



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 04:30 pm GMT

PDB ID : 4UI9
EMDB ID : EMD-2924
Title : Atomic structure of the human Anaphase-Promoting Complex
Authors : Chang, L.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D.
Deposited on : 2015-03-27
Resolution : 3.60 Å(reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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) : 2.31.3

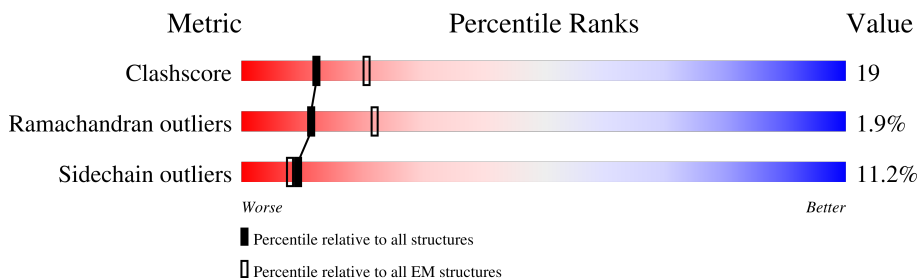
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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






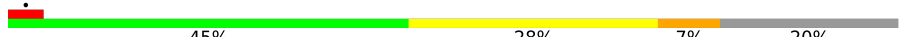


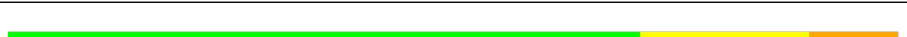

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1944	
2	B	84	
3	C	591	
3	P	591	
4	D	121	
5	E	110	
6	F	824	
6	H	824	

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Mol	Chain	Length	Quality of chain
7	G	85	
8	I	808	
9	J	620	
10	K	620	
11	L	183	
12	M	74	
13	N	822	
14	O	756	
15	R	493	
16	S	447	
17	T	21	
18	U	24	
19	W	85	
20	X	565	
20	Y	565	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 66453 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1441	10947	7043	1853	1977	74	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PHE	THR	conflict	UNP Q9H1A4
A	940	ILE	THR	conflict	UNP Q9H1A4
A	1059	GLU	ASP	conflict	UNP Q9H1A4
A	1358	LEU	ILE	conflict	UNP Q9H1A4
A	1637	LEU	THR	conflict	UNP Q9H1A4
A	1880	PRO	LEU	conflict	UNP Q9H1A4
A	1881	LEU	GLU	conflict	UNP Q9H1A4

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	84	650	418	117	98	17	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LEU	THR	conflict	UNP Q9NYG5

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	524	4305	2774	726	781	24	0	0
3	P	491	4042	2611	678	729	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	161	LEU	LYS	conflict	UNP Q9UJX2
P	161	LEU	LYS	conflict	UNP Q9UJX2

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	55	Total	C	N	O	0	0
			437	277	73	87		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	TYR	PHE	conflict	UNP P60006

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			450	290	74	85	1		

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	498	Total	C	N	O	S	0	0
			3923	2514	664	719	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	403	GLU	LYS	conflict	UNP P30260
F	475	SER	ALA	conflict	UNP P30260
F	484	SER	ALA	conflict	UNP P30260
H	403	GLU	LYS	conflict	UNP P30260
H	475	SER	ALA	conflict	UNP P30260
H	484	SER	ALA	conflict	UNP P30260

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			214	134	40	39	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	14	GLU	ASP	conflict	UNP Q8NHZ8

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	730	Total	C	N	O	S	0	0
			5709	3660	950	1066	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	430	ASP	GLU	conflict	UNP Q9UJX5

- Molecule 9 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2602	685	735	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	225	ASN	ASP	conflict	UNP Q13042
J	228	GLU	GLN	conflict	UNP Q13042
J	229	LYS	GLU	conflict	UNP Q13042

- Molecule 10 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	493	Total	C	N	O	S	0	0
			3988	2565	673	726	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	228	GLU	GLN	conflict	UNP Q13042

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Chain	Residue	Modelled	Actual	Comment	Reference
K	229	LYS	GLU	conflict	UNP Q13042
K	265	LYS	ALA	conflict	UNP Q13042

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	182	1435	898	263	268	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	GLU	deletion	UNP Q9UM13

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	59	493	310	79	102	2	0	0

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	631	4831	3064	877	868	22	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	410	ILE	LEU	conflict	UNP Q9UJX6

- Molecule 14 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	685	5396	3439	939	991	27	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	42	SER	ASN	conflict	UNP Q9UJX4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	55	VAL	MET	conflict	UNP Q9UJX4
O	63	GLN	LEU	conflict	UNP Q9UJX4
O	75	VAL	LEU	conflict	UNP Q9UJX4
O	79	LEU	TYR	conflict	UNP Q9UJX4
O	164	SER	ASN	conflict	UNP Q9UJX4
O	165	ASP	GLY	conflict	UNP Q9UJX4
O	167	ASN	-	insertion	UNP Q9UJX4

- Molecule 15 is a protein called FIZZY-RELATED PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	387	3003	1895	541	557	10	0	0

- Molecule 16 is a protein called F-BOX ONLY PROTEIN 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	94	648	396	119	124	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	323	ILE	THR	conflict	UNP Q9UKT4
S	326	LYS	ALA	conflict	UNP Q9UKT4

