wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 04:35 pm GMT

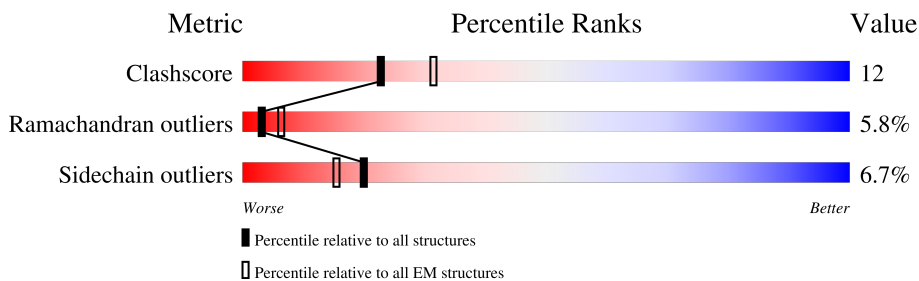|		
PDB ID	:	4A7L
EMDB ID	:	EMD-1989
Title	:	Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 1)
Authors	:	Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.; Raunser, S.
Deposited on	:	2011-11-14
Resolution	:	8.10 Å(reported)
Based on initial models	:	1LKX, 3MFP

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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 8.10 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.
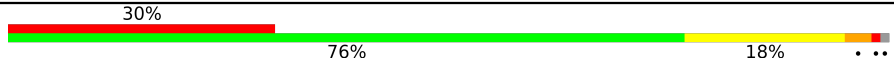
Metric	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		5.8%
Sidechain outliers		6.7%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=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	375	5% 71% 21% 6% •
1	D	375	6% 69% 22% 5% •
1	E	375	6% 70% 22% 6% •
1	F	375	6% 70% 21% 6% •
1	I	375	6% 70% 22% 6% •
2	B	136	18% 97% •
2	H	136	26% 96% •
3	C	697	31% 78% 17% • ••

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Mol	Chain	Length	Quality of chain
3	G	697	30% 76% 18%
3	J	697	29% 77% 18%

2   Entity composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 33500 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 ACTIN, ALPHA SKELETON MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1 ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		
2	H	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		

- Molecule 3 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	G	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	J	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	conflict	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	conflict	UNP Q03479
C	334	GLU	SER	engineered mutation	UNP Q03479
G	77	MET	ILE	conflict	UNP Q03479
G	215	ASP	ASN	conflict	UNP Q03479
G	334	GLU	SER	engineered mutation	UNP Q03479
J	77	MET	ILE	conflict	UNP Q03479
J	215	ASP	ASN	conflict	UNP Q03479
J	334	GLU	SER	engineered mutation	UNP Q03479

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
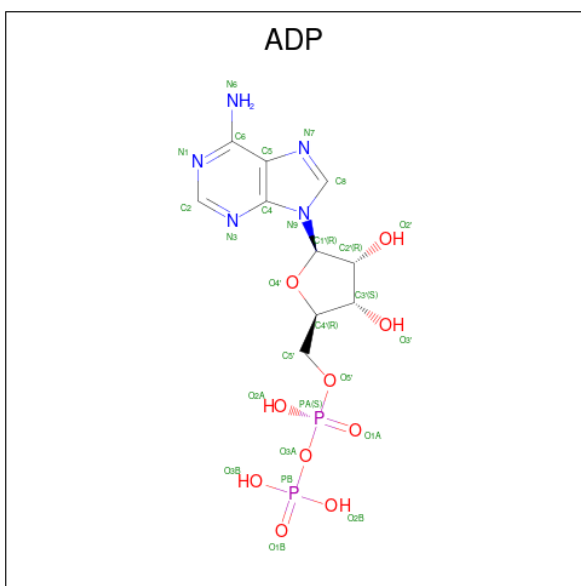
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

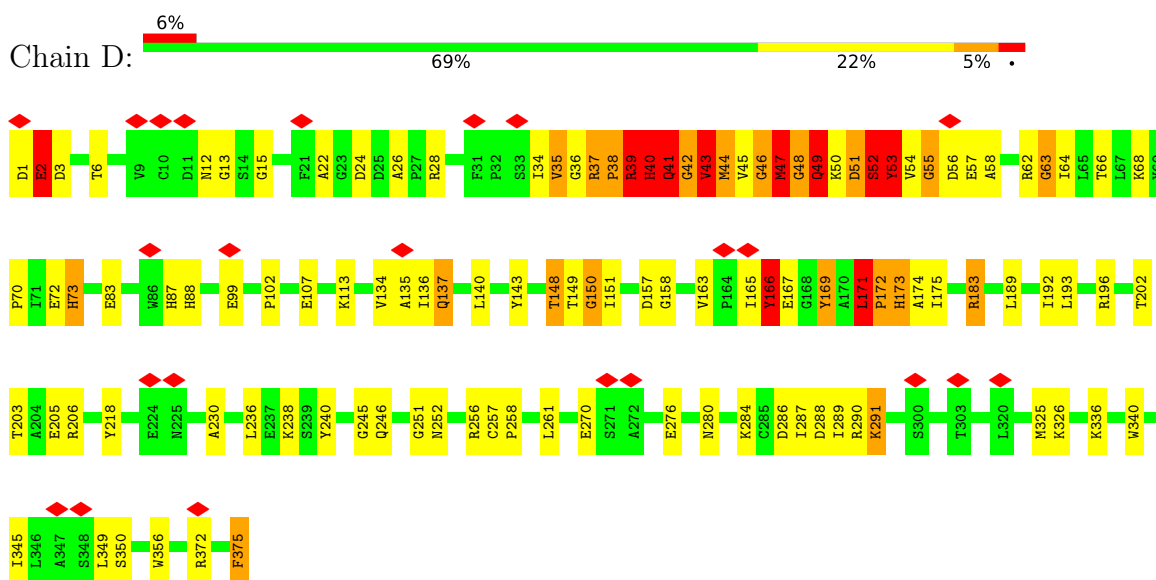| Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0
5	E	1	Total 1	Ca 1	0
5	F	1	Total 1	Ca 1	0
5	I	1	Total 1	Ca 1	0

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.
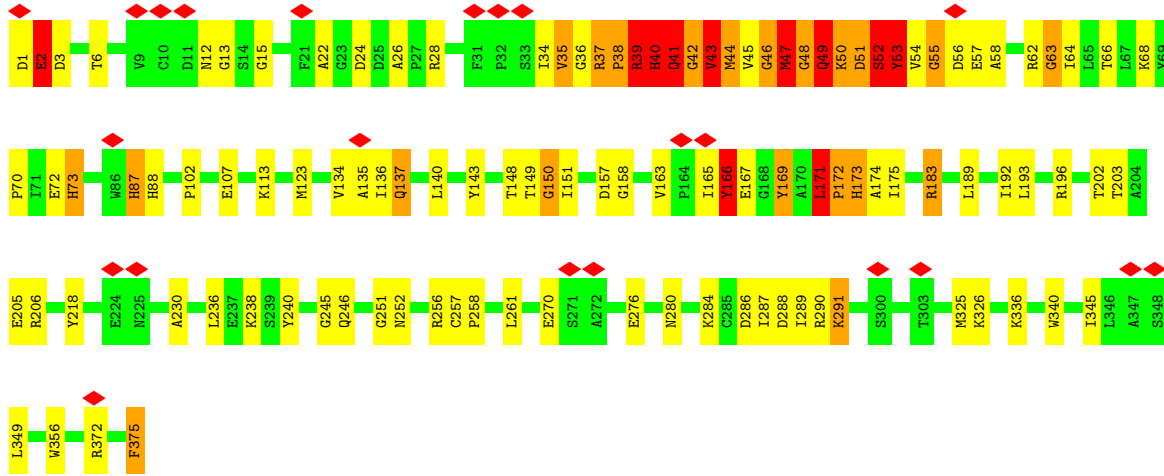
- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

