



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 08:28 PM EST

PDB ID : 6CP3
EMDB ID : EMD-7546
Title : Monomer yeast ATP synthase (F1Fo) reconstituted in nanodisc with inhibitor of oligomycin bound.
Authors : Srivastava, A.P.; Luo, M.; Symersky, J.; Liao, M.F.; Mueller, D.M.
Deposited on : 2018-03-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

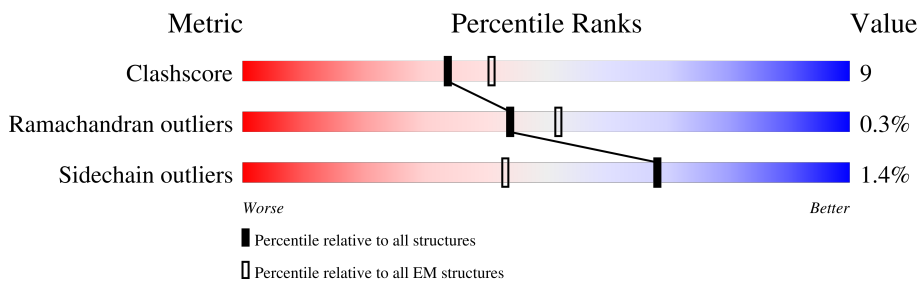
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	K	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">61%</div> </div>
1	L	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">58%</div> </div>
1	M	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">61%</div> </div>
1	N	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">59%</div> </div>
1	O	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">51%</div> </div>
1	P	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">70%</div> </div>
1	Q	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">62%</div> </div>
1	R	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">57%</div> </div>
1	R	76	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">61%</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	76	43% 62% 36% .
1	T	76	53% 67% 30% .
2	Y	195	11% 58% 33%
3	A	510	7% 80% 19% .
3	B	510	8% 80% 19% .
3	C	510	8% 79% 20% .
4	D	478	6% 80% 18% .
4	E	478	9% 81% 18% .
4	F	478	5% 82% 17% .
5	G	278	10% 83% 14% .
6	H	138	26% 73% 22% .
7	I	61	15% 90% 7% .
8	Z	209	27% 60% 14% 26%
9	7	173	41% 79% 18% ..
10	6	92	78% 71% 26% .
11	U	95	53% 61% 27% . 11%
12	8	48	42% 67% 19% . 12%
13	X	249	60% 69% 21% 10%
14	J	37	76% 95% 5%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 38882 atoms, of which 0 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 subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	74	Total 535	C 358	N 82	O 91	S 4	0	0
1	L	74	Total 532	C 356	N 82	O 91	S 3	0	0
1	M	75	Total 537	C 359	N 83	O 92	S 3	0	0
1	N	74	Total 532	C 356	N 82	O 91	S 3	0	0
1	O	74	Total 533	C 357	N 82	O 91	S 3	0	0
1	P	74	Total 535	C 358	N 82	O 91	S 4	0	0
1	Q	74	Total 532	C 356	N 82	O 91	S 3	0	0
1	R	75	Total 537	C 359	N 83	O 92	S 3	0	0
1	S	74	Total 532	C 356	N 82	O 91	S 3	0	0
1	T	74	Total 533	C 357	N 82	O 91	S 3	0	0

- Molecule 2 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Y	187	Total 1317	C 828	N 226	O 262	S 1	0	0

- Molecule 3 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	507	Total 3852	C 2432	N 676	O 741	S 3	0	0
3	B	506	Total 3836	C 2420	N 678	O 735	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	508	Total	C	N	O	S	0	0
			3865	2439	680	743	3		

- Molecule 4 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
4	E	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	F	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

- Molecule 5 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		

- Molecule 6 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	132	Total	C	N	O	S	0	0
			990	624	165	199	2		

- Molecule 7 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	59	Total	C	N	O	0	0
			392	243	71	78		

- Molecule 8 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	155	Total	C	N	O	S	0	0
			1232	778	211	242	1		

- Molecule 9 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	7	171	1363	856	236	268	3	0	0

- Molecule 10 is a protein called ATP synthase subunit H, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	6	89	710	441	114	155		0	0

- Molecule 11 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	U	85	639	420	109	109	1	0	0

- Molecule 12 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	8	42	364	256	52	53	3	0	0

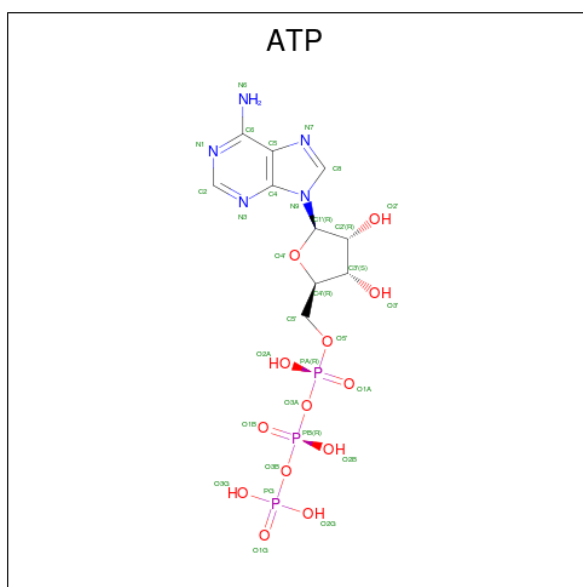
- Molecule 13 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	X	224	1772	1210	265	287	10	0	0

- Molecule 14 is a protein called ATP synthase subunit J, mitochondrial.

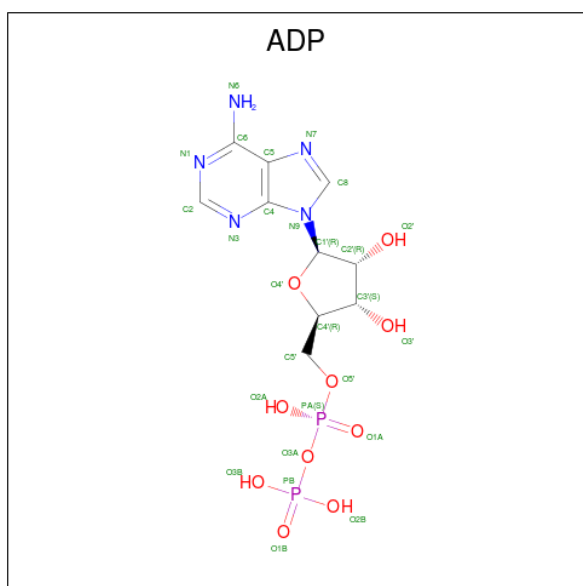
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	37	292	197	45	48	2	0	0

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

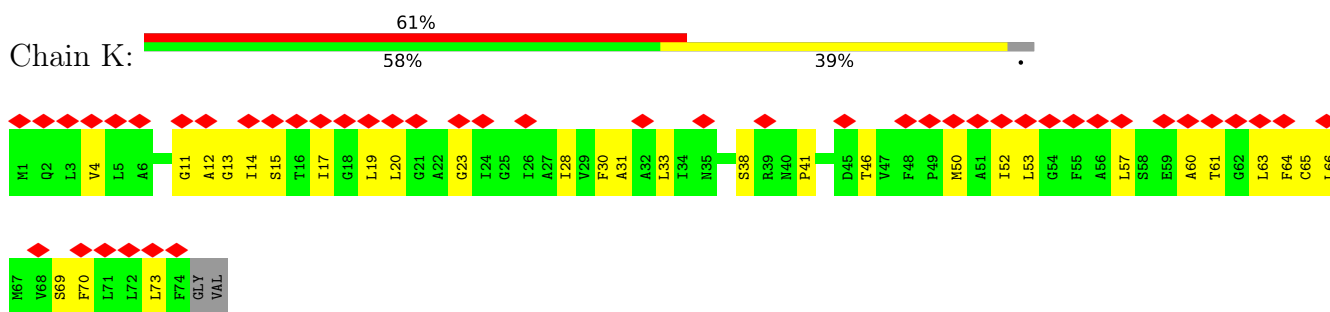


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	D	1	27	10	5	10	2	0
16	F	1	27	10	5	10	2	0

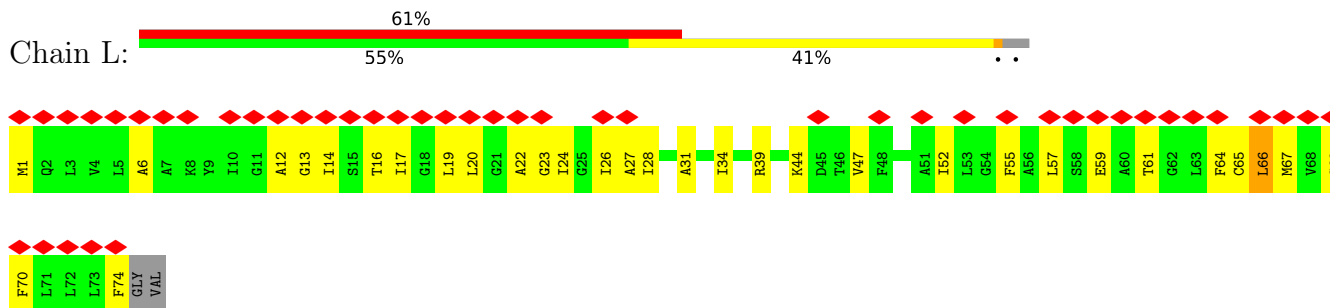
3 Residue-property plots [i](#)

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.

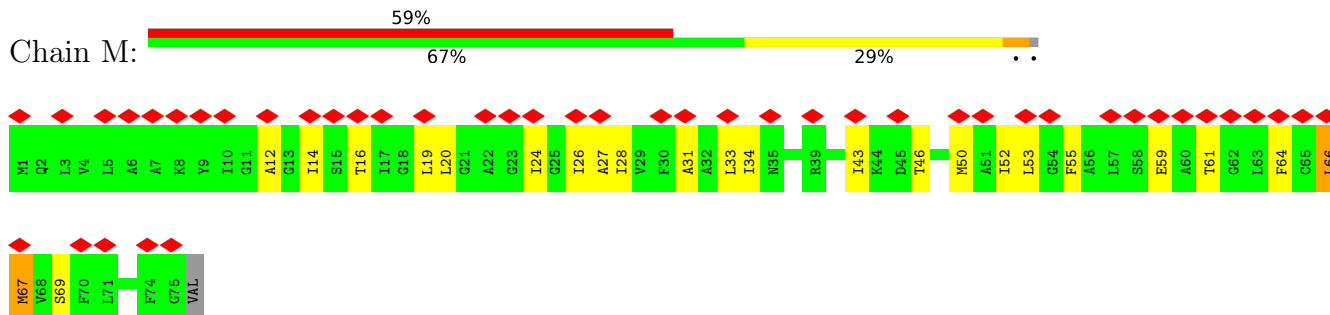
- Molecule 1: ATP synthase subunit 9, mitochondrial



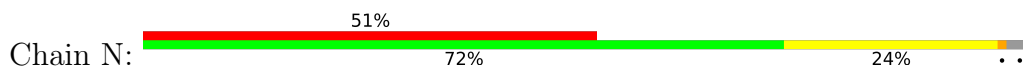
- Molecule 1: ATP synthase subunit 9, mitochondrial

