wwPDB EM Validation Summary Report (i)

Feb 24, 2024 – 04:16 PM EST

PDB ID	:	7JH7
EMDB ID	:	EMD-22335
Title	:	cardiac actomyosin complex
Authors	:	Galkin, V.E.; Schroeder, G.F.
Deposited on	:	2020-07-20
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

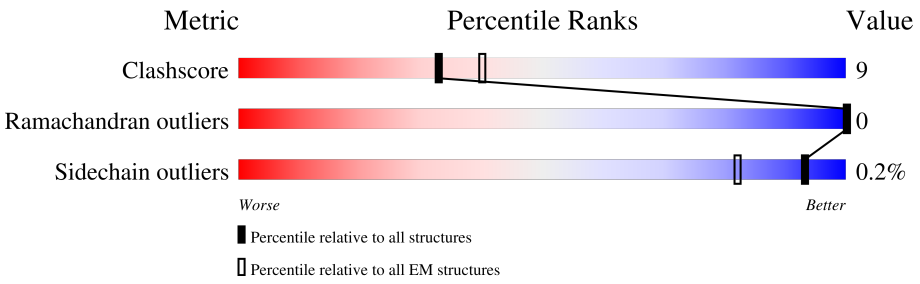
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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 <=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	377	77% 21%
1	B	377	77% 21%
1	C	377	79% 20%
1	D	377	77% 21%
1	E	377	78% 20%
2	F	1935	8% 30% 8% 62%
2	G	1935	9% 30% 8% 62%
2	H	1935	9% 30% 8% 62%

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Mol	Chain	Length	Quality of chain
3	I	135	33% 100%
3	J	135	41% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	C	401	-	-	X	-
4	ADP	E	401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33924 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 cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	371	2903	1840	489	553	21	1	0
1	B	371	2903	1840	489	553	21	1	0
1	C	371	2903	1840	489	553	21	1	0
1	E	371	2903	1840	489	553	21	1	0
1	D	371	2903	1840	489	553	21	1	0

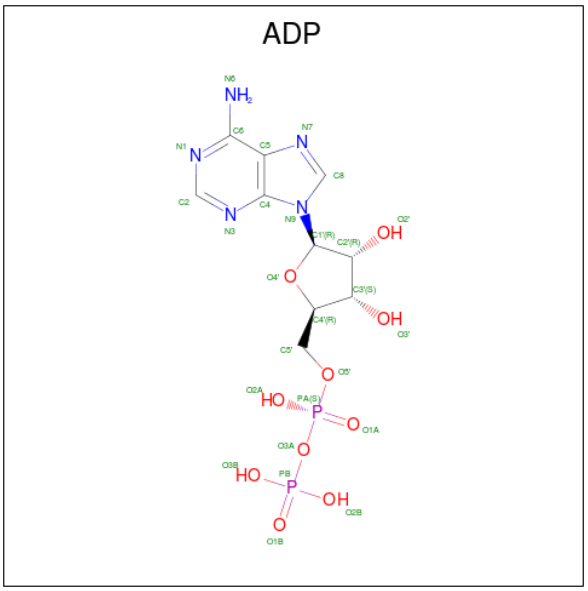
- Molecule 2 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	742	5973	3816	1017	1109	31	0	0
2	G	742	5973	3816	1017	1109	31	0	0
2	H	742	5973	3816	1017	1109	31	0	0

- Molecule 3 is a protein called tropomyosin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	I	135	675	405	135	135	0	0
3	J	135	675	405	135	135	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

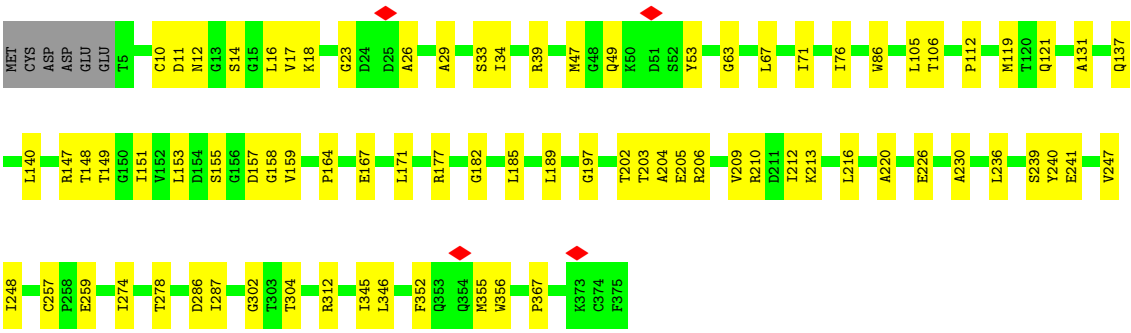
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

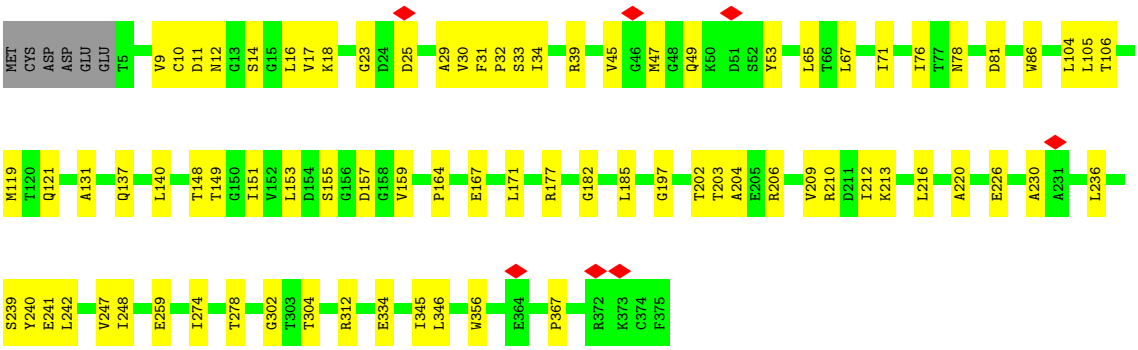
• Molecule 1: Actin, alpha cardiac muscle 1

Chain A:



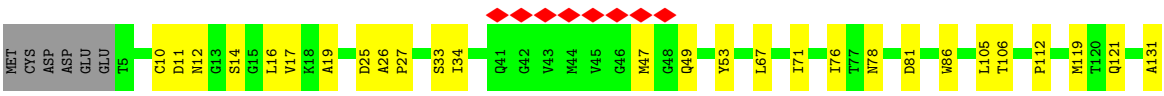
• Molecule 1: Actin, alpha cardiac muscle 1

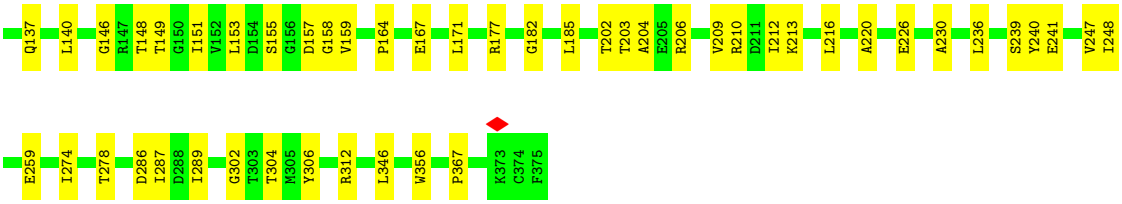
Chain B:



• Molecule 1: Actin, alpha cardiac muscle 1

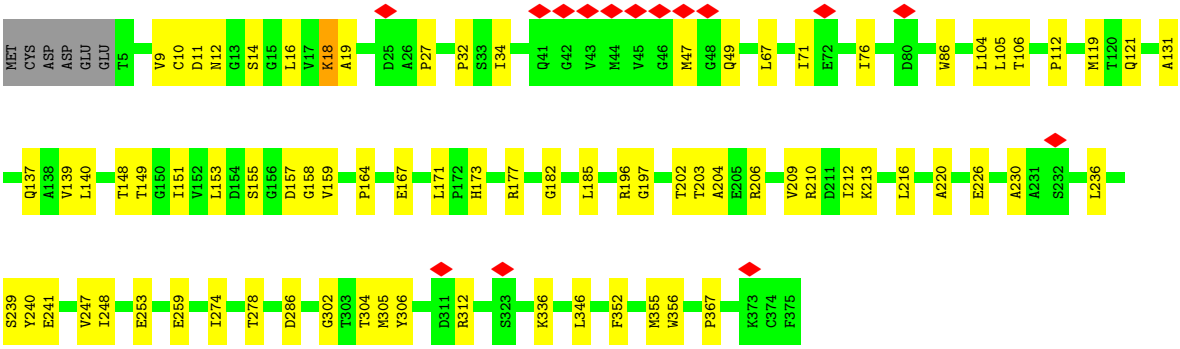
Chain C:





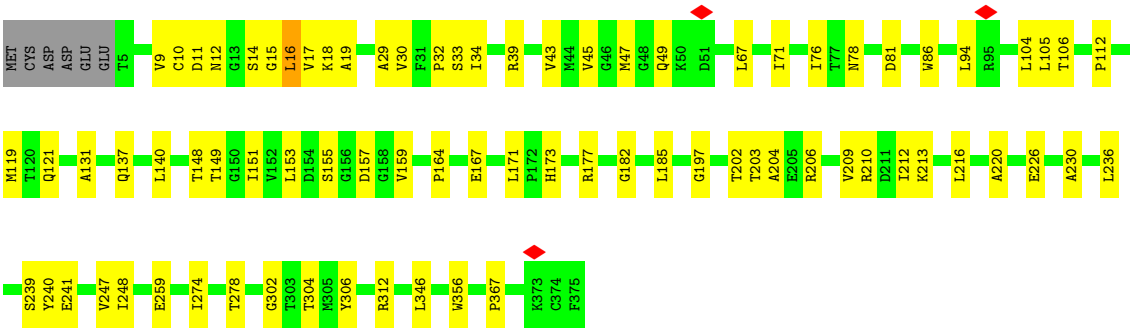
- Molecule 1: Actin, alpha cardiac muscle 1