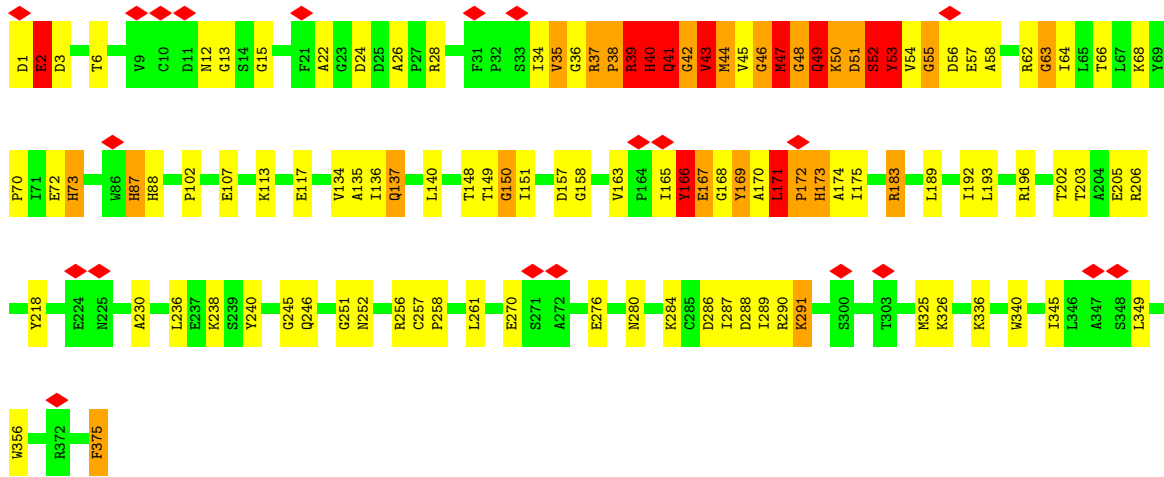- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE
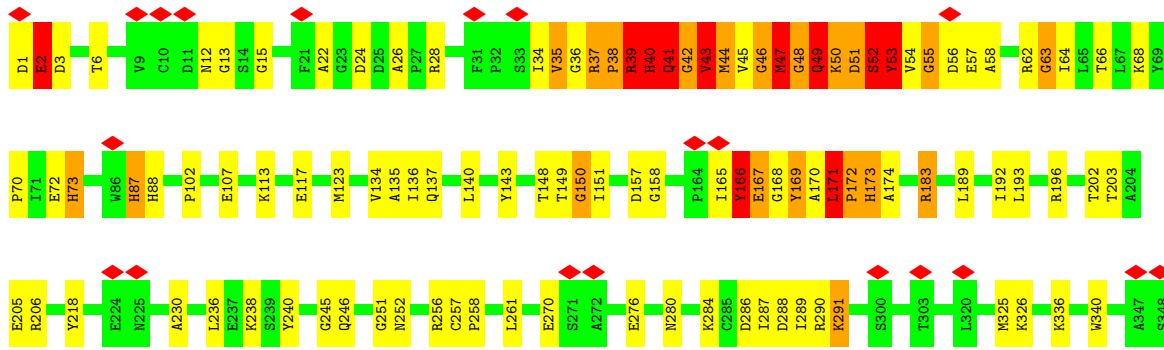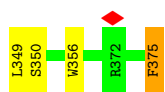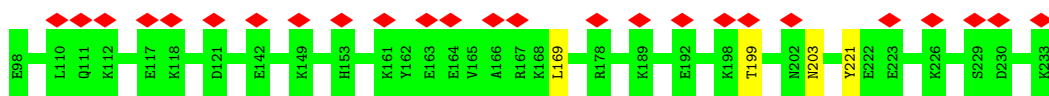

- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

Chain F:

• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

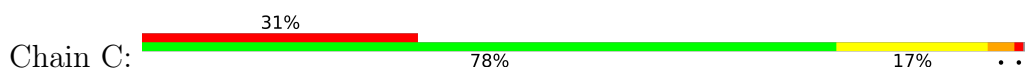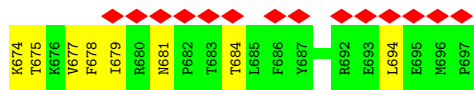Chain I:

L349 S350 W356 R372 F375

• Molecule 2: TROPOMYOSIN 1 ALPHA

18%

Chain B: 97%

E98 L110 Q111 K112 E117 K118 D121 E142 K149 H153 K161 Y162 E163 E164 V165 A166 R167 K168 L169 R178 K189 E192 K198 T199 N202 N203 Y221 E222 E223 K226 S229 D230 K233

• Molecule 2: TROPOMYOSIN 1 ALPHA

26%

Chain H: 96%

E98 A107 Q111 E114 D121 E122 S123 E124 R125 G126 M127 E138 E142 E145 L148 K149 E150 A151 K152 H153 E156 D159 R160 V165 D175 R178 G188 A191 E194 E195 N202 N203 K204 K205 S206 E218 D219 K220 Y221 E222 E223

K226 S229 D230 K231 L232 K233

• Molecule 3: MYOSIN IE HEAVY CHAIN

31%

Chain C: 78% 17%

MET ILE PRO LYS THR LYS ALA GLU G9 V10 P11 D12 F13 V14 L15 L16 N17 Q18 I19 L28 T29 M30 R31 H32 K33 S34 D35 Y38 T39 Y40 I41 G42 D43 V44 S47 T48 K52 N53 L54 N55 I56 Y57 K58 E59 S60 K63 A64 Y65 N66 G67 R68 P74 P75 H76

M77 Y78 A79 L80 A81 N82 D83 A84 Y85 R89 Q90 S91 Q92 E93 N94 I98 I99 S100 G106 K107 T108 L118 V121 S122 S123 N124 Q125 S126 R131 M135 L136 S139 N140 P141 L142 L143 E144 A145 A149 L152 R153 N154 D155 F160 Y163 M166

S173 P174 I175 N181 Y182 L183 L184 E185 K186 T193 E196 H200 I201 L206 K207 G208 L209 S210 Q211 S212 D215 L229 K230 K231 S232 G233 C234 F235 S238 T239 K247 I248 I249 T255 L256 G257 L270 A271 L274 A282 E283 A284 A285 R288 T289 G290

T291 D298 T299 K300 K310 L320 C321 Y322 I325 S326 T327 G328 V329 G330 K331 E334 V335 I336 S337 V338 D350 N362 V365 N369 I372 N373 K378 G379 P380 I384 L385 Y388 G389 F390 E391 V392 P393 Q394 N395 F405 C406 L410 F414

T418 R428 E429 G430 I431 E432 W433 K434 N435 I436 E437 V438 F439 N440 M441 K442 P443 L447 I448 P452 I453 G454 L455 I456 L459 D460 E461 A462 C463 K467 S468 T469 D470 D475 E482 K483 H486 S489 Y490 V491 V492 S493 K494 D495 R496 S497 I498 T501 C502 F503

R504 H507 Y508 A509 G510 D511 V512 D515 V516 R517 G518 F519 L520 K524 G529 D530 L531 I532 S539 F547 P548 P549 T550 R551 R558 P559 E560 A572 L573 L578 A579 C580 V585 R586 C587 I588 K589 S590 K594 Q595 A596 E601 D602 R605 H606 Q607 V608

R609 Y610 E615 R618 V619 R620 R621 A622 G623 F624 A625 G626 R627 I628 E629 Y630 T631 R632 F633 Y634 N635 R636 Y637 K638 M639 K642 K643 T644 W645 P646 S647 F648 N649 G650 T651 A652 K653 Q654 A655 T656 E657 L658 I659 L660 Q661 Q662 H663 N664 I665 D666 K667 E668 E669 I670 R671 M672 G673

