



Full wwPDB EM Validation Report ⓘ

Oct 1, 2026 – 05:22 PM EDT

PDB ID : 9ZB4 / pdb_00009zb4
EMDB ID : EMD-73974
Title : Cryo-EM structure of Leishmania tarentolae respiratory complex V (ATP synthase) membrane region
Authors : Liao, Y.T.; Chao, L.
Deposited on : 2025-11-20
Resolution : 3.73 Å(reported)
Based on initial model : .

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:

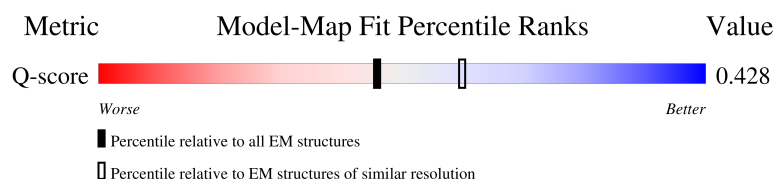
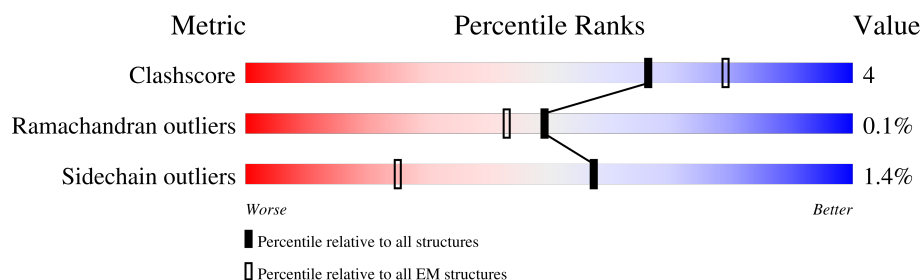
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.73 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10415 (3.23 - 4.23)

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	O	55	5% 89% 11%
1	o	55	89% 9% •
2	C	76	87% 80% 18% •
2	P	76	86% 82% 18%

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Mol	Chain	Length	Quality of chain
2	Q	76	84% 83% 16% .
2	R	76	82% 84% 14% .
2	S	76	71% 83% 17%
2	U	76	57% 88% 12%
2	V	76	64% 83% 17%
2	W	76	76% 92% 7% .
2	X	76	83% 75% 25%
2	Y	76	67% 87% 13%
2	c	76	86% 75% 25%
2	p	76	86% 83% 17%
2	q	76	84% 79% 20% .
2	r	76	84% 80% 20%
2	s	76	79% 88% 11% .
2	u	76	71% 95% . .
2	v	76	59% 95% 5%
2	w	76	72% 92% 8%
2	x	76	78% 92% 8%
2	y	76	76% 75% 25%
3	L	231	11% 87% 13%
3	l	231	11% 87% 12% .
4	B	102	9% 89% 10% .
4	b	102	7% 94% 6%
5	D	384	10% 92% 8%
5	d	384	10% 96% .
6	H	163	17% 87% 12% .

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Mol	Chain	Length	Quality of chain
6	h	163	
7	I	127	
7	i	127	
8	E	123	
8	e	123	
9	J	66	
9	j	66	
10	K	75	
10	k	75	
11	M	59	
11	m	59	
12	G	104	
12	g	104	
13	A	99	
13	a	99	
14	F	136	
14	f	136	
15	N	78	
15	n	78	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 41236 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 LtaP27_632926_633111, LtATPEG4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	55	Total	C	N	O	S	0	0
			481	322	83	74	2		
1	O	55	Total	C	N	O	S	0	0
			481	322	83	74	2		

- Molecule 2 is a protein called Mitochondrial ATP synthase subunit c-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	x	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	c	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	p	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	q	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	r	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	s	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	y	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	u	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	v	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	w	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	X	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	C	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	P	76	Total	C	N	O	S	0	0
			550	367	86	91	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	R	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	S	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	Y	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	U	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	V	76	Total	C	N	O	S	0	0
			550	367	86	91	6		
2	W	76	Total	C	N	O	S	0	0
			550	367	86	91	6		

- Molecule 3 is a protein called ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	l	231	Total	C	N	O	S	0	0
			1983	1401	257	288	37		
3	L	231	Total	C	N	O	S	0	0
			1983	1401	257	288	37		

- Molecule 4 is a protein called Mitochondrial ATP synthase subunit i/j.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	102	Total	C	N	O	S	0	0
			865	557	152	151	5		
4	B	102	Total	C	N	O	S	0	0
			865	557	152	151	5		

- Molecule 5 is a protein called Mitochondrial ATP synthase subunit ATPTB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	384	Total	C	N	O	S	0	0
			3196	2047	551	578	20		
5	D	384	Total	C	N	O	S	0	0
			3196	2047	551	578	20		

- Molecule 6 is a protein called Mitochondrial ATP synthase subunit ATPTB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	163	Total	C	N	O	S	0	0
			1349	860	247	235	7		
6	H	163	Total	C	N	O	S	0	0
			1349	860	247	235	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	109	ASP	VAL	conflict	UNP A0A640KJ33
h	110	VAL	ASP	conflict	UNP A0A640KJ33
H	109	ASP	VAL	conflict	UNP A0A640KJ33
H	110	VAL	ASP	conflict	UNP A0A640KJ33

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit g.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	127	Total	C	N	O	S	0	0
			1030	658	184	179	9		
7	I	127	Total	C	N	O	S	0	0
			1030	658	184	179	9		

- Molecule 8 is a protein called Mitochondrial ATP synthase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	123	Total	C	N	O	S	0	0
			1012	660	176	171	5		
8	E	123	Total	C	N	O	S	0	0
			1012	660	176	171	5		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	66	Total	C	N	O	S	0	0
			590	402	91	94	3		
9	J	66	Total	C	N	O	S	0	0
			590	402	91	94	3		

- Molecule 10 is a protein called Mitochondrial ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	75	Total	C	N	O	S	0	0
			642	423	100	118	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	75	Total	C	N	O	S	0	0
			642	423	100	118	1		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	59	Total	C	N	O	S	0	0
			490	307	96	85	2		
11	M	59	Total	C	N	O	S	0	0
			490	307	96	85	2		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit k.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	g	104	Total	C	N	O	S	0	0
			848	558	139	145	6		
12	G	104	Total	C	N	O	S	0	0
			848	558	139	145	6		

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit ATPTB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	99	Total	C	N	O	S	0	0
			804	500	149	150	5		
13	A	99	Total	C	N	O	S	0	0
			804	500	149	150	5		

- Molecule 14 is a protein called Mitochondrial ATP synthase subunit ATPTB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	136	Total	C	N	O	S	0	0
			1108	715	178	209	6		
14	F	136	Total	C	N	O	S	0	0
			1108	715	178	209	6		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit ATPEG3.

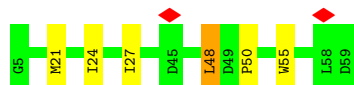
Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	78	Total	C	N	O	S	0	0
			720	471	130	116	3		
15	N	78	Total	C	N	O	S	0	0
			720	471	130	116	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

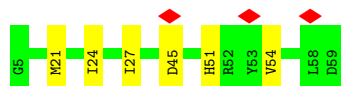
- Molecule 1: LtaP27_632926_633111, LtATPEG4

Chain o: 

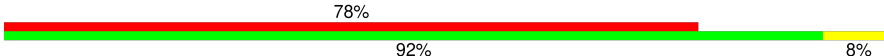


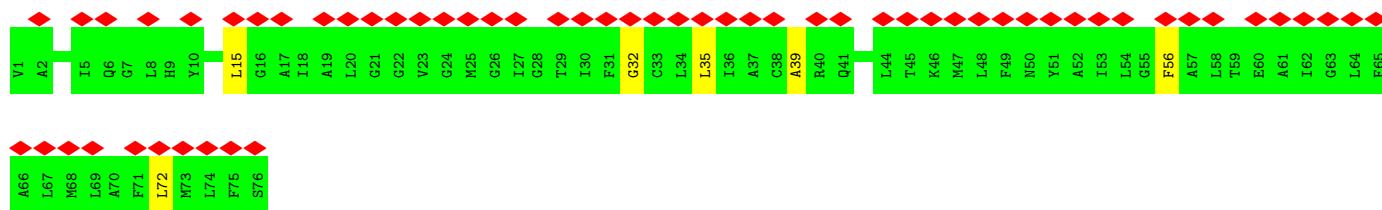
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Chain O: 



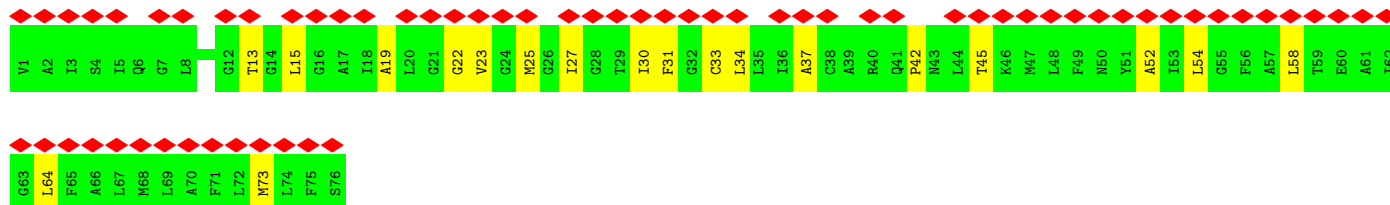
- Molecule 2: Mitochondrial ATP synthase subunit c-1

Chain x: 

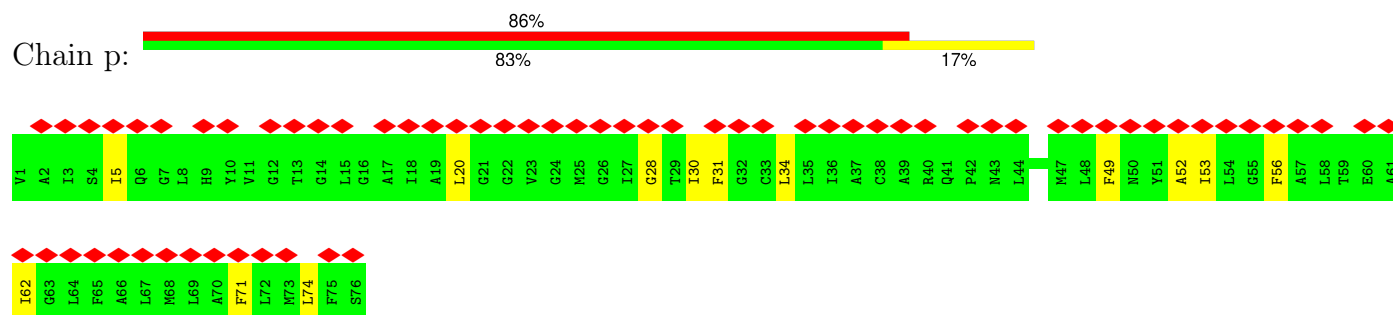


- Molecule 2: Mitochondrial ATP synthase subunit c-1

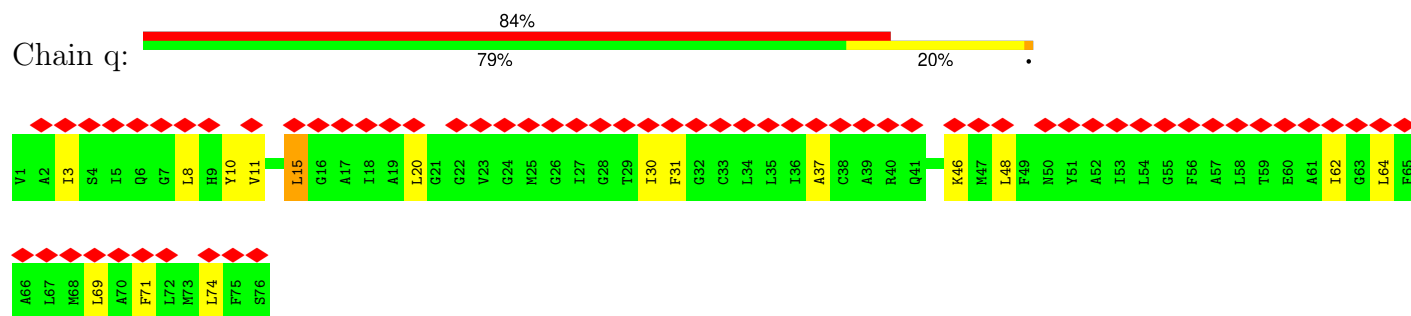
Chain c: 



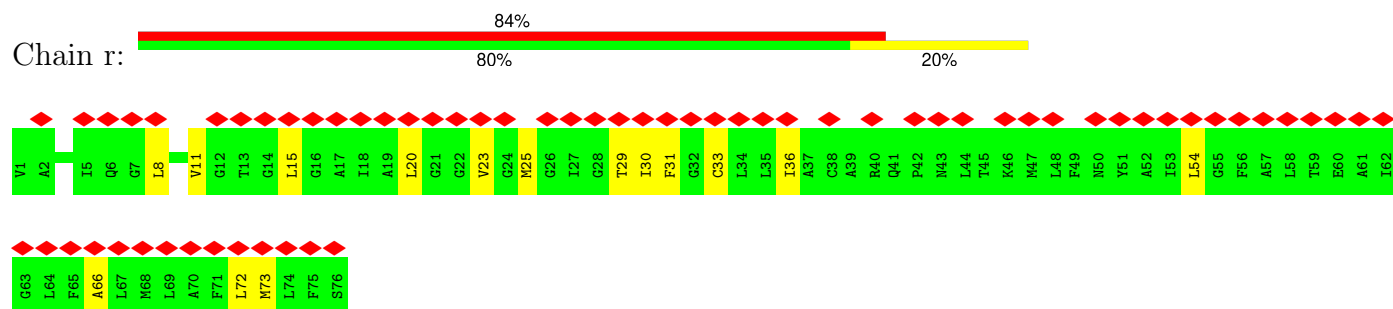
• Molecule 2: Mitochondrial ATP synthase subunit c-1



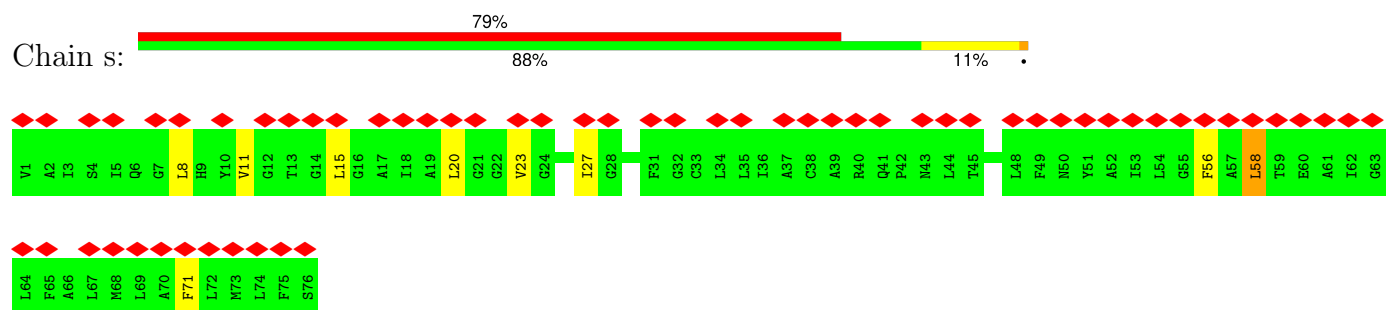
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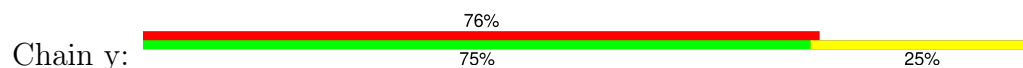
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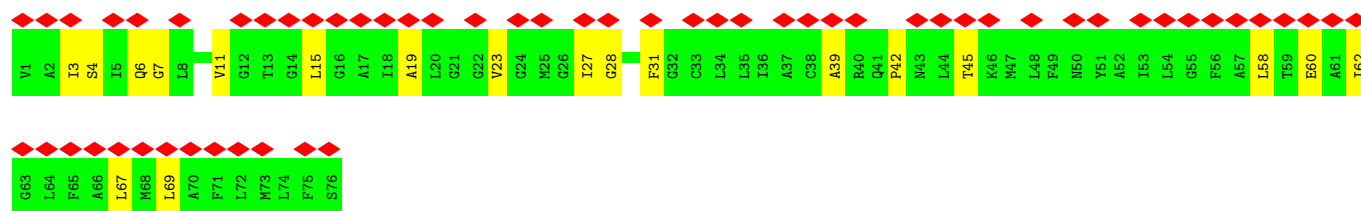