- Molecule 17 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	T	21	109	65	22	22	0	0

- Molecule 18 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	U	24	120	72	24	24	0	0

- Molecule 19 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	W	25	213	133	40	39	1	0	0

- Molecule 20 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	X	484	3770	2394	650	705	21	0	0
20	Y	496	3865	2450	667	725	23	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	63	LEU	MET	conflict	UNP Q9UJX3
X	142	LEU	MET	conflict	UNP Q9UJX3
X	148	VAL	MET	conflict	UNP Q9UJX3
X	466	ASN	ASP	conflict	UNP Q9UJX3
X	472	GLU	ARG	conflict	UNP Q9UJX3
Y	63	LEU	MET	conflict	UNP Q9UJX3
Y	142	LEU	MET	conflict	UNP Q9UJX3
Y	148	VAL	MET	conflict	UNP Q9UJX3
Y	466	ASN	ASP	conflict	UNP Q9UJX3
Y	472	GLU	ARG	conflict	UNP Q9UJX3

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	B	3	Total	Zn	0
			3	3	
21	S	2	Total	Zn	0
			2	2	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202084	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.400	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	359.04, 359.04, 359.04	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	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:
ZN

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	0.75	0/11190	0.99	21/15238 (0.1%)
2	B	0.52	0/675	0.86	1/914 (0.1%)
3	C	0.75	1/4403 (0.0%)	0.95	9/5945 (0.2%)
3	P	0.70	1/4137 (0.0%)	0.92	3/5587 (0.1%)
4	D	0.71	0/447	0.98	1/612 (0.2%)
5	E	0.65	0/459	0.86	0/619
6	F	0.70	3/4013 (0.1%)	0.90	7/5428 (0.1%)
6	H	0.70	2/3943 (0.1%)	0.90	4/5329 (0.1%)
7	G	0.62	0/215	1.03	1/285 (0.4%)
8	I	0.58	0/5827	0.85	3/7899 (0.0%)
9	J	0.75	3/4146 (0.1%)	0.97	9/5615 (0.2%)
10	K	0.89	3/4086 (0.1%)	0.96	5/5532 (0.1%)
11	L	0.71	0/1468	0.96	5/1993 (0.3%)
12	M	0.73	0/502	1.05	1/680 (0.1%)
13	N	0.63	1/4913 (0.0%)	1.01	18/6650 (0.3%)
14	O	0.73	5/5494 (0.1%)	0.96	5/7425 (0.1%)
15	R	2.23	11/3068 (0.4%)	2.62	75/4162 (1.8%)
16	S	0.54	0/654	0.81	3/880 (0.3%)
17	T	1.02	0/108	1.11	0/149
18	U	0.91	0/119	1.10	3/165 (1.8%)
19	W	0.64	0/214	1.02	0/284
20	X	0.60	4/3830 (0.1%)	0.84	6/5187 (0.1%)
20	Y	0.54	0/3925	0.85	4/5311 (0.1%)
All	All	0.83	34/67836 (0.1%)	1.07	184/91889 (0.2%)

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	9
8	I	0	2
9	J	0	1
13	N	0	26
15	R	0	5
17	T	0	1
20	X	0	1
All	All	0	45

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	431	PRO	N-CD	53.78	2.23	1.47
15	R	392	PRO	N-CD	50.89	2.19	1.47
15	R	302	PRO	N-CD	48.99	2.16	1.47
15	R	301	PRO	N-CD	47.51	2.14	1.47
10	K	229	LYS	CB-CG	33.09	2.42	1.52

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	431	PRO	O-C-N	-52.04	39.44	122.70
15	R	310	GLN	O-C-N	-29.51	73.03	123.20
15	R	240	ARG	NE-CZ-NH2	-25.22	107.69	120.30
15	R	307	ARG	NE-CZ-NH2	-25.20	107.70	120.30
15	R	313	ARG	NE-CZ-NH2	-25.18	107.71	120.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	MET	Peptide
1	A	124	GLN	Peptide
1	A	14	ALA	Peptide
1	A	83	ILE	Peptide
1	A	86	ASP	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10947	0	10690	367	0
2	B	650	0	600	33	0
3	C	4305	0	4273	121	0
3	P	4042	0	3998	137	0
4	D	437	0	396	14	0
5	E	450	0	435	12	0
6	F	3923	0	3813	95	0
6	H	3853	0	3788	95	0
7	G	214	0	222	2	0
8	I	5709	0	5597	124	0
9	J	4047	0	3956	138	0
10	K	3988	0	3917	126	0
11	L	1435	0	1382	69	0
12	M	493	0	469	28	0
13	N	4831	0	4527	292	0
14	O	5396	0	5425	160	0
15	R	3003	0	2951	432	0
16	S	648	0	543	31	0
17	T	109	0	107	9	0
18	U	120	0	80	1	0
19	W	213	0	220	8	0
20	X	3770	0	3829	254	0
20	Y	3865	0	3925	168	0
21	B	3	0	0	0	0
21	S	2	0	0	0	0
All	All	66453	0	65143	2494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 2494 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:404:ASN:CB	15:R:449:LEU:HD21	1.22	1.60
15:R:404:ASN:HB2	15:R:449:LEU:CD2	1.35	1.53
15:R:292:MET:CE	15:R:309:LEU:HD21	1.42	1.47
20:X:358:ALA:HB3	20:X:382:ALA:CB	1.43	1.46
20:X:355:TYR:CD2	20:X:386:MET:N	1.83	1.46