Chain E:



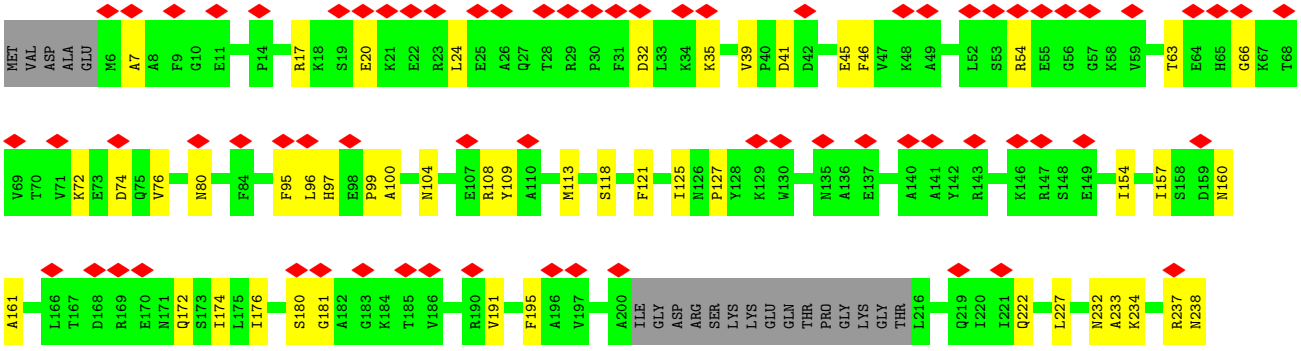
- Molecule 1: Actin, alpha cardiac muscle 1

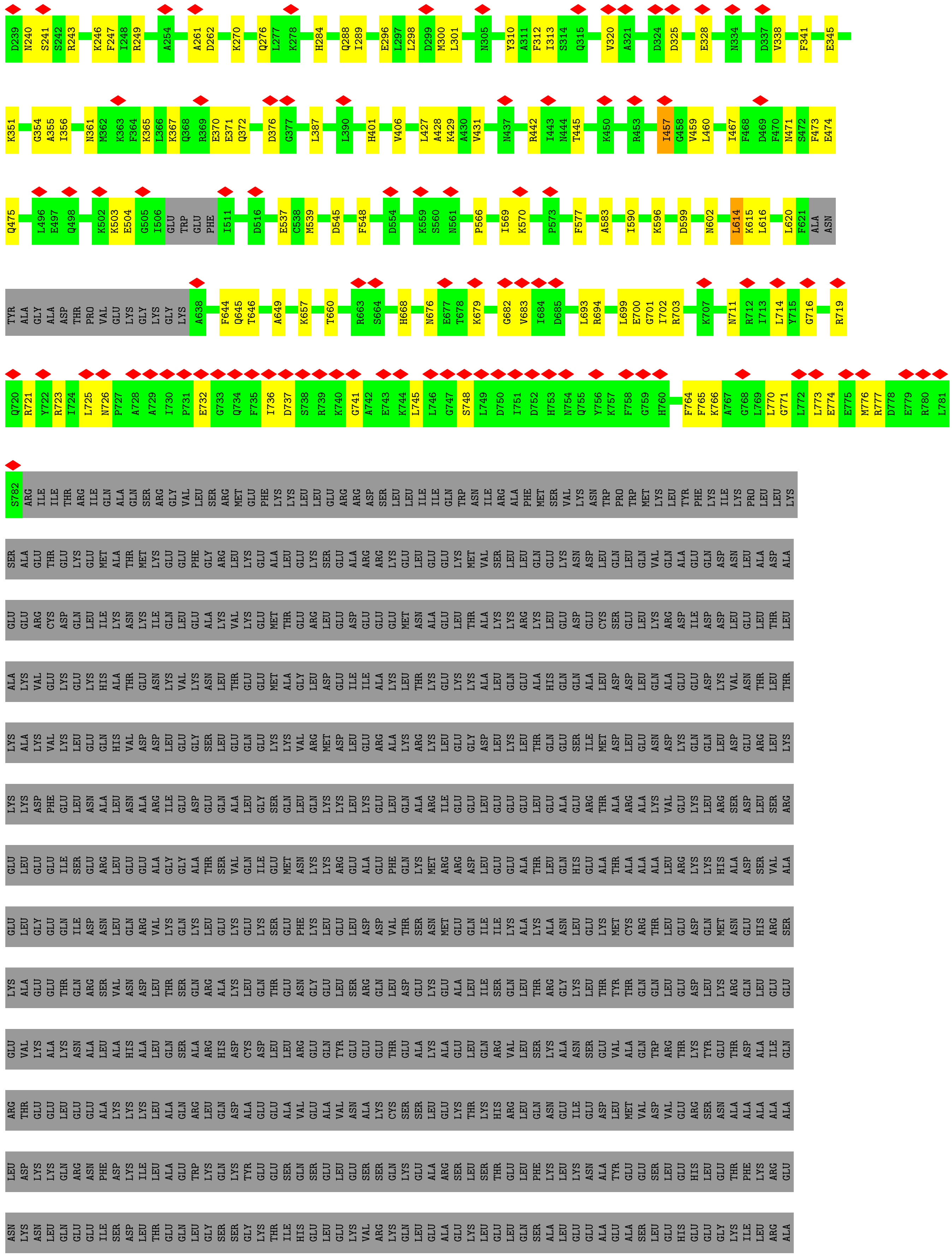
Chain D:



- Molecule 2: Myosin-7

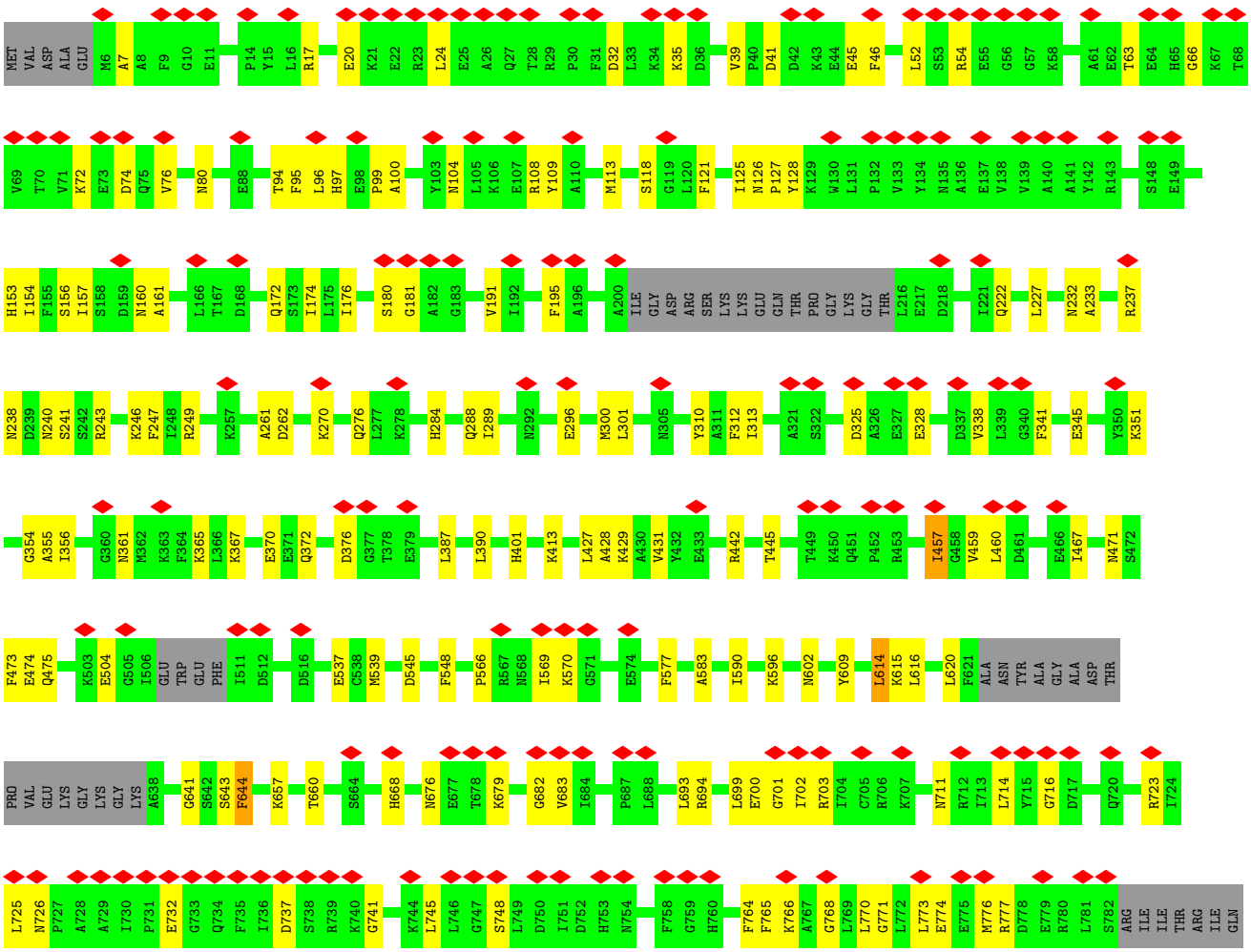
Chain F:




D239 N240 S241 S242 R243 K246 F247 I248 R249 A254 A261 D262 K270 Q276 L277 K278 H284 Q288 I289 E296 L297 L298 D299 M300 L301 N305 Y310 A311 F312 I313 S314 Q315 V320 A321 D324 D325 E328 N334 D337 V338 F341 E345
K351 G354 A355 I356 N361 M362 K363 F364 K365 L366 K367 Q368 R369 E370 E371 Q372 D376 G377 L387 L390 H401 V406 L427 A428 K429 A430 V431 N437 R442 I443 N444 T445 K450 R453 I457 G458 V459 L460 I467 F468 D469 F470 N471 S472 F473 E474
Q475 L496 E497 Q498 K502 K503 E504 G505 I506 GLU TRP GLU PHE I511 D516 E537 C538 M539 D545 F548 D554 K559 S560 N561 P566 I569 K570 P573 F577 A583 I590 K596 D599 N602 L614 K615 L616 L620 F621 ALA ASN
TYR ALA GLY ALA ASP THR PRO VAL GLU LYS GLY LYS GLY LYS A638 F644 Q645 T646 A649 K657 T660 R663 S664 H668 N676 E677 T678 K679 G682 V683 I684 D685 L693 R694 L699 E700 G701 I702 R703 K707 N711 R712 I713 L714 Y715 G716 R719
Q720 R721 Y722 R723 I724 L725 N726 P727 A728 A729 I730 P731 E732 G733 Q734 F735 I736 D737 S738 R739 K740 G741 A742 E743 K744 L745 L746 G747 S748 L749 D750 I751 D752 H753 N754 Q755 Y756 K757 F758 G759 H760 F764 F765 K766 A767 G768 L769 L770 G771 L772 L773 E774 E775 M776 R777 D778 E779 R780 L781
S782

- Molecule 2: Myosin-7

Chain G:



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

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

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

ALA THR GLU ASN LYS VAL LYS ASN LEU THR GLU GLU MET ALA GLY LEU ASP GLU ILE ILE ALA LYS LEU THR LYS GLU LYS LYS ALA LEU GLN GLU ALA HIS GLN GLN ALA LEU ASP ASP LEU GLN ALA GLU GLU ASP LYS VAL ASN THR LEU THR LYS ALA LYS VAL LYS LEU GLU GLN

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

LEU ASN ALA ARG ILE GLU ASP GLU GLN ALA LEU GLY SER GLN LEU GLN LYS LYS LEU LYS GLU LEU GLN ALA ARG ILE GLU GLU LEU GLU GLU GLU LEU GLU ALA GLU ARG THR ALA ARG ALA LYS VAL GLU LYS LEU ARG SER ASP LEU SER ARG GLU LEU GLU GLU ILE SER GLU ARG

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

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

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

ALA HIS ALA LEU GLN SER ALA ARG HIS ASP CYS ASP LEU LEU ARG GLU GLN TYR GLU GLU THR GLU ALA LYS ALA GLU LEU GLN ARG VAL LEU SER LYS ALA ASN SER GLU VAL ALA GLN TRP ARG THR LYS TYR GLU THR ASP ALA ILE GLN ARG THR GLU GLU LEU GLU GLU ALA

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

ASP LYS ILE LEU ALA GLU TRP LYS GLN LYS TYR GLU GLU SER GLN SER GLU LEU GLU SER SER GLN LYS GLU ALA ARG SER LEU SER THR GLU LEU PHE LYS LEU LYS ASN ALA TYR GLU GLU SER LEU GLU HIS LEU GLU THR PHE LYS ARG GLU ASN LYS ASN LEU GLN GLU GLU ILE

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

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

SER HIS ALA ASN ARG MET ALA ALA GLU ALA GLN LYS GLN VAL LYS SER LEU GLN SER LEU LEU LYS ASP THR GLN ILE GLN LEU ASP ASP ALA VAL ARG ALA ASN ASP ASP LEU LYS GLU ASN ILE ALA ILE VAL GLU ARG ARG ASN ASN LEU LEU GLN ALA GLU LEU GLU GLU LEU ARG

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

ASN ALA GLU GLU LYS ALA LYS LYS ALA ILE THR ASP ALA ALA MET MET ALA GLU GLU LEU LYS LYS GLU GLN ASP THR SER ALA HIS LEU GLU ARG MET LYS LYS ASN MET GLU GLN THR ILE LYS ASP LEU GLN HIS ARG LEU ASP GLU ALA GLU GLN ILE ALA LEU LYS GLY GLY LYS

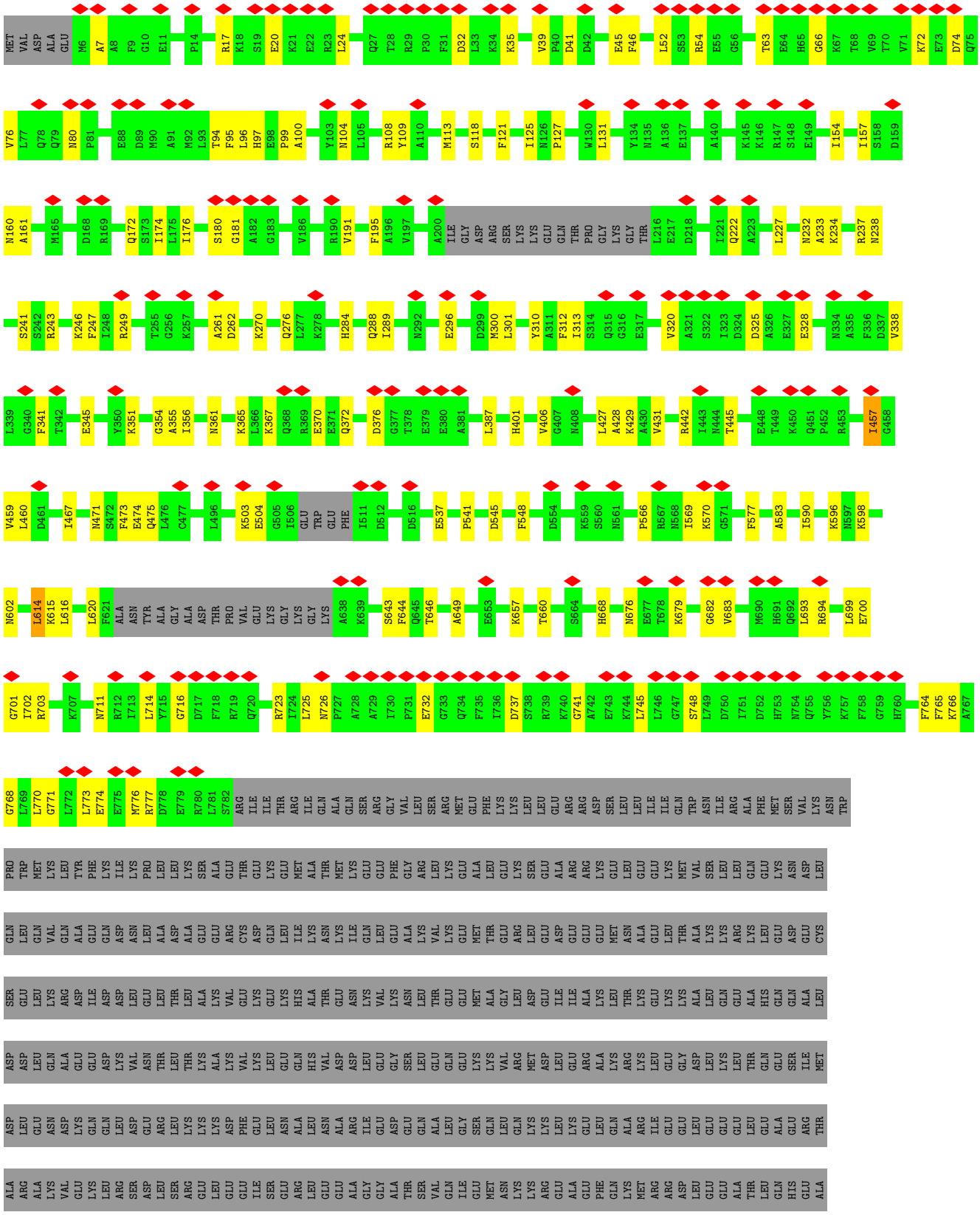
LYS GLN LEU GLN LYS LEU GLU ALA ARG VAL ARG GLU LEU GLU ASN GLU LEU GLU ALA GLU GLN LYS ARG ASN ALA GLU SER VAL LYS GLY MET ARG LYS SER GLU ARG ARG ILE LYS GLU LEU THR TYR GLN THR GLU GLU ASP ARG LYS ASN LEU LEU ARG LEU GLN ASP LEU VAL ASP