• Molecule 2: Mitochondrial ATP synthase subunit c-1

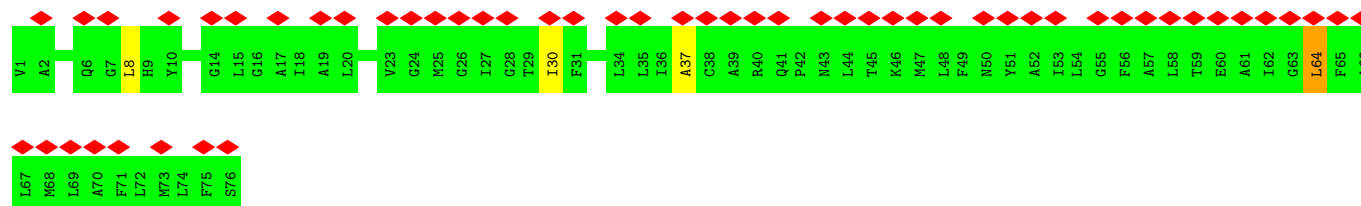


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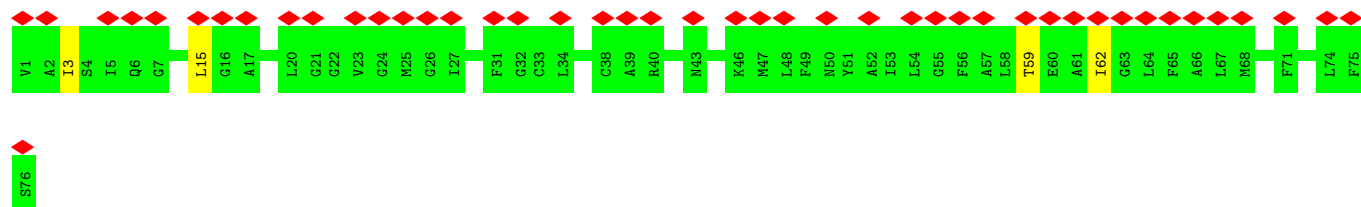




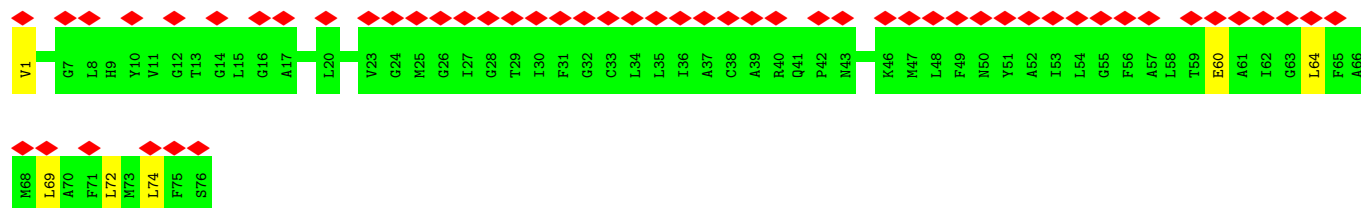
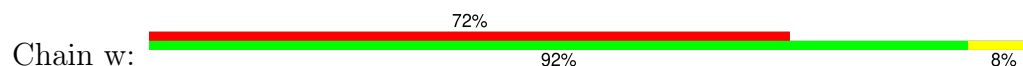
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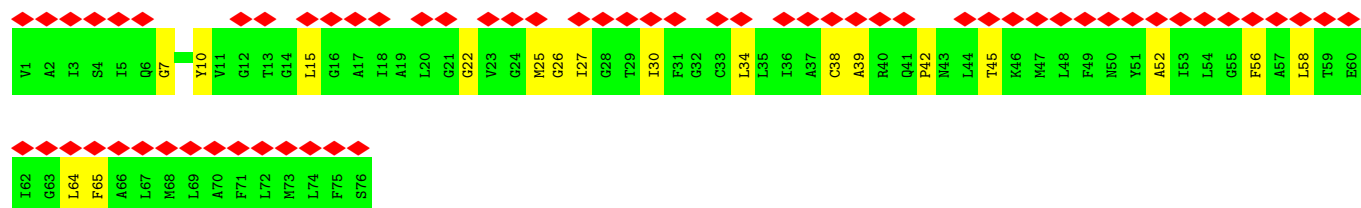
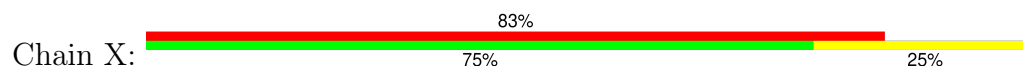
• Molecule 2: Mitochondrial ATP synthase subunit c-1



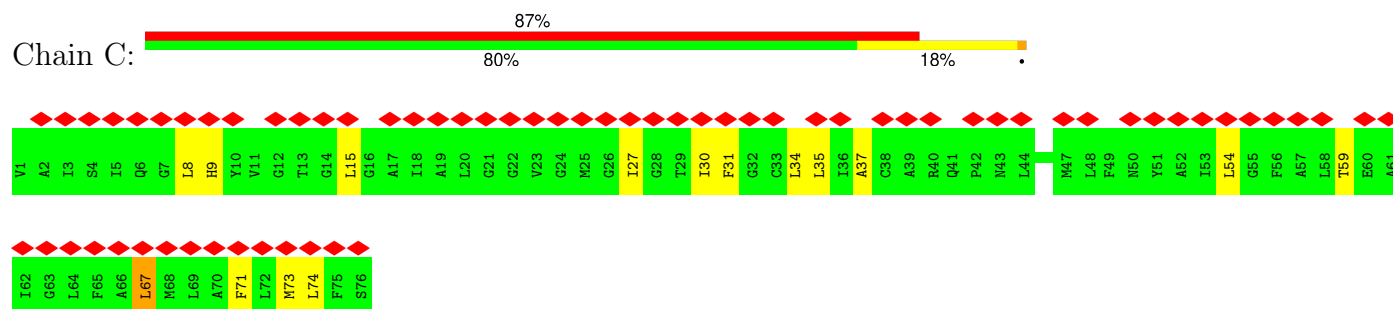
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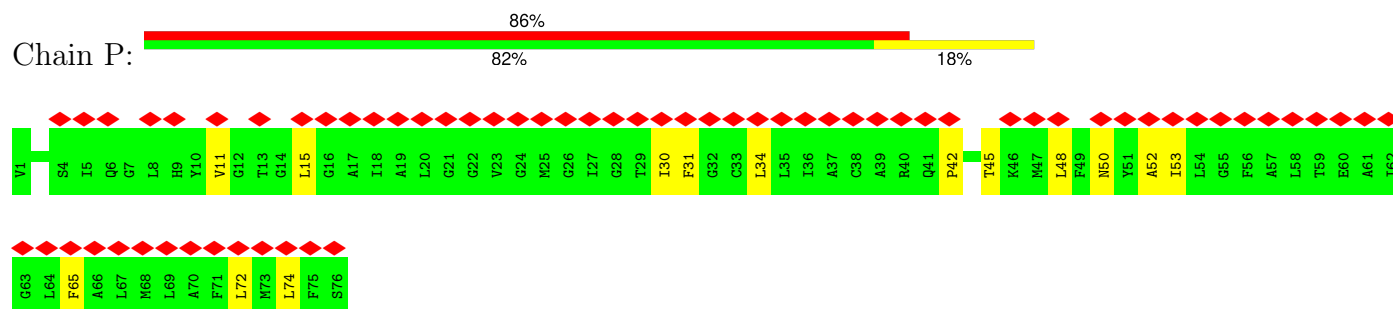
• Molecule 2: Mitochondrial ATP synthase subunit c-1



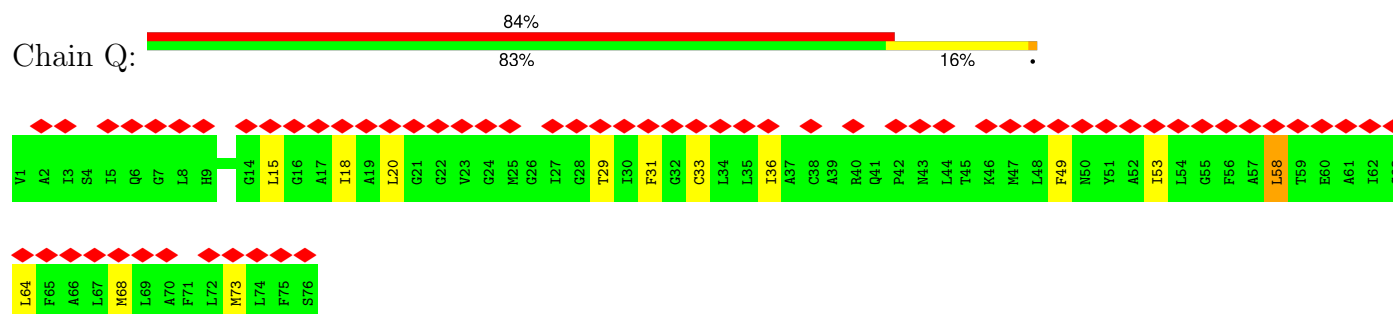
● Molecule 2: Mitochondrial ATP synthase subunit c-1



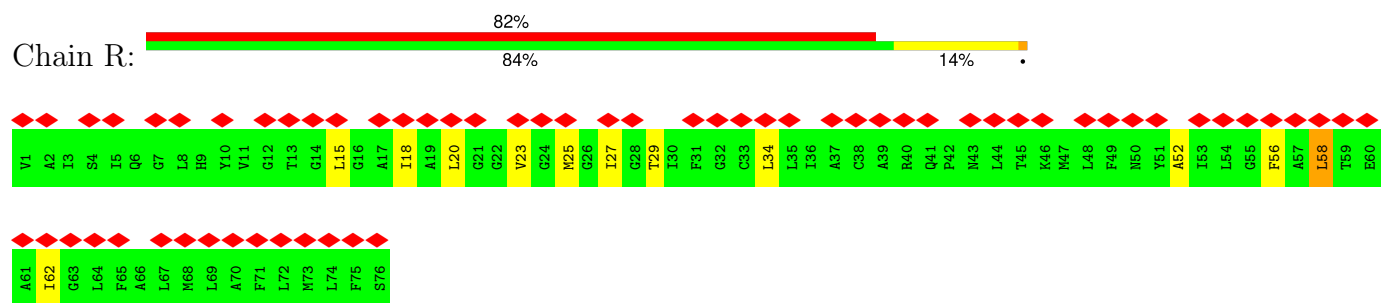
● Molecule 2: Mitochondrial ATP synthase subunit c-1



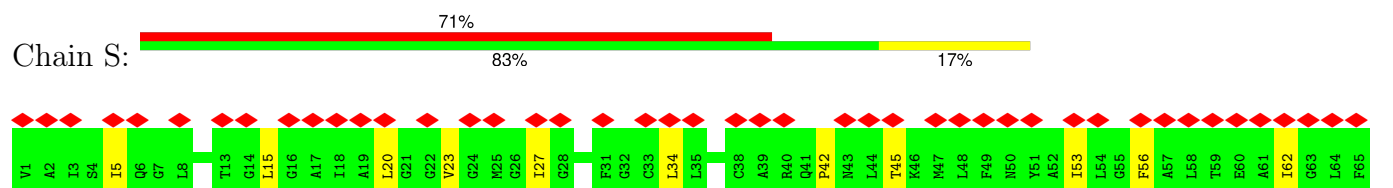
● Molecule 2: Mitochondrial ATP synthase subunit c-1



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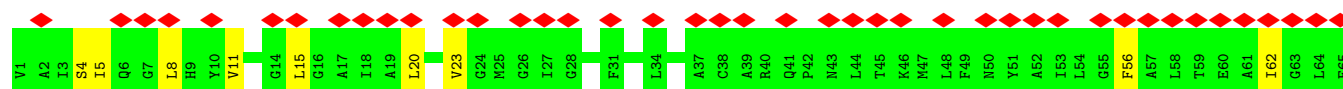
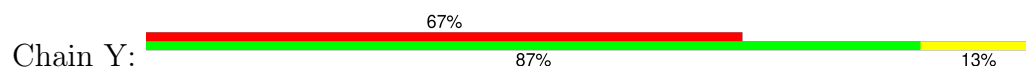


● Molecule 2: Mitochondrial ATP synthase subunit c-1

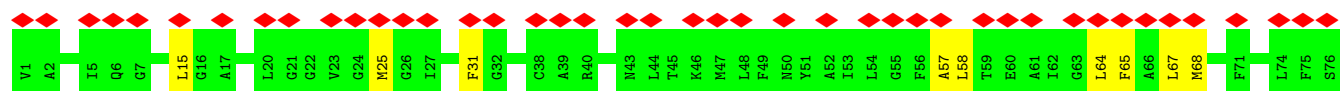
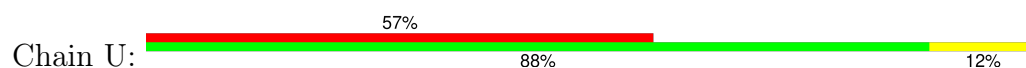




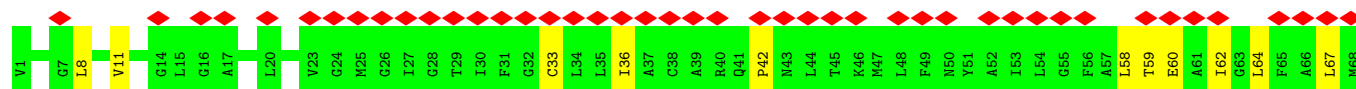
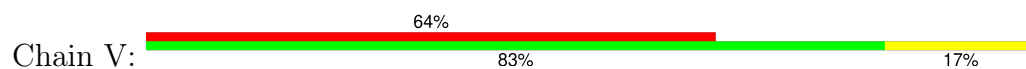
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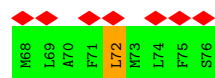
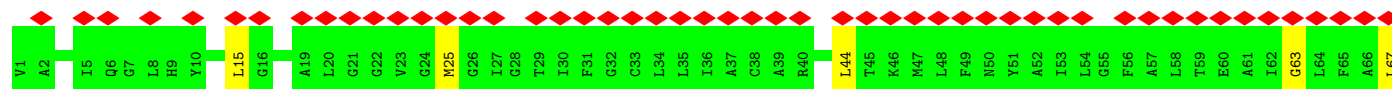
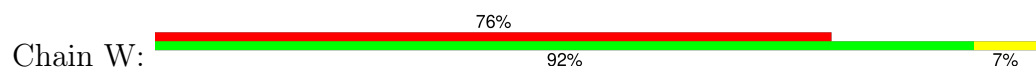
• Molecule 2: Mitochondrial ATP synthase subunit c-1



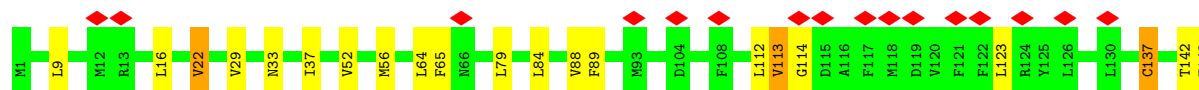
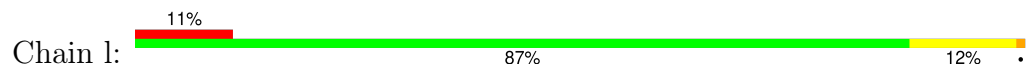
• Molecule 2: Mitochondrial ATP synthase subunit c-1