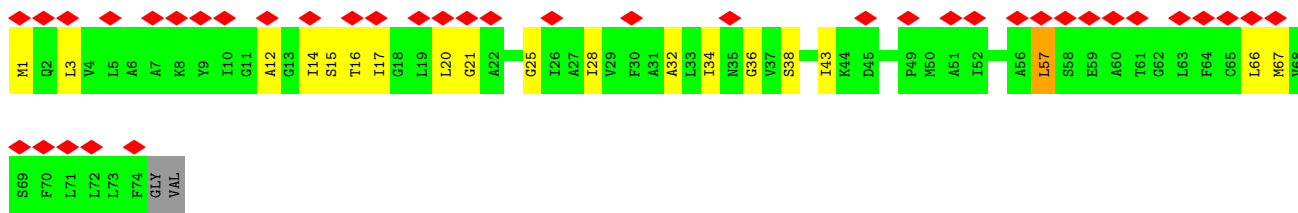


- Molecule 1: ATP synthase subunit 9, mitochondrial

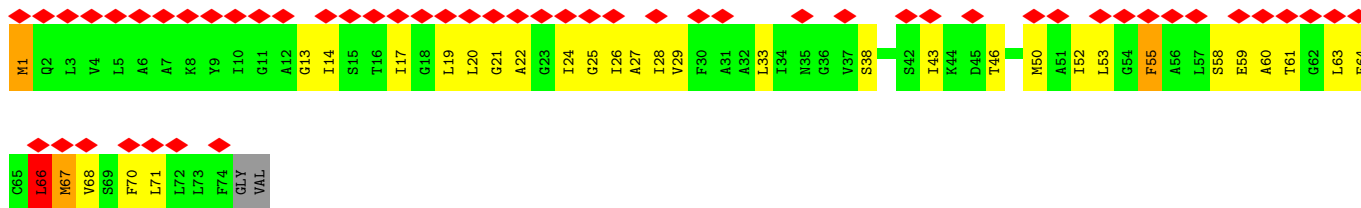


- Molecule 1: ATP synthase subunit 9, mitochondrial

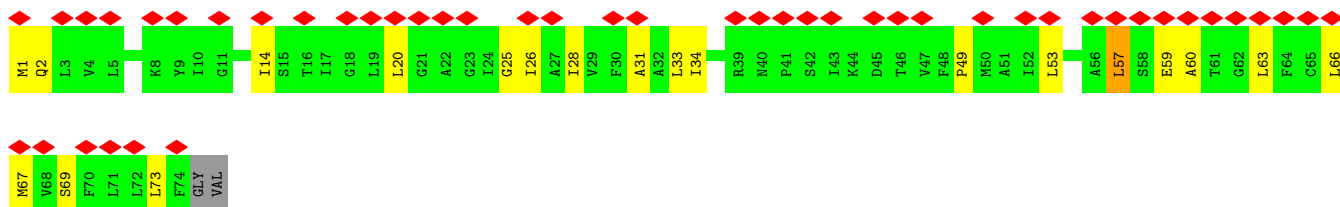




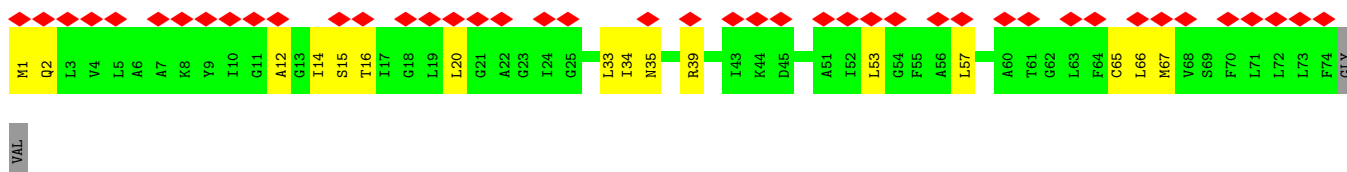
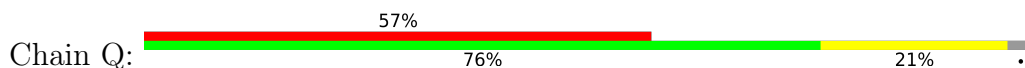
• Molecule 1: ATP synthase subunit 9, mitochondrial



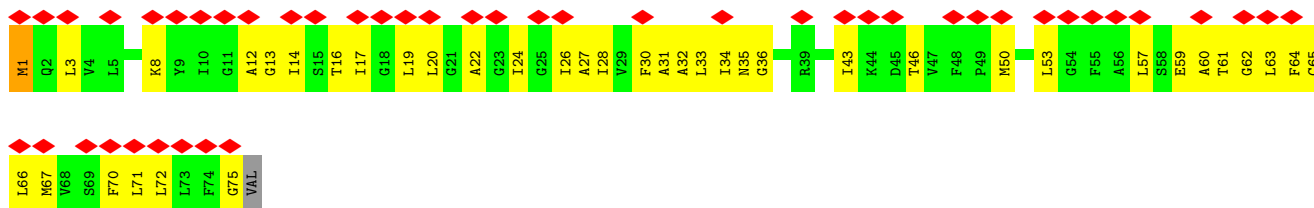
• Molecule 1: ATP synthase subunit 9, mitochondrial



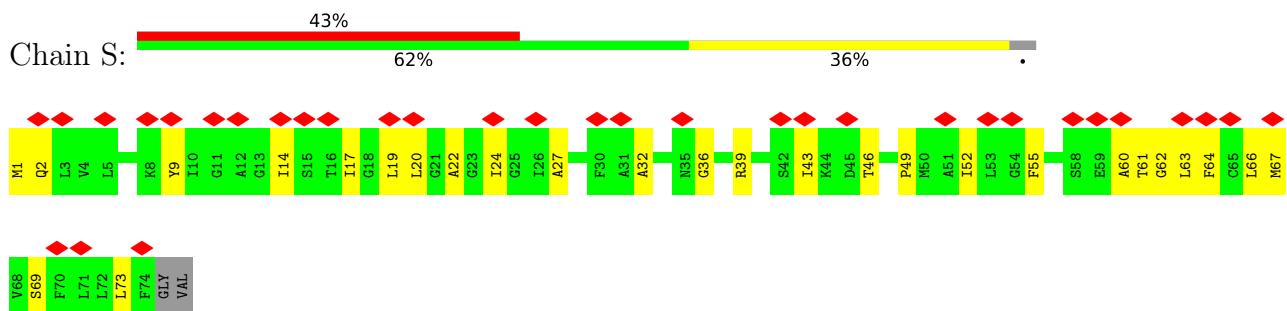
• Molecule 1: ATP synthase subunit 9, mitochondrial



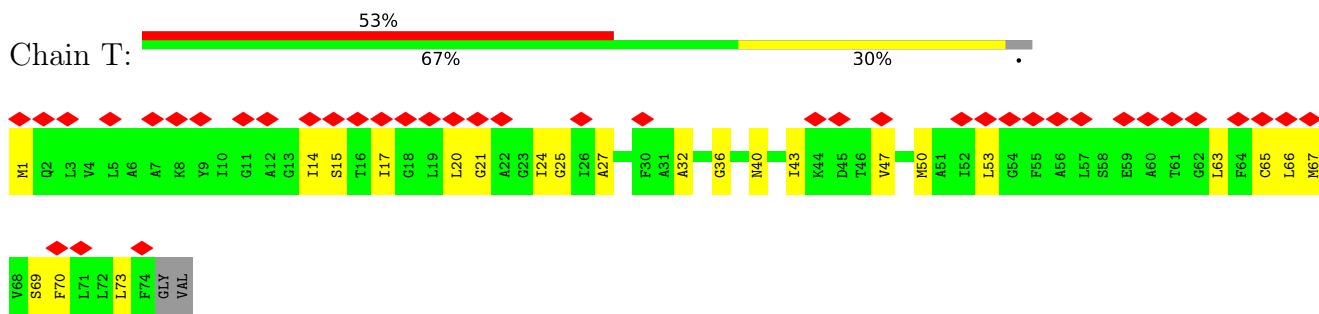
• Molecule 1: ATP synthase subunit 9, mitochondrial



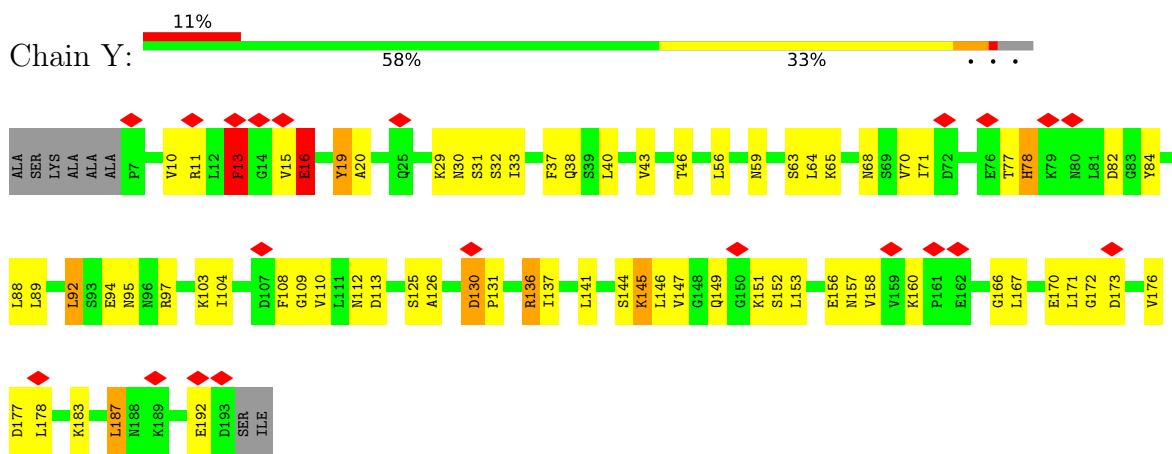
• Molecule 1: ATP synthase subunit 9, mitochondrial



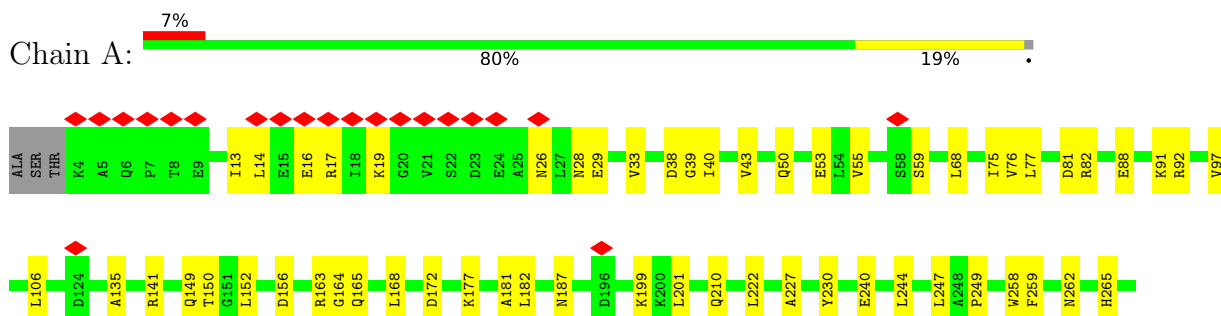
• Molecule 1: ATP synthase subunit 9, mitochondrial

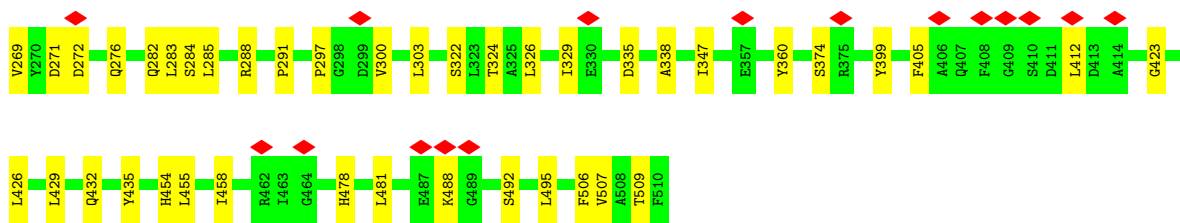


• Molecule 2: ATP synthase subunit 5, mitochondrial

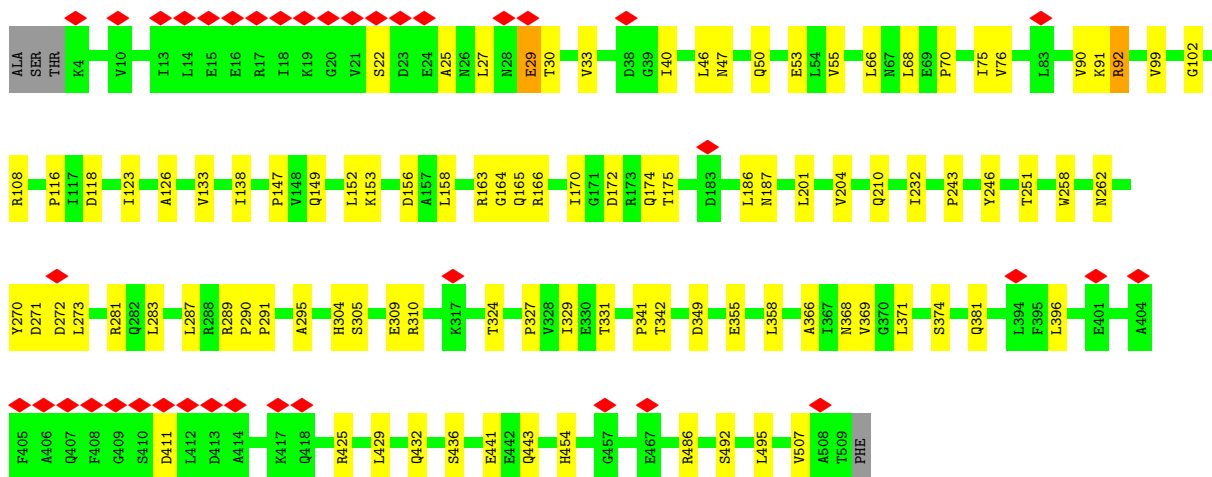
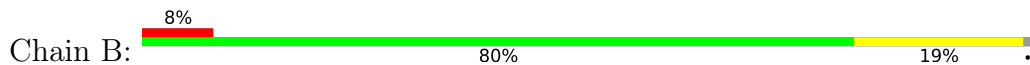


