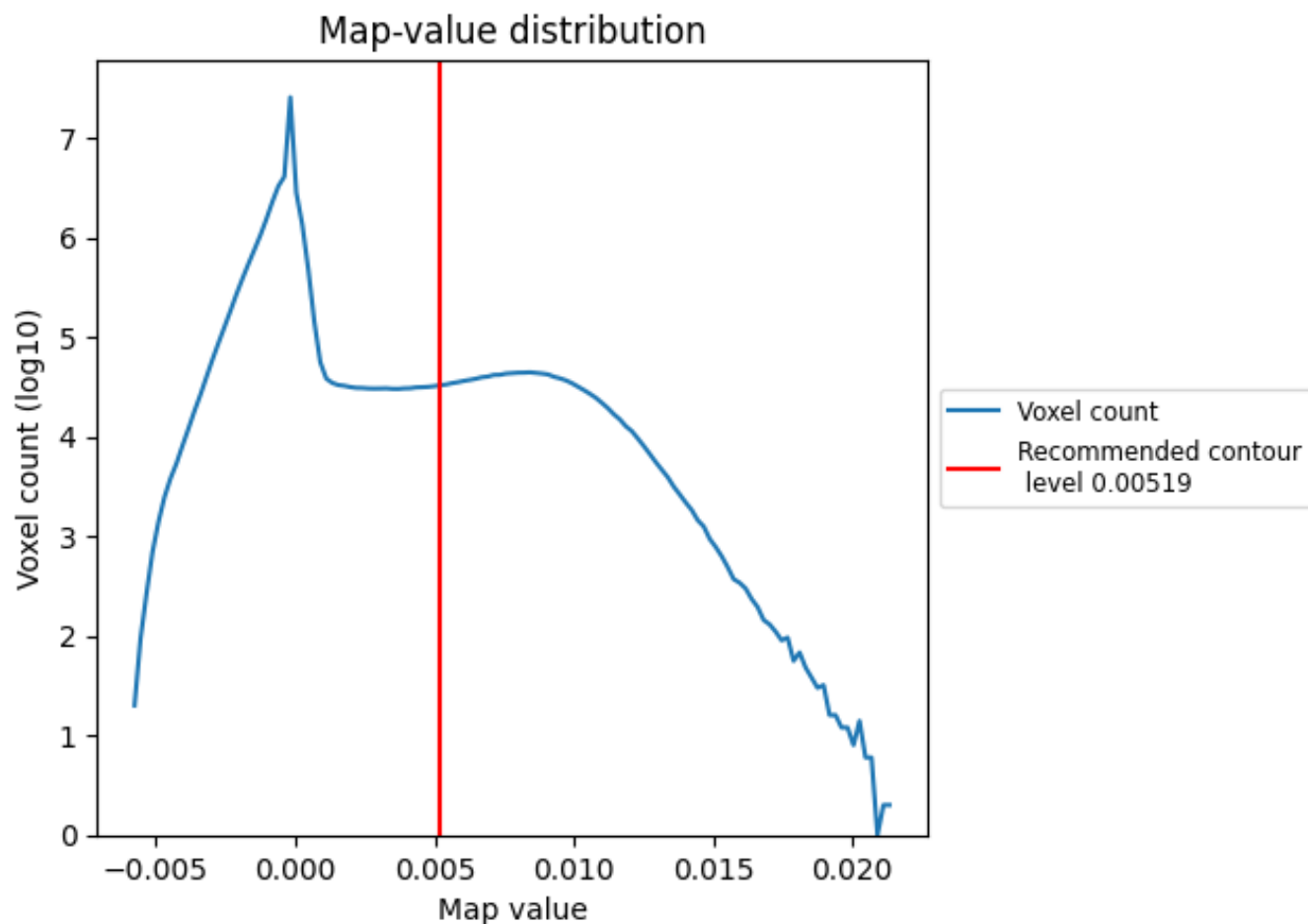


Z

7 Map analysis [i](#)

