Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:26 am GMT

PDB ID	:	8RUY
EMDB ID	:	EMD-19515
Title	:	Structure of IFTA and IFTB in Retrograde Intraflagellar transport trains
Authors	:	Lacey, S.; Pigino, G.
Deposited on	:	2024-01-31
Resolution	:	15.40 Å(reported)

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:

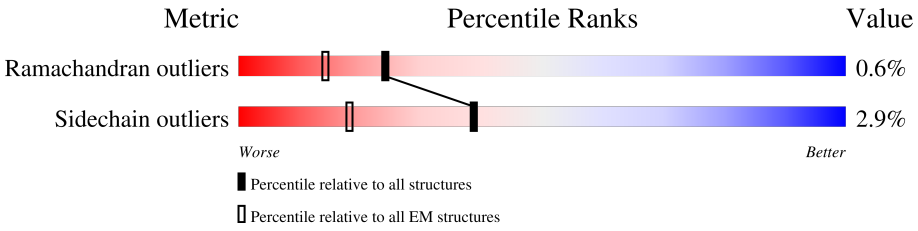
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 15.40 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	A	1367	16% 98%
2	B	1409	21% 96%
3	H	454	19% 93% 6%
3	h	454	13% 93%
4	J	765	7% 97%
4	j	765	15% 96%
5	K	510	21% 79%
5	k	510	21% 79%
6	L	135	7% 82% 16%

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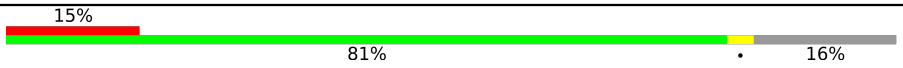
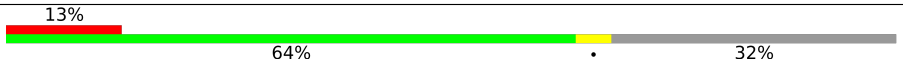
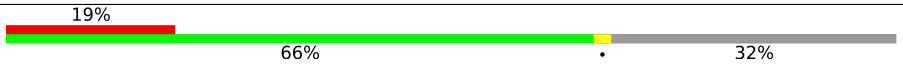
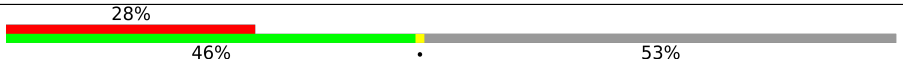
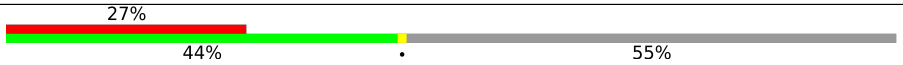
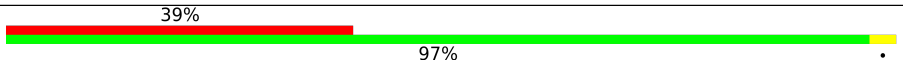
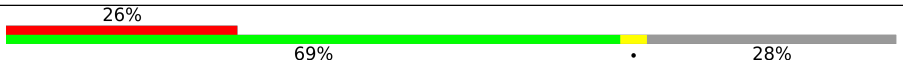
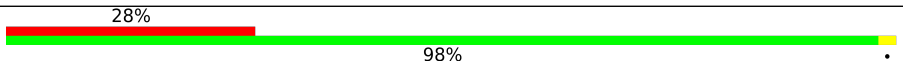
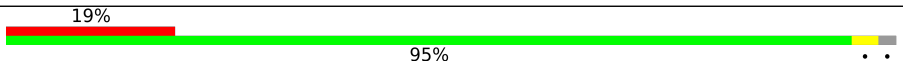
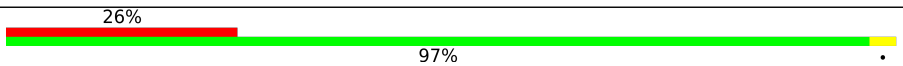
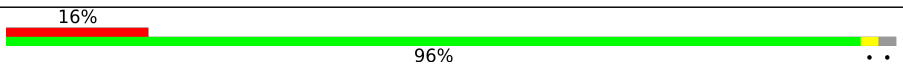
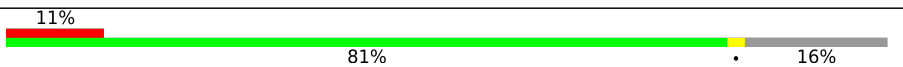
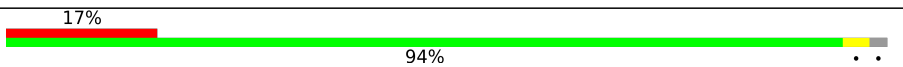
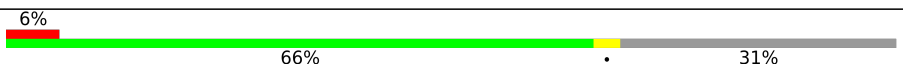
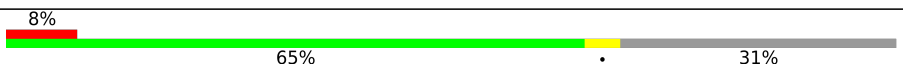
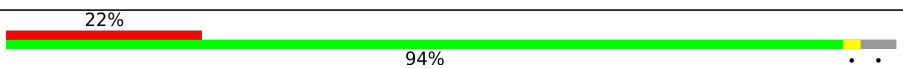
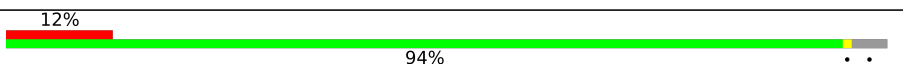
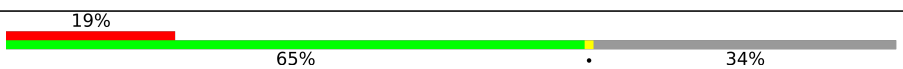
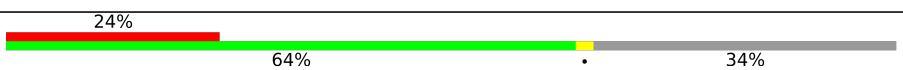
Mol	Chain	Length	Quality of chain
6	l	135	
7	N	443	
7	n	443	
8	O	641	
9	P	683	
10	Q	204	
11	R	189	
12	S	344	
12	s	344	
13	T	192	
14	I	1755	
14	i	1755	
15	C	1239	
16	D	1224	
17	E	1355	
18	F	782	
18	f	782	
19	G	647	
19	g	647	
20	M	469	
20	m	469	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 139391 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 Intraflagellar transport protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1367	10579	6654	1857	1998	70	0	0

- Molecule 2 is a protein called Intraflagellar transport particle protein 140.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1374	10764	6763	1893	2029	79	0	0

- Molecule 3 is a protein called Osm-6-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	454	3553	2269	591	680	13	0	0
3	h	440	Total	C	N	O	S	0	0
			3443	2199	574	657	13		

- Molecule 4 is a protein called Intraflagellar transport protein 80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	765	6025	3807	1053	1132	33	0	0
4	j	765	Total	C	N	O	S	0	0
			6025	3807	1053	1132	33		

- Molecule 5 is a protein called IFT54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	106	849	524	155	164	6	0	0
5	k	106	Total	C	N	O	S	0	0
			849	524	155	164	6		

- Molecule 6 is a protein called Intraflagellar transport particle protein IFT20.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	114	Total	C	N	O	S	0	0
			919	562	166	187	4		
6	l	114	Total	C	N	O	S	0	0
			919	562	166	187	4		

- Molecule 7 is a protein called Clusterin-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	303	Total	C	N	O	S	0	0
			2472	1547	439	476	10		
7	n	303	Total	C	N	O	S	0	0
			2472	1547	439	476	10		

- Molecule 8 is a protein called Intraflagellar transport protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	299	Total	C	N	O	S	0	0
			2411	1485	437	474	15		

- Molecule 9 is a protein called Intraflagellar transport protein 81.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	306	Total	C	N	O	S	0	0
			2439	1512	436	482	9		

- Molecule 10 is a protein called Intraflagellar transport protein 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	204	Total	C	N	O	S	0	0
			1602	1025	262	307	8		

- Molecule 11 is a protein called Intraflagellar transport protein 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	136	Total	C	N	O	S	0	0
			1086	681	190	208	7		

- Molecule 12 is a protein called Intraflagellar transport protein 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	133	Total	C	N	O	S	0	0
			1045	666	172	197	10		
12	s	141	Total	C	N	O	S	0	0
			1138	727	190	213	8		

- Molecule 13 is a protein called Intraflagellar transport protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	192	Total	C	N	O	S	0	0
			1500	946	261	285	8		

- Molecule 14 is a protein called Intraflagellar transport protein 172.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	1755	Total	C	N	O	S	0	0
			13906	8752	2439	2639	76		
14	I	1714	Total	C	N	O	S	0	0
			13615	8578	2384	2577	76		

- Molecule 15 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	1210	Total	C	N	O	S	0	0
			9609	6108	1671	1773	57		

- Molecule 16 is a protein called Intraflagellar transport protein 121.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	1027	Total	C	N	O	S	0	0
			8154	5184	1401	1509	60		

- Molecule 17 is a protein called Intraflagellar transport protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	1325	Total	C	N	O	S	0	0
			10464	6587	1860	1956	61		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	variant	UNP A9XPA6

- Molecule 18 is a protein called IFT88.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	539	Total	C	N	O	S	0	0
			4337	2747	762	795	33		
18	f	538	Total	C	N	O	S	0	0
			4328	2741	760	794	33		

- Molecule 19 is a protein called IFT70.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	619	Total	C	N	O	S	0	0
			4978	3171	826	948	33		
19	g	619	Total	C	N	O	S	0	0
			4978	3171	826	948	33		

- Molecule 20 is a protein called Intraflagellar transport protein 57.

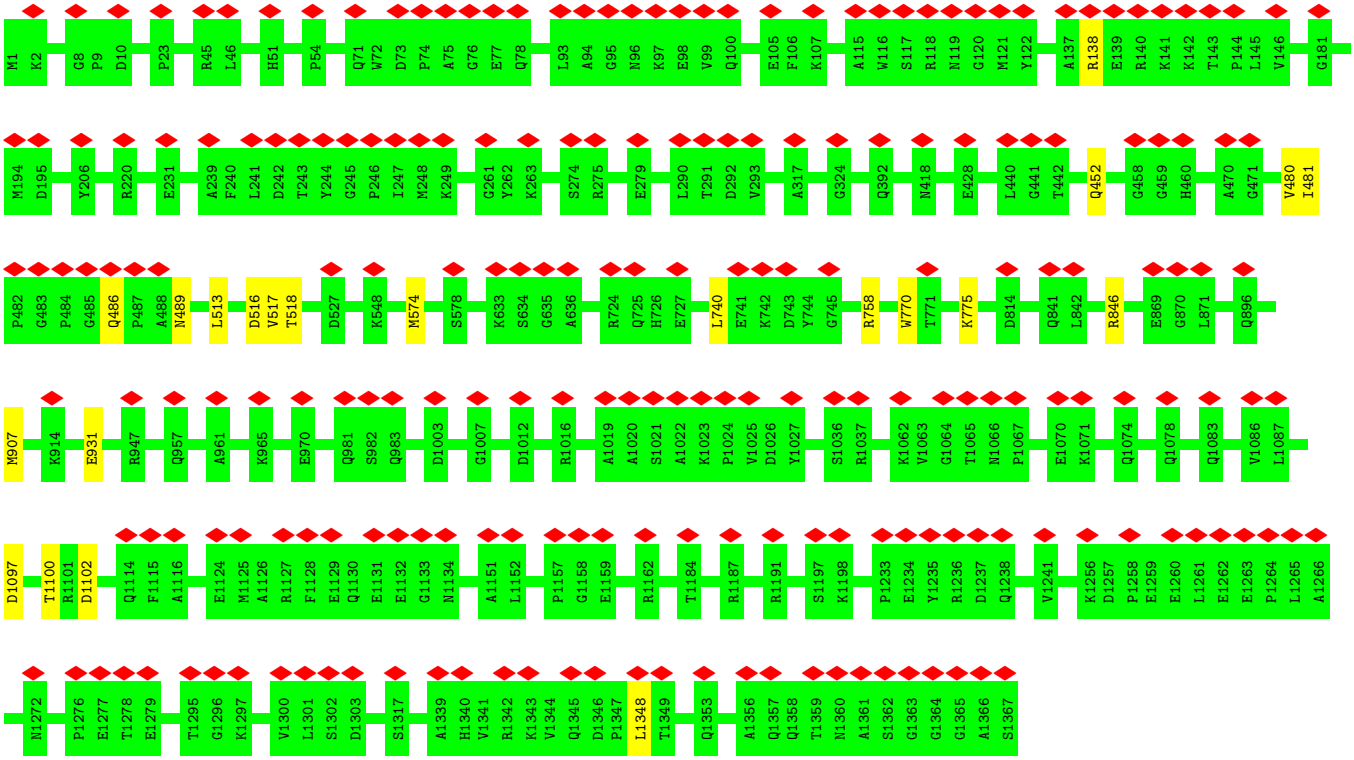
Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	309	Total	C	N	O	S	0	0
			2466	1552	438	466	10		
20	m	309	Total	C	N	O	S	0	0
			2466	1552	438	466	10		

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.

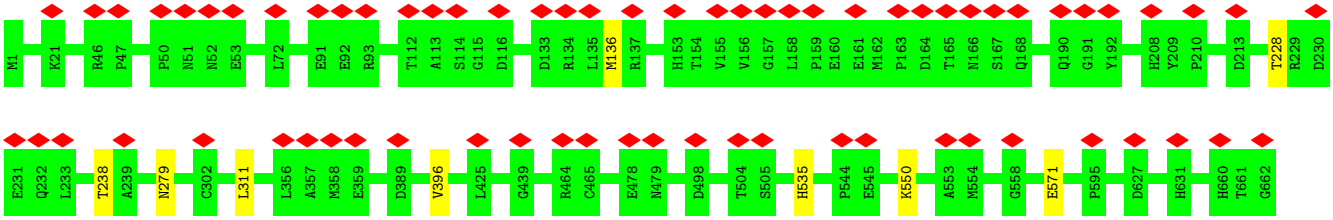
• Molecule 1: Intraflagellar transport protein 144

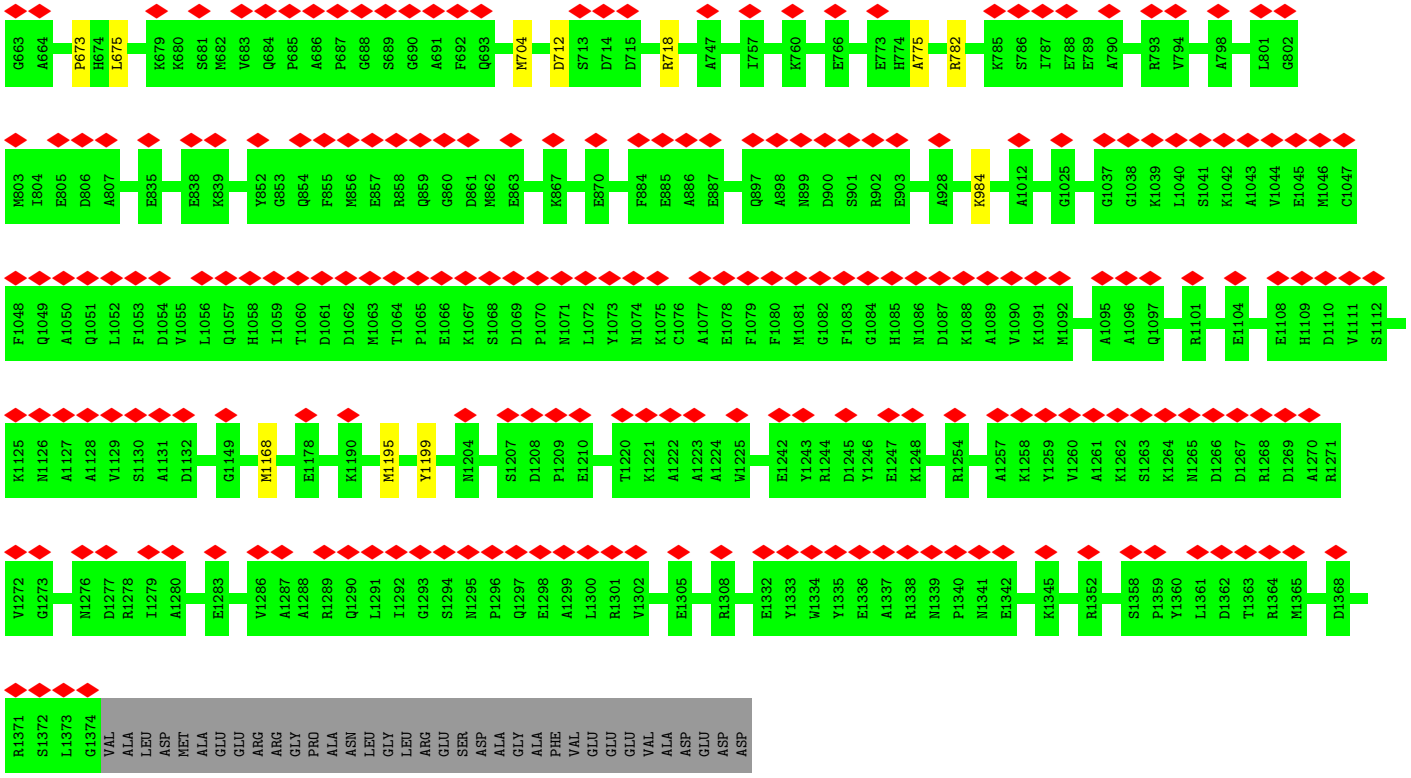
Chain A:



• Molecule 2: Intraflagellar transport particle protein 140

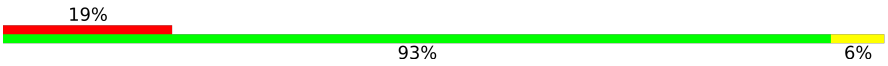
Chain B:

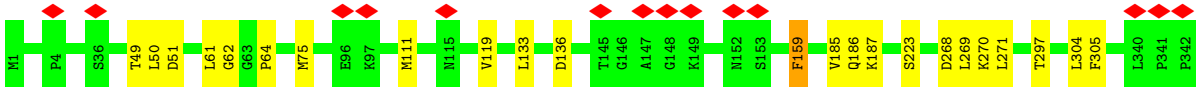


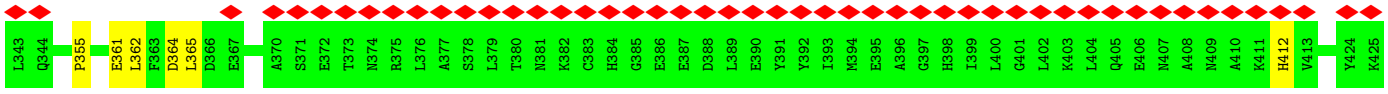


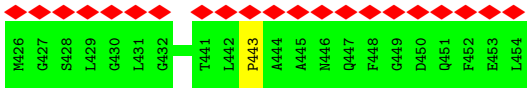
• Molecule 3: Osm-6-like protein

Chain H:



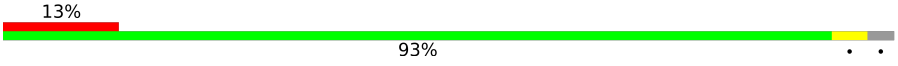


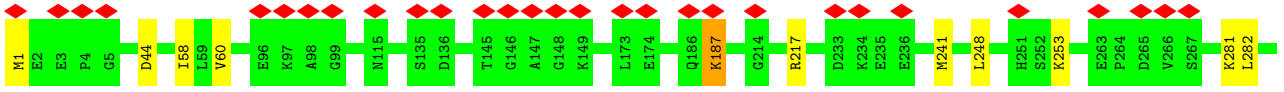


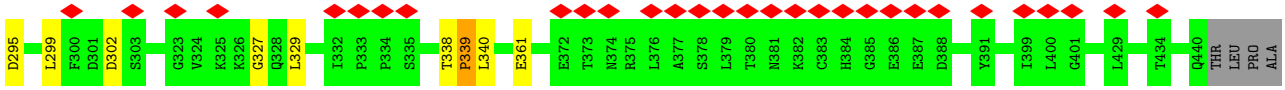


• Molecule 3: Osm-6-like protein

Chain h:

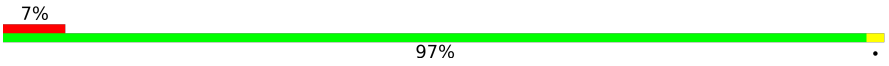


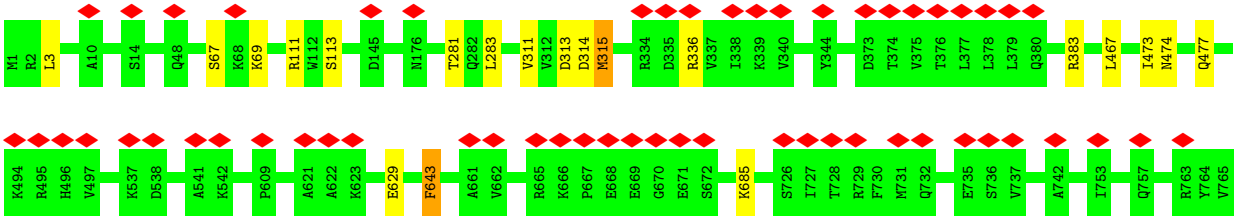




• Molecule 4: Intraflagellar transport protein 80

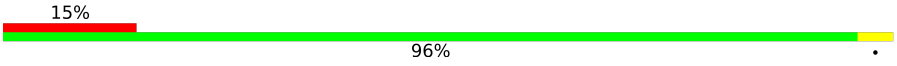
Chain J:

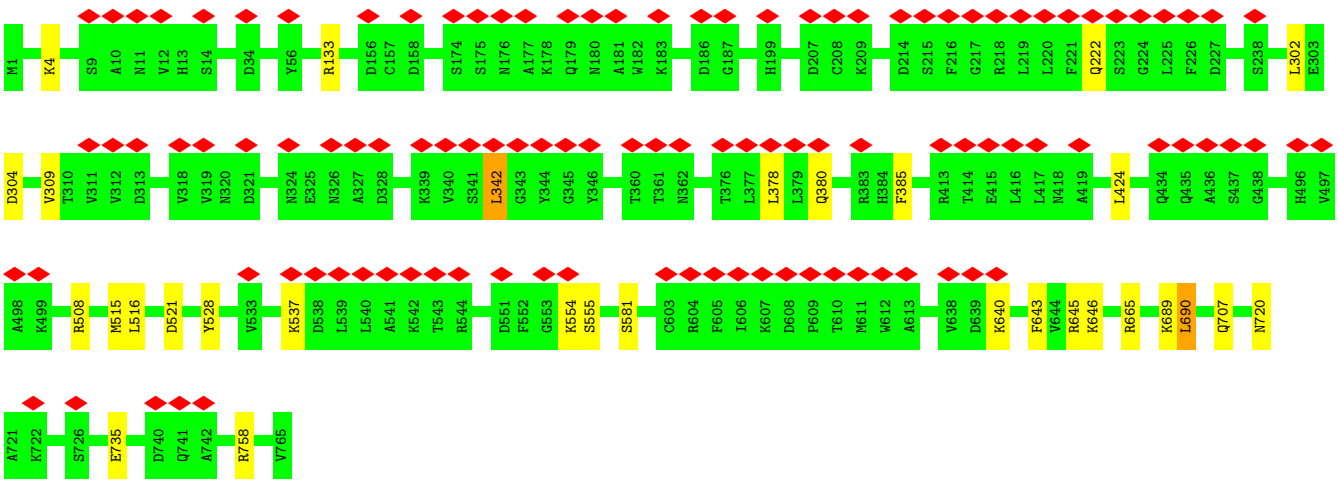




• Molecule 4: Intraflagellar transport protein 80

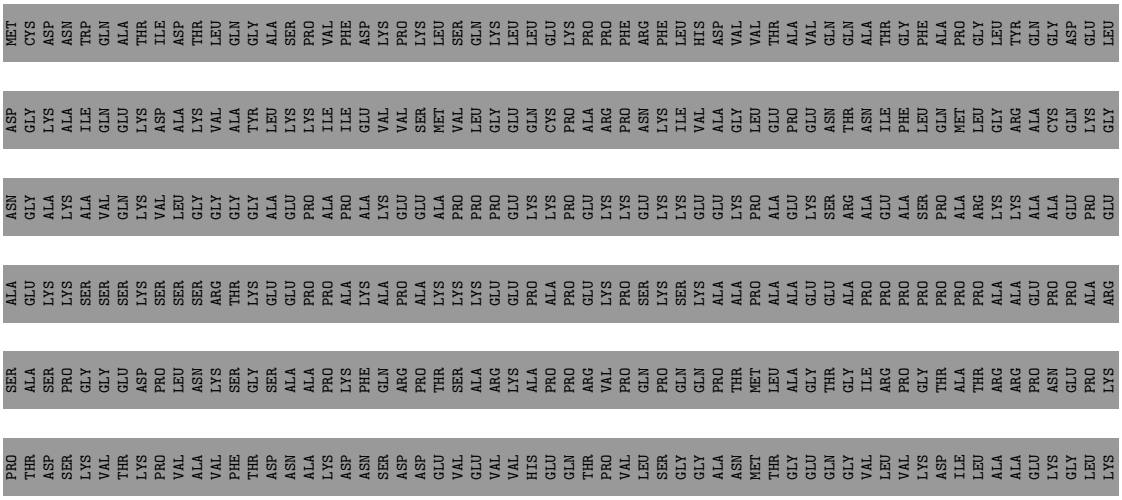
Chain j:

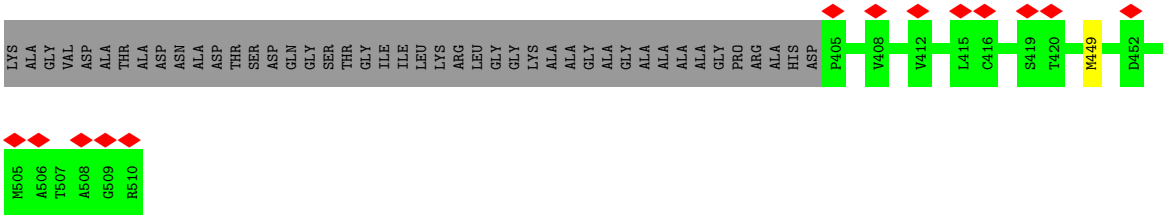




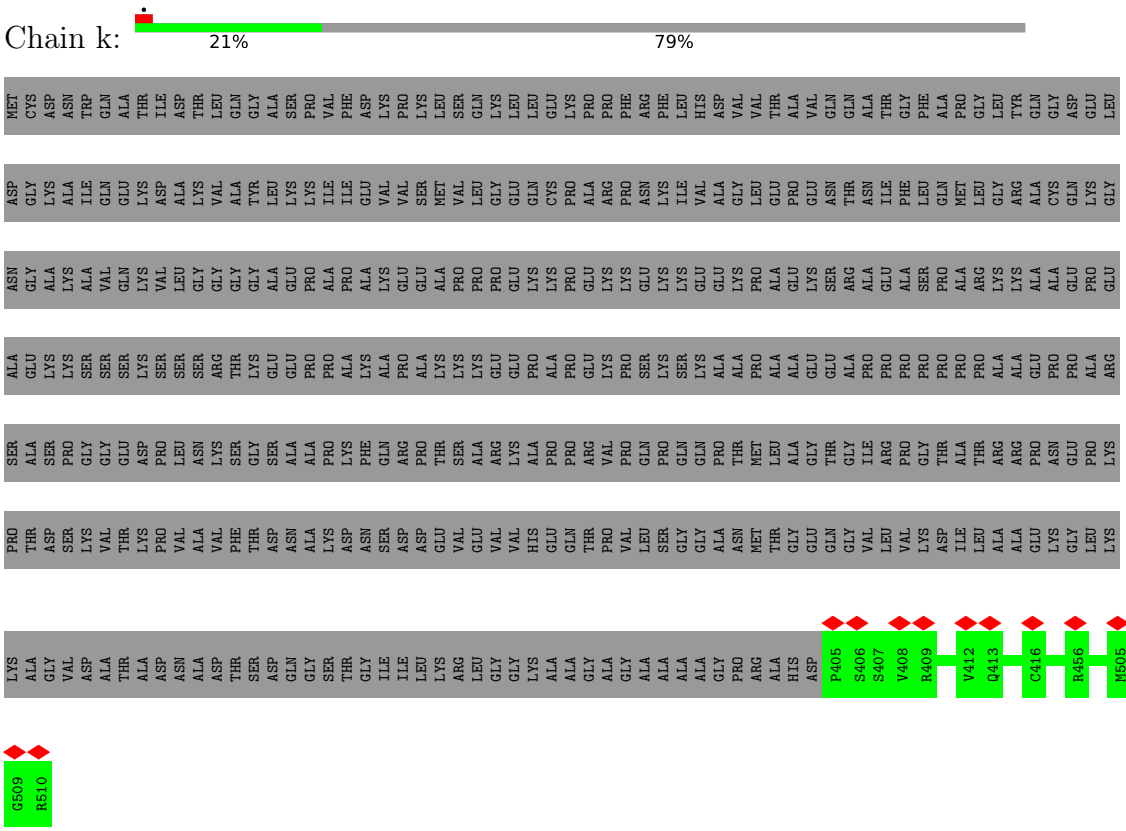
• Molecule 5: IFT54

Chain K:

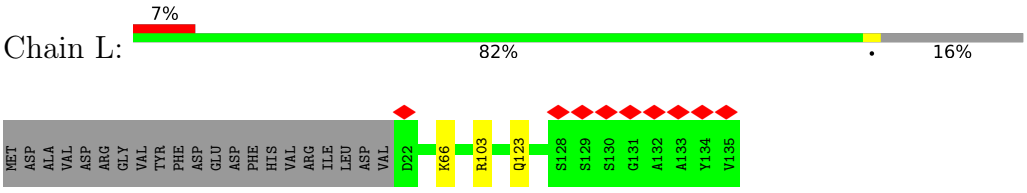




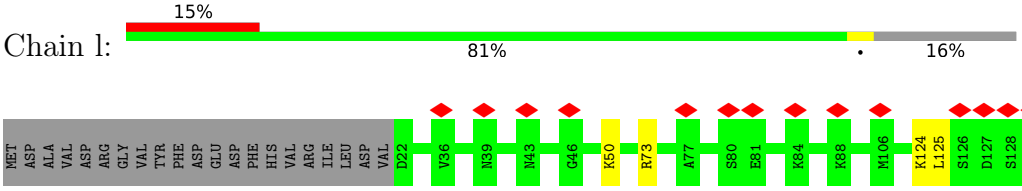
• Molecule 5: IFT54



• Molecule 6: Intraflagellar transport particle protein IFT20

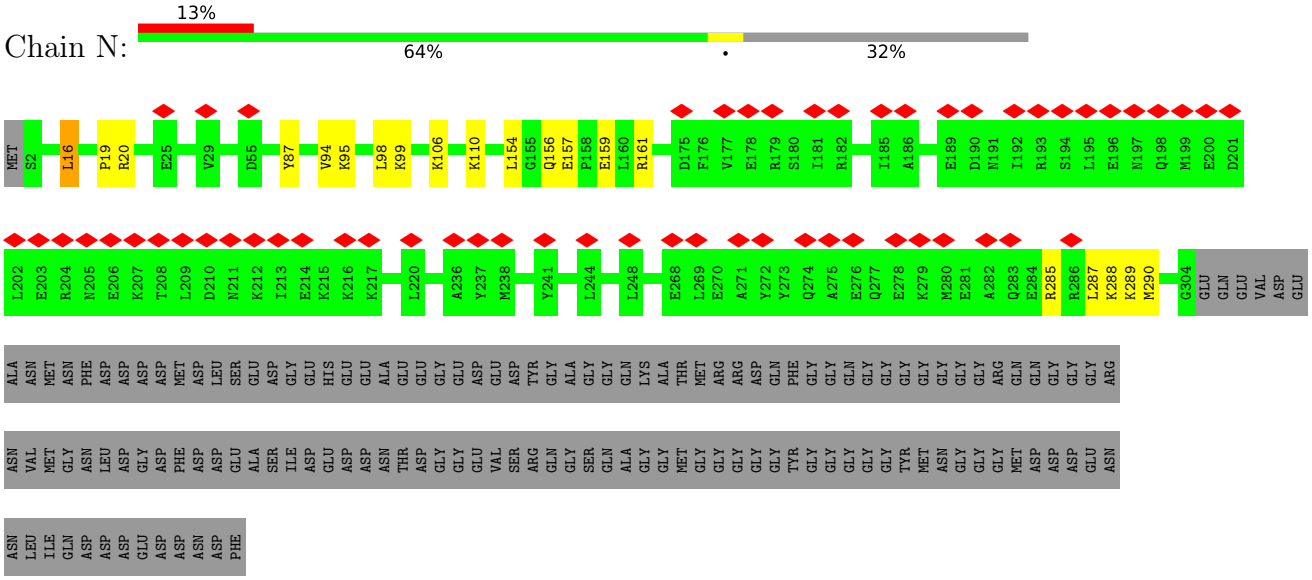


• Molecule 6: Intraflagellar transport particle protein IFT20



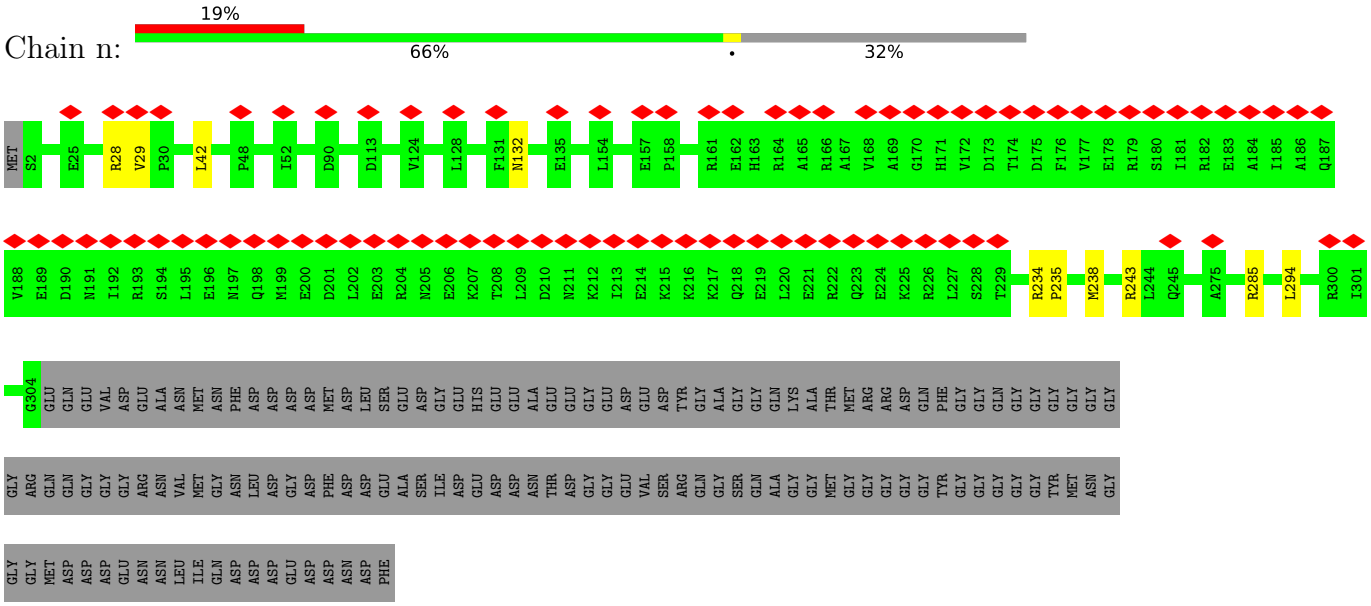
• Molecule 7: Clusterin-associated protein 1

Chain N:



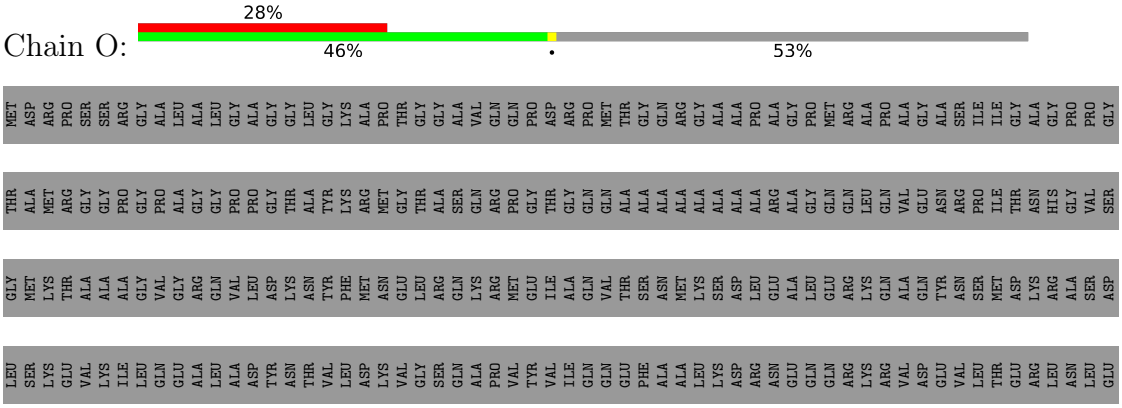
• Molecule 7: Clusterin-associated protein 1

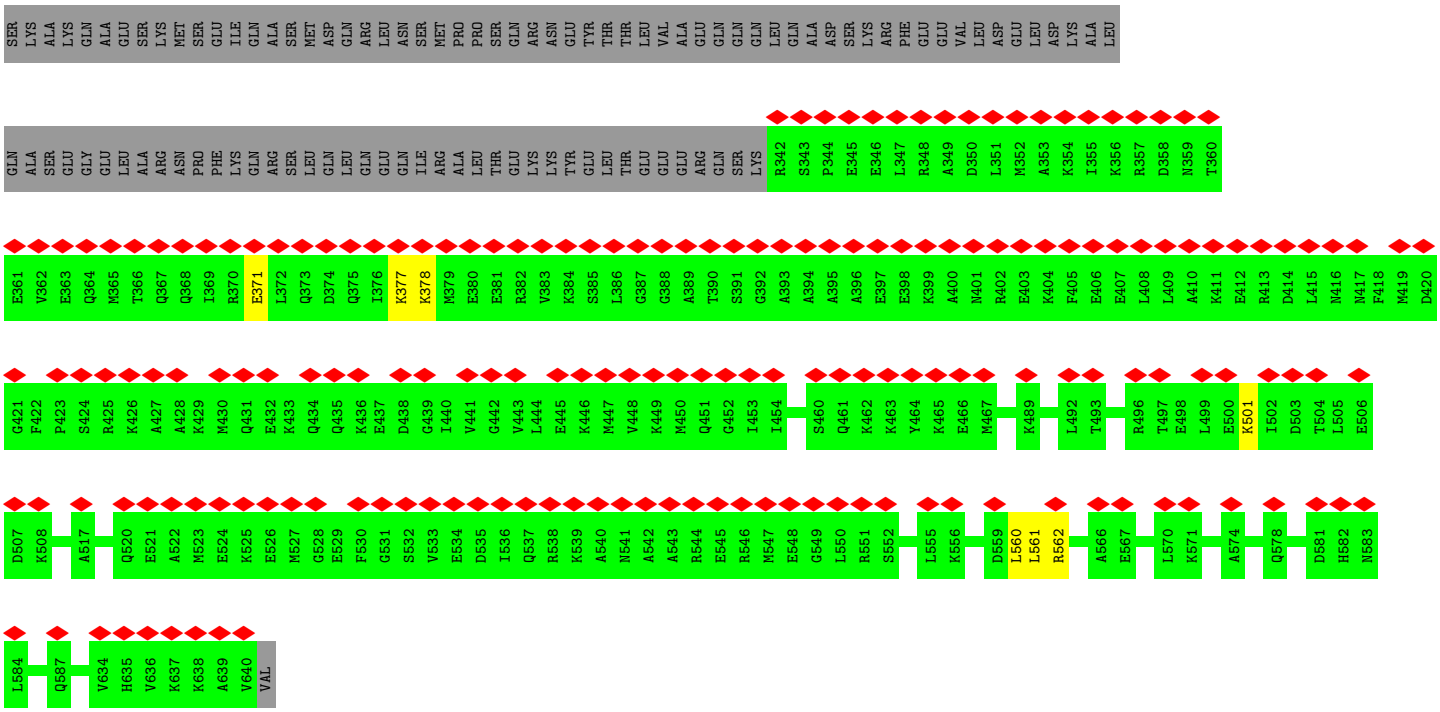
Chain n:



• Molecule 8: Intraflagellar transport protein 74

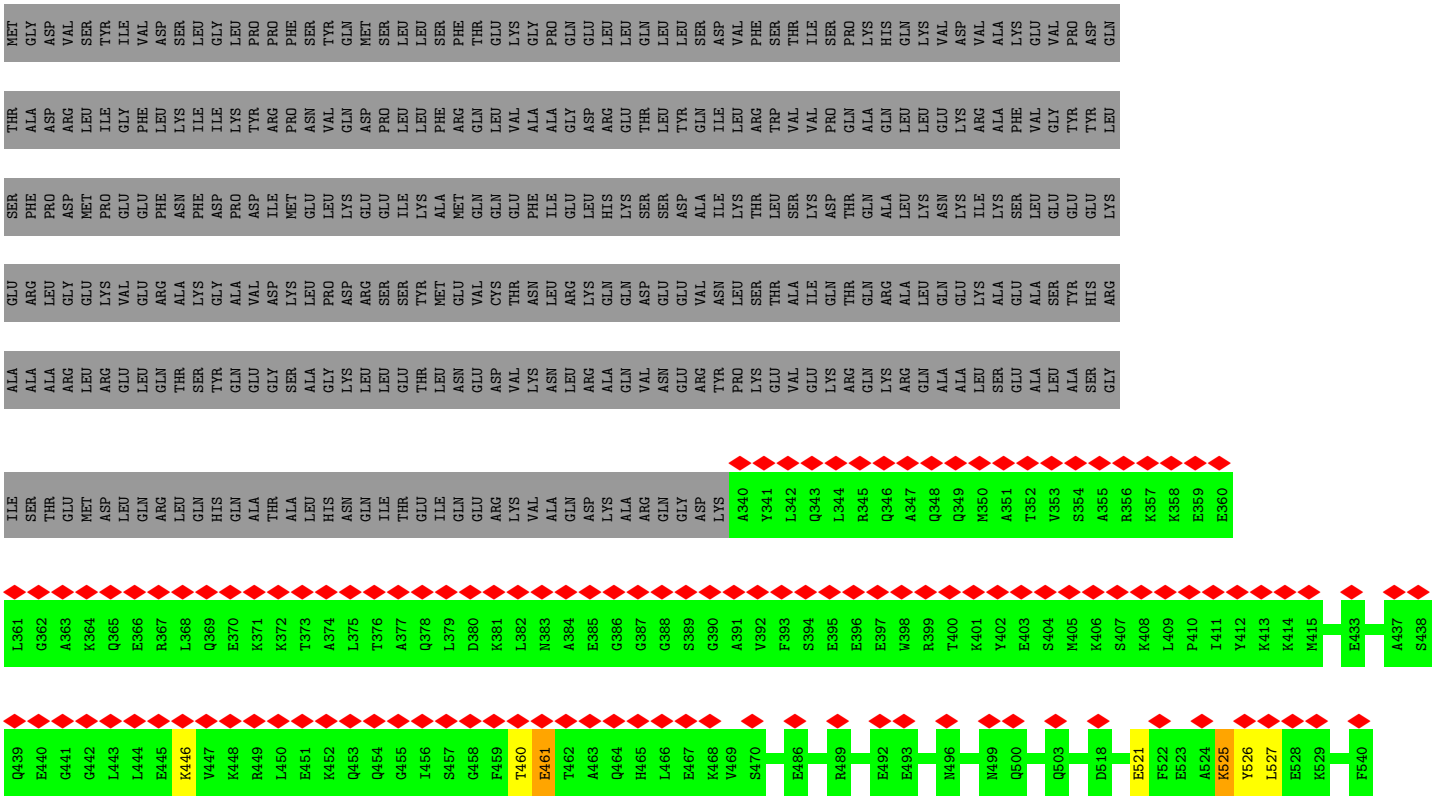
Chain O:

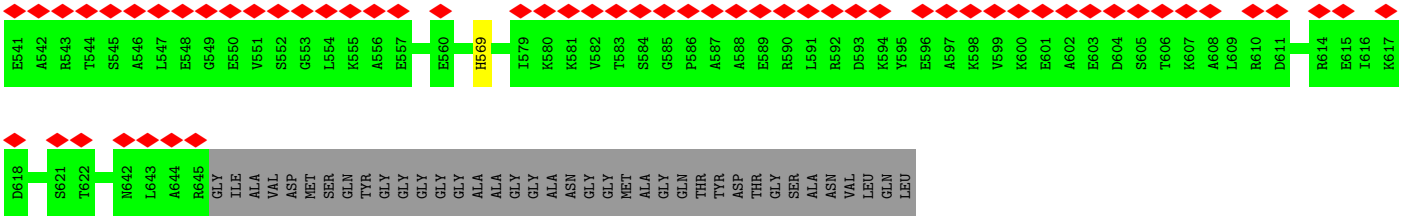




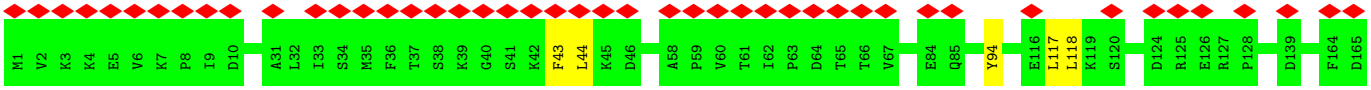
• Molecule 9: Intraflagellar transport protein 81

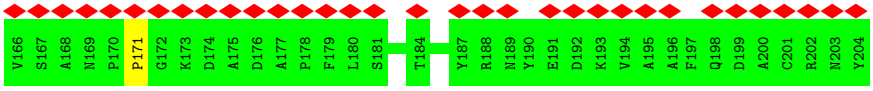
Chain P:



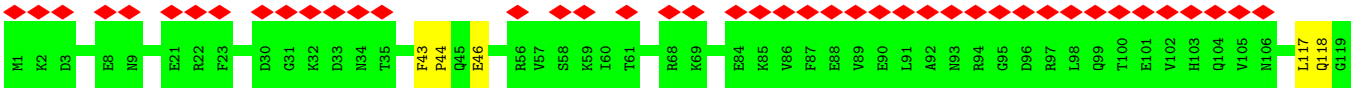


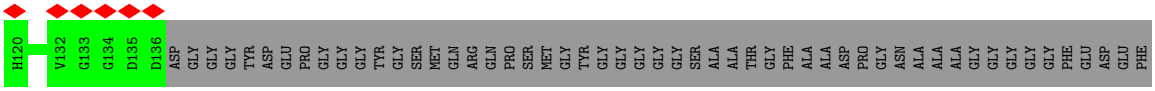
• Molecule 10: Intraflagellar transport protein 27



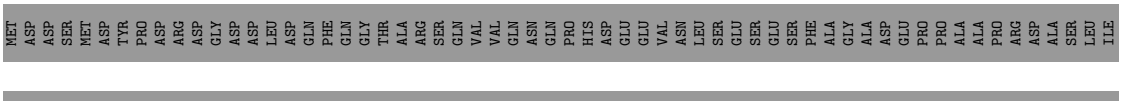


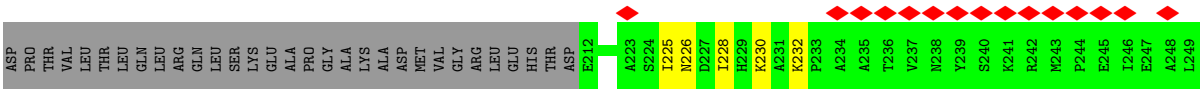
• Molecule 11: Intraflagellar transport protein 25

