Full wwPDB EM Validation Report (i)

May 19, 2024 – 12:54 am BST

PDB ID	:	6Z47
EMDB ID	:	EMD-11069
Title	:	Smooth muscle myosin shutdown state heads region
Authors	:	Scarff, C.A.; Carrington, G.; Casas Mao, D.; Chalovich, J.M.; Knight, P.J.; Ranson, N.A.; Peckham, M.
Deposited on	:	2020-05-22
Resolution	:	6.30 Å(reported)

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

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

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

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

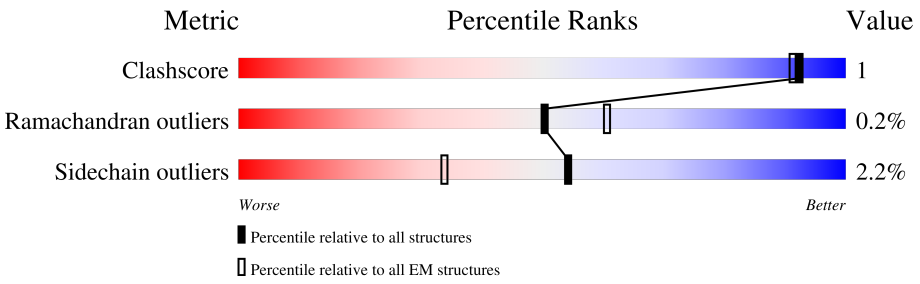
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.30 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	1979	42% • 55%
1	B	1979	43% • 55%
1	G	1979	12% • 87%
1	H	1979	13% 87%
2	C	151	95% • •
2	D	151	99% •
3	E	172	81% • • 13%
3	F	172	81% 5% 13%

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
5	ADP	A	2002	-	-	X	-
6	PO4	A	2003	-	-	X	-
6	PO4	B	2003	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23468 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 Myosin heavy chain 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	888	7213	4572	1256	1350	35	0	0
1	B	888	7213	4572	1256	1350	35	0	0
1	G	257	2108	1278	382	441	7	0	0
1	H	257	2108	1278	382	441	7	0	0

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	PHE	conflict	UNP G1N5L2
A	250	LYS	VAL	conflict	UNP G1N5L2
A	251	PHE	LEU	conflict	UNP G1N5L2
A	252	ILE	LEU	conflict	UNP G1N5L2
A	253	ARG	LEU	conflict	UNP G1N5L2
A	?	-	CYS	deletion	UNP G1N5L2
A	254	ILE	LEU	conflict	UNP G1N5L2
A	255	ASN	HIS	conflict	UNP G1N5L2
A	257	ASP	GLN	conflict	UNP G1N5L2
A	259	THR	SER	conflict	UNP G1N5L2
A	260	GLY	PHE	conflict	UNP G1N5L2
A	261	TYR	LEU	conflict	UNP G1N5L2
A	263	VAL	TYR	conflict	UNP G1N5L2
A	264	GLY	ARG	conflict	UNP G1N5L2
A	265	ALA	SER	conflict	UNP G1N5L2
A	266	ASN	GLN	conflict	UNP G1N5L2
A	267	ILE	VAL	conflict	UNP G1N5L2
A	268	GLU	LEU	conflict	UNP G1N5L2
A	269	THR	SER	conflict	UNP G1N5L2
A	270	TYR	CYS	conflict	UNP G1N5L2
A	271	LEU	MET	conflict	UNP G1N5L2
A	272	LEU	GLY	conflict	UNP G1N5L2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLU	GLN	conflict	UNP G1N5L2
A	274	LYS	SER	conflict	UNP G1N5L2
A	276	ARG	SER	conflict	UNP G1N5L2
A	277	ALA	LEU	conflict	UNP G1N5L2
A	278	ILE	SER	conflict	UNP G1N5L2
A	279	ARG	SER	conflict	UNP G1N5L2
A	280	GLN	THR	conflict	UNP G1N5L2
A	281	ALA	PHE	conflict	UNP G1N5L2
A	282	LYS	PRO	conflict	UNP G1N5L2
A	283	ASP	ASN	conflict	UNP G1N5L2
A	284	GLU	ILE	conflict	UNP G1N5L2
A	285	ARG	LYS	conflict	UNP G1N5L2
A	286	THR	ARG	conflict	UNP G1N5L2
A	288	HIS	GLU	conflict	UNP G1N5L2
A	289	ILE	THR	conflict	UNP G1N5L2
A	291	TYR	LEU	conflict	UNP G1N5L2
A	292	TYR	PHE	conflict	UNP G1N5L2
A	295	ALA	SER	conflict	UNP G1N5L2
A	296	GLY	ALA	conflict	UNP G1N5L2
A	297	ALA	VAL	conflict	UNP G1N5L2
A	298	SER	ARG	conflict	UNP G1N5L2
A	300	GLN	SER	conflict	UNP G1N5L2
A	301	MET	PHE	conflict	UNP G1N5L2
A	302	ARG	GLY	conflict	UNP G1N5L2
B	249	GLY	PHE	conflict	UNP G1N5L2
B	250	LYS	VAL	conflict	UNP G1N5L2
B	251	PHE	LEU	conflict	UNP G1N5L2
B	252	ILE	LEU	conflict	UNP G1N5L2
B	253	ARG	LEU	conflict	UNP G1N5L2
B	?	-	CYS	deletion	UNP G1N5L2
B	254	ILE	LEU	conflict	UNP G1N5L2
B	255	ASN	HIS	conflict	UNP G1N5L2
B	257	ASP	GLN	conflict	UNP G1N5L2
B	259	THR	SER	conflict	UNP G1N5L2
B	260	GLY	PHE	conflict	UNP G1N5L2
B	261	TYR	LEU	conflict	UNP G1N5L2
B	263	VAL	TYR	conflict	UNP G1N5L2
B	264	GLY	ARG	conflict	UNP G1N5L2
B	265	ALA	SER	conflict	UNP G1N5L2
B	266	ASN	GLN	conflict	UNP G1N5L2
B	267	ILE	VAL	conflict	UNP G1N5L2
B	268	GLU	LEU	conflict	UNP G1N5L2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	THR	SER	conflict	UNP G1N5L2
B	270	TYR	CYS	conflict	UNP G1N5L2
B	271	LEU	MET	conflict	UNP G1N5L2
B	272	LEU	GLY	conflict	UNP G1N5L2
B	273	GLU	GLN	conflict	UNP G1N5L2
B	274	LYS	SER	conflict	UNP G1N5L2
B	276	ARG	SER	conflict	UNP G1N5L2
B	277	ALA	LEU	conflict	UNP G1N5L2
B	278	ILE	SER	conflict	UNP G1N5L2
B	279	ARG	SER	conflict	UNP G1N5L2
B	280	GLN	THR	conflict	UNP G1N5L2
B	281	ALA	PHE	conflict	UNP G1N5L2
B	282	LYS	PRO	conflict	UNP G1N5L2
B	283	ASP	ASN	conflict	UNP G1N5L2
B	284	GLU	ILE	conflict	UNP G1N5L2
B	285	ARG	LYS	conflict	UNP G1N5L2
B	286	THR	ARG	conflict	UNP G1N5L2
B	288	HIS	GLU	conflict	UNP G1N5L2
B	289	ILE	THR	conflict	UNP G1N5L2
B	291	TYR	LEU	conflict	UNP G1N5L2
B	292	TYR	PHE	conflict	UNP G1N5L2
B	295	ALA	SER	conflict	UNP G1N5L2
B	296	GLY	ALA	conflict	UNP G1N5L2
B	297	ALA	VAL	conflict	UNP G1N5L2
B	298	SER	ARG	conflict	UNP G1N5L2
B	300	GLN	SER	conflict	UNP G1N5L2
B	301	MET	PHE	conflict	UNP G1N5L2
B	302	ARG	GLY	conflict	UNP G1N5L2
G	249	GLY	PHE	conflict	UNP G1N5L2
G	250	LYS	VAL	conflict	UNP G1N5L2
G	251	PHE	LEU	conflict	UNP G1N5L2
G	252	ILE	LEU	conflict	UNP G1N5L2
G	253	ARG	LEU	conflict	UNP G1N5L2
G	?	-	CYS	deletion	UNP G1N5L2
G	254	ILE	LEU	conflict	UNP G1N5L2
G	255	ASN	HIS	conflict	UNP G1N5L2
G	257	ASP	GLN	conflict	UNP G1N5L2
G	259	THR	SER	conflict	UNP G1N5L2
G	260	GLY	PHE	conflict	UNP G1N5L2
G	261	TYR	LEU	conflict	UNP G1N5L2
G	263	VAL	TYR	conflict	UNP G1N5L2
G	264	GLY	ARG	conflict	UNP G1N5L2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	265	ALA	SER	conflict	UNP G1N5L2
G	266	ASN	GLN	conflict	UNP G1N5L2
G	267	ILE	VAL	conflict	UNP G1N5L2
G	268	GLU	LEU	conflict	UNP G1N5L2
G	269	THR	SER	conflict	UNP G1N5L2
G	270	TYR	CYS	conflict	UNP G1N5L2
G	271	LEU	MET	conflict	UNP G1N5L2
G	272	LEU	GLY	conflict	UNP G1N5L2
G	273	GLU	GLN	conflict	UNP G1N5L2
G	274	LYS	SER	conflict	UNP G1N5L2
G	276	ARG	SER	conflict	UNP G1N5L2
G	277	ALA	LEU	conflict	UNP G1N5L2
G	278	ILE	SER	conflict	UNP G1N5L2
G	279	ARG	SER	conflict	UNP G1N5L2
G	280	GLN	THR	conflict	UNP G1N5L2
G	281	ALA	PHE	conflict	UNP G1N5L2
G	282	LYS	PRO	conflict	UNP G1N5L2
G	283	ASP	ASN	conflict	UNP G1N5L2
G	284	GLU	ILE	conflict	UNP G1N5L2
G	285	ARG	LYS	conflict	UNP G1N5L2
G	286	THR	ARG	conflict	UNP G1N5L2
G	288	HIS	GLU	conflict	UNP G1N5L2
G	289	ILE	THR	conflict	UNP G1N5L2
G	291	TYR	LEU	conflict	UNP G1N5L2
G	292	TYR	PHE	conflict	UNP G1N5L2
G	295	ALA	SER	conflict	UNP G1N5L2
G	296	GLY	ALA	conflict	UNP G1N5L2
G	297	ALA	VAL	conflict	UNP G1N5L2
G	298	SER	ARG	conflict	UNP G1N5L2
G	300	GLN	SER	conflict	UNP G1N5L2
G	301	MET	PHE	conflict	UNP G1N5L2
G	302	ARG	GLY	conflict	UNP G1N5L2
H	249	GLY	PHE	conflict	UNP G1N5L2
H	250	LYS	VAL	conflict	UNP G1N5L2
H	251	PHE	LEU	conflict	UNP G1N5L2
H	252	ILE	LEU	conflict	UNP G1N5L2
H	253	ARG	LEU	conflict	UNP G1N5L2
H	?	-	CYS	deletion	UNP G1N5L2
H	254	ILE	LEU	conflict	UNP G1N5L2
H	255	ASN	HIS	conflict	UNP G1N5L2
H	257	ASP	GLN	conflict	UNP G1N5L2
H	259	THR	SER	conflict	UNP G1N5L2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	260	GLY	PHE	conflict	UNP G1N5L2
H	261	TYR	LEU	conflict	UNP G1N5L2
H	263	VAL	TYR	conflict	UNP G1N5L2
H	264	GLY	ARG	conflict	UNP G1N5L2
H	265	ALA	SER	conflict	UNP G1N5L2
H	266	ASN	GLN	conflict	UNP G1N5L2
H	267	ILE	VAL	conflict	UNP G1N5L2
H	268	GLU	LEU	conflict	UNP G1N5L2
H	269	THR	SER	conflict	UNP G1N5L2
H	270	TYR	CYS	conflict	UNP G1N5L2
H	271	LEU	MET	conflict	UNP G1N5L2
H	272	LEU	GLY	conflict	UNP G1N5L2
H	273	GLU	GLN	conflict	UNP G1N5L2
H	274	LYS	SER	conflict	UNP G1N5L2
H	276	ARG	SER	conflict	UNP G1N5L2
H	277	ALA	LEU	conflict	UNP G1N5L2
H	278	ILE	SER	conflict	UNP G1N5L2
H	279	ARG	SER	conflict	UNP G1N5L2
H	280	GLN	THR	conflict	UNP G1N5L2
H	281	ALA	PHE	conflict	UNP G1N5L2
H	282	LYS	PRO	conflict	UNP G1N5L2
H	283	ASP	ASN	conflict	UNP G1N5L2
H	284	GLU	ILE	conflict	UNP G1N5L2
H	285	ARG	LYS	conflict	UNP G1N5L2
H	286	THR	ARG	conflict	UNP G1N5L2
H	288	HIS	GLU	conflict	UNP G1N5L2
H	289	ILE	THR	conflict	UNP G1N5L2
H	291	TYR	LEU	conflict	UNP G1N5L2
H	292	TYR	PHE	conflict	UNP G1N5L2
H	295	ALA	SER	conflict	UNP G1N5L2
H	296	GLY	ALA	conflict	UNP G1N5L2
H	297	ALA	VAL	conflict	UNP G1N5L2
H	298	SER	ARG	conflict	UNP G1N5L2
H	300	GLN	SER	conflict	UNP G1N5L2
H	301	MET	PHE	conflict	UNP G1N5L2
H	302	ARG	GLY	conflict	UNP G1N5L2