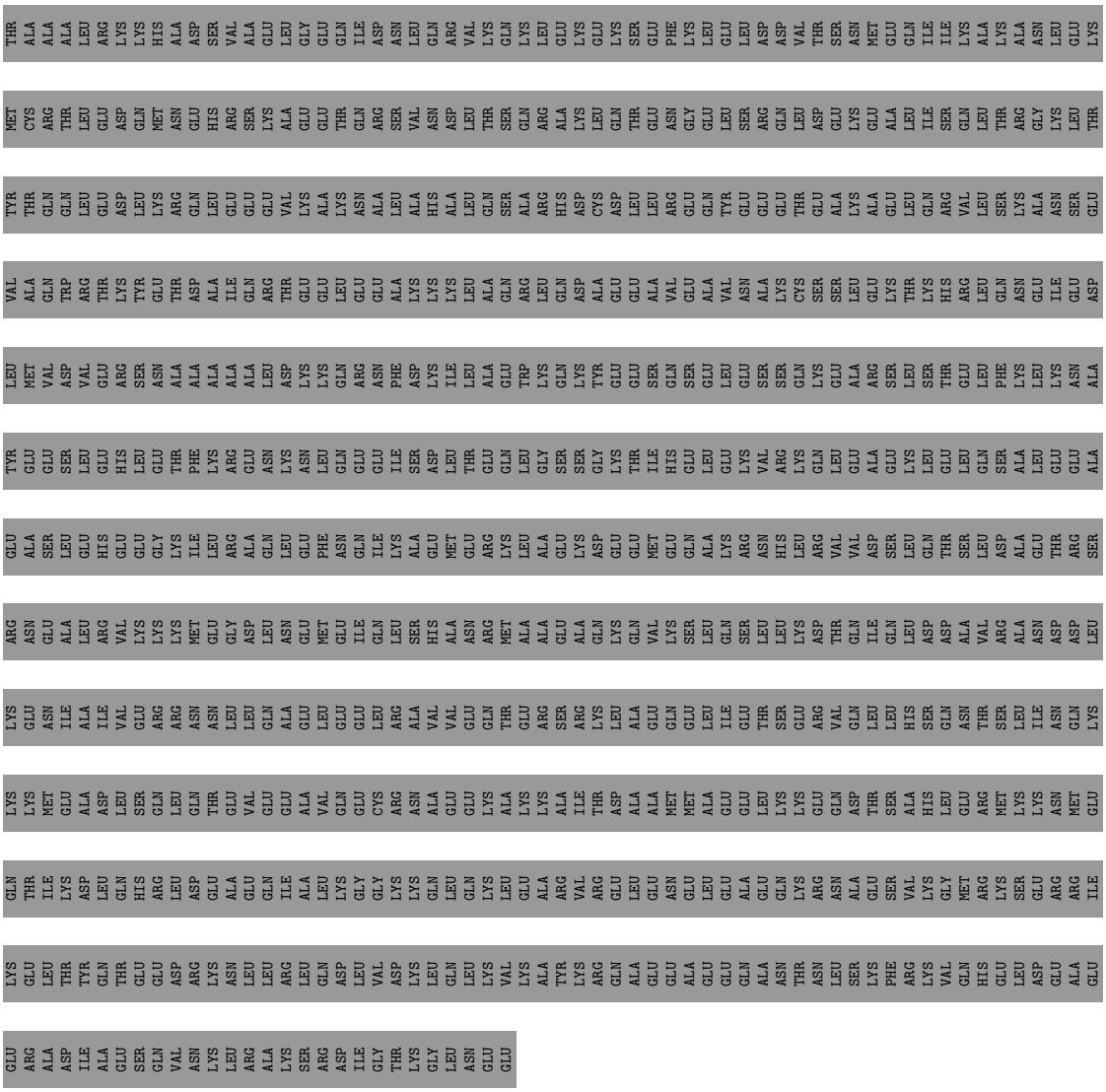
LYS LEU GLN LEU LYS VAL LYS ALA TYR LYS ARG GLN ALA GLU GLU ALA GLU GLU GLN ALA ASN THR ASN LEU SER LYS PHE ARG LYS VAL GLN HIS GLU LEU ASP GLU ALA GLU GLU ARG ALA ASP ILE ALA GLU SER GLN VAL ASN LYS LEU ARG ALA LYS SER ARG ASP ILE GLY THR

LYS GLY LEU ASN GLU GLU

• Molecule 2: Myosin-7

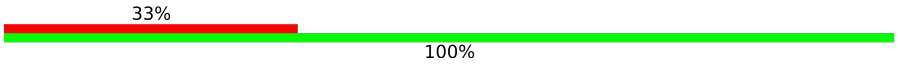
Chain H: 9% 30% 8% 62%

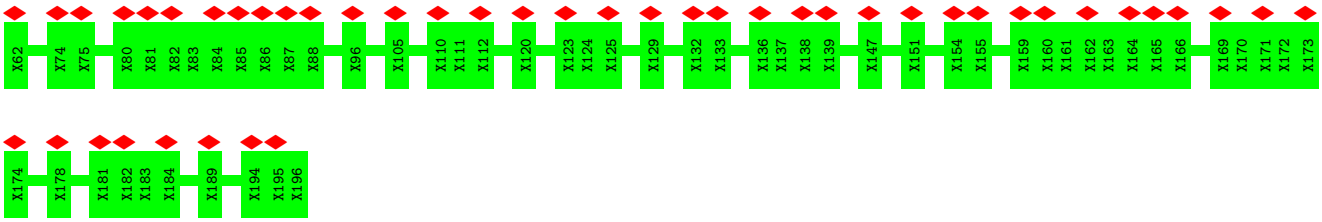




• Molecule 3: tropomyosin

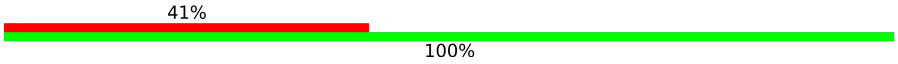
Chain I:

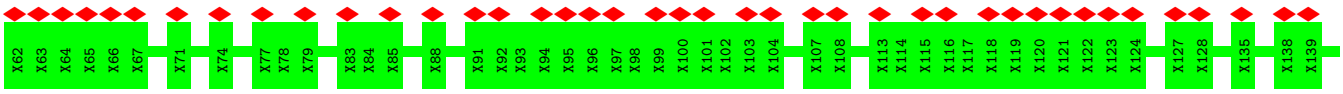


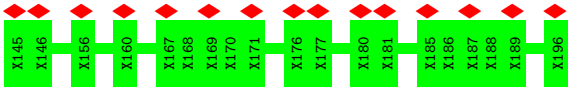


• Molecule 3: tropomyosin

Chain J:






X145
X146
X156
X160
X167
X168
X169
X170
X171
X176
X177
X180
X181
X185
X186
X187
X188
X189
X196

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.7°, rise=27.3 Å, axial sym=C1	Depositor
Number of segments used	115746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	18.425	Depositor
Minimum map value	-7.830	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	140.448, 163.68, 235.48799	wwPDB
Map dimensions	133, 155, 223	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.36	0/2969	0.58	0/4021
1	B	0.36	0/2969	0.58	0/4021
1	C	0.36	0/2969	0.58	0/4021
1	D	0.36	0/2969	0.58	0/4021
1	E	0.36	0/2969	0.58	0/4021
2	F	0.33	0/6097	0.58	1/8213 (0.0%)
2	G	0.33	0/6097	0.58	1/8213 (0.0%)
2	H	0.33	0/6097	0.58	1/8213 (0.0%)
All	All	0.34	0/33136	0.58	3/44744 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	457	ILE	N-CA-C	-5.77	95.42	111.00
2	F	457	ILE	N-CA-C	-5.76	95.46	111.00
2	G	457	ILE	N-CA-C	-5.74	95.51	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2903	0	2880	61	0
1	B	2903	0	2880	71	0
1	C	2903	0	2880	73	0
1	D	2903	0	2880	61	0
1	E	2903	0	2880	70	0
2	F	5973	0	5953	104	0
2	G	5973	0	5953	110	0
2	H	5973	0	5953	99	0
3	I	675	0	137	0	0
3	J	675	0	137	0	0
4	A	27	0	12	3	0
4	B	27	0	12	4	0
4	C	27	0	12	13	0
4	D	27	0	12	6	0
4	E	27	0	12	11	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	33924	0	32593	612	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 9.

The worst 5 of 612 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:C:14:SER:OG	1:C:158:GLY:HA3	1.28	1.26
1:C:12:ASN:OD1	1:C:119:MET:CE	1.90	1.19
1:C:14:SER:OG	1:C:158:GLY:CA	1.94	1.15
1:C:12:ASN:OD1	1:C:119:MET:HE1	0.95	1.11
1:B:23:GLY:HA2	2:G:644:PHE:CE2	1.85	1.10

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/377 (98%)	350 (95%)	20 (5%)	0	100	100
1	B	370/377 (98%)	350 (95%)	20 (5%)	0	100	100
1	C	370/377 (98%)	350 (95%)	20 (5%)	0	100	100
1	D	370/377 (98%)	350 (95%)	20 (5%)	0	100	100
1	E	370/377 (98%)	351 (95%)	19 (5%)	0	100	100
2	F	734/1935 (38%)	677 (92%)	57 (8%)	0	100	100
2	G	734/1935 (38%)	677 (92%)	57 (8%)	0	100	100
2	H	734/1935 (38%)	677 (92%)	57 (8%)	0	100	100
All	All	4052/7690 (53%)	3782 (93%)	270 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/320 (98%)	314 (100%)	1 (0%)	92	96
1	B	315/320 (98%)	315 (100%)	0	100	100
1	C	315/320 (98%)	314 (100%)	1 (0%)	92	96
1	D	315/320 (98%)	314 (100%)	1 (0%)	92	96
1	E	315/320 (98%)	314 (100%)	1 (0%)	92	96
2	F	644/1697 (38%)	643 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	644/1697 (38%)	642 (100%)	2 (0%)	92	96
2	H	644/1697 (38%)	643 (100%)	1 (0%)	93	97
All	All	3507/6691 (52%)	3499 (100%)	8 (0%)	93	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	16	LEU
1	E	18	LYS
1	C	16	LEU
2	G	644	PHE
2	H	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	HIS
2	H	401	HIS
1	C	296	ASN
2	H	171	ASN
2	H	676	ASN

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 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	401	5	24,29,29	1.17	3 (12%)	29,45,45	1.51	5 (17%)
4	ADP	B	401	5	24,29,29	1.15	3 (12%)	29,45,45	1.51	5 (17%)
4	ADP	D	401	5	24,29,29	1.16	3 (12%)	29,45,45	1.52	5 (17%)
4	ADP	A	401	5	24,29,29	1.16	3 (12%)	29,45,45	1.51	5 (17%)
4	ADP	C	401	5	24,29,29	1.16	3 (12%)	29,45,45	1.51	5 (17%)

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	401	5	-	0/12/32/32	0/3/3/3
4	ADP	B	401	5	-	0/12/32/32	0/3/3/3
4	ADP	D	401	5	-	0/12/32/32	0/3/3/3
4	ADP	A	401	5	-	0/12/32/32	0/3/3/3
4	ADP	C	401	5	-	0/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-C4	2.71	1.48	1.40
4	B	401	ADP	C5-C4	2.68	1.48	1.40
4	E	401	ADP	C5-C4	2.66	1.48	1.40
4	E	401	ADP	C2'-C1'	-2.66	1.49	1.53
4	A	401	ADP	C5-C4	2.66	1.48	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401	ADP	PA-O3A-PB	-4.01	119.08	132.83
4	B	401	ADP	PA-O3A-PB	-4.00	119.09	132.83
4	C	401	ADP	PA-O3A-PB	-4.00	119.09	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	ADP	PA-O3A-PB	-3.99	119.12	132.83
4	D	401	ADP	PA-O3A-PB	-3.98	119.18	132.83

There are no chirality outliers.