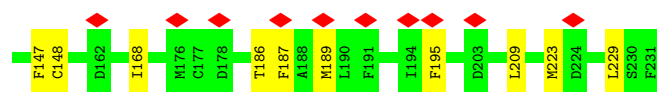


• Molecule 2: Mitochondrial ATP synthase subunit c-1

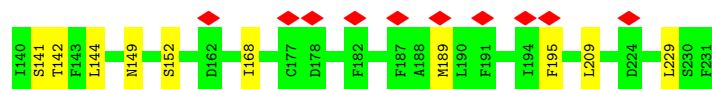
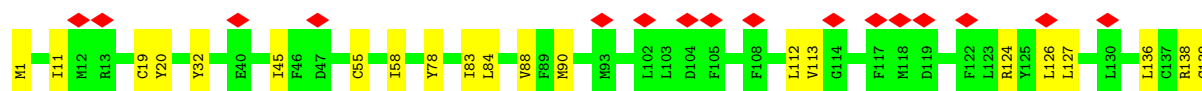
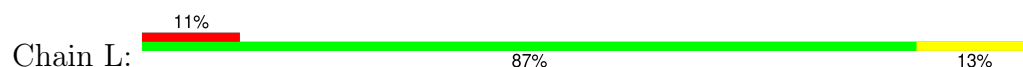


• Molecule 3: ATPase 6

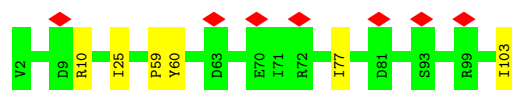




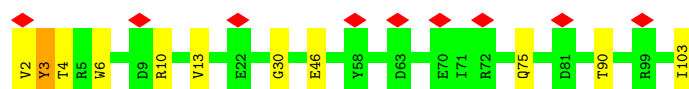
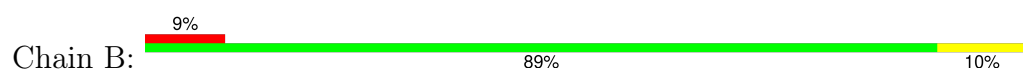
- Molecule 3: ATPase 6



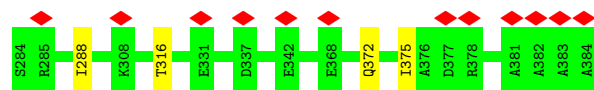
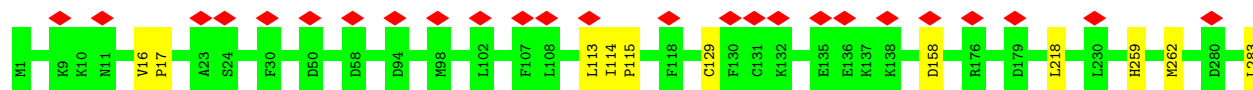
- Molecule 4: Mitochondrial ATP synthase subunit i/j



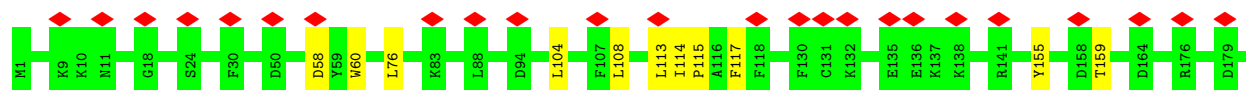
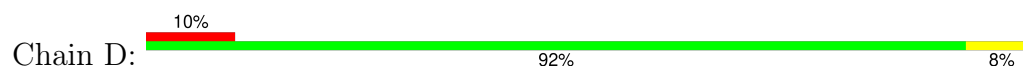
- Molecule 4: Mitochondrial ATP synthase subunit i/j

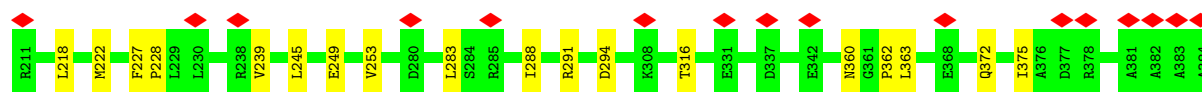


- Molecule 5: Mitochondrial ATP synthase subunit ATPTB1

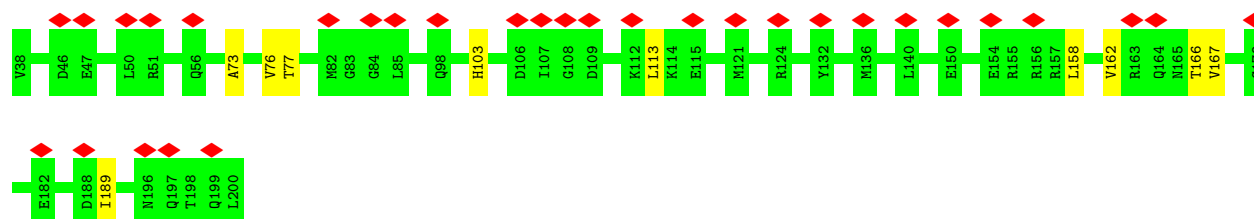


- Molecule 5: Mitochondrial ATP synthase subunit ATPTB1

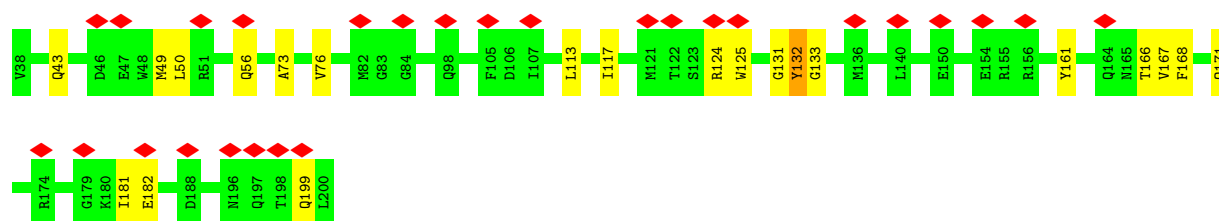
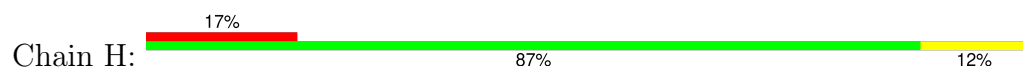




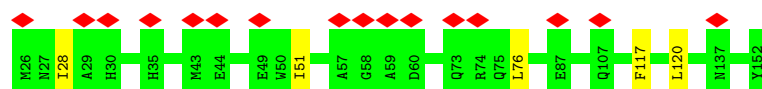
- Molecule 6: Mitochondrial ATP synthase subunit ATPTB6



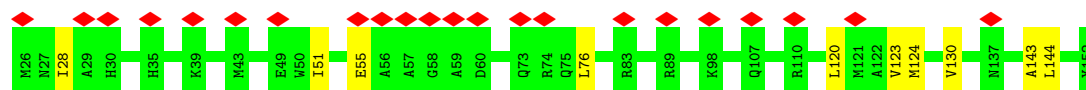
- Molecule 6: Mitochondrial ATP synthase subunit ATPTB6



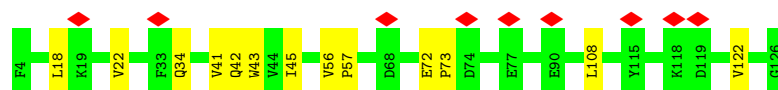
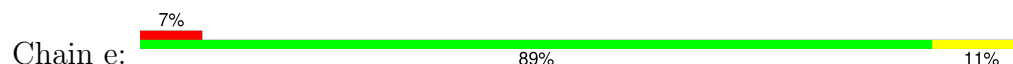
- Molecule 7: Mitochondrial ATP synthase subunit g



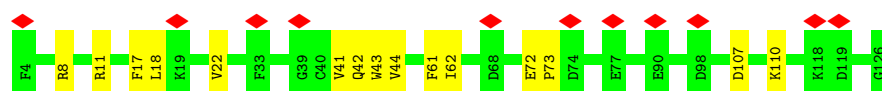
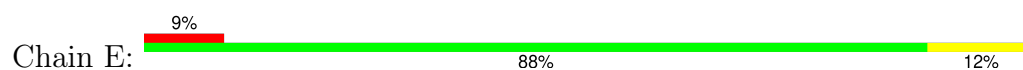
- Molecule 7: Mitochondrial ATP synthase subunit g



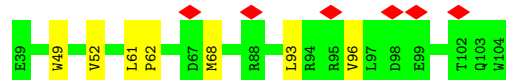
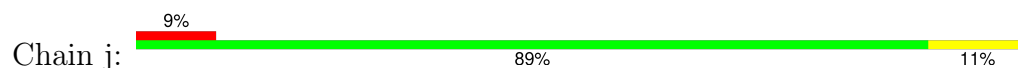
- Molecule 8: Mitochondrial ATP synthase subunit f



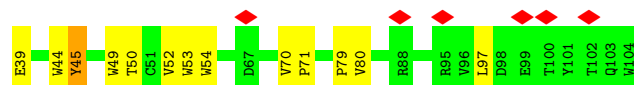
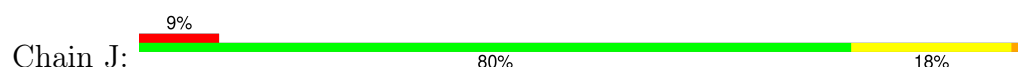
- Molecule 8: Mitochondrial ATP synthase subunit f



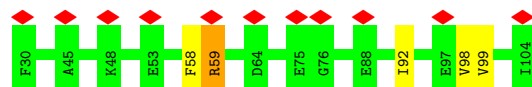
- Molecule 9: Mitochondrial ATP synthase subunit 8



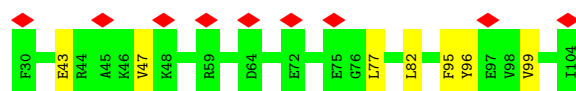
- Molecule 9: Mitochondrial ATP synthase subunit 8



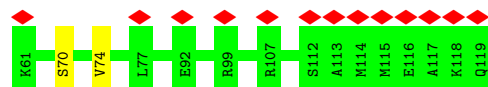
- Molecule 10: Mitochondrial ATP synthase subunit b



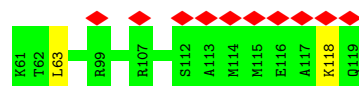
- Molecule 10: Mitochondrial ATP synthase subunit b



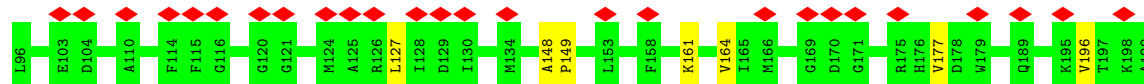
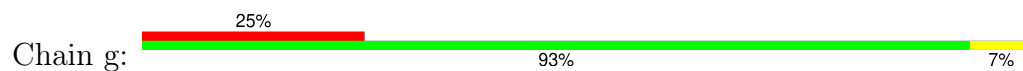
- Molecule 11: Mitochondrial ATP synthase subunit e



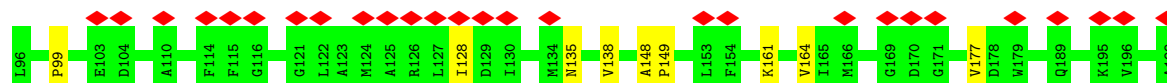
- Molecule 11: Mitochondrial ATP synthase subunit e



- Molecule 12: Mitochondrial ATP synthase subunit k



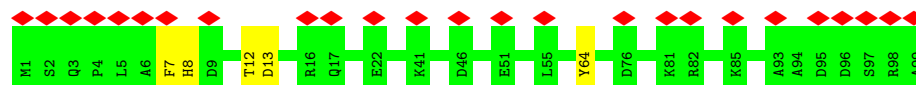
- Molecule 12: Mitochondrial ATP synthase subunit k



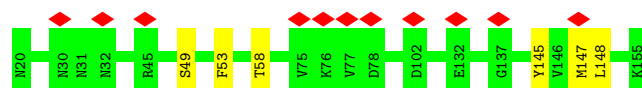
- Molecule 13: Mitochondrial ATP synthase subunit ATPTB12



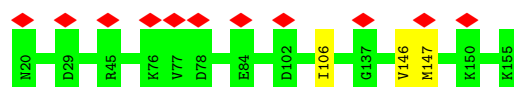
- Molecule 13: Mitochondrial ATP synthase subunit ATPTB12



- Molecule 14: Mitochondrial ATP synthase subunit ATPTB11

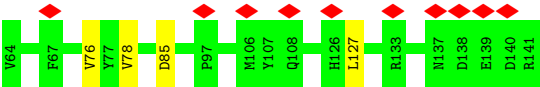


- Molecule 14: Mitochondrial ATP synthase subunit ATPTB11

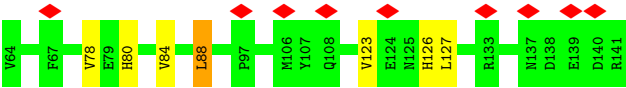
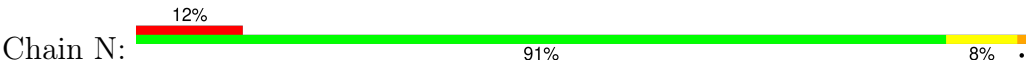


- Molecule 15: Mitochondrial ATP synthase subunit ATPEG3





• Molecule 15: Mitochondrial ATP synthase subunit ATPEG3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	4649	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	565.248, 565.248, 565.248	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.736, 0.736, 0.736	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	O	0.18	0/503	0.33	0/685
1	o	0.18	0/503	0.35	0/685
2	C	0.14	0/559	0.30	0/753
2	P	0.14	0/559	0.31	0/753
2	Q	0.17	0/559	0.30	0/753
2	R	0.14	0/559	0.27	0/753
2	S	0.15	0/559	0.34	0/753
2	U	0.14	0/559	0.28	0/753
2	V	0.14	0/559	0.29	0/753
2	W	0.16	0/559	0.30	0/753
2	X	0.15	0/559	0.29	0/753
2	Y	0.15	0/559	0.31	0/753
2	c	0.15	0/559	0.33	0/753
2	p	0.14	0/559	0.32	0/753
2	q	0.14	0/559	0.34	0/753
2	r	0.15	0/559	0.29	0/753
2	s	0.14	0/559	0.30	0/753
2	u	0.13	0/559	0.25	0/753
2	v	0.14	0/559	0.29	0/753
2	w	0.13	0/559	0.28	0/753
2	x	0.14	0/559	0.25	0/753
2	y	0.15	0/559	0.31	0/753
3	L	0.15	0/2052	0.36	0/2775
3	l	0.15	0/2052	0.36	0/2775
4	B	0.14	0/888	0.33	0/1202
4	b	0.14	0/888	0.33	0/1202
5	D	0.13	0/3292	0.32	0/4453
5	d	0.12	0/3292	0.30	0/4453
6	H	0.13	0/1380	0.32	0/1863
6	h	0.12	0/1380	0.28	0/1863
7	I	0.12	0/1054	0.29	0/1421
7	i	0.12	0/1054	0.26	0/1421
8	E	0.15	0/1046	0.35	0/1419
8	e	0.16	0/1046	0.37	0/1419

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	J	0.16	0/617	0.33	0/846
9	j	0.15	0/617	0.31	0/846
10	K	0.14	0/666	0.34	0/907
10	k	0.14	0/666	0.30	0/907
11	M	0.14	0/500	0.27	0/670
11	m	0.13	0/500	0.22	0/670
12	G	0.14	0/878	0.29	0/1190
12	g	0.14	0/878	0.33	0/1190
13	A	0.14	0/823	0.30	0/1110
13	a	0.13	0/823	0.32	0/1110
14	F	0.16	0/1145	0.34	0/1556
14	f	0.16	0/1145	0.33	0/1556
15	N	0.14	0/750	0.34	0/1023
15	n	0.14	0/750	0.32	0/1023
All	All	0.14	0/42368	0.32	0/57300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	481	0	449	3	0
1	o	481	0	449	4	0
2	C	550	0	587	17	0
2	P	550	0	587	12	0
2	Q	550	0	587	13	0
2	R	550	0	587	12	0
2	S	550	0	587	12	0
2	U	550	0	587	10	0
2	V	550	0	587	11	0
2	W	550	0	587	11	0
2	X	550	0	587	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	550	0	587	10	0
2	c	550	0	587	18	0
2	p	550	0	587	11	0
2	q	550	0	587	12	0
2	r	550	0	587	13	0
2	s	550	0	587	10	0
2	u	550	0	587	5	0
2	v	550	0	587	2	0
2	w	550	0	587	7	0
2	x	550	0	587	9	0
2	y	550	0	587	14	0
3	L	1983	0	1997	25	0
3	l	1983	0	1997	21	0
4	B	865	0	859	7	0
4	b	865	0	859	4	0
5	D	3196	0	3050	15	0
5	d	3196	0	3050	7	0
6	H	1349	0	1341	16	0
6	h	1349	0	1341	4	0
7	I	1030	0	1029	9	0
7	i	1030	0	1029	6	0
8	E	1012	0	991	8	0
8	e	1012	0	991	9	0
9	J	590	0	566	8	0
9	j	590	0	566	5	0
10	K	642	0	604	4	0
10	k	642	0	604	5	0
11	M	490	0	475	1	0
11	m	490	0	475	1	0
12	G	848	0	828	6	0
12	g	848	0	828	7	0
13	A	804	0	779	2	0
13	a	804	0	779	2	0
14	F	1108	0	1061	3	0
14	f	1108	0	1061	3	0
15	N	720	0	681	5	0
15	n	720	0	681	4	0
All	All	41236	0	41160	322	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 4.