- Molecule 2 is a protein called Myosin light chain smooth muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	150	1174	727	195	240	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	150	1174	727	195	240	12	0	0

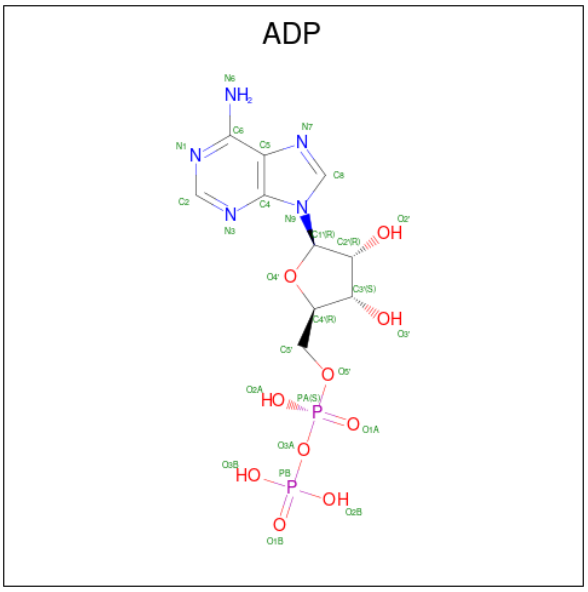
- Molecule 3 is a protein called Myosin light chain 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	149	1205	756	196	242	11	0	0
3	F	149	1205	756	196	242	11	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

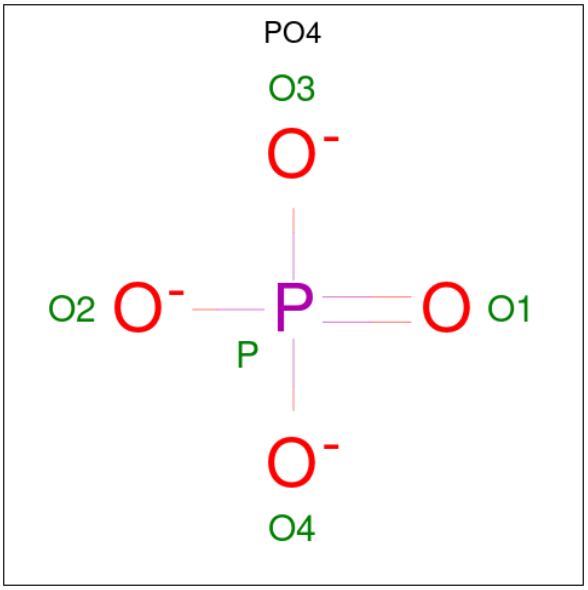
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0
4	E	1	1	1	0
4	F	1	1	1	0

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



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



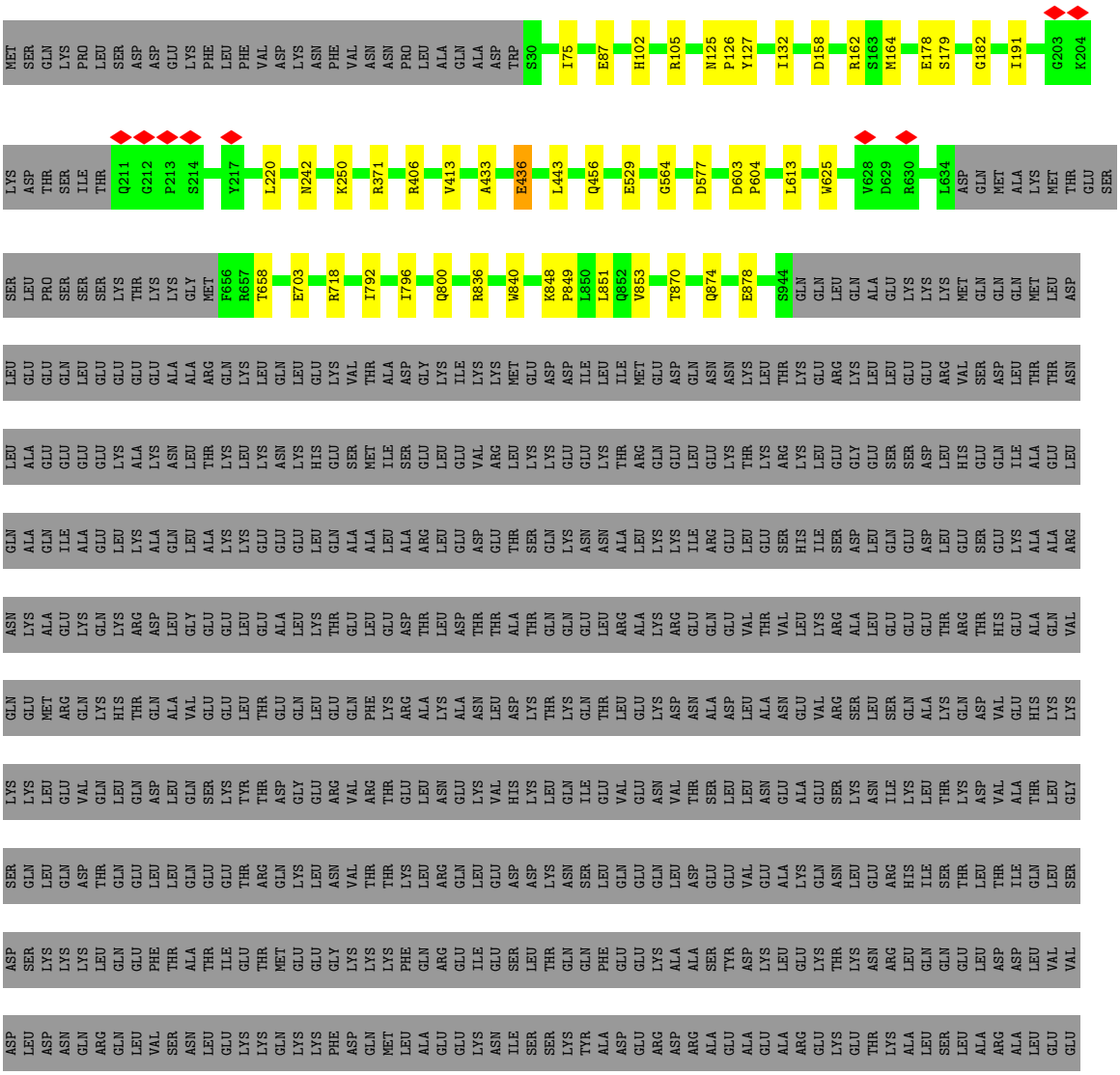
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
6	A	1	5	4	1	0
6	B	1	5	4	1	0

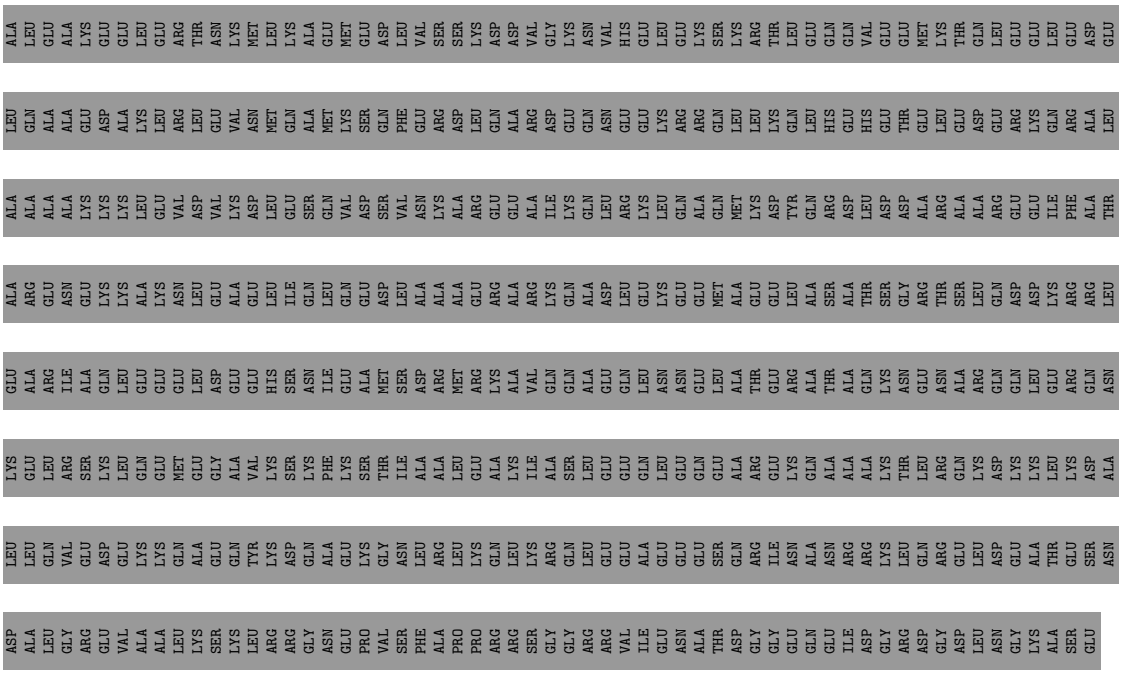
3 Residue-property plots (i)

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

- Molecule 1: Myosin heavy chain 11

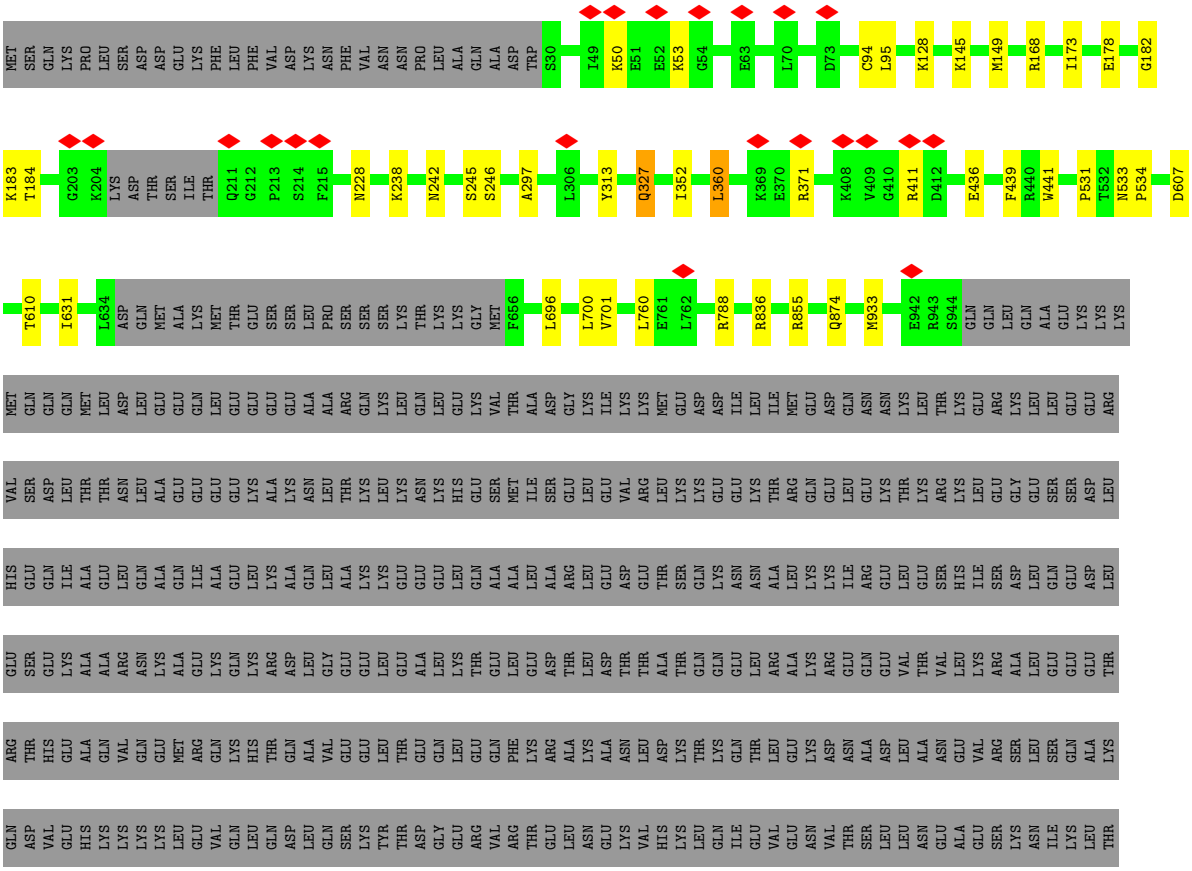
Chain A:





• Molecule 1: Myosin heavy chain 11

Chain B:



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

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

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

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

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

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

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

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

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

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

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

ASN GLY LYS ALA SER GLU

- Molecule 1: Myosin heavy chain 11

Chain G:

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

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

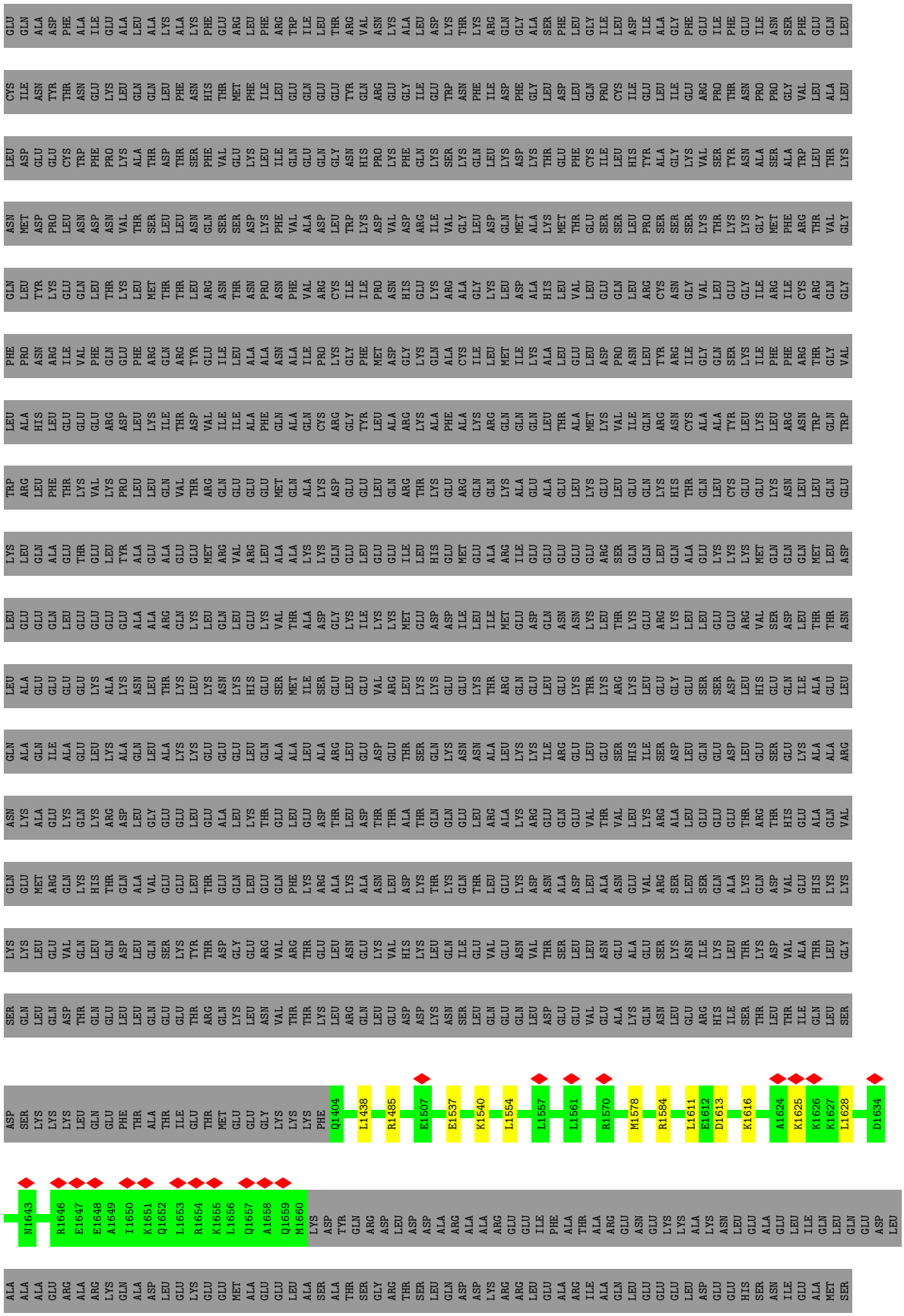
CYS VAL VAL VAL ASN PRO TYR LYS GLN LEU PRO ILE TYR SER GLU LYS ILE ILE ASP MET TYR LYS GLY LYS LYS ARG HIS GLU MET PRO PRO HIS ILE TYR ALA ILE ALA ASP THR ALA TYR ARG SER MET LEU GLN ASP ARG GLU ASP GLN SER ILE LEU CYS THR GLY GLU SER GLY

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

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

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

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


GLU GLN ALA ASP PHE ALA ILE GLU ALA LEU ALA LYS ALA LYS PHE GLU ARG LEU PHE ARG TRP ILE LEU THR ARG VAL ASN LYS ALA LEU ASP LYS THR LYS ARG GLN GLY ALA SER PHE LEU GLY ILE LEU ASP ILE ALA GLY PHE GLU ILE PHE GLU ILE ASN SER PHE GLU GLN LEU
CYS ILE ASN TYR THR ASN GLU LYS LEU GLN GLN LEU PHE ASN HIS THR MET PHE ILE LEU GLU ILE GLN GLN GLU GLU TYR GLN ARG GLU GLY ILE GLU TRP ASN PHE ILE ASP PHE GLY LEU ASP GLU LEU GLN PRO CYS ILE GLU LEU ILE GLU ARG PRO THR ASN PRO PRO GLY VAL LEU ALA LEU
LEU ASP GLU GLU CYS TRP PHE PRO LYS ALA THR ASP THR SER PHE VAL GLU LYS LEU ILE GLN GLU GLN GLY ASN HIS PRO LYS PHE GLN LYS SER LYS GLN LEU LYS ASP LYS THR GLU PHE CYS ILE LEU HIS TYR ALA GLY LYS VAL SER TYR ASN ALA SER ALA TRP LEU THR LYS
ASN MET ASP PRO LEU ASN ASP ASN VAL THR SER LEU LEU ASN GLN SER SER ASP LYS PHE VAL ALA ASP LEU TRP LYS ASP VAL ASP ARG ILE VAL GLY LEU ASP GLN MET ALA LYS MET THR GLU SER SER LEU PRO SER SER SER LYS THR LYS LYS GLY MET PHE ARG THR VAL GLY
GLN LEU TYR LYS GLU GLN LEU THR LYS LEU MET THR THR LEU ARG ASN THR ASN PRO ASN PHE VAL ARG CYS ILE ILE PRO ASN HIS GLU LYS ARG ALA GLY LYS LEU ASP ALA HIS LEU VAL LEU GLU GLN LEU ARG CYS ASN GLY VAL LEU GLU GLY ILE ARG ILE CYS ARG GLN GLY
PHE PRO ASN ARG ILE VAL PHE GLN GLU PHE ARG GLN ARG TYR GLU ILE LEU ALA ALA ASN ALA ILE PRO LYS GLY PHE MET ASP GLY LYS GLN ALA CYS ILE LEU LYS ALA ILE LYS ALA LEU GLU LEU ASP PRO ASN LEU TYR ARG ILE GLY GLN SER LYS ILE PHE ARG THR GLY VAL
LEU ALA HIS LEU GLU GLU GLU ARG ASP LEU LYS ILE THR ASP VAL ILE ILE ALA PHE GLN ALA GLN CYS ARG GLY TYR LEU ALA ARG LYS ALA PHE ALA ALA GLN GLN LEU THR ALA MET LYS VAL ILE GLN LEU ARG ASN CYS ASN GLY VAL LEU GLU GLN GLN SER LYS LEU LYS LEU ARG ASN TRP GLN TRP
TRP ARG LEU PHE THR LYS VAL LYS PRO LEU LEU GLN VAL THR ARG GLN GLU GLU GLU MET GLN ALA LYS ASP GLU GLU LEU GLN GLN ARG THR LYS GLU ARG GLN LYS ALA GLU ALA GLU LEU LYS GLU LEU GLU GLN GLU GLU LYS ASN LEU LEU GLN GLU
LYS LEU GLN ALA GLU THR GLU LEU TYR ALA ALA GLU GLU MET GLU ALA ALA ALA LYS LYS GLN GLU GLU LEU GLU GLU ILE LEU HIS GLU MET GLU ALA ARG ILE GLU GLU GLU GLU GLU ARG SER GLN GLN LEU GLN ALA GLU LYS LYS LYS MET GLN GLN GLN MET LEU ASP
LEU GLU GLU GLN LEU GLU GLU GLU ALA ALA ARG GLN LYS LEU GLU VAL THR ALA ASP GLY LYS LYS ILE LYS LYS MET GLU ASP ILE LEU ILE MET GLU ASP GLN ASN ASN LYS LEU THR LYS GLU ARG LYS LEU LEU LEU GLU GLU ARG VAL SER ASP LEU THR THR ASN
LEU ALA GLU GLU GLU LYS ALA LYS ASN ASN LEU THR LYS LEU GLU LYS HIS GLU SER MET ILE SER GLU LEU GLU VAL ARG LEU LYS LYS GLU GLU VAL ARG GLN GLU LEU GLU GLU LYS THR LYS ARG GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLN ALA GLN ILE ALA GLU LEU LYS ALA GLN LEU LYS LYS ALA LEU ALA ALA LEU LEU LEU ARG LEU GLU ASP GLU THR SER GLN LYS ASN ASN LEU LEU LYS ILE ARG GLU LEU GLU LEU GLU SER HIS ILE SER ASP LEU GLU GLU ASP LEU GLU SER GLN GLN GLU ASP LEU GLU GLN GLU ARG
ASN LYS ALA GLU LYS GLN LYS ARG ASP LEU GLU GLU GLU LEU GLU GLU LYS THR GLU LEU ASP THR THR ALA THR GLN GLN GLU LYS ASN ASN ALA LYS ARG GLU GLN GLN VAL THR VAL LEU LYS ARG ARG GLY ALA LEU GLU GLU GLU GLU GLU GLU ARG GLN VAL
GLN GLU MET ARG GLN LYS HIS THR GLN ALA VAL GLU GLU GLU LEU GLU GLU LEU GLU GLN GLU PHE LYS ARG ALA LYS ALA ASN LEU ASP LYS THR LYS GLN THR LEU GLU LYS ASN ALA ASP LEU ALA ASN GLU VAL ARG SER LEU SER GLN ALA LYS GLN LYS LYS
LYS LYS LEU GLU VAL GLN LYS LEU GLN SER LYS TYR THR ASP GLY GLU ARG VAL ARG THR GLU LEU ASN VAL LEU GLU ASN VAL THR SER LEU LEU ASN GLU ALA GLU SER LYS ASN ILE LYS LEU THR LYS ASP VAL ALA THR LEU GLY
SER GLN LEU GLN ASP THR GLN GLU LEU LEU GLN GLN GLU THR ARG GLN LYS LEU ASN VAL THR THR LYS LEU ARG GLN LEU ASP LYS SER ASN LEU GLN GLN GLU GLU VAL GLU ALA LYS GLN LEU GLU ILE ARG HIS ILE SER THR LEU THR ILE GLN LEU SER
ASP SER LYS LYS LYS LEU LEU PHE THR ALA THR ILE GLU THR MET GLU GLU GLY LYS LYS LYS PHE Q1404 L1438 R1485 E1507 E1537 K1540 L1554 L1557 L1561 R1570 M1578 R1584 L1611 E1612 D1613 K1616 A1624 K1625 K1626 K1627 L1628 D1634
M1643 R1646 E1647 E1648 A1649 I1650 K1651 Q1652 L1653 R1654 K1655 L1656 Q1657 A1658 Q1659 M1660 LYS ASP TYR GLN ARG ASP LEU ASP ASP ALA ARG ALA ALA ARG GLU GLU ILE PHE ALA THR ALA ARG GLU ASN GLU LYS LYS ALA ASN LYS GLU ASN LEU GLU ALA GLU LEU ILE GLN LEU LEU GLN GLU LEU
ALA ALA ALA GLU ARG ALA ARG LYS GLN LYS ALA ALA LEU GLU LYS GLU GLU MET ALA GLU GLU LEU ALA SER ALA THR SER GLY ARG THR SER LEU GLN ASP ASP LYS ASN ASP ALA ARG ILE ALA ALA GLN LEU GLU GLU GLU LEU ASP GLU GLU ILE GLU HIS SER ASN GLU GLU ILE GLU ALA ASN GLU GLU GLU LEU GLU GLU ARG GLU LEU GLU ILE ALA MET SER