• Molecule 3: ATP synthase subunit alpha, mitochondrial

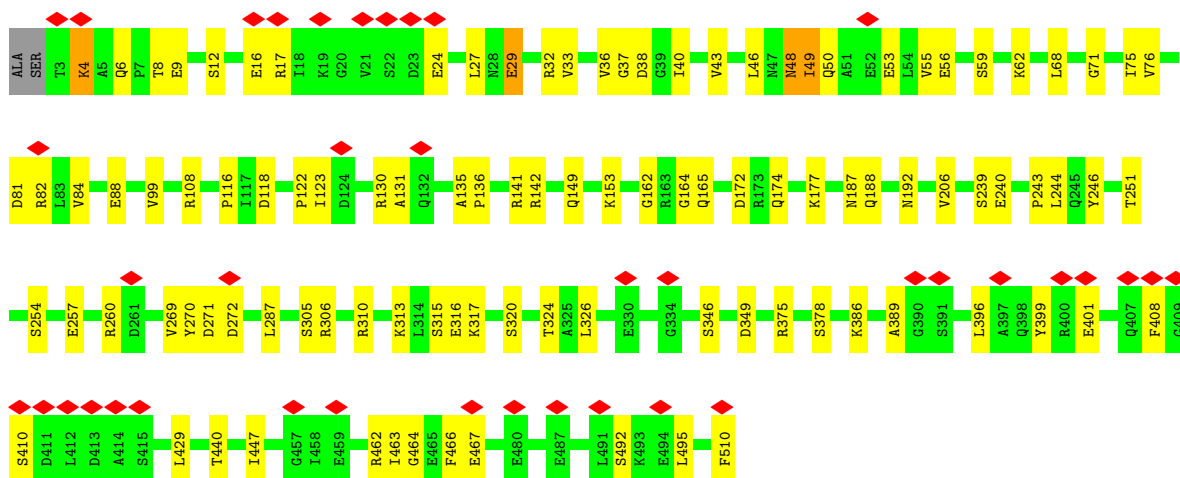
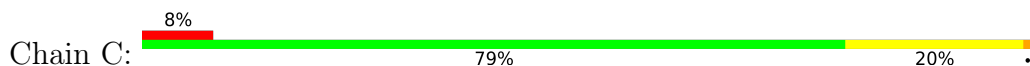




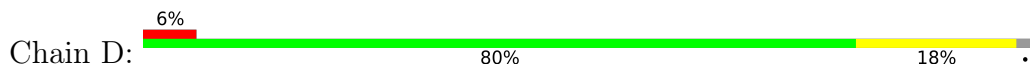
• Molecule 3: ATP synthase subunit alpha, mitochondrial

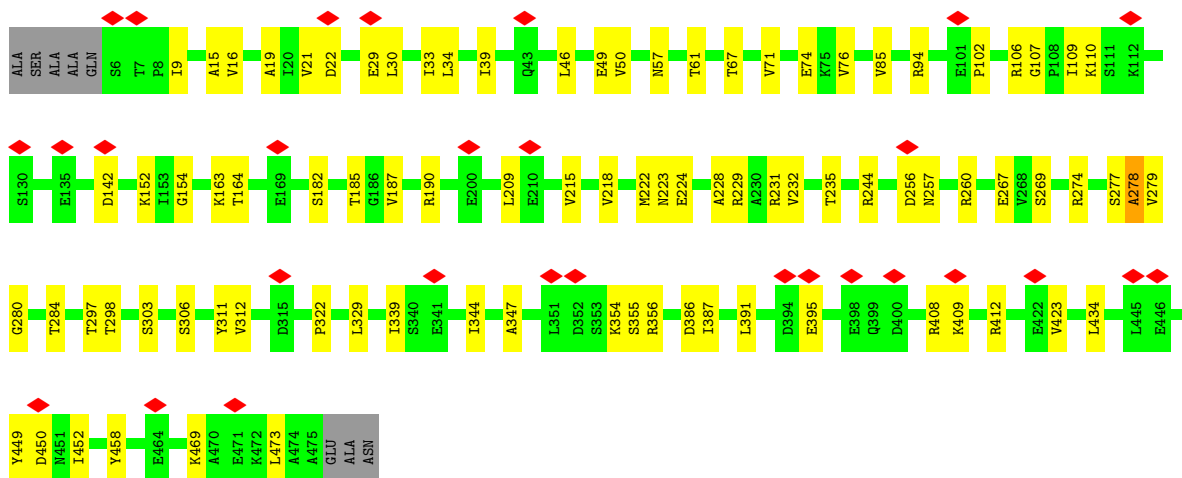


• Molecule 3: ATP synthase subunit alpha, mitochondrial

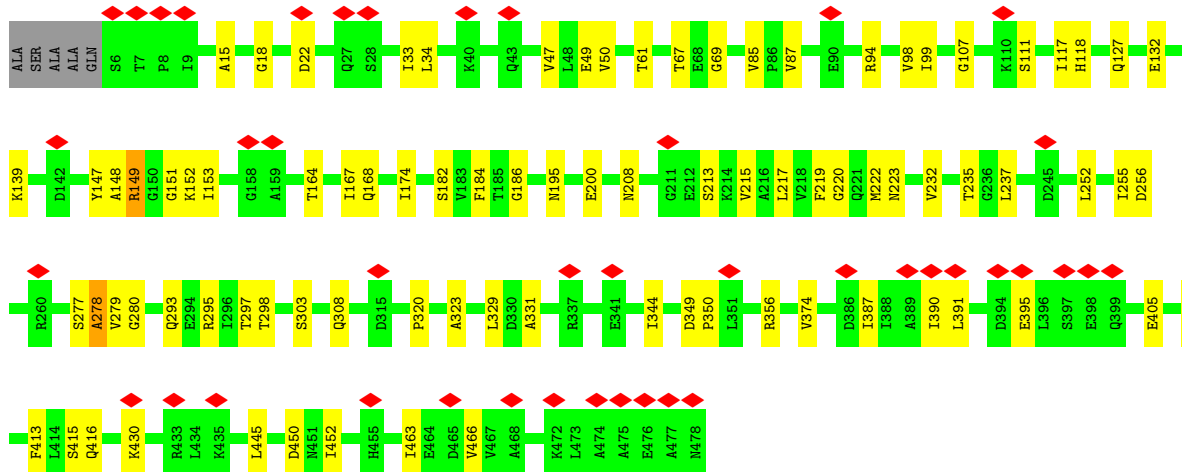
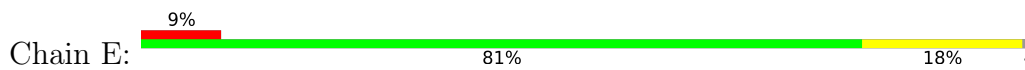


• Molecule 4: ATP synthase subunit beta, mitochondrial

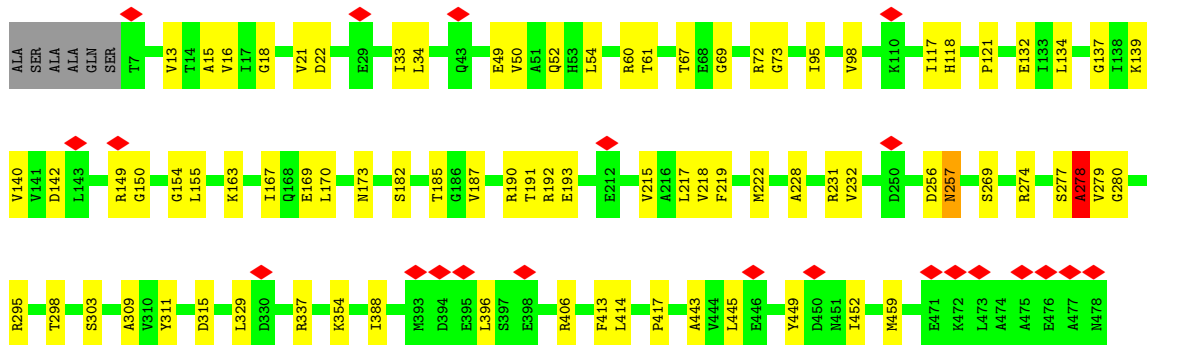
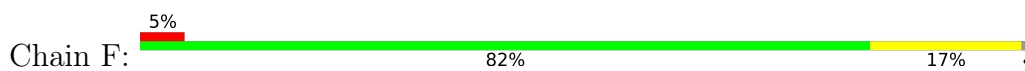




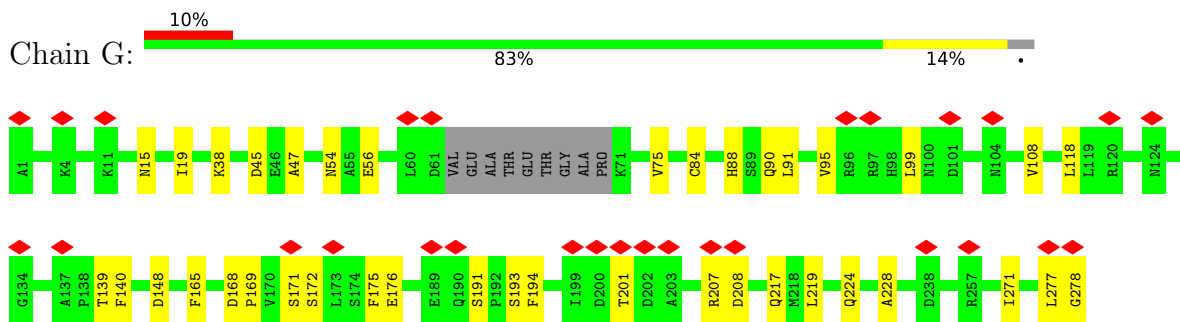
• Molecule 4: ATP synthase subunit beta, mitochondrial



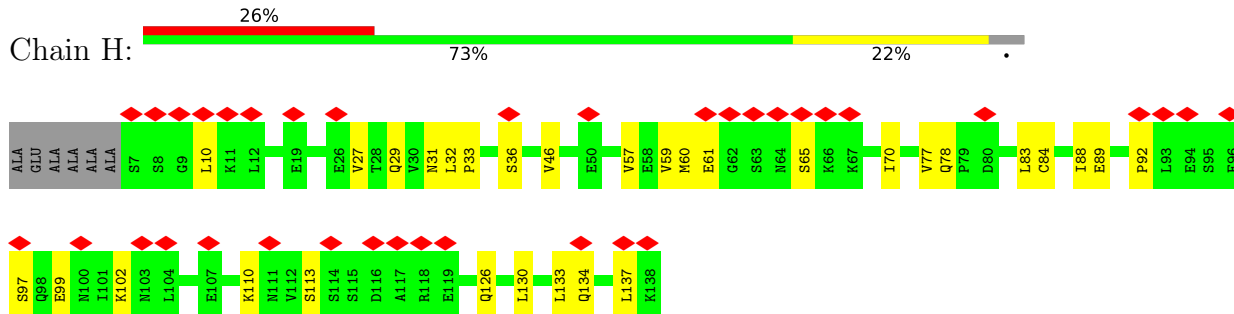
• Molecule 4: ATP synthase subunit beta, mitochondrial



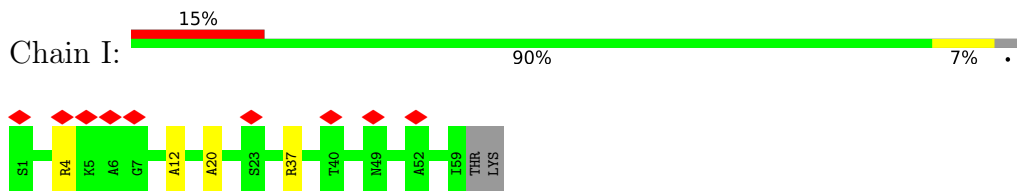
• Molecule 5: ATP synthase subunit gamma, mitochondrial