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1399/1944 (72%)	1260 (90%)	107 (8%)	32 (2%)	6	38
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	22
3	C	520/591 (88%)	495 (95%)	23 (4%)	2 (0%)	34	71
3	P	485/591 (82%)	460 (95%)	24 (5%)	1 (0%)	47	79
4	D	53/121 (44%)	46 (87%)	6 (11%)	1 (2%)	8	42
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	494/824 (60%)	477 (97%)	11 (2%)	6 (1%)	13	51
6	H	479/824 (58%)	462 (96%)	12 (2%)	5 (1%)	15	55
7	G	23/85 (27%)	23 (100%)	0	0	100	100
8	I	722/808 (89%)	690 (96%)	28 (4%)	4 (1%)	25	64
9	J	500/620 (81%)	467 (93%)	28 (6%)	5 (1%)	15	55
10	K	489/620 (79%)	458 (94%)	26 (5%)	5 (1%)	15	55
11	L	180/183 (98%)	170 (94%)	8 (4%)	2 (1%)	14	53
12	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
13	N	609/822 (74%)	501 (82%)	50 (8%)	58 (10%)	0	8
14	O	677/756 (90%)	644 (95%)	25 (4%)	8 (1%)	13	51
15	R	375/493 (76%)	343 (92%)	25 (7%)	7 (2%)	8	42
16	S	88/447 (20%)	68 (77%)	15 (17%)	5 (6%)	1	18
17	T	19/21 (90%)	14 (74%)	3 (16%)	2 (10%)	0	7
18	U	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	23
19	W	23/85 (27%)	23 (100%)	0	0	100	100
20	X	480/565 (85%)	462 (96%)	15 (3%)	3 (1%)	25	64
20	Y	492/565 (87%)	471 (96%)	16 (3%)	5 (1%)	15	55
All	All	8321/11257 (74%)	7725 (93%)	440 (5%)	156 (2%)	11	42

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	860	TYR
1	A	1125	ILE

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	1150/1720 (67%)	988 (86%)	162 (14%)	3	21
2	B	65/75 (87%)	55 (85%)	10 (15%)	2	18
3	C	452/516 (88%)	399 (88%)	53 (12%)	5	29
3	P	422/516 (82%)	373 (88%)	49 (12%)	5	29
4	D	46/115 (40%)	42 (91%)	4 (9%)	10	41
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	7
6	F	407/729 (56%)	367 (90%)	40 (10%)	8	36
6	H	408/729 (56%)	372 (91%)	36 (9%)	10	40
7	G	23/77 (30%)	21 (91%)	2 (9%)	10	41
8	I	620/730 (85%)	572 (92%)	48 (8%)	13	45
9	J	424/548 (77%)	368 (87%)	56 (13%)	4	23
10	K	423/549 (77%)	381 (90%)	42 (10%)	8	35
11	L	155/168 (92%)	140 (90%)	15 (10%)	8	36
12	M	55/67 (82%)	44 (80%)	11 (20%)	1	8
13	N	459/724 (63%)	403 (88%)	56 (12%)	5	26
14	O	578/652 (89%)	491 (85%)	87 (15%)	3	19
15	R	324/428 (76%)	306 (94%)	18 (6%)	21	56
16	S	56/404 (14%)	43 (77%)	13 (23%)	1	5
17	T	1/2 (50%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	W	23/77 (30%)	22 (96%)	1 (4%)	29	63
20	X	407/484 (84%)	378 (93%)	29 (7%)	14	48
20	Y	418/484 (86%)	382 (91%)	36 (9%)	10	41
All	All	6963/9883 (70%)	6185 (89%)	778 (11%)	9	30

5 of 778 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	12	ASP
14	O	328	ILE
11	L	177	PHE
10	K	522	CYS
13	N	410	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	71	GLN
3	P	299	ASN
20	X	106	GLN
6	H	595	GLN
6	H	545	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	2
16	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	419:CYS	C	420:SER	N	27.15
1	N	92:TRP	C	93:ASN	N	3.02
1	N	563:ASP	C	564:MET	N	2.52

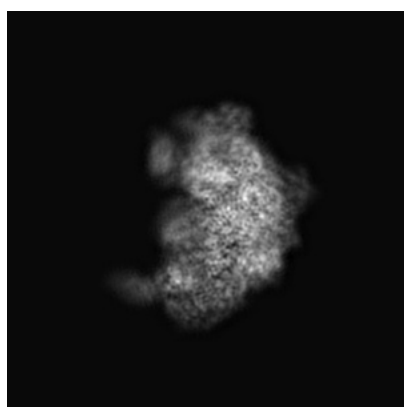
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2924. These allow visual inspection of the internal detail of the map and identification of artifacts.