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

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

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

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

• Molecule 1: Myosin heavy chain 11

Chain H: 13% 87%

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

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

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

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

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

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

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

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

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

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

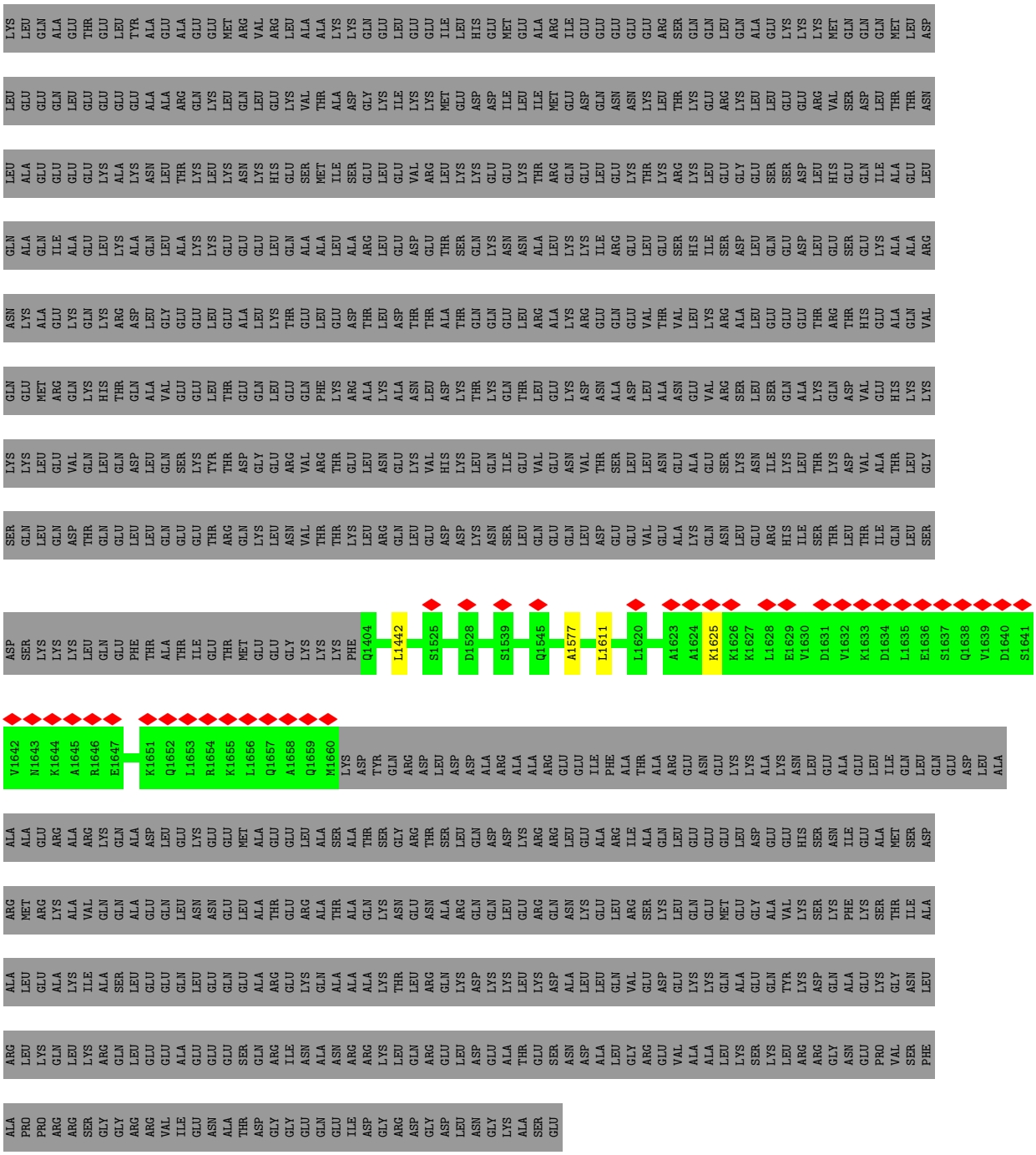
ASN MET ASP PRO LEU ASN ASP ASN VAL THR SER LEU LEU ASN GLN SER SER ASP LYS PHE VAL ALA ASP LEU TRP LYS ASP VAL ASP ARG ILE VAL GLY LEU ASP GLN MET ALA LYS MET THR GLU SER SER LEU PRO SER SER SER LYS THR LYS LYS GLY MET PHE ARG THR VAL GLY

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

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

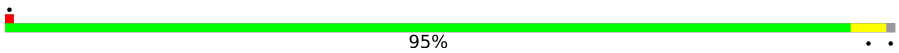
LEU ALA HIS LEU GLU GLU GLU ARG ASP LEU LYS ILE THR ASP VAL ILE ILE ALA PHE GLN ALA GLN CYS ARG GLY TYR LEU ALA ARG LYS ALA PHE ALA LYS ARG GLN GLN GLN LEU THR ALA MET LYS VAL ILE GLN ARG ASN CYS ALA ALA TYR LEU LYS LEU ARG ASN TRP GLN TRP

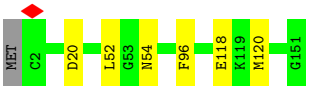
TRP ARG LEU PHE THR LYS VAL LYS PRO LEU LEU GLN VAL THR ARG GLN GLU GLU GLU MET GLN ALA LYS ASP GLU GLU LEU GLN ARG THR LYS GLU ARG GLN GLN LYS ALA GLU ALA GLU LEU LYS GLU LEU GLU GLN LYS HIS THR GLN LEU CYS GLU GLU LYS ASN LEU LEU GLN GLU



• Molecule 2: Myosin light chain smooth muscle isoform

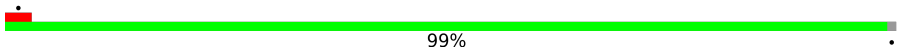
Chain C:

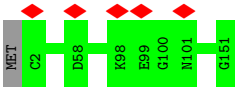




• Molecule 2: Myosin light chain smooth muscle isoform

Chain D:





• Molecule 3: Myosin light chain 9

Chain E:

• Molecule 3: Myosin light chain 9

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.671	Depositor
Minimum map value	-0.537	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	376.64, 376.64, 376.64	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, PO4, 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	0.35	0/7339	0.58	0/9875
1	B	0.35	0/7339	0.58	0/9875
1	G	0.34	0/2115	0.51	0/2814
1	H	0.33	0/2115	0.49	0/2814
2	C	0.31	0/1189	0.55	0/1594
2	D	0.31	0/1189	0.51	0/1594
3	E	0.35	0/1230	0.61	0/1651
3	F	0.35	0/1230	0.58	0/1651
All	All	0.34	0/23746	0.56	0/31868

There are no bond length outliers.

There are no bond angle outliers.

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	7213	0	7252	34	0
1	B	7213	0	7251	18	0
1	G	2108	0	2115	5	0
1	H	2108	0	2115	5	0
2	C	1174	0	1128	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1174	0	1128	0	0
3	E	1205	0	1119	4	0
3	F	1205	0	1119	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	27	0	12	17	0
5	B	27	0	12	7	0
6	A	5	0	0	4	0
6	B	5	0	0	5	0
All	All	23468	0	23251	64	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 1.

All (64) 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:A:179:SER:O	6:A:2003:PO4:O3	1.70	1.08
1:A:242:ASN:ND2	5:A:2002:ADP:O1B	2.10	0.83
1:B:242:ASN:ND2	6:B:2003:PO4:O1	2.11	0.83
1:B:242:ASN:ND2	5:B:2002:ADP:O1B	2.14	0.81
1:B:184:THR:OG1	5:B:2002:ADP:O2B	1.98	0.81
1:A:179:SER:O	5:A:2002:ADP:O1B	2.00	0.78
5:B:2002:ADP:O1B	6:B:2003:PO4:P	2.42	0.76
1:A:182:GLY:HA2	5:A:2002:ADP:PA	2.31	0.70
1:B:245:SER:HA	6:B:2003:PO4:O1	1.91	0.69
1:A:127:TYR:HA	5:A:2002:ADP:H1'	1.75	0.67
1:A:126:PRO:HD2	5:A:2002:ADP:C5	2.35	0.62
1:B:182:GLY:HA2	5:B:2002:ADP:PA	2.42	0.60
1:A:179:SER:HA	6:A:2003:PO4:O2	2.01	0.60
1:B:246:SER:H	6:B:2003:PO4:P	2.26	0.58
5:A:2002:ADP:O1B	6:A:2003:PO4:O3	2.21	0.58
1:B:327:GLN:HA	1:B:327:GLN:HE21	1.68	0.57
1:B:183:LYS:NZ	5:B:2002:ADP:O3B	2.36	0.55
1:A:125:ASN:OD1	5:A:2002:ADP:O4'	2.24	0.55
1:A:132:ILE:HG22	1:A:132:ILE:O	2.07	0.53
1:A:125:ASN:OD1	5:A:2002:ADP:C1'	2.56	0.53
1:A:182:GLY:HA2	5:A:2002:ADP:O3A	2.08	0.53
1:A:179:SER:O	6:A:2003:PO4:P	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:H	5:A:2002:ADP:PB	2.33	0.51
1:A:182:GLY:CA	5:A:2002:ADP:O3A	2.59	0.50
1:A:126:PRO:HD2	5:A:2002:ADP:C4	2.46	0.50
5:B:2002:ADP:O1B	6:B:2003:PO4:O2	2.29	0.50
1:A:125:ASN:OD1	5:A:2002:ADP:C8	2.66	0.49
1:G:1611:LEU:CB	1:H:1611:LEU:HD23	2.43	0.49
3:E:146:ALA:HB1	3:E:147:PRO:HD2	1.95	0.48
1:A:126:PRO:HD2	5:A:2002:ADP:C8	2.49	0.48
1:A:158:ASP:O	1:A:162:ARG:HG2	2.15	0.47
1:A:870:THR:HG23	1:B:874:GLN:OE1	2.15	0.47
1:A:800:GLN:NE2	2:C:118:GLU:O	2.46	0.47
1:A:874:GLN:O	1:A:878:GLU:HG2	2.14	0.47
1:A:433:ALA:O	1:A:436:GLU:HG3	2.16	0.46
1:A:125:ASN:HD21	5:A:2002:ADP:C5'	2.29	0.45
1:A:848:LYS:N	1:A:849:PRO:HD2	2.32	0.45
1:A:182:GLY:N	5:A:2002:ADP:O3A	2.49	0.45
1:B:313:TYR:CZ	1:B:360:LEU:HD21	2.52	0.44
1:A:851:LEU:HD22	3:E:36:GLU:HG3	1.99	0.44
1:B:696:LEU:HD11	1:B:701:VAL:HG11	1.99	0.44
1:A:125:ASN:ND2	5:A:2002:ADP:O4'	2.52	0.43
1:A:603:ASP:N	1:A:604:PRO:HD3	2.34	0.43
1:A:800:GLN:HE21	2:C:120:MET:HG3	1.83	0.43
1:B:436:GLU:HA	1:B:439:PHE:CE2	2.53	0.43
3:E:49:ILE:HG23	3:E:54:LEU:CD2	2.49	0.43
1:A:792:ILE:HG22	1:A:796:ILE:HG12	1.99	0.43
1:B:533:ASN:HB3	1:B:534:PRO:HD2	2.01	0.43
1:G:1613:ASP:HA	1:G:1616:LYS:HE3	2.01	0.43
1:A:792:ILE:HG21	2:C:96:PHE:CZ	2.54	0.43
1:G:1611:LEU:HB3	1:H:1611:LEU:HD23	2.00	0.43
1:G:1628:LEU:HD12	1:H:1625:LYS:HG2	2.02	0.42
1:A:102:HIS:HA	1:A:105:ARG:HG2	2.02	0.42
1:B:182:GLY:HA2	5:B:2002:ADP:O5'	2.20	0.42
3:F:116:GLY:HA2	3:F:156:TYR:CZ	2.55	0.42
3:F:146:ALA:HB1	3:F:147:PRO:CD	2.50	0.42
3:E:105:ASN:CG	1:H:1577:ALA:HB2	2.41	0.42
1:A:613:LEU:HD23	1:A:625:TRP:CE2	2.55	0.41
1:B:94:CYS:SG	1:B:95:LEU:N	2.88	0.41
1:B:352:ILE:HD11	1:B:441:TRP:CZ3	2.56	0.41
1:B:610:THR:HG21	1:B:631:ILE:HD11	2.02	0.41
1:B:533:ASN:O	1:B:534:PRO:C	2.57	0.40
1:G:1438:LEU:HD22	1:H:1442:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ARG:HG2	1:A:413:VAL:HG22	2.03	0.40