All (322) 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:P:34:LEU:HD11	2:P:52:ALA:HB2	1.65	0.78
2:x:72:LEU:HD11	2:w:74:LEU:HD21	1.69	0.75
2:s:15:LEU:HD22	2:y:15:LEU:HD13	1.73	0.71
7:i:120:LEU:HD13	10:k:99:VAL:HG21	1.74	0.70
2:C:67:LEU:HD11	2:P:65:PHE:HB3	1.72	0.69
8:E:18:LEU:O	8:E:22:VAL:HG22	1.93	0.69
2:V:74:LEU:HD21	2:W:72:LEU:HD11	1.74	0.69
2:C:73:MET:HE3	2:C:73:MET:O	1.94	0.68
7:I:120:LEU:HD13	10:K:99:VAL:HG21	1.75	0.68
2:r:11:VAL:HG13	2:s:8:LEU:HD21	1.76	0.68
2:S:5:ILE:HG23	2:Y:5:ILE:HD13	1.76	0.67
2:Q:20:LEU:HD21	2:R:62:ILE:HG23	1.76	0.67
6:H:171:GLN:HE21	6:H:181:ILE:HD13	1.60	0.66
2:p:5:ILE:HD13	2:q:3:ILE:HG23	1.79	0.64
3:l:189:MET:HE3	3:l:189:MET:HA	1.79	0.64
3:L:189:MET:HA	3:L:189:MET:HE3	1.79	0.64
8:e:18:LEU:O	8:e:22:VAL:HG22	1.98	0.63
12:g:177:VAL:HG23	15:n:127:LEU:HD21	1.80	0.63
2:r:25:MET:O	2:r:29:THR:HG23	2.00	0.62
2:P:31:PHE:CZ	2:Q:58:LEU:HD21	2.34	0.62
2:W:25:MET:HE2	2:W:25:MET:HA	1.81	0.62
3:l:84:LEU:HD12	3:l:147:PHE:HB2	1.81	0.61
5:D:218:LEU:CD1	5:D:316:THR:HG21	2.30	0.61
3:L:149:ASN:HA	2:U:64:LEU:HD13	1.82	0.60
12:G:177:VAL:HG21	15:N:127:LEU:HD12	1.84	0.59
2:R:25:MET:O	2:R:29:THR:HG23	2.04	0.58
2:R:20:LEU:HA	2:R:23:VAL:HG12	1.86	0.58
2:Q:18:ILE:CD1	2:R:18:ILE:HD11	2.34	0.58
2:c:34:LEU:HD21	2:c:52:ALA:HB2	1.85	0.58
2:y:42:PRO:O	2:y:45:THR:HG23	2.04	0.58
6:h:158:LEU:O	6:h:162:VAL:HG23	2.04	0.57
2:S:42:PRO:O	2:S:45:THR:HG23	2.04	0.57
7:i:117:PHE:HA	10:k:92:ILE:HD11	1.86	0.57
2:c:27:ILE:HA	2:c:30:ILE:HG22	1.86	0.56
2:c:34:LEU:CD2	2:c:52:ALA:HB2	2.35	0.56
2:W:63:GLY:O	2:W:67:LEU:HD13	2.04	0.56
2:Y:5:ILE:HD12	2:Y:5:ILE:N	2.21	0.55
5:D:104:LEU:O	5:D:108:LEU:HD23	2.07	0.55
2:C:67:LEU:HD12	2:C:71:PHE:CE2	2.41	0.55
2:x:56:PHE:CZ	2:c:58:LEU:HD12	2.43	0.54
9:j:61:LEU:HD23	9:j:61:LEU:C	2.33	0.54
4:B:4:THR:HG1	4:B:6:TRP:CD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:49:TRP:O	9:J:52:VAL:HG12	2.08	0.54
1:o:48:LEU:HD22	1:o:48:LEU:H	1.71	0.54
3:l:16:LEU:HD11	9:j:68:MET:HE1	1.90	0.54
3:L:168:ILE:HD11	3:L:189:MET:HE1	1.90	0.54
3:l:168:ILE:HD11	3:l:189:MET:HE1	1.89	0.53
2:x:35:LEU:HD13	2:c:34:LEU:HD23	1.91	0.53
2:y:27:ILE:HD11	2:y:60:GLU:OE2	2.09	0.53
2:P:74:LEU:HD22	2:Q:73:MET:HE1	1.89	0.53
2:S:20:LEU:HD12	2:Y:62:ILE:HG23	1.90	0.53
2:V:59:THR:O	2:V:62:ILE:HG22	2.08	0.53
2:x:72:LEU:HD11	2:w:74:LEU:CD2	2.38	0.52
2:Y:15:LEU:HD23	2:U:15:LEU:HD21	1.90	0.52
3:L:90:MET:HE2	4:B:30:GLY:HA2	1.91	0.52
6:H:117:ILE:HD12	6:H:117:ILE:C	2.35	0.52
2:r:8:LEU:HD12	2:r:8:LEU:O	2.10	0.52
2:R:27:ILE:HD12	2:R:56:PHE:HD2	1.73	0.52
8:e:108:LEU:HD23	8:e:108:LEU:O	2.09	0.52
2:X:42:PRO:O	2:X:45:THR:HG23	2.10	0.51
2:R:20:LEU:HD12	2:S:62:ILE:HG23	1.93	0.51
2:c:64:LEU:C	2:c:64:LEU:HD23	2.34	0.51
12:G:161:LYS:HA	12:G:164:VAL:HG12	1.92	0.51
2:s:56:PHE:CZ	2:y:58:LEU:HD12	2.46	0.51
6:H:181:ILE:HD12	6:H:182:GLU:H	1.75	0.51
2:P:34:LEU:HD11	2:P:52:ALA:CB	2.38	0.51
2:X:25:MET:HE3	2:W:25:MET:SD	2.51	0.51
2:X:15:LEU:HG	2:C:15:LEU:HD21	1.91	0.51
2:X:15:LEU:HD13	2:W:15:LEU:HG	1.93	0.50
2:r:31:PHE:CE1	2:s:58:LEU:HD11	2.46	0.50
2:s:27:ILE:HD12	2:s:56:PHE:HD1	1.75	0.50
2:X:26:GLY:N	2:W:25:MET:HE1	2.27	0.50
6:h:113:LEU:HD23	6:h:113:LEU:C	2.36	0.50
2:q:8:LEU:O	2:q:11:VAL:HG12	2.12	0.50
2:X:7:GLY:O	2:C:8:LEU:HD23	2.12	0.50
5:d:114:ILE:HB	5:d:115:PRO:HD3	1.94	0.50
8:e:41:VAL:HG23	8:e:42:GLN:N	2.27	0.50
10:k:98:VAL:HG12	10:k:98:VAL:O	2.12	0.50
2:X:26:GLY:CA	2:W:25:MET:HE1	2.42	0.50
5:D:218:LEU:HD11	5:D:316:THR:HG21	1.93	0.50
2:q:15:LEU:HD22	2:r:15:LEU:HD13	1.93	0.49
7:i:76:LEU:HD21	7:I:51:ILE:HD11	1.95	0.49
9:j:49:TRP:O	9:j:52:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:77:ILE:HG21	13:a:50:VAL:HG22	1.95	0.49
2:s:20:LEU:HA	2:s:23:VAL:HG12	1.94	0.49
2:Q:15:LEU:HD22	2:Q:15:LEU:H	1.78	0.49
6:H:166:THR:HG22	6:H:167:VAL:N	2.29	0.48
2:Y:73:MET:HE2	2:Y:73:MET:N	2.28	0.48
2:c:22:GLY:HA2	2:c:25:MET:HE2	1.95	0.48
10:K:95:PHE:O	10:K:96:TYR:HB3	2.14	0.48
3:l:88:VAL:HG21	3:l:143:PHE:HB3	1.94	0.48
2:R:15:LEU:CD2	2:S:15:LEU:HD21	2.43	0.48
2:U:31:PHE:CZ	2:V:58:LEU:HD12	2.48	0.48
3:l:37:ILE:HD11	3:l:223:MET:SD	2.54	0.48
2:r:31:PHE:CZ	2:s:58:LEU:HD21	2.48	0.48
2:q:71:PHE:HA	2:q:74:LEU:HD23	1.96	0.48
2:X:39:ALA:HB2	2:C:37:ALA:HB1	1.95	0.48
1:O:21:MET:O	1:O:24:ILE:HG22	2.13	0.48
5:d:218:LEU:HD13	5:d:316:THR:HG21	1.95	0.48
2:X:61:ALA:HA	2:X:64:LEU:HD23	1.96	0.48
5:D:222:MET:HE1	5:D:239:VAL:HG13	1.96	0.48
2:u:64:LEU:HD13	3:l:137:CYS:SG	2.54	0.48
2:Q:18:ILE:HD11	2:R:18:ILE:HD11	1.96	0.48
8:E:72:GLU:N	8:E:73:PRO:CD	2.77	0.47
1:O:51:HIS:O	1:O:54:VAL:HG23	2.14	0.47
6:h:166:THR:HG22	6:h:167:VAL:N	2.29	0.47
8:e:72:GLU:N	8:e:73:PRO:HD2	2.29	0.47
3:l:229:LEU:HD12	3:l:229:LEU:O	2.15	0.47
14:f:145:TYR:HB3	14:f:148:LEU:HD21	1.95	0.47
3:l:9:LEU:HD11	3:l:65:PHE:CE2	2.49	0.47
6:H:49:MET:HE2	6:H:161:TYR:OH	2.14	0.47
2:Y:8:LEU:O	2:Y:11:VAL:HG12	2.14	0.47
2:V:72:LEU:HD23	2:V:72:LEU:C	2.39	0.47
2:C:74:LEU:HD21	2:P:72:LEU:HD21	1.97	0.47
6:H:132:TYR:CG	6:H:133:GLY:N	2.83	0.47
2:V:8:LEU:O	2:V:11:VAL:HG22	2.15	0.47
2:V:67:LEU:C	2:V:67:LEU:HD23	2.40	0.47
2:X:27:ILE:HG23	2:C:59:THR:HG22	1.96	0.47
5:D:283:LEU:HD13	5:D:288:ILE:HD11	1.97	0.46
1:o:21:MET:O	1:o:24:ILE:HG22	2.15	0.46
2:y:67:LEU:C	2:y:67:LEU:HD13	2.41	0.46
4:B:103:ILE:HD12	4:B:103:ILE:H	1.80	0.46
7:I:28:ILE:HD12	7:I:28:ILE:N	2.31	0.46
2:Q:49:PHE:CZ	2:Q:53:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:20:LEU:HA	2:S:23:VAL:HG22	1.98	0.46
7:i:51:ILE:HD11	7:I:76:LEU:HD21	1.98	0.46
3:L:112:LEU:HD23	3:L:124:ARG:NH2	2.31	0.46
2:P:31:PHE:HZ	2:Q:58:LEU:HD21	1.80	0.46
4:b:59:PRO:O	4:b:60:TYR:HB2	2.16	0.46
3:L:11:ILE:HD12	3:L:11:ILE:H	1.81	0.46
2:U:31:PHE:HZ	2:V:58:LEU:HD12	1.80	0.46
4:b:25:ILE:N	4:b:25:ILE:HD12	2.31	0.46
12:g:177:VAL:HG23	15:n:127:LEU:CD2	2.44	0.46
4:B:10:ARG:O	4:B:13:VAL:HG12	2.16	0.46
2:x:15:LEU:HD22	2:c:15:LEU:HD13	1.98	0.46
6:H:43:GLN:CD	15:N:88:LEU:HD12	2.40	0.46
5:D:114:ILE:HB	5:D:115:PRO:HD3	1.97	0.46
12:G:128:ILE:C	12:G:128:ILE:HD12	2.41	0.46
2:c:27:ILE:HD13	2:p:62:ILE:HD12	1.98	0.45
3:l:52:VAL:O	3:l:56:MET:HG2	2.16	0.45
3:L:127:LEU:HD13	2:S:53:ILE:CG2	2.46	0.45
2:p:34:LEU:HD12	2:p:52:ALA:CB	2.46	0.45
1:O:24:ILE:HA	1:O:27:ILE:HG22	1.97	0.45
1:o:24:ILE:HA	1:o:27:ILE:HG22	1.98	0.45
2:C:27:ILE:HA	2:C:30:ILE:HG22	1.98	0.45
2:Y:56:PHE:CZ	2:U:58:LEU:HD11	2.52	0.45
15:N:123:VAL:HG22	15:N:123:VAL:O	2.16	0.45
2:r:54:LEU:C	2:r:54:LEU:HD23	2.42	0.45
5:d:283:LEU:HD13	5:d:288:ILE:HD11	1.99	0.45
3:L:55:CYS:HA	3:L:58:ILE:HG22	1.99	0.45
2:Q:31:PHE:CE1	2:R:58:LEU:HD21	2.51	0.45
5:D:227:PHE:HB3	5:D:228:PRO:HD3	1.97	0.45
2:x:35:LEU:HD13	2:c:34:LEU:CD2	2.47	0.45
2:x:39:ALA:HB2	2:c:37:ALA:HB1	1.97	0.45
9:J:52:VAL:HG13	9:J:53:TRP:N	2.32	0.45
15:N:80:HIS:O	15:N:84:VAL:HG23	2.17	0.45
2:p:71:PHE:CE1	2:q:69:LEU:HD21	2.52	0.45
5:d:372:GLN:HA	5:d:375:ILE:HG22	1.99	0.45
3:L:45:ILE:HD12	3:L:45:ILE:O	2.17	0.45
9:J:44:TRP:O	9:J:45:TYR:CD1	2.70	0.45
7:i:117:PHE:CA	10:k:92:ILE:HD11	2.47	0.45
3:L:78:TYR:HE1	3:L:84:LEU:HD21	1.82	0.45
3:L:126:LEU:C	3:L:126:LEU:HD23	2.42	0.45
2:q:37:ALA:HB3	2:q:48:LEU:HD21	1.99	0.44
10:k:58:PHE:O	10:k:59:ARG:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:38:CYS:SG	2:X:45:THR:HG22	2.57	0.44
2:U:67:LEU:C	2:U:67:LEU:HD13	2.43	0.44
2:S:27:ILE:HD12	2:S:56:PHE:HD2	1.82	0.44
3:l:29:VAL:CG2	3:l:56:MET:HE1	2.47	0.44
7:i:28:ILE:HD12	7:i:28:ILE:N	2.32	0.44
9:j:93:LEU:O	9:j:96:VAL:HG12	2.18	0.44
3:L:45:ILE:HD12	3:L:45:ILE:C	2.42	0.44
3:L:83:ILE:HD12	9:J:50:THR:HA	2.00	0.44
10:K:43:GLU:O	10:K:47:VAL:HG13	2.16	0.44
13:A:12:THR:HG23	13:A:13:ASP:N	2.33	0.44
8:e:41:VAL:HG22	8:e:45:ILE:HB	2.00	0.44
2:U:65:PHE:O	2:U:68:MET:HG3	2.18	0.44
5:D:372:GLN:HA	5:D:375:ILE:HG22	1.99	0.44
2:X:7:GLY:C	2:C:8:LEU:HD23	2.42	0.44
2:C:9:HIS:HA	2:C:73:MET:HE2	1.99	0.44
7:I:130:VAL:HG12	7:I:130:VAL:O	2.17	0.44
2:q:11:VAL:HG22	2:q:15:LEU:HD23	1.99	0.44
11:M:63:LEU:N	11:M:63:LEU:HD22	2.33	0.44
2:C:31:PHE:HB2	2:P:30:ILE:HD11	1.98	0.44
2:r:72:LEU:C	2:r:72:LEU:HD12	2.43	0.43
3:L:229:LEU:HD11	5:D:58:ASP:HB3	2.00	0.43
3:L:229:LEU:HD12	3:L:229:LEU:N	2.33	0.43
6:H:171:GLN:NE2	6:H:181:ILE:HD13	2.32	0.43
8:E:11:ARG:NE	14:F:106:ILE:HD13	2.33	0.43
9:J:97:LEU:C	9:J:97:LEU:HD13	2.43	0.43
2:X:22:GLY:O	2:W:25:MET:HE3	2.18	0.43
2:s:11:VAL:HG22	2:y:11:VAL:HG23	2.00	0.43
14:f:49:SER:HA	14:f:58:THR:HG21	2.01	0.43
3:L:209:LEU:HD21	2:U:57:ALA:HB2	1.99	0.43
2:C:67:LEU:HD12	2:C:71:PHE:HE2	1.83	0.43
2:Y:4:SER:C	2:Y:5:ILE:HD12	2.43	0.43
5:D:249:GLU:O	5:D:253:VAL:HG23	2.17	0.43
5:D:291:ARG:HA	5:D:294:ASP:OD2	2.18	0.43
2:y:39:ALA:HB2	2:u:37:ALA:HB1	1.99	0.43
2:w:72:LEU:O	2:w:72:LEU:HD23	2.19	0.43
14:f:147:MET:HB2	15:n:78:VAL:HG23	1.98	0.43
3:L:112:LEU:C	3:L:113:VAL:HG12	2.43	0.43
6:H:73:ALA:O	6:H:76:VAL:HG12	2.17	0.43
1:o:50:PRO:HD3	7:I:143:ALA:HB2	2.00	0.43
6:h:73:ALA:O	6:h:76:VAL:HG12	2.16	0.43
12:g:161:LYS:HA	12:g:164:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:ASN:O	2:P:53:ILE:HG22	2.17	0.43
2:Q:64:LEU:O	2:Q:68:MET:HE2	2.18	0.43
2:y:28:GLY:HA2	2:u:30:ILE:HD11	2.00	0.43
6:H:113:LEU:N	6:H:113:LEU:HD22	2.33	0.43
2:c:31:PHE:C	2:p:30:ILE:HD13	2.44	0.43
3:l:16:LEU:HD23	3:l:16:LEU:C	2.44	0.43
6:H:181:ILE:HD12	6:H:182:GLU:N	2.33	0.43
2:w:64:LEU:HD22	3:l:195:PHE:CE2	2.54	0.43
3:L:88:VAL:HG11	3:L:139:CYS:O	2.18	0.43
2:W:25:MET:HE2	2:W:25:MET:CA	2.48	0.43
2:c:42:PRO:O	2:c:45:THR:HG23	2.17	0.43
2:q:31:PHE:HB2	2:r:30:ILE:HD11	2.00	0.43
2:v:59:THR:O	2:v:62:ILE:HG22	2.18	0.43
3:l:113:VAL:HG23	3:l:114:GLY:H	1.83	0.43
13:a:35:HIS:HD1	13:a:56:THR:HG23	1.83	0.43
9:J:70:VAL:N	9:J:71:PRO:HD2	2.33	0.43
2:X:10:TYR:CD1	2:C:73:MET:HE1	2.53	0.43
2:r:20:LEU:HA	2:r:23:VAL:HG12	2.01	0.43
9:j:61:LEU:HB3	9:j:62:PRO:HD3	2.01	0.43
4:B:2:VAL:HG23	4:B:3:TYR:N	2.34	0.43
12:G:135:ASN:HA	12:G:138:VAL:HG12	1.99	0.43
2:s:71:PHE:CE1	2:y:69:LEU:HD21	2.54	0.42
3:l:9:LEU:HD11	3:l:65:PHE:CZ	2.53	0.42
3:l:186:THR:HG23	3:l:187:PHE:N	2.34	0.42
12:g:177:VAL:CG2	15:n:127:LEU:HD21	2.49	0.42
2:Q:15:LEU:HD22	2:Q:15:LEU:N	2.34	0.42
2:Q:20:LEU:HD11	2:R:62:ILE:CG2	2.49	0.42
2:R:15:LEU:HG	2:S:15:LEU:HD21	2.01	0.42
3:l:29:VAL:CG1	3:l:56:MET:HE1	2.49	0.42
3:L:32:TYR:O	3:L:32:TYR:CG	2.72	0.42
6:H:124:ARG:C	6:H:125:TRP:CG	2.97	0.42
6:H:131:GLY:O	6:H:133:GLY:N	2.53	0.42
7:I:120:LEU:O	7:I:123:VAL:HG12	2.19	0.42
8:E:41:VAL:HG22	8:E:41:VAL:O	2.18	0.42
2:Q:33:CYS:HA	2:Q:36:ILE:HG22	2.01	0.42
2:c:54:LEU:O	2:c:58:LEU:HD23	2.20	0.42
2:y:3:ILE:HG22	2:y:4:SER:N	2.33	0.42
3:l:22:VAL:HG23	8:e:34:GLN:NE2	2.34	0.42
12:g:127:LEU:HD23	12:g:127:LEU:C	2.44	0.42
2:V:42:PRO:HB3	2:W:44:LEU:HD11	2.01	0.42
2:w:72:LEU:HD23	2:w:72:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:152:SER:OG	2:U:67:LEU:HD12	2.18	0.42
2:P:42:PRO:O	2:P:45:THR:HG22	2.20	0.42
2:c:13:THR:HG22	2:c:73:MET:HG3	2.00	0.42
6:H:56:GLN:HA	6:H:168:PHE:CE2	2.54	0.42
3:L:152:SER:CB	2:U:67:LEU:HD12	2.49	0.42
9:J:45:TYR:O	9:J:45:TYR:CD2	2.73	0.42
2:x:72:LEU:HD12	2:x:72:LEU:C	2.45	0.42
2:y:31:PHE:HB2	2:u:30:ILE:CD1	2.49	0.42
8:e:122:VAL:HG23	8:e:122:VAL:O	2.20	0.42
6:H:166:THR:HG22	6:H:167:VAL:H	1.85	0.42
8:E:61:PHE:O	8:E:62:ILE:HB	2.20	0.42
5:D:362:PRO:O	5:D:363:LEU:HB2	2.20	0.42
2:Y:20:LEU:O	2:Y:23:VAL:HG22	2.20	0.42
5:D:113:LEU:C	5:D:113:LEU:HD13	2.45	0.42
4:b:103:ILE:HD12	4:b:103:ILE:H	1.85	0.42
5:d:113:LEU:HD13	5:d:113:LEU:O	2.20	0.42
12:g:196:VAL:O	12:g:196:VAL:HG13	2.20	0.42
7:I:144:LEU:H	7:I:144:LEU:HD22	1.84	0.42
8:E:42:GLN:HG3	8:E:43:TRP:H	1.84	0.42
2:p:20:LEU:HD11	2:q:62:ILE:O	2.20	0.41
2:V:33:CYS:HA	2:V:36:ILE:HG22	2.01	0.41
8:e:56:VAL:HB	8:e:57:PRO:HD3	2.02	0.41
3:L:141:SER:O	3:L:142:THR:C	2.63	0.41
2:p:34:LEU:O	2:p:34:LEU:HD23	2.20	0.41
2:q:20:LEU:HD21	2:r:66:ALA:HB2	2.02	0.41
2:X:65:PHE:CG	2:W:67:LEU:HD21	2.55	0.41
2:x:32:GLY:HA2	2:c:33:CYS:SG	2.60	0.41
2:c:19:ALA:O	2:c:23:VAL:HG23	2.20	0.41
2:w:60:GLU:O	2:w:64:LEU:HG	2.20	0.41
10:K:77:LEU:HB3	10:K:82:LEU:HD21	2.03	0.41
2:R:34:LEU:HD12	2:R:52:ALA:HB2	2.03	0.41
8:E:11:ARG:CZ	14:F:106:ILE:HD13	2.50	0.41
13:A:7:PHE:O	13:A:7:PHE:CD2	2.74	0.41
12:G:148:ALA:HB3	12:G:149:PRO:HD3	2.02	0.41
2:s:20:LEU:HD12	2:y:62:ILE:HG23	2.02	0.41
3:L:19:CYS:O	3:L:20:TYR:HB2	2.20	0.41
9:J:79:PRO:O	9:J:80:VAL:HB	2.21	0.41
2:X:27:ILE:HD13	2:X:56:PHE:HD1	1.86	0.41
2:V:60:GLU:O	2:V:64:LEU:HG	2.20	0.41
2:c:31:PHE:HB3	2:p:30:ILE:HD13	2.02	0.41
4:B:90:THR:HG22	4:B:90:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:16:VAL:N	5:d:17:PRO:HD2	2.36	0.41
3:L:136:LEU:C	3:L:138:ARG:H	2.29	0.41
7:I:120:LEU:O	7:I:124:MET:HG2	2.21	0.41
8:E:107:ASP:O	8:E:110:LYS:HG2	2.20	0.41
2:p:28:GLY:HA2	2:q:30:ILE:HG12	2.03	0.41
2:y:7:GLY:C	2:u:8:LEU:HD23	2.46	0.41
2:y:19:ALA:O	2:y:23:VAL:HG22	2.20	0.41
3:l:123:LEU:HD12	3:l:123:LEU:C	2.46	0.41
5:d:259:HIS:HA	5:d:262:MET:SD	2.61	0.41
2:C:34:LEU:O	2:C:34:LEU:HD23	2.21	0.41
2:S:67:LEU:HD13	2:S:67:LEU:C	2.46	0.41
2:q:10:TYR:CD1	2:r:73:MET:HE1	2.55	0.41
2:v:3:ILE:HG22	2:w:1:VAL:CG1	2.51	0.41
2:X:27:ILE:HA	2:X:30:ILE:HG22	2.02	0.41
2:C:54:LEU:HD13	2:C:54:LEU:C	2.46	0.41
3:l:56:MET:HE3	8:e:43:TRP:CZ3	2.56	0.40
2:X:34:LEU:HD22	2:X:52:ALA:CB	2.51	0.40
2:X:64:LEU:HD12	2:X:64:LEU:C	2.46	0.40
2:r:33:CYS:HA	2:r:36:ILE:HG22	2.04	0.40
2:P:11:VAL:HG22	2:P:15:LEU:HD13	2.03	0.40
2:S:20:LEU:HD12	2:Y:62:ILE:CG2	2.51	0.40
2:S:62:ILE:HD12	2:S:62:ILE:N	2.36	0.40
5:D:60:TRP:CZ2	12:G:99:PRO:HD3	2.56	0.40
3:l:112:LEU:C	3:l:113:VAL:HG22	2.46	0.40
14:F:147:MET:HB2	15:N:78:VAL:HG23	2.03	0.40
2:p:49:PHE:O	2:p:53:ILE:HD13	2.22	0.40
11:m:70:SER:O	11:m:74:VAL:HG23	2.21	0.40
12:g:148:ALA:HB3	12:g:149:PRO:HD3	2.03	0.40
3:L:195:PHE:CZ	2:V:64:LEU:HD13	2.56	0.40
4:B:103:ILE:HD12	4:B:103:ILE:N	2.37	0.40
2:C:35:LEU:HD12	2:P:48:LEU:HB2	2.03	0.40
5:D:155:TYR:O	5:D:159:THR:HG22	2.22	0.40
2:p:31:PHE:CZ	2:p:52:ALA:HB1	2.57	0.40
6:H:124:ARG:C	6:H:125:TRP:CD1	2.99	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	O	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	o	53/55 (96%)	52 (98%)	0	1 (2%)	6	33
2	C	74/76 (97%)	74 (100%)	0	0	100	100
2	P	74/76 (97%)	74 (100%)	0	0	100	100
2	Q	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	R	74/76 (97%)	74 (100%)	0	0	100	100
2	S	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	U	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	V	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	W	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	X	74/76 (97%)	74 (100%)	0	0	100	100
2	Y	74/76 (97%)	74 (100%)	0	0	100	100
2	c	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	p	74/76 (97%)	74 (100%)	0	0	100	100
2	q	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	r	74/76 (97%)	74 (100%)	0	0	100	100
2	s	74/76 (97%)	74 (100%)	0	0	100	100
2	u	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	v	74/76 (97%)	74 (100%)	0	0	100	100
2	w	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	x	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
3	L	229/231 (99%)	217 (95%)	12 (5%)	0	100	100
3	l	229/231 (99%)	215 (94%)	13 (6%)	1 (0%)	30	60
4	B	100/102 (98%)	96 (96%)	3 (3%)	1 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	b	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
5	D	382/384 (100%)	367 (96%)	15 (4%)	0	100	100
5	d	382/384 (100%)	372 (97%)	10 (3%)	0	100	100
6	H	161/163 (99%)	149 (92%)	11 (7%)	1 (1%)	21	52
6	h	161/163 (99%)	156 (97%)	5 (3%)	0	100	100
7	I	125/127 (98%)	125 (100%)	0	0	100	100
7	i	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
8	E	121/123 (98%)	110 (91%)	10 (8%)	1 (1%)	16	47
8	e	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
9	J	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
9	j	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
10	K	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
10	k	73/75 (97%)	70 (96%)	2 (3%)	1 (1%)	9	37
11	M	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
11	m	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
12	G	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
12	g	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
13	A	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
13	a	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
14	F	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
14	f	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
15	N	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
15	n	76/78 (97%)	73 (96%)	3 (4%)	0	100	100
All	All	5028/5124 (98%)	4853 (96%)	169 (3%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	k	59	ARG
6	H	132	TYR
1	o	55	TRP
4	B	3	TYR
8	E	17	PHE
3	l	113	VAL

