Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 01:05 AM EST

PDB ID	:	7JTK
EMDB ID	:	EMD-22475
Title	:	Radial spoke 1 isolated from Chlamydomonas reinhardtii
Authors	:	Gui, M.; Ma, M.; Sze-Tu, E.; Wang, X.; Koh, F.; Zhong, E.; Berger, B.; Davis, J.; Dutcher, S.; Zhang, R.; Brown, A.
Deposited on	:	2020-08-17
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

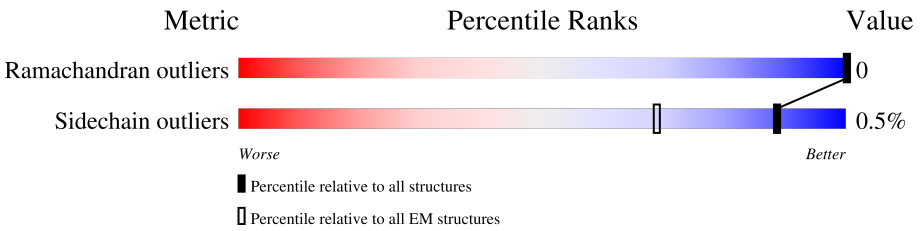
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	814	91% 8%
1	B	814	92% 8%
2	C	738	57% 42%
2	D	738	58% 42%
3	E	516	55% 45%
3	F	516	55% 44%
4	G	465	90% 9%
4	H	465	91% 9%
5	I	521	92% 7%

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Mol	Chain	Length	Quality of chain
5	J	521	92% 7%
6	K	459	93% 7%
6	L	459	93% 7%
7	M	500	9% 91%
7	N	500	8% 92%
8	O	269	93% 7%
8	P	269	92% 7%
8	Q	269	92% 7%
8	R	269	93% 7%
9	S	216	92% 8%
9	T	216	92% 8%
10	U	204	24% 76%
10	V	204	89% 11%
11	W	181	88% 10%
12	X	387	97%
13	Y	346	62% 38%
13	Z	346	62% 38%
13	y	346	18% 82%
13	z	346	18% 82%
14	a	91	92% 8%
14	b	91	92% 8%
14	c	91	92% 8%
14	d	91	92% 8%
15	e	34	100%
16	i	586	34% 66%

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Mol	Chain	Length	Quality of chain
16	j	586	34% 66%
17	k	230	92% 7%
18	s	682	5% 95%
19	u	70	69% 29%
19	v	70	70% 29%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 72807 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 Flagellar radial spoke protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	749	5698	3611	962	1111	14	0	0
1	B	749	5698	3611	962	1111	14	0	0

- Molecule 2 is a protein called Flagellar radial spoke protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	427	3248	2048	577	614	9	0	0
2	D	427	3248	2048	577	614	9	0	0

- Molecule 3 is a protein called Flagellar radial spoke protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	284	2216	1378	398	431	9	0	0
3	F	287	2232	1386	401	436	9	0	0

- Molecule 4 is a protein called Flagellar radial spoke protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	421	3207	2043	535	621	8	0	0
4	H	421	3207	2043	535	621	8	0	0

- Molecule 5 is a protein called Flagellar radial spoke protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	483	3644	2330	623	679	12	0	0
5	J	483	3644	2330	623	679	12	0	0

- Molecule 6 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	428	3214	2043	544	614	13	0	0
6	L	428	3214	2043	544	614	13	0	0

- Molecule 7 is a protein called Flagellar radial spoke protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	47	373	243	62	67	1	0	0
			Total	C	N	O			
7	N	40	316	208	53	55		0	0

- Molecule 8 is a protein called Flagellar radial spoke protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	249	1930	1233	327	365	5	0	0
8	P	249	1930	1233	327	365	5	0	0
8	Q	249	1930	1233	327	365	5	0	0
8	R	249	1930	1233	327	365	5	0	0

- Molecule 9 is a protein called Flagellar radial spoke protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	199	1530	977	257	287	9	0	0
9	T	199	1530	977	257	287	9	0	0

- Molecule 10 is a protein called Flagellar radial spoke protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	U	48	382	250	64	67	1	0	0
			Total	C	N	O	S		
10	V	182	1055	649	198	206	2	0	0

- Molecule 11 is a protein called Flagellar radial spoke protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	163	1241	796	210	231	4	0	0

- Molecule 12 is a protein called Flagellar radial spoke protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	X	379	2787	1753	506	518	10	0	0

- Molecule 13 is a protein called Flagellar radial spoke protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Y	213	1693	1092	296	301	4	0	0
			Total	C	N	O	S		
13	Z	213	1693	1092	296	301	4	0	0
			Total	C	N	O	S		
13	y	64	528	335	90	100	3	0	0
			Total	C	N	O	S		
13	z	64	528	335	90	100	3	0	0

- Molecule 14 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	a	84	686	442	115	125	4	0	0
			Total	C	N	O	S		
14	b	84	686	442	115	125	4	0	0
			Total	C	N	O	S		
14	c	84	686	442	115	125	4	0	0
			Total	C	N	O	S		
14	d	84	686	442	115	125	4	0	0

- Molecule 15 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	e	34	170	102	34	34	0	0

- Molecule 16 is a protein called Flagellar radial spoke protein 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	i	201	1558	1010	267	276	5	0	0
			Total	C	N	O	S		
16	j	201	1558	1010	267	276	5	0	0

- Molecule 17 is a protein called Cytochrome b5 heme-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	k	213	1756	1130	299	320	7	0	0

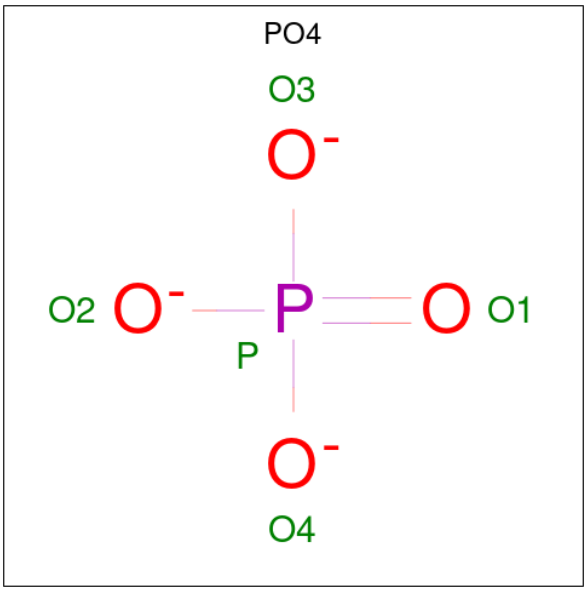
- Molecule 18 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	s	37	301	183	57	60	1	0	0

- Molecule 19 is a protein called Predicted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	50	427	273	73	78	3	0	0
			Total	C	N	O	S		
19	v	50	427	273	73	78	3	0	0

- Molecule 20 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



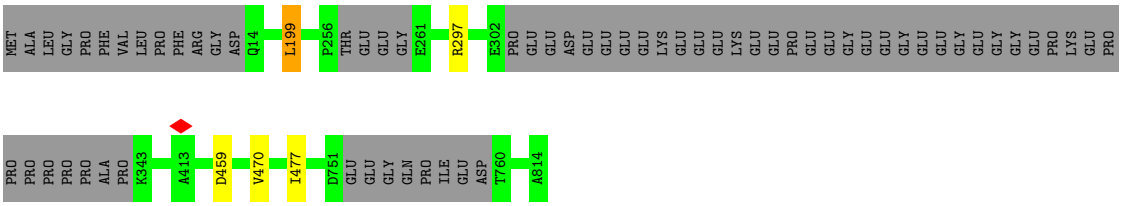
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
20	G	1	5	4	1	0
20	H	1	5	4	1	0
20	K	1	5	4	1	0
20	L	1	5	4	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

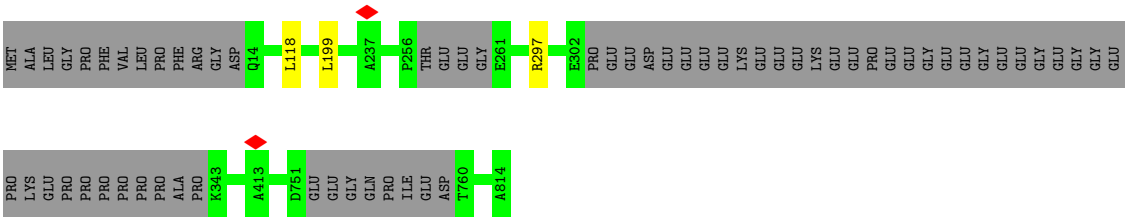
• Molecule 1: Flagellar radial spoke protein 1

Chain A:



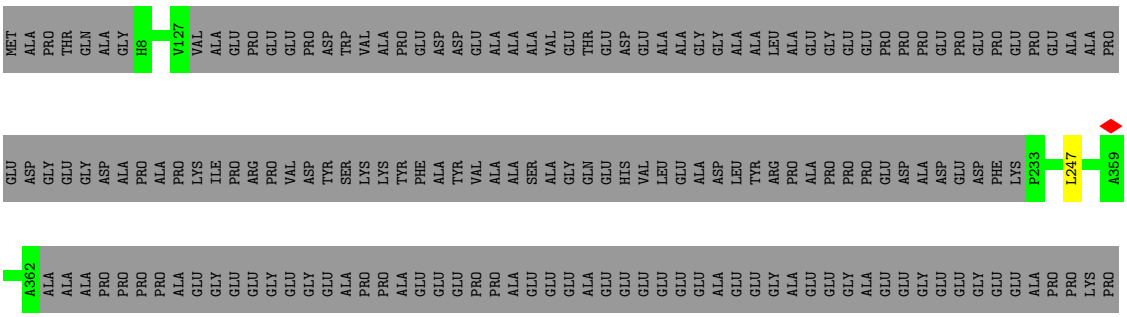
• Molecule 1: Flagellar radial spoke protein 1

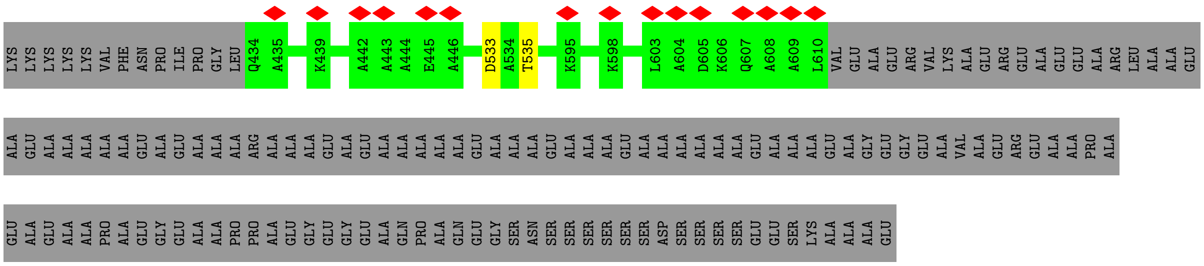
Chain B:



• Molecule 2: Flagellar radial spoke protein 2

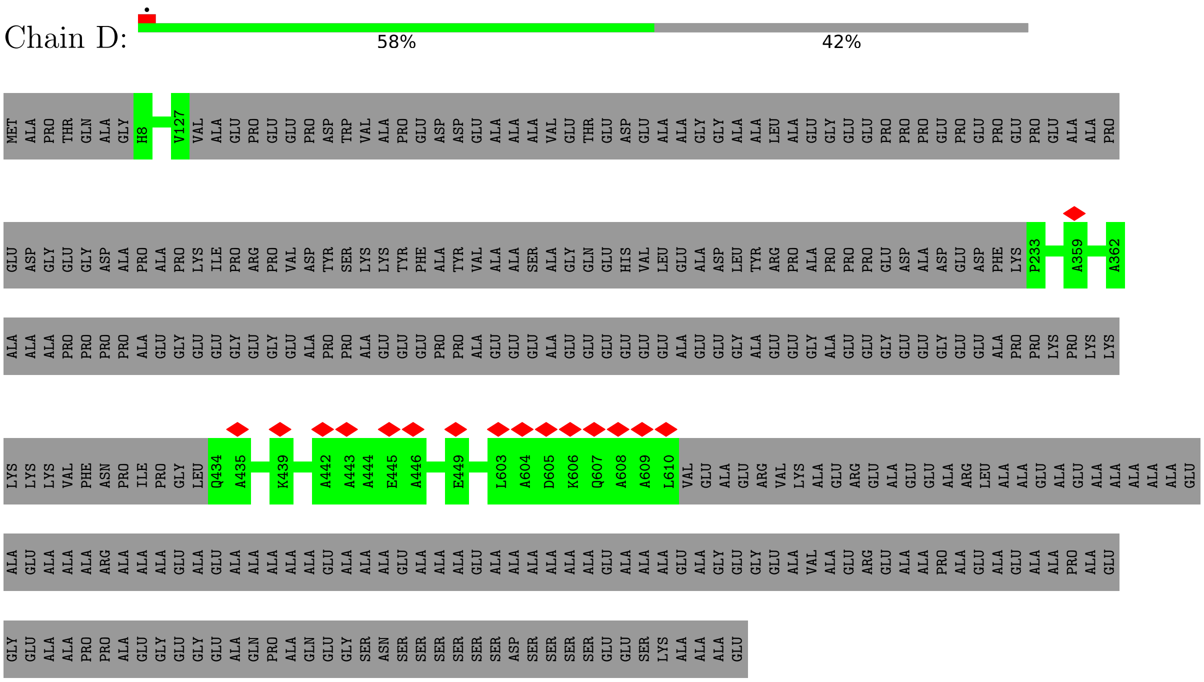
Chain C:





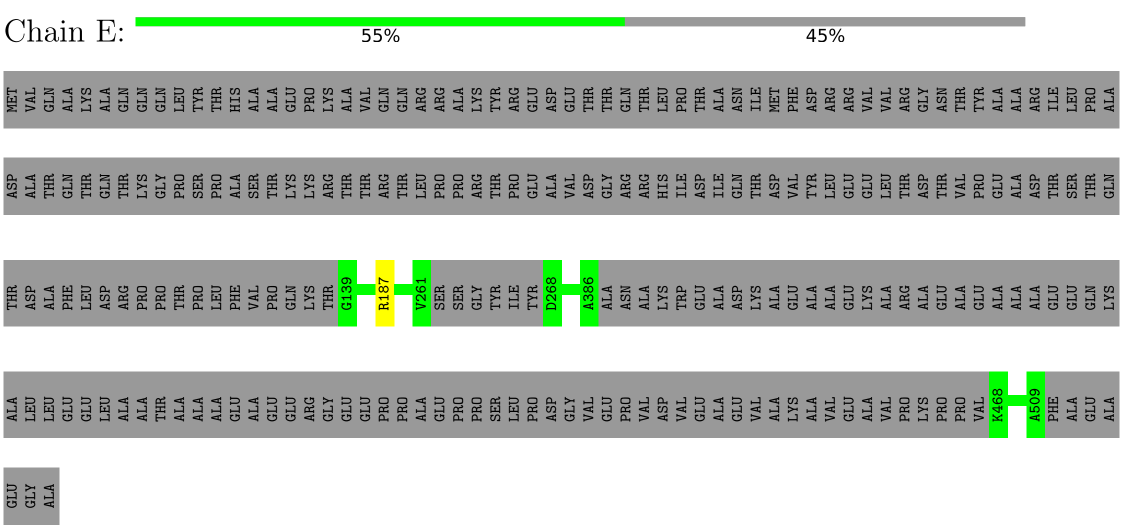
• Molecule 2: Flagellar radial spoke protein 2

Chain D:



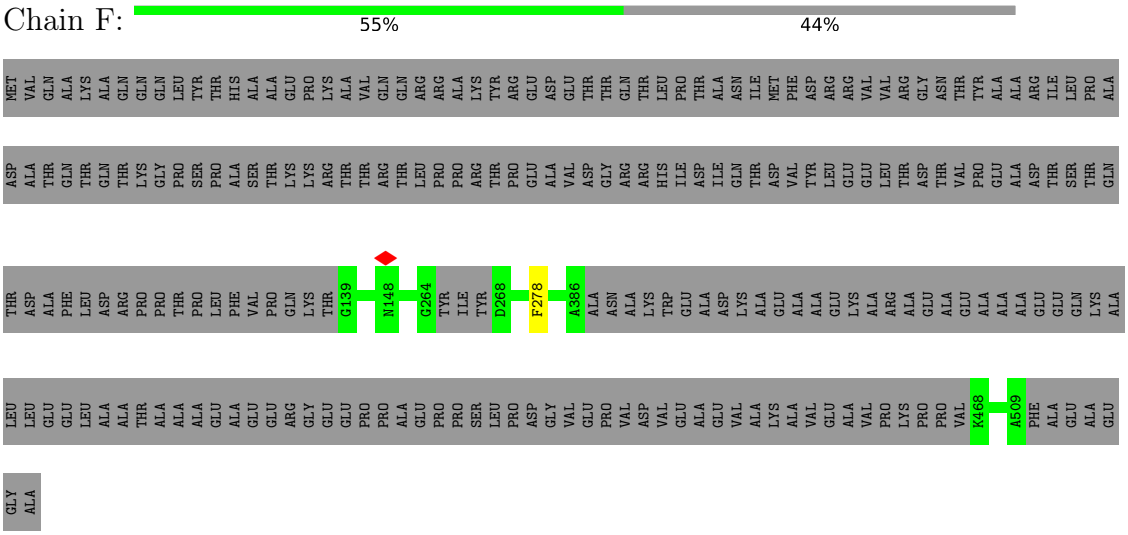
• Molecule 3: Flagellar radial spoke protein 3

Chain E:



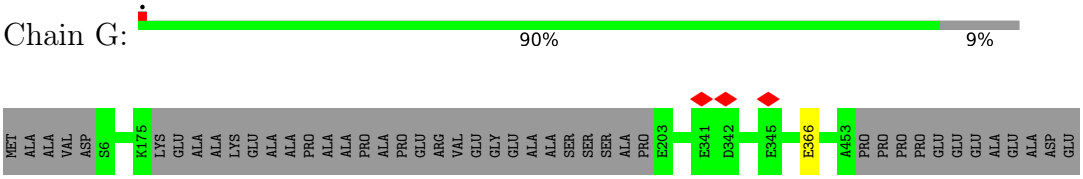
• Molecule 3: Flagellar radial spoke protein 3

Chain F:



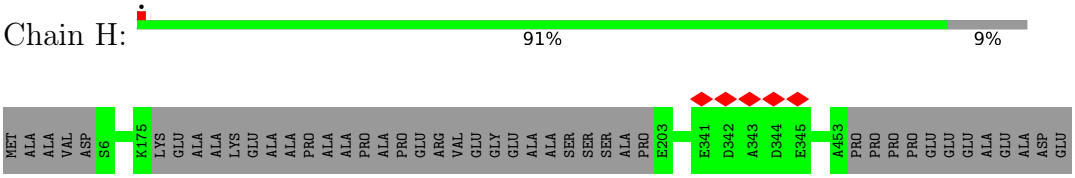
• Molecule 4: Flagellar radial spoke protein 4

Chain G:



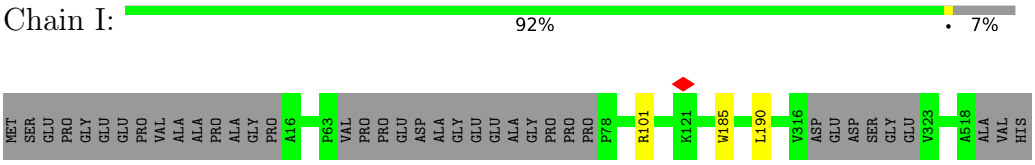
• Molecule 4: Flagellar radial spoke protein 4

Chain H:



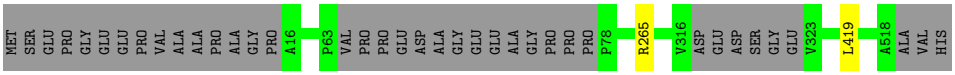
• Molecule 5: Flagellar radial spoke protein 5

Chain I:



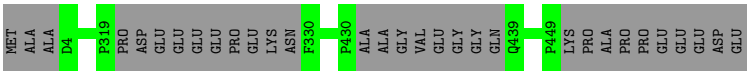
• Molecule 5: Flagellar radial spoke protein 5

Chain J:



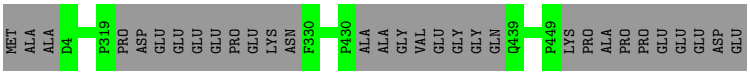
• Molecule 6: Flagellar radial spoke protein 6

Chain K:



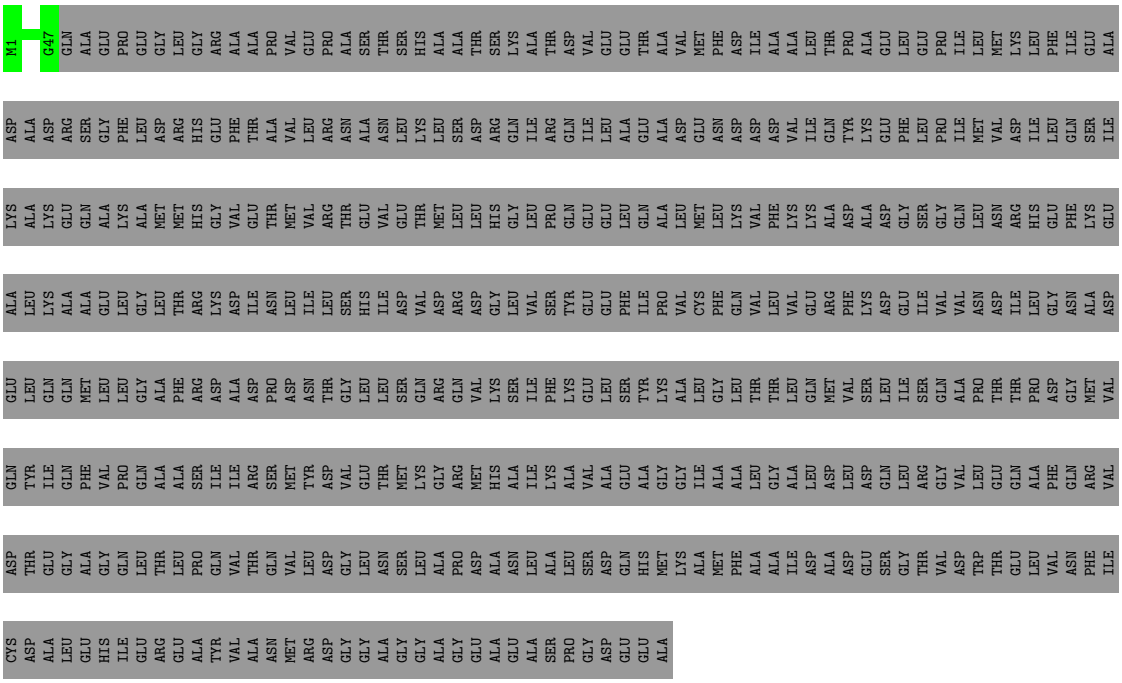
• Molecule 6: Flagellar radial spoke protein 6

Chain L: 93% 7%



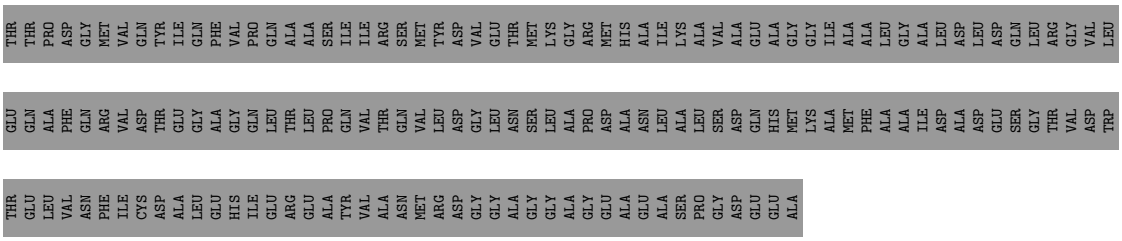
• Molecule 7: Flagellar radial spoke protein 7

Chain M: 9% 91%



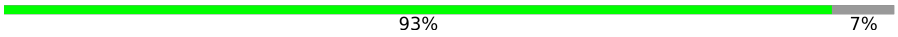
• Molecule 7: Flagellar radial spoke protein 7

Chain N: 8% 92%



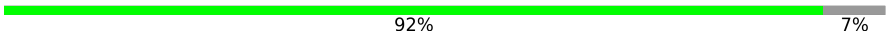
• Molecule 8: Flagellar radial spoke protein 9

Chain O:



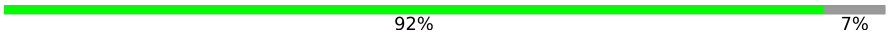
• Molecule 8: Flagellar radial spoke protein 9

Chain P:



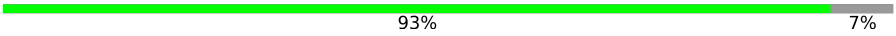
• Molecule 8: Flagellar radial spoke protein 9

Chain Q:



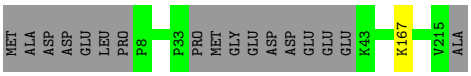
• Molecule 8: Flagellar radial spoke protein 9

Chain R:



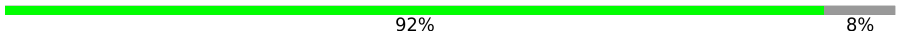
• Molecule 9: Flagellar radial spoke protein 10

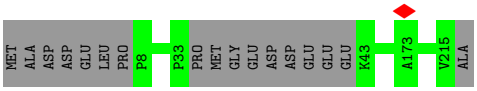
Chain S:



• Molecule 9: Flagellar radial spoke protein 10

Chain T:





- Molecule 10: Flagellar radial spoke protein 11

Chain U: 24% 76%

MET ASP VAL GLU P5 A52 SER GLY VAL SER ASN SER SER ALA PRO ALA LYS GLU GLN LEU ARG GLN VAL TYR THR ARG GLY GLY SER GLY GLY ALA THR LEU THR GLU SER GLN VAL THR GLY LEU CYS GLN GLN ALA GLY ILE ALA ASP ALA VAL VAL ALA LYS VAL MET GLU VAL

GLY ALA PHE THR PRO ALA ALA VAL ASP LEU SER LYS PHE VAL PHE LEU CYS LEU ALA MET SER CYS GLU ASP PHE ASN ARG VAL CYS MET GLY VAL PHE ASP VAL PHE SER ASP ASN GLY SER LEU PRO ALA GLN ASP LEU LEU THR LEU ILE ALA HIS LEU GLY PRO ASP MET ASP PRO

GLU VAL THR PRO ALA PHE LEU ASP ALA VAL ALA ALA GLU LEU PRO ALA GLY GLY GLY ALA VAL THR TYR MET GLU LEU CYS GLU ALA PRO SER LEU LYS PRO LYS LEU GLY LEU SER

- Molecule 10: Flagellar radial spoke protein 11

Chain V: 89% 11%

M1 G54 VAL SER ASN SER SER A60 G73 GLY SER GLY GLY ALA T79 Q90 GLN ALA GLY ILE A95 F108 THR PRO ALA ALA VAL D114 D143 D151 L172 A176 L179 L201 GLY LEU SER

- Molecule 11: Flagellar radial spoke protein 12

Chain W: 88% 10%

MET ASP PHE GLU SER ASN GLY ALA MET MET GLU TYR CYS LYS SER THR G17 S126 L131 D167 I176 Y177 N178 P179 ASN SER

- Molecule 12: Flagellar radial spoke protein 14

Chain X: 97%

MET D2 T32 G162 I205 F370 G380 ALA PRO PRO ILE ASN GLU GLU

- Molecule 13: Flagellar radial spoke protein 16

Chain Y: 62% 38%

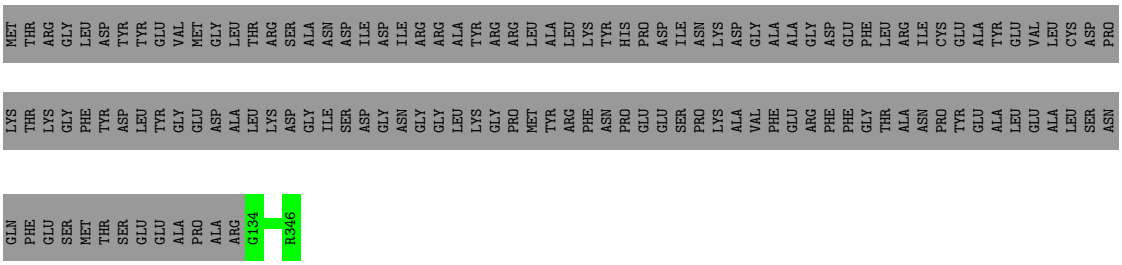
MET THR ARG GLY LEU ASP TYR TYR GLU VAL MET GLY LEU THR ARG SER ALA ASN ASP ILE ASP ILE ARG ARG ALA TYR ARG ARG LEU ALA LEU LYS TYR HIS PRO ASP ILE ASN LYS ASP GLY ALA ALA GLY ASP GLU PHE LEU ARG ILE CYS GLU ALA TYR GLU VAL LEU CYS ASP PRO

LYS THR LYS GLY PHE TYR ASP LEU TYR GLY GLU ASP ALA LEU LYS ASP GLY ILE SER ASP GLY ASN GLY GLY LEU LYS GLY PRO MET TYR ARG PHE ASN PRO GLU GLU SER PRO LYS ALA VAL PHE GLU ARG PHE PHE GLY THR ALA ASN PRO TYR GLU ALA LEU GLU ALA LEU SER ASN

GLN PHE GLU SER MET THR SER GLU GLU ALA PRO ALA ARG G134 R346

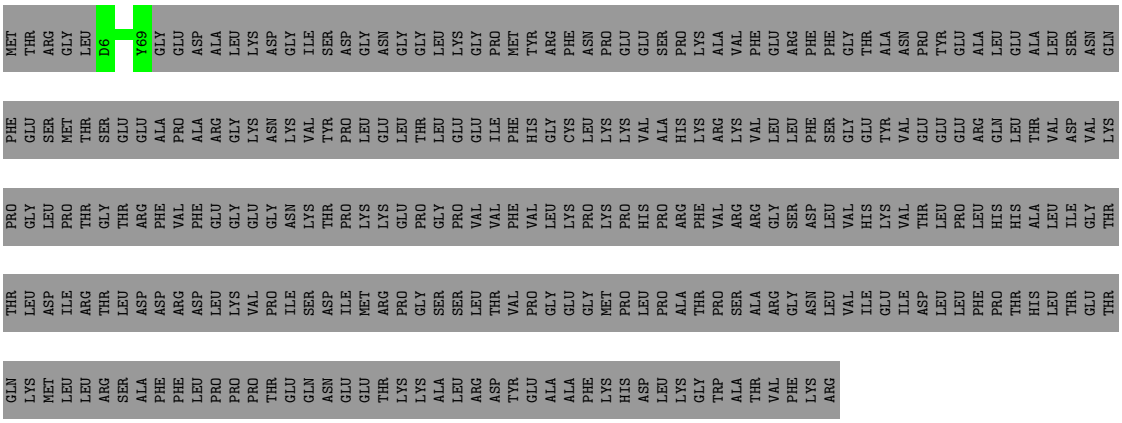
- Molecule 13: Flagellar radial spoke protein 16

Chain Z: 62% 38%



• Molecule 13: Flagellar radial spoke protein 16

Chain y: 18% 82%



• Molecule 13: Flagellar radial spoke protein 16

Chain z: 18% 82%

• Molecule 14: Dynein 8 kDa light chain, flagellar outer arm

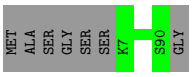
Chain a: 92% 8%

• Molecule 14: Dynein 8 kDa light chain, flagellar outer arm

Chain b: 92% 8%

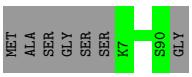
• Molecule 14: Dynein 8 kDa light chain, flagellar outer arm

Chain c: 92% 8%



• Molecule 14: Dynein 8 kDa light chain, flagellar outer arm

Chain d: 92% 8%



• Molecule 15: Unknown protein

Chain e: 100%

There are no outlier residues recorded for this chain.