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	882/1979 (45%)	855 (97%)	24 (3%)	3 (0%)	41	76
1	B	882/1979 (45%)	842 (96%)	38 (4%)	2 (0%)	47	81
1	G	255/1979 (13%)	253 (99%)	2 (1%)	0	100	100
1	H	255/1979 (13%)	254 (100%)	1 (0%)	0	100	100
2	C	148/151 (98%)	142 (96%)	5 (3%)	1 (1%)	22	63
2	D	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
3	E	147/172 (86%)	139 (95%)	8 (5%)	0	100	100
3	F	147/172 (86%)	135 (92%)	11 (8%)	1 (1%)	22	63
All	All	2864/8562 (34%)	2759 (96%)	98 (3%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	GLY
1	A	87	GLU
1	B	297	ALA
1	A	853	VAL
2	C	54	ASN
1	B	531	PRO
3	F	22	VAL

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	782/1746 (45%)	765 (98%)	17 (2%)	52	71
1	B	782/1746 (45%)	761 (97%)	21 (3%)	44	65
1	G	229/1746 (13%)	222 (97%)	7 (3%)	40	62
1	H	229/1746 (13%)	229 (100%)	0	100	100
2	C	129/130 (99%)	127 (98%)	2 (2%)	62	79
2	D	129/130 (99%)	129 (100%)	0	100	100
3	E	130/150 (87%)	125 (96%)	5 (4%)	33	57
3	F	130/150 (87%)	126 (97%)	4 (3%)	40	62
All	All	2540/7544 (34%)	2484 (98%)	56 (2%)	54	71

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	164	MET
1	A	178	GLU
1	A	191	ILE
1	A	220	LEU
1	A	250	LYS
1	A	371	ARG
1	A	436	GLU
1	A	443	LEU
1	A	456	GLN
1	A	529	GLU
1	A	577	ASP
1	A	658	THR
1	A	703	GLU
1	A	718	ARG
1	A	836	ARG
1	A	840	TRP
1	B	50	LYS
1	B	53	LYS

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	145	LYS
1	B	149	MET
1	B	168	ARG
1	B	173	ILE
1	B	178	GLU
1	B	228	ASN
1	B	238	LYS
1	B	327	GLN
1	B	360	LEU
1	B	371	ARG
1	B	411	ARG
1	B	607	ASP
1	B	700	LEU
1	B	760	LEU
1	B	788	ARG
1	B	836	ARG
1	B	855	ARG
1	B	933	MET
2	C	20	ASP
2	C	52	LEU
3	E	45	ARG
3	E	54	LEU
3	E	105	ASN
3	E	110	PHE
3	E	112	GLU
3	F	43	GLN
3	F	44	ASN
3	F	49	ILE
3	F	120	GLU
1	G	1485	ARG
1	G	1537	GLU
1	G	1540	LYS
1	G	1554	LEU
1	G	1578	MET
1	G	1584	ARG
1	G	1625	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN

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Mol	Chain	Res	Type
1	B	327	GLN
1	B	723	ASN
3	E	55	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	PO4	A	2003	4	4,4,4	0.74	0	6,6,6	0.46	0
5	ADP	A	2002	4	24,29,29	0.68	0	29,45,45	0.78	0
6	PO4	B	2003	4	4,4,4	1.95	1 (25%)	6,6,6	1.18	1 (16%)
5	ADP	B	2002	4	24,29,29	0.91	0	29,45,45	0.79	0

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
5	ADP	A	2002	4	-	3/12/32/32	0/3/3/3
5	ADP	B	2002	4	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2003	PO4	P-O1	3.49	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	2003	PO4	O3-P-O1	-2.07	103.34	110.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	ADP	C5'-O5'-PA-O1A
5	B	2002	ADP	C5'-O5'-PA-O1A
5	A	2002	ADP	C5'-O5'-PA-O3A
5	B	2002	ADP	C5'-O5'-PA-O3A
5	A	2002	ADP	C5'-O5'-PA-O2A
5	B	2002	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

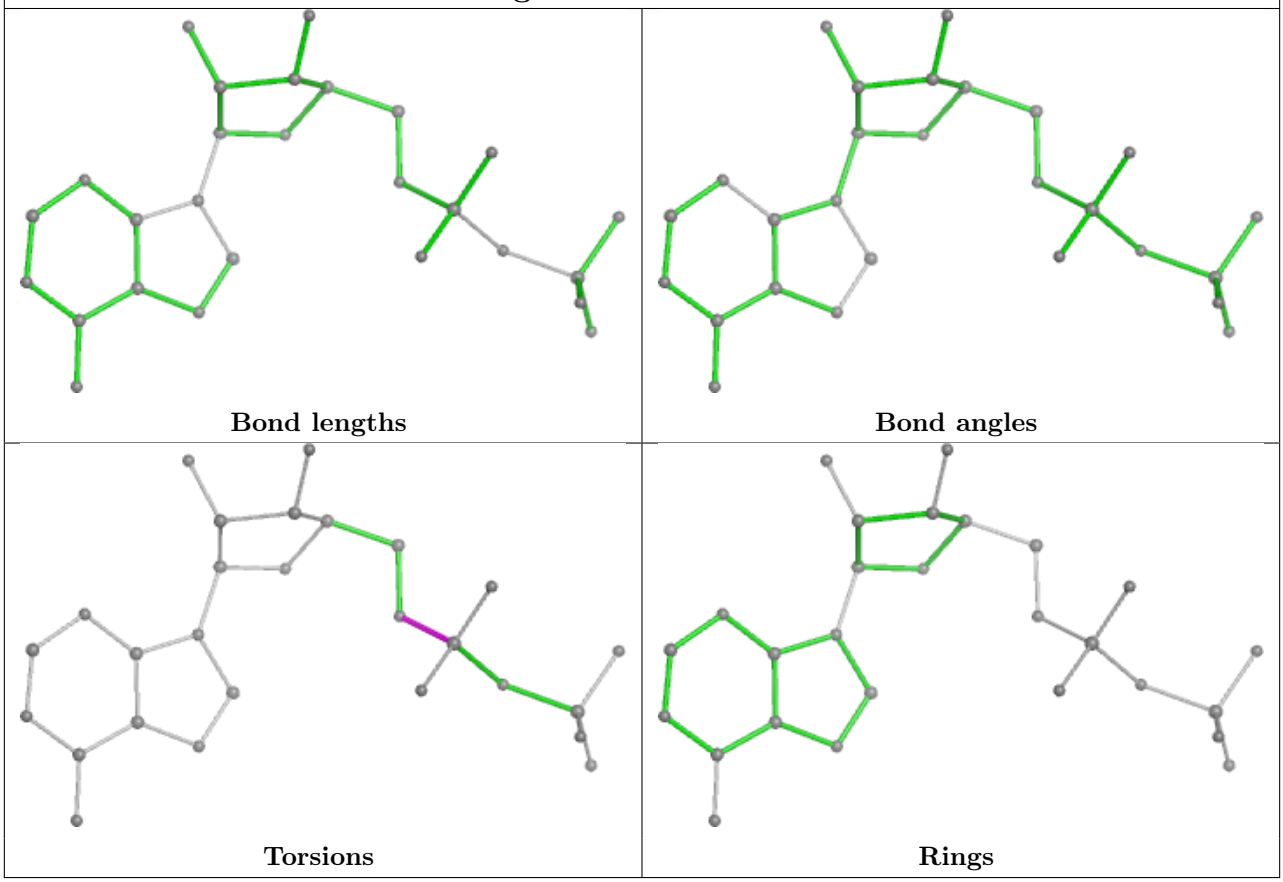
4 monomers are involved in 30 short contacts:

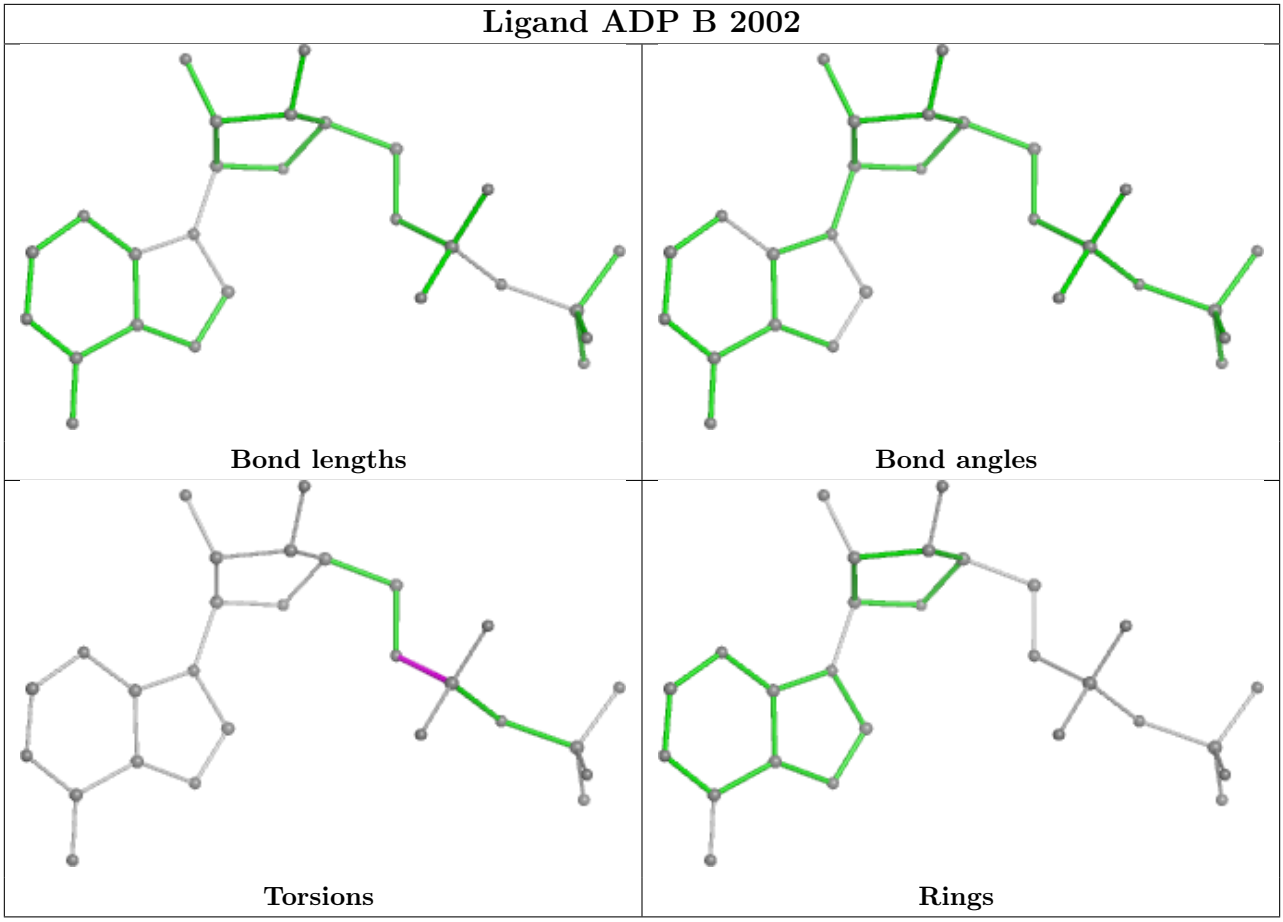
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2003	PO4	4	0
5	A	2002	ADP	17	0
6	B	2003	PO4	5	0
5	B	2002	ADP	7	0

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 2002





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.