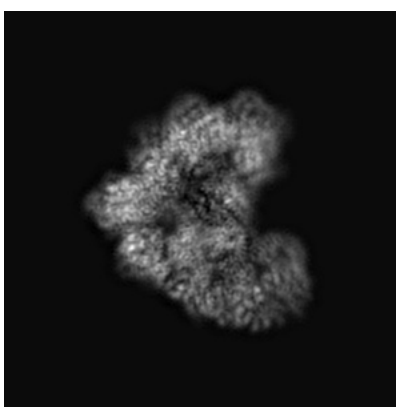
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

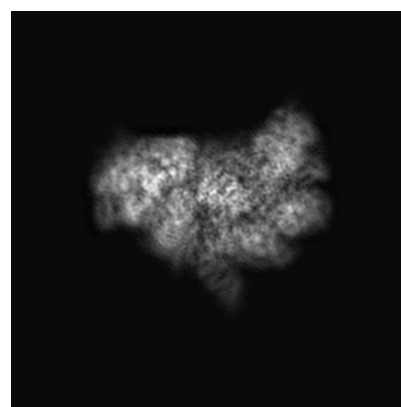
6.1.1 Primary map



X



Y

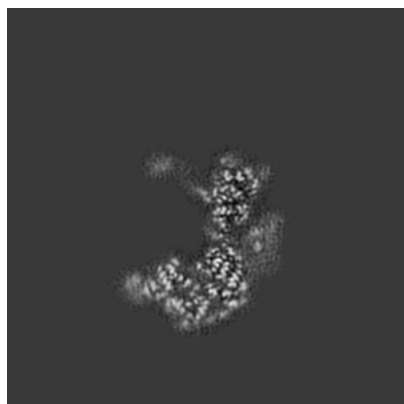


Z

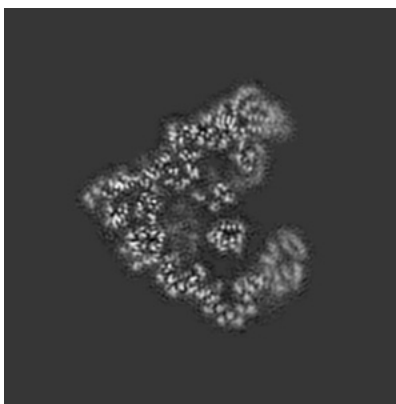
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

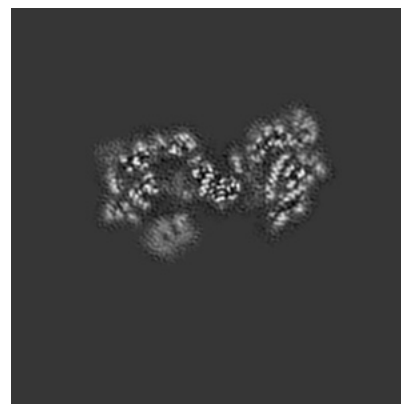
6.2.1 Primary map



X Index: 132



Y Index: 132

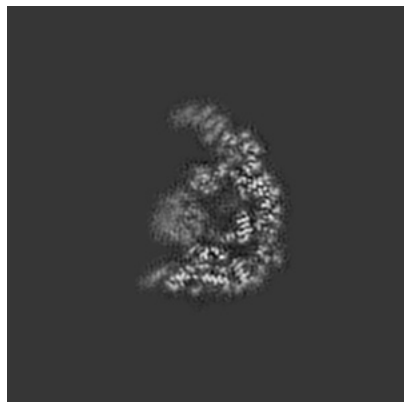


Z Index: 132

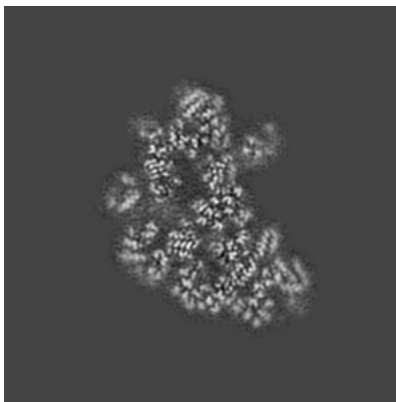
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