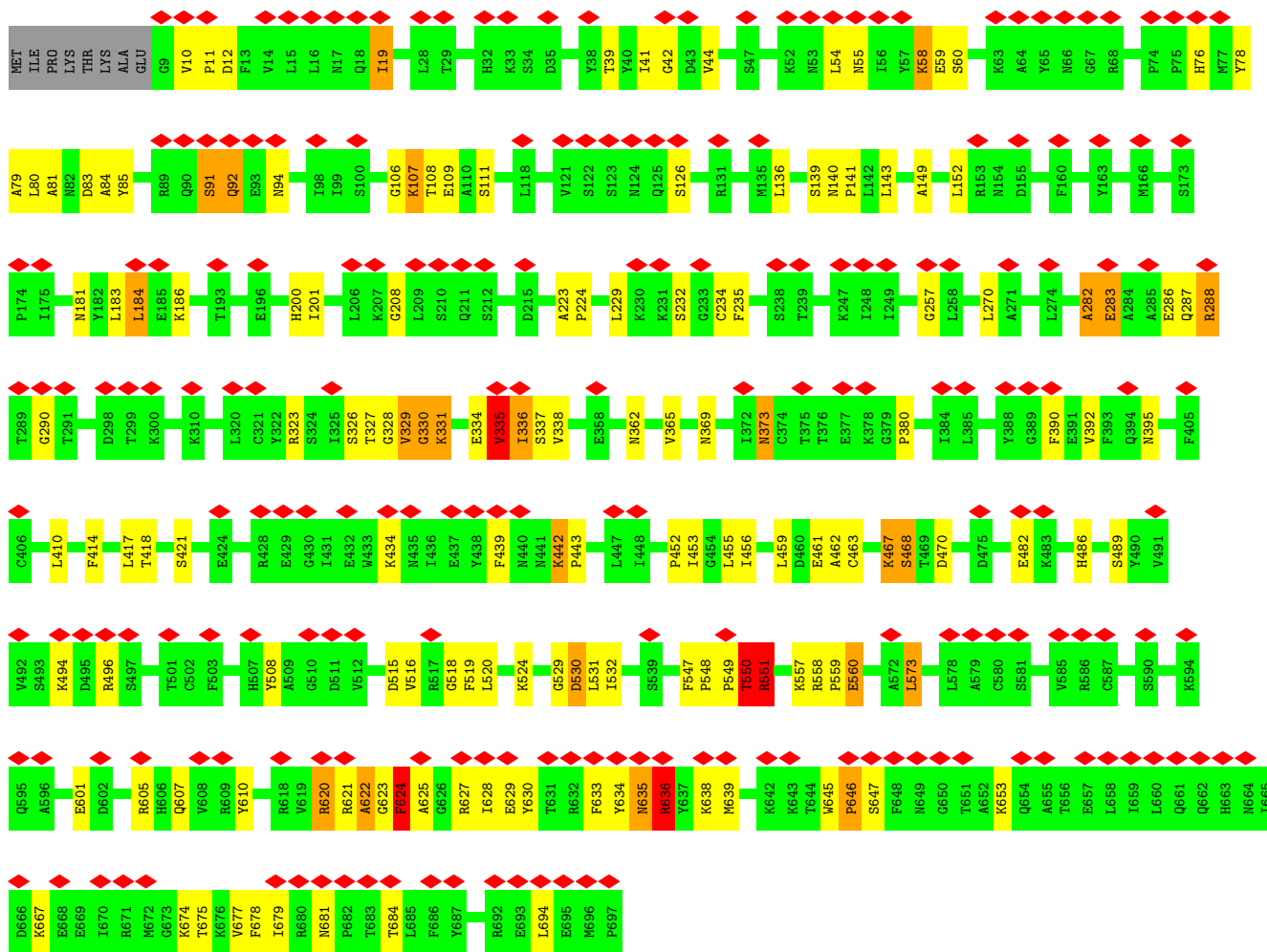K674 T675 K676 V677 F678 I679 R680 N681 P682 T683 T684 L685 F686 Y687 R692 E693 L694 E695 M696 P697

• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain G:

30%

76%　　　　　18%

MET ILE PRO THR LYS ALA GLU G9 V10 P11 D12 F13 V14 L15 L16 N17 Q18 I19 L28 T29 H32 K33 S34 D35 Y38 T39 Y40 I41 G42 D43 V44 S47 K52 N53 L54 N55 I56 Y57 K58 E59 S60 K63 A64 Y65 N66 G67 R68 P74 P75 H76 M77 Y78

A79 L80 A81 N82 D83 A84 Y85 R89 Q90 S91 Q92 E93 N94 I98 I99 S100 G106 K107 T108 E109 A110 S111 L118 V121 S122 S123 N124 Q125 S126 R131 M135 L136 S139 N140 P141 L142 L143 A149 L152 R153 N154 D155 F160 Y163 M166 S173

P174 I175 N181 Y182 L183 L184 E185 K186 T193 E196 H200 I201 L206 K207 G208 L209 S210 Q211 S212 D215 A223 P224 L229 K230 K231 S232 G233 C234 F235 S238 T239 K247 I248 I249 G257 L258 L270 A271 L274 A282 E283 A284 A285 E286 Q287 R288

T289 G290 T291 D298 T299 K300 K310 L320 C321 Y322 R323 S324 I325 S326 T327 G328 V329 G330 K331 E334 V335 I336 S337 V338 E358 N362 V365 N369 I372 N373 C374 T375 T376 E377 K378 G379 P380 I384 L385 Y388 G389 E391 V392 F393 Q394 N395 F405

C406 L410 F414 L417 T418 S421 E424 R428 E429 G430 I431 E432 W433 K434 N435 I436 E437 Y438 F439 N440 N441 K442 P443 L447 I448 P452 I453 G454 L455 I456 L459 D460 E461 A462 C463 K467 S468 T469 D470 D475 E482 K483 H486 S489 Y490 V491

V492 S493 K494 D495 R496 S497 T501 C502 F503 H507 Y508 A509 G510 D511 V512 D515 V516 R517 G518 F519 L520 K524 G529 D530 L531 I532 S539 F547 P548 P549 T550 R551 K557 R558 P559 E560 A572 L573 L578 A579 C580 S581 V585 R586 C587 S590 K594

Q595 A596 E601 D602 R605 H606 Q607 V608 R609 Y610 R618 V619 R620 R621 A622 G623 P624 A625 G626 R627 I628 E629 Y630 T631 R632 F633 Y634 N635 R636 Y637 K638 M639 K642 K643 T644 W645 P646 S647 F648 N649 G650 T651 A652 K653 Q654 A655 T656 E657 L658 I659 L660 Q661 Q662 H663 N664 I665

D666 K667 E668 K669 I670 R671 M672 G673 K674 T675 K676 V677 F678 I679 R680 N681 P682 T683 T684 L685 F686 Y687 R692 E693 L694 E695 M696 P697

• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J:

29%

77%　　　　　18%

MET ILE PRO THR LYS ALA GLU G9 V10 P11 D12 F13 V14 L15 L16 N17 Q18 I19 L28 T29 H32 K33 S34 D35 Y38 T39 Y40 I41 G42 D43 V44 S47 T48 K52 N53 L54 N55 I56 Y57 K58 E59 S60 K63 A64 Y65 N66 G67 R68 P74 P75 H76 M77

Y78 A79 L80 A81 N82 D83 A84 Y85 R89 Q90 S91 Q92 E93 N94 I98 I99 S100 G106 K107 T108 E109 A110 S111 L118 V121 S122 S123 N124 Q125 S126 R131 M135 L136 S139 N140 P141 L142 L143 A149 L152 R153 N154 D155 F160 Y163 M166

S173 P174 I175 N181 Y182 L183 L184 E185 K186 T193 E196 H200 I201 L206 K207 G208 L209 S210 Q211 S212 D215 A223 P224 K230 K231 S232 G233 C234 F235 S238 T239 K247 I248 I249 G257 L258 L270 A271 L274 A282 E283 A284 A285 E286 Q287 R288

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	5555	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.7	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	169644	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	294.4, 294.4, 404.80002	wwPDB
Map dimensions	160, 160, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.84, 1.84, 1.84	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, HIC, CA

