WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Nov 13, 2024 – 02:22 PM EST

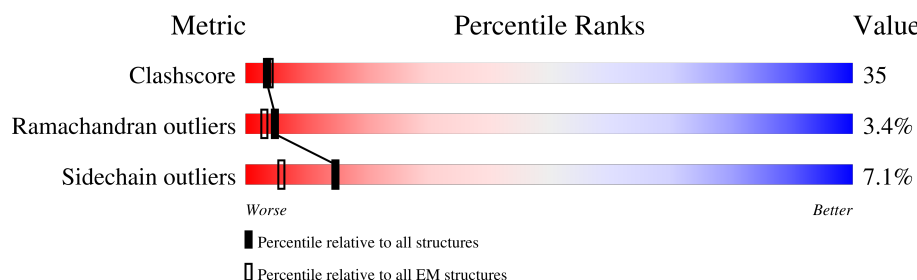|		
PDB ID	:	3J0J
EMDB ID	:	EMD-5335
Title	:	Fitted atomic models of Thermus thermophilus V-ATPase subunits into cryo-EM map
Authors	:	Lau, W.C.Y.; Rubinstein, J.L.
Deposited on	:	2011-08-24
Resolution	:	9.70 Å(reported)
Based on initial models	:	3K5B, 1R5Z, 3A5C

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1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 9.70 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	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		3.4%
Sidechain outliers		7.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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	578	82% 13% • • •
1	B	578	10% 85% 10% • •
1	C	578	6% 83% 12% • • •
2	D	478	6% 83% 10% • 6%
2	E	478	5% 82% 11% • 6%
2	F	478	5% 82% 12% • 6%
3	G	223	23% 24% 8% 42%
4	H	104	19% 79% 14% 7%

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Mol	Chain	Length	Quality of chain
5	I	104	12% · 70% · 24% · · · ·
5	K	104	10% · 73% · 22% · ·
6	J	188	11% · 64% · 25% · 7% · ·
6	L	188	17% · 64% · 26% · 6% · ·
7	M	323	7% · 30% · 63% · 5% · ·

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 22726 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	561	Total 2752	C 1630	N 561	O 561	0	0
1	B	561	Total 2752	C 1630	N 561	O 561	0	0
1	C	561	Total 2752	C 1630	N 561	O 561	0	0

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	450	Total 2212	C 1312	N 450	O 450	0	0
2	E	450	Total 2212	C 1312	N 450	O 450	0	0
2	F	450	Total 2212	C 1312	N 450	O 450	0	0

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	129	Total 639	C 381	N 129	O 129	0	0

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	104	Total 509	C 301	N 104	O 104	0	0

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	100	Total 747	C 460	N 136	O 150	S 1	0	0
5	K	100	Total 747	C 460	N 136	O 150	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	17	GLY	-	expression tag	UNP Q5SIT5
K	17	GLY	-	expression tag	UNP Q5SIT5

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	184	Total 1312	C 815	N 242	O 252	S 3	0	0
6	L	184	Total 1312	C 815	N 242	O 252	S 3	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total 2514	C 1599	N 460	O 451	S 4	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots ⓘ

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

- Molecule 1: V-type ATP synthase alpha chain

- Molecule 1: V-type ATP synthase alpha chain


- Molecule 1: V-type ATP synthase alpha chain

Chain C:

6%

83% 12% • • •

M1 V5 A10 G11 P12 A13 G18 M19 Y25 D26 I27 G44 Y52 E53 S56 P63 L69 P70 L71 A72 V73 E74 L75 M79 I87 Q88 L91 GLU ARG ILE ARG GLU LYS THR GLY ILE TYR ILE THR ARG GLY VAL VAL V108 H109 G126 D127

E128 V129 M133 F141 G142 F143 L148 P151 D152 G155 R156 V173 V174 L175 E176 D177 G178 T179 E180 Y184 H185 T186 V189 R190 R191 P194 G208 M209 R210 F216 G221 A224 A225 I226 P227 G228 P229 F230 G231 S232 G233 L241 W244 S245

C255 G256 G259 N260 L266 P275 N290 P295 V296 A297 Y304 V305 G306 R314 F318 D325 A333 P345 P352 G366 E374 V384 S385 P386 P387 G388 P394 V395 A405 F406 F419 P420 S429 L430 F431 R440 A444 Q469

Q496 Q497 C507 K531 R532 G533 E557 E558 F559 F563 K575 A576 L577 ALA

• Molecule 2: V-type ATP synthase beta chain

Chain D:

6%

83% 10% • 6%

MET ASP LEU LEU LYS LYS E7 G16 P17 A24 K25 D26 L27 A28 E49 V50 S51 E52 T64 G65 L66 A69 I70 V76 E77 D78 V79 A80 G102 I106 R124 R125 K126 F130 G134 L144 K149 L150 F153 L158 P175 ASP LEU SER

GLY GLU GLY GLU K183 E184 V189 G195 L201 I205 S217 T258 D259 E269 A272 A273 R274 E275 E276 I277 P278 P284 T289 Y295 M316 P317 D318 I332 T333 E334 G335 Q338 L339 E342 Y349 P350 P351 L355 P356 S359 R360 L361

M362 K370 I392 R393 K394 I398 E401 D402 Q427 Q428 N429 R430 Y463 GLY GLN LYS LEU GLU GLU ILE TRP GLY ALA PRO GLN ALA LEU ASP

• Molecule 2: V-type ATP synthase beta chain

Chain E:

5%

82% 11% • 6%

MET ASP LEU LEU LYS LYS E7 Y8 G16 P17 A24 K25 D26 L27 A28 Y29 G30 G40 R41 V42 E49 V50 S51 E52 E61 G65 L66 D67 L68 A69 T70 T71 V76 E77 D78 V79 A80 R81 L82 K86 G102 L117 P118 L119 N120 P121 R124 V140

K149 L150 F153 G157 V173 R174 P175 ASP LEU SER GLY GLU GLY GLU K183 V189 G212 S217 P227 T228 I229 P235 L239 R274 E275 E276 I277 P284 T289 Y295 E296 R297 A298 M316 P317 I332 T333 E334 G335 Q338 L339 Y349

P350 P351 L355 P356 S359 R360 L361 M362 E401 D402 Q427 Q428 S435 K452 Y463 GLY GLN LYS LEU GLU GLU ILE TRP GLY ALA PRO GLN ALA LEU ASP

• Molecule 2: V-type ATP synthase beta chain

Chain F:

5%

82% 12% • 6%

• Molecule 3: V-type ATP synthase subunit D

Chain G: 23%   24%   8%   42%

• Molecule 4: V-type ATP synthase subunit F
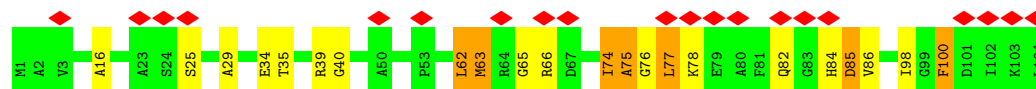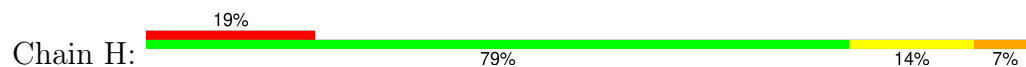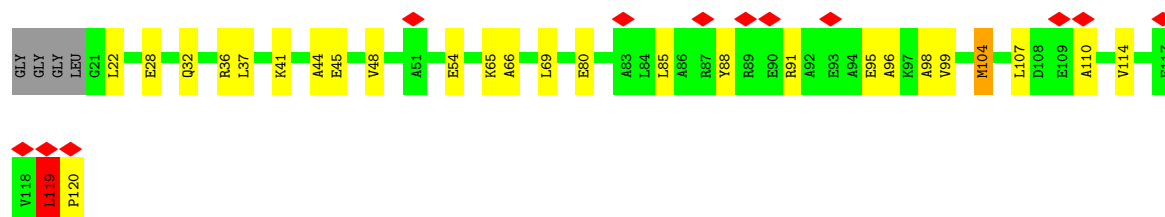
Chain H: 19%   79%   14%   7%

• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain I: 12%   70%   24%

• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K: 10%   73%   22%

• Molecule 6: V-type ATP synthase subunit E

Chain J:

• Molecule 6: V-type ATP synthase subunit E

Chain L:
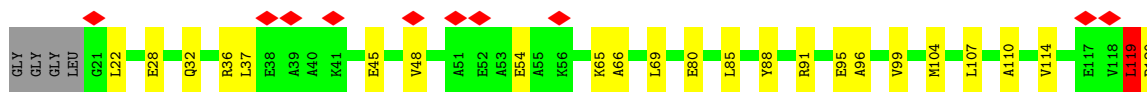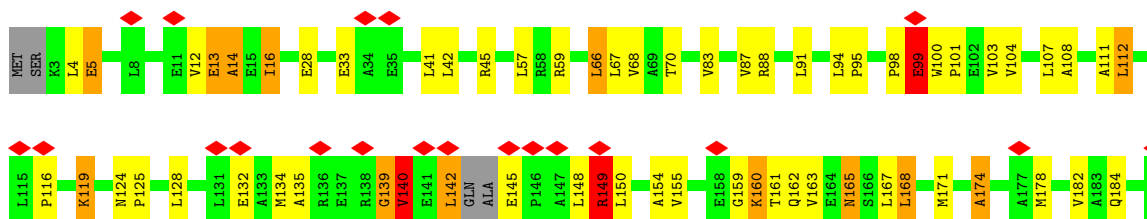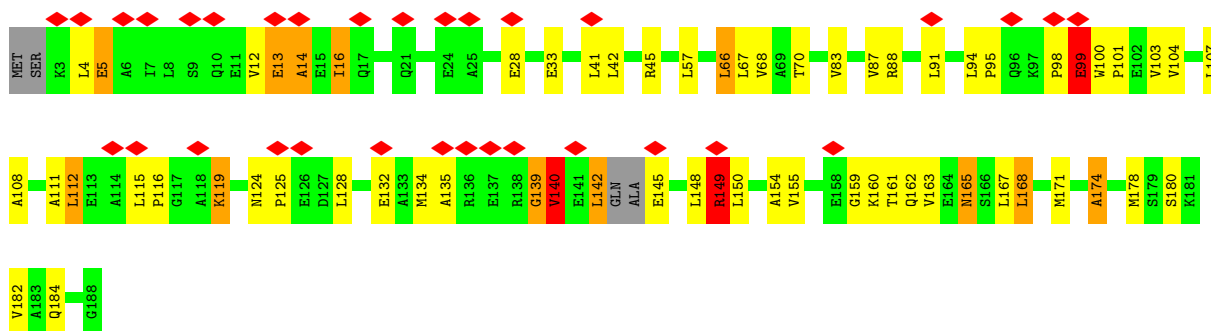
• Molecule 7: V-type ATP synthase subunit C

Chain M:
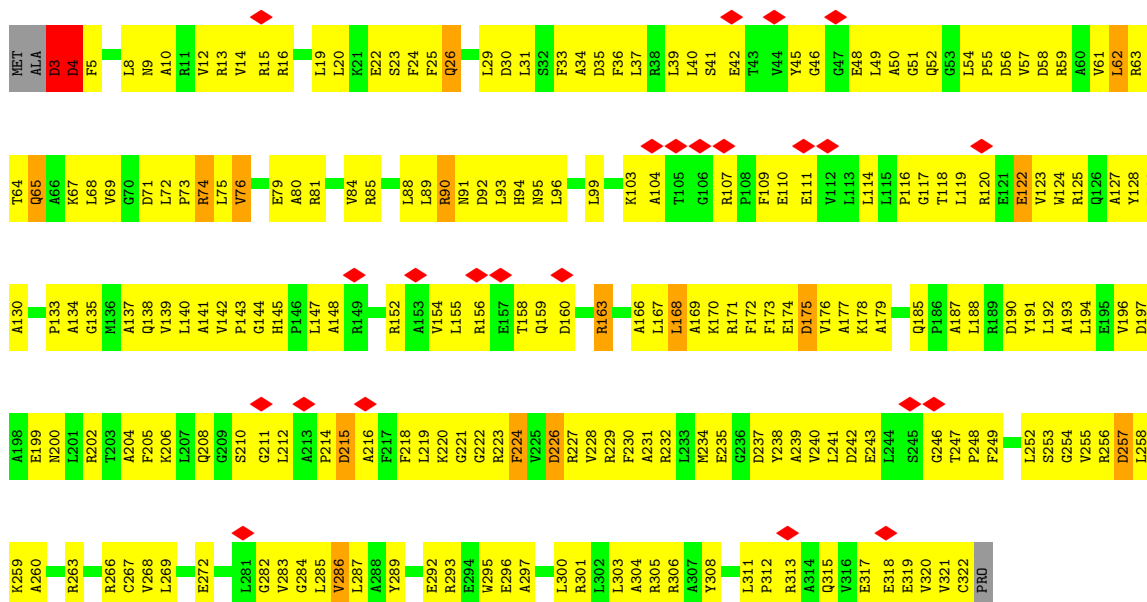
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46105	Depositor
Resolution determination method	Not provided	
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	0.18	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50000	Depositor
Image detector	GENERIC FILM	Depositor
Maximum map value	1.571	Depositor
Minimum map value	-0.417	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.548	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: ADP

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	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	B	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	C	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	E	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	125/637 (19.6%)	2.63	50/885 (5.6%)
4	H	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
5	I	0.42	1/749 (0.1%)	0.48	0/1004
5	K	0.42	1/749 (0.1%)	0.48	0/1004
6	J	0.45	2/1325 (0.2%)	0.53	0/1798
6	L	0.45	2/1325 (0.2%)	0.53	0/1798
7	M	1.22	5/2553 (0.2%)	1.11	12/3447 (0.3%)
All	All	1.02	164/22726 (0.7%)	1.19	138/31288 (0.4%)

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	6
1	B	0	6
1	C	0	6
2	D	0	4
2	E	0	3
2	F	0	3
4	H	0	2
7	M	0	1
All	All	0	31

The worst 5 of 164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	47	MET	CA-CB	-24.99	0.98	1.53
3	G	27	LEU	CA-CB	14.81	1.87	1.53
4	H	75	ALA	N-CA	13.46	1.73	1.46
3	G	7	THR	CA-CB	12.79	1.86	1.53
3	G	31	LYS	N-CA	12.37	1.71	1.46

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	ASP	O-C-N	-39.91	58.85	122.70
1	B	325	ASP	O-C-N	-39.91	58.85	122.70
1	C	325	ASP	O-C-N	-39.84	58.95	122.70
1	C	70	PRO	C-N-CA	-27.46	53.06	121.70
4	H	76	GLY	N-CA-C	26.73	179.94	113.10

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	69	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1300	122	0
1	B	2752	0	1303	59	0
1	C	2752	0	1302	86	0
2	D	2212	0	1009	80	0
2	E	2212	0	1009	84	0
2	F	2212	0	1009	83	0
3	G	639	0	299	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	509	0	255	23	0
5	I	747	0	726	21	0
5	K	747	0	726	18	0
6	J	1312	0	1240	74	0
6	L	1312	0	1240	56	0
7	M	2514	0	2583	624	0
8	A	27	0	12	0	0
8	C	27	0	12	4	0
All	All	22726	0	14025	1287	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 35.