• Molecule 16: Flagellar radial spoke protein 23

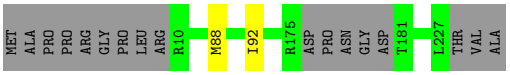
Chain i: 34% 66%

• Molecule 16: Flagellar radial spoke protein 23

Chain j: 34% 66%

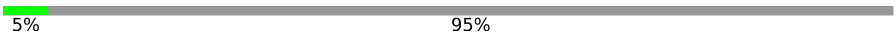
- Molecule 17: Cytochrome b5 heme-binding domain-containing protein

Chain k:



- Molecule 18: Uncharacterized protein

Chain s:



THR ILE ASP ARG LEU LYS ILE ASN ALA ASN GLN GLU ASN LYS GLU ALA ARG ILE GLN HIS THR LEU ASN GLU MET SER LYS PRO LYS LYS PHE ALA LEU ARG ASN GLY GLY LYS VAL ASP VAL HIS THR PRO PHE THR THR ARG ALA LYS GLU LEU GLN GLN LEU TYR ASN GLY LEU ASN

LEU PRO LEU LEU THR VAL ASP GLU ARG LEU ASP VAL LEU LEU HIS VAL LYS TRP THR VAL LYS GLU PHE ASP CYS ASP LEU THR ARG GLU LEU VAL ASP LEU ILE ASP ARG GLU ALA ASP LEU LEU ASN ARG GLY ARG ASN PRO LYS MET LEU GLU GLY LEU ARG LYS ARG ILE SER SER

LEU PHE LEU ASN PHE ILE GLU THR PRO GLU PHE ASN PRO GLU ALA VAL ARG PHE GLN ILE VAL PRO MET ASP PHE GLU ALA TYR LEU TYR GLU GLN VAL GLY LYS ALA THR ALA LYS ALA GLY THR SER VAL GLY THR ARG THR LEU SER

- Molecule 19: Predicted protein

Chain u:

MET SER SER GLN TYR SER GLU SER ARG PRO LEU HIS GLY SER ALA ALA Q17 T18 R66 SER GLY THR ALA

- Molecule 19: Predicted protein

Chain v:

MET SER SER GLN TYR SER GLU SER ARG PRO LEU HIS GLY SER ALA ALA Q17 Q38 R66 SER GLY THR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	610.4, 610.4, 610.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.35	0/5844	0.52	0/7949
1	B	0.33	0/5844	0.51	0/7949
2	C	0.36	0/3301	0.48	0/4467
2	D	0.29	0/3301	0.44	0/4467
3	E	0.28	0/2239	0.44	0/3018
3	F	0.36	0/2255	0.47	0/3039
4	G	0.30	0/3289	0.47	0/4493
4	H	0.33	0/3289	0.49	0/4493
5	I	0.29	0/3733	0.44	0/5092
5	J	0.31	0/3733	0.45	0/5092
6	K	0.29	0/3305	0.44	0/4527
6	L	0.29	0/3305	0.45	0/4527
7	M	0.27	0/383	0.42	0/517
7	N	0.27	0/325	0.41	0/439
8	O	0.31	0/1971	0.46	0/2681
8	P	0.30	0/1971	0.46	0/2681
8	Q	0.30	0/1971	0.45	0/2681
8	R	0.29	0/1971	0.47	0/2681
9	S	0.31	0/1585	0.47	0/2140
9	T	0.30	0/1585	0.49	0/2140
10	U	0.27	0/390	0.41	0/530
10	V	0.26	0/1059	0.43	0/1453
11	W	0.33	0/1273	0.51	0/1737
12	X	0.31	0/2830	0.49	0/3851
13	Y	0.26	0/1736	0.43	0/2352
13	Z	0.26	0/1736	0.43	0/2352
13	y	0.26	0/539	0.39	0/726
13	z	0.29	0/539	0.42	0/726
14	a	0.31	0/702	0.50	0/945
14	b	0.32	0/702	0.53	0/945
14	c	0.32	0/702	0.56	0/945
14	d	0.27	0/702	0.52	0/945

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	i	0.26	0/1594	0.43	0/2157
16	j	0.31	0/1594	0.46	0/2157
17	k	0.32	0/1813	0.49	0/2482
18	s	0.25	0/305	0.47	0/411
19	u	0.35	0/437	0.46	0/589
19	v	0.32	0/437	0.46	0/589
All	All	0.31	0/74290	0.47	0/100965

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	LEU	Mainchain

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	741/814 (91%)	710 (96%)	31 (4%)	0	100	100
1	B	741/814 (91%)	713 (96%)	28 (4%)	0	100	100
2	C	421/738 (57%)	417 (99%)	4 (1%)	0	100	100
2	D	421/738 (57%)	411 (98%)	10 (2%)	0	100	100
3	E	278/516 (54%)	276 (99%)	2 (1%)	0	100	100
3	F	281/516 (54%)	278 (99%)	3 (1%)	0	100	100
4	G	417/465 (90%)	396 (95%)	21 (5%)	0	100	100
4	H	417/465 (90%)	400 (96%)	17 (4%)	0	100	100
5	I	477/521 (92%)	466 (98%)	11 (2%)	0	100	100
5	J	477/521 (92%)	464 (97%)	13 (3%)	0	100	100
6	K	422/459 (92%)	413 (98%)	9 (2%)	0	100	100
6	L	422/459 (92%)	415 (98%)	7 (2%)	0	100	100
7	M	45/500 (9%)	42 (93%)	3 (7%)	0	100	100
7	N	38/500 (8%)	37 (97%)	1 (3%)	0	100	100
8	O	245/269 (91%)	237 (97%)	8 (3%)	0	100	100
8	P	245/269 (91%)	238 (97%)	7 (3%)	0	100	100
8	Q	245/269 (91%)	240 (98%)	5 (2%)	0	100	100
8	R	245/269 (91%)	239 (98%)	6 (2%)	0	100	100
9	S	195/216 (90%)	190 (97%)	5 (3%)	0	100	100
9	T	195/216 (90%)	187 (96%)	8 (4%)	0	100	100
10	U	46/204 (22%)	45 (98%)	1 (2%)	0	100	100
10	V	172/204 (84%)	167 (97%)	5 (3%)	0	100	100
11	W	161/181 (89%)	150 (93%)	11 (7%)	0	100	100
12	X	377/387 (97%)	359 (95%)	18 (5%)	0	100	100
13	Y	211/346 (61%)	206 (98%)	5 (2%)	0	100	100
13	Z	211/346 (61%)	206 (98%)	5 (2%)	0	100	100
13	y	62/346 (18%)	62 (100%)	0	0	100	100
13	z	62/346 (18%)	61 (98%)	1 (2%)	0	100	100
14	a	82/91 (90%)	80 (98%)	2 (2%)	0	100	100
14	b	82/91 (90%)	75 (92%)	7 (8%)	0	100	100
14	c	82/91 (90%)	74 (90%)	8 (10%)	0	100	100
14	d	82/91 (90%)	78 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	i	199/586 (34%)	190 (96%)	9 (4%)	0	100	100
16	j	199/586 (34%)	186 (94%)	13 (6%)	0	100	100
17	k	209/230 (91%)	202 (97%)	7 (3%)	0	100	100
18	s	35/682 (5%)	33 (94%)	2 (6%)	0	100	100
19	u	48/70 (69%)	46 (96%)	2 (4%)	0	100	100
19	v	48/70 (69%)	46 (96%)	2 (4%)	0	100	100
All	All	9336/14482 (64%)	9035 (97%)	301 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	586/640 (92%)	581 (99%)	5 (1%)	78	91
1	B	586/640 (92%)	583 (100%)	3 (0%)	88	95
2	C	320/517 (62%)	317 (99%)	3 (1%)	78	91
2	D	320/517 (62%)	320 (100%)	0	100	100
3	E	223/406 (55%)	222 (100%)	1 (0%)	91	95
3	F	225/406 (55%)	224 (100%)	1 (0%)	91	95
4	G	342/371 (92%)	341 (100%)	1 (0%)	92	96
4	H	342/371 (92%)	342 (100%)	0	100	100
5	I	376/403 (93%)	373 (99%)	3 (1%)	81	93
5	J	376/403 (93%)	374 (100%)	2 (0%)	88	95
6	K	334/357 (94%)	334 (100%)	0	100	100
6	L	334/357 (94%)	334 (100%)	0	100	100
7	M	39/406 (10%)	39 (100%)	0	100	100
7	N	32/406 (8%)	32 (100%)	0	100	100
8	O	203/221 (92%)	203 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	P	203/221 (92%)	202 (100%)	1 (0%)	88	95
8	Q	203/221 (92%)	202 (100%)	1 (0%)	88	95
8	R	203/221 (92%)	203 (100%)	0	100	100
9	S	150/164 (92%)	149 (99%)	1 (1%)	84	94
9	T	150/164 (92%)	150 (100%)	0	100	100
10	U	41/162 (25%)	41 (100%)	0	100	100
10	V	46/162 (28%)	46 (100%)	0	100	100
11	W	136/152 (90%)	132 (97%)	4 (3%)	42	74
12	X	281/288 (98%)	278 (99%)	3 (1%)	73	88
13	Y	189/297 (64%)	189 (100%)	0	100	100
13	Z	189/297 (64%)	189 (100%)	0	100	100
13	y	54/297 (18%)	54 (100%)	0	100	100
13	z	54/297 (18%)	54 (100%)	0	100	100
14	a	72/76 (95%)	72 (100%)	0	100	100
14	b	72/76 (95%)	72 (100%)	0	100	100
14	c	72/76 (95%)	72 (100%)	0	100	100
14	d	72/76 (95%)	72 (100%)	0	100	100
16	i	158/433 (36%)	157 (99%)	1 (1%)	86	94
16	j	158/433 (36%)	157 (99%)	1 (1%)	86	94
17	k	191/204 (94%)	189 (99%)	2 (1%)	76	90
18	s	33/553 (6%)	33 (100%)	0	100	100
19	u	47/62 (76%)	45 (96%)	2 (4%)	29	64
19	v	47/62 (76%)	46 (98%)	1 (2%)	53	79
All	All	7459/11415 (65%)	7423 (100%)	36 (0%)	89	95