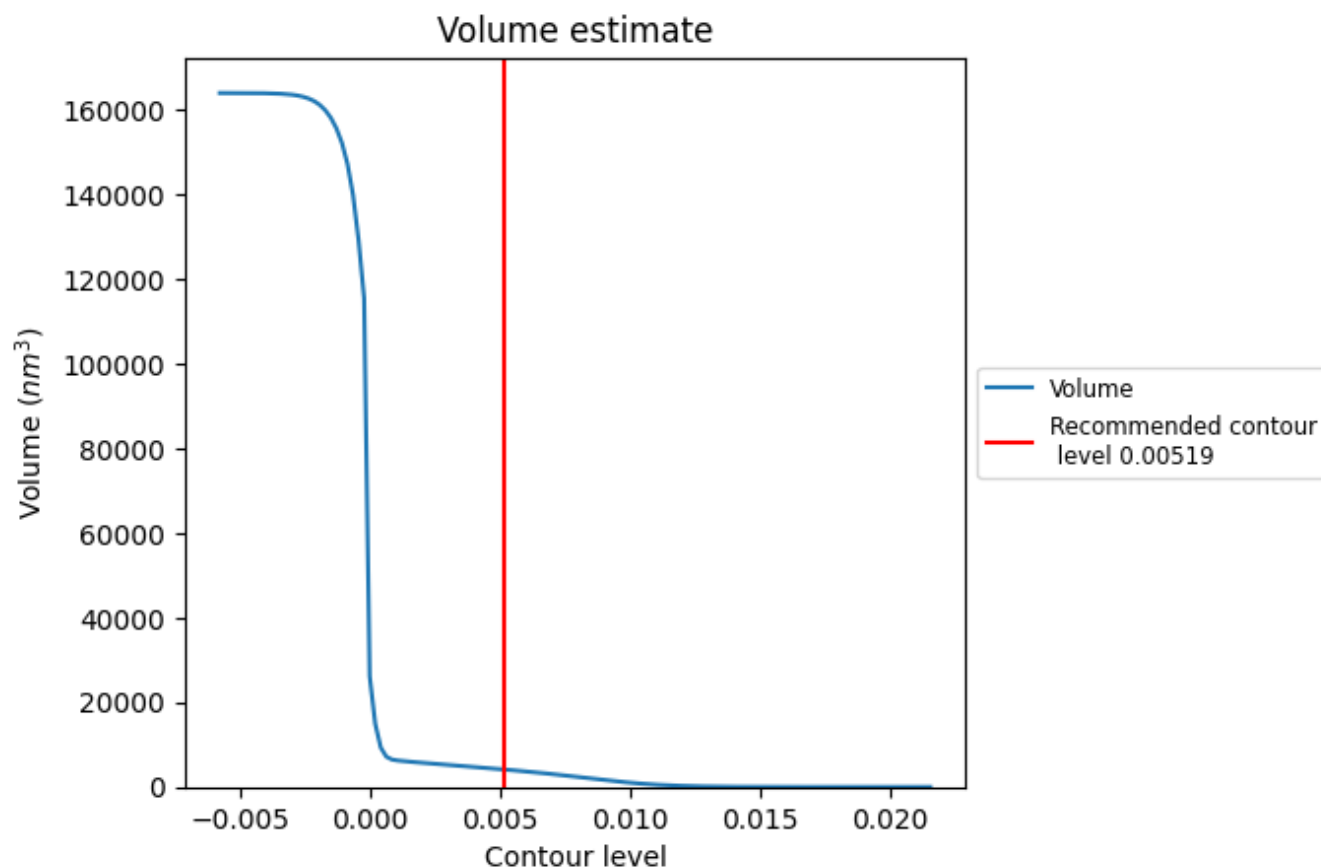
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