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	0.97	18/2984 (0.6%)	0.72	15/4040 (0.4%)
1	D	0.93	17/2984 (0.6%)	0.68	13/4040 (0.3%)
1	E	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
1	F	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
1	I	0.93	17/2984 (0.6%)	0.71	15/4040 (0.4%)
2	B	0.36	0/1107	0.31	0/1471
2	H	0.21	0/1107	0.33	0/1471
3	C	0.26	0/5594	0.39	0/7539
3	G	0.22	0/5594	0.38	0/7539
3	J	0.22	0/5594	0.38	0/7539
All	All	0.65	86/33916 (0.3%)	0.55	73/45759 (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	1
1	D	0	1
1	E	0	1
1	F	0	1
1	I	0	1
All	All	0	5

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	166	TYR	CD2-CE2	19.09	1.68	1.39
1	E	166	TYR	CD2-CE2	19.08	1.68	1.39
1	A	166	TYR	CD2-CE2	19.07	1.68	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	TYR	CD2-CE2	19.05	1.68	1.39
1	D	166	TYR	CD2-CE2	19.03	1.67	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	E	149	THR	C-N-CA	9.42	142.07	122.30
1	E	39	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	F	39	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	I	149	THR	C-N-CA	9.40	142.04	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	HIS	Sidechain
1	D	40	HIS	Sidechain
1	E	40	HIS	Sidechain
1	F	40	HIS	Sidechain
1	I	40	HIS	Sidechain

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	2934	0	2895	150	0
1	D	2934	0	2895	131	0
1	E	2934	0	2895	125	0
1	F	2934	0	2895	123	0
1	I	2934	0	2895	127	0
2	B	1104	0	1104	3	0
2	H	1104	0	1104	18	0
3	C	5494	0	5492	79	0
3	G	5494	0	5492	89	0
3	J	5494	0	5492	97	0
4	A	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	0	12	4	0
4	E	27	0	12	4	0
4	F	27	0	12	4	0
4	I	27	0	12	4	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	33500	0	33219	834	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 12.

The worst 5 of 834 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)
1:D:54:VAL:HG22	1:D:55:GLY:H	1.10	1.14
1:A:54:VAL:HG22	1:A:55:GLY:H	1.10	1.10
1:I:54:VAL:HG22	1:I:55:GLY:H	1.10	1.10
1:F:54:VAL:HG22	1:F:55:GLY:H	1.10	1.08
1:E:54:VAL:HG22	1:E:55:GLY:H	1.10	1.07

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	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	13
1	D	372/375 (99%)	288 (77%)	56 (15%)	28 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	13
1	F	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	13
1	I	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	13
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	687/697 (99%)	574 (84%)	78 (11%)	35 (5%)	2	19
3	G	687/697 (99%)	573 (83%)	80 (12%)	34 (5%)	2	20
3	J	687/697 (99%)	574 (84%)	79 (12%)	34 (5%)	2	20
All	All	4189/4238 (99%)	3433 (82%)	513 (12%)	243 (6%)	3	18

5 of 243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	51	ASP

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/317 (100%)	289 (91%)	28 (9%)	10	31
1	D	317/317 (100%)	289 (91%)	28 (9%)	10	31
1	E	317/317 (100%)	286 (90%)	31 (10%)	8	26
1	F	317/317 (100%)	286 (90%)	31 (10%)	8	26
1	I	317/317 (100%)	286 (90%)	31 (10%)	8	26
2	B	118/118 (100%)	118 (100%)	0	100	100
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	580 (95%)	29 (5%)	25	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	609/616 (99%)	575 (94%)	34 (6%)	21	46
3	J	609/616 (99%)	575 (94%)	34 (6%)	21	46
All	All	3648/3669 (99%)	3402 (93%)	246 (7%)	20	41

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	375	PHE
3	J	184	LEU
1	F	326	LYS
3	J	143	LEU
3	J	550	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
3	J	200	HIS
3	G	76	HIS
3	J	181	ASN
3	J	395	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	HIC	A	73	1	8,11,12	1.59	2 (25%)	6,14,16	1.88	2 (33%)
1	HIC	F	73	1	8,11,12	1.60	2 (25%)	6,14,16	1.89	2 (33%)
1	HIC	E	73	1	8,11,12	1.60	2 (25%)	6,14,16	1.89	2 (33%)
1	HIC	D	73	1	8,11,12	1.59	2 (25%)	6,14,16	1.87	2 (33%)
1	HIC	I	73	1	8,11,12	1.60	2 (25%)	6,14,16	1.88	2 (33%)

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
1	HIC	A	73	1	-	2/5/6/8	0/1/1/1
1	HIC	F	73	1	-	2/5/6/8	0/1/1/1
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1
1	HIC	I	73	1	-	2/5/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	HIC	CA-N	2.80	1.56	1.48
1	I	73	HIC	CA-N	2.79	1.56	1.48
1	F	73	HIC	CA-N	2.79	1.56	1.48
1	A	73	HIC	CA-N	2.79	1.56	1.48
1	D	73	HIC	CA-N	2.78	1.56	1.48

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	73	HIC	CB-CA-C	-3.75	104.43	111.47
1	D	73	HIC	CB-CA-C	-3.75	104.44	111.47
1	E	73	HIC	CB-CA-C	-3.75	104.44	111.47
1	A	73	HIC	CB-CA-C	-3.74	104.45	111.47
1	F	73	HIC	CB-CA-C	-3.74	104.47	111.47

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

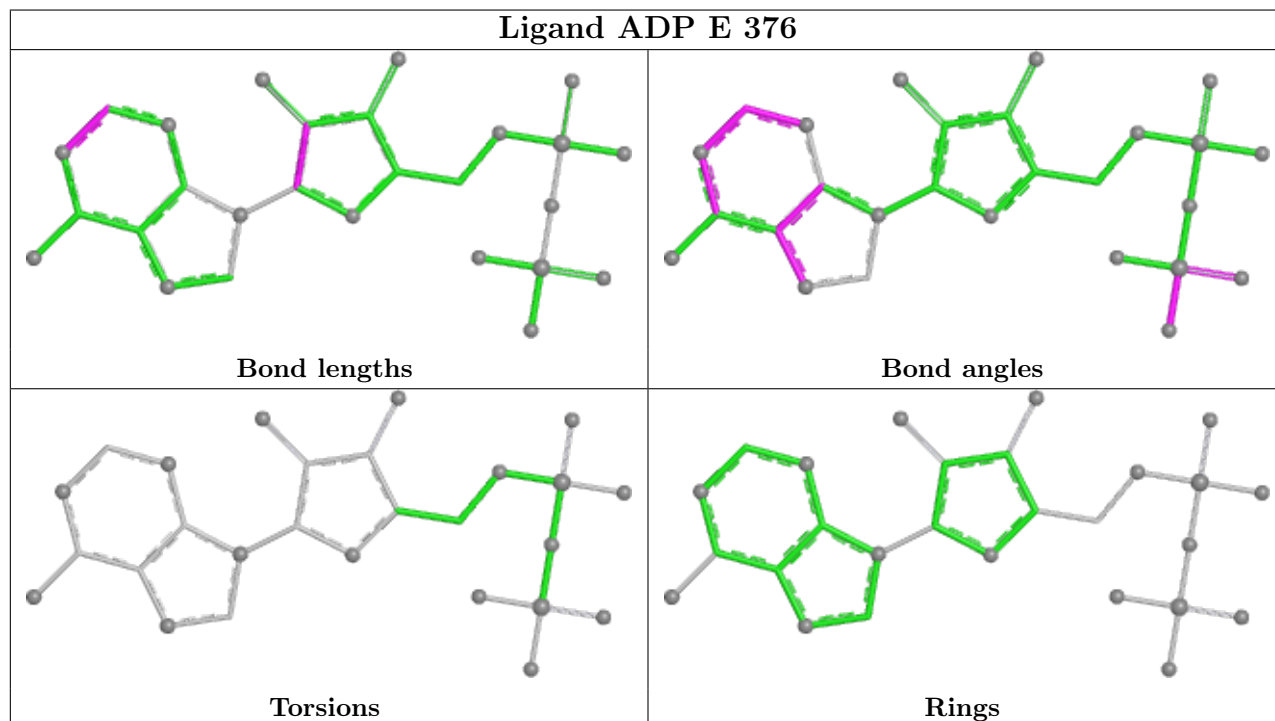| Mol	Chain	Res	Type	Atoms
1	A	73	HIC	N-CA-CB-CG
1	A	73	HIC	C-CA-CB-CG
1	D	73	HIC	N-CA-CB-CG
1	D	73	HIC	C-CA-CB-CG
1	E	73	HIC	N-CA-CB-CG