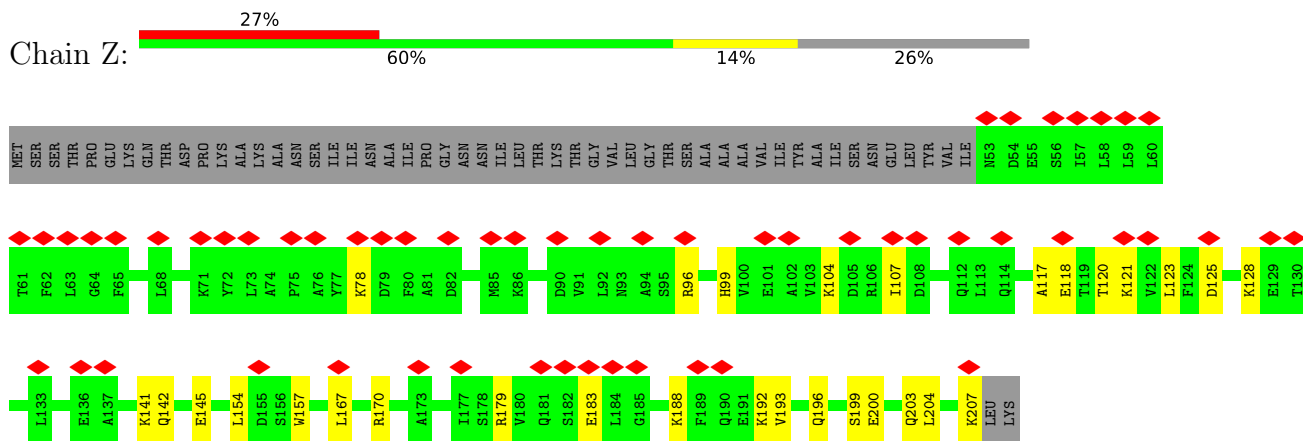
• Molecule 6: ATP synthase subunit delta, mitochondrial



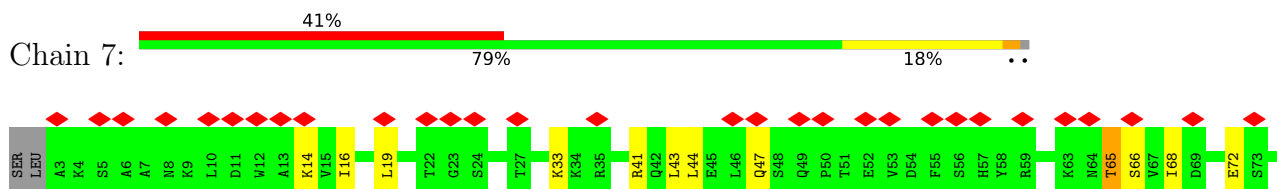
• Molecule 7: ATP synthase subunit epsilon, mitochondrial

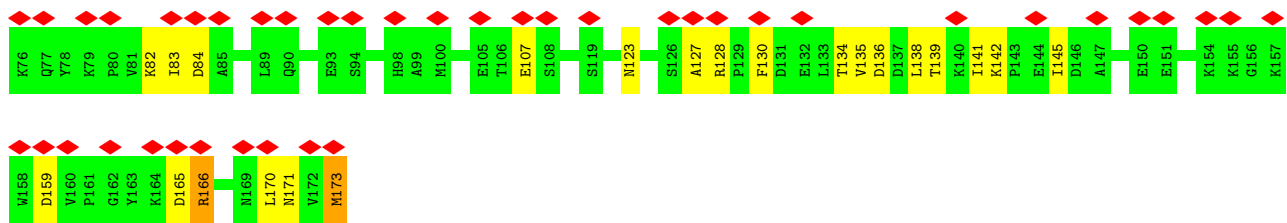


• Molecule 8: ATP synthase subunit 4, mitochondrial

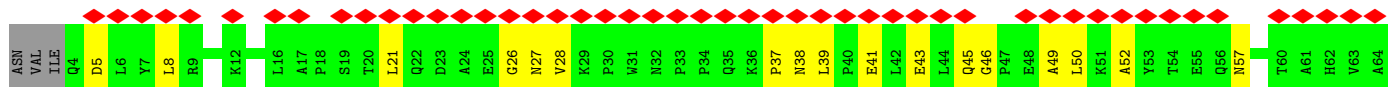
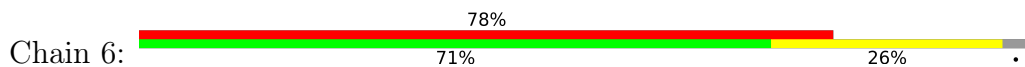


• Molecule 9: ATP synthase subunit d, mitochondrial

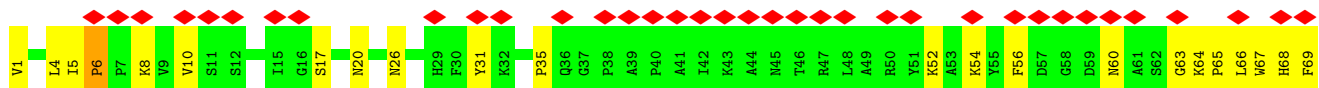




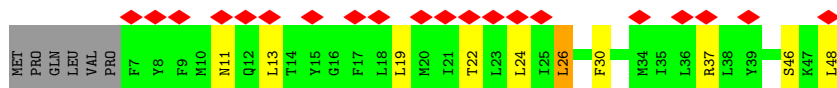
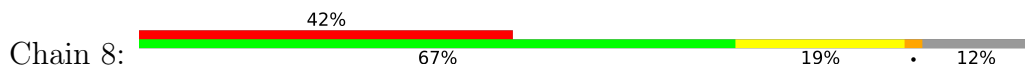
• Molecule 10: ATP synthase subunit H, mitochondrial



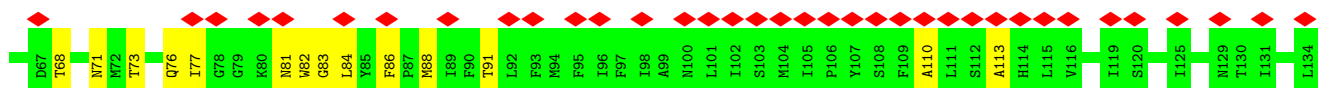
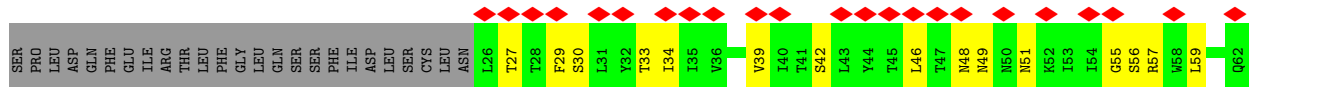
• Molecule 11: ATP synthase subunit f, mitochondrial

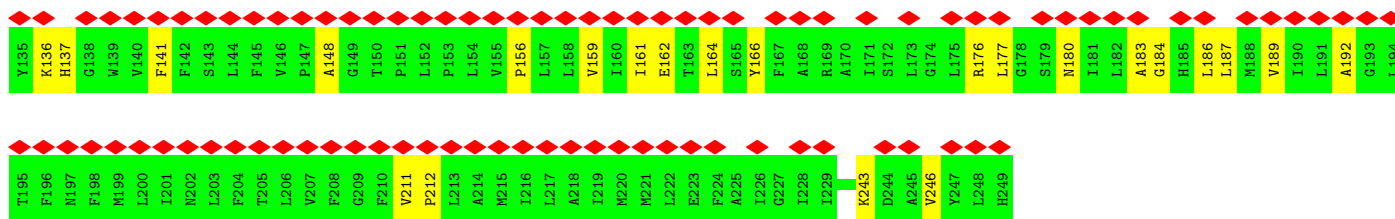


• Molecule 12: ATP synthase protein 8

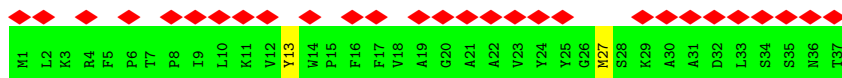
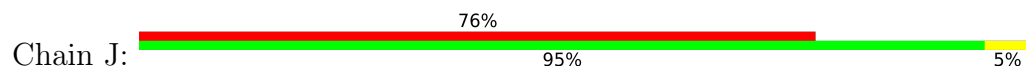


• Molecule 13: ATP synthase subunit a





- Molecule 14: ATP synthase subunit J, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0324	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FME, ADP, ATP

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	K	0.37	0/533	0.65	1/722 (0.1%)
1	L	0.37	0/533	0.76	2/722 (0.3%)
1	M	0.36	0/537	0.71	0/727
1	N	0.34	0/533	0.80	3/722 (0.4%)
1	O	0.37	0/533	0.74	1/722 (0.1%)
1	P	0.34	0/533	0.76	1/722 (0.1%)
1	Q	0.34	0/533	0.74	2/722 (0.3%)
1	R	0.37	0/537	0.76	2/727 (0.3%)
1	S	0.37	0/533	0.72	0/722
1	T	0.39	0/533	0.69	0/722
2	Y	0.36	0/1334	0.68	4/1814 (0.2%)
3	A	0.47	0/3910	0.60	0/5291
3	B	0.50	0/3893	0.63	1/5269 (0.0%)
3	C	0.45	0/3923	0.59	0/5308
4	D	0.48	0/3605	0.60	0/4889
4	E	0.46	0/3628	0.58	0/4919
4	F	0.51	1/3622 (0.0%)	0.61	0/4911
5	G	0.40	0/2111	0.56	0/2838
6	H	0.37	0/1004	0.55	0/1359
7	I	0.33	0/398	0.50	0/547
8	Z	0.35	0/1246	0.55	0/1678
9	7	0.33	0/1382	0.61	1/1858 (0.1%)
10	6	0.33	0/725	0.67	0/988
11	U	0.34	0/659	0.62	0/895
12	8	0.38	0/374	0.66	1/503 (0.2%)
13	X	0.35	0/1820	0.62	0/2483
14	J	0.34	0/302	0.56	0/410
All	All	0.43	1/39274 (0.0%)	0.62	19/53190 (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
1	O	0	1
1	P	0	1
3	A	0	1
4	D	0	1
4	E	0	1
4	F	0	1
10	6	0	2
12	8	0	1
13	X	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	155	LEU	CA-CB	-5.20	1.41	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	57	LEU	CA-CB-CG	7.90	133.46	115.30
1	P	57	LEU	CA-CB-CG	6.86	131.08	115.30
2	Y	145	LYS	CB-CA-C	-6.69	97.02	110.40
1	N	57	LEU	CA-CB-CG	6.55	130.36	115.30
1	R	57	LEU	CA-CB-CG	6.00	129.09	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	26	ASN	Peptide
4	D	278	ALA	Peptide
4	E	278	ALA	Peptide
1	O	55	PHE	Peptide
1	P	57	LEU	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	K	535	0	578	27	0
1	L	532	0	571	23	0
1	M	537	0	576	17	0
1	N	532	0	571	13	0
1	O	533	0	573	27	0
1	P	535	0	578	15	0
1	Q	532	0	571	11	0
1	R	537	0	576	25	0
1	S	532	0	571	21	0
1	T	533	0	573	16	0
2	Y	1317	0	1260	74	0
3	A	3852	0	3930	63	0
3	B	3836	0	3917	86	0
3	C	3865	0	3948	69	0
4	D	3549	0	3621	57	0
4	E	3572	0	3638	50	0
4	F	3566	0	3633	53	0
5	G	2086	0	2156	29	0
6	H	990	0	999	20	0
7	I	392	0	306	5	0
8	Z	1232	0	1256	36	0
9	7	1363	0	1389	28	0
10	6	710	0	668	11	0
11	U	639	0	615	19	0
12	8	364	0	390	9	0
13	X	1772	0	1873	38	0
14	J	292	0	298	2	0
15	A	31	0	12	0	0
15	B	31	0	12	0	0
15	C	31	0	12	0	0
16	D	27	0	12	2	0
16	F	27	0	12	2	0
All	All	38882	0	39695	707	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 9.