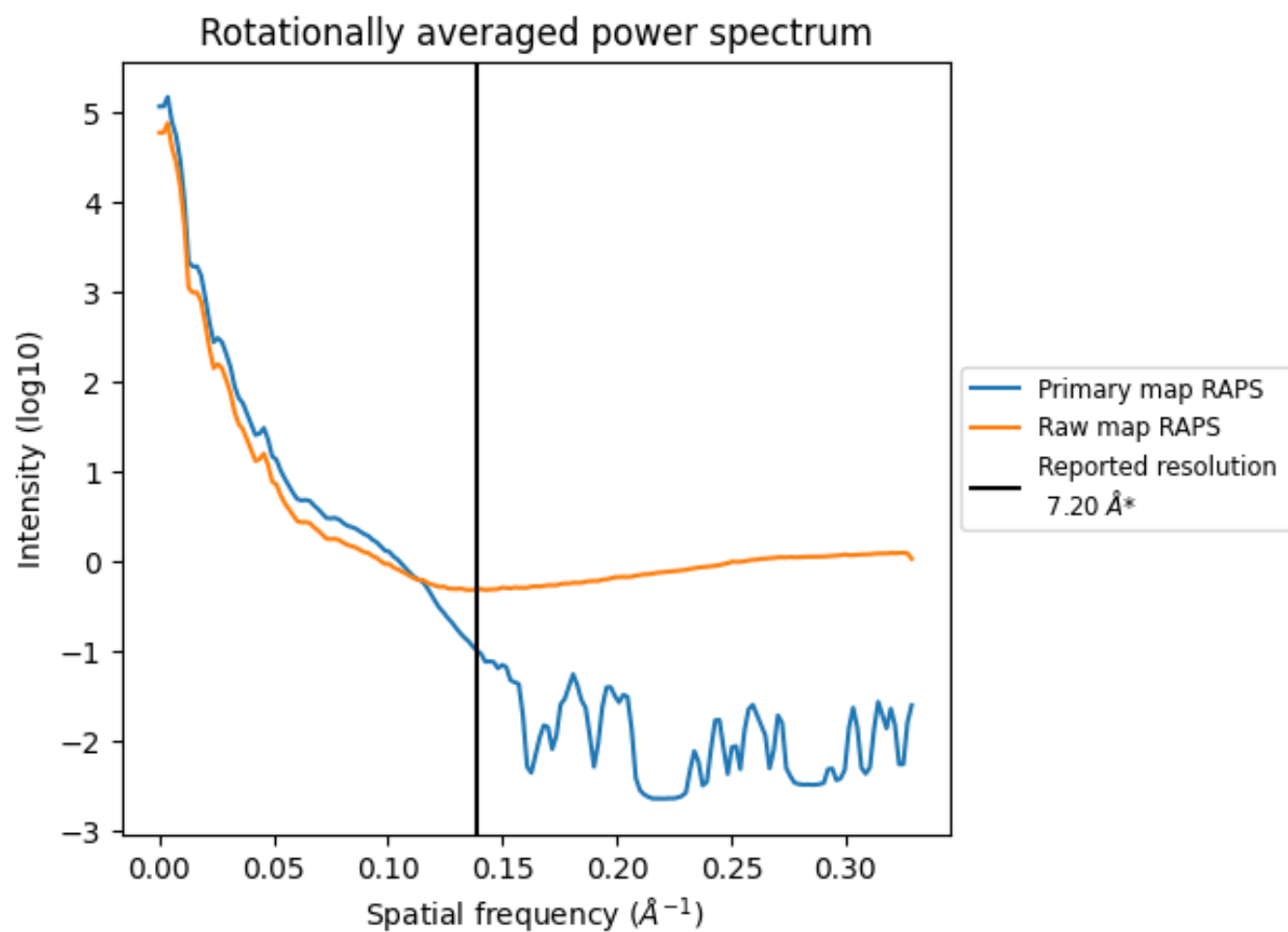
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4114 nm³; this corresponds to an approximate mass of 3716 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