There are no ring outliers.
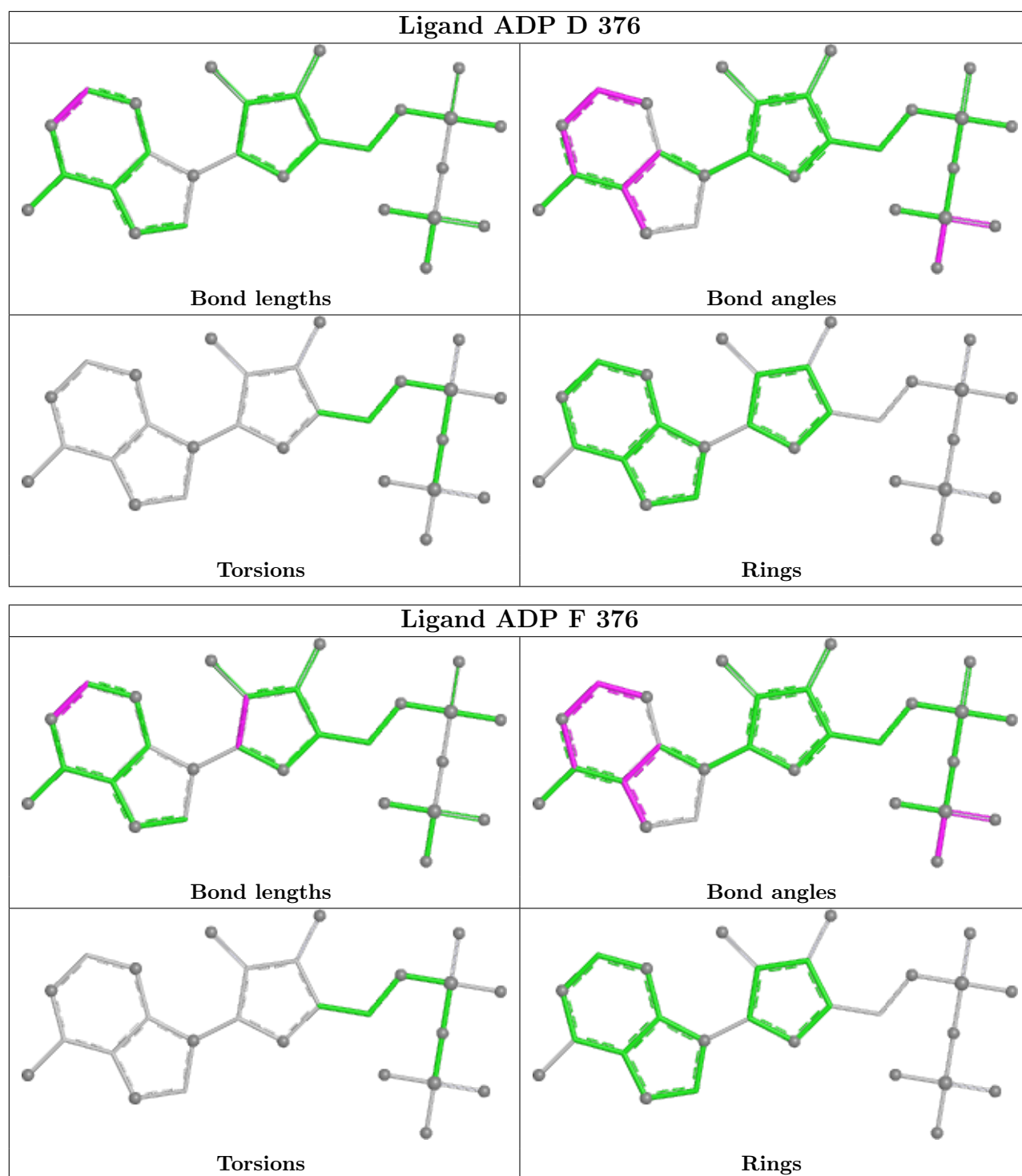
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0
1	F	73	HIC	2	0
1	E	73	HIC	2	0
1	D	73	HIC	2	0
1	I	73	HIC	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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	$\#|Z| > 2$
4	ADP	E	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (13%)
4	ADP	A	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (13%)
4	ADP	I	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (13%)
4	ADP	D	376	-	24,29,29	1.20	1 (4%)	29,45,45	1.40	4 (13%)
4	ADP	F	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	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
4	ADP	E	376	-	-	0/12/32/32	0/3/3/3
4	ADP	A	376	-	-	0/12/32/32	0/3/3/3
4	ADP	I	376	-	-	0/12/32/32	0/3/3/3
4	ADP	D	376	-	-	0/12/32/32	0/3/3/3
4	ADP	F	376	-	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	376	ADP	C2-N1	3.02	1.39	1.33
4	D	376	ADP	C2-N1	3.00	1.39	1.33
4	I	376	ADP	C2-N1	2.99	1.39	1.33
4	F	376	ADP	C2-N1	2.98	1.39	1.33
4	E	376	ADP	C2-N1	2.95	1.39	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	376	ADP	C4-C5-N7	3.96	113.52	109.40
4	I	376	ADP	C4-C5-N7	3.94	113.50	109.40
4	F	376	ADP	C4-C5-N7	3.92	113.49	109.40
4	A	376	ADP	C4-C5-N7	3.89	113.45	109.40
4	D	376	ADP	C4-C5-N7	3.87	113.43	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	376	ADP	4	0
4	A	376	ADP	4	0
4	I	376	ADP	4	0
4	D	376	ADP	4	0
4	F	376	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 E 376