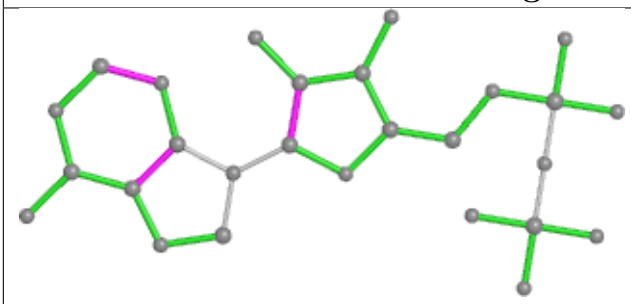
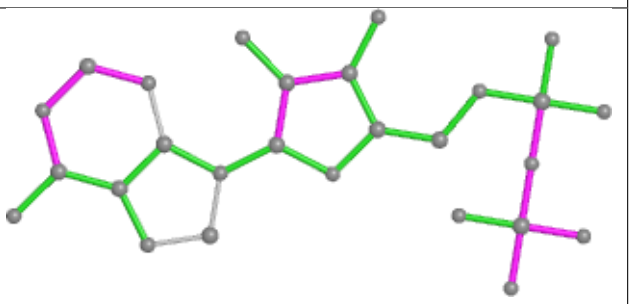
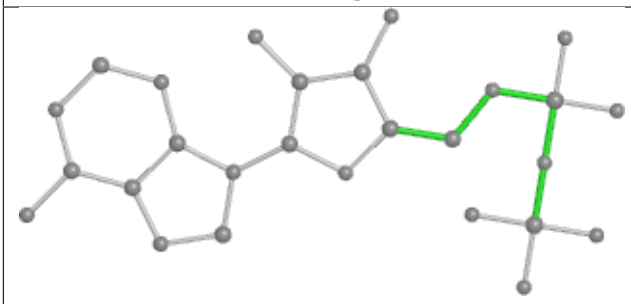
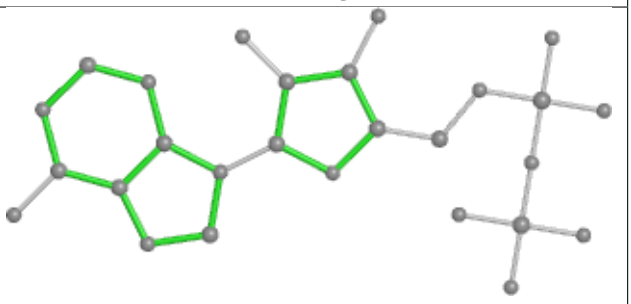
There are no torsion outliers.

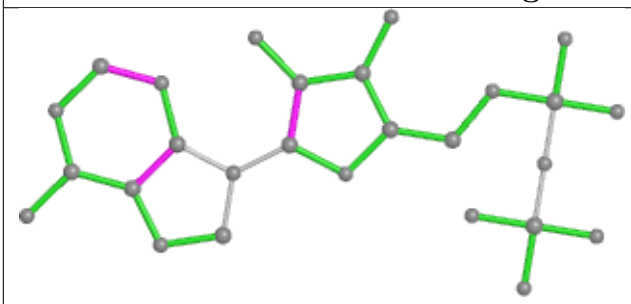
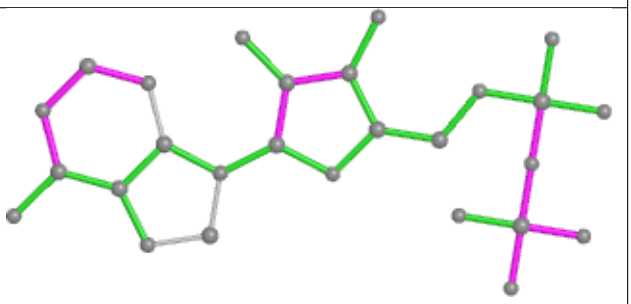
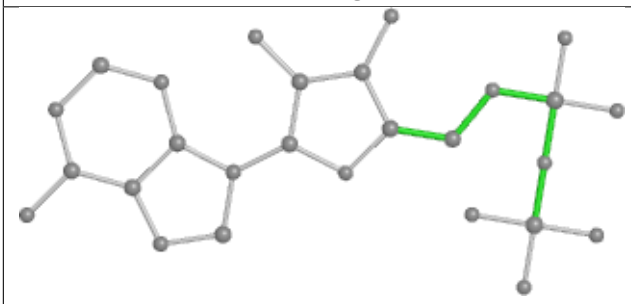
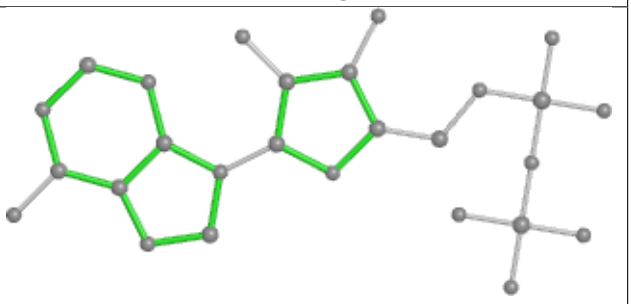
There are no ring outliers.

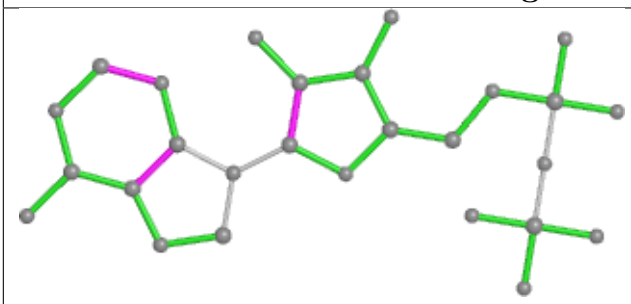
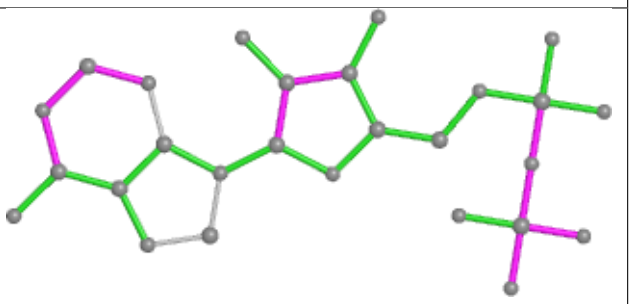
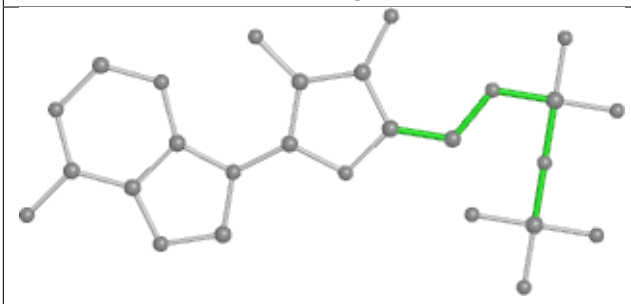
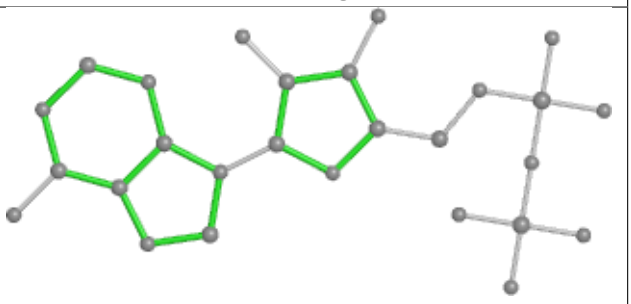
5 monomers are involved in 37 short contacts:

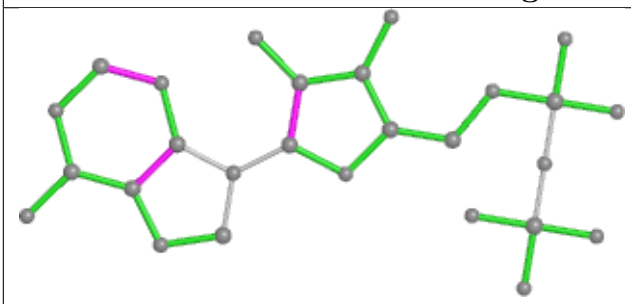
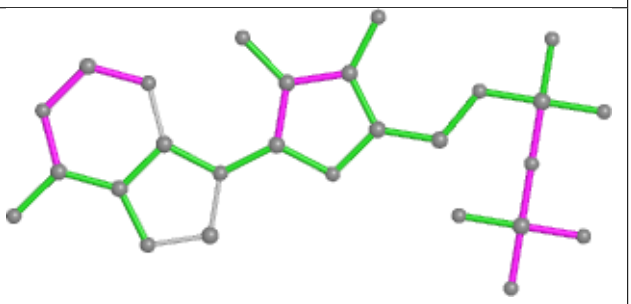
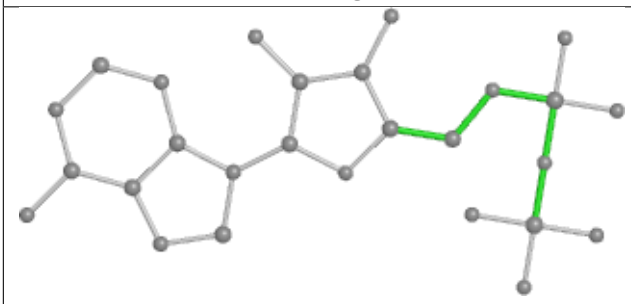
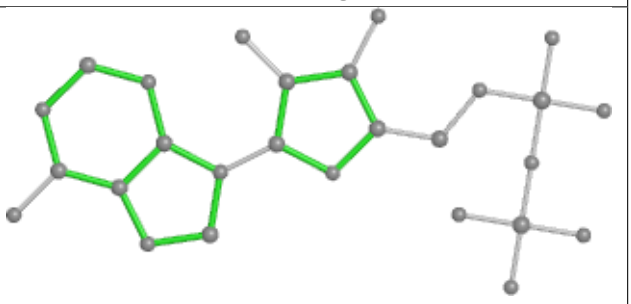
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	ADP	11	0
4	B	401	ADP	4	0
4	D	401	ADP	6	0
4	A	401	ADP	3	0
4	C	401	ADP	13	0