The worst 5 of 1287 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)
7:M:33:PHE:CG	7:M:308:TYR:HD1	1.08	1.66
7:M:33:PHE:CD2	7:M:308:TYR:CD1	1.83	1.64
7:M:20:LEU:HD23	7:M:24:PHE:CD1	1.11	1.61
2:E:25:LYS:CA	6:J:161:THR:HG23	1.14	1.61
3:G:189:GLU:CA	3:G:189:GLU:CB	1.76	1.61

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	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	3	23
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	3	21
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	6	32
2	E	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	6	32
2	F	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	5	29
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	6	32
5	I	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	6	32
5	K	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	6	32
6	J	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	1	14
6	L	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	1	14
7	M	318/323 (98%)	281 (88%)	32 (10%)	5 (2%)	8	38
All	All	4110/4402 (93%)	3678 (90%)	293 (7%)	139 (3%)	5	21

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	62/76 (82%)	59 (95%)	3 (5%)	21	43
5	K	62/76 (82%)	59 (95%)	3 (5%)	21	43
6	J	108/141 (77%)	94 (87%)	14 (13%)	3	14
6	L	108/141 (77%)	94 (87%)	14 (13%)	3	14
7	M	254/256 (99%)	246 (97%)	8 (3%)	35	54
All	All	594/690 (86%)	552 (93%)	42 (7%)	15	32

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	L	140	VAL
7	M	4	ASP
6	L	142	LEU
6	L	168	LEU
7	M	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	M	9	ASN
7	M	52	GLN
7	M	65	GLN
7	M	94	HIS
7	M	185	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 oligosaccharides in this entry.

5.6   Ligand geometry (i)

2 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
8	ADP	A	600	-	24,29,29	1.38	4 (16%)	29,45,45	0.91	1 (3%)
8	ADP	C	600	-	24,29,29	1.08	2 (8%)	29,45,45	1.09	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	600	-	-	2/12/32/32	0/3/3/3
8	ADP	C	600	-	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	PA-O3A	4.05	1.63	1.59
8	A	600	ADP	O4'-C1'	2.90	1.44	1.40
8	C	600	ADP	PB-O2B	-2.52	1.45	1.54
8	A	600	ADP	PB-O2B	-2.42	1.45	1.54
8	C	600	ADP	PA-O1A	-2.35	1.42	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	600	ADP	C5-C6-N6	2.39	123.95	120.31
8	C	600	ADP	O3B-PB-O2B	2.38	116.74	107.80
8	A	600	ADP	O3A-PA-O1A	2.09	116.99	110.70
8	C	600	ADP	O4'-C4'-C3'	-2.06	101.06	105.15
8	C	600	ADP	O5'-PA-O1A	2.06	117.09	108.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	600	ADP	PA-O3A-PB-O2B
8	A	600	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	600	ADP	4	0