Bond lengths — Bond angles — Torsions — Rings

Ligand ADP A 376

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP I 376

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 376

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 376

Bond lengths

Bond angles

Torsions

Rings
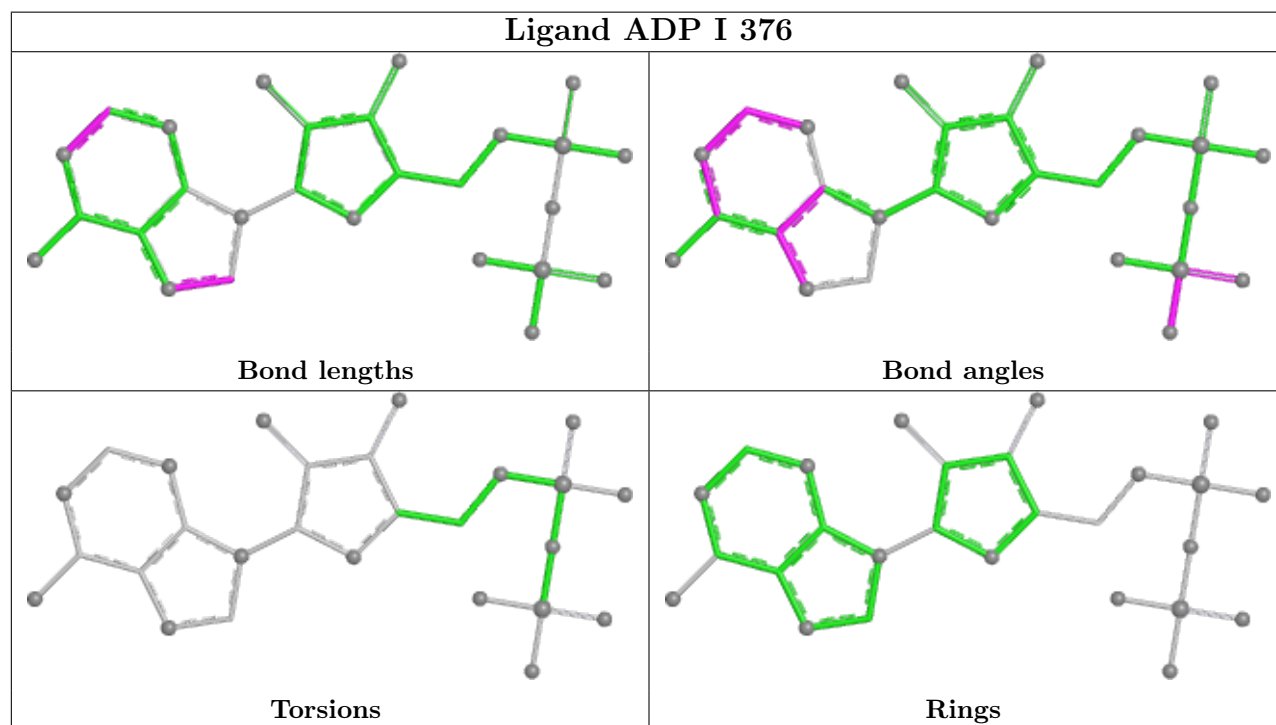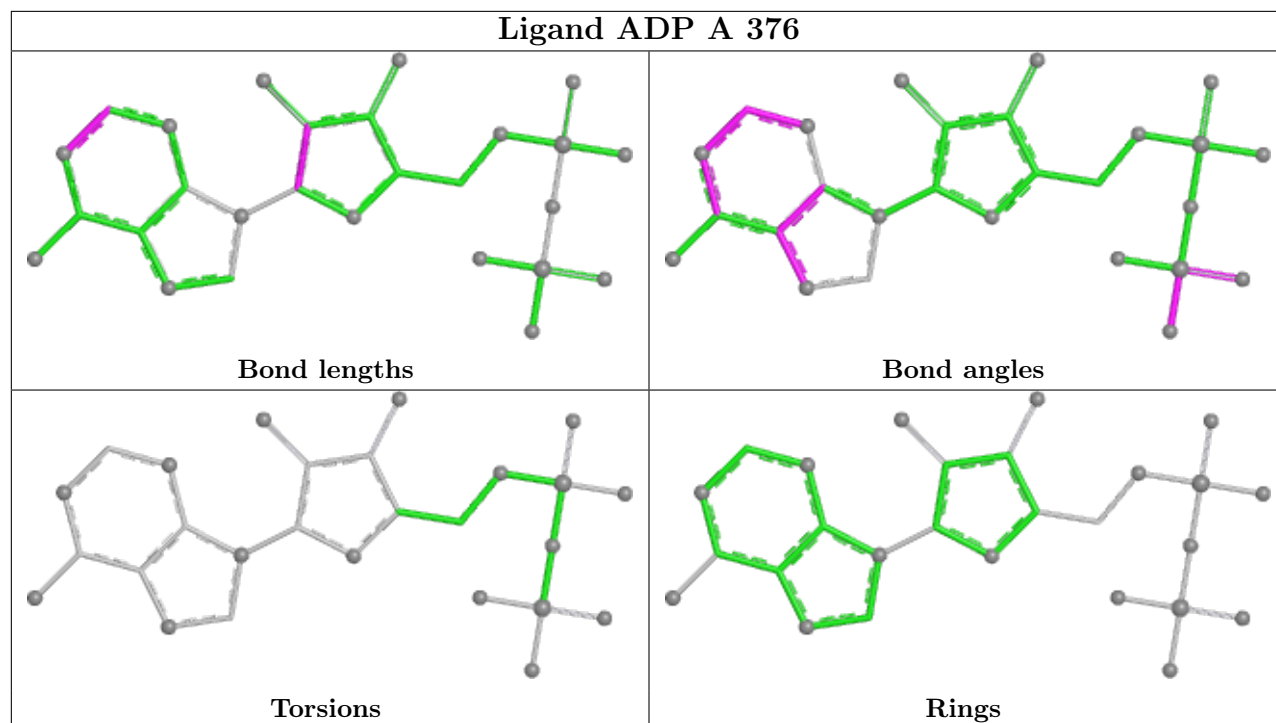
5.7   Other polymers ⓘ

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-1989. 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
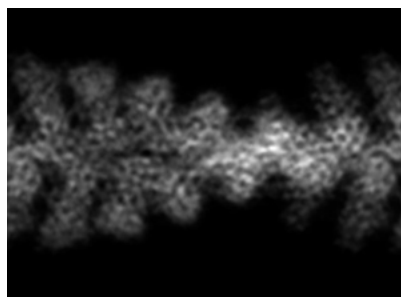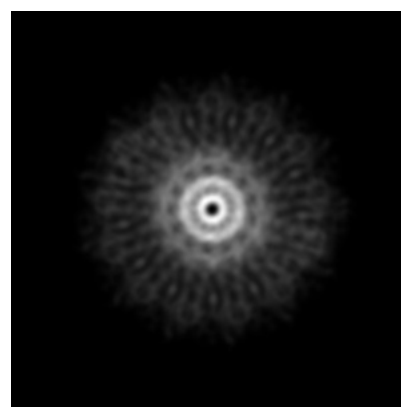
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
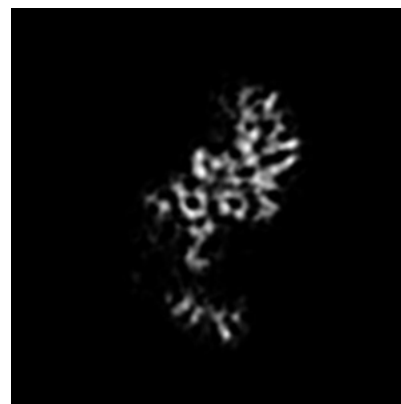
X Index: 80	Y Index: 80	Z Index: 110