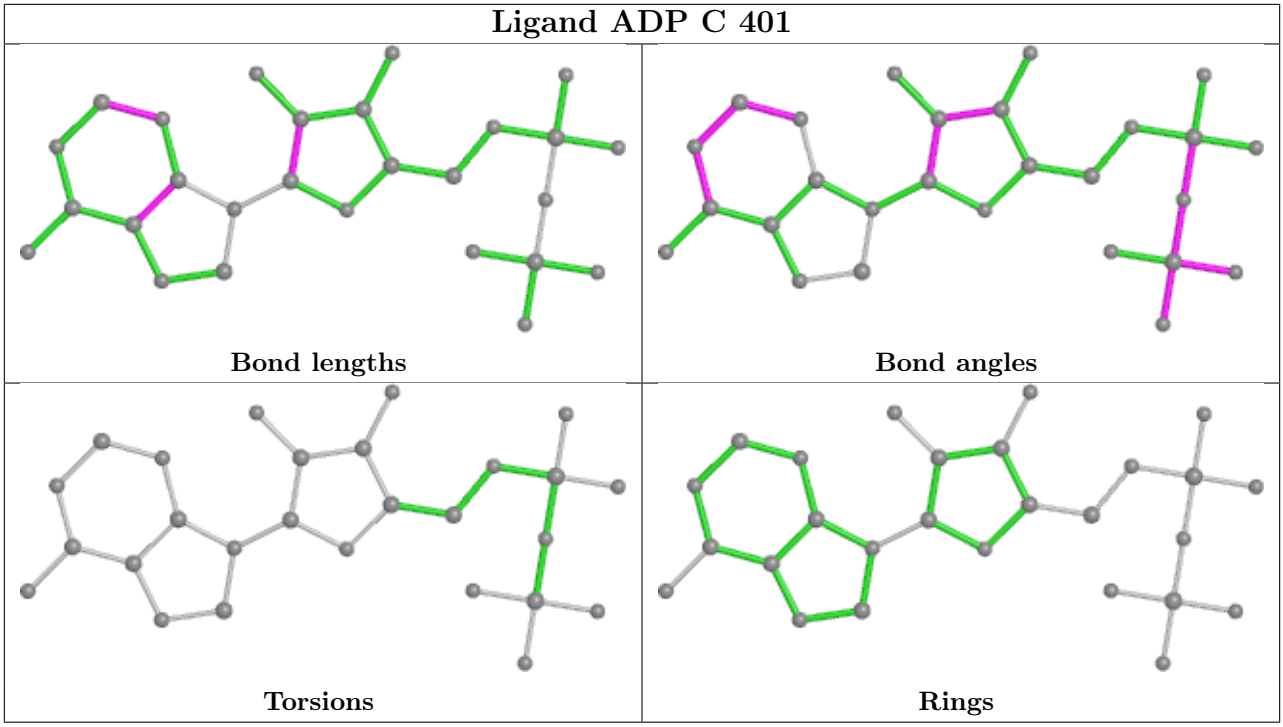
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

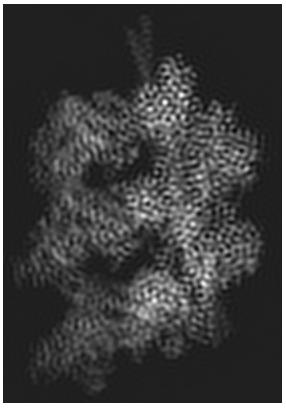
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22335. These allow visual inspection of the internal detail of the map and identification of artifacts.

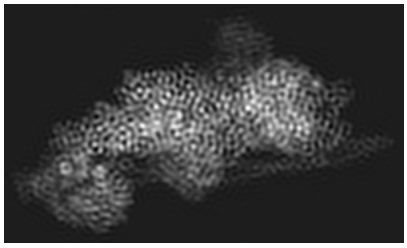
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

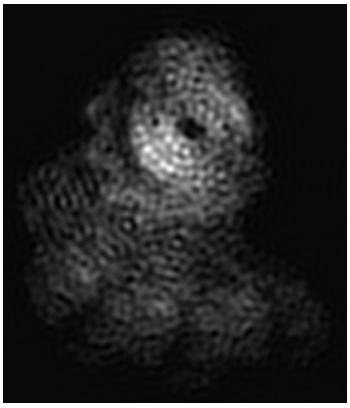
6.1.1 Primary map



X



Y

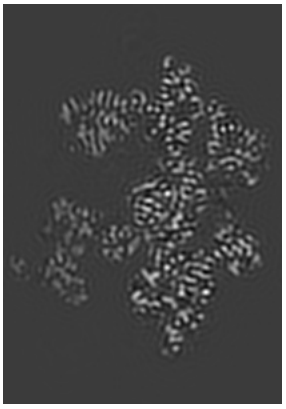


Z

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

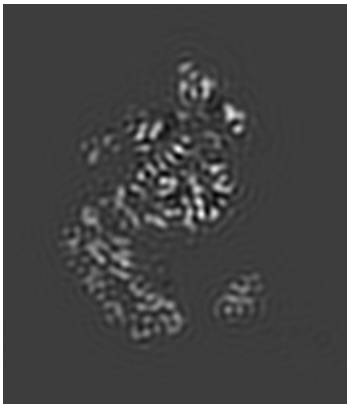
6.2 Central slices (i)

6.2.1 Primary map



X Index: 66

Y Index: 77



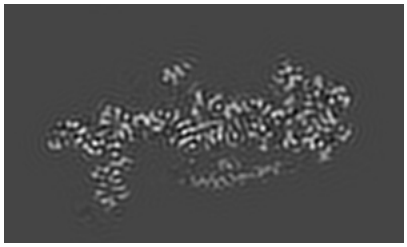
Z Index: 111

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

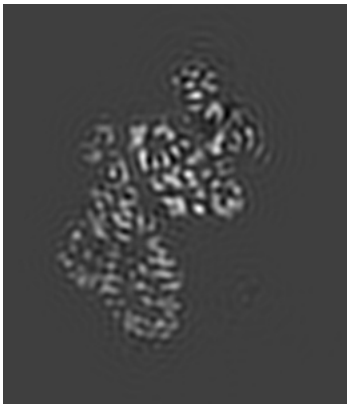
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 64



Y Index: 94

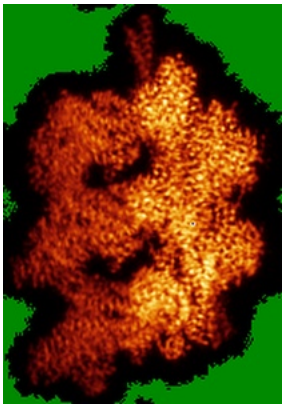


Z Index: 105

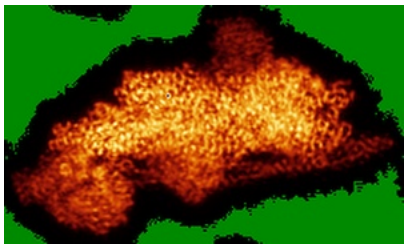
The images above show the largest variance slices of the map in three orthogonal directions.

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

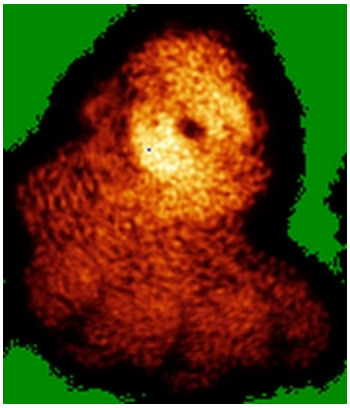
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