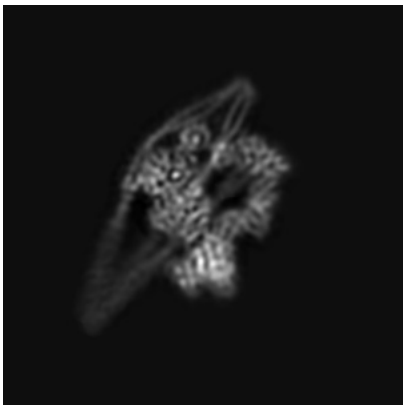
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11069. These allow visual inspection of the internal detail of the map and identification of artifacts.

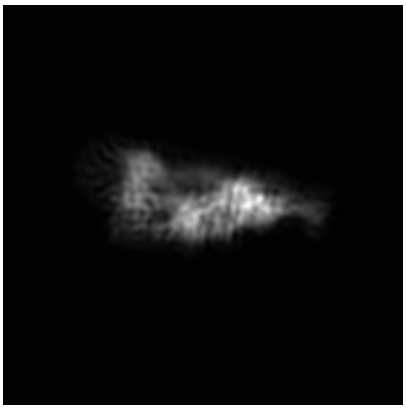
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



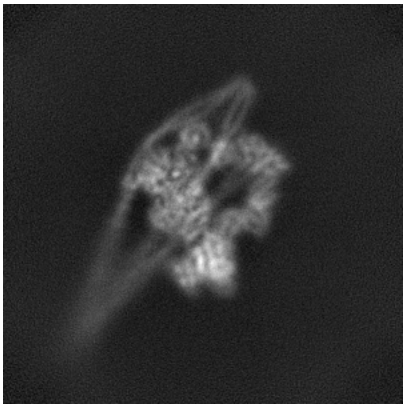
X



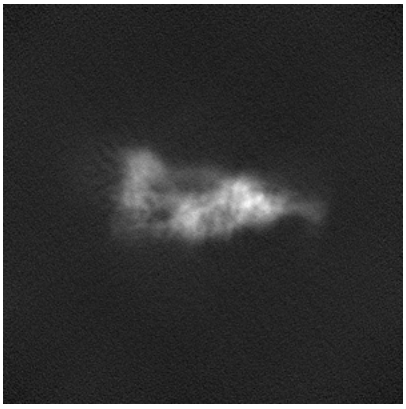
Y

Z

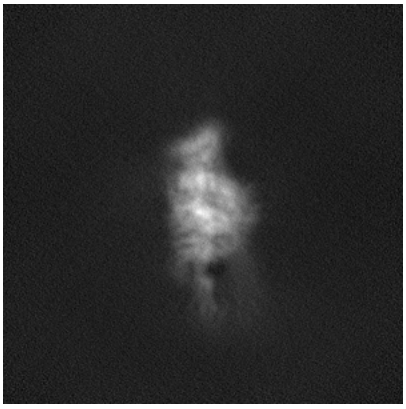
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

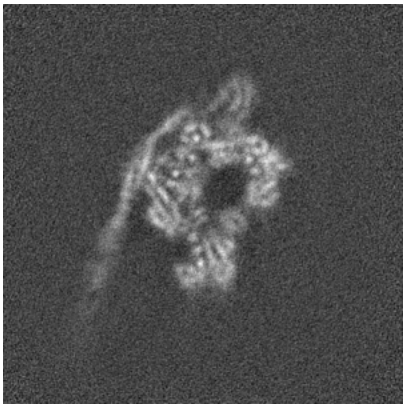
6.2.1 Primary map

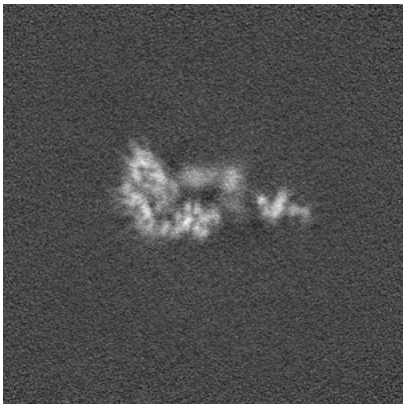
X Index: 176

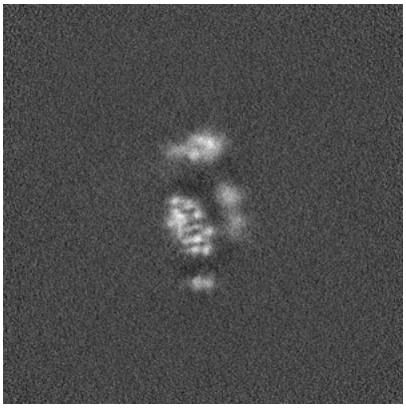
Y Index: 176

Z Index: 176

6.2.2 Raw map


X Index: 176


Y Index: 176


Z Index: 176

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

6.3 Largest variance slices (i)

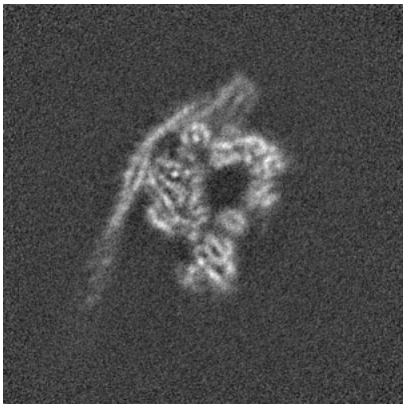
6.3.1 Primary map

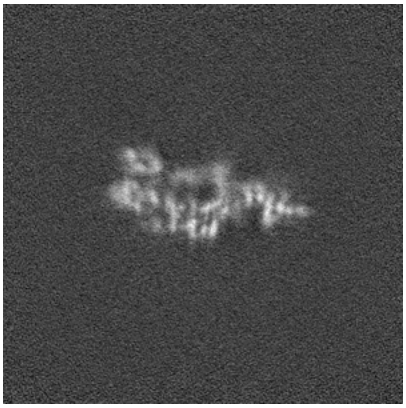
X Index: 173

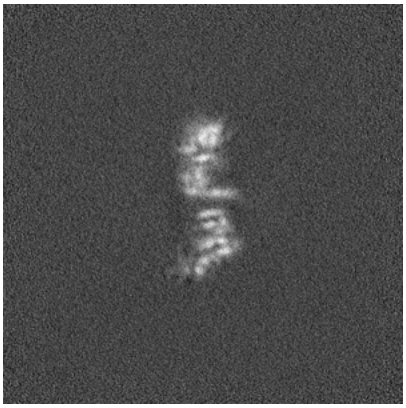
Y Index: 168

Z Index: 202

6.3.2 Raw map


X Index: 173


Y Index: 168

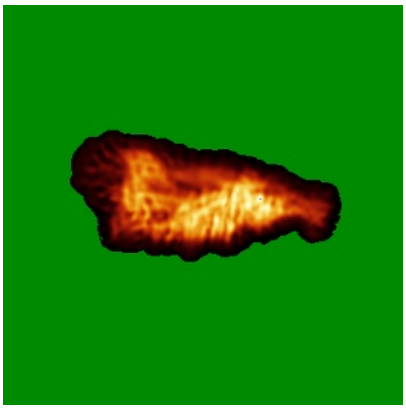

Z Index: 215

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

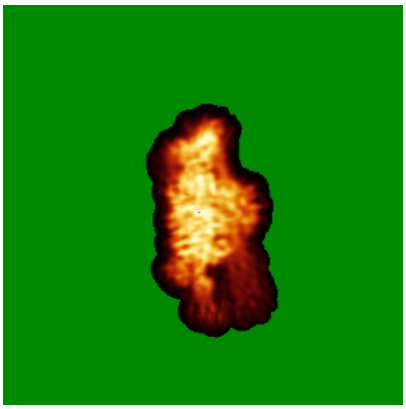
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