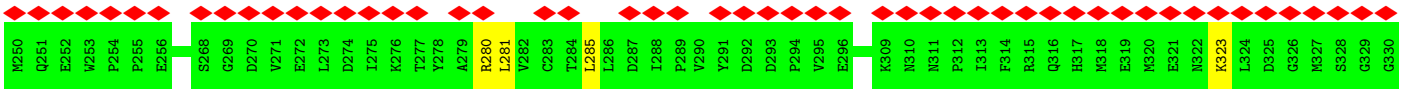


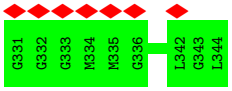


• Molecule 12: Intraflagellar transport protein 46



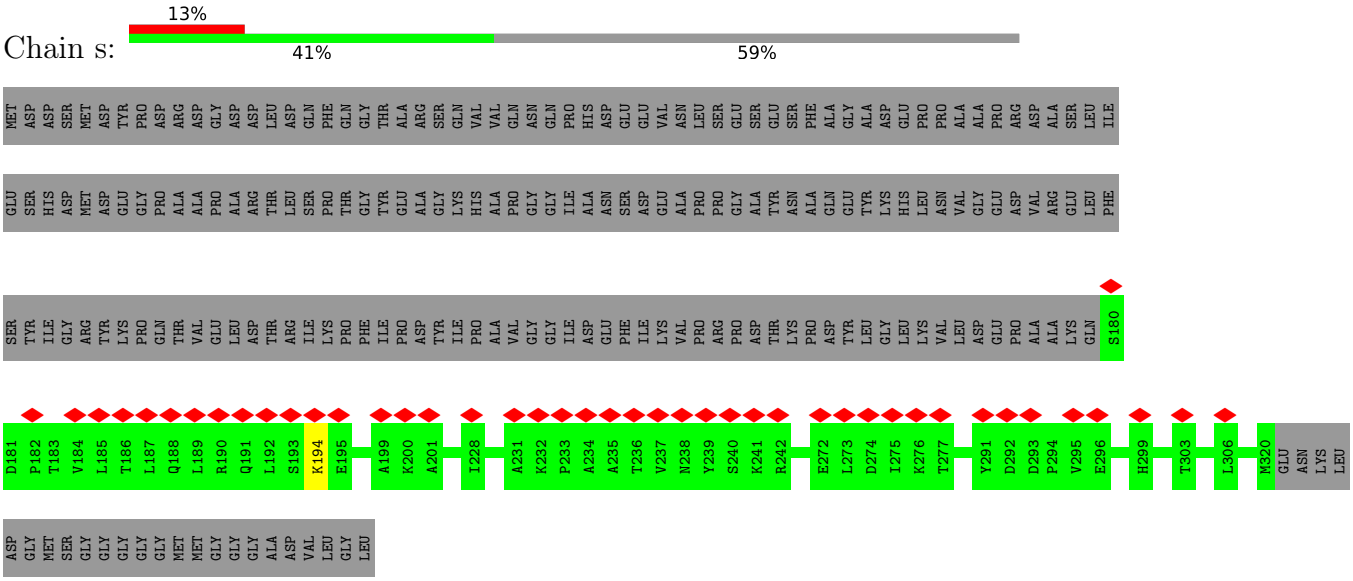






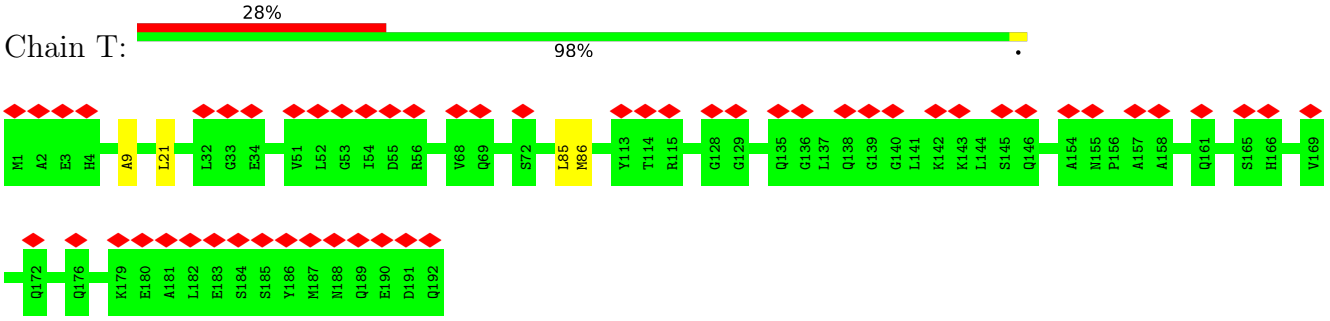
• Molecule 12: Intraflagellar transport protein 46

Chain s:



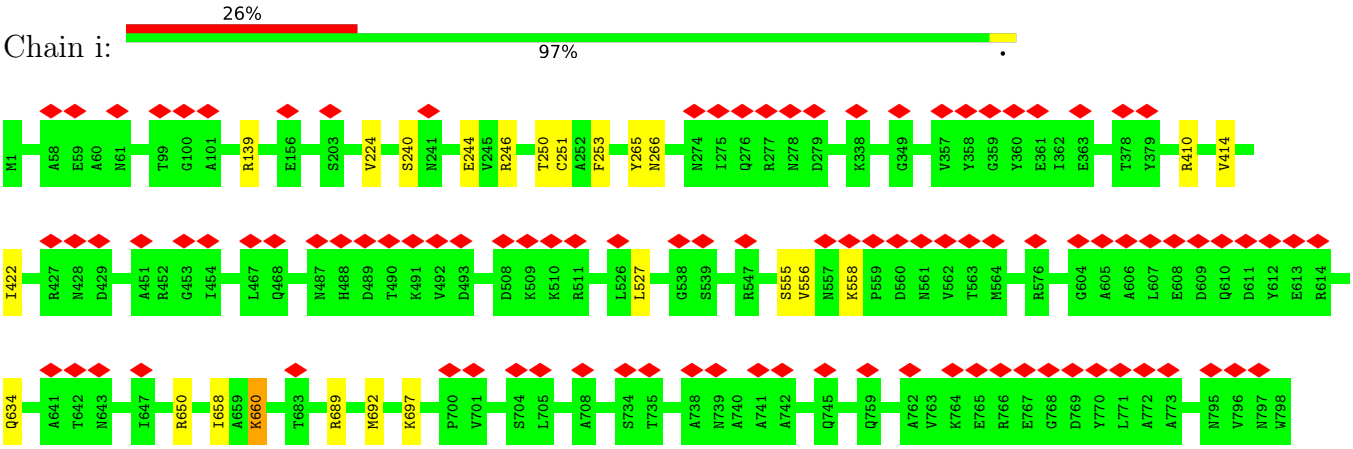
• Molecule 13: Intraflagellar transport protein 22

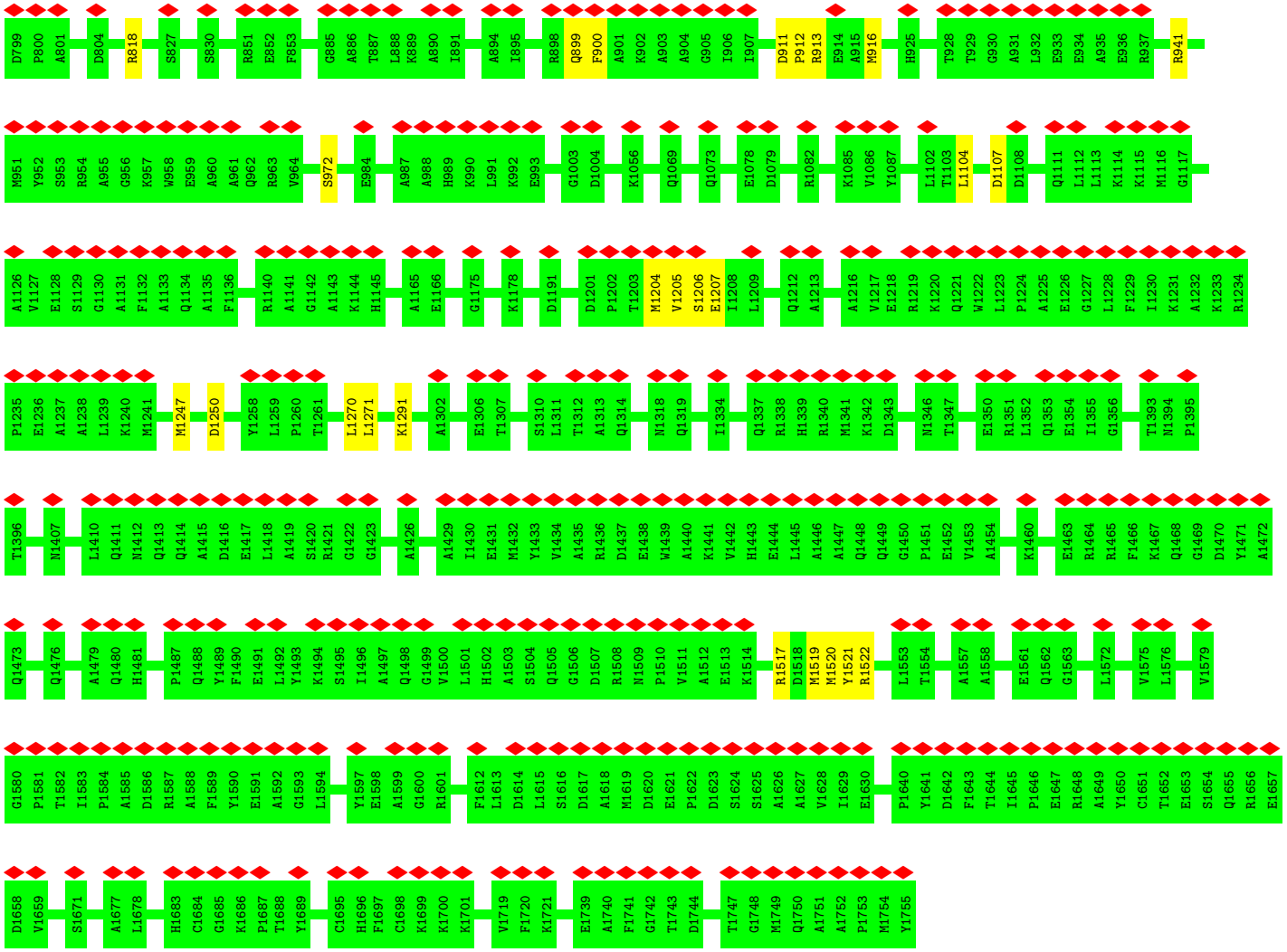
Chain T:



• Molecule 14: Intraflagellar transport protein 172

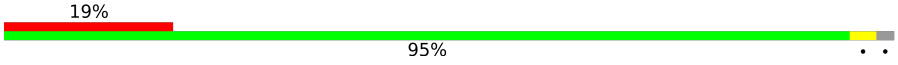
Chain i:

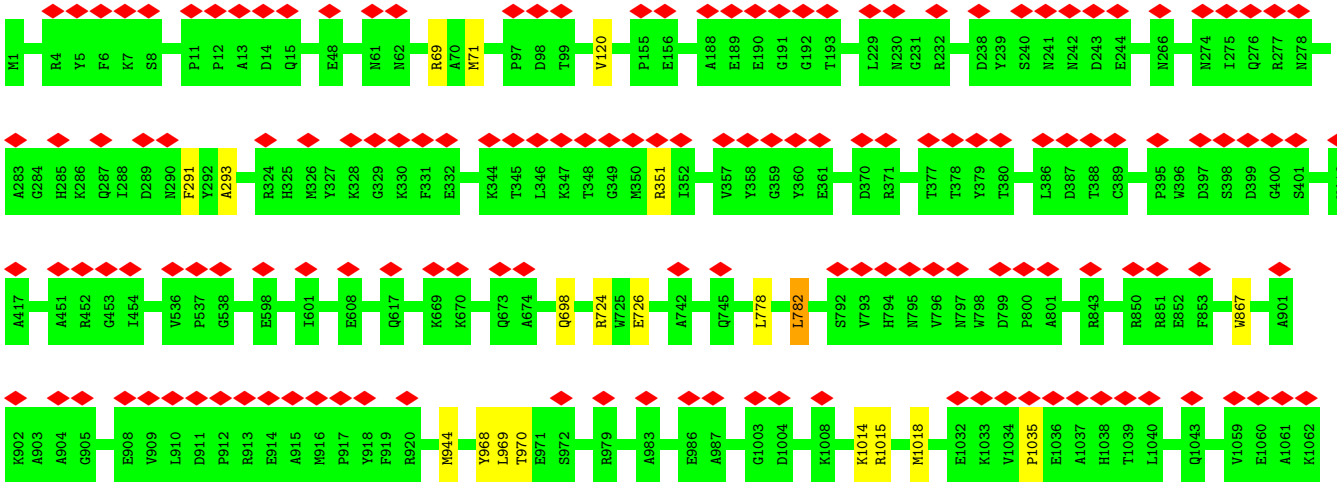


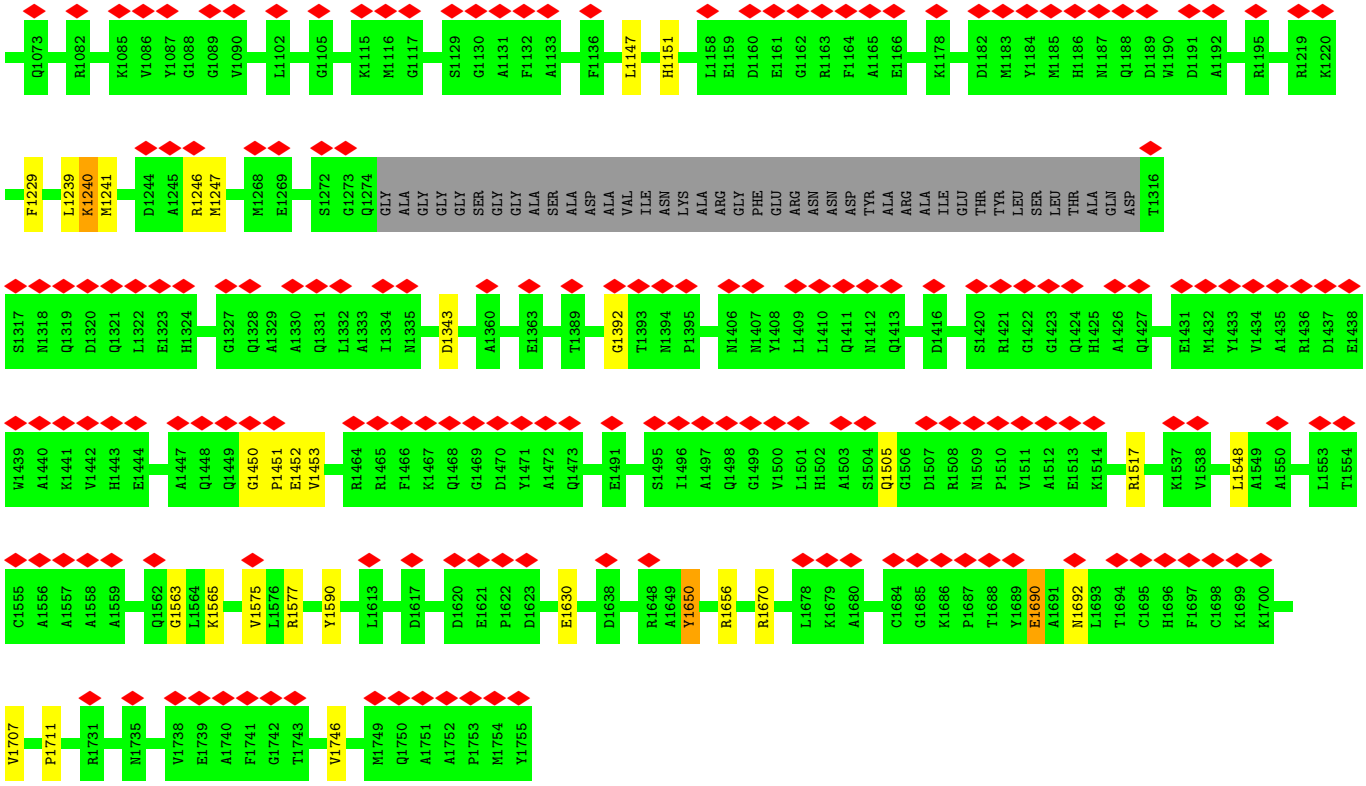


• Molecule 14: Intraflagellar transport protein 172

Chain I:

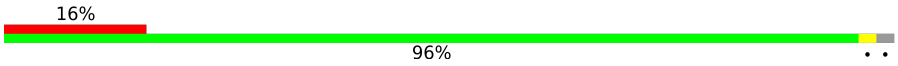




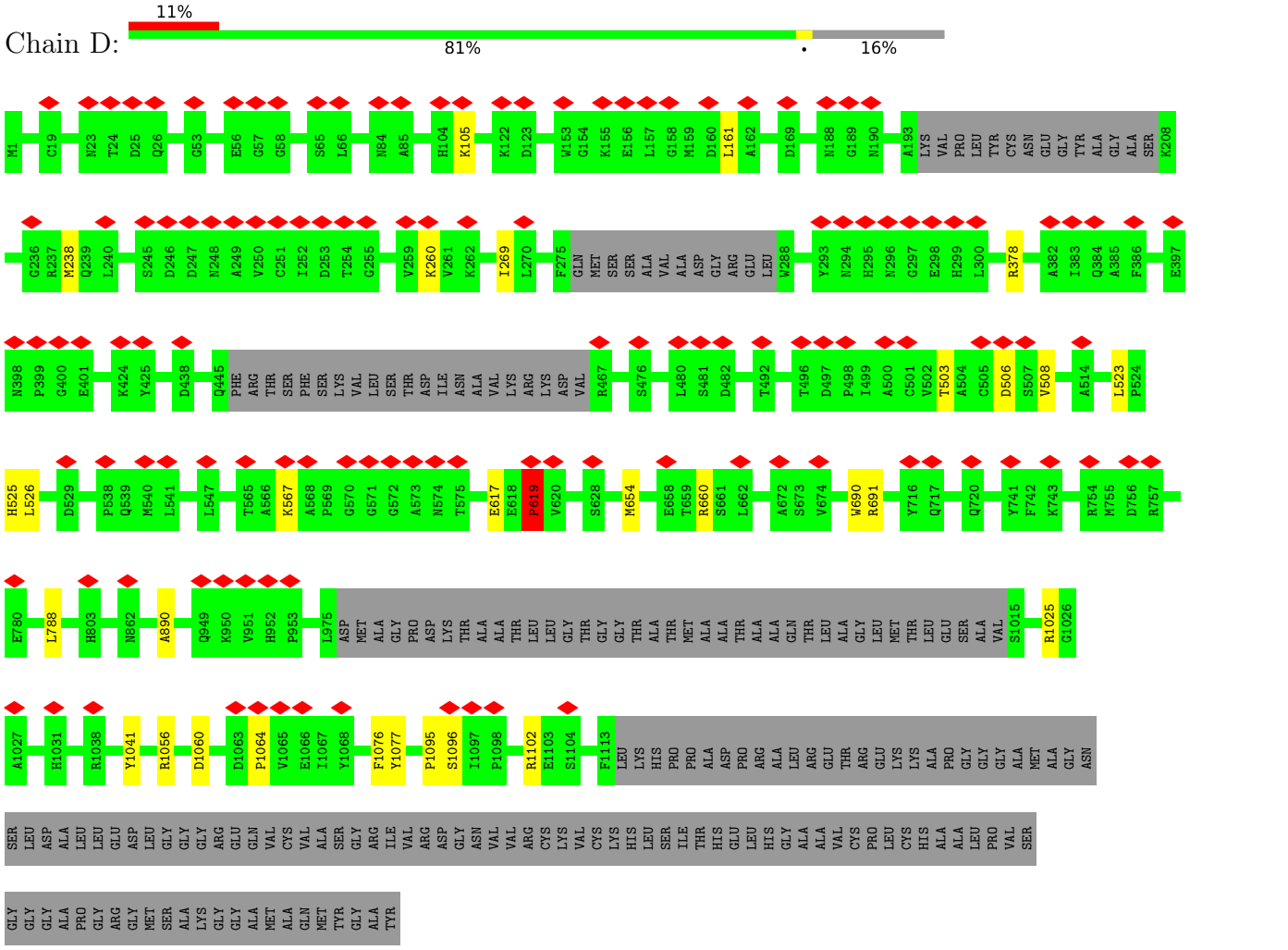


• Molecule 15: Intraflagellar transport protein 122 homolog

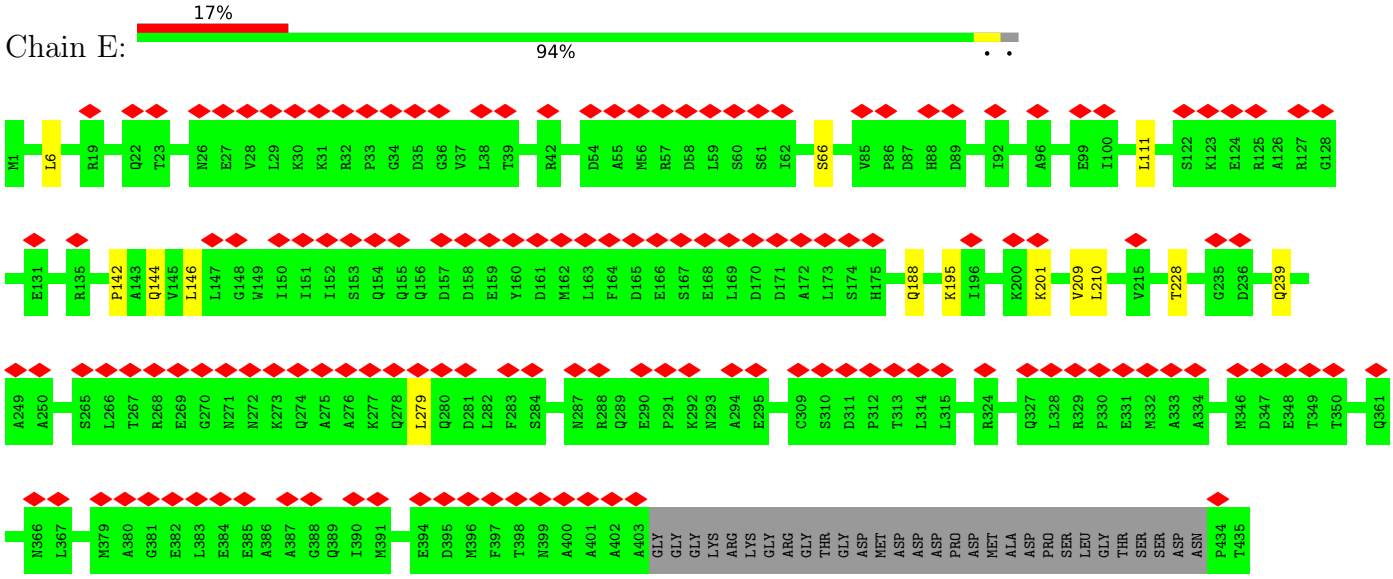
Chain C:

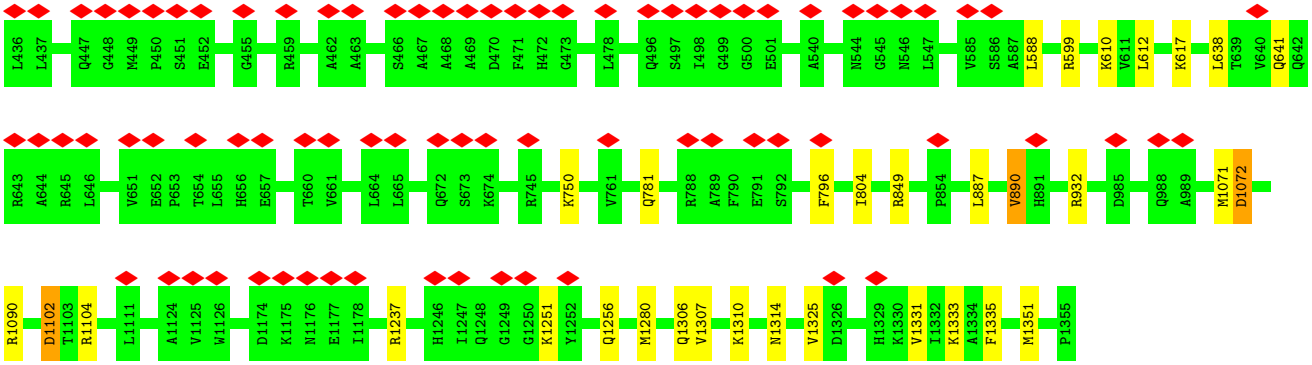


• Molecule 16: Intraflagellar transport protein 121

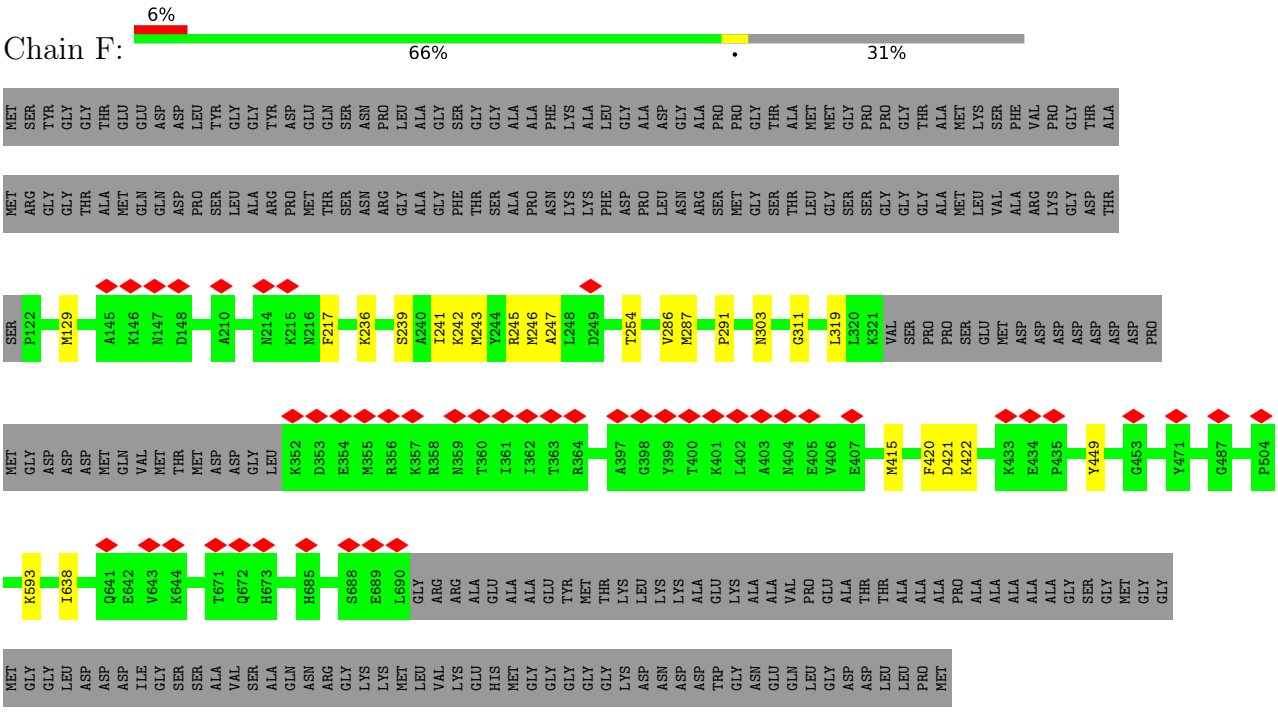


• Molecule 17: Intraflagellar transport protein 139

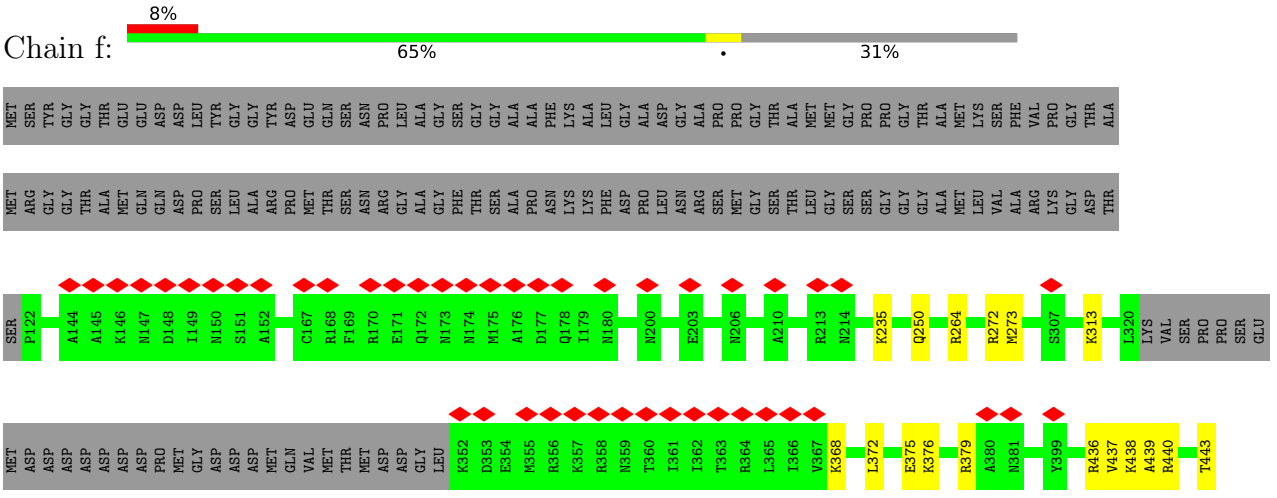


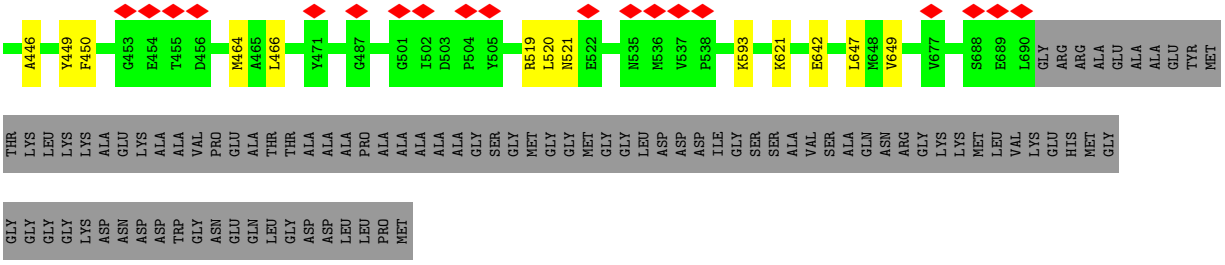


• Molecule 18: IFT88



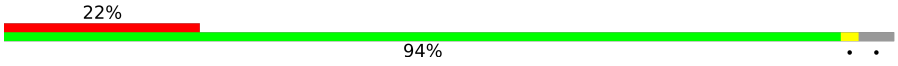
• Molecule 18: IFT88

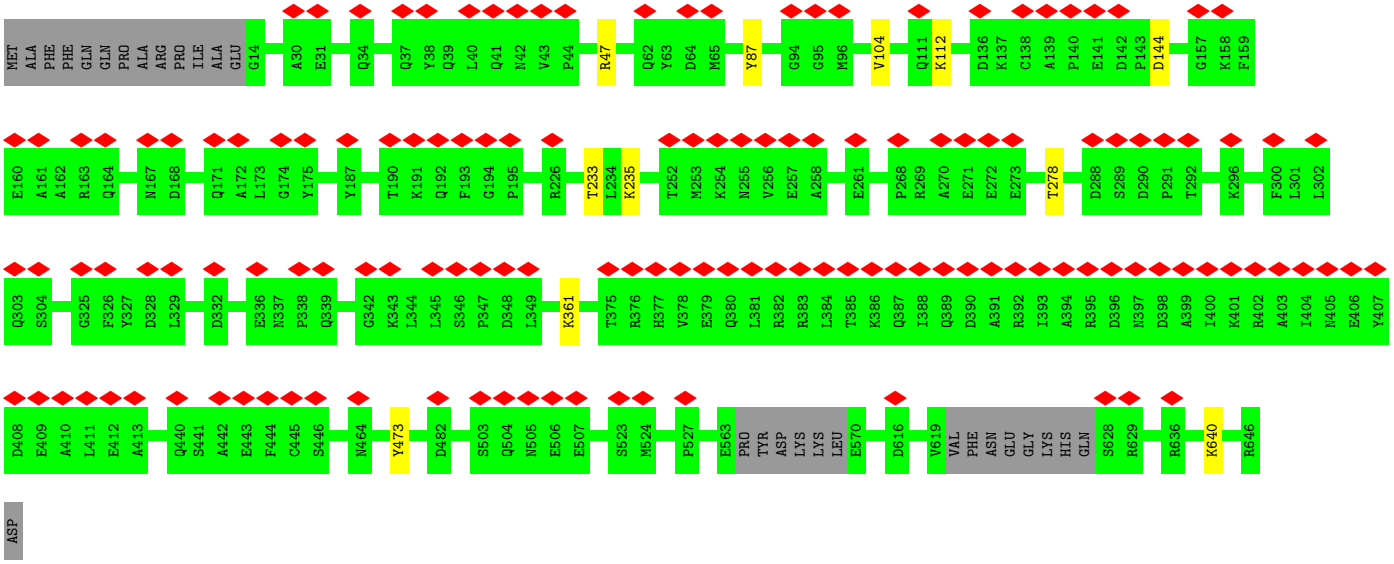




• Molecule 19: IFT70

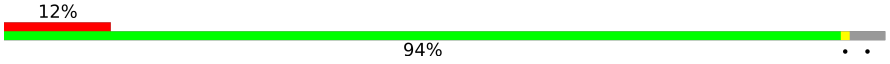
Chain G:

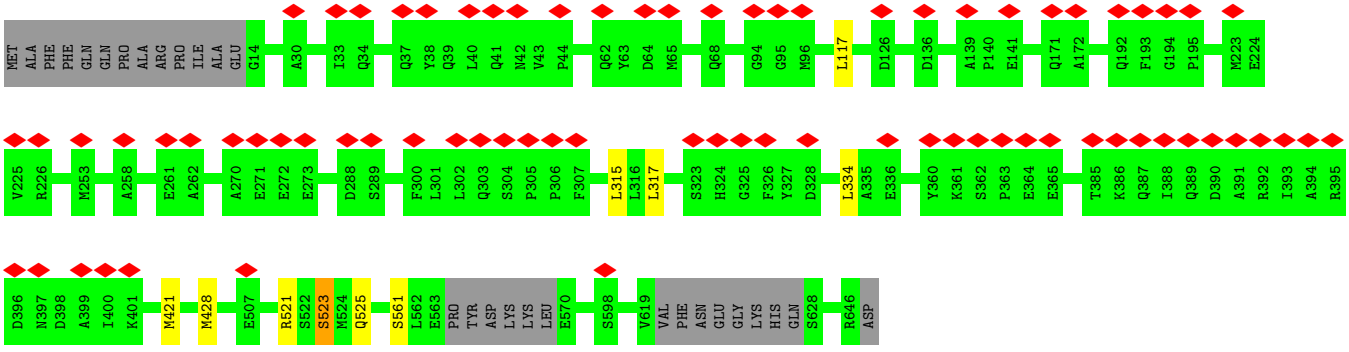




• Molecule 19: IFT70

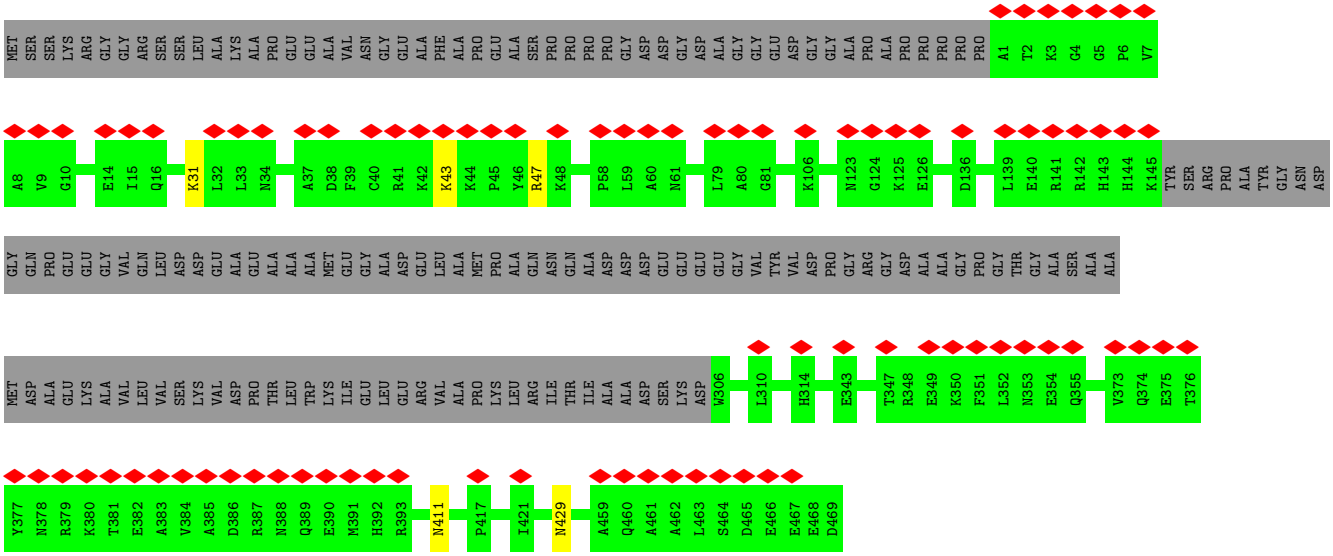
Chain g:





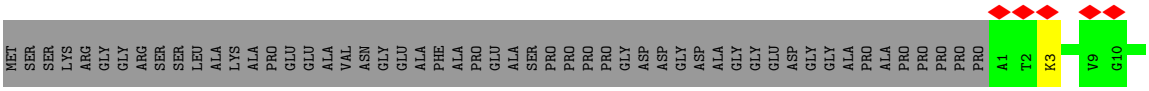
• Molecule 20: Intraflagellar transport protein 57

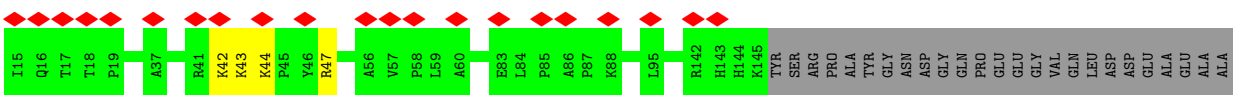
Chain M:



• Molecule 20: Intraflagellar transport protein 57

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	5896	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 ($e^-/Å^2$)	104	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	11.329	Depositor
Minimum map value	0.000	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.478	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	1357.44, 2090.7, 1357.44	wwPDB
Map dimensions	224, 345, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.06, 6.06, 6.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	0/10781	0.65	0/14601
2	B	0.36	0/10982	0.65	0/14878
3	H	0.41	0/3635	0.69	0/4918
3	h	0.39	0/3522	0.70	0/4765
4	J	0.40	0/6147	0.69	0/8333
4	j	0.37	0/6147	0.70	1/8333 (0.0%)
5	K	0.31	0/857	0.69	0/1144
5	k	0.30	0/857	0.61	0/1144
6	L	0.36	0/922	0.65	0/1226
6	l	0.37	0/922	0.63	0/1226
7	N	0.41	0/2504	0.69	0/3356
7	n	0.38	0/2504	0.66	0/3356
8	O	0.36	0/2425	0.71	0/3223
9	P	0.37	0/2462	0.67	0/3290
10	Q	0.41	0/1637	0.63	0/2224
11	R	0.36	0/1103	0.67	0/1485
12	S	0.42	0/1068	0.73	0/1441
12	s	0.31	0/1164	0.66	0/1579
13	T	0.34	0/1528	0.63	0/2066
14	I	0.40	0/13910	0.68	0/18827
14	i	0.34	0/14205	0.64	0/19226
15	C	0.34	0/9820	0.62	0/13292
16	D	0.38	0/8336	0.67	1/11273 (0.0%)
17	E	0.39	0/10649	0.69	0/14397
18	F	0.41	0/4423	0.70	0/5956
18	f	0.39	0/4414	0.67	0/5945
19	G	0.40	0/5080	0.70	0/6863
19	g	0.37	0/5080	0.65	0/6863
20	M	0.34	0/2510	0.61	0/3385
20	m	0.31	0/2510	0.61	0/3385
All	All	0.37	0/142104	0.67	2/192000 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	j	665	ARG	N-CA-C	-5.25	96.81	111.00
16	D	619	PRO	N-CA-CB	-5.09	97.00	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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	A	1365/1367 (100%)	1263 (92%)	99 (7%)	3 (0%)	44	78
2	B	1372/1409 (97%)	1244 (91%)	122 (9%)	6 (0%)	30	68
3	H	452/454 (100%)	361 (80%)	80 (18%)	11 (2%)	5	27
3	h	438/454 (96%)	370 (84%)	63 (14%)	5 (1%)	12	47
4	J	763/765 (100%)	652 (86%)	107 (14%)	4 (0%)	25	64
4	j	763/765 (100%)	658 (86%)	101 (13%)	4 (0%)	25	64
5	K	104/510 (20%)	101 (97%)	3 (3%)	0	100	100
5	k	104/510 (20%)	100 (96%)	4 (4%)	0	100	100
6	L	112/135 (83%)	111 (99%)	1 (1%)	0	100	100
6	l	112/135 (83%)	107 (96%)	5 (4%)	0	100	100
7	N	301/443 (68%)	267 (89%)	32 (11%)	2 (1%)	19	57
7	n	301/443 (68%)	274 (91%)	25 (8%)	2 (1%)	19	57
8	O	297/641 (46%)	285 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	P	304/683 (44%)	288 (95%)	13 (4%)	3 (1%)	13 49
10	Q	202/204 (99%)	175 (87%)	25 (12%)	2 (1%)	13 49
11	R	134/189 (71%)	119 (89%)	13 (10%)	2 (2%)	8 40
12	S	131/344 (38%)	110 (84%)	19 (14%)	2 (2%)	8 40
12	s	139/344 (40%)	131 (94%)	8 (6%)	0	100 100
13	T	190/192 (99%)	178 (94%)	11 (6%)	1 (0%)	25 64
14	I	1710/1755 (97%)	1505 (88%)	191 (11%)	14 (1%)	16 55
14	i	1753/1755 (100%)	1554 (89%)	191 (11%)	8 (0%)	25 64
15	C	1206/1239 (97%)	1076 (89%)	120 (10%)	10 (1%)	16 55
16	D	1017/1224 (83%)	872 (86%)	136 (13%)	9 (1%)	14 52
17	E	1321/1355 (98%)	1148 (87%)	165 (12%)	8 (1%)	22 60
18	F	535/782 (68%)	468 (88%)	60 (11%)	7 (1%)	10 43
18	f	534/782 (68%)	470 (88%)	62 (12%)	2 (0%)	30 68
19	G	613/647 (95%)	567 (92%)	46 (8%)	0	100 100
19	g	613/647 (95%)	544 (89%)	67 (11%)	2 (0%)	37 73
20	M	305/469 (65%)	285 (93%)	20 (7%)	0	100 100
20	m	305/469 (65%)	274 (90%)	29 (10%)	2 (1%)	19 57
All	All	17496/21111 (83%)	15557 (89%)	1830 (10%)	109 (1%)	24 60

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	297	THR
3	H	412	HIS
4	J	315	MET
9	P	525	LYS
3	h	187	LYS
3	h	339	PRO
14	i	1205	VAL
15	C	692	SER
17	E	66	SER
17	E	890	VAL
17	E	1102	ASP
18	F	247	ALA
14	I	293	ALA
14	I	698	GLN

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Mol	Chain	Res	Type
14	I	1690	GLU
3	H	62	GLY
3	H	136	ASP
4	J	643	PHE
12	S	226	ASN
12	S	228	ILE
3	h	327	GLY
3	h	329	LEU
14	i	658	ILE
4	j	555	SER
15	C	554	ILE
15	C	694	GLN
16	D	691	ARG
16	D	890	ALA
16	D	1077	TYR
18	F	303	ASN
14	I	1450	GLY
14	I	1451	PRO
14	I	1453	VAL
19	g	523	SER
2	B	675	LEU
3	H	64	PRO
3	H	159	PHE
3	H	271	LEU
4	J	313	ASP
7	N	19	PRO
9	P	460	THR
10	Q	44	LEU
11	R	44	PRO
14	i	251	CYS
14	i	912	PRO
4	j	342	LEU
15	C	311	THR
15	C	557	PRO
16	D	619	PRO
16	D	654	MET
16	D	1095	PRO
18	F	593	LYS
14	I	1240	LYS
14	I	1711	PRO
18	f	439	ALA
18	f	446	ALA

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Mol	Chain	Res	Type
20	m	467	GLU
20	m	468	GLU
1	A	770	TRP
2	B	775	ALA
3	H	187	LYS
4	J	314	ASP
7	N	16	LEU
14	i	266	ASN
14	i	1271	LEU
15	C	918	ARG
17	E	188	GLN
14	I	1035	PRO
14	I	1392	GLY
14	I	1563	GLY
14	I	1650	TYR
1	A	1097	ASP
2	B	238	THR
2	B	571	GLU
2	B	673	PRO
2	B	984	LYS
3	H	133	LEU
3	H	443	PRO
10	Q	171	PRO
11	R	43	PHE
13	T	9	ALA
3	h	44	ASP
14	i	660	LYS
4	j	690	LEU
15	C	1018	PRO
16	D	523	LEU
16	D	1096	SER
17	E	142	PRO
17	E	1072	ASP
18	F	449	TYR
18	F	638	ILE
14	I	782	LEU
19	g	525	GLN
9	P	461	GLU
4	j	528	TYR
7	n	234	ARG
7	n	235	PRO
15	C	916	PRO

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Mol	Chain	Res	Type
1	A	517	VAL
16	D	1064	PRO
17	E	1307	VAL
3	H	355	PRO
18	F	311	GLY
15	C	697	ILE
17	E	1325	VAL
15	C	938	PRO
18	F	291	PRO
14	i	556	VAL
14	I	1575	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	A	1119/1119 (100%)	1100 (98%)	19 (2%)	56	72
2	B	1136/1162 (98%)	1122 (99%)	14 (1%)	67	78
3	H	388/388 (100%)	368 (95%)	20 (5%)	19	40
3	h	377/388 (97%)	360 (96%)	17 (4%)	23	45
4	J	648/648 (100%)	630 (97%)	18 (3%)	38	57
4	j	648/648 (100%)	620 (96%)	28 (4%)	25	46
5	K	90/401 (22%)	89 (99%)	1 (1%)	70	80
5	k	90/401 (22%)	90 (100%)	0	100	100
6	L	101/120 (84%)	98 (97%)	3 (3%)	36	55
6	l	101/120 (84%)	97 (96%)	4 (4%)	27	47
7	N	261/358 (73%)	242 (93%)	19 (7%)	11	31
7	n	261/358 (73%)	253 (97%)	8 (3%)	35	54
8	O	260/526 (49%)	253 (97%)	7 (3%)	40	58
9	P	262/581 (45%)	255 (97%)	7 (3%)	40	58
10	Q	176/176 (100%)	172 (98%)	4 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	R	121/147 (82%)	118 (98%)	3 (2%)	42	61
12	S	114/288 (40%)	107 (94%)	7 (6%)	15	37
12	s	128/288 (44%)	127 (99%)	1 (1%)	79	85
13	T	159/159 (100%)	156 (98%)	3 (2%)	52	69
14	I	1405/1431 (98%)	1364 (97%)	41 (3%)	37	56
14	i	1431/1431 (100%)	1389 (97%)	42 (3%)	37	56
15	C	1020/1035 (99%)	1005 (98%)	15 (2%)	60	75
16	D	865/1005 (86%)	842 (97%)	23 (3%)	40	58
17	E	1092/1114 (98%)	1050 (96%)	42 (4%)	28	49
18	F	457/627 (73%)	440 (96%)	17 (4%)	29	49
18	f	456/627 (73%)	428 (94%)	28 (6%)	15	37
19	G	534/558 (96%)	523 (98%)	11 (2%)	48	66
19	g	534/558 (96%)	525 (98%)	9 (2%)	56	72
20	M	268/381 (70%)	263 (98%)	5 (2%)	52	69
20	m	268/381 (70%)	258 (96%)	10 (4%)	29	49
All	All	14770/17424 (85%)	14344 (97%)	426 (3%)	39	56

All (426) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	452	GLN
1	A	480	VAL
1	A	481	ILE
1	A	486	GLN
1	A	489	ASN
1	A	513	LEU
1	A	516	ASP
1	A	518	THR
1	A	574	MET
1	A	740	LEU
1	A	758	ARG
1	A	775	LYS
1	A	846	ARG
1	A	907	MET
1	A	931	GLU
1	A	1100	THR

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Mol	Chain	Res	Type
1	A	1102	ASP
1	A	1348	LEU
2	B	136	MET
2	B	228	THR
2	B	279	ASN
2	B	311	LEU
2	B	396	VAL
2	B	535	HIS
2	B	550	LYS
2	B	704	MET
2	B	712	ASP
2	B	718	ARG
2	B	782	ARG
2	B	1168	MET
2	B	1195	MET
2	B	1199	TYR
3	H	49	THR
3	H	50	LEU
3	H	51	ASP
3	H	61	LEU
3	H	75	MET
3	H	111	MET
3	H	119	VAL
3	H	159	PHE
3	H	185	VAL
3	H	186	GLN
3	H	223	SER
3	H	268	ASP
3	H	269	LEU
3	H	270	LYS
3	H	304	LEU
3	H	305	PHE
3	H	361	GLU
3	H	362	LEU
3	H	364	ASP
3	H	365	LEU
4	J	3	LEU
4	J	67	SER
4	J	69	LYS
4	J	111	ARG
4	J	113	SER
4	J	281	THR

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Mol	Chain	Res	Type
4	J	283	LEU
4	J	311	VAL
4	J	315	MET
4	J	336	ARG
4	J	383	ARG
4	J	467	LEU
4	J	473	ILE
4	J	474	ASN
4	J	477	GLN
4	J	629	GLU
4	J	643	PHE
4	J	685	LYS
5	K	449	MET
6	L	66	LYS
6	L	103	ARG
6	L	123	GLN
7	N	16	LEU
7	N	20	ARG
7	N	87	TYR
7	N	94	VAL
7	N	95	LYS
7	N	98	LEU
7	N	99	LYS
7	N	106	LYS
7	N	110	LYS
7	N	154	LEU
7	N	156	GLN
7	N	157	GLU
7	N	159	GLU
7	N	161	ARG
7	N	285	ARG
7	N	287	LEU
7	N	288	LYS
7	N	289	LYS
7	N	290	MET
8	O	371	GLU
8	O	377	LYS
8	O	378	LYS
8	O	501	LYS
8	O	560	LEU
8	O	561	LEU
8	O	562	ARG