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	LEU
1	A	297	ARG
1	A	459	ASP
1	A	470	VAL
1	A	477	ILE
1	B	118	LEU

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Mol	Chain	Res	Type
1	B	199	LEU
1	B	297	ARG
2	C	247	LEU
2	C	533	ASP
2	C	535	THR
3	E	187	ARG
3	F	278	PHE
4	G	366	GLU
5	I	101	ARG
5	I	185	TRP
5	I	190	LEU
5	J	265	ARG
5	J	419	LEU
8	P	202	PHE
8	Q	112	LEU
9	S	167	LYS
11	W	126	SER
11	W	131	LEU
11	W	176	ILE
11	W	178	ASN
12	X	32	THR
12	X	205	ILE
12	X	370	PHE
16	i	56	LYS
16	j	161	ILE
17	k	88	MET
17	k	92	ILE
19	u	17	GLN
19	u	18	THR
19	v	38	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	290	ASN
1	A	479	GLN
1	A	487	GLN
1	B	290	ASN
2	C	302	GLN
2	D	32	GLN
3	E	285	GLN

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Mol	Chain	Res	Type
4	G	329	GLN
5	I	288	GLN
5	I	358	GLN
5	J	183	GLN
5	J	423	ASN
6	K	309	GLN
8	R	183	ASN
9	S	54	HIS
11	W	113	GLN
11	W	178	ASN
12	X	233	HIS
12	X	367	GLN
13	Y	236	HIS
13	Z	216	HIS
14	b	57	HIS
14	d	57	HIS
17	k	45	GLN
19	v	31	ASN
19	v	34	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	PO4	G	501	-	4,4,4	0.96	0	6,6,6	0.44	0
20	PO4	H	501	-	4,4,4	0.95	0	6,6,6	0.41	0
20	PO4	K	501	-	4,4,4	0.96	0	6,6,6	0.43	0
20	PO4	L	501	-	4,4,4	0.96	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

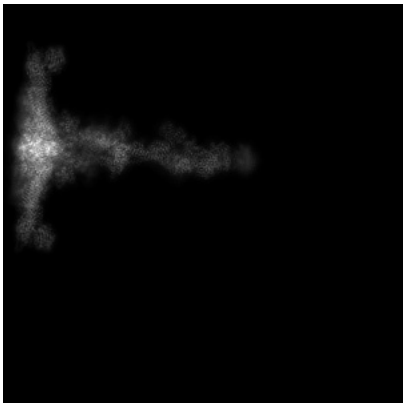
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22475. These allow visual inspection of the internal detail of the map and identification of artifacts.

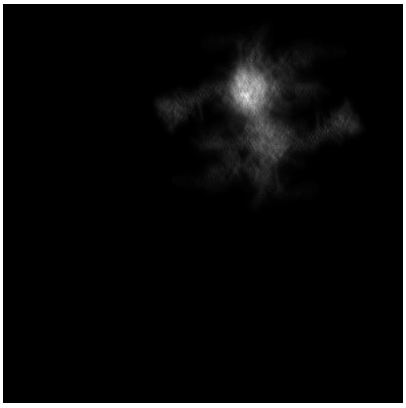
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

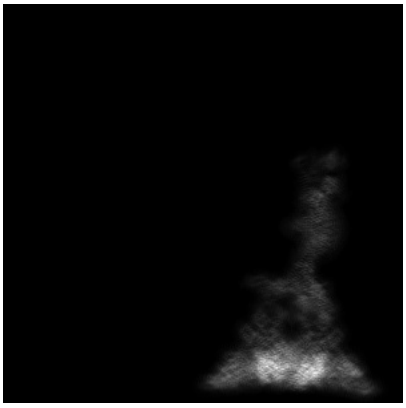
6.1.1 Primary map



X



Y

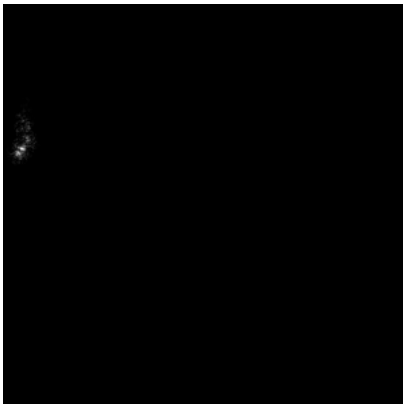


Z

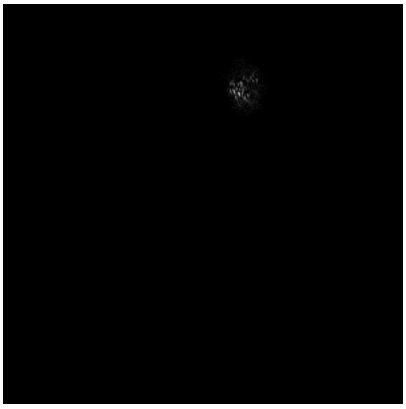
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 280



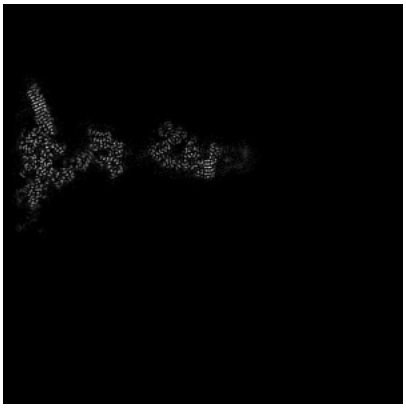
Y Index: 280

Z Index: 280

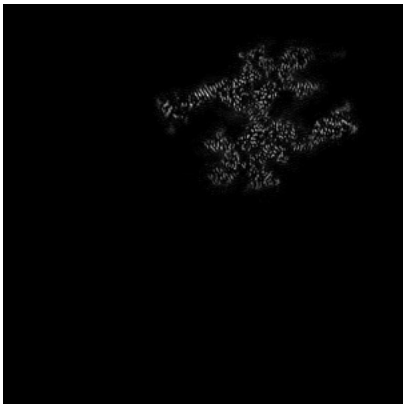
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 443



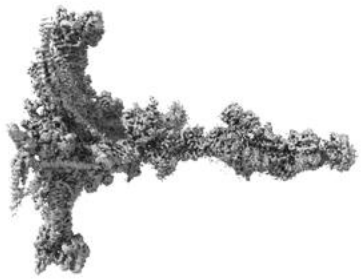
Y Index: 48

Z Index: 355

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

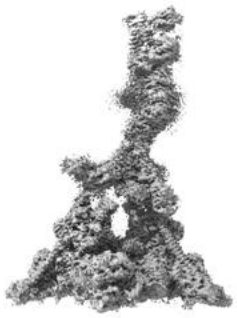
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

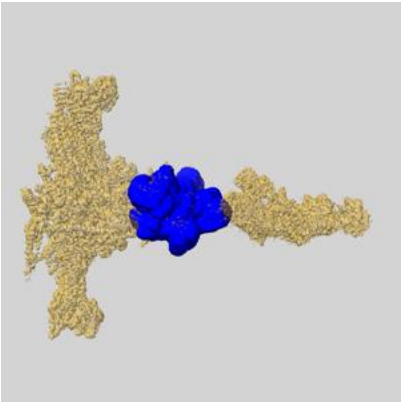
6.5 Mask visualisation (i)

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

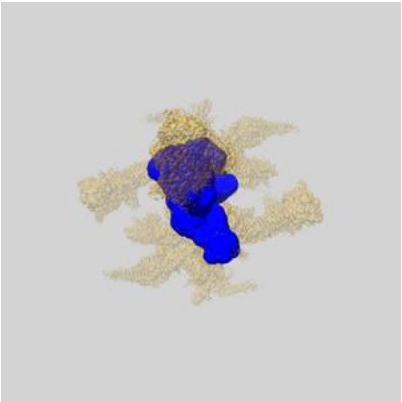
A mask typically either:

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

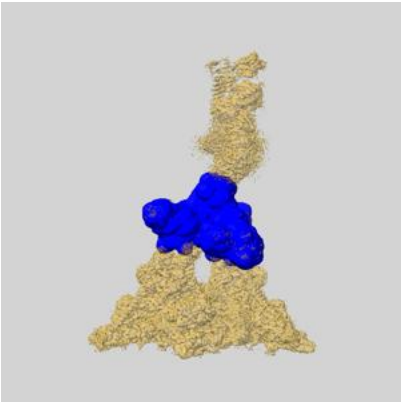
6.5.1 emd_22475_msk_3.map (i)



X

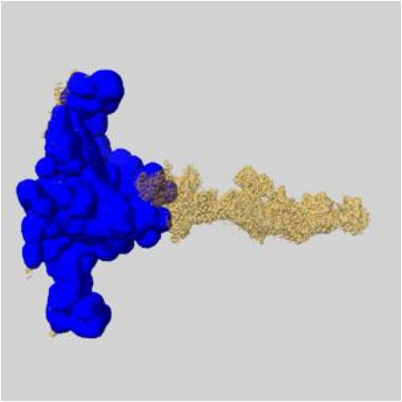


Y

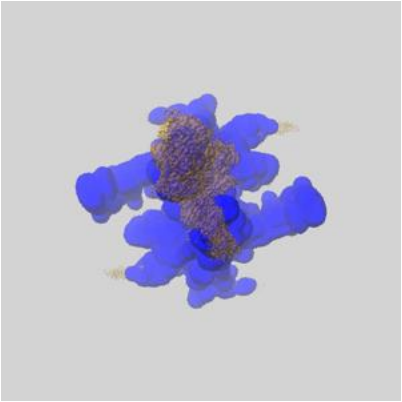


Z

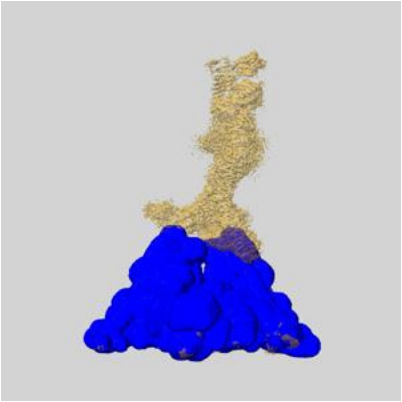
6.5.2 emd_22475_msk_2.map (i)