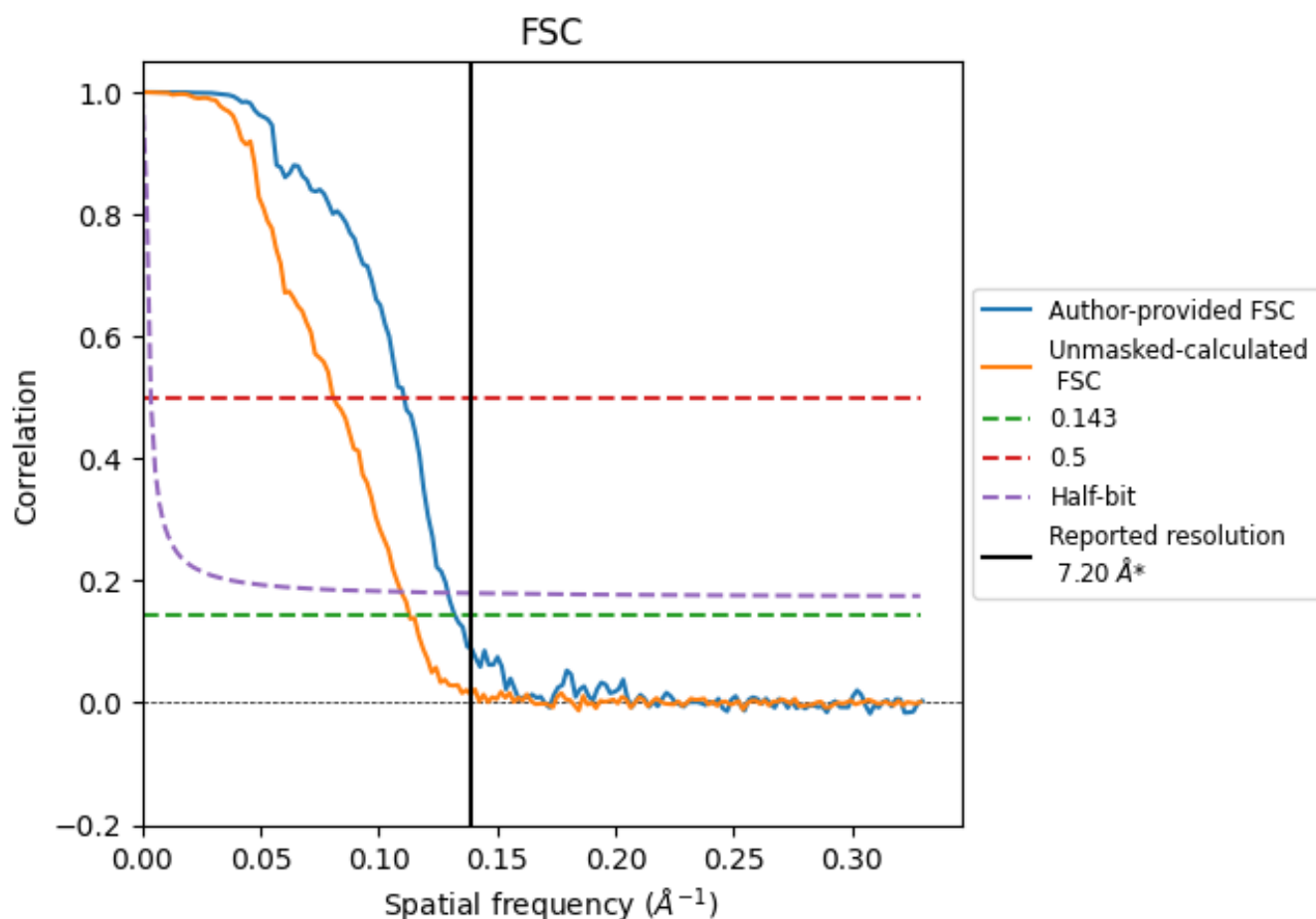


*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

8.2 Resolution estimates [i](#)

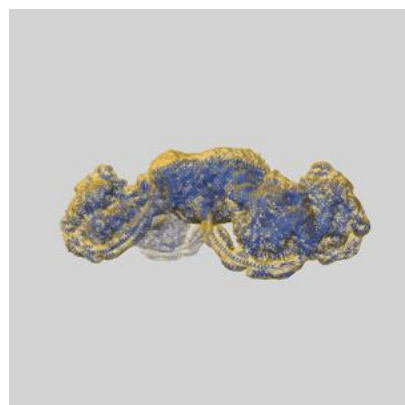
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.56	9.03	7.73
Unmasked-calculated*	8.86	12.36	9.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.86 differs from the reported value 7.2 by more than 10 %

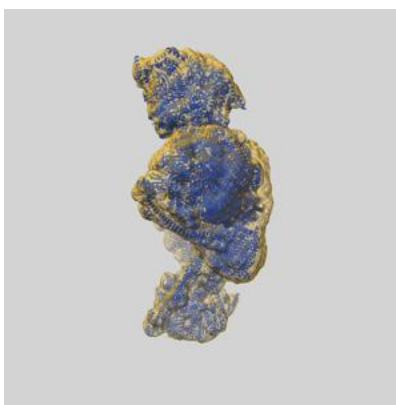
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65238 and PDB model 9VPC. Per-residue inclusion information can be found in section 3 on page 16.