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

Ligand ADP A 600

Bond lengths   Bond angles

Torsions   Rings

Ligand ADP C 600

Bond lengths

Bond angles

Torsions

Rings
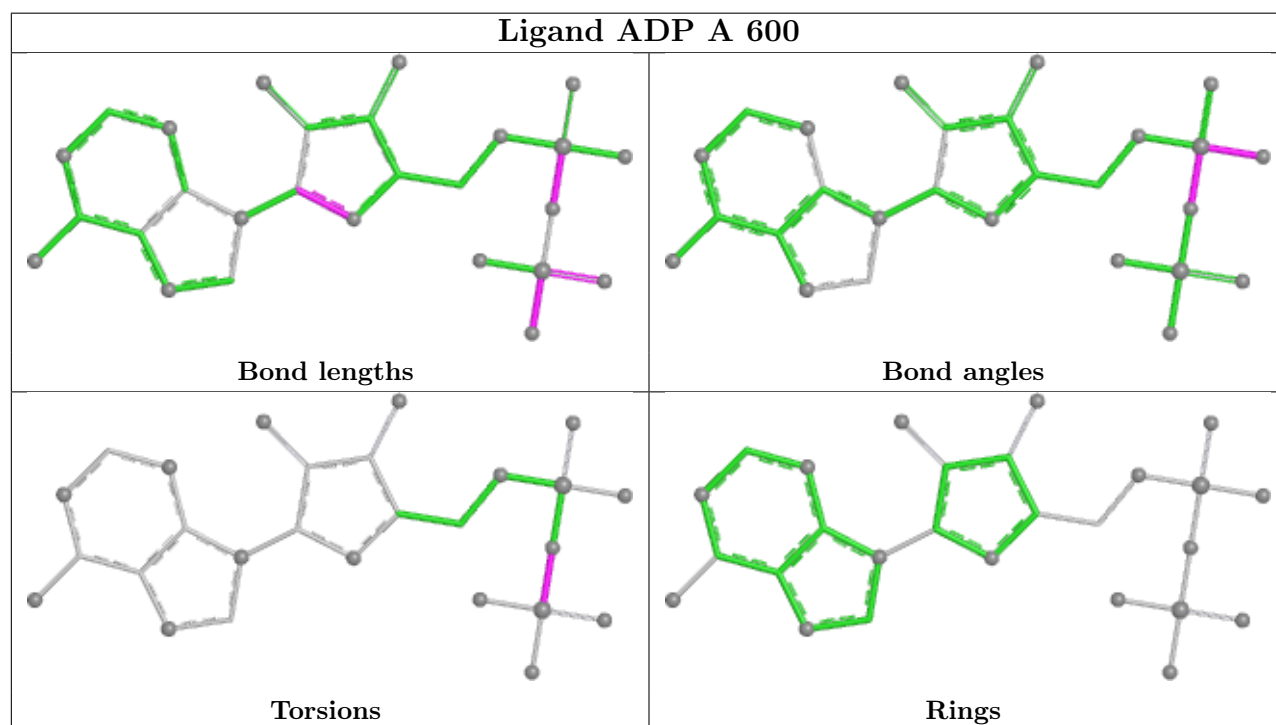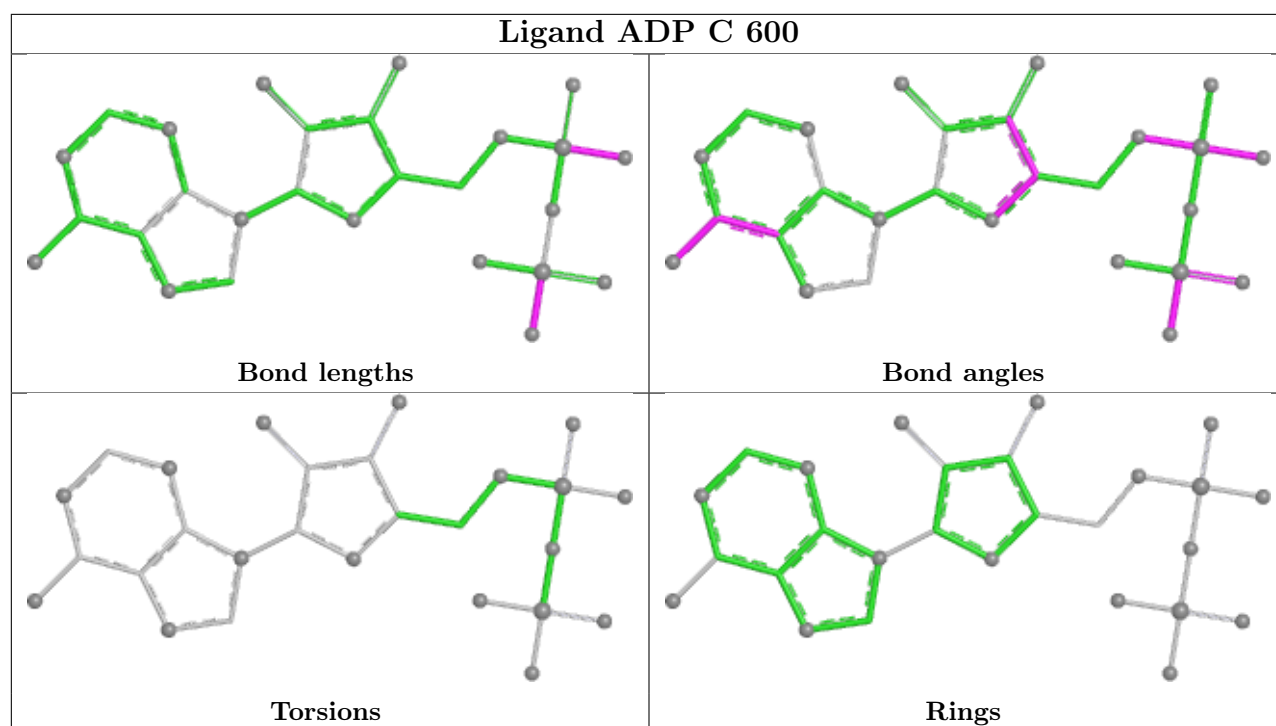
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-5335. 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 |
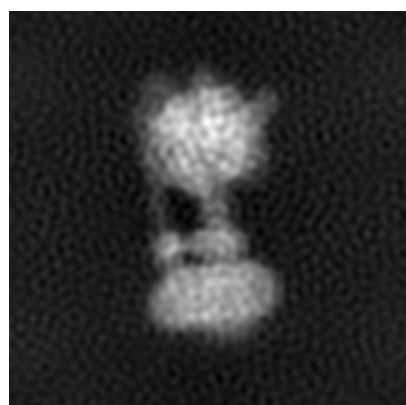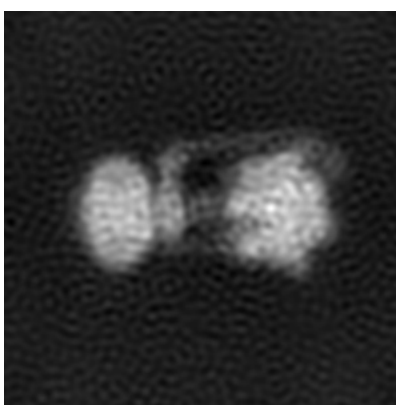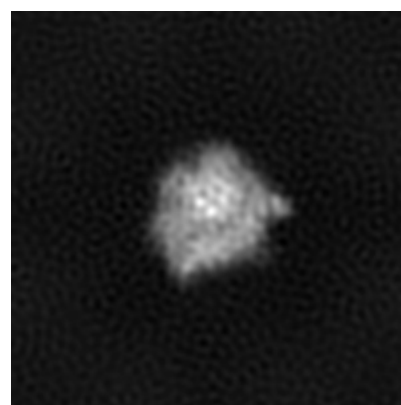
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
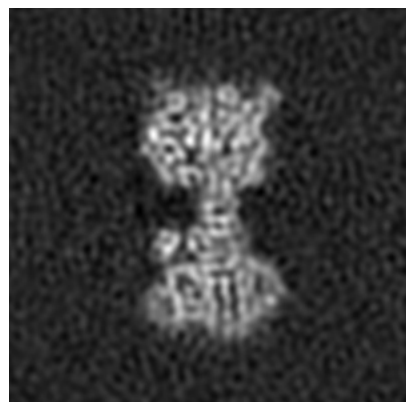
6.2.1   Primary map
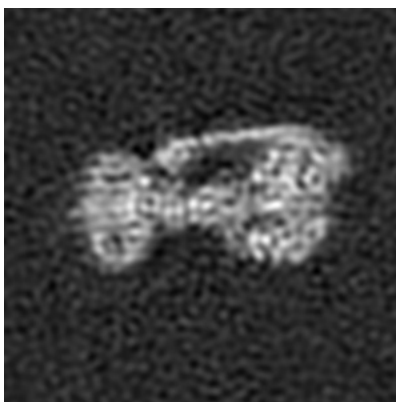
| X Index: 128 | Y Index: 128 | Z Index: 128 |
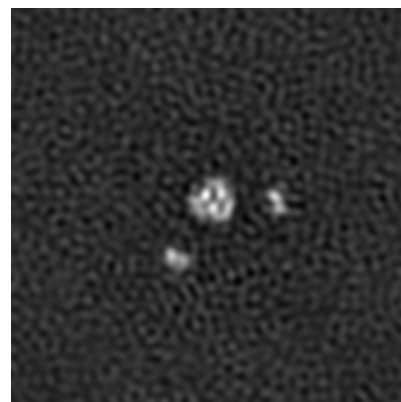
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
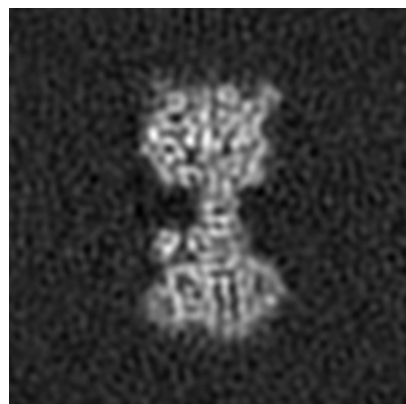
6.3.1 Primary map
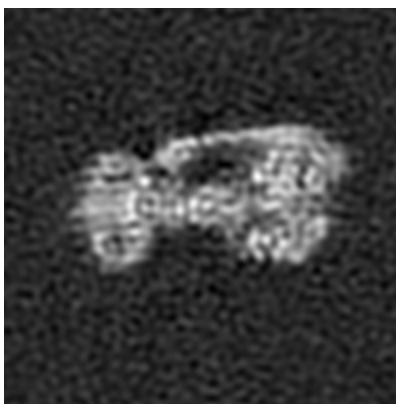
| X Index: 128 | Y Index: 129 | Z Index: 181 |
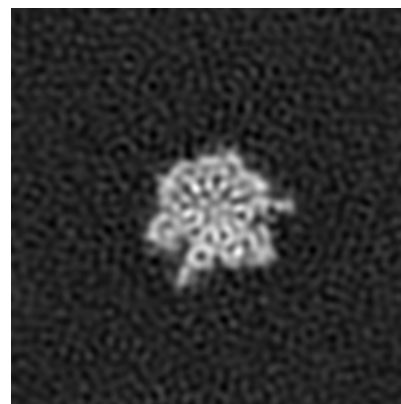
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