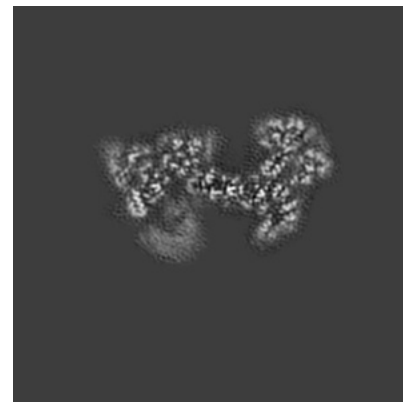
6.3.1 Primary map



X Index: 107



Y Index: 156



Z Index: 124

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

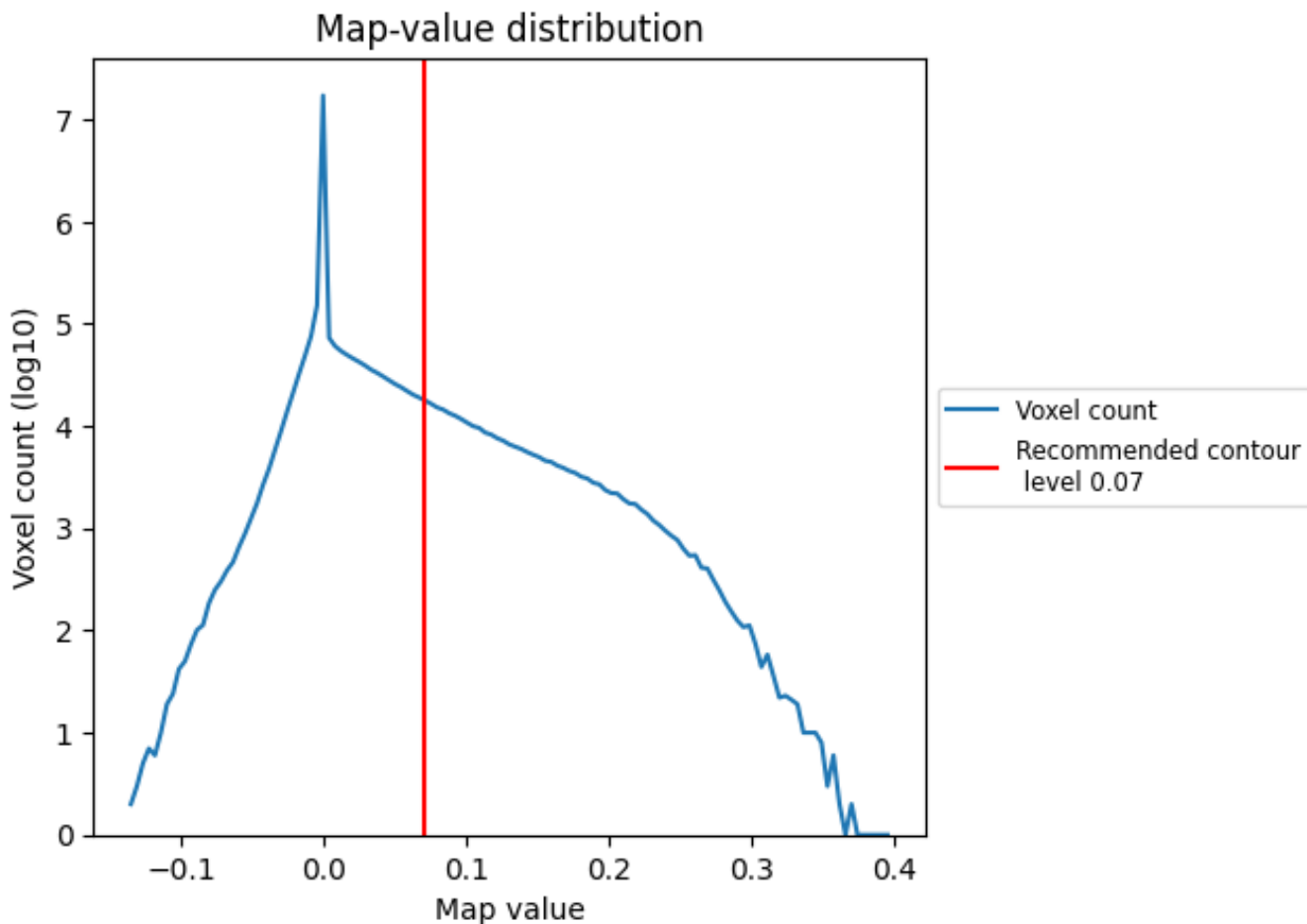
6.5 Mask visualisation

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

7 Map analysis [i](#)

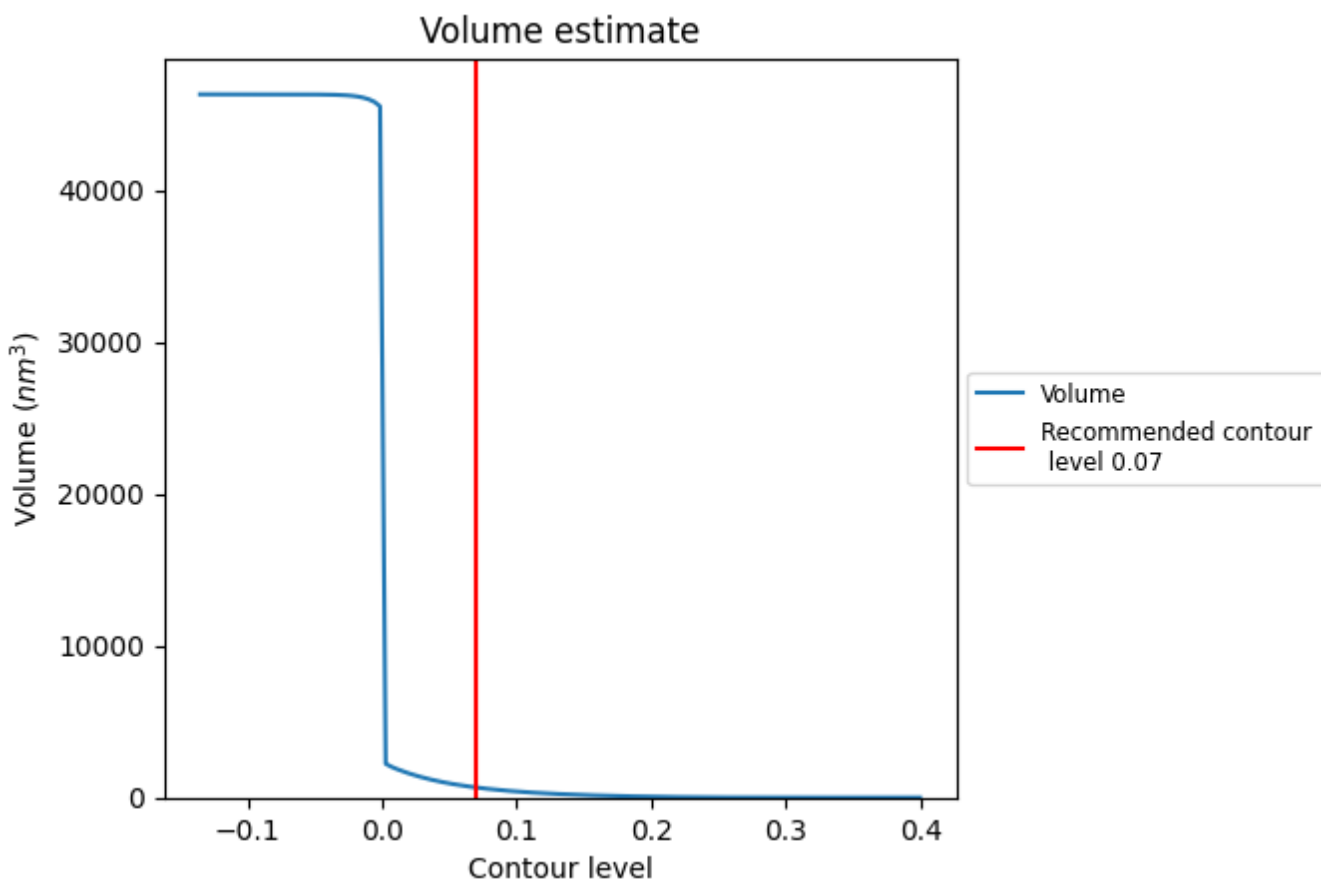
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