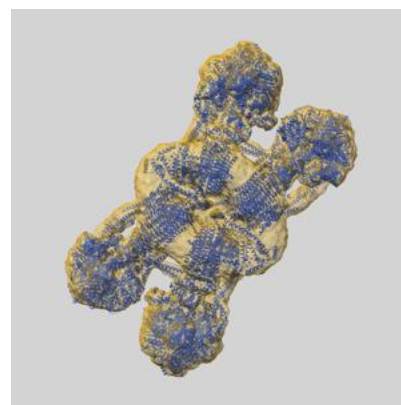
9.1 Map-model overlay [i](#)



X



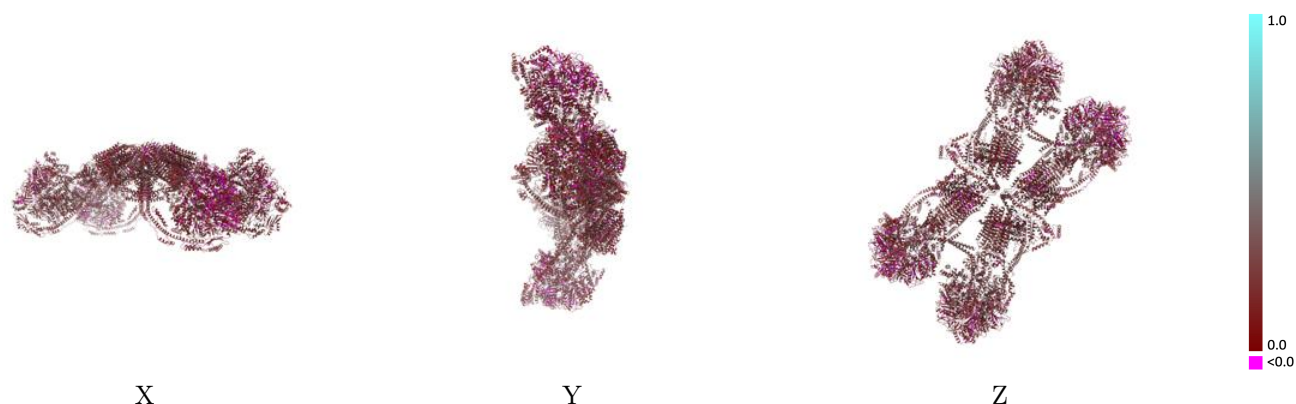
Y



Z

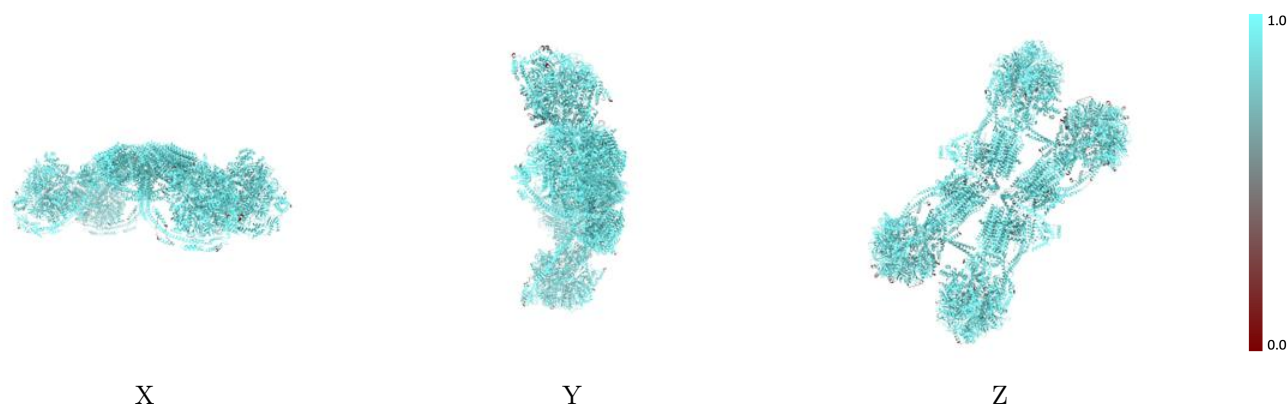
The images above show the 3D surface view of the map at the recommended contour level 0.00519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