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Mol	Chain	Res	Type
9	P	446	LYS
9	P	461	GLU
9	P	521	GLU
9	P	525	LYS
9	P	526	TYR
9	P	527	LEU
9	P	569	HIS
10	Q	43	PHE
10	Q	94	TYR
10	Q	117	LEU
10	Q	118	LEU
11	R	46	GLU
11	R	117	LEU
11	R	118	GLN
12	S	225	ILE
12	S	230	LYS
12	S	232	LYS
12	S	280	ARG
12	S	281	LEU
12	S	285	LEU
12	S	323	LYS
13	T	21	LEU
13	T	85	LEU
13	T	86	MET
3	h	1	MET
3	h	58	ILE
3	h	60	VAL
3	h	187	LYS
3	h	217	ARG
3	h	241	MET
3	h	248	LEU
3	h	253	LYS
3	h	281	LYS
3	h	282	LEU
3	h	295	ASP
3	h	299	LEU
3	h	302	ASP
3	h	338	THR
3	h	339	PRO
3	h	340	LEU
3	h	361	GLU
14	i	139	ARG

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Mol	Chain	Res	Type
14	i	224	VAL
14	i	240	SER
14	i	244	GLU
14	i	246	ARG
14	i	250	THR
14	i	253	PHE
14	i	265	TYR
14	i	410	ARG
14	i	414	VAL
14	i	422	ILE
14	i	527	LEU
14	i	555	SER
14	i	558	LYS
14	i	634	GLN
14	i	650	ARG
14	i	660	LYS
14	i	689	ARG
14	i	692	MET
14	i	697	LYS
14	i	818	ARG
14	i	899	GLN
14	i	900	PHE
14	i	911	ASP
14	i	913	ARG
14	i	916	MET
14	i	941	ARG
14	i	972	SER
14	i	1104	LEU
14	i	1107	ASP
14	i	1204	MET
14	i	1206	SER
14	i	1207	GLU
14	i	1247	MET
14	i	1250	ASP
14	i	1270	LEU
14	i	1291	LYS
14	i	1517	ARG
14	i	1519	MET
14	i	1520	MET
14	i	1521	TYR
14	i	1522	ARG
4	j	4	LYS

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Mol	Chain	Res	Type
4	j	133	ARG
4	j	222	GLN
4	j	302	LEU
4	j	304	ASP
4	j	309	VAL
4	j	342	LEU
4	j	378	LEU
4	j	380	GLN
4	j	385	PHE
4	j	424	LEU
4	j	508	ARG
4	j	515	MET
4	j	516	LEU
4	j	521	ASP
4	j	537	LYS
4	j	554	LYS
4	j	581	SER
4	j	640	LYS
4	j	643	PHE
4	j	645	ARG
4	j	646	LYS
4	j	689	LYS
4	j	690	LEU
4	j	707	GLN
4	j	720	ASN
4	j	735	GLU
4	j	758	ARG
6	l	50	LYS
6	l	73	ARG
6	l	124	LYS
6	l	125	LEU
7	n	28	ARG
7	n	29	VAL
7	n	42	LEU
7	n	132	ASN
7	n	238	MET
7	n	243	ARG
7	n	285	ARG
7	n	294	LEU
12	s	194	LYS
15	C	250	ARG
15	C	295	THR

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Mol	Chain	Res	Type
15	C	310	MET
15	C	406	ARG
15	C	415	ARG
15	C	467	ARG
15	C	645	ARG
15	C	670	ARG
15	C	691	ARG
15	C	842	ARG
15	C	877	ASN
15	C	937	LEU
15	C	940	ARG
15	C	941	GLU
15	C	942	VAL
16	D	105	LYS
16	D	161	LEU
16	D	238	MET
16	D	260	LYS
16	D	269	ILE
16	D	378	ARG
16	D	503	THR
16	D	506	ASP
16	D	508	VAL
16	D	525	HIS
16	D	526	LEU
16	D	567	LYS
16	D	617	GLU
16	D	619	PRO
16	D	660	ARG
16	D	690	TRP
16	D	788	LEU
16	D	1025	ARG
16	D	1041	TYR
16	D	1056	ARG
16	D	1060	ASP
16	D	1076	PHE
16	D	1102	ARG
17	E	6	LEU
17	E	111	LEU
17	E	144	GLN
17	E	146	LEU
17	E	195	LYS
17	E	201	LYS

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Mol	Chain	Res	Type
17	E	209	VAL
17	E	210	LEU
17	E	228	THR
17	E	239	GLN
17	E	279	LEU
17	E	588	LEU
17	E	599	ARG
17	E	610	LYS
17	E	612	LEU
17	E	617	LYS
17	E	638	LEU
17	E	641	GLN
17	E	750	LYS
17	E	781	GLN
17	E	796	PHE
17	E	804	ILE
17	E	849	ARG
17	E	887	LEU
17	E	890	VAL
17	E	932	ARG
17	E	1071	MET
17	E	1072	ASP
17	E	1090	ARG
17	E	1102	ASP
17	E	1104	ARG
17	E	1237	ARG
17	E	1251	LYS
17	E	1256	GLN
17	E	1280	MET
17	E	1306	GLN
17	E	1310	LYS
17	E	1314	ASN
17	E	1331	VAL
17	E	1333	LYS
17	E	1335	PHE
17	E	1351	MET
18	F	129	MET
18	F	217	PHE
18	F	236	LYS
18	F	239	SER
18	F	241	ILE
18	F	242	LYS

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Mol	Chain	Res	Type
18	F	243	MET
18	F	245	ARG
18	F	246	MET
18	F	254	THR
18	F	286	VAL
18	F	287	MET
18	F	319	LEU
18	F	415	MET
18	F	420	PHE
18	F	421	ASP
18	F	422	LYS
19	G	47	ARG
19	G	87	TYR
19	G	104	VAL
19	G	112	LYS
19	G	144	ASP
19	G	233	THR
19	G	235	LYS
19	G	278	THR
19	G	361	LYS
19	G	473	TYR
19	G	640	LYS
14	I	69	ARG
14	I	71	MET
14	I	120	VAL
14	I	291	PHE
14	I	351	ARG
14	I	724	ARG
14	I	726	GLU
14	I	778	LEU
14	I	782	LEU
14	I	867	TRP
14	I	944	MET
14	I	968	TYR
14	I	969	LEU
14	I	970	THR
14	I	1014	LYS
14	I	1015	ARG
14	I	1018	MET
14	I	1147	LEU
14	I	1151	HIS
14	I	1229	PHE

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Mol	Chain	Res	Type
14	I	1239	LEU
14	I	1240	LYS
14	I	1241	MET
14	I	1246	ARG
14	I	1247	MET
14	I	1343	ASP
14	I	1452	GLU
14	I	1505	GLN
14	I	1517	ARG
14	I	1548	LEU
14	I	1565	LYS
14	I	1577	ARG
14	I	1590	TYR
14	I	1630	GLU
14	I	1650	TYR
14	I	1656	ARG
14	I	1670	ARG
14	I	1690	GLU
14	I	1692	ASN
14	I	1707	VAL
14	I	1746	VAL
20	M	31	LYS
20	M	43	LYS
20	M	47	ARG
20	M	411	ASN
20	M	429	ASN
18	f	235	LYS
18	f	250	GLN
18	f	264	ARG
18	f	272	ARG
18	f	273	MET
18	f	313	LYS
18	f	368	LYS
18	f	372	LEU
18	f	375	GLU
18	f	376	LYS
18	f	379	ARG
18	f	436	ARG
18	f	437	VAL
18	f	438	LYS
18	f	440	ARG
18	f	443	THR

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Mol	Chain	Res	Type
18	f	449	TYR
18	f	450	PHE
18	f	464	MET
18	f	466	LEU
18	f	519	ARG
18	f	520	LEU
18	f	521	ASN
18	f	593	LYS
18	f	621	LYS
18	f	642	GLU
18	f	647	LEU
18	f	649	VAL
19	g	117	LEU
19	g	315	LEU
19	g	317	LEU
19	g	334	LEU
19	g	421	MET
19	g	428	MET
19	g	521	ARG
19	g	523	SER
19	g	561	SER
20	m	3	LYS
20	m	42	LYS
20	m	43	LYS
20	m	44	LYS
20	m	47	ARG
20	m	333	ARG
20	m	408	LYS
20	m	412	ILE
20	m	468	GLU
20	m	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	86	ASN
1	A	282	HIS
1	A	320	ASN
1	A	449	ASN
1	A	489	ASN
1	A	1139	HIS

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Mol	Chain	Res	Type
1	A	1168	HIS
1	A	1345	GLN
2	B	70	HIS
2	B	225	ASN
2	B	279	ASN
2	B	292	GLN
2	B	346	GLN
2	B	500	HIS
2	B	535	HIS
2	B	745	ASN
2	B	941	GLN
2	B	962	HIS
3	H	257	ASN
3	H	287	GLN
4	J	251	GLN
4	J	564	ASN
5	K	461	GLN
6	L	31	GLN
7	N	26	ASN
9	P	566	HIS
9	P	613	GLN
13	T	28	GLN
3	h	140	ASN
3	h	287	GLN
3	h	328	GLN
14	i	222	ASN
14	i	634	GLN
14	i	1267	GLN
14	i	1722	ASN
4	j	222	GLN
4	j	354	GLN
4	j	384	HIS
4	j	510	HIS
4	j	707	GLN
7	n	71	GLN
7	n	277	GLN
15	C	290	GLN
15	C	532	GLN
15	C	709	ASN
15	C	950	ASN
15	C	976	GLN
15	C	1110	GLN

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Mol	Chain	Res	Type
16	D	432	HIS
16	D	519	ASN
16	D	532	HIS
16	D	792	HIS
16	D	886	GLN
17	E	274	GLN
17	E	361	GLN
17	E	496	GLN
17	E	608	GLN
17	E	641	GLN
17	E	642	GLN
17	E	781	GLN
17	E	876	ASN
17	E	1108	GLN
17	E	1131	ASN
17	E	1256	GLN
17	E	1278	GLN
17	E	1306	GLN
18	F	314	ASN
18	F	518	GLN
18	F	546	GLN
19	G	39	GLN
19	G	148	ASN
19	G	211	HIS
14	I	722	ASN
14	I	723	HIS
14	I	1151	HIS
14	I	1505	GLN
14	I	1525	ASN
14	I	1692	ASN
20	M	353	ASN
18	f	162	ASN
18	f	198	ASN
18	f	404	ASN
18	f	444	ASN
18	f	546	GLN
18	f	608	ASN
18	f	668	GLN
18	f	672	GLN
19	g	494	ASN
19	g	533	HIS
19	g	591	HIS

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Mol	Chain	Res	Type
19	g	613	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.

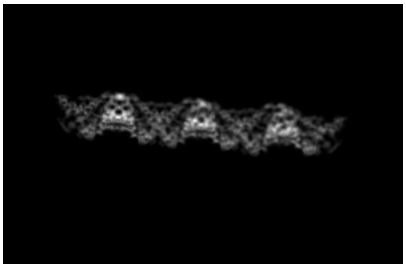
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19515. These allow visual inspection of the internal detail of the map and identification of artifacts.

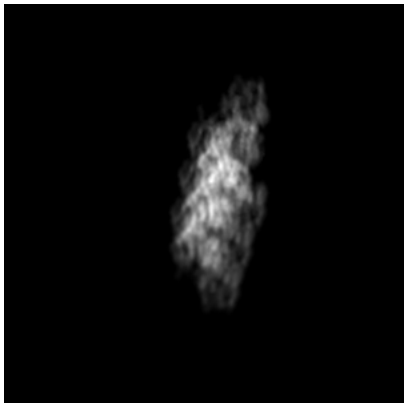
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

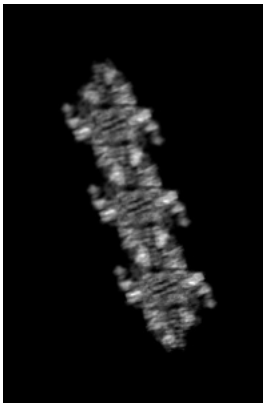
6.1.1 Primary map



X



Y



Z

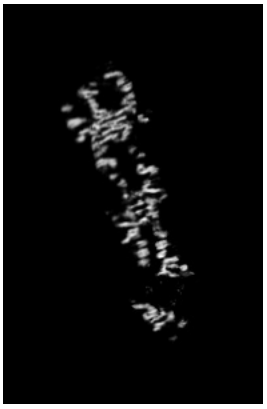
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 112

Y Index: 172



Z Index: 112

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: 117

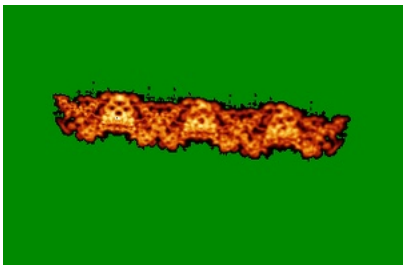
Y Index: 104

Z Index: 117

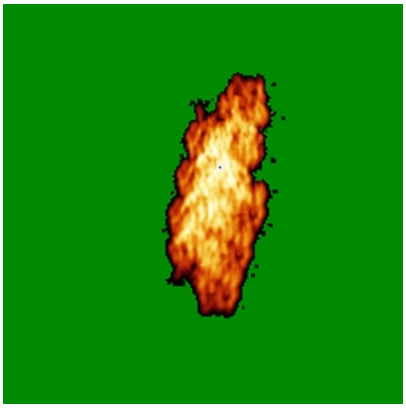
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