X

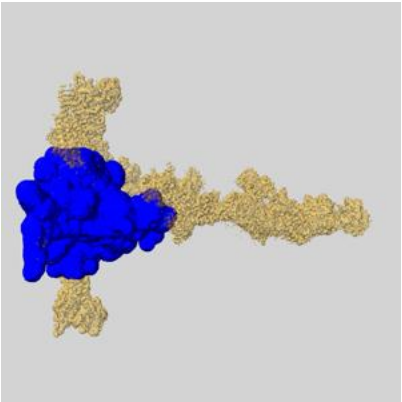


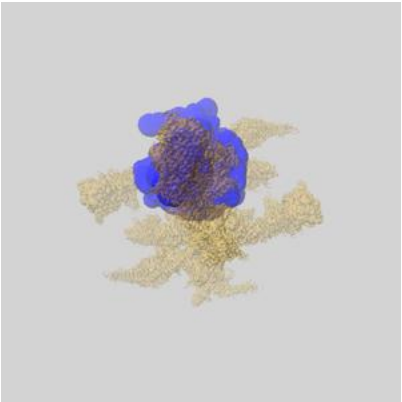
Y

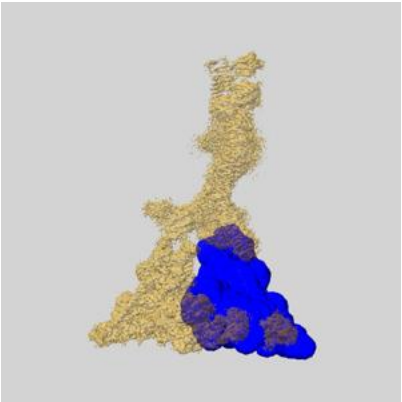


Z

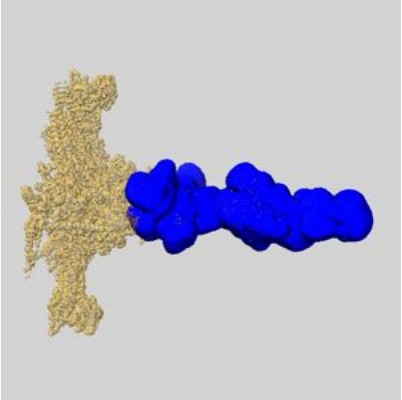
6.5.3 emd_22475_msk_5.map ⓘ

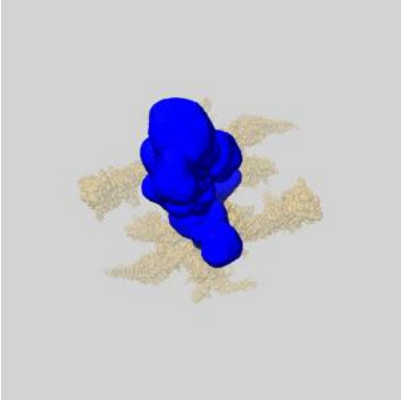

X

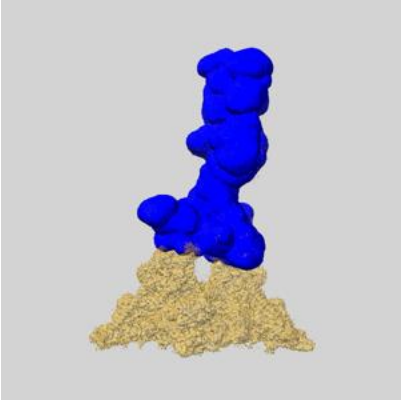

Y


Z

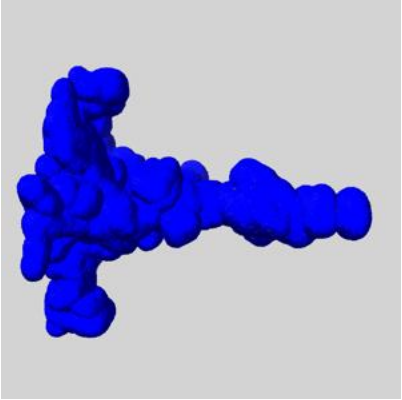
6.5.4 emd_22475_msk_4.map ⓘ

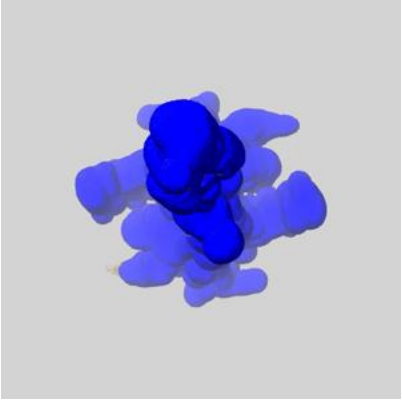

X

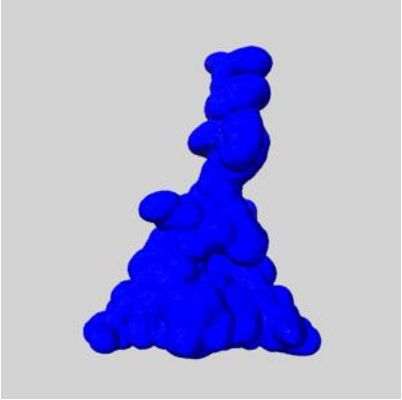

Y


Z

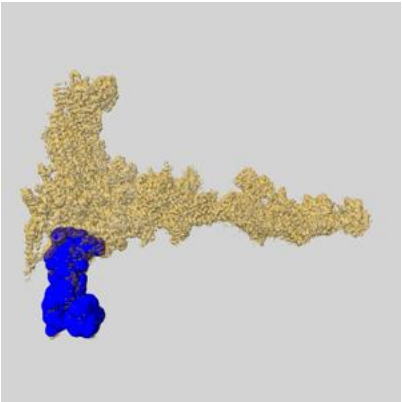
6.5.5 emd_22475_msk_1.map ⓘ

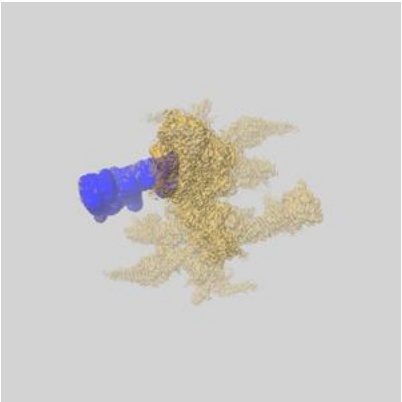

X


Y


Z

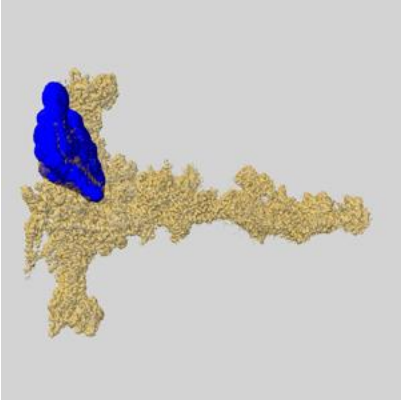
6.5.6 emd_22475_msk_7.map (i)

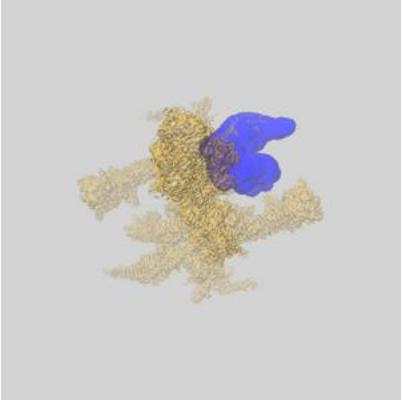

X

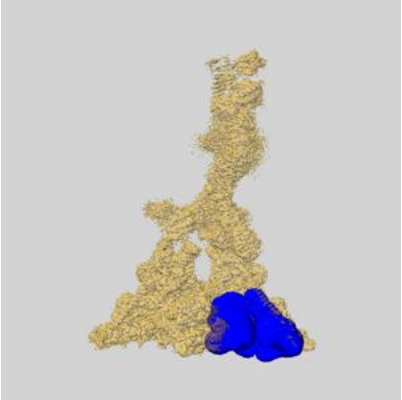

Y

Z

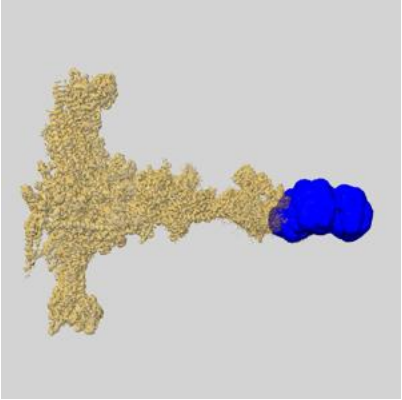
6.5.7 emd_22475_msk_6.map (i)

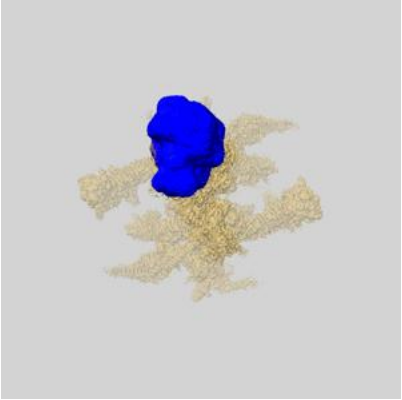

X

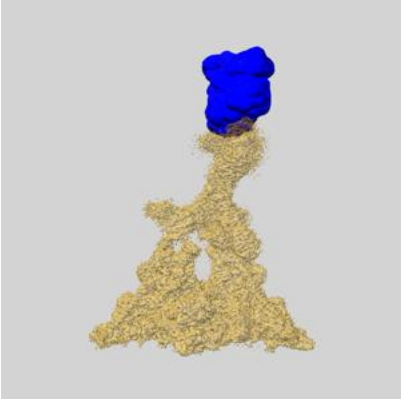

Y


Z

6.5.8 emd_22475_msk_8.map (i)