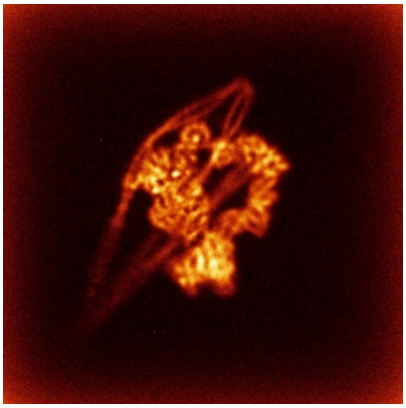


Y

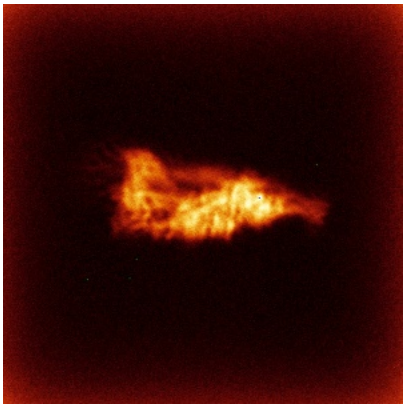


Z

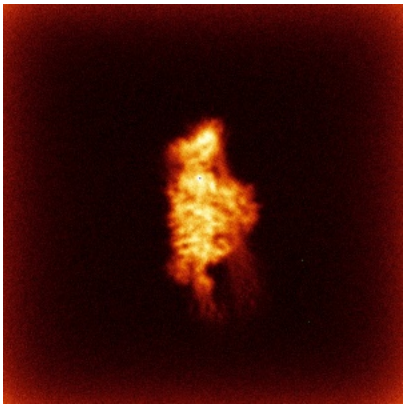
6.4.2 Raw map



X



Y

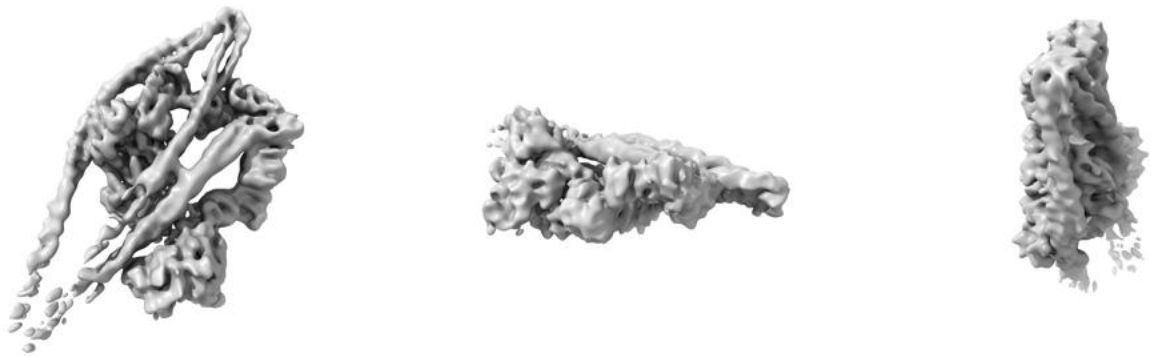


Z

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

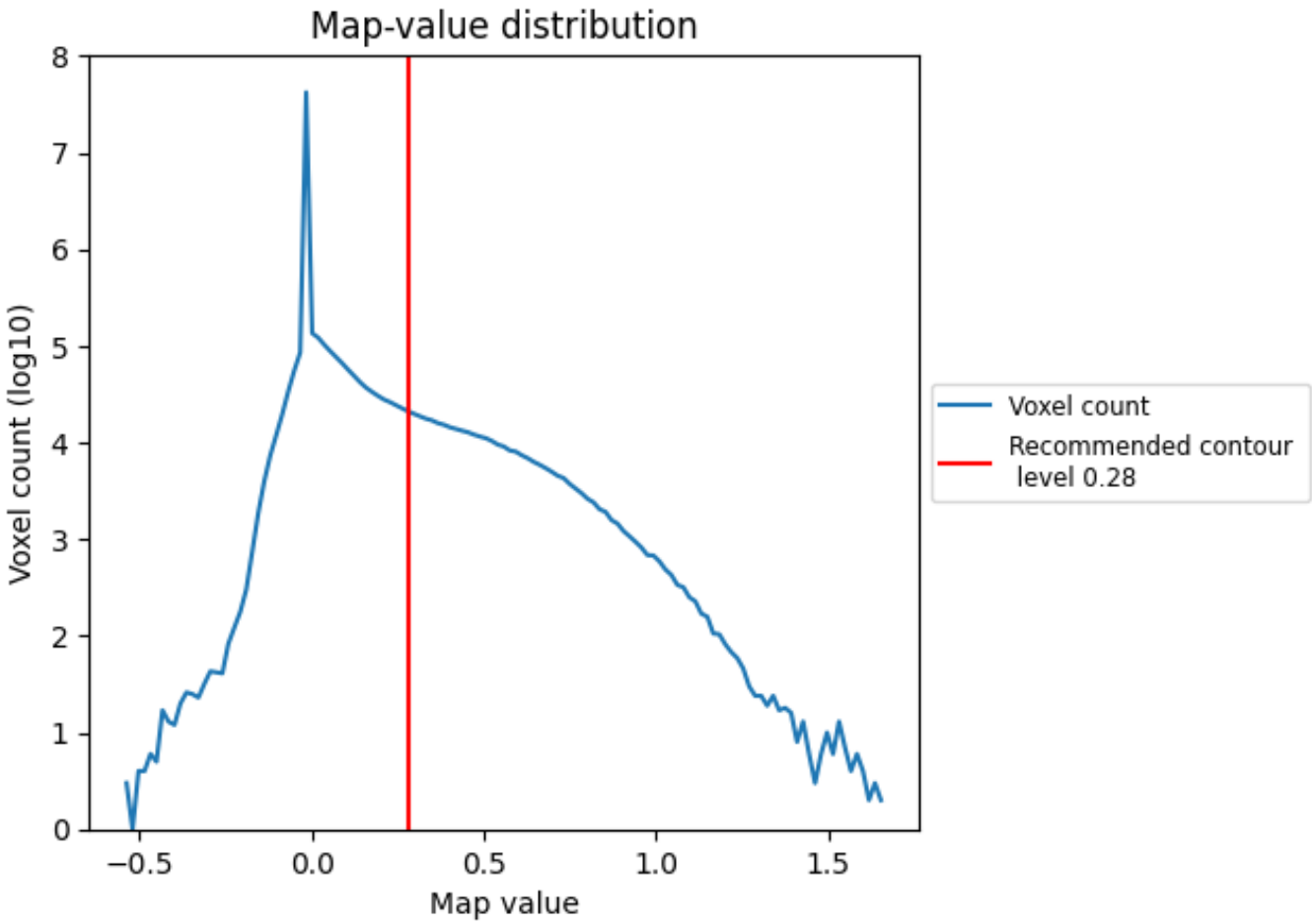
6.6 Mask visualisation (i)

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

7 Map analysis (i)

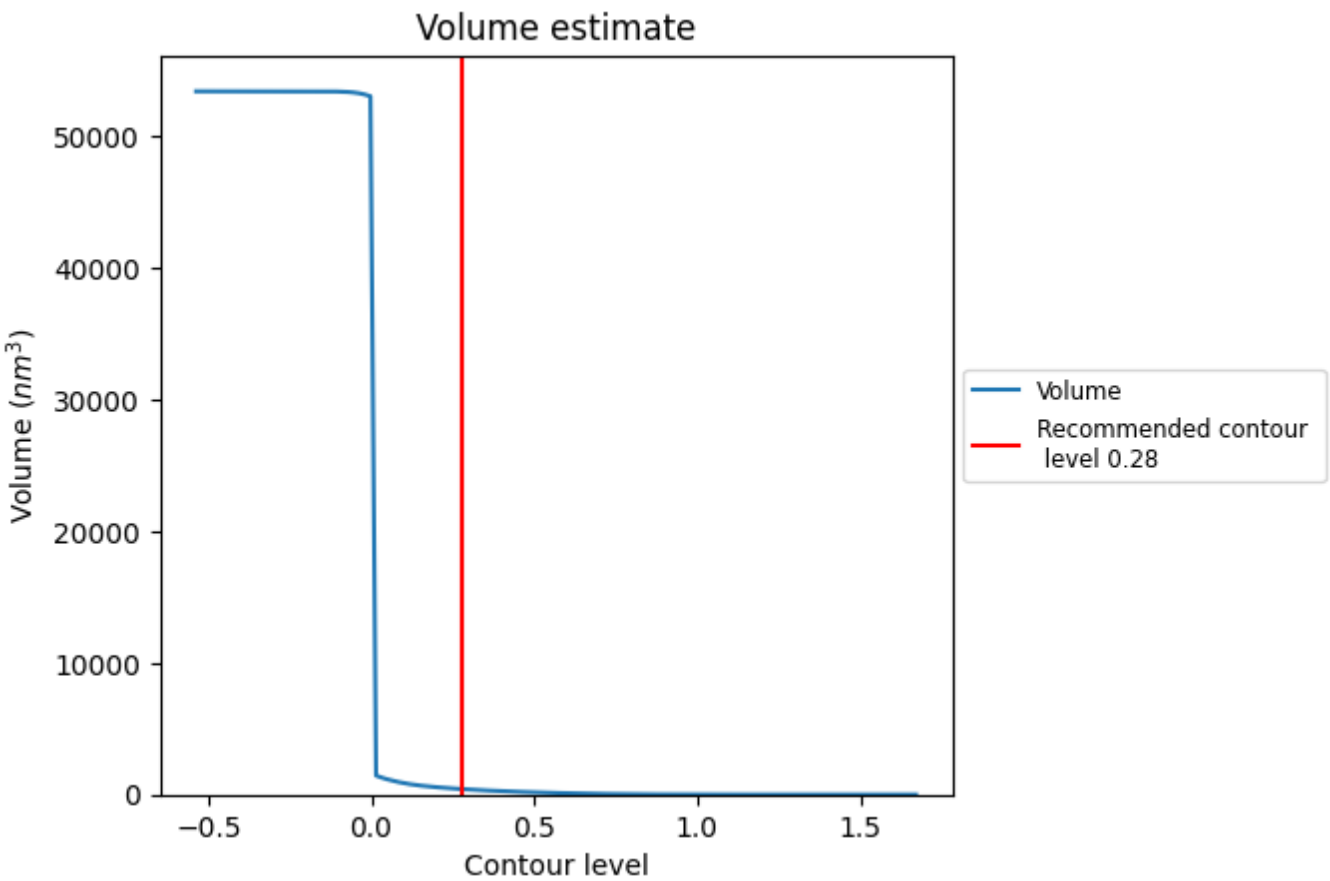
This section contains the results of statistical analysis of the map.

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.

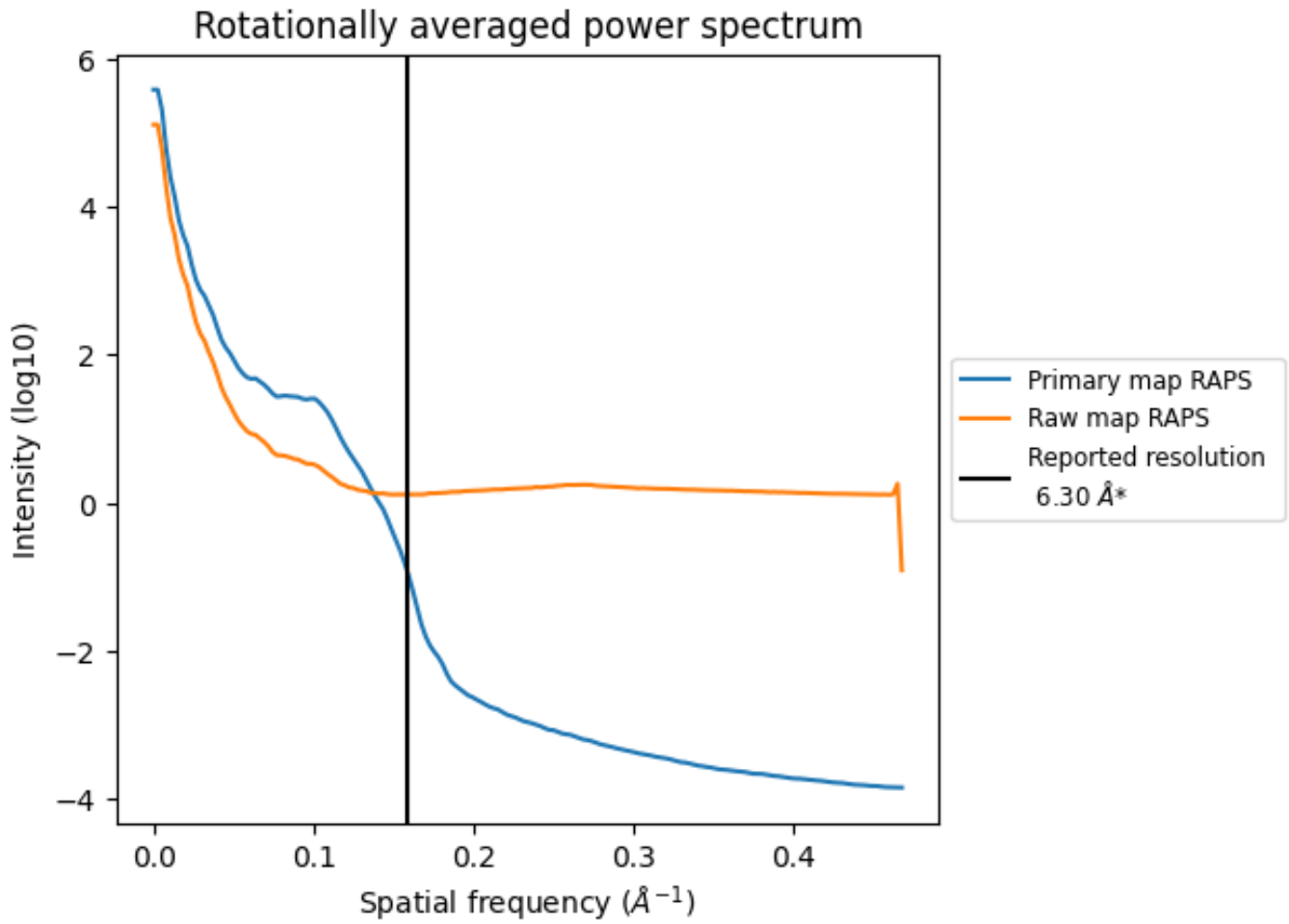
7.2 Volume estimate (i)



The volume at the recommended contour level is 413 nm^3; this corresponds to an approximate mass of 373 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)