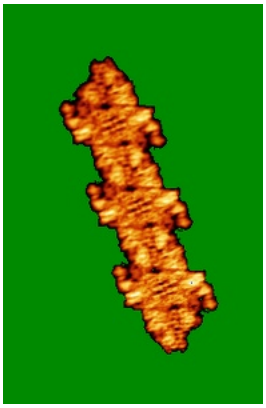
6.4.1 Primary map



X



Y

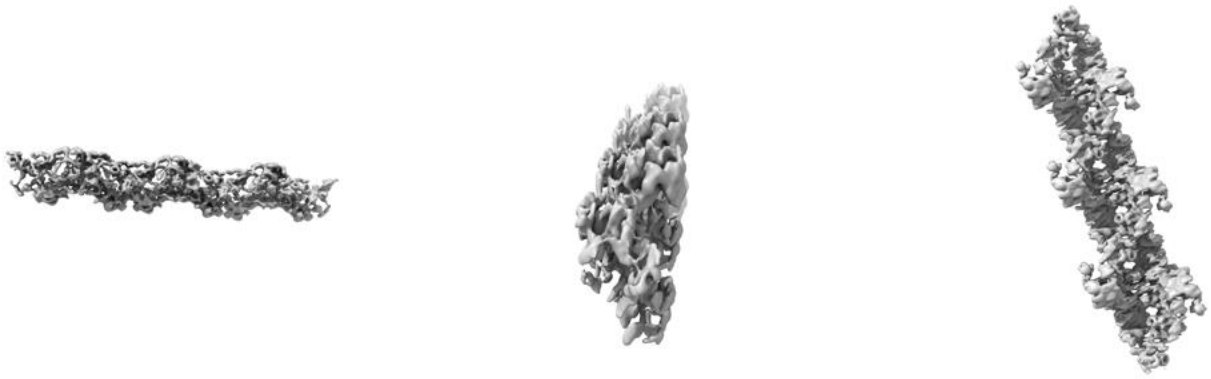


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

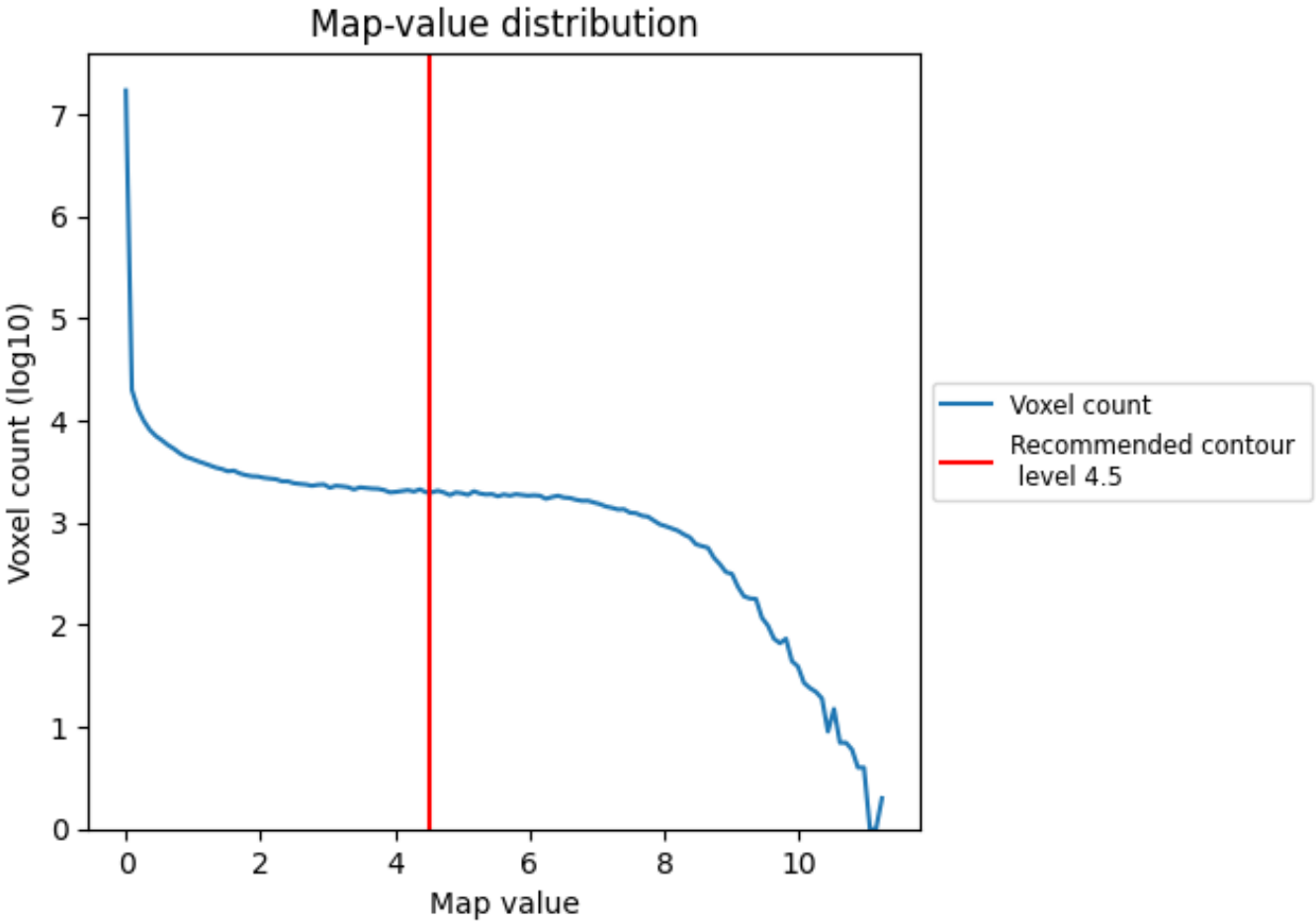
6.6 Mask visualisation (i)

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

7 Map analysis

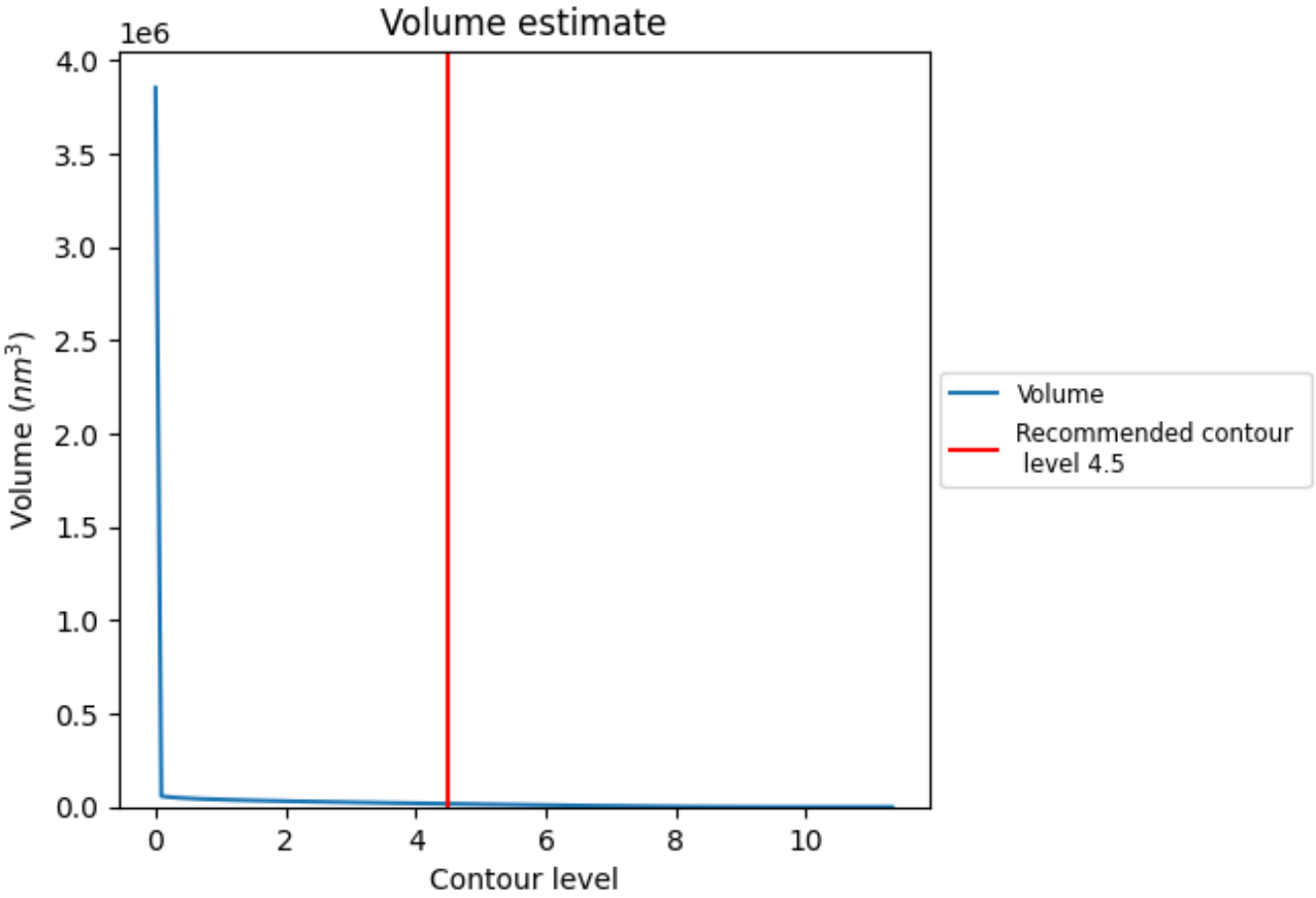
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 16773 nm^3; this corresponds to an approximate mass of 15151 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

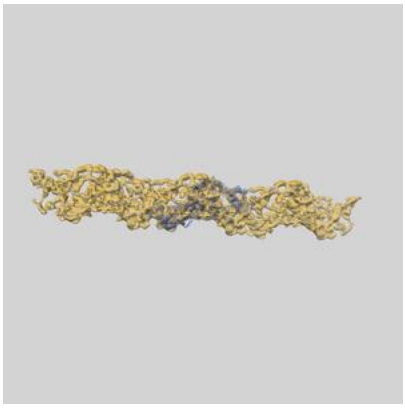
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

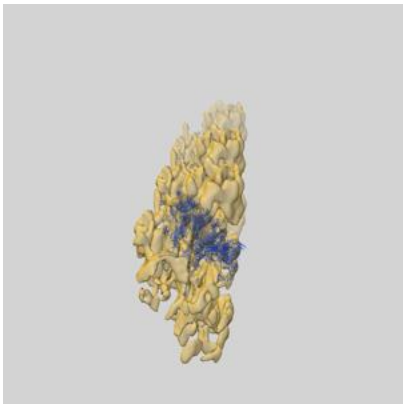
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19515 and PDB model 8RUY. Per-residue inclusion information can be found in section 3 on page 8.

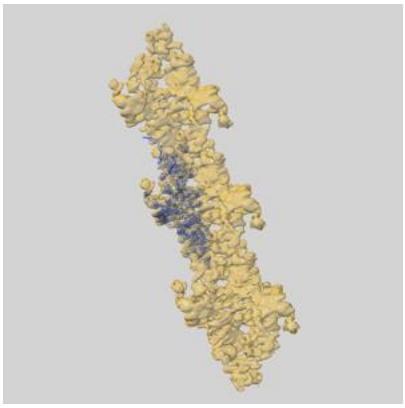
9.1 Map-model overlay



X



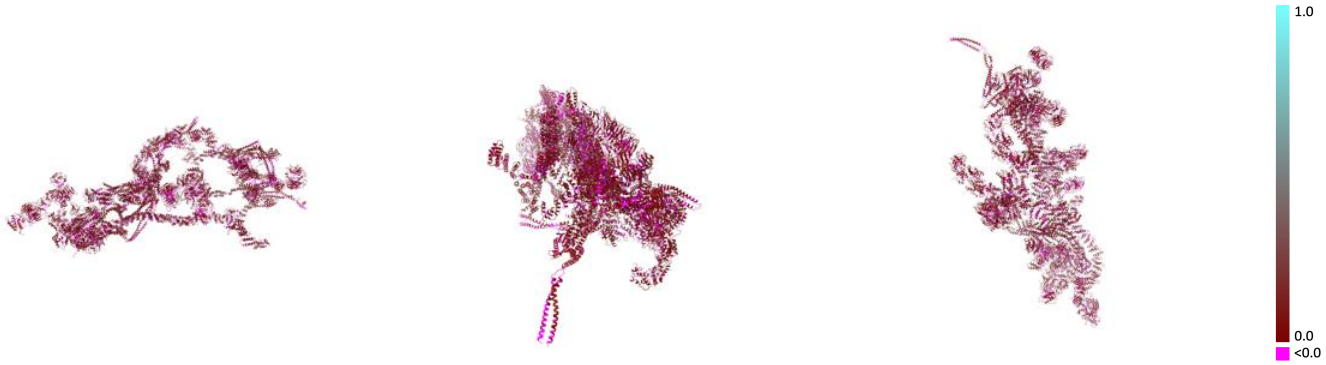
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

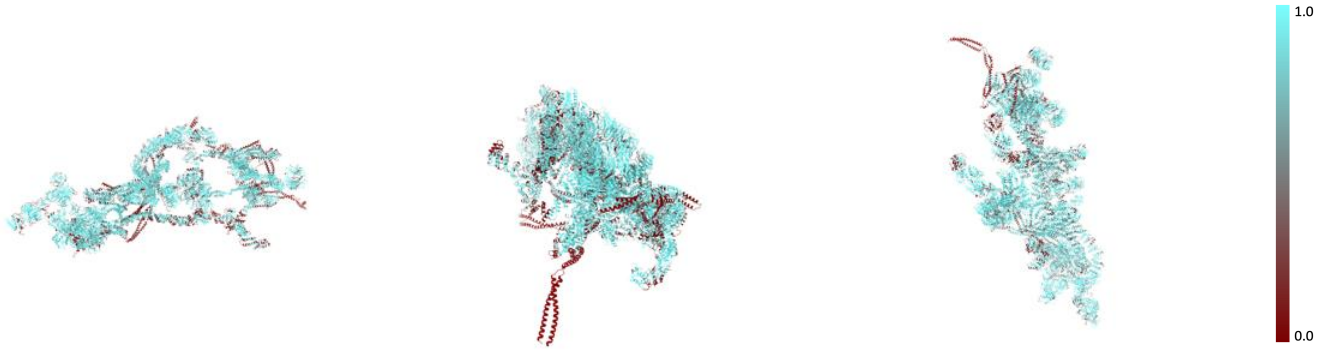
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

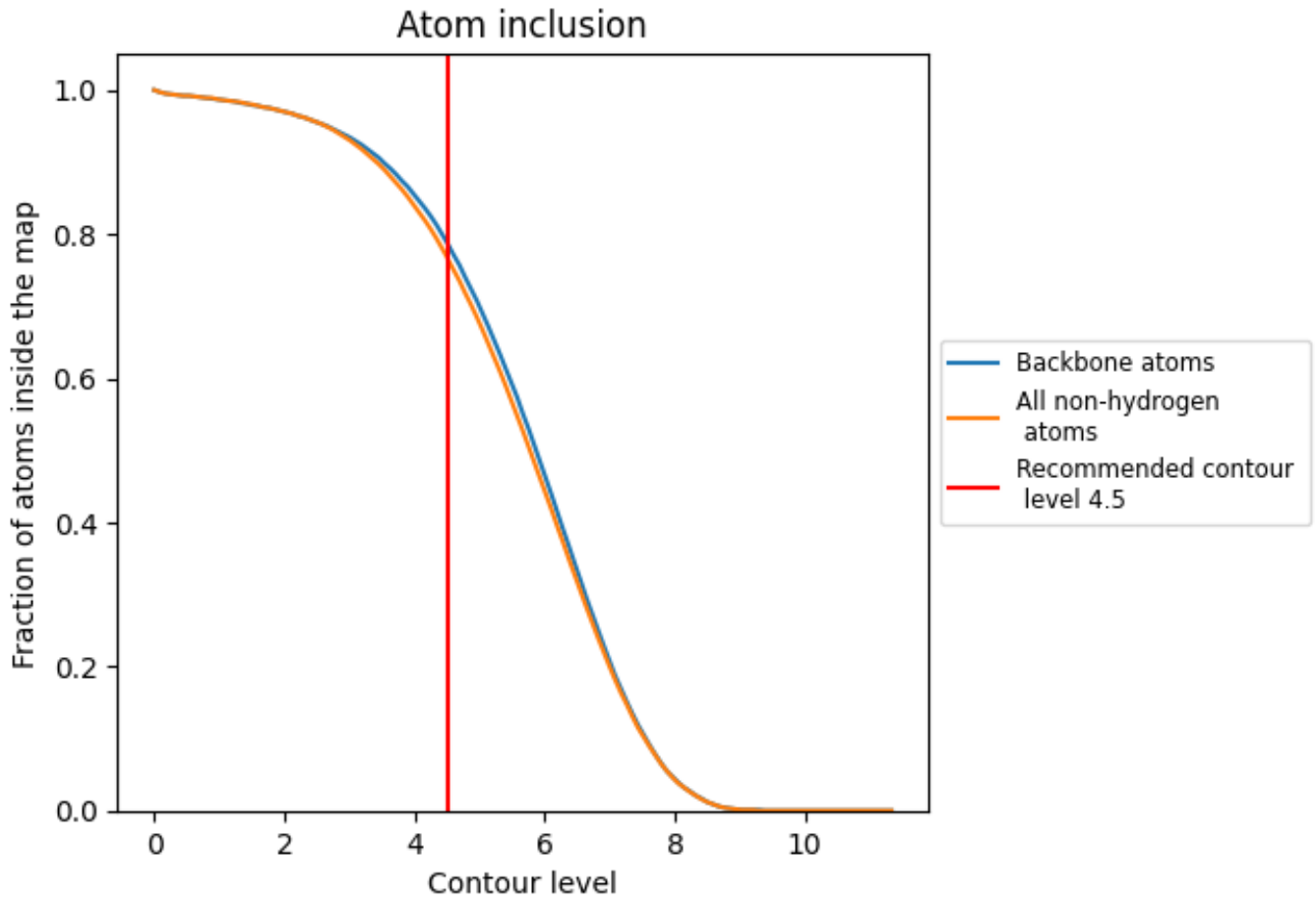
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 77% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.0720
A	0.7990	0.0770
B	0.7640	0.0730
C	0.8050	0.0670
D	0.8520	0.0730
E	0.7930	0.0780
F	0.8880	0.0850
G	0.7460	0.0680
H	0.8080	0.0660
I	0.7700	0.0700
J	0.8970	0.0690
K	0.8400	0.0750
L	0.9110	0.0910
M	0.6770	0.0720
N	0.7590	0.0800
O	0.3700	0.0650
P	0.3780	0.0450
Q	0.5860	0.0620
R	0.5770	0.0840
S	0.4310	0.0780
T	0.6860	0.0630
f	0.8640	0.0770
g	0.8510	0.0740
h	0.8310	0.0660
i	0.7120	0.0770
j	0.8300	0.0650
k	0.8380	0.1210
l	0.7890	0.0560
m	0.6010	0.0630
n	0.6800	0.0720
s	0.6600	0.0770