5.3.2 Protein sidechains ⓘ

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	O	48/48 (100%)	47 (98%)	1 (2%)	47	64
1	o	48/48 (100%)	47 (98%)	1 (2%)	47	64
2	C	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	P	54/54 (100%)	54 (100%)	0	100	100
2	Q	54/54 (100%)	52 (96%)	2 (4%)	30	53
2	R	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	S	54/54 (100%)	52 (96%)	2 (4%)	30	53
2	U	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	V	54/54 (100%)	54 (100%)	0	100	100
2	W	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	X	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	Y	54/54 (100%)	54 (100%)	0	100	100
2	c	54/54 (100%)	54 (100%)	0	100	100
2	p	54/54 (100%)	52 (96%)	2 (4%)	30	53
2	q	54/54 (100%)	51 (94%)	3 (6%)	19	45
2	r	54/54 (100%)	54 (100%)	0	100	100
2	s	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	u	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	v	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	w	54/54 (100%)	53 (98%)	1 (2%)	50	65
2	x	54/54 (100%)	54 (100%)	0	100	100
2	y	54/54 (100%)	53 (98%)	1 (2%)	50	65
3	L	222/222 (100%)	220 (99%)	2 (1%)	70	74
3	l	222/222 (100%)	213 (96%)	9 (4%)	27	52
4	B	93/93 (100%)	91 (98%)	2 (2%)	45	63
4	b	93/93 (100%)	92 (99%)	1 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	331/331 (100%)	327 (99%)	4 (1%)	63	71
5	d	331/331 (100%)	329 (99%)	2 (1%)	78	79
6	H	139/139 (100%)	137 (99%)	2 (1%)	59	70
6	h	139/139 (100%)	136 (98%)	3 (2%)	45	63
7	I	108/108 (100%)	107 (99%)	1 (1%)	70	74
7	i	108/108 (100%)	108 (100%)	0	100	100
8	E	106/106 (100%)	104 (98%)	2 (2%)	50	65
8	e	106/106 (100%)	106 (100%)	0	100	100
9	J	64/64 (100%)	61 (95%)	3 (5%)	23	48
9	j	64/64 (100%)	64 (100%)	0	100	100
10	K	70/70 (100%)	70 (100%)	0	100	100
10	k	70/70 (100%)	70 (100%)	0	100	100
11	M	48/48 (100%)	47 (98%)	1 (2%)	47	64
11	m	48/48 (100%)	48 (100%)	0	100	100
12	G	87/87 (100%)	87 (100%)	0	100	100
12	g	87/87 (100%)	87 (100%)	0	100	100
13	A	83/83 (100%)	81 (98%)	2 (2%)	43	62
13	a	83/83 (100%)	82 (99%)	1 (1%)	63	71
14	F	123/123 (100%)	122 (99%)	1 (1%)	73	76
14	f	123/123 (100%)	122 (99%)	1 (1%)	73	76
15	N	77/77 (100%)	75 (97%)	2 (3%)	40	60
15	n	77/77 (100%)	75 (97%)	2 (3%)	40	60
All	All	4278/4278 (100%)	4216 (99%)	62 (1%)	57	70