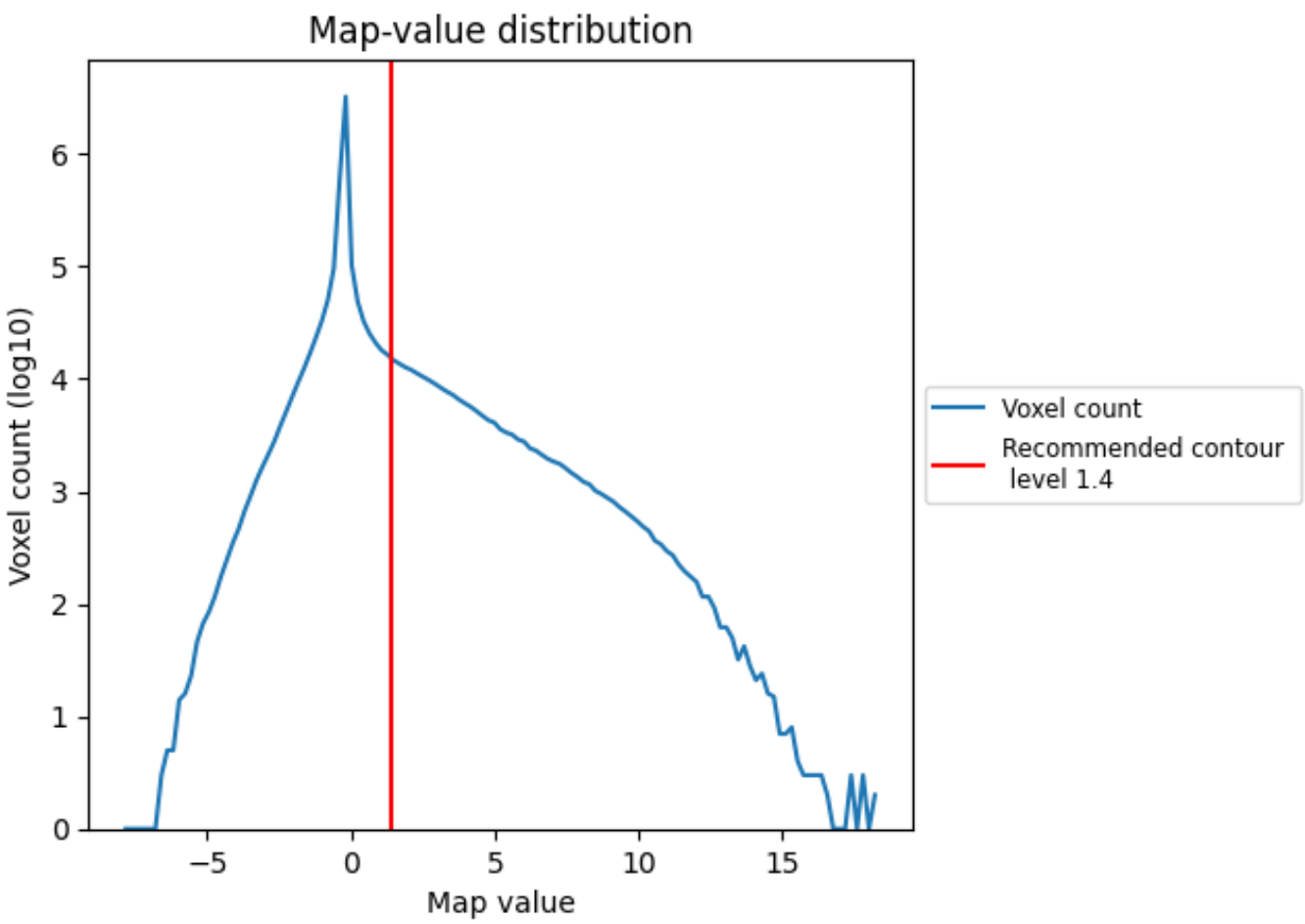
6.6 Mask visualisation (i)

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

7 Map analysis (i)

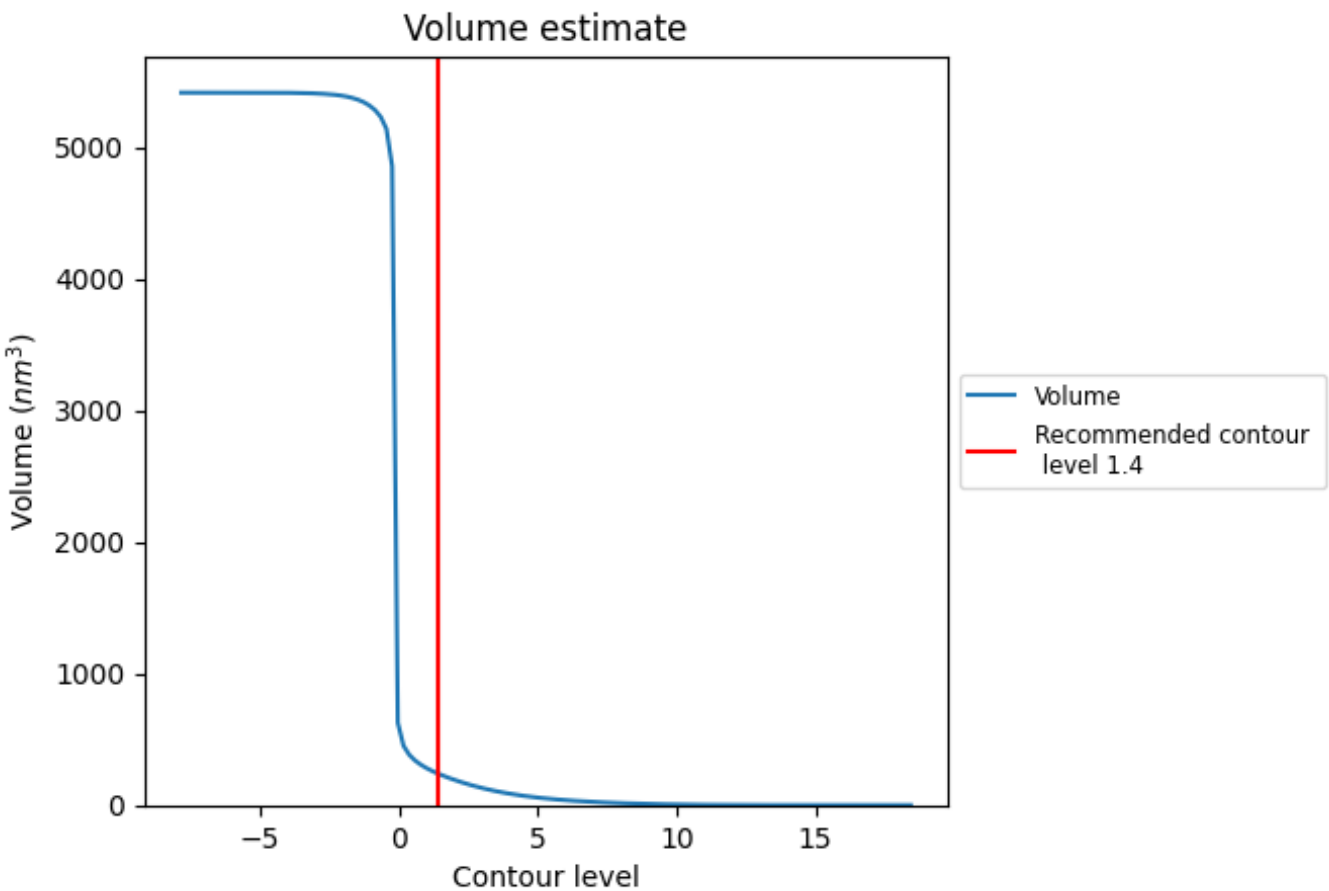
This section contains the results of statistical analysis of the map.

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 240 nm^3; this corresponds to an approximate mass of 217 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.

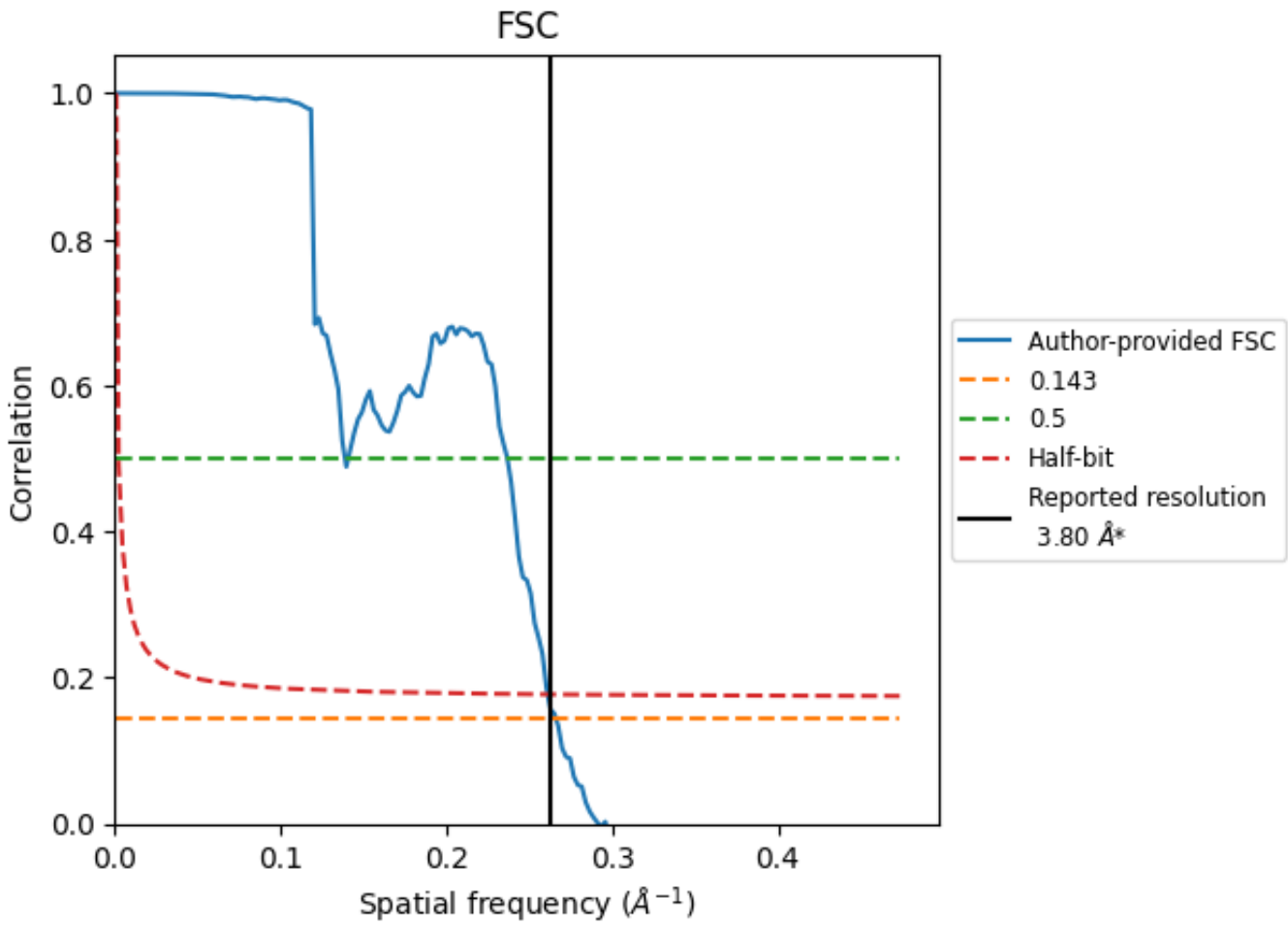
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