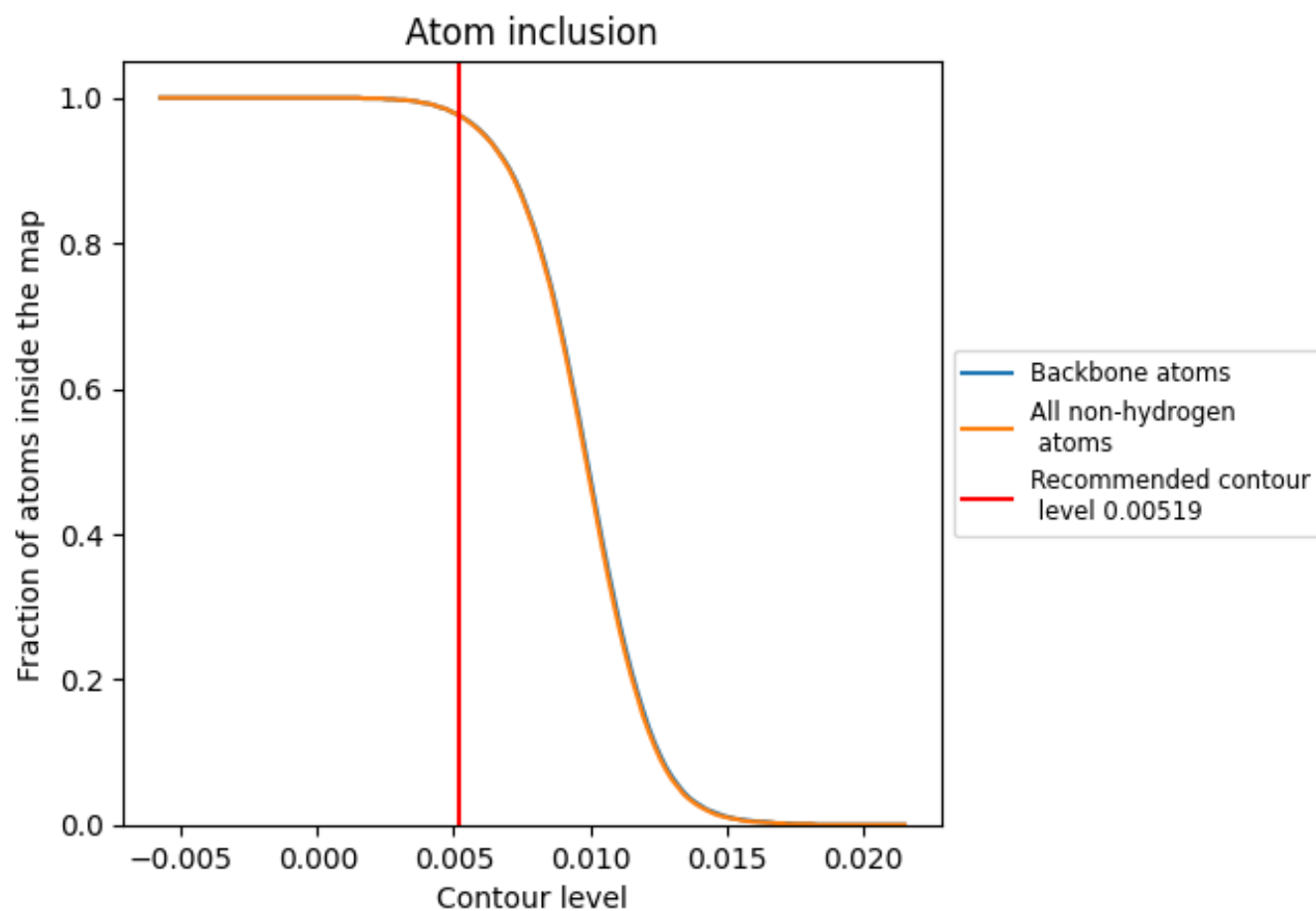
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00519).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.1880
18	 0.9950	 0.2070
1A	 0.9720	 0.1700
1B	 0.9700	 0.2020
1C	 0.9970	 0.2190
1D	 0.9880	 0.1870
1E	 0.9820	 0.1870
1F	 0.9930	 0.2210
1G	 0.9870	 0.2480
1H	 0.9990	 0.2350
1I	 0.9790	 0.2120
1J	 0.9710	 0.2680
1K	 1.0000	 0.2250
1L	 0.9940	 0.2450
1M	 0.9920	 0.2000
1N	 0.9970	 0.2350
1O	 1.0000	 0.2360
1P	 1.0000	 0.2240
1Q	 1.0000	 0.2210
1R	 1.0000	 0.2370
1S	 0.9420	 0.1930
1a	 0.9990	 0.2410
1b	 0.9920	 0.2480
1d	 0.9960	 0.2390
1e	 0.9820	 0.1910
1f	 0.9880	 0.2100
1g	 0.9970	 0.1980
1h	 0.9950	 0.2370
1j	 0.9750	 0.2650
1k	 1.0000	 0.2420
28	 0.9950	 0.2220
2A	 0.9290	 0.1300
2B	 0.9900	 0.1410
2C	 0.9810	 0.1560
2D	 0.9600	 0.1430