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	48	LEU
2	p	56	PHE
2	p	74	LEU
2	q	15	LEU
2	q	46	LYS
2	q	64	LEU
2	s	58	LEU

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Mol	Chain	Res	Type
2	y	6	GLN
2	u	64	LEU
2	v	15	LEU
2	w	69	LEU
3	l	22	VAL
3	l	33	ASN
3	l	64	LEU
3	l	79	LEU
3	l	89	PHE
3	l	137	CYS
3	l	142	THR
3	l	148	CYS
3	l	209	LEU
4	b	10	ARG
5	d	129	CYS
5	d	158	ASP
6	h	77	THR
6	h	103	HIS
6	h	189	ILE
13	a	64	TYR
14	f	53	PHE
15	n	76	VAL
15	n	85	ASP
3	L	1	MET
3	L	144	LEU
4	B	46	GLU
4	B	75	GLN
6	H	50	LEU
6	H	199	GLN
7	I	55	GLU
8	E	8	ARG
8	E	44	VAL
9	J	39	GLU
9	J	45	TYR
9	J	54	TRP
11	M	118	LYS
13	A	8	HIS
13	A	64	TYR
14	F	146	VAL
2	X	58	LEU
2	C	67	LEU
2	Q	29	THR

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Mol	Chain	Res	Type
2	Q	58	LEU
2	R	58	LEU
2	S	34	LEU
2	S	71	PHE
2	U	25	MET
2	W	72	LEU
5	D	76	LEU
5	D	117	PHE
5	D	245	LEU
5	D	360	ASN
15	N	88	LEU
15	N	126	HIS
1	O	45	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	o	51	HIS
1	o	57	HIS
2	u	41	GLN
2	u	43	ASN
3	l	154	HIS
4	b	52	ASN
5	d	166	HIS
5	d	346	HIS
5	d	372	GLN
6	h	151	HIS
6	h	196	ASN
6	h	197	GLN
6	h	199	GLN
8	e	34	GLN
8	e	66	HIS
8	e	67	ASN
13	a	27	HIS
4	B	80	ASN
6	H	56	GLN
2	X	9	HIS
2	R	41	GLN
5	D	100	HIS
5	D	174	GLN
5	D	268	HIS
5	D	339	ASN

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Mol	Chain	Res	Type
12	G	119	ASN
15	N	89	HIS
1	O	51	HIS

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.

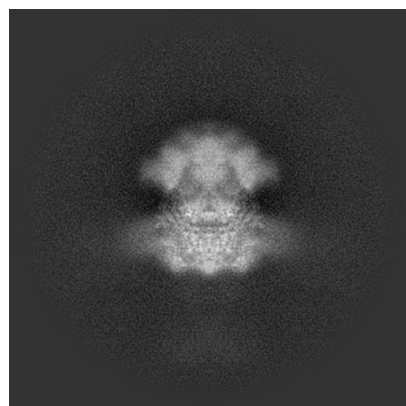
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73974. These allow visual inspection of the internal detail of the map and identification of artifacts.

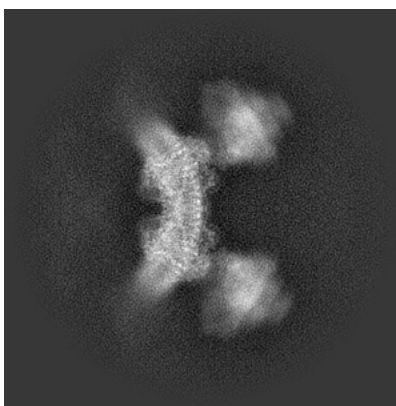
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

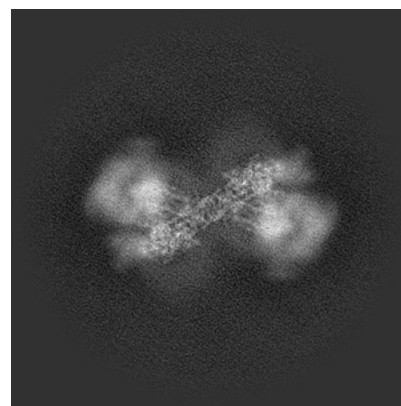
6.1.1 Primary map



X

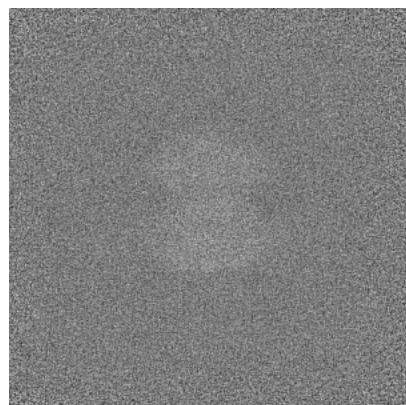


Y

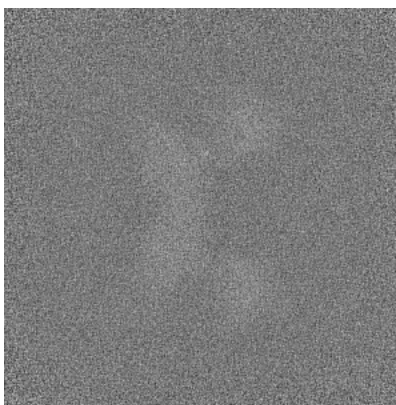


Z

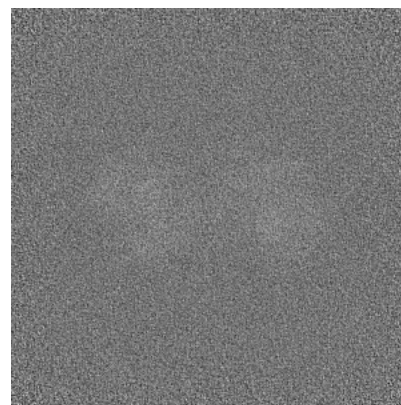
6.1.2 Raw map



X



Y

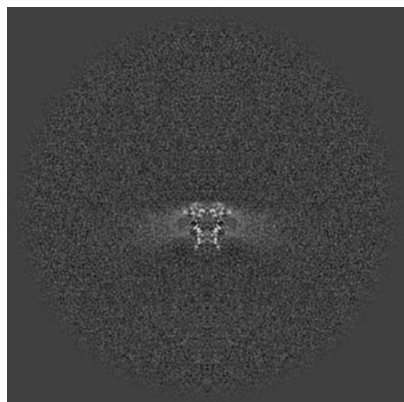


Z

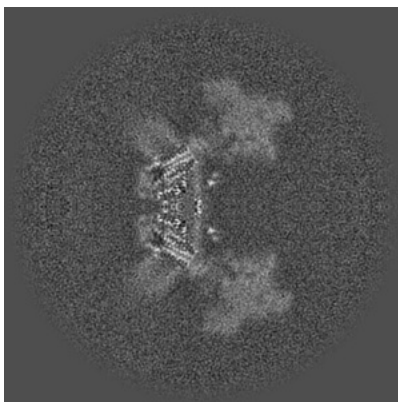
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

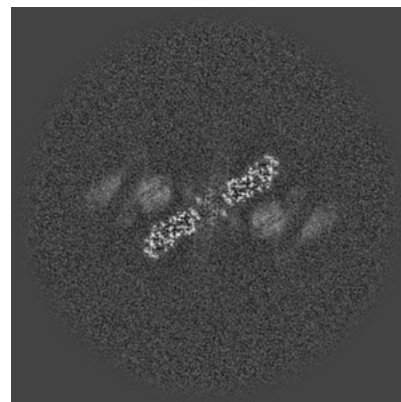
6.2.1 Primary map



X Index: 384

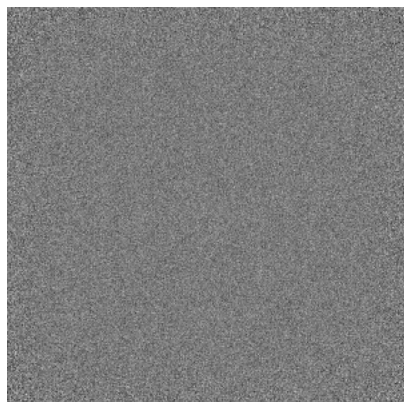


Y Index: 384

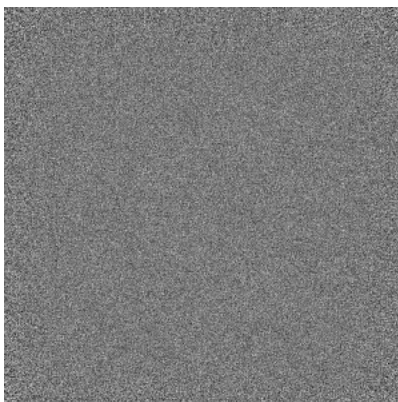


Z Index: 384

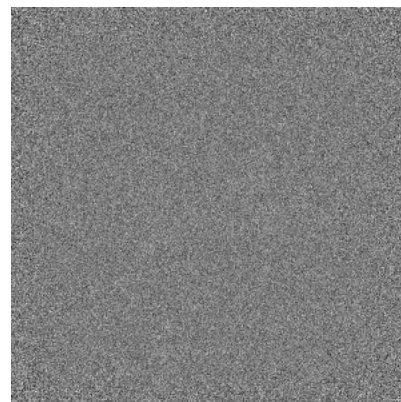
6.2.2 Raw map



X Index: 384



Y Index: 384

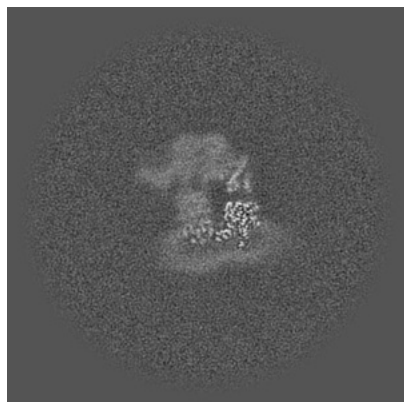


Z Index: 384

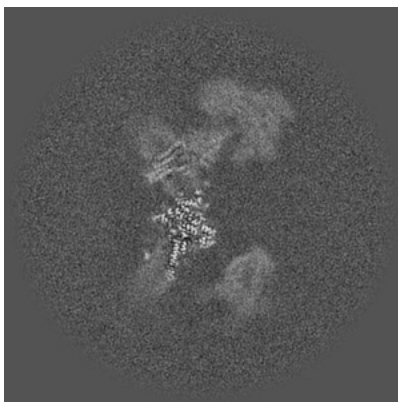
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

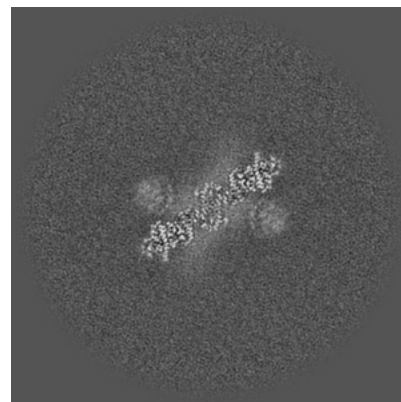
6.3.1 Primary map



X Index: 493

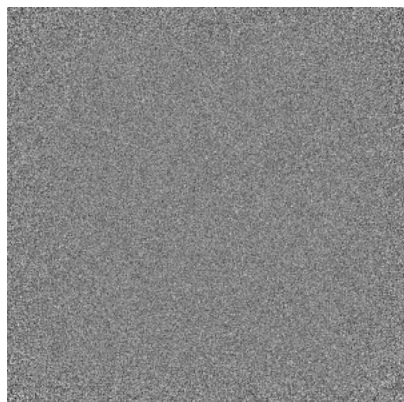


Y Index: 360

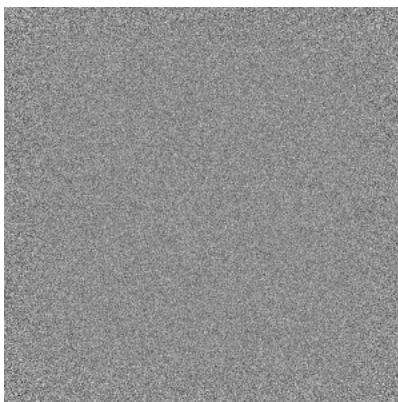


Z Index: 371

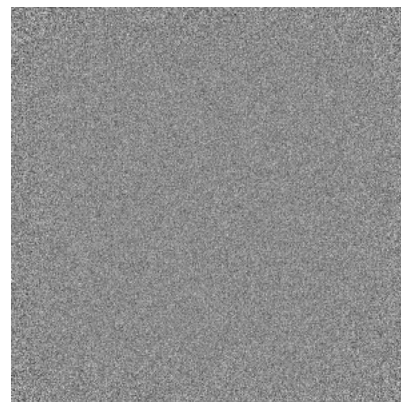
6.3.2 Raw map



X Index: 0



Y Index: 0

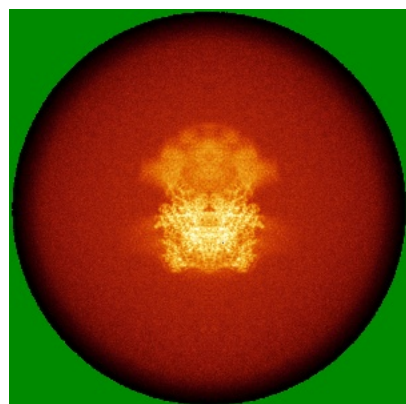


Z Index: 0

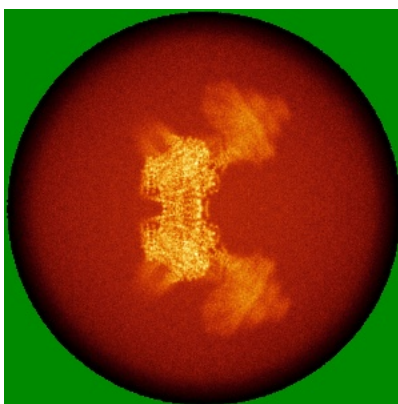
The images above show the largest variance slices of the map in three orthogonal directions.