| X | Y | Z |
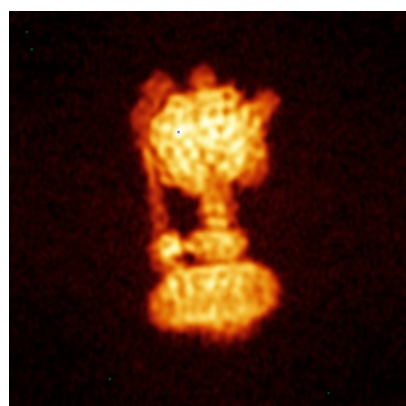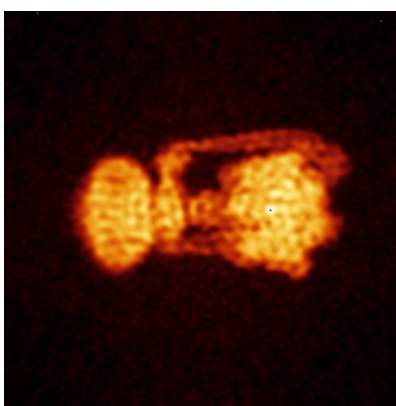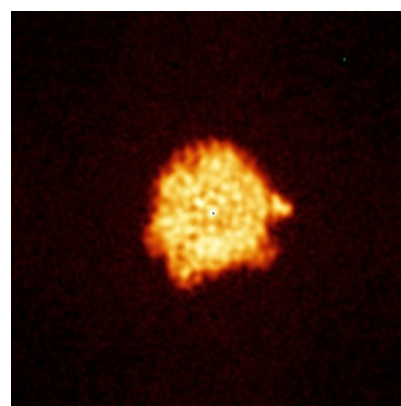
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ
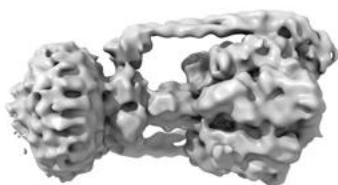
6.5.1 Primary map

X	Y	Z
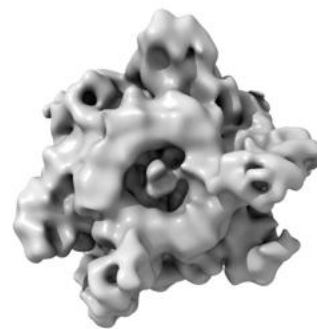
The images above show the 3D surface view of the map at the recommended contour level 0.548. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6   Mask visualisation (i)

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

A mask typically either:

- Encompasses the whole structure

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

6.6.1   emd_5335_msk_2.map (i)
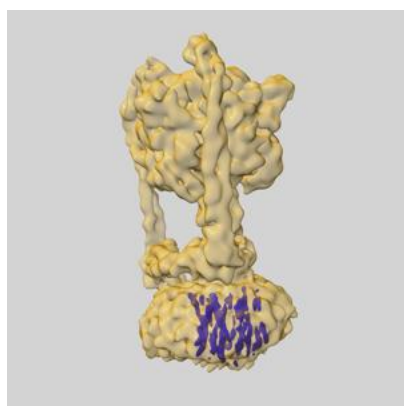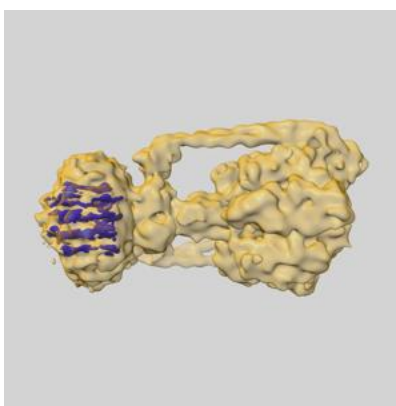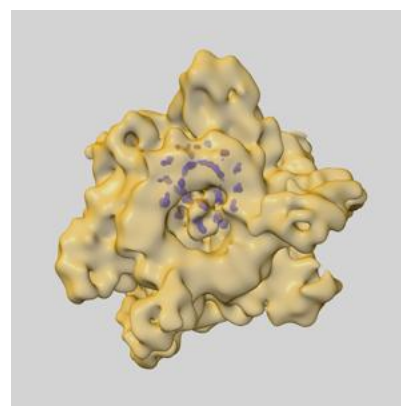
X   Y   Z

6.6.2   emd_5335_msk_1.map (i)
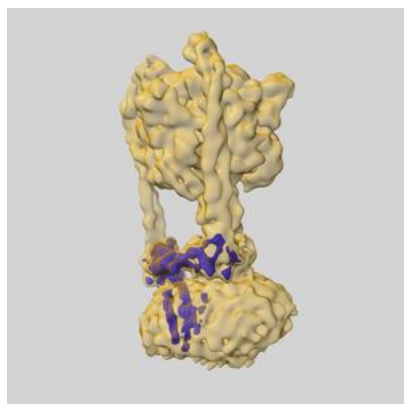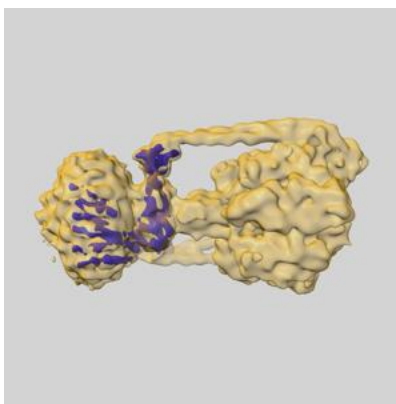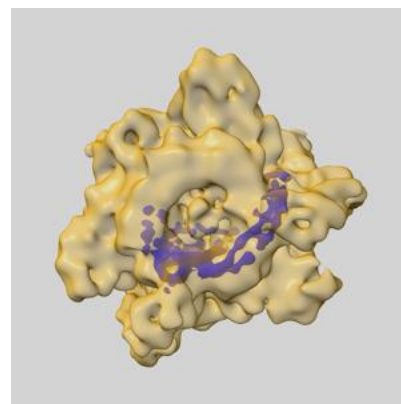
X   Y   Z

6.6.3　emd_5335_msk_3.map ⓘ

X　　　　　　　　　　　　　　　Y　　　　　　　　　　　　　　　Z
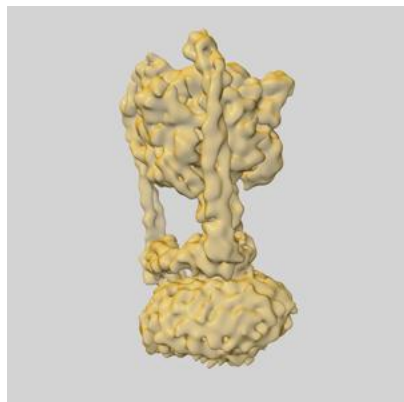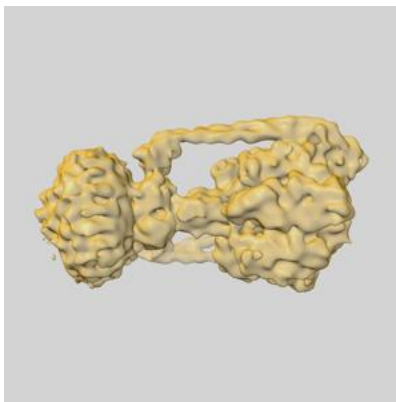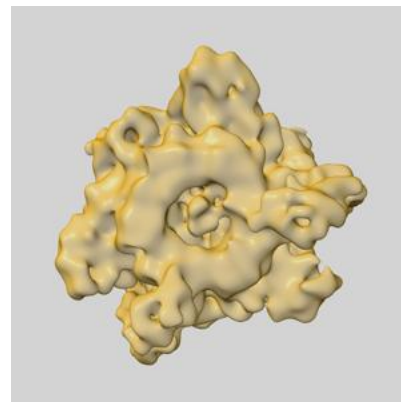
7 Map analysis ⓘ