The worst 5 of 707 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)
2:Y:19:TYR:CD2	2:Y:92:LEU:HD21	1.50	1.45
2:Y:19:TYR:CE2	2:Y:92:LEU:HD21	1.76	1.18
2:Y:19:TYR:CE2	2:Y:92:LEU:CD2	2.28	1.17
3:C:40:ILE:CD1	3:C:76:VAL:HG12	1.81	1.11
2:Y:19:TYR:CD2	2:Y:92:LEU:CD2	2.41	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	K	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
1	L	72/76 (95%)	65 (90%)	7 (10%)	0	100	100
1	M	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
1	N	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
1	O	72/76 (95%)	65 (90%)	7 (10%)	0	100	100
1	P	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
1	Q	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	R	73/76 (96%)	67 (92%)	6 (8%)	0	100	100
1	S	72/76 (95%)	68 (94%)	4 (6%)	0	100	100
1	T	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
2	Y	185/195 (95%)	156 (84%)	23 (12%)	6 (3%)	4	32
3	A	505/510 (99%)	467 (92%)	38 (8%)	0	100	100
3	B	504/510 (99%)	472 (94%)	31 (6%)	1 (0%)	47	79
3	C	506/510 (99%)	465 (92%)	41 (8%)	0	100	100
4	D	468/478 (98%)	439 (94%)	28 (6%)	1 (0%)	47	79
4	E	471/478 (98%)	444 (94%)	26 (6%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	470/478 (98%)	438 (93%)	30 (6%)	2 (0%)	34	70
5	G	265/278 (95%)	254 (96%)	11 (4%)	0	100	100
6	H	130/138 (94%)	117 (90%)	12 (9%)	1 (1%)	19	57
7	I	57/61 (93%)	54 (95%)	3 (5%)	0	100	100
8	Z	153/209 (73%)	149 (97%)	4 (3%)	0	100	100
9	7	169/173 (98%)	150 (89%)	17 (10%)	2 (1%)	13	50
10	6	87/92 (95%)	67 (77%)	20 (23%)	0	100	100
11	U	83/95 (87%)	70 (84%)	12 (14%)	1 (1%)	13	50
12	8	40/48 (83%)	38 (95%)	2 (5%)	0	100	100
13	X	222/249 (89%)	203 (91%)	19 (9%)	0	100	100
14	J	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
All	All	5072/5299 (96%)	4688 (92%)	369 (7%)	15 (0%)	44	74

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	32	SER
4	D	279	VAL
4	E	279	VAL
4	F	279	VAL
2	Y	10	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	54/55 (98%)	54 (100%)	0	100	100
1	L	54/55 (98%)	53 (98%)	1 (2%)	57	76
1	M	54/55 (98%)	52 (96%)	2 (4%)	34	62
1	N	54/55 (98%)	52 (96%)	2 (4%)	34	62
1	O	54/55 (98%)	52 (96%)	2 (4%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	54/55 (98%)	52 (96%)	2 (4%)	34	62
1	Q	54/55 (98%)	52 (96%)	2 (4%)	34	62
1	R	54/55 (98%)	53 (98%)	1 (2%)	57	76
1	S	54/55 (98%)	53 (98%)	1 (2%)	57	76
1	T	54/55 (98%)	53 (98%)	1 (2%)	57	76
2	Y	131/164 (80%)	114 (87%)	17 (13%)	4	23
3	A	409/412 (99%)	408 (100%)	1 (0%)	93	97
3	B	406/412 (98%)	403 (99%)	3 (1%)	84	91
3	C	411/412 (100%)	397 (97%)	14 (3%)	37	64
4	D	380/384 (99%)	379 (100%)	1 (0%)	92	96
4	E	382/384 (100%)	381 (100%)	1 (0%)	92	96
4	F	381/384 (99%)	380 (100%)	1 (0%)	92	96
5	G	230/236 (98%)	230 (100%)	0	100	100
6	H	111/112 (99%)	111 (100%)	0	100	100
7	I	25/48 (52%)	25 (100%)	0	100	100
8	Z	137/182 (75%)	136 (99%)	1 (1%)	84	91
9	7	154/158 (98%)	151 (98%)	3 (2%)	57	76
10	6	79/82 (96%)	77 (98%)	2 (2%)	47	70
11	U	60/76 (79%)	60 (100%)	0	100	100
12	8	41/47 (87%)	41 (100%)	0	100	100
13	X	193/217 (89%)	192 (100%)	1 (0%)	88	94
14	J	30/30 (100%)	30 (100%)	0	100	100
All	All	4100/4290 (96%)	4041 (99%)	59 (1%)	68	81

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	177	ASP
9	7	173	MET
3	C	4	LYS
9	7	166	ARG
4	D	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
10	6	38	ASN
13	X	180	ASN
10	6	57	ASN
12	8	11	ASN
3	C	332	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	L	1	1	5,6,10	1.38	1 (20%)	3,6,11	1.43	1 (33%)
1	FME	S	1	1	5,6,10	1.47	1 (20%)	3,6,11	1.71	1 (33%)
1	FME	M	1	1	6,7,10	1.03	0	6,7,11	1.09	0
1	FME	K	1	1	8,9,10	0.92	0	7,9,11	0.69	0
1	FME	O	1	1	6,7,10	0.99	0	6,7,11	1.25	1 (16%)
1	FME	R	1	1	6,7,10	0.96	0	6,7,11	1.47	1 (16%)
1	FME	N	1	1	5,6,10	1.32	1 (20%)	3,6,11	1.82	1 (33%)
1	FME	T	1	1	6,7,10	0.94	0	6,7,11	1.90	2 (33%)
1	FME	Q	1	1	5,6,10	1.38	1 (20%)	3,6,11	1.49	1 (33%)
1	FME	P	1	1	8,9,10	0.94	0	7,9,11	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	L	1	1	-	0/2/5/11	-
1	FME	S	1	1	-	0/2/5/11	-
1	FME	M	1	1	-	2/5/7/11	-
1	FME	K	1	1	-	1/7/9/11	-
1	FME	O	1	1	-	3/5/7/11	-
1	FME	R	1	1	-	3/5/7/11	-
1	FME	N	1	1	-	0/2/5/11	-
1	FME	T	1	1	-	3/5/7/11	-
1	FME	Q	1	1	-	0/2/5/11	-
1	FME	P	1	1	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	1	FME	CA-N	-2.61	1.43	1.46
1	L	1	FME	CA-N	-2.36	1.44	1.46
1	Q	1	FME	CA-N	-2.29	1.44	1.46
1	N	1	FME	CA-N	-2.10	1.44	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	1	FME	CB-CA-C	-3.28	106.59	111.29
1	N	1	FME	CB-CA-N	2.88	112.81	109.61
1	R	1	FME	CB-CA-C	-2.86	107.20	111.29
1	T	1	FME	C-CA-N	2.80	114.79	109.73
1	S	1	FME	CB-CA-N	2.76	112.69	109.61

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	M	1	FME	CB-CA-N-CN
1	O	1	FME	CB-CA-N-CN
1	O	1	FME	C-CA-CB-CG
1	P	1	FME	C-CA-CB-CG
1	P	1	FME	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	1	FME	1	0
1	R	1	FME	1	0
1	P	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	ATP	B	600	-	26,33,33	0.96	1 (3%)	31,52,52	1.86	5 (16%)
16	ADP	F	600	-	24,29,29	0.97	1 (4%)	29,45,45	1.41	3 (10%)
15	ATP	A	600	-	26,33,33	0.93	1 (3%)	31,52,52	1.80	5 (16%)
15	ATP	C	600	-	26,33,33	0.92	1 (3%)	31,52,52	1.82	5 (16%)
16	ADP	D	600	-	24,29,29	0.99	1 (4%)	29,45,45	1.54	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ATP	B	600	-	-	2/18/38/38	0/3/3/3
16	ADP	F	600	-	-	4/12/32/32	0/3/3/3
15	ATP	A	600	-	-	1/18/38/38	0/3/3/3
15	ATP	C	600	-	-	0/18/38/38	0/3/3/3
16	ADP	D	600	-	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	600	ADP	C5-C4	2.16	1.46	1.40
15	B	600	ATP	C5-C4	2.12	1.46	1.40
15	A	600	ATP	C5-C4	2.05	1.46	1.40
15	C	600	ATP	C5-C4	2.02	1.46	1.40
16	F	600	ADP	C2'-C1'	-2.00	1.50	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	600	ATP	PA-O3A-PB	-5.13	115.23	132.83
15	C	600	ATP	PB-O3B-PG	-4.98	115.75	132.83
15	B	600	ATP	PB-O3B-PG	-4.92	115.94	132.83
15	A	600	ATP	PA-O3A-PB	-4.74	116.57	132.83
15	C	600	ATP	PA-O3A-PB	-4.73	116.60	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	600	ATP	C5'-O5'-PA-O3A
16	D	600	ADP	C5'-O5'-PA-O1A
16	D	600	ADP	C5'-O5'-PA-O3A
16	F	600	ADP	C5'-O5'-PA-O1A
16	F	600	ADP	C5'-O5'-PA-O2A

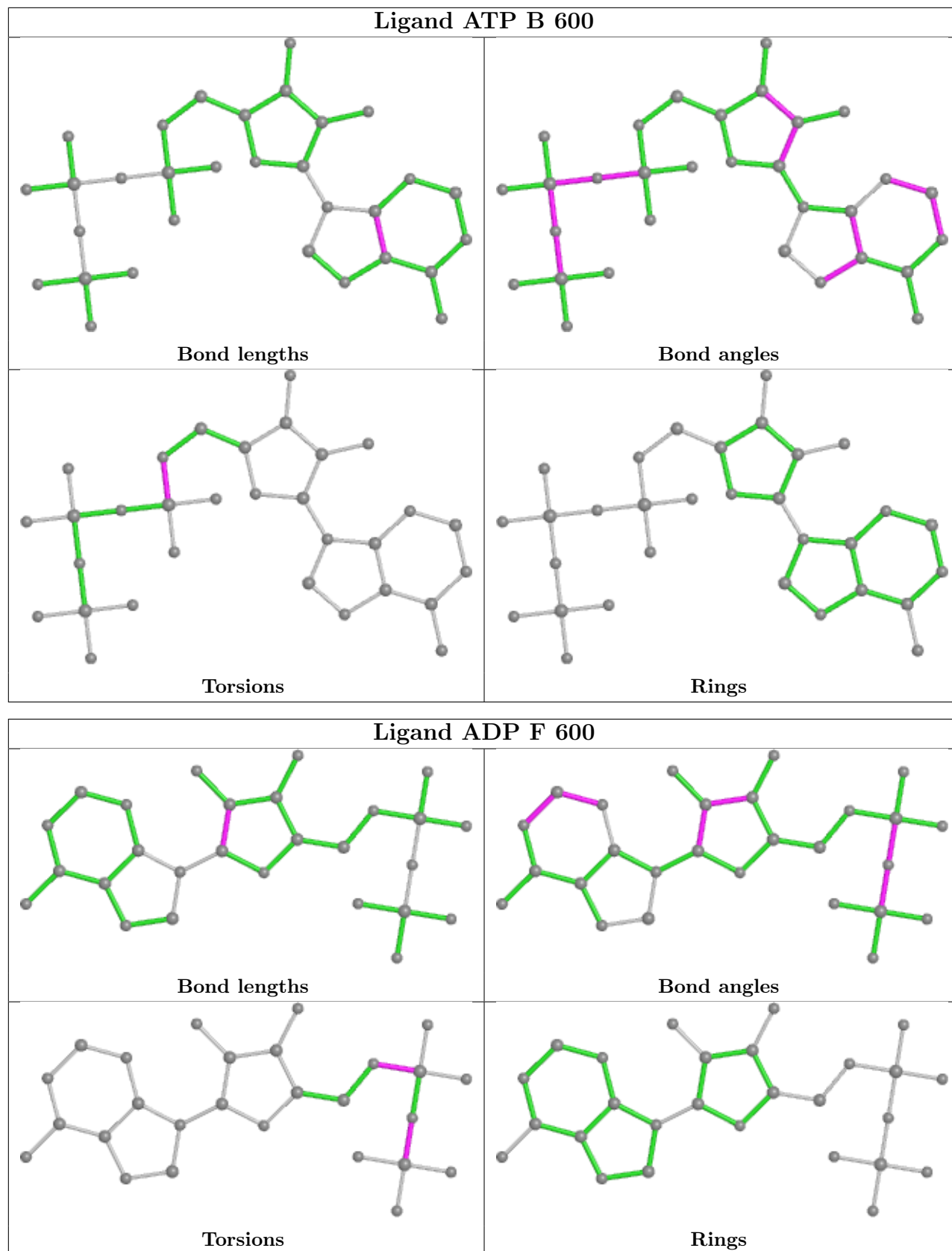
There are no ring outliers.