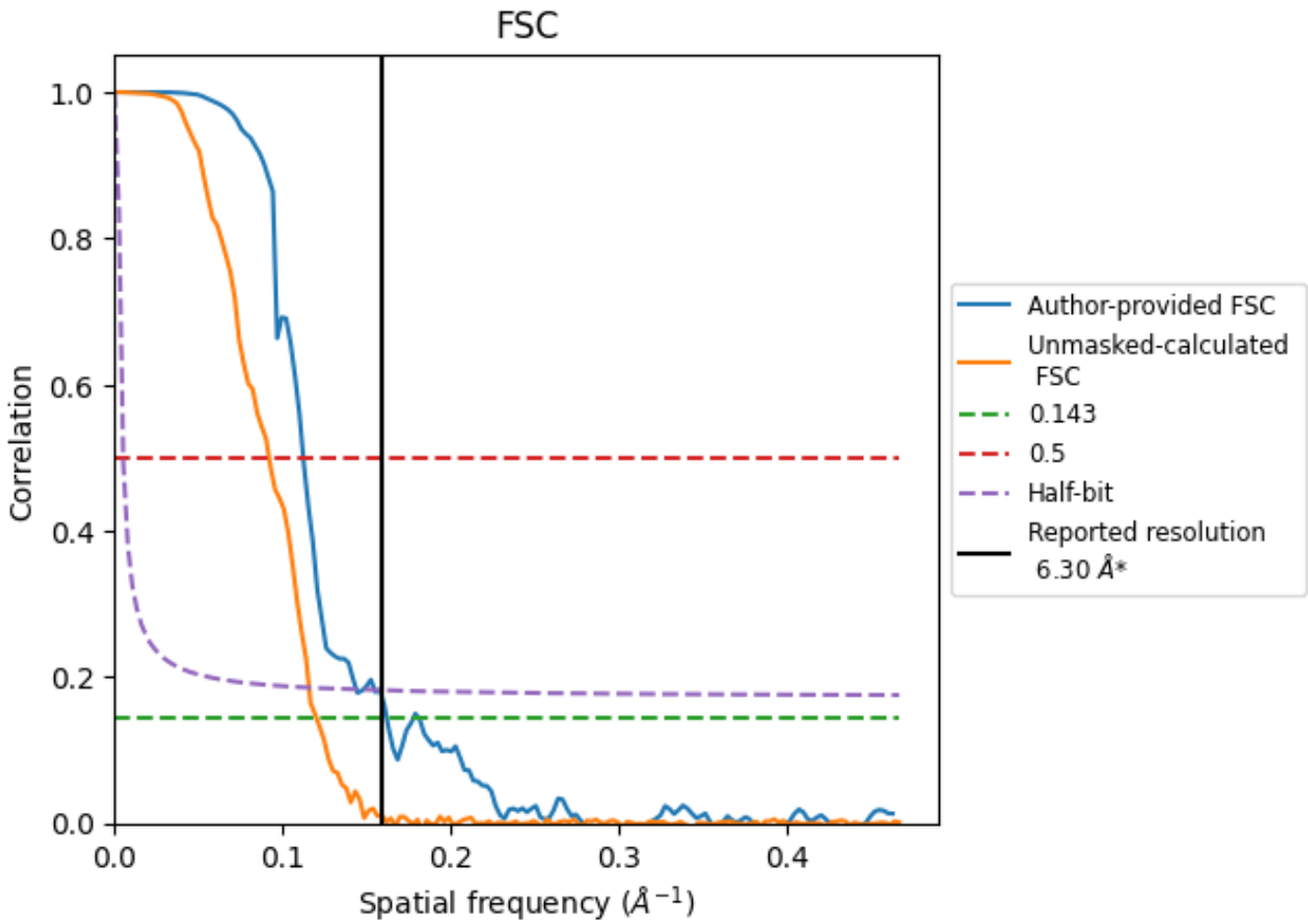


*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

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 0.159 Å^{-1}

8.2 Resolution estimates (i)

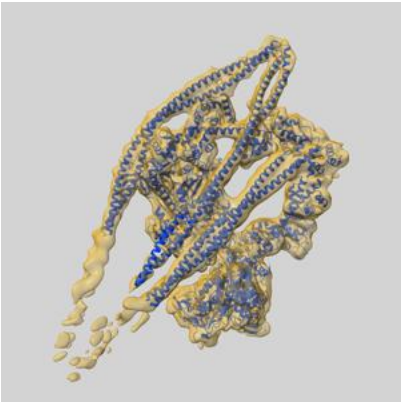
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.17	8.89	6.94
Unmasked-calculated*	8.31	10.87	8.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.31 differs from the reported value 6.3 by more than 10 %

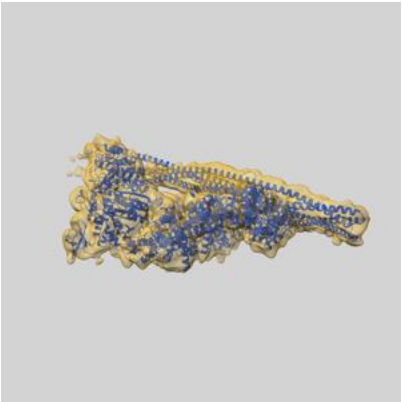
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11069 and PDB model 6Z47. Per-residue inclusion information can be found in section 3 on page 11.

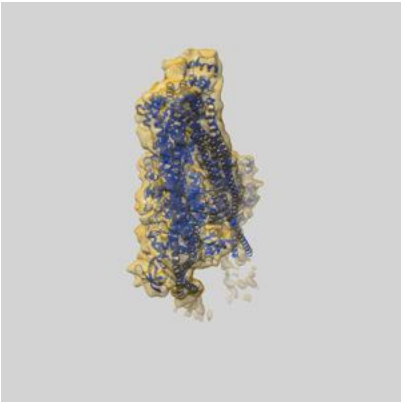
9.1 Map-model overlay (i)



X



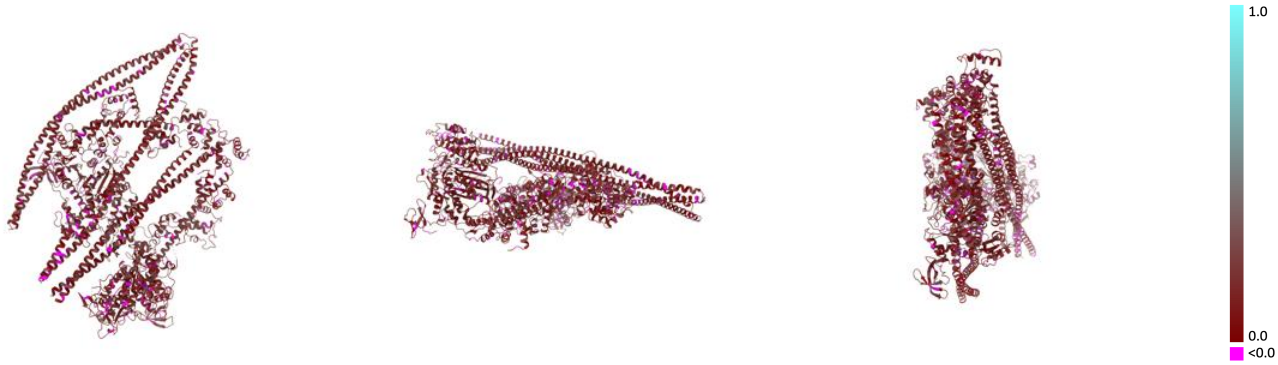
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 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.

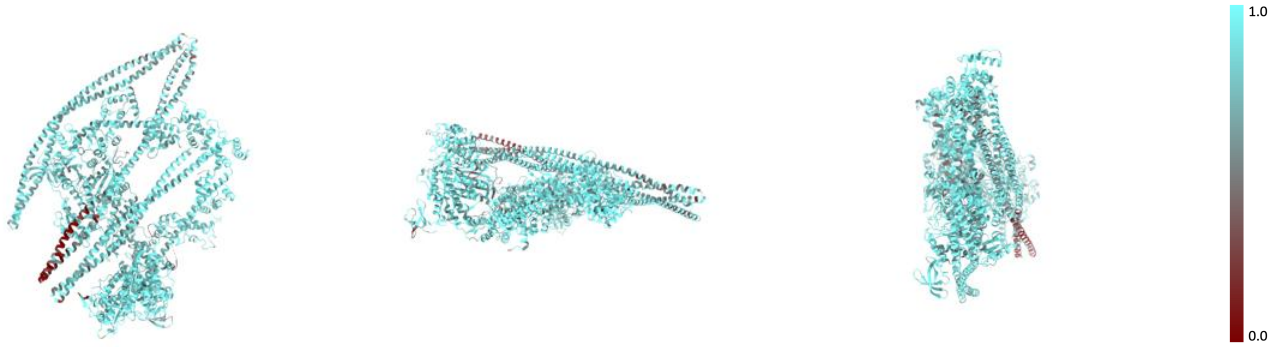
9.2 Q-score mapped to coordinate model (i)



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.

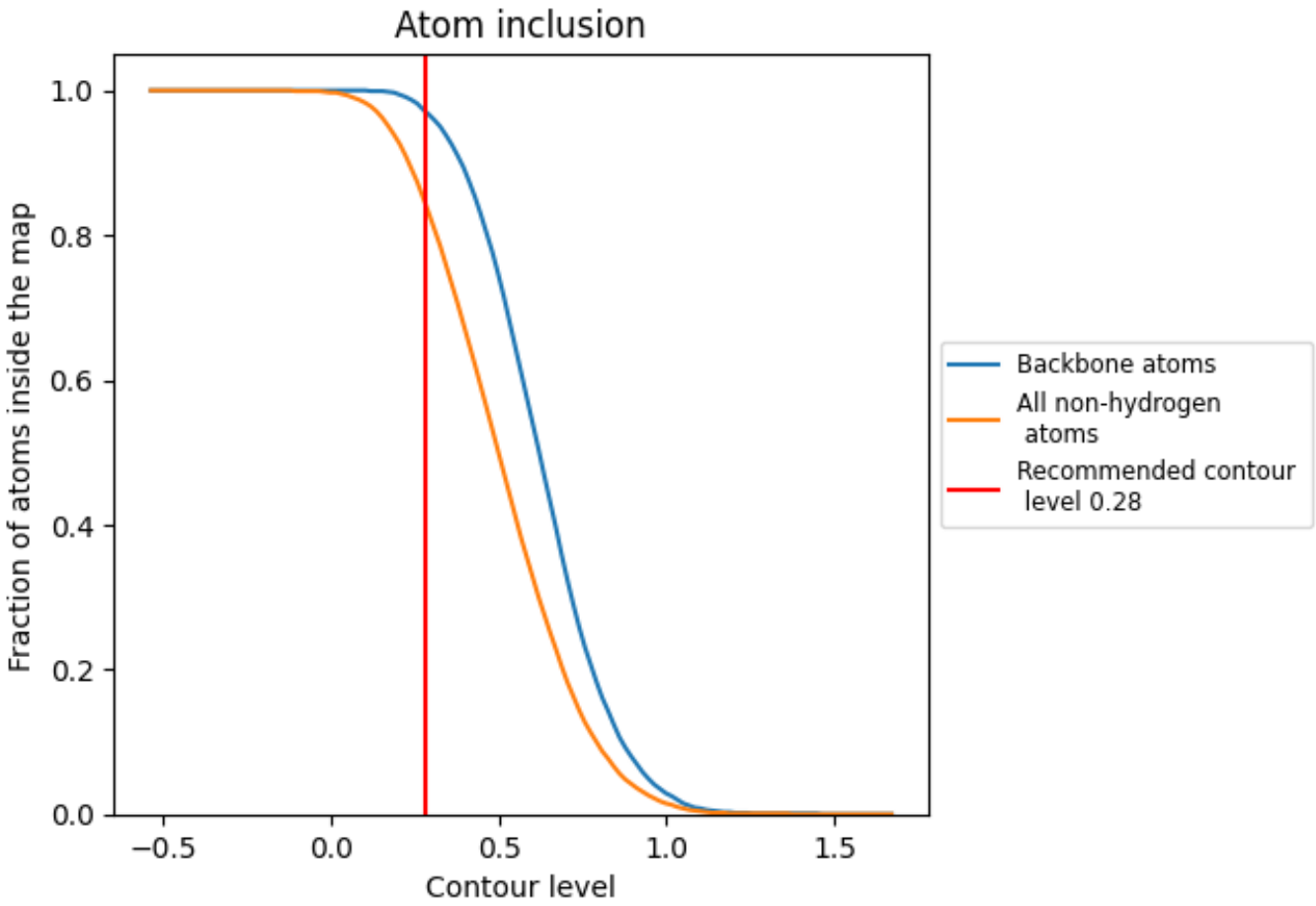
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 84% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.1550
A	0.8650	0.1630
B	0.8640	0.1520
C	0.8650	0.1570
D	0.8720	0.1470
E	0.9140	0.1570
F	0.9340	0.1470
G	0.7310	0.1530
H	0.7060	0.1440