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

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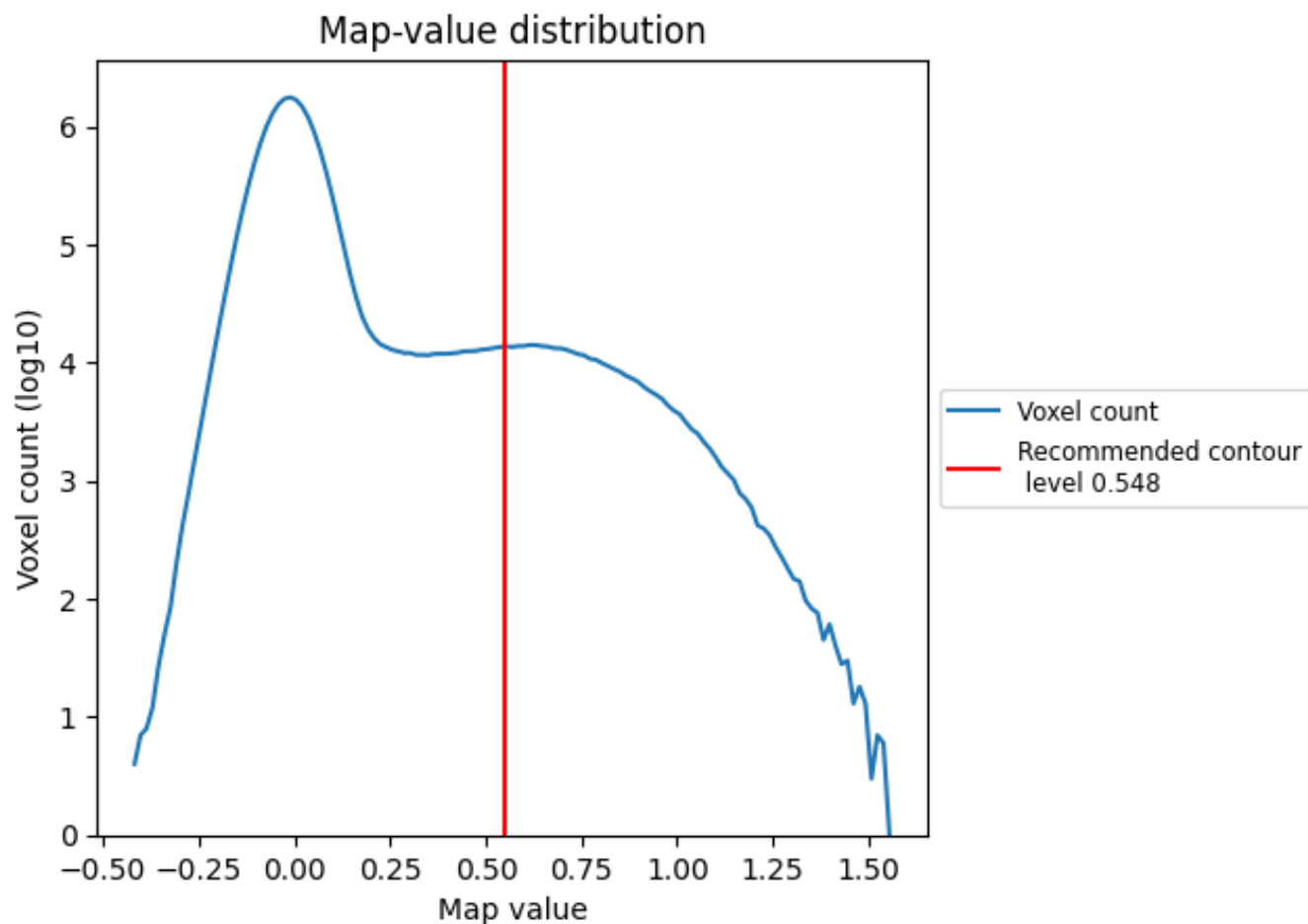
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
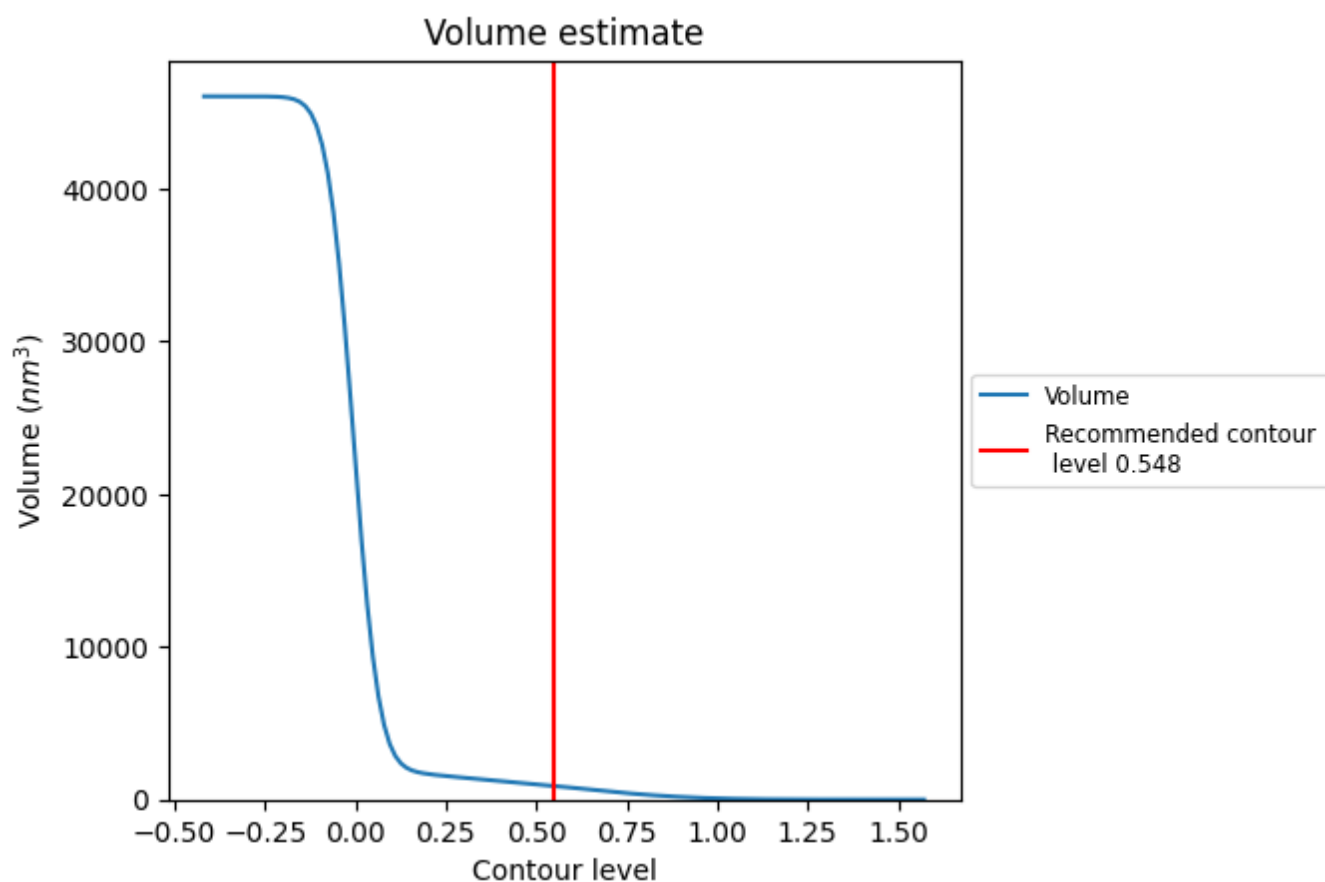
The volume at the recommended contour level is 897 nm^3; this corresponds to an approximate mass of 810 kDa.