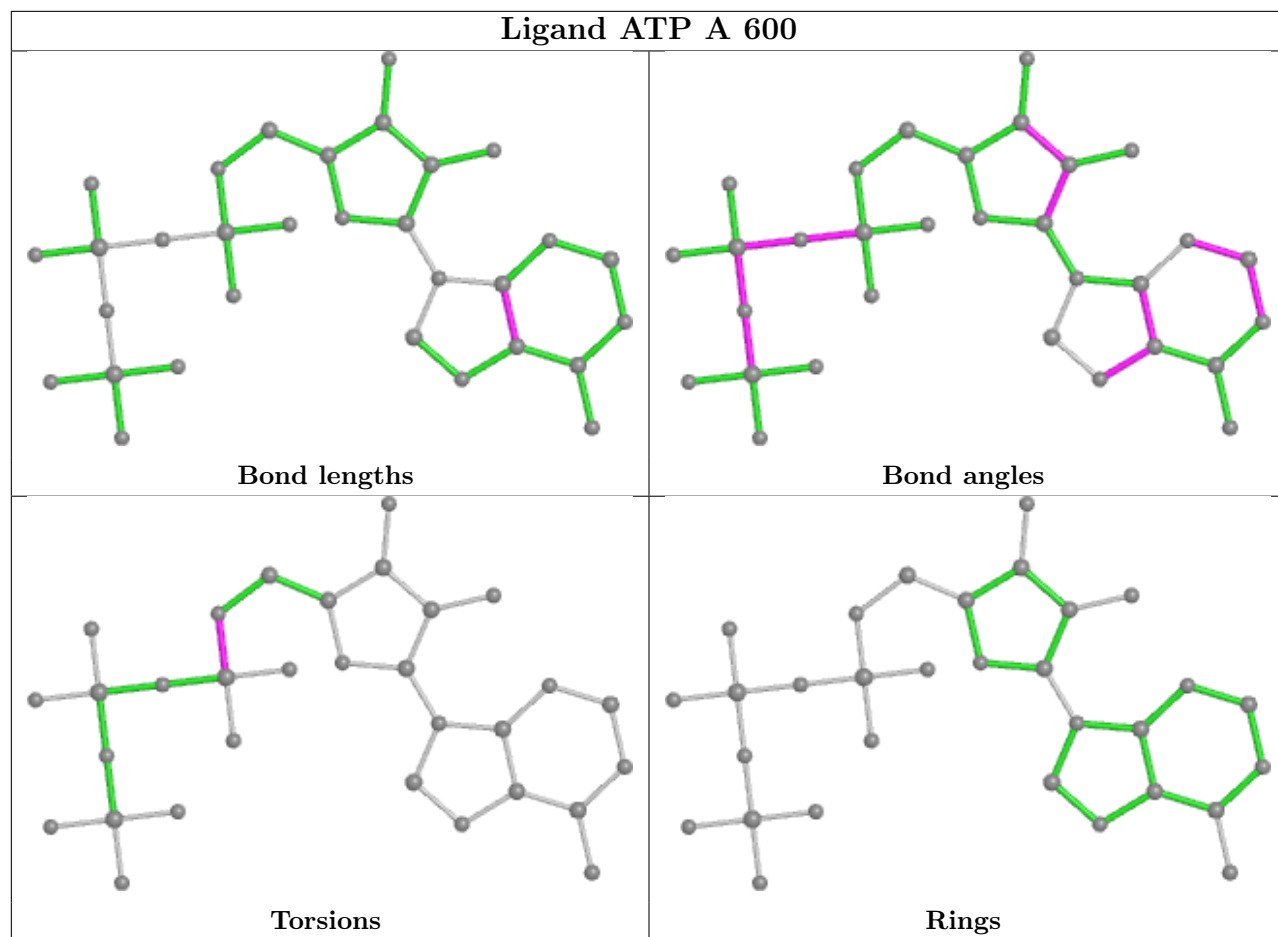
2 monomers are involved in 4 short contacts:

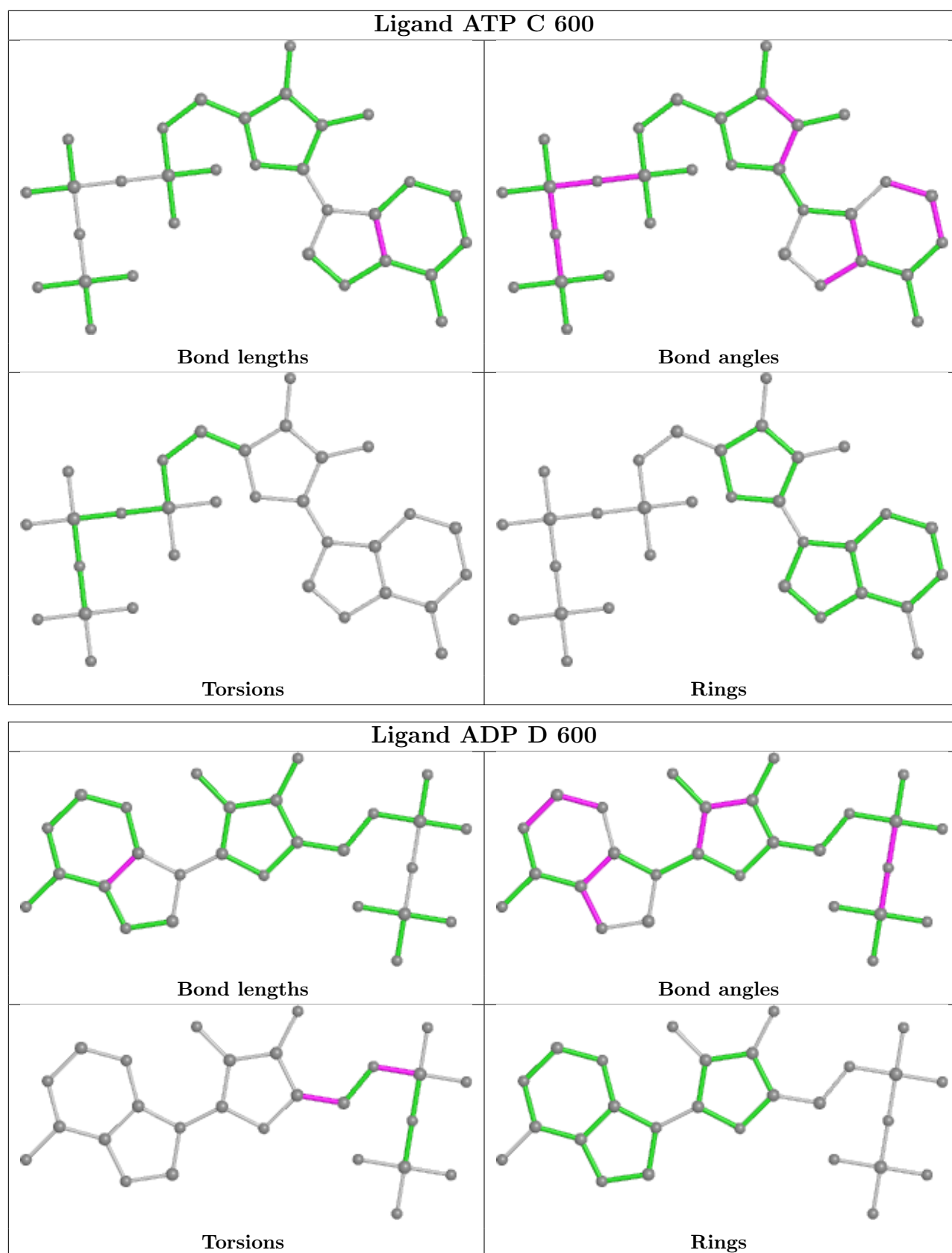
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	F	600	ADP	2	0
16	D	600	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.







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.

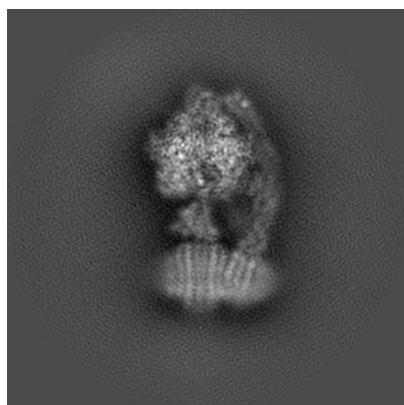
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7546. These allow visual inspection of the internal detail of the map and identification of artifacts.

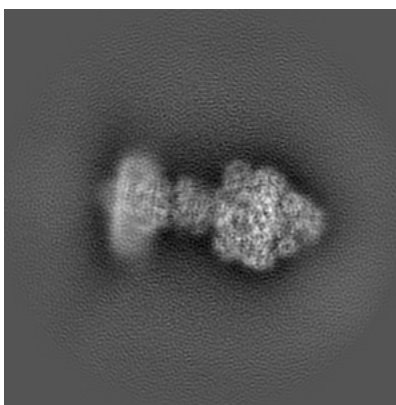
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

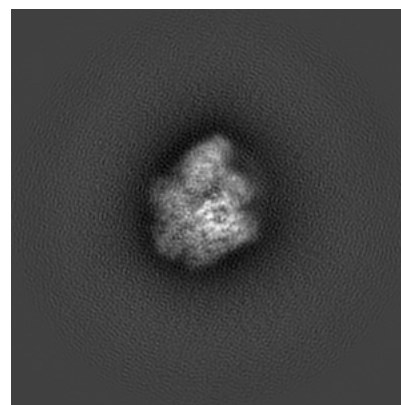
6.1.1 Primary map



X



Y

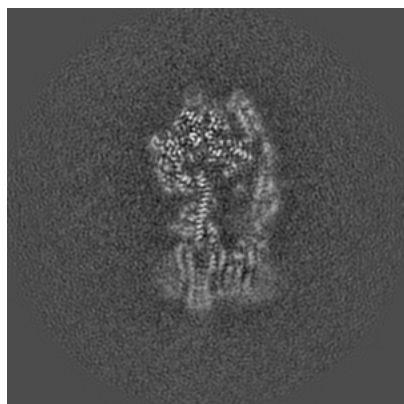


Z

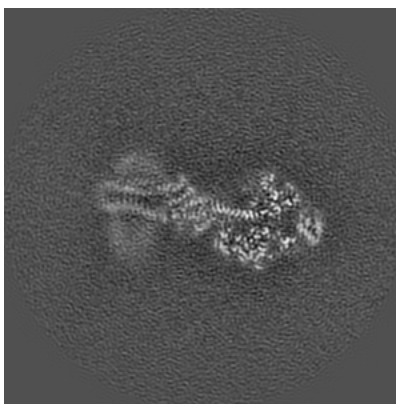
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

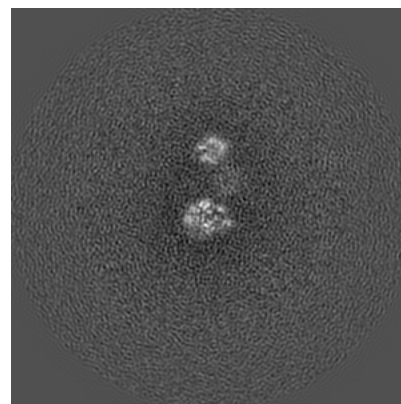
6.2.1 Primary map



X Index: 160



Y Index: 160

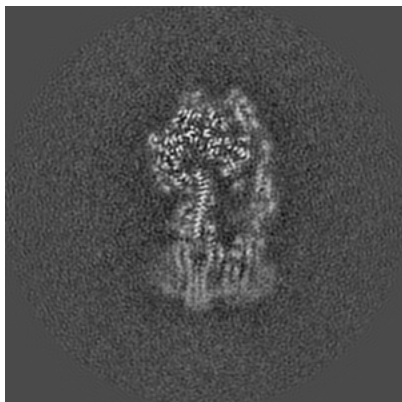


Z Index: 160

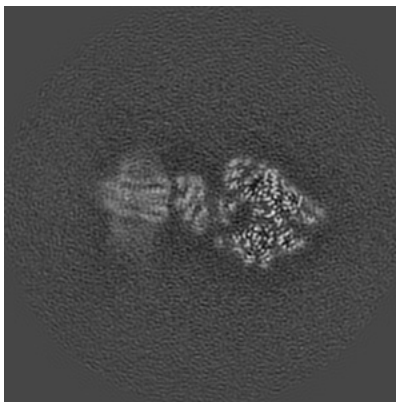
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

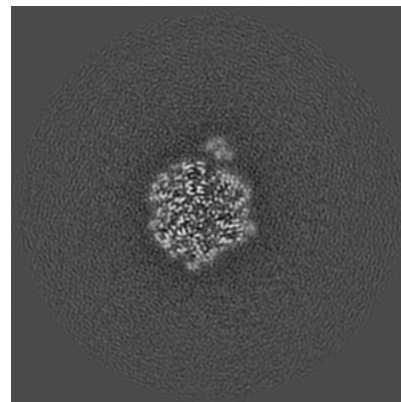
6.3.1 Primary map



X Index: 159



Y Index: 145



Z Index: 208

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

6.4 Orthogonal surface views [i](#)

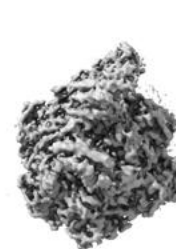
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0324. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