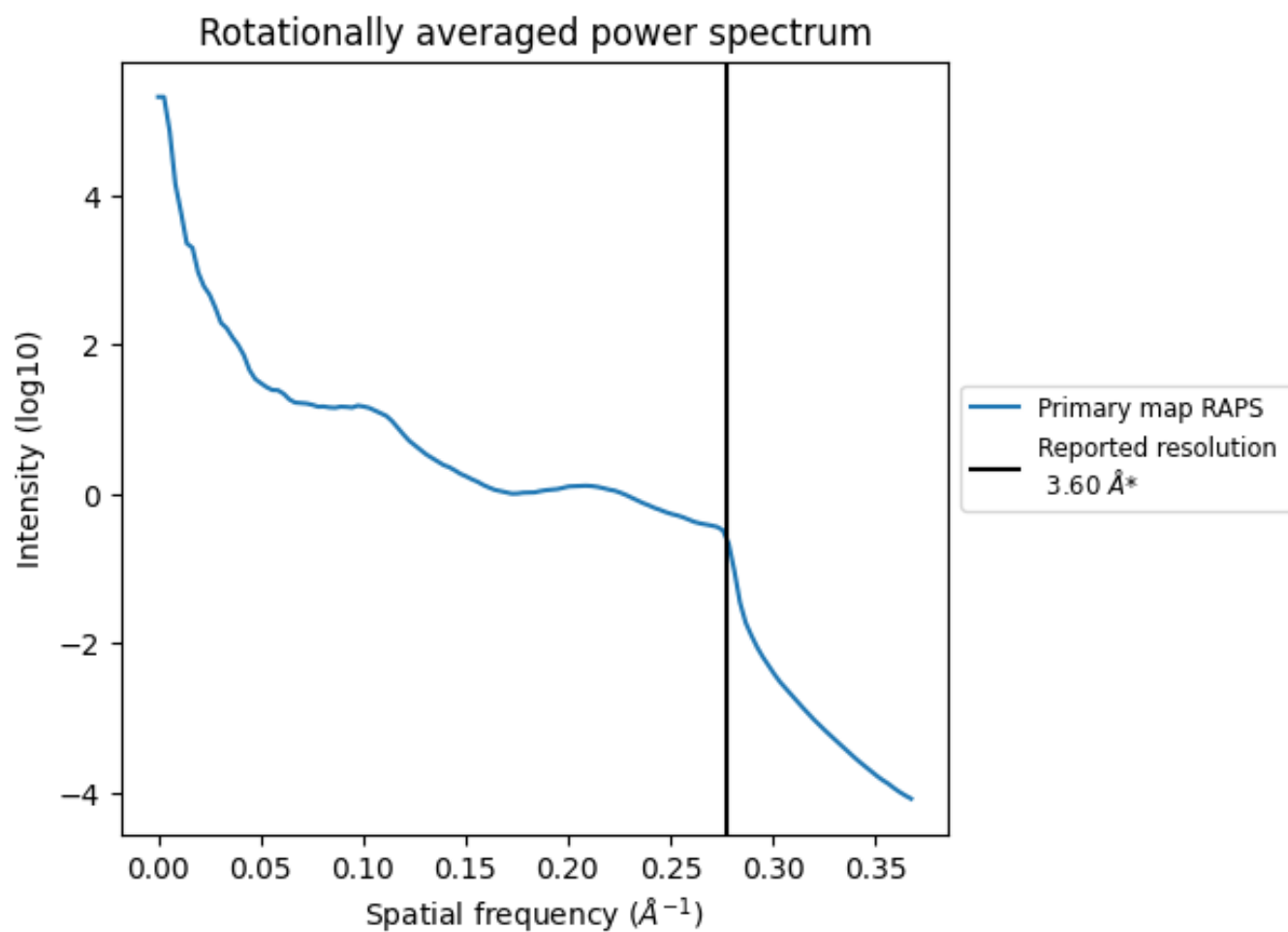
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 663 nm³; this corresponds to an approximate mass of 599 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 0.278 Å⁻¹