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Chain	Atom inclusion	Q-score
2E	 0.9780	 0.1350
2F	 0.9900	 0.1680
2G	 0.9840	 0.2150
2H	 0.9540	 0.1980
2I	 0.8580	 0.1680
2J	 1.0000	 0.2820
2K	 1.0000	 0.2080
2L	 1.0000	 0.1860
2M	 1.0000	 0.2110
2N	 0.9970	 0.1990
2O	 0.9950	 0.2020
2P	 0.9920	 0.1970
2Q	 0.9970	 0.1990
2R	 1.0000	 0.1960
2S	 0.8550	 0.1210
2a	 1.0000	 0.2410
2b	 0.9860	 0.2230
2d	 0.8540	 0.1710
2e	 0.9930	 0.2160
2f	 0.9930	 0.2200
2g	 1.0000	 0.2060
2h	 0.9740	 0.1890
2j	 1.0000	 0.2100
2k	 0.9320	 0.1630
38	 1.0000	 0.1900
3A	 0.9720	 0.1640
3B	 0.9790	 0.1780
3C	 0.9980	 0.2220
3D	 0.9820	 0.1910
3E	 0.9850	 0.1570
3F	 0.9900	 0.2050
3G	 0.9930	 0.2140
3H	 0.9890	 0.2090
3I	 0.9700	 0.2010
3J	 0.9680	 0.2460
3K	 1.0000	 0.1890
3L	 0.9920	 0.2330
3M	 0.9700	 0.2050
3N	 0.9810	 0.2190
3O	 0.9950	 0.2390
3P	 1.0000	 0.2190
3Q	 1.0000	 0.2190

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Chain	Atom inclusion	Q-score
3R	 0.9950	 0.2200
3S	 0.9770	 0.1890
3a	 0.9970	 0.2300
3b	 0.9960	 0.2310
3d	 0.9950	 0.2410
3e	 0.9750	 0.1980
3f	 0.9930	 0.2220
3g	 1.0000	 0.2250
3h	 0.9950	 0.2230
3j	 0.9370	 0.2410
3k	 1.0000	 0.2440
48	 1.0000	 0.2070
4A	 0.9230	 0.1160
4B	 0.9700	 0.1290
4C	 0.9690	 0.1710
4D	 0.9490	 0.1490
4E	 0.9740	 0.1120
4F	 0.9870	 0.1670
4G	 0.9700	 0.2110
4H	 0.9510	 0.1900
4I	 0.8460	 0.1670
4J	 1.0000	 0.2910
4K	 1.0000	 0.1960
4L	 0.9970	 0.1910
4M	 0.9970	 0.2160
4N	 0.9920	 0.2060
4O	 0.9840	 0.2080
4P	 0.9780	 0.1920
4Q	 1.0000	 0.2050
4R	 1.0000	 0.2000
4S	 0.9140	 0.1220
4a	 1.0000	 0.2540
4b	 0.9810	 0.2190
4d	 0.8310	 0.1550
4e	 1.0000	 0.2270
4f	 0.9930	 0.2420
4g	 0.9970	 0.2080
4h	 0.9740	 0.1800
4j	 0.9920	 0.2100
4k	 0.9890	 0.1730