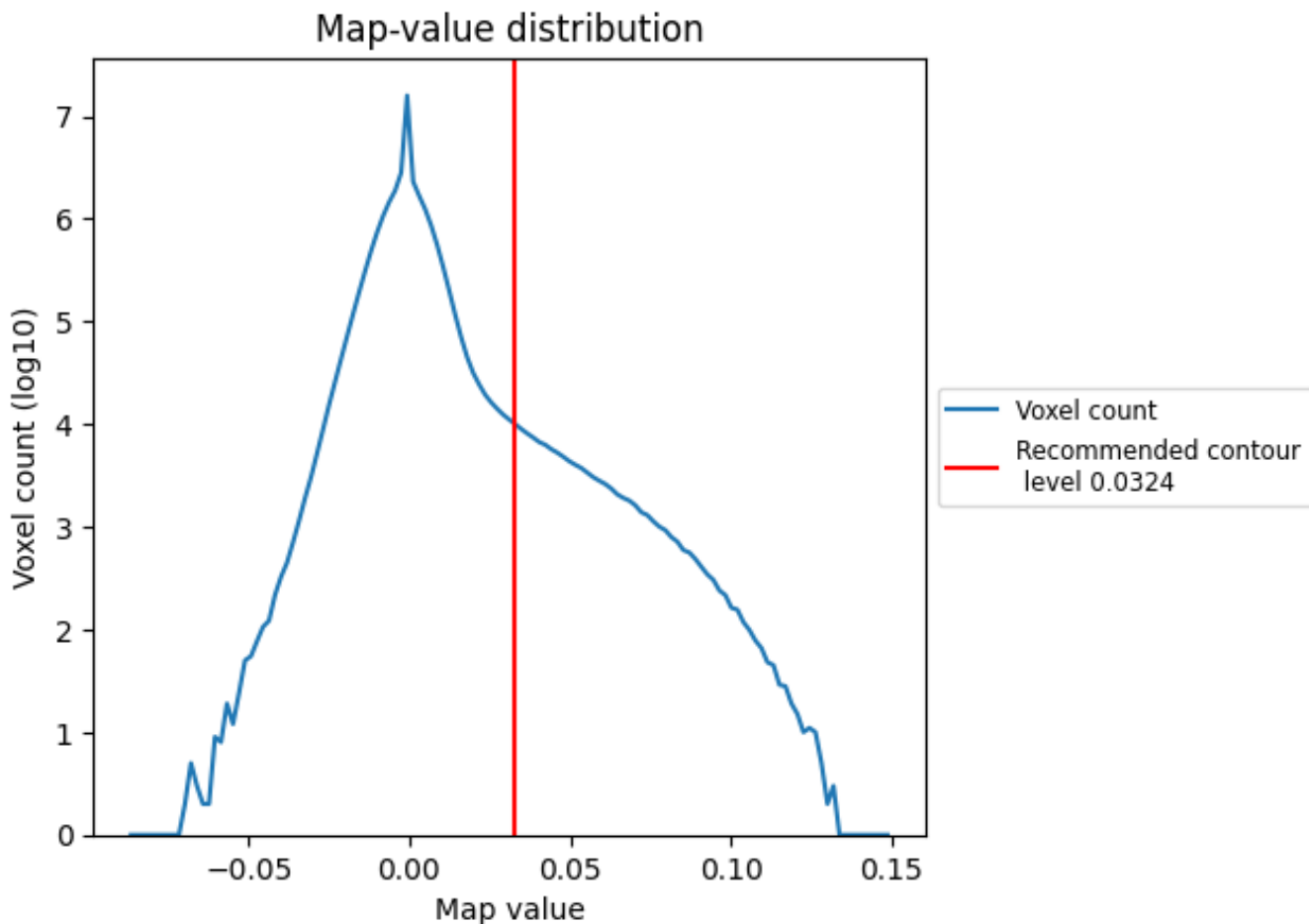
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

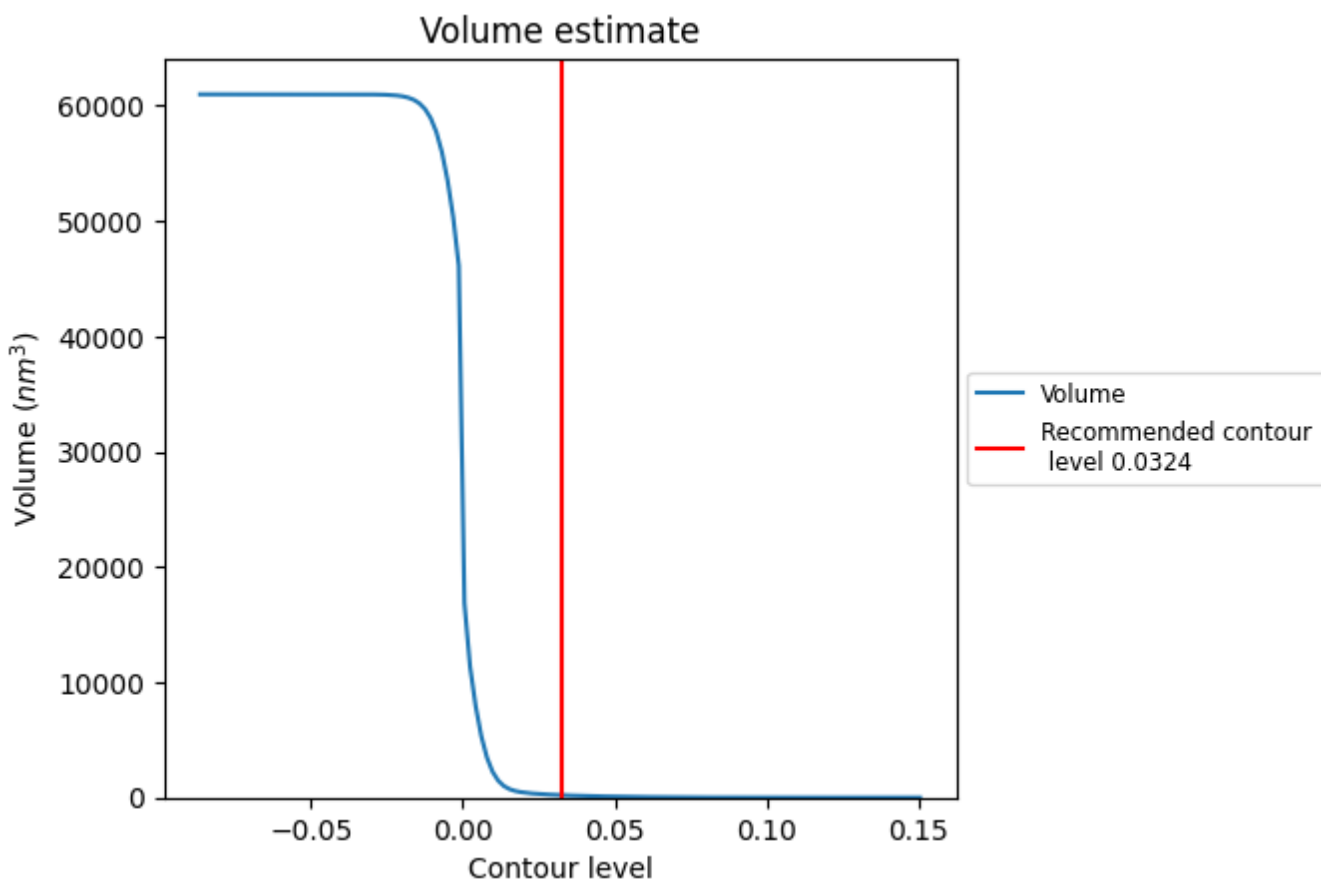
This section contains the results of statistical analysis of the map.

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.

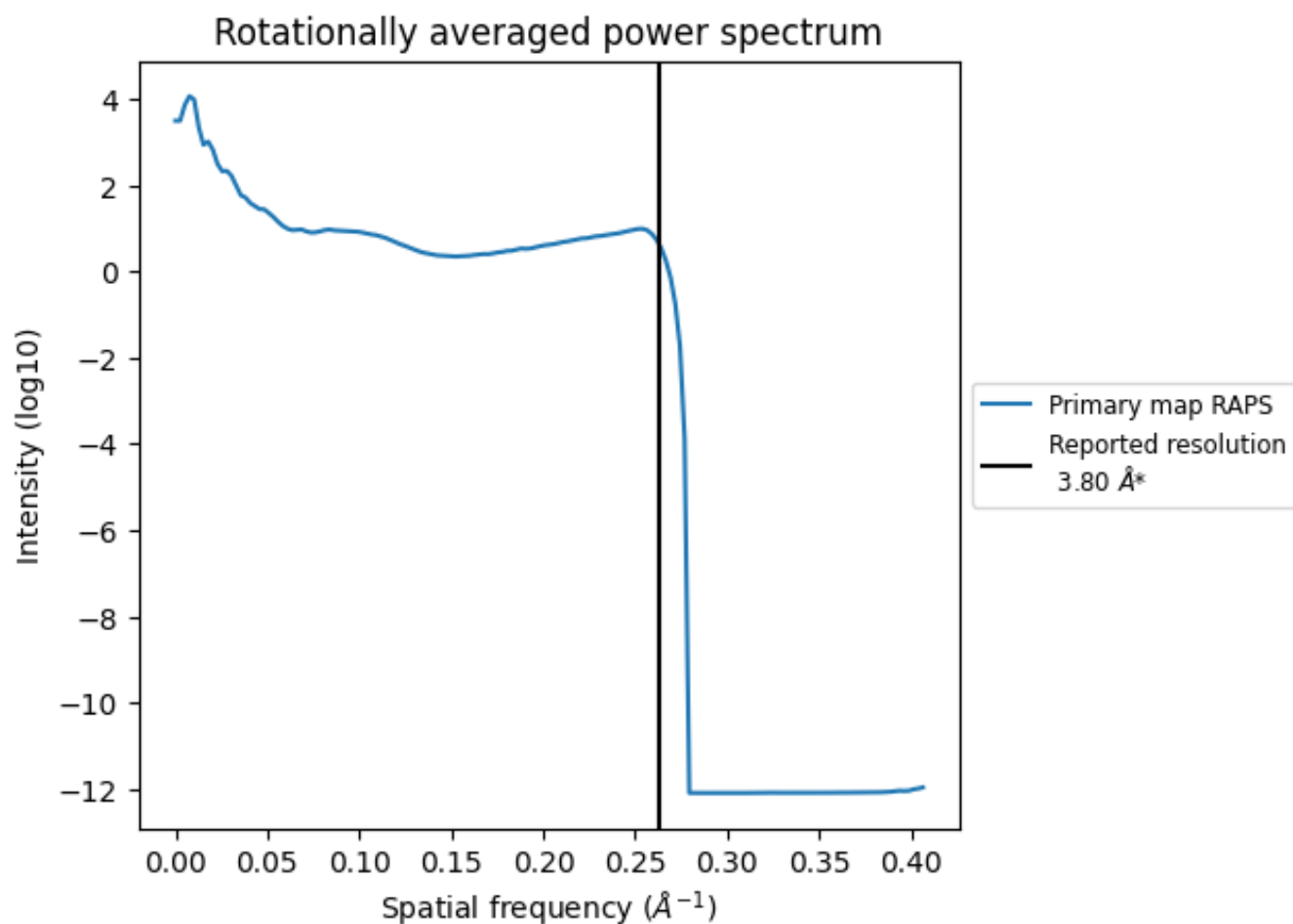
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 [\(i\)](#)