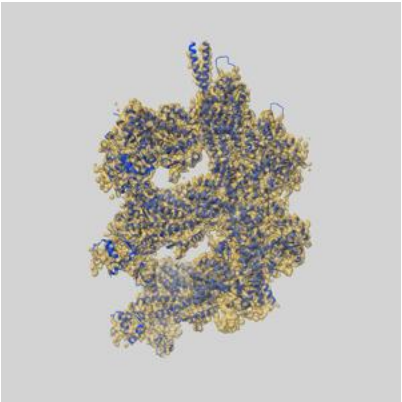
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	7.20	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

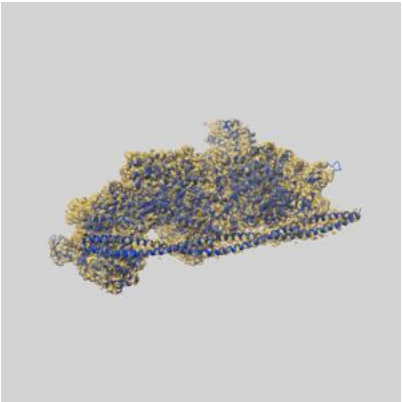
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22335 and PDB model 7JH7. Per-residue inclusion information can be found in section 3 on page 6.

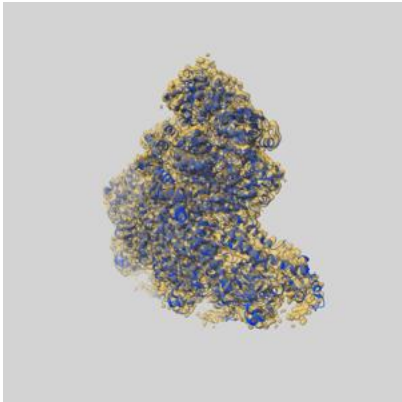
9.1 Map-model overlay (i)



X



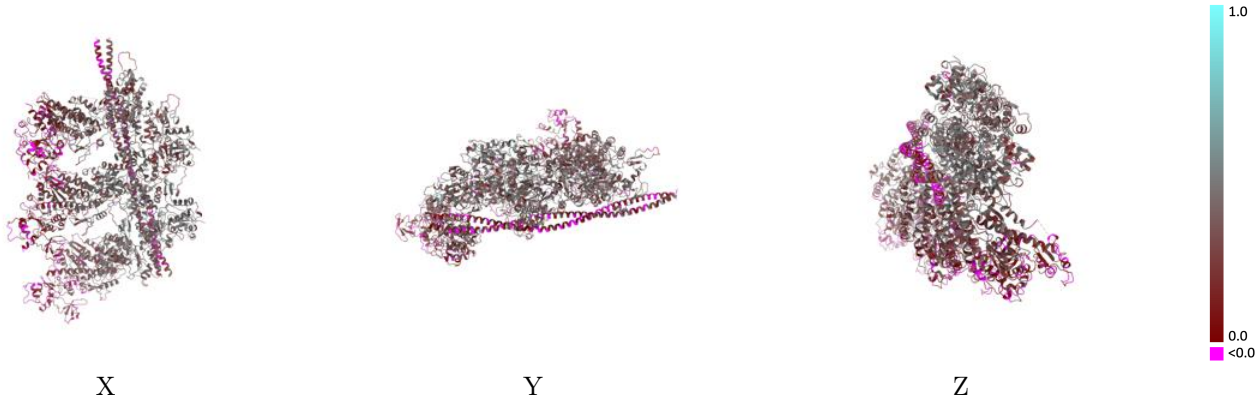
Y



Z

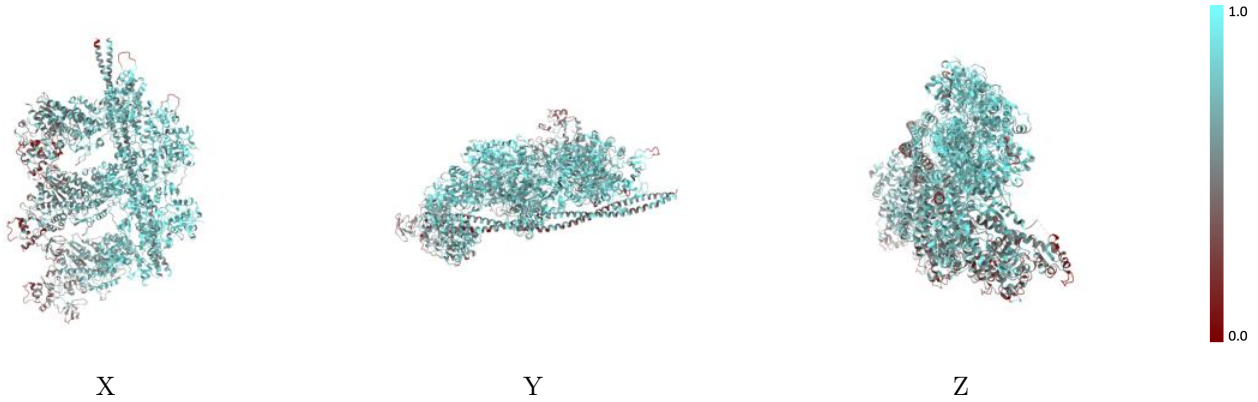
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



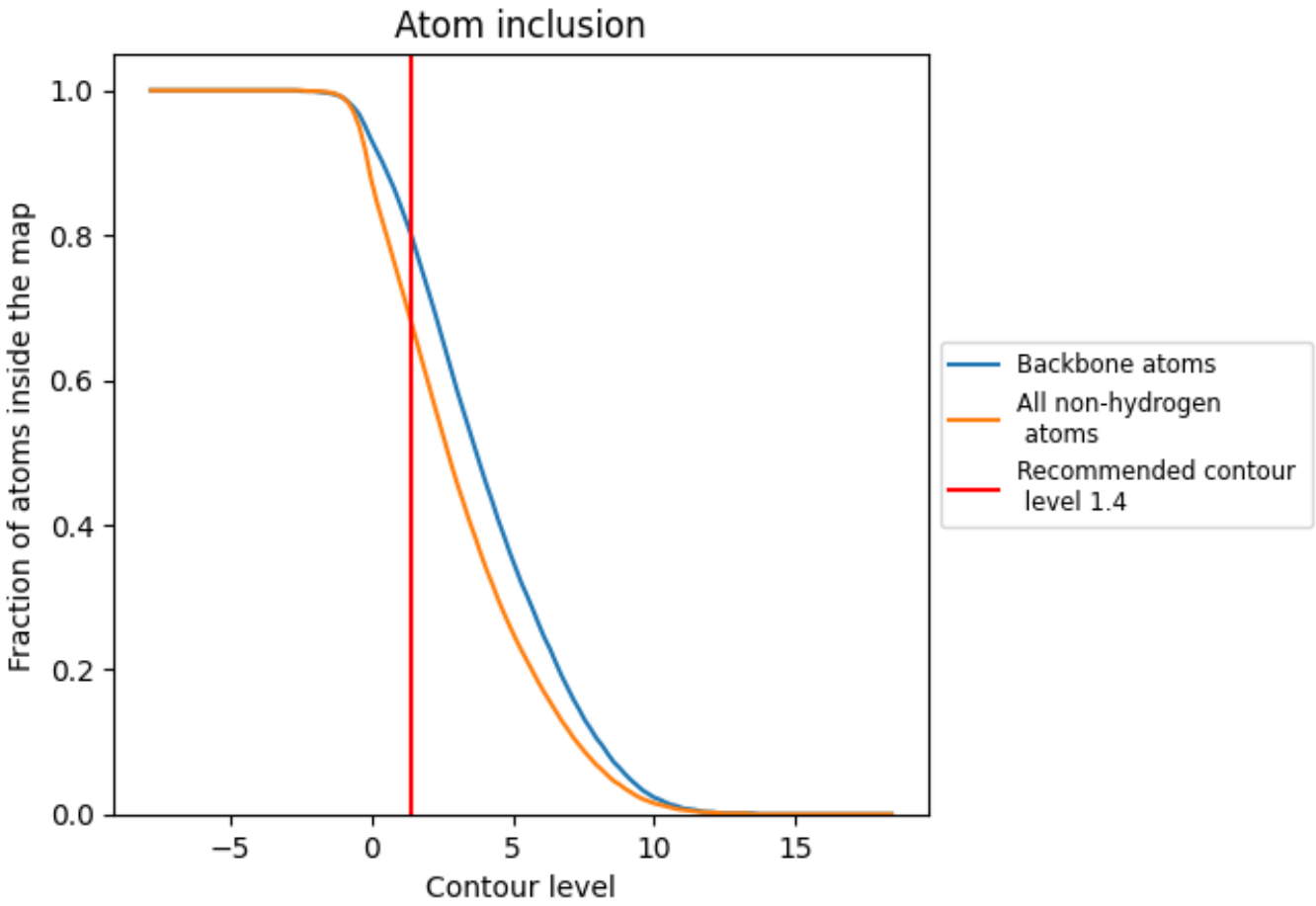
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.4).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.3080
A	0.8190	0.4190
B	0.8030	0.4070
C	0.7920	0.4000
D	0.8190	0.4320
E	0.7720	0.3690
F	0.6040	0.2600
G	0.5780	0.2350
H	0.5860	0.2330
I	0.5990	0.1520
J	0.5450	0.0780