X

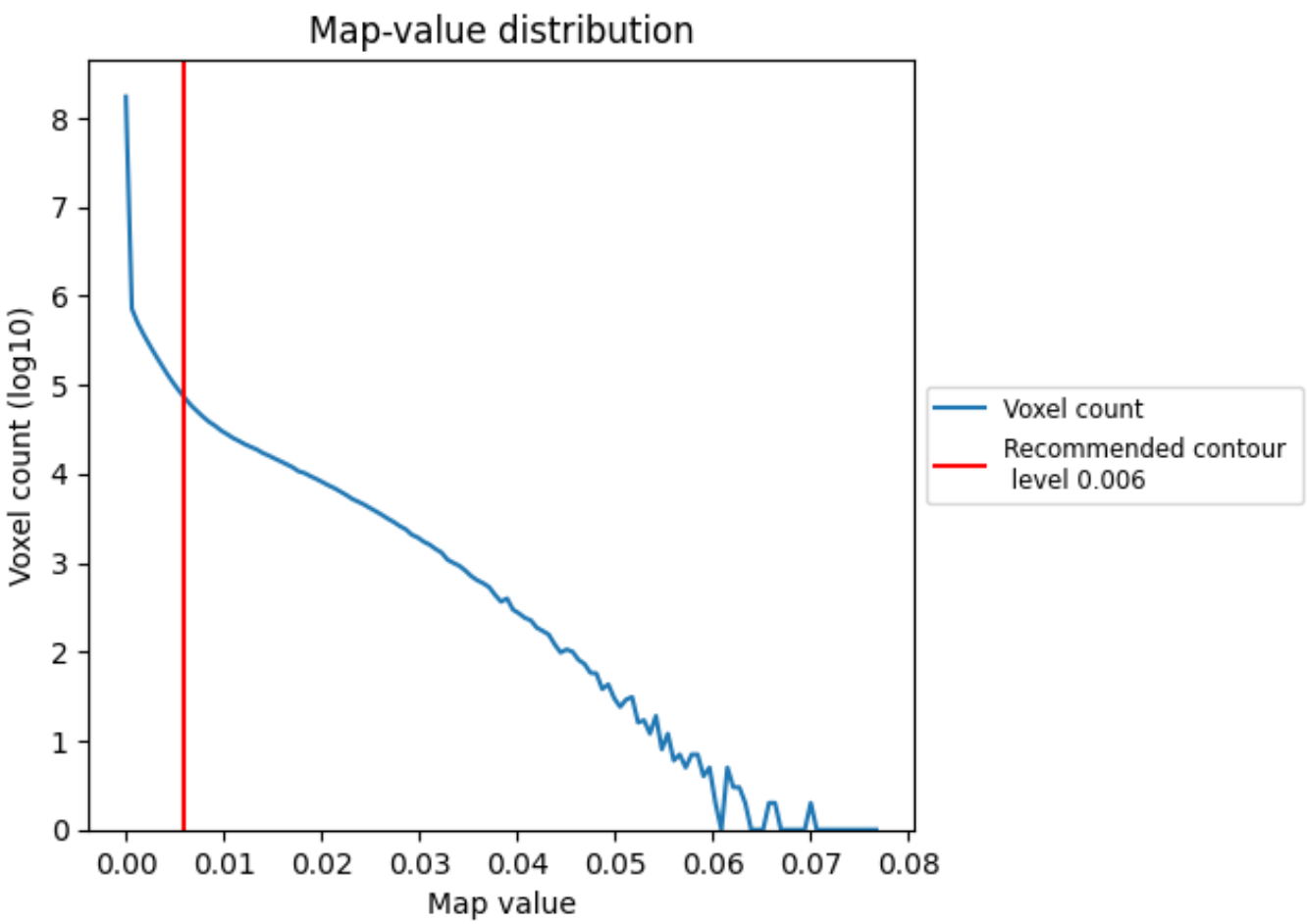

Y


Z

7 Map analysis (i)

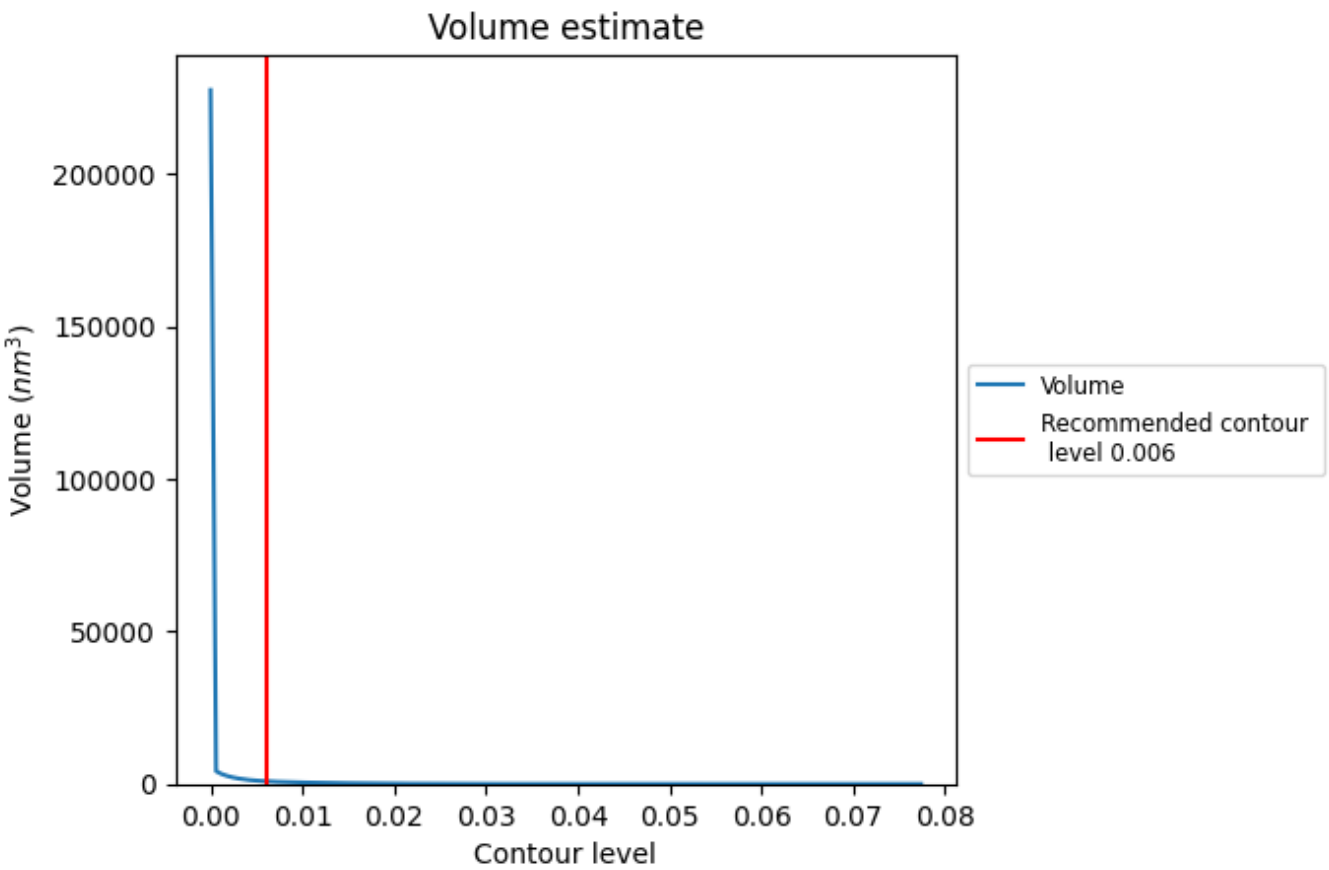
This section contains the results of statistical analysis of the map.

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.

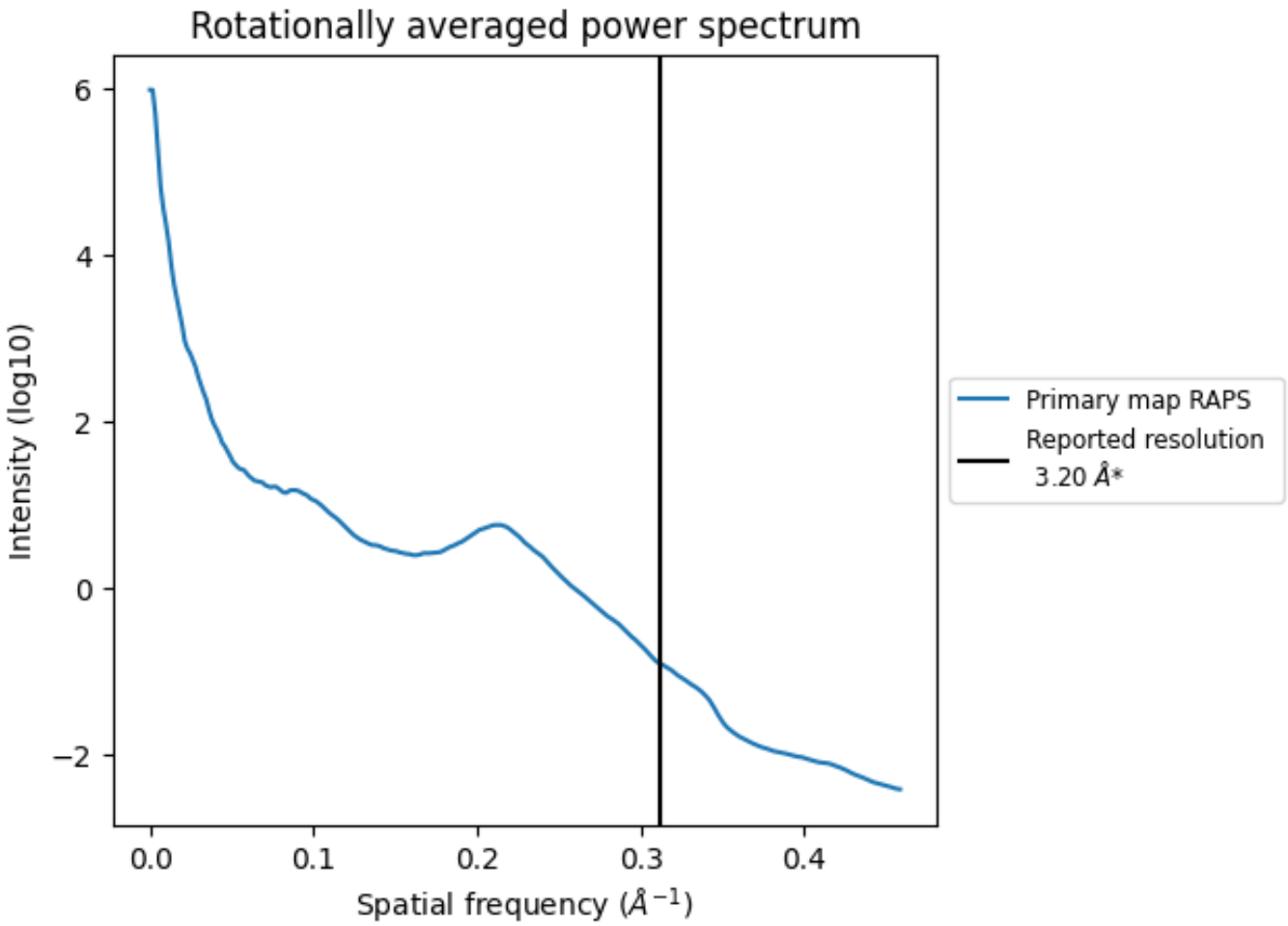
7.2 Volume estimate (i)



The volume at the recommended contour level is 893 nm^3; this corresponds to an approximate mass of 806 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

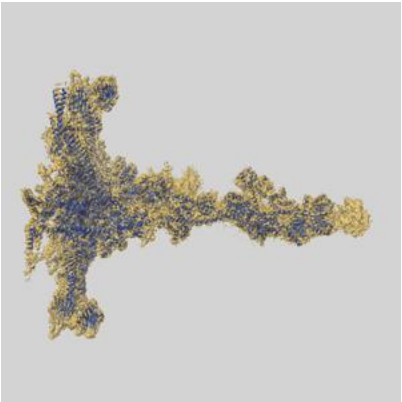
8 Fourier-Shell correlation (i)

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

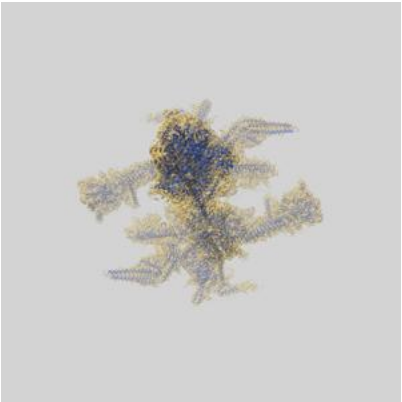
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22475 and PDB model 7JTK. Per-residue inclusion information can be found in section 3 on page 10.