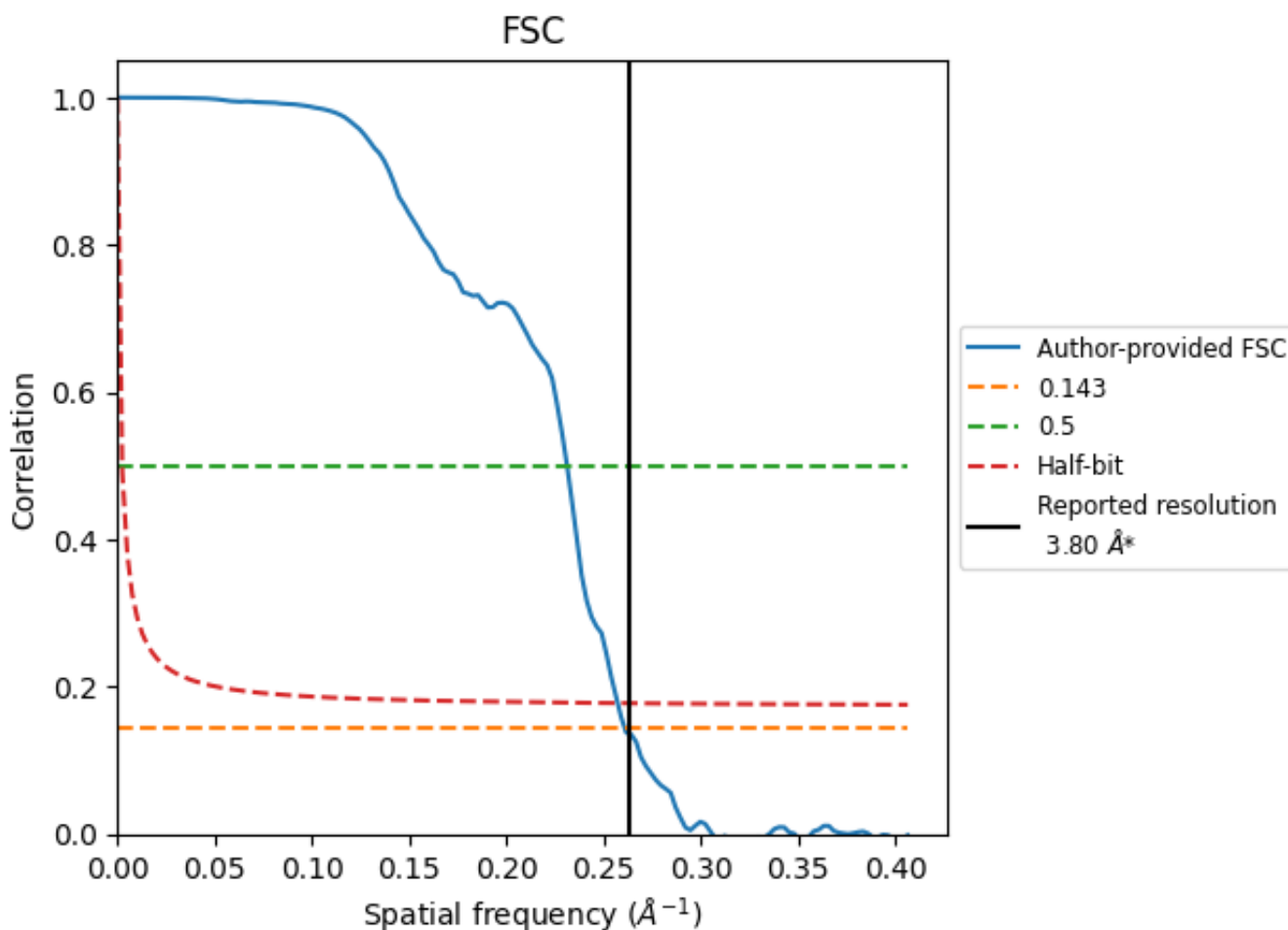


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

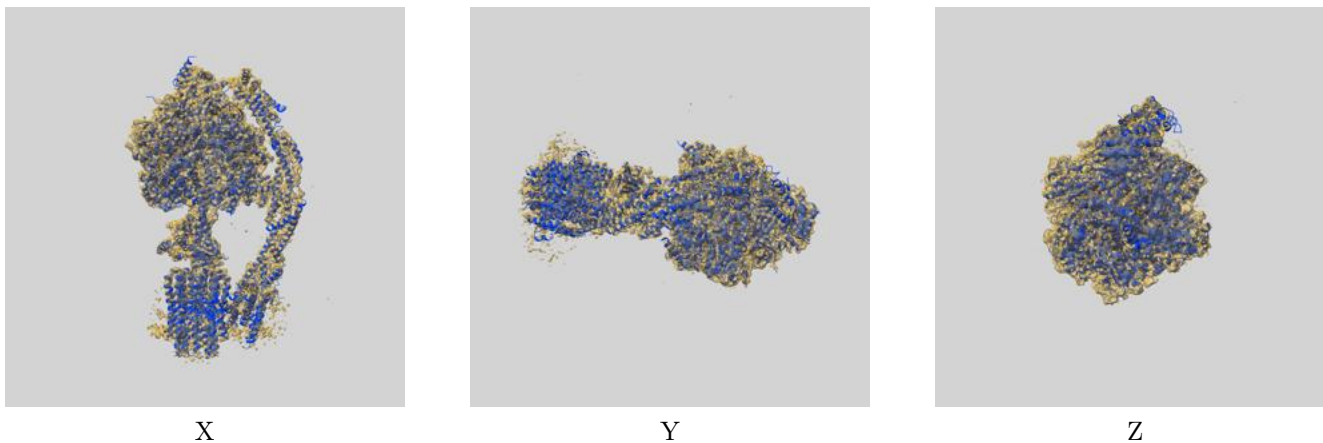
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.32	3.89
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

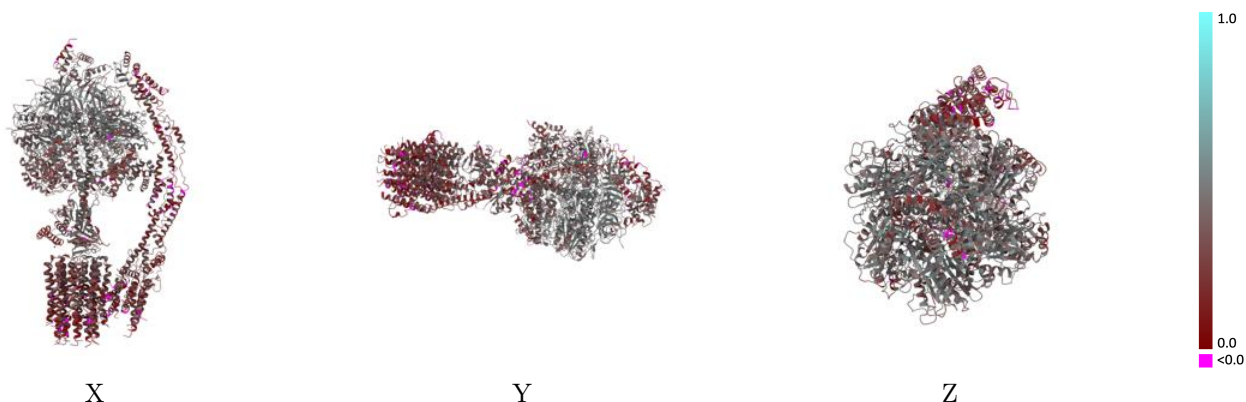
This section contains information regarding the fit between EMDB map EMD-7546 and PDB model 6CP3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



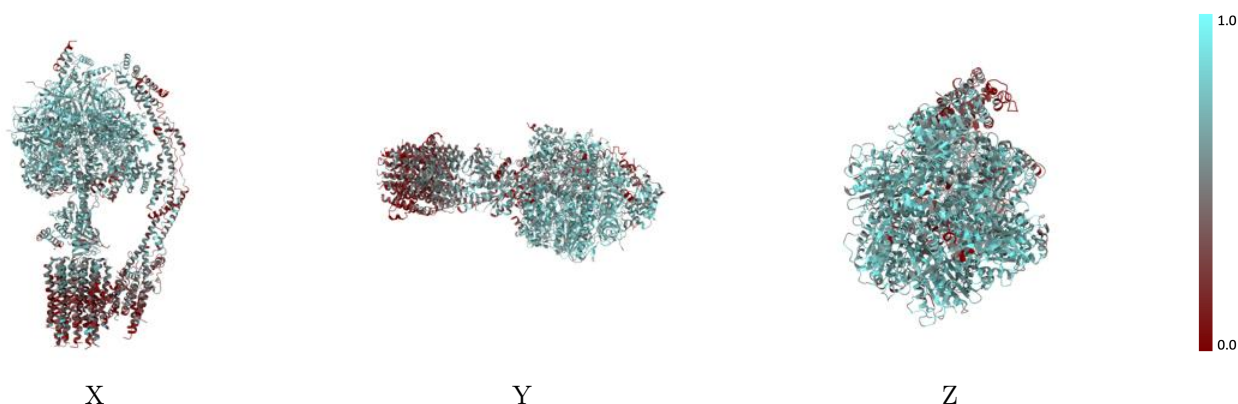
The images above show the 3D surface view of the map at the recommended contour level 0.0324 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



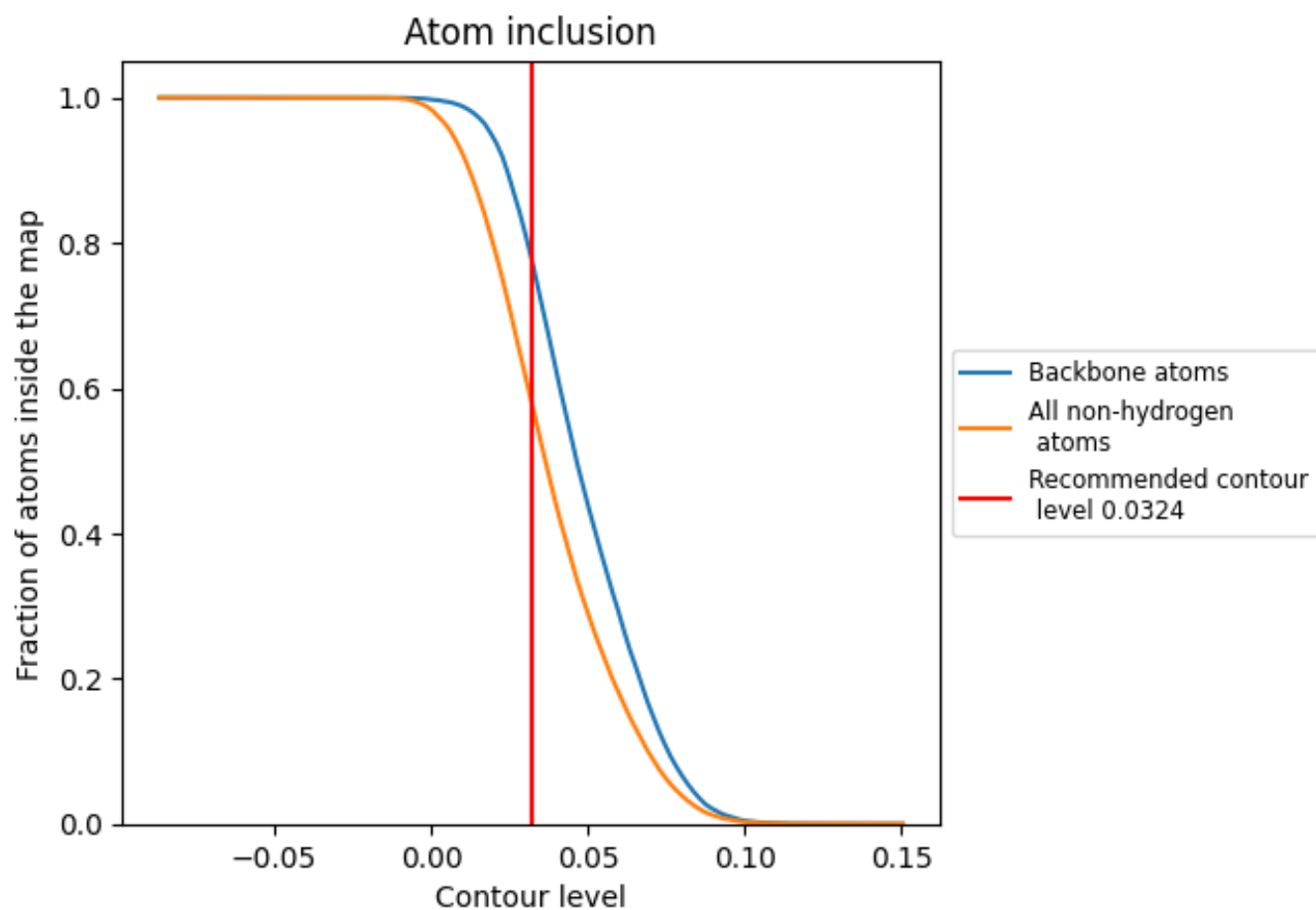
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0324).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 58% 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 (0.0324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5752	 0.3550
6	 0.1847	 0.1390
7	 0.4371	 0.2440
8	 0.4062	 0.2470
A	 0.6969	 0.4160
B	 0.6849	 0.4240
C	 0.6805	 0.4100
D	 0.6834	 0.4200
E	 0.6509	 0.4070
F	 0.6996	 0.4370
G	 0.6193	 0.3850
H	 0.5259	 0.3010
I	 0.6580	 0.3200
J	 0.2448	 0.2020
K	 0.3722	 0.2590
L	 0.3516	 0.2670
M	 0.3727	 0.2350
N	 0.3951	 0.2420
O	 0.3019	 0.2230
P	 0.3026	 0.1940
Q	 0.3138	 0.2240
R	 0.3371	 0.2640
S	 0.4329	 0.2850
T	 0.4057	 0.2800
U	 0.3455	 0.2530
X	 0.2975	 0.2100
Y	 0.6427	 0.3630
Z	 0.4613	 0.2420