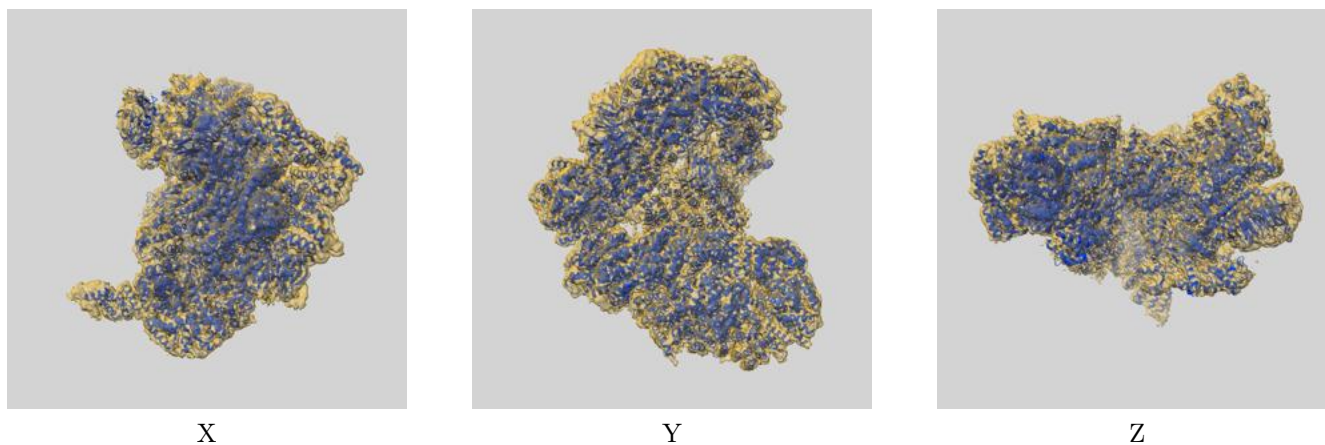
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

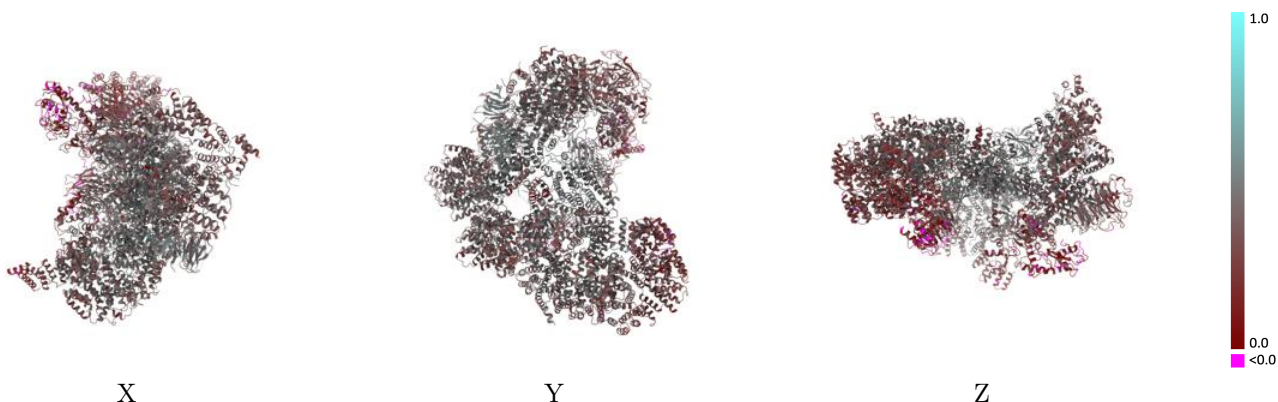
This section contains information regarding the fit between EMDB map EMD-2924 and PDB model 4UI9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



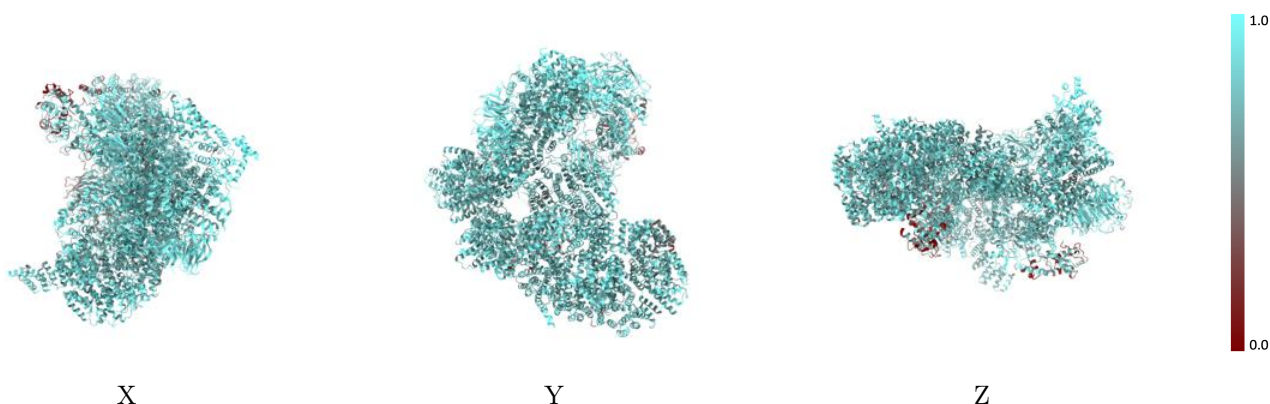
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