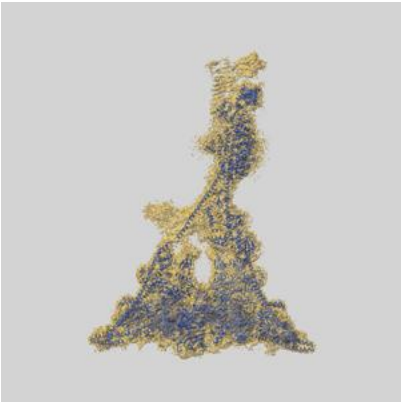
9.1 Map-model overlay (i)



X



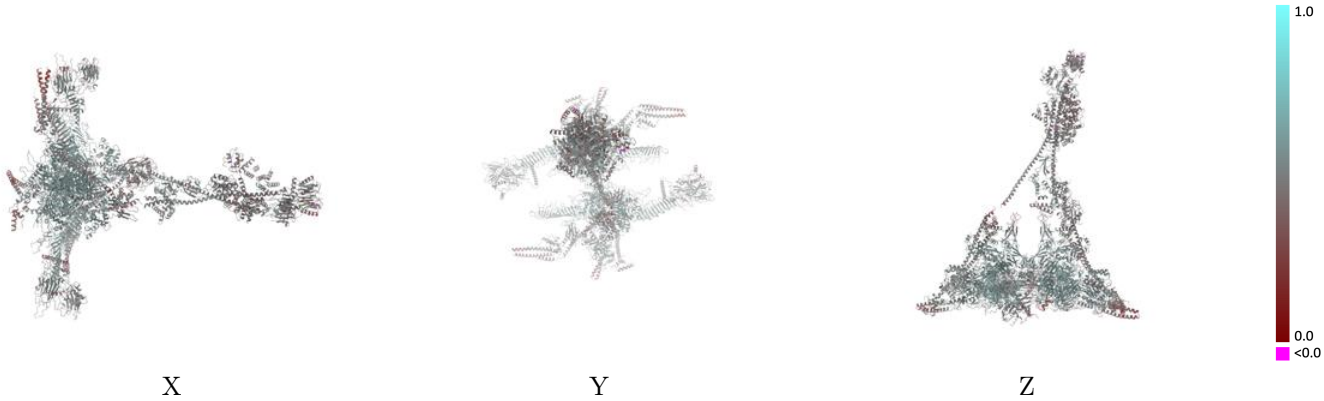
Y



Z

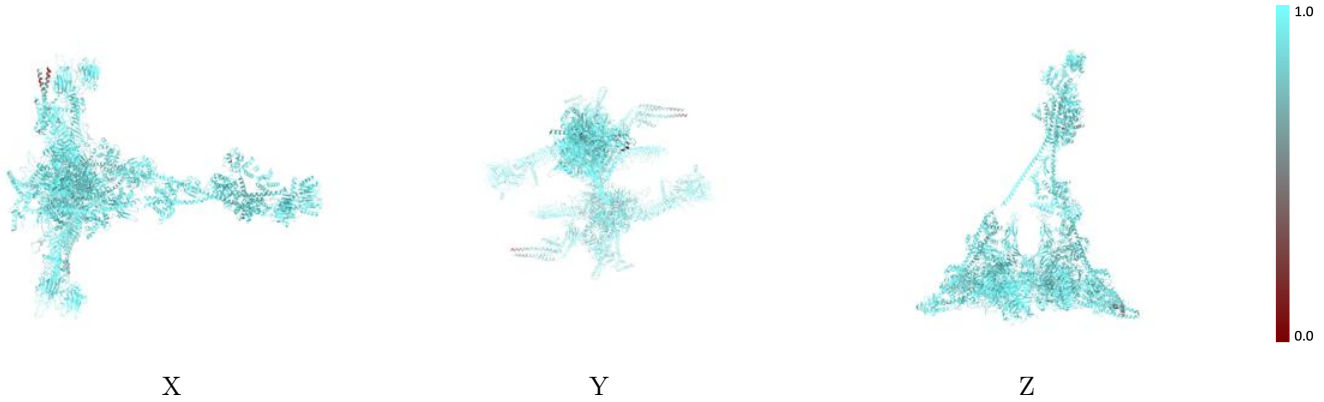
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



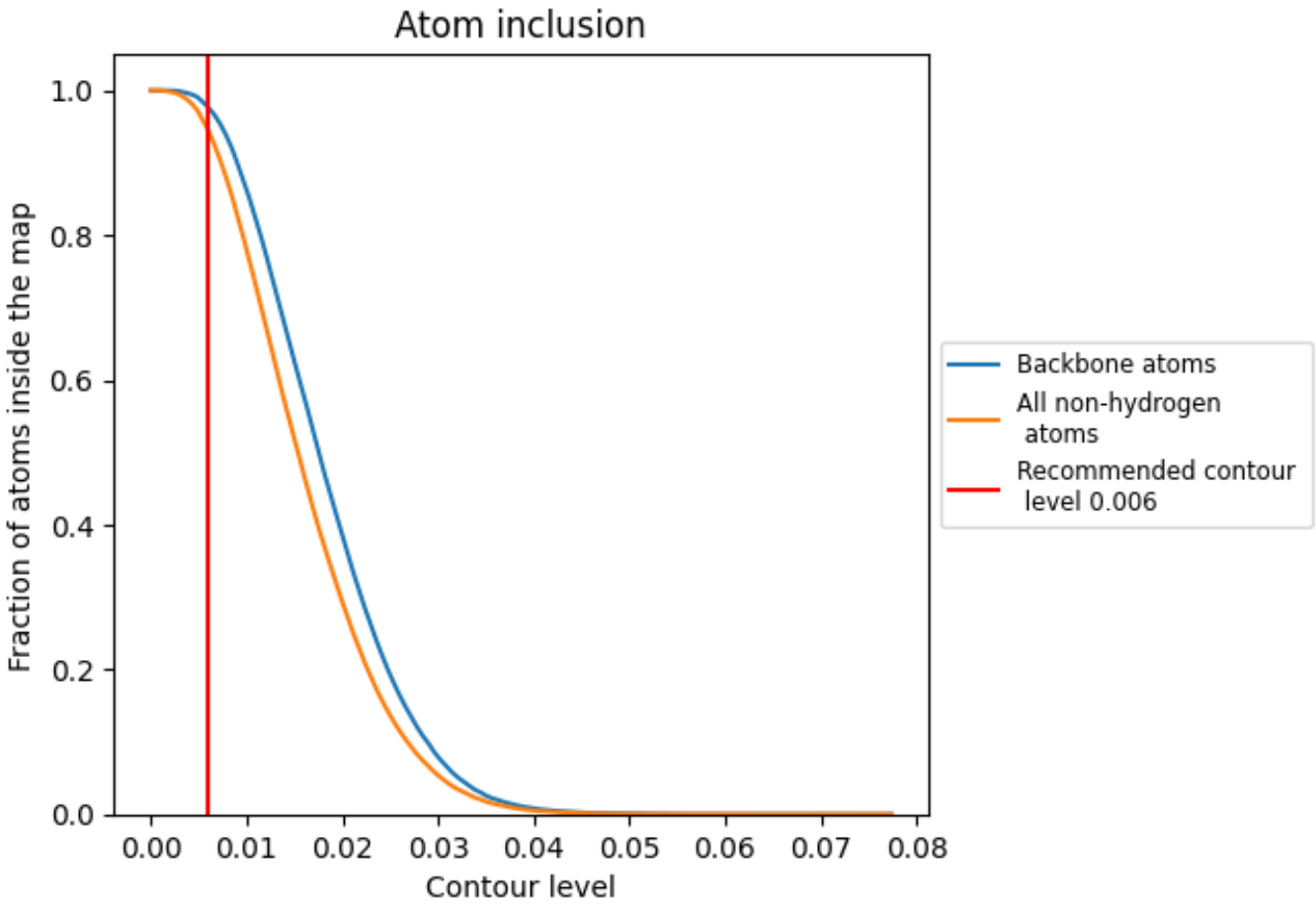
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9451	0.5010
A	0.9441	0.4840
B	0.9459	0.4830
C	0.8796	0.4600
D	0.8818	0.4630
E	0.9278	0.4510
F	0.9141	0.4550
G	0.9469	0.5350
H	0.9513	0.5350
I	0.9572	0.5080
J	0.9603	0.5090
K	0.9598	0.5420
L	0.9604	0.5440
M	0.9231	0.4580
N	0.9416	0.5000
O	0.9793	0.5580
P	0.9788	0.5580
Q	0.9815	0.5600
R	0.9820	0.5540
S	0.9773	0.5350
T	0.9740	0.5280
U	0.9388	0.4470
V	0.8761	0.4490
W	0.9273	0.4640
X	0.9178	0.4620
Y	0.9699	0.5220
Z	0.9735	0.5230
a	0.9704	0.4600
b	0.9364	0.4650
c	0.9275	0.4480
d	0.8905	0.4240
e	0.9000	0.4650
i	0.9426	0.5030
j	0.9583	0.5100
k	0.9697	0.5060

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
s	0.9078	0.4380
u	0.9472	0.4800
v	0.9400	0.4560
y	0.9686	0.4370
z	0.9764	0.5030