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

6.3 Largest variance slices (i)

6.3.1 Primary map
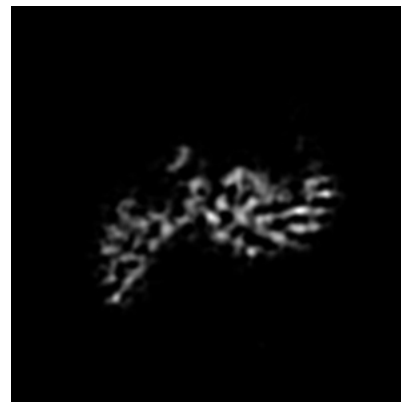
| X Index: 83 | Y Index: 77 | Z Index: 56 |

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 |
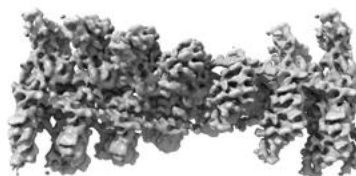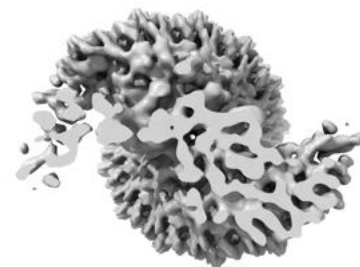
The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5　Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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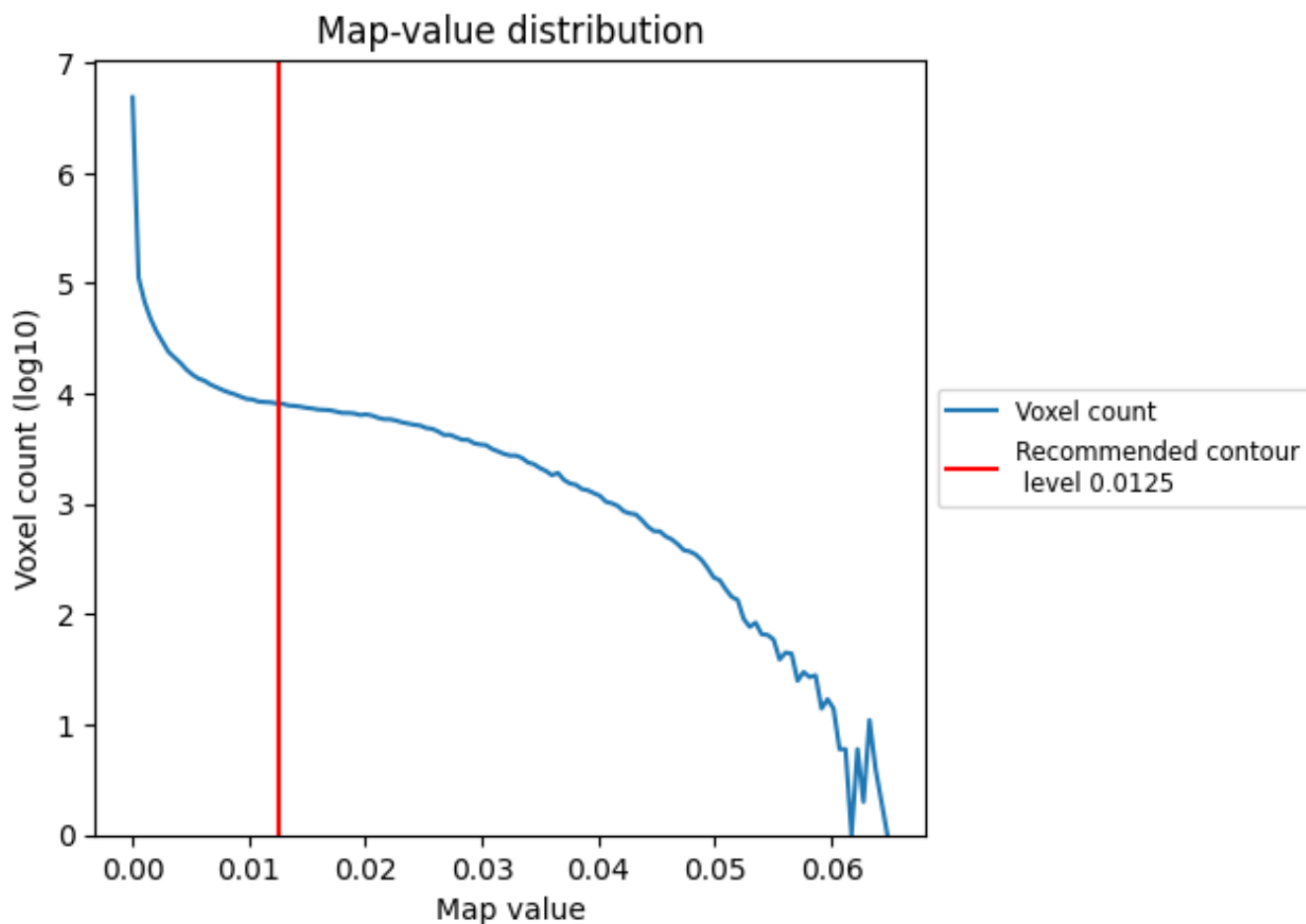
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
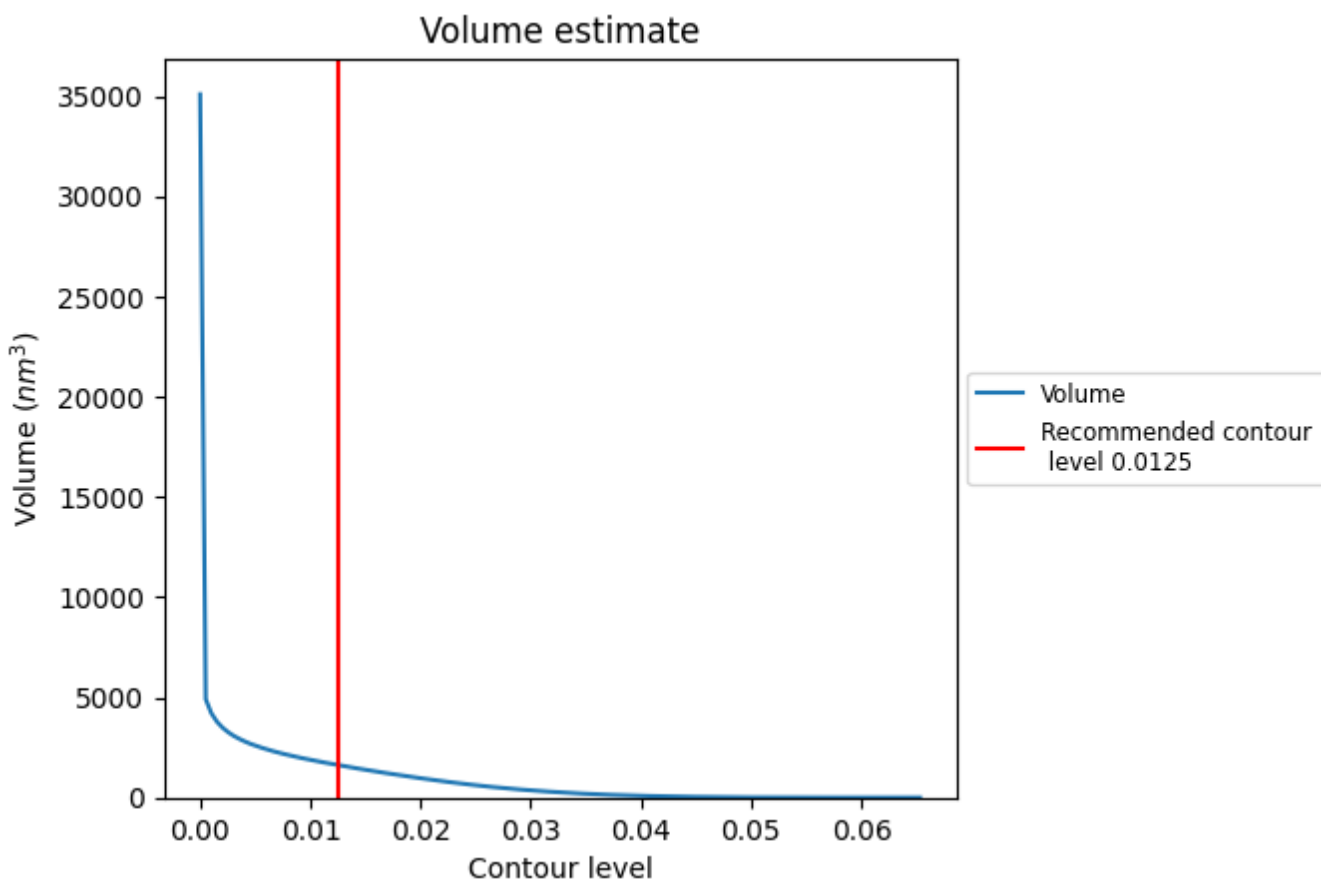
The volume at the recommended contour level is 1624 nm^3; this corresponds to an approximate mass of 1467 kDa.