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

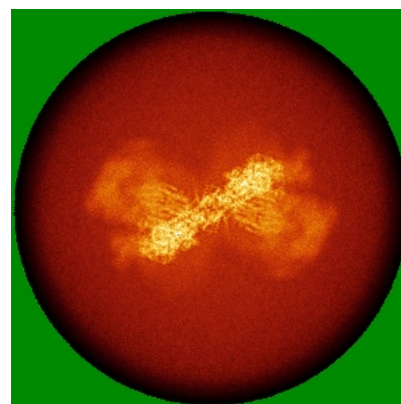
6.4.1 Primary map



X

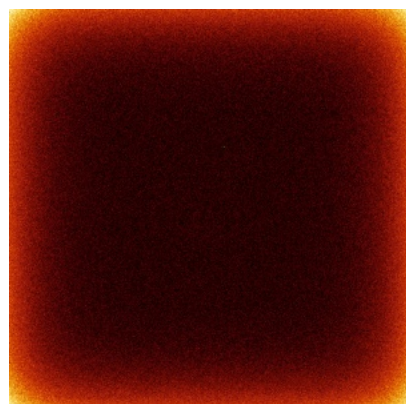


Y

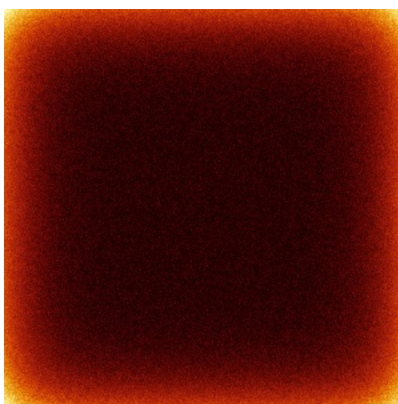


Z

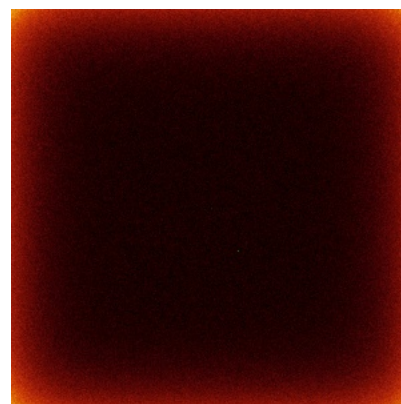
6.4.2 Raw map



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.

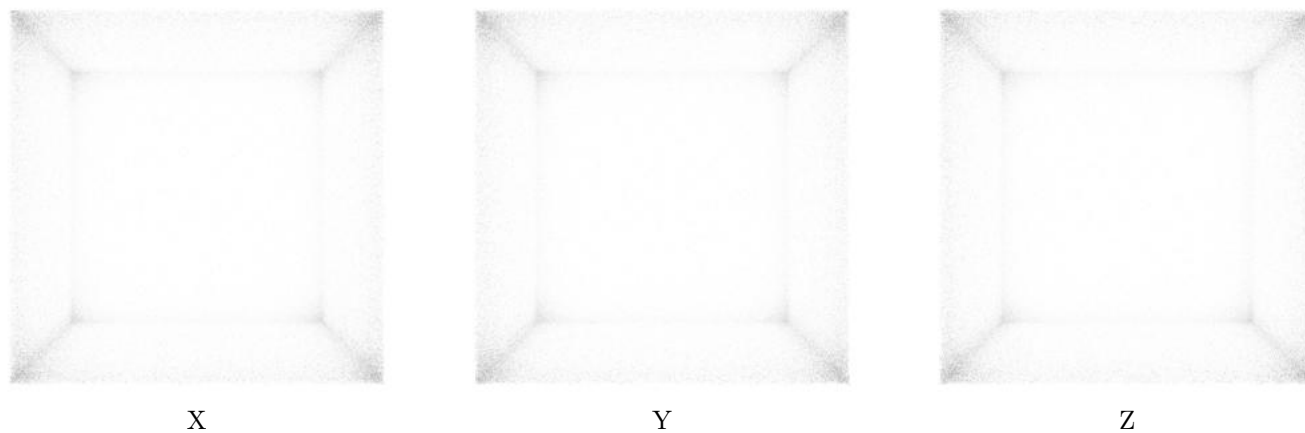
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

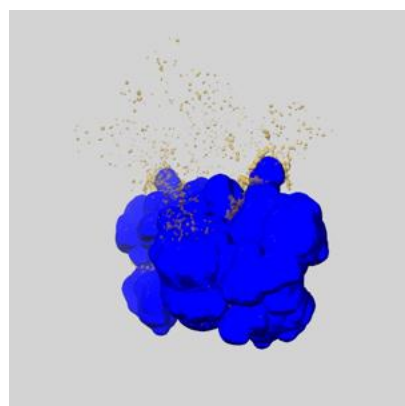
6.6 Mask visualisation [i](#)

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

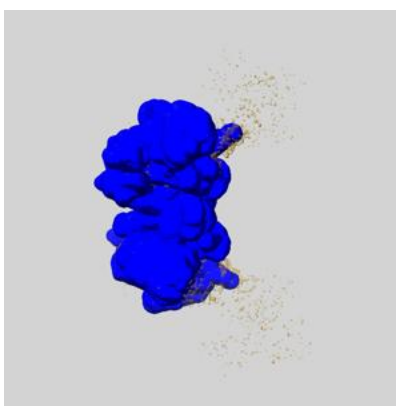
A mask typically either:

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

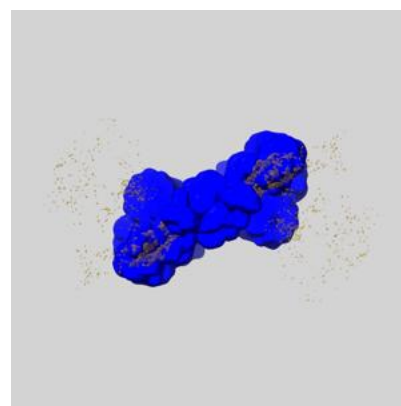
6.6.1 emd_73974_msk_1.map [i](#)



X



Y

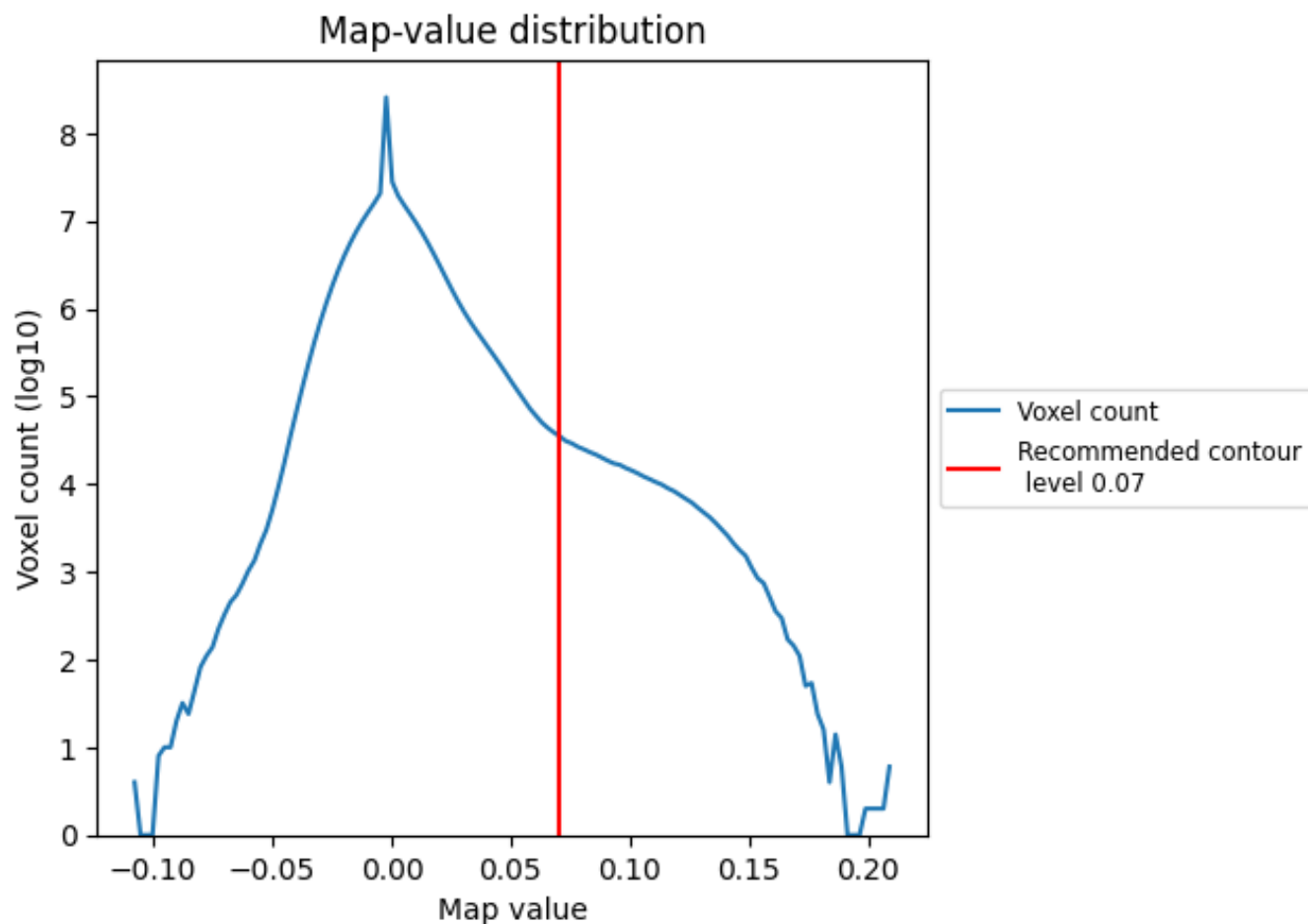


Z

7 Map analysis [i](#)

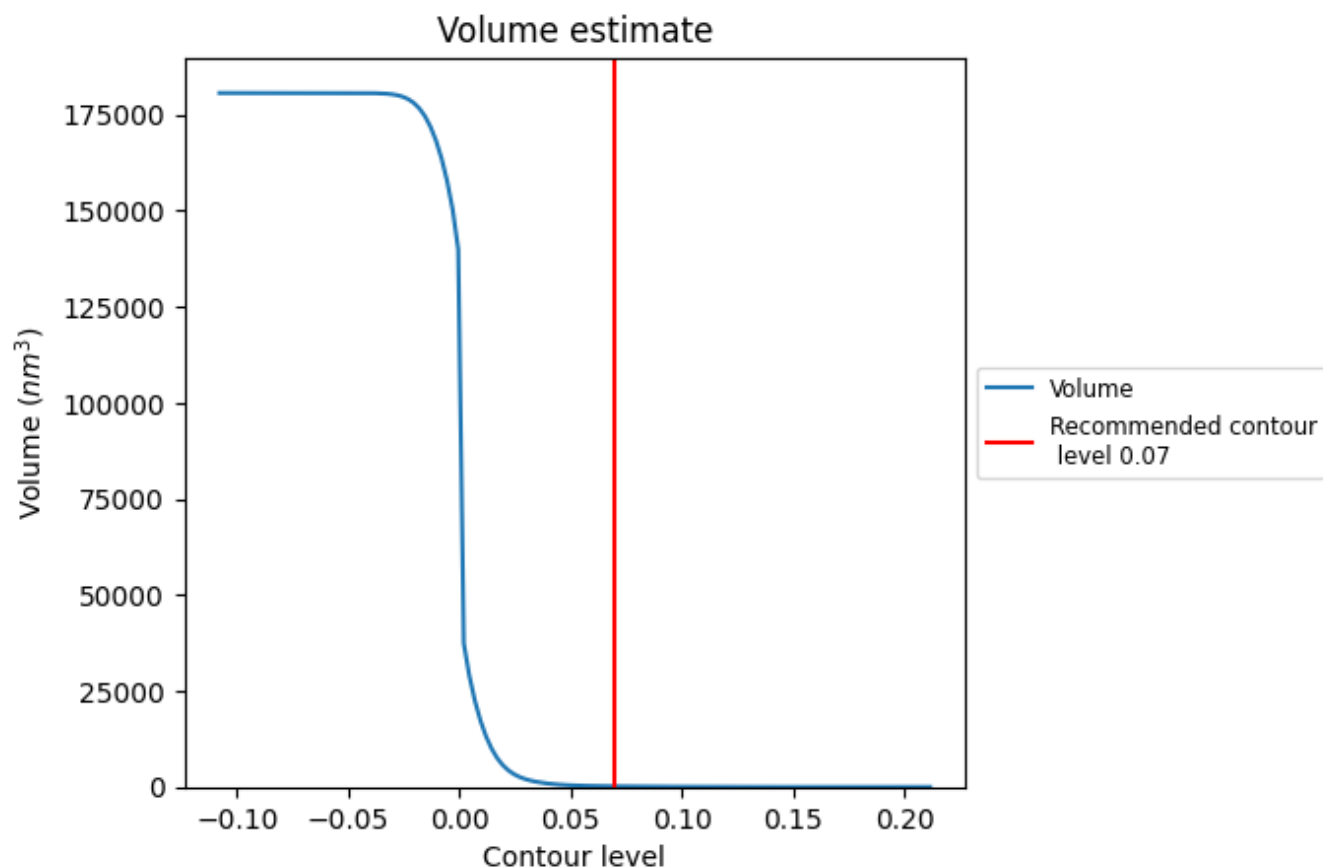
This section contains the results of statistical analysis of the map.

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.

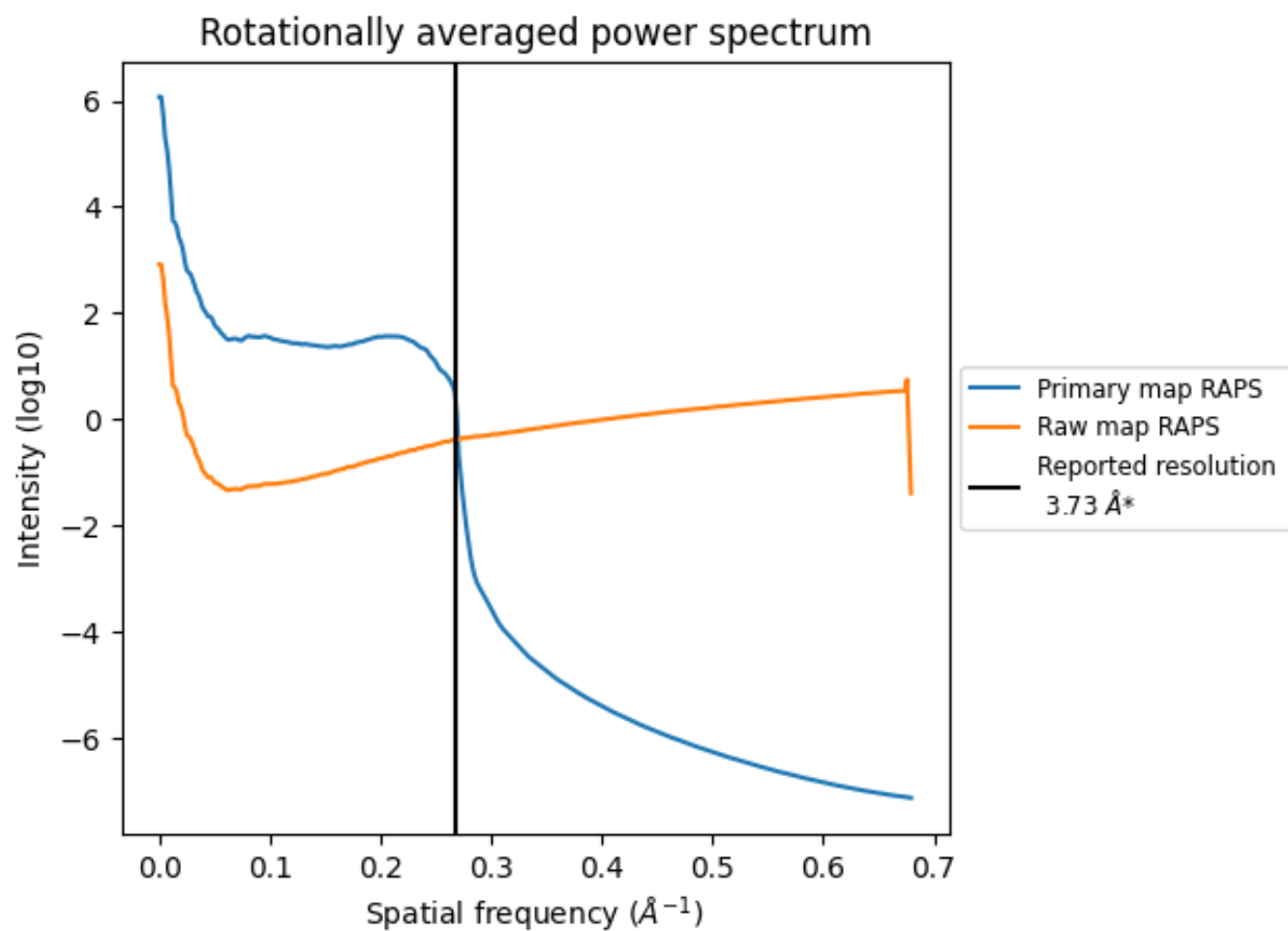
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