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)
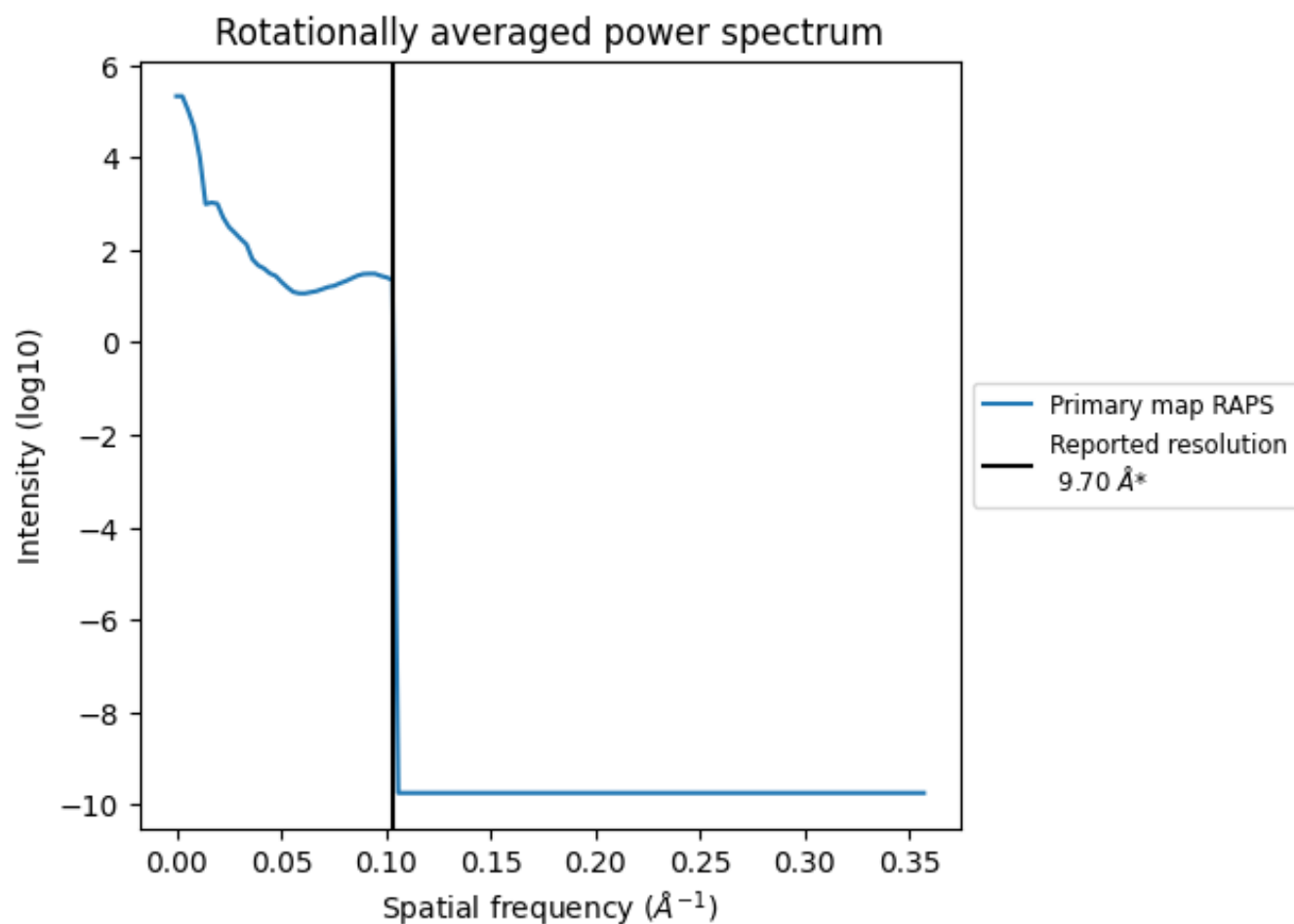
*Reported resolution corresponds to spatial frequency of 0.103 Å^{-1}

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-5335 and PDB model 3J0J. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay ⓘ
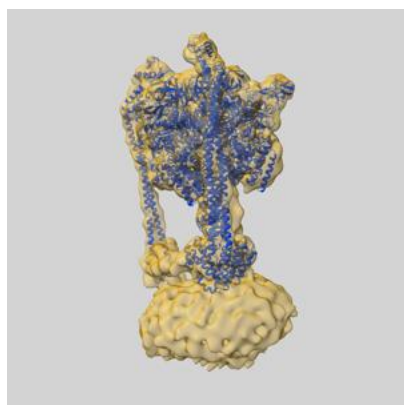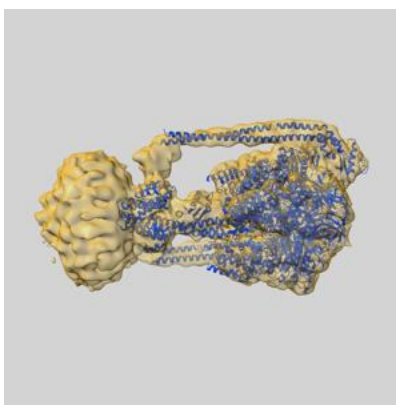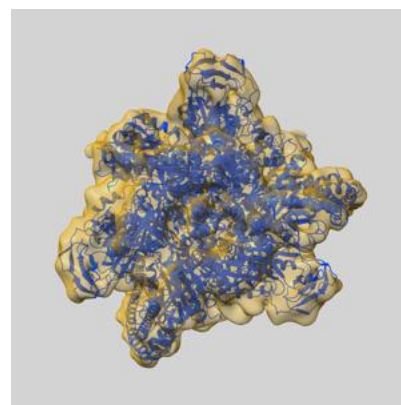
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.548 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 ⓘ