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

7.3   Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-1989 and PDB model 4A7L. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ
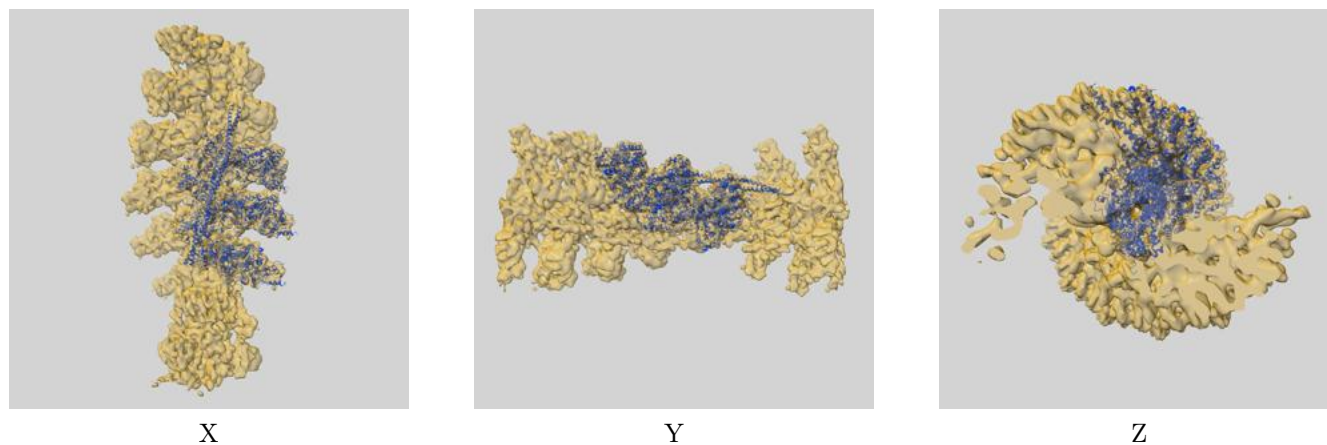
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0125 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   ⓘ
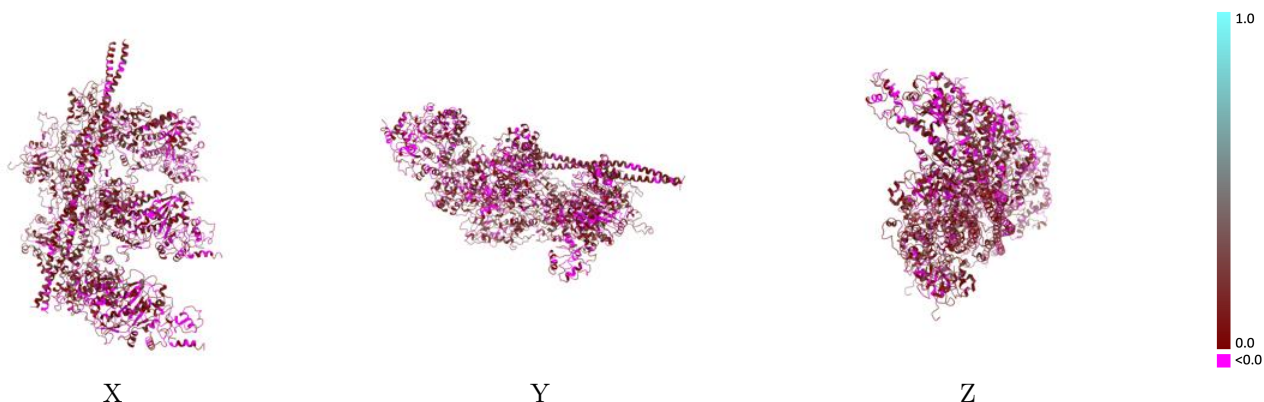
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
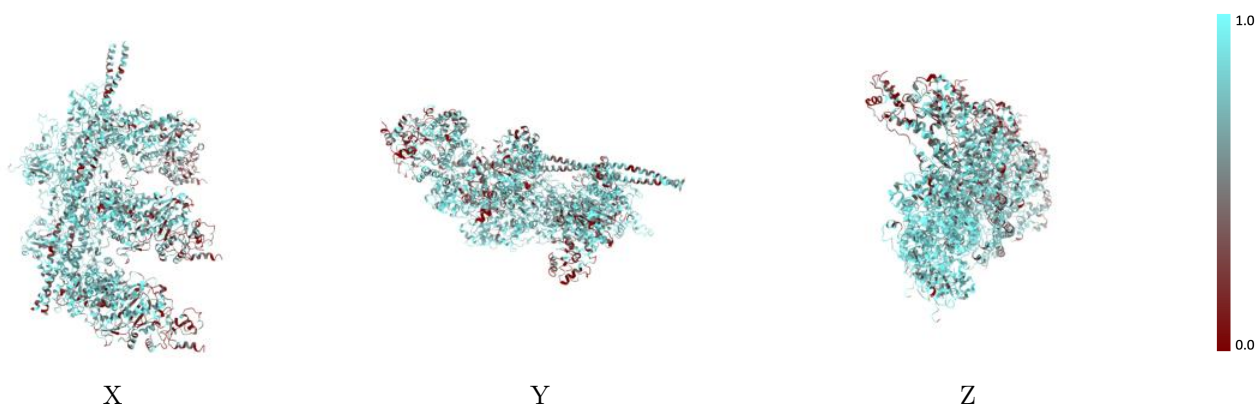
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

9.4   Atom inclusion ⓘ
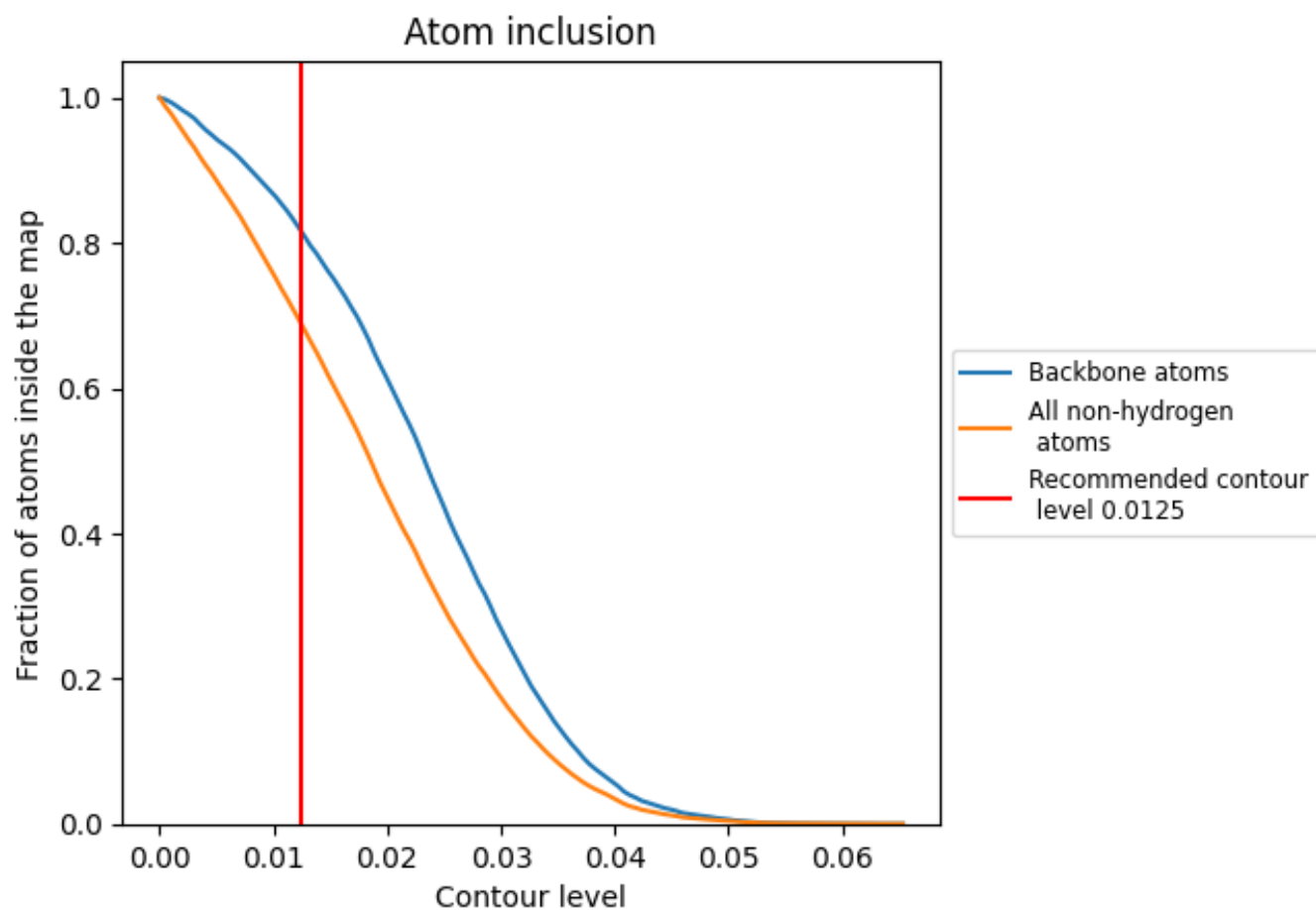
At the recommended contour level, 81% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.0880
A	0.8076	0.1160
B	0.6258	0.1070
C	0.5852	0.0650
D	0.8070	0.1120
E	0.8056	0.1130
F	0.8100	0.1120
G	0.5898	0.0650
H	0.6046	0.0780
I	0.8083	0.1130
J	0.5896	0.0650

1.0

0.0
<0.0