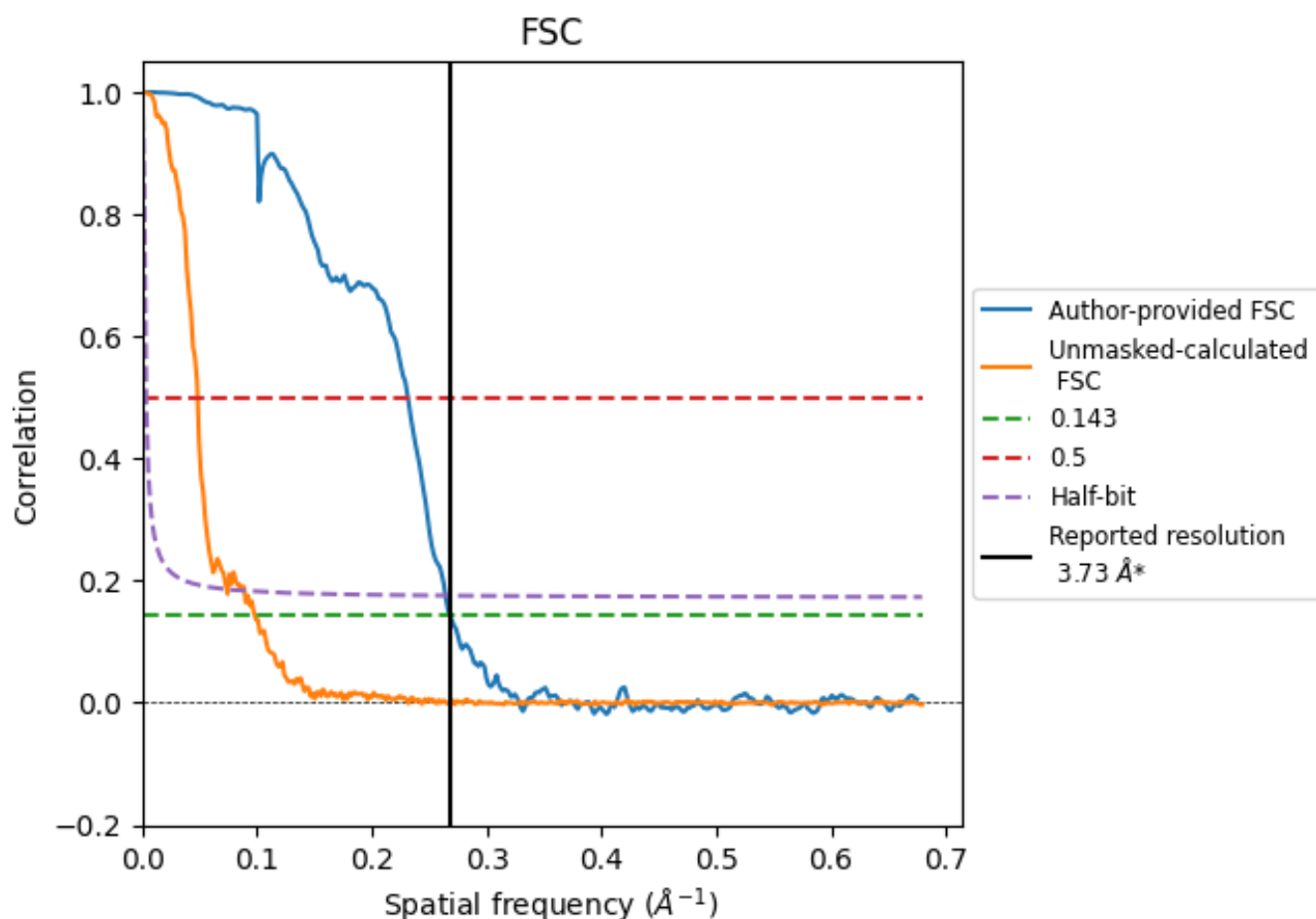


*Reported resolution corresponds to spatial frequency of 0.268 $\text{\AA}^{-1}$

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 $0.268 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

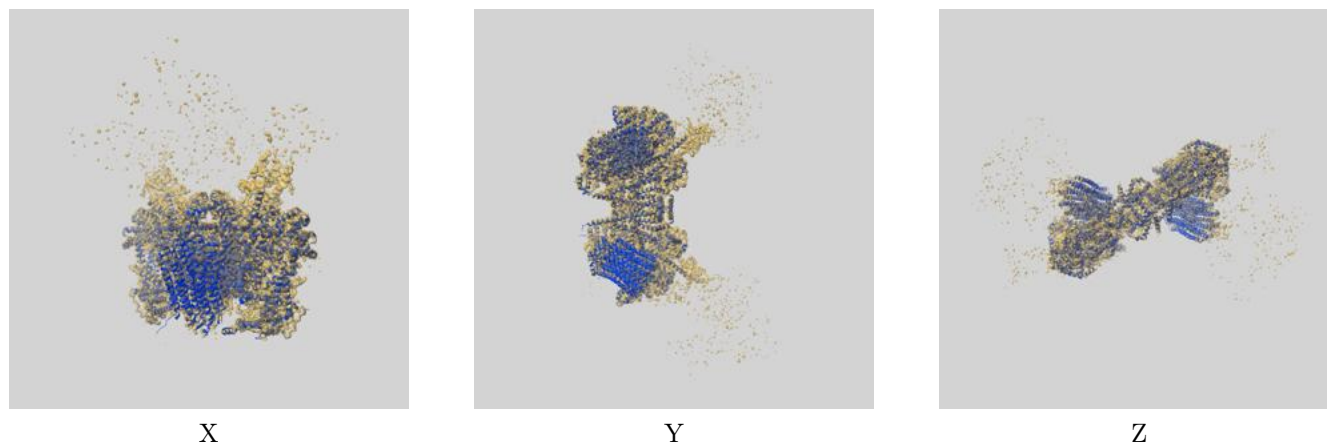
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.73	4.32	3.79
Unmasked-calculated*	10.20	20.75	13.59

*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 10.20 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

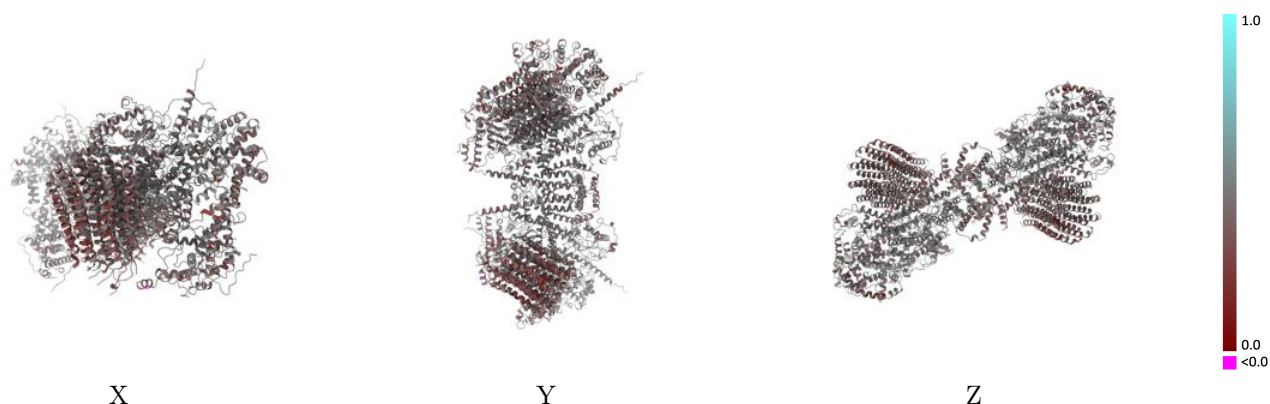
This section contains information regarding the fit between EMDB map EMD-73974 and PDB model 9ZB4. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



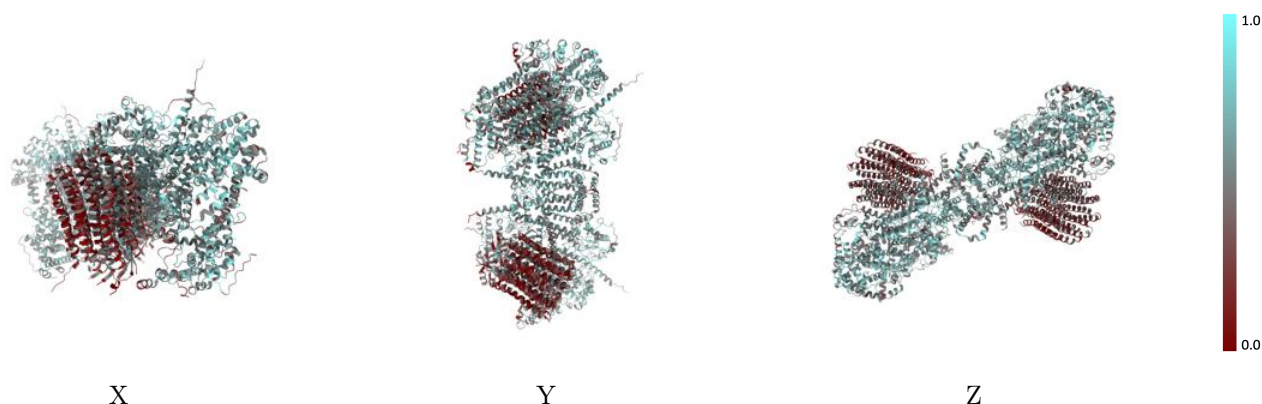
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



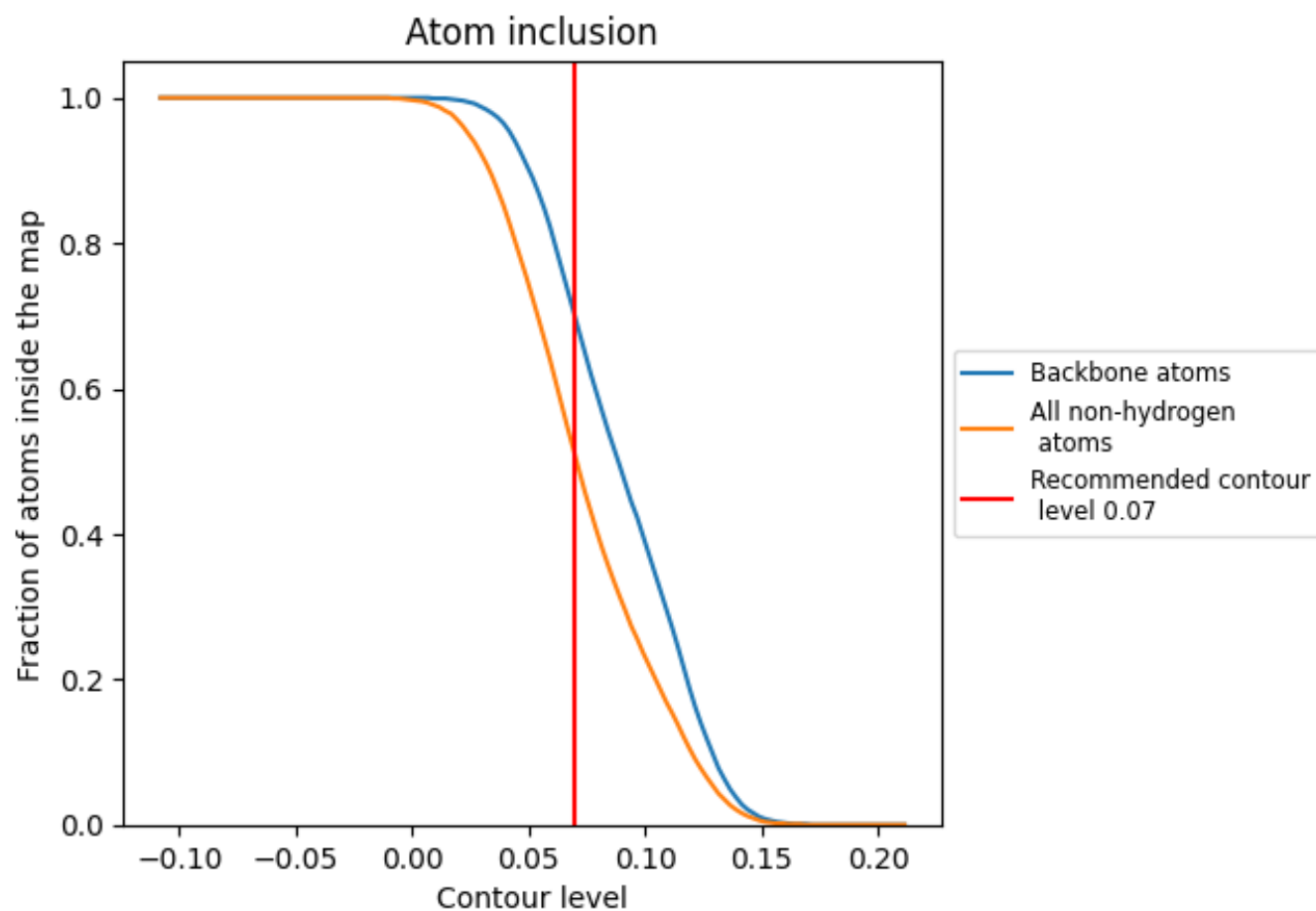
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 51% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5090	 0.4280
A	 0.5530	 0.4090
B	 0.6100	 0.4470
C	 0.2310	 0.3250
D	 0.6220	 0.4480
E	 0.6340	 0.4680
F	 0.6170	 0.4620
G	 0.5140	 0.4320
H	 0.5790	 0.4190
I	 0.5740	 0.4300
J	 0.6300	 0.4600
K	 0.6410	 0.4640
L	 0.5650	 0.4620
M	 0.5320	 0.4360
N	 0.6300	 0.4690
O	 0.6510	 0.4690
P	 0.2290	 0.3420
Q	 0.2420	 0.3740
R	 0.2490	 0.3670
S	 0.3000	 0.3790
U	 0.3860	 0.4030
V	 0.3280	 0.4060
W	 0.2560	 0.3700
X	 0.1870	 0.3450
Y	 0.3550	 0.3980
a	 0.5470	 0.4080
b	 0.6180	 0.4490
c	 0.2020	 0.3510
d	 0.6150	 0.4470
e	 0.6340	 0.4750
f	 0.6220	 0.4640
g	 0.5220	 0.4340
h	 0.5780	 0.4330
i	 0.5700	 0.4320
j	 0.6250	 0.4620



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Chain	Atom inclusion	Q-score
k	 0.6330	 0.4620
l	 0.5580	 0.4630
m	 0.5410	 0.4340
n	 0.6170	 0.4620
o	 0.6490	 0.4730
p	 0.2270	 0.3250
q	 0.2310	 0.3350
r	 0.2330	 0.3590
s	 0.2360	 0.3590
u	 0.3590	 0.4020
v	 0.3770	 0.4030
w	 0.3210	 0.4040
x	 0.2550	 0.3740
y	 0.2980	 0.3850