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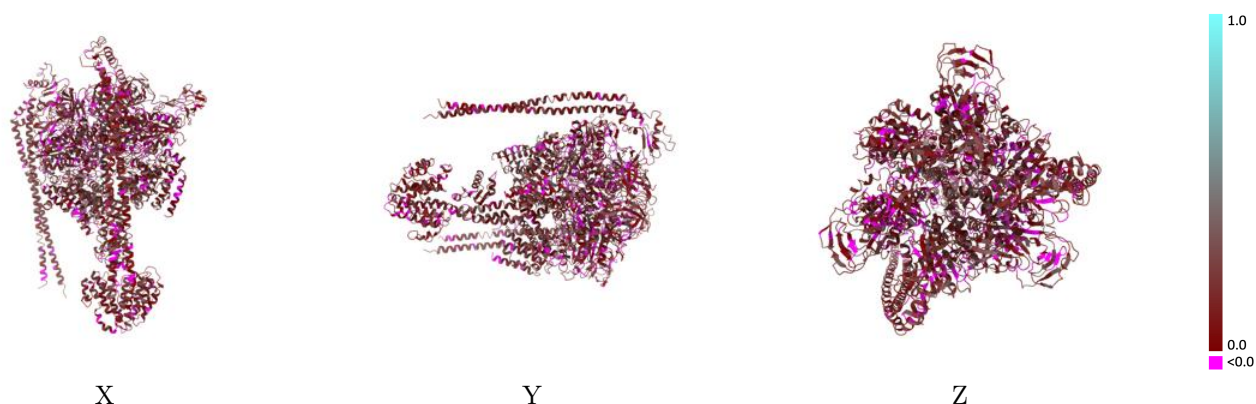
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
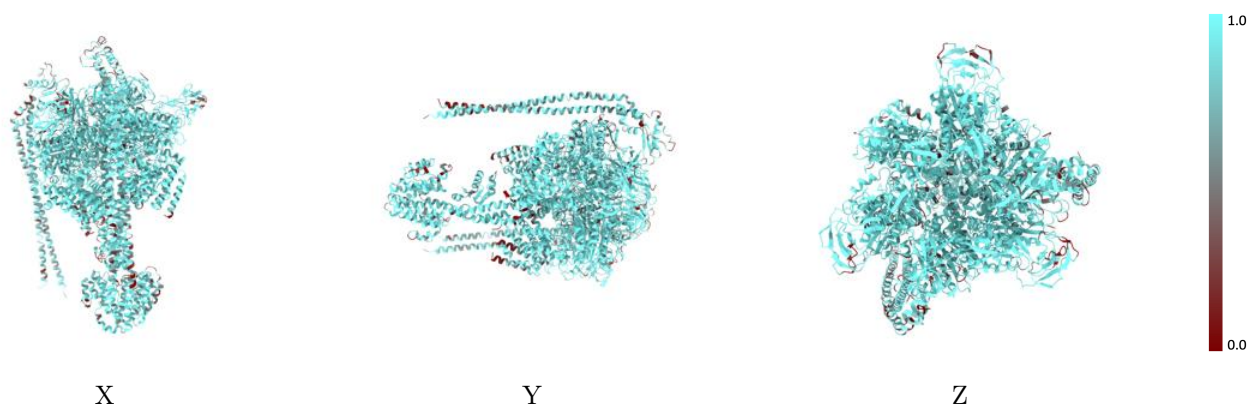
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.548).

9.4 Atom inclusion ⓘ
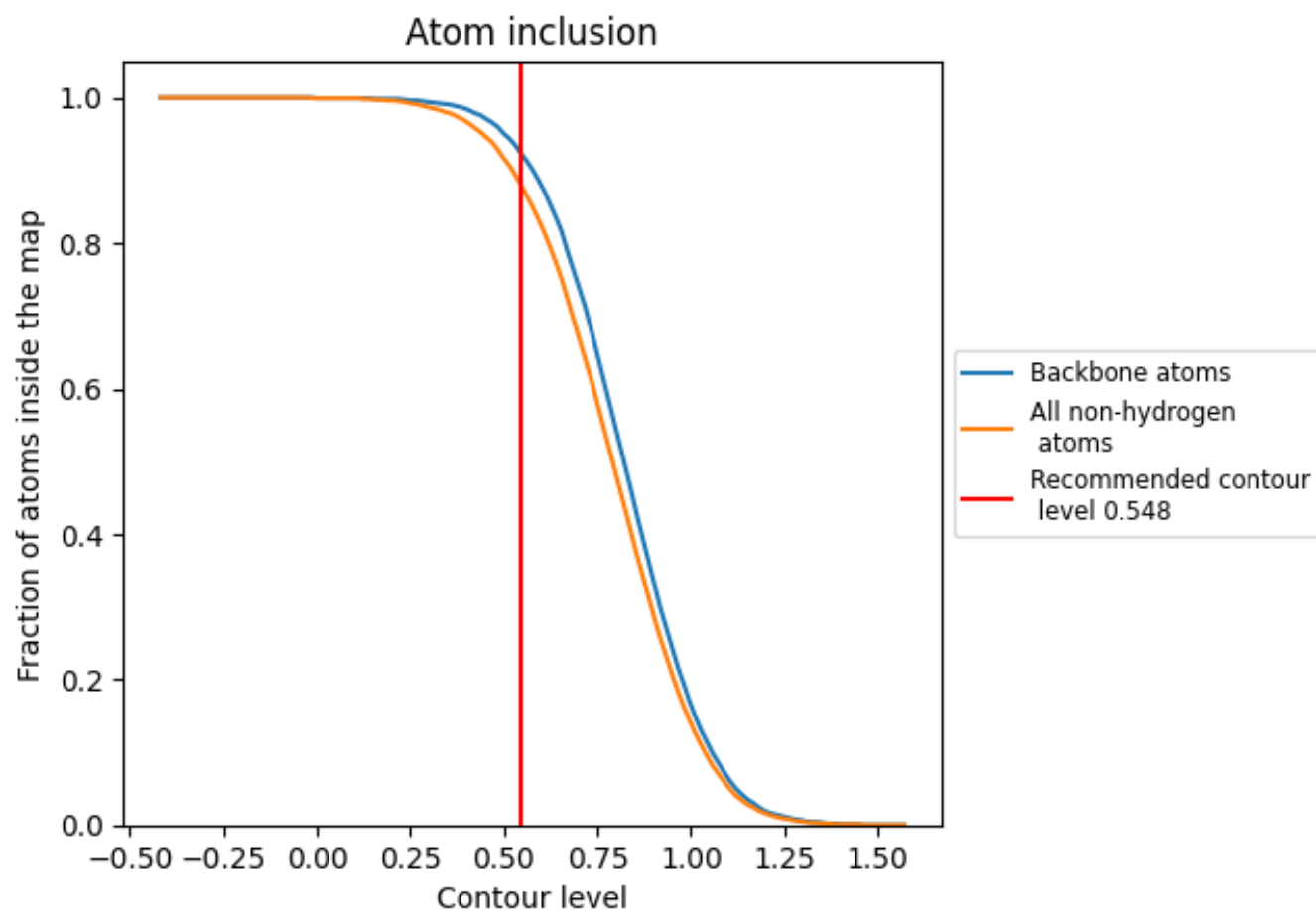
At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary　ⓘ

The table lists the average atom inclusion at the recommended contour level (0.548) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.1440
A	0.9290	0.1400
B	0.8820	0.1230
C	0.9210	0.1560
D	0.9210	0.1460
E	0.9320	0.1560
F	0.9220	0.1460
G	0.9530	0.2040
H	0.7860	0.1280
I	0.7140	0.1430
J	0.7770	0.1530
K	0.7610	0.1440
L	0.7340	0.1470
M	0.8460	0.1260

1.0

0.0
<0.0