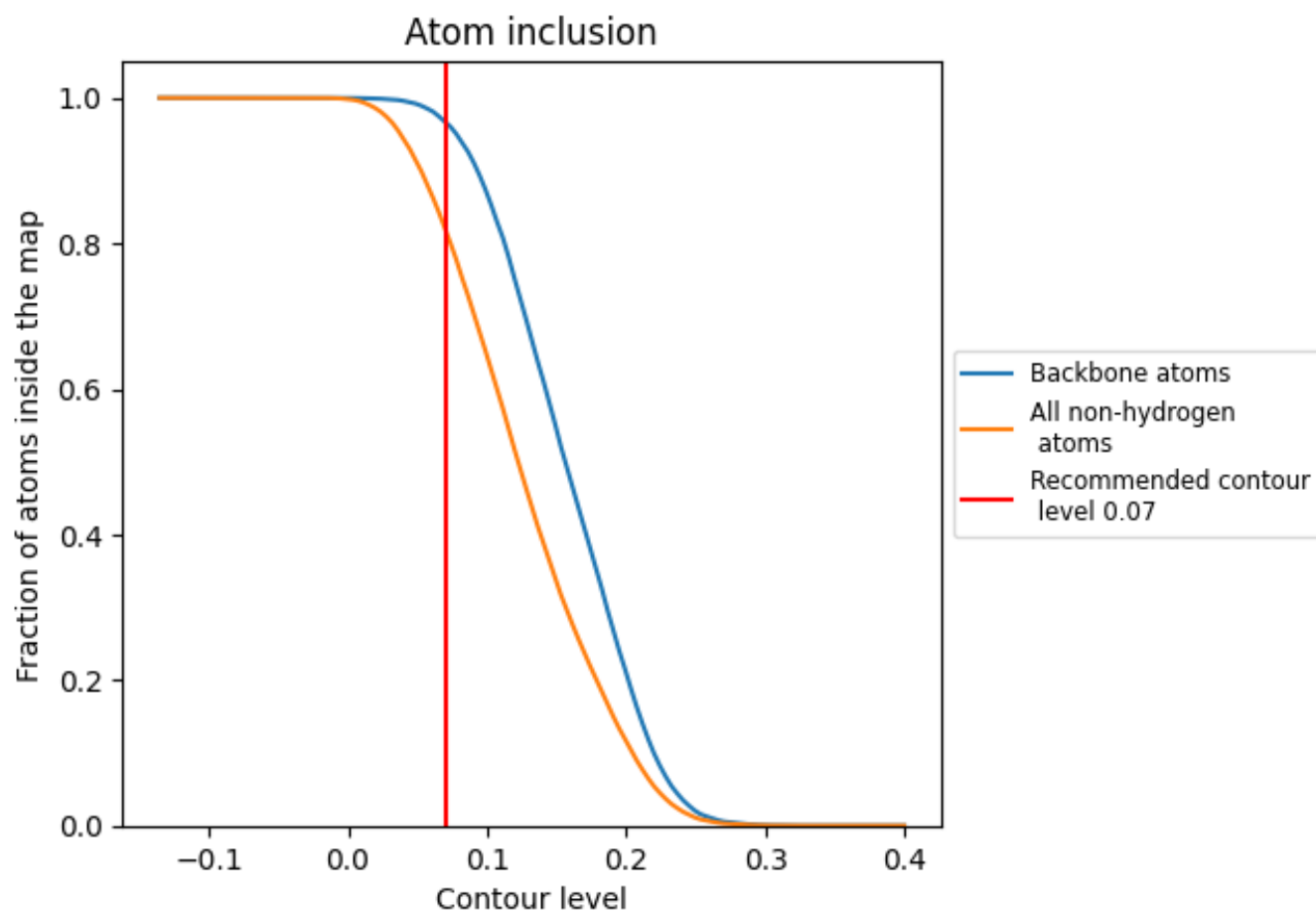
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8188	 0.3780
A	 0.8687	 0.4460
B	 0.7696	 0.2160
C	 0.8343	 0.4160
D	 0.8241	 0.4390
E	 0.8266	 0.4250
F	 0.8418	 0.4090
G	 0.7816	 0.3900
H	 0.8386	 0.4120
I	 0.8310	 0.3690
J	 0.8581	 0.4080
K	 0.8509	 0.4150
L	 0.8424	 0.4330
M	 0.7329	 0.4210
N	 0.7594	 0.2790
O	 0.8522	 0.4330
P	 0.8423	 0.3750
R	 0.6537	 0.2250
S	 0.6254	 0.2370
T	 0.9450	 0.4510
U	 0.9833	 0.3890
W	 0.7805	 0.4170
X	 0.7258	 0.2580
Y	 0.7833	 0.3200

