



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 11:52 PM EDT

PDB ID : 9YRG / pdb_00009yrg
EMDB ID : EMD-73367
Title : Cryo-EM structure of human beta-cardiac myosin in the interacting-heads motif and S2-FH undocked state
Authors : Somavarapu, A.K.; Ge, J.; Yengo, C.M.; Craig, R.; Padron, R.
Deposited on : 2025-10-16
Resolution : 3.20 Å (reported)
Based on initial models : 2FXM, 8ACT

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 ⓘ symbol.

The types of validation reports are described at

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

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

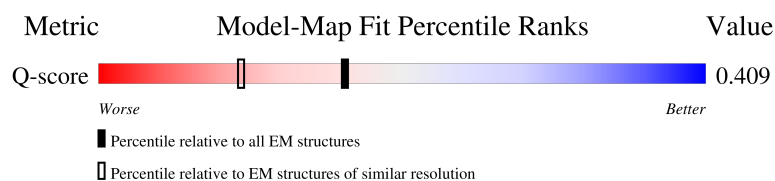
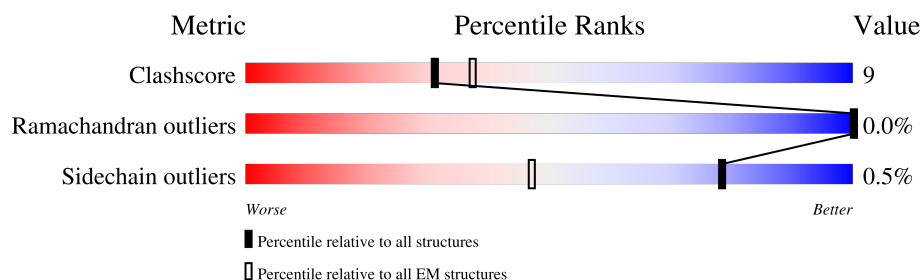
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1315	
1	B	1315	
2	C	188	
2	D	188	

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Mol	Chain	Length	Quality of chain
3	E	169	
3	F	169	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19443 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-7, General control transcription factor GCN4, Enhanced Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	912	Total	C	N	O	S	0	0
			7387	4709	1266	1371	41		
1	B	908	Total	C	N	O	S	0	0
			7362	4693	1262	1366	41		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1049	GLY	-	linker	UNP P03069
A	1050	SER	-	linker	UNP P03069
A	1051	GLY	-	linker	UNP P03069
A	1052	LYS	-	linker	UNP P03069
A	1053	LEU	-	linker	UNP P03069
A	1054	GLY	-	linker	UNP P03069
A	1055	VAL	MET	engineered mutation	UNP P42212
A	1118	LEU	PHE	engineered mutation	UNP P42212
A	1119	THR	SER	engineered mutation	UNP P42212
A	1285	LEU	HIS	engineered mutation	UNP P42212
A	1293	GLY	-	expression tag	UNP P42212
A	1294	LEU	-	expression tag	UNP P42212
A	1295	ASN	-	expression tag	UNP P42212
A	1296	ASP	-	expression tag	UNP P42212
A	1297	ILE	-	expression tag	UNP P42212
A	1298	PHE	-	expression tag	UNP P42212
A	1299	GLU	-	expression tag	UNP P42212
A	1300	ALA	-	expression tag	UNP P42212
A	1301	GLN	-	expression tag	UNP P42212
A	1302	LYS	-	expression tag	UNP P42212
A	1303	ILE	-	expression tag	UNP P42212
A	1304	GLU	-	expression tag	UNP P42212
A	1305	TRP	-	expression tag	UNP P42212
A	1306	HIS	-	expression tag	UNP P42212
A	1307	GLU	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1308	ASP	-	expression tag	UNP P42212
A	1309	TYR	-	expression tag	UNP P42212
A	1310	LYS	-	expression tag	UNP P42212
A	1311	ASP	-	expression tag	UNP P42212
A	1312	ASP	-	expression tag	UNP P42212
A	1313	ASP	-	expression tag	UNP P42212
A	1314	ASP	-	expression tag	UNP P42212
A	1315	LYS	-	expression tag	UNP P42212
B	1049	GLY	-	linker	UNP P03069
B	1050	SER	-	linker	UNP P03069
B	1051	GLY	-	linker	UNP P03069
B	1052	LYS	-	linker	UNP P03069
B	1053	LEU	-	linker	UNP P03069
B	1054	GLY	-	linker	UNP P03069
B	1055	VAL	MET	engineered mutation	UNP P42212
B	1118	LEU	PHE	engineered mutation	UNP P42212
B	1119	THR	SER	engineered mutation	UNP P42212
B	1285	LEU	HIS	engineered mutation	UNP P42212
B	1293	GLY	-	expression tag	UNP P42212
B	1294	LEU	-	expression tag	UNP P42212
B	1295	ASN	-	expression tag	UNP P42212
B	1296	ASP	-	expression tag	UNP P42212
B	1297	ILE	-	expression tag	UNP P42212
B	1298	PHE	-	expression tag	UNP P42212
B	1299	GLU	-	expression tag	UNP P42212
B	1300	ALA	-	expression tag	UNP P42212
B	1301	GLN	-	expression tag	UNP P42212
B	1302	LYS	-	expression tag	UNP P42212
B	1303	ILE	-	expression tag	UNP P42212
B	1304	GLU	-	expression tag	UNP P42212
B	1305	TRP	-	expression tag	UNP P42212
B	1306	HIS	-	expression tag	UNP P42212
B	1307	GLU	-	expression tag	UNP P42212
B	1308	ASP	-	expression tag	UNP P42212
B	1309	TYR	-	expression tag	UNP P42212
B	1310	LYS	-	expression tag	UNP P42212
B	1311	ASP	-	expression tag	UNP P42212
B	1312	ASP	-	expression tag	UNP P42212
B	1313	ASP	-	expression tag	UNP P42212
B	1314	ASP	-	expression tag	UNP P42212
B	1315	LYS	-	expression tag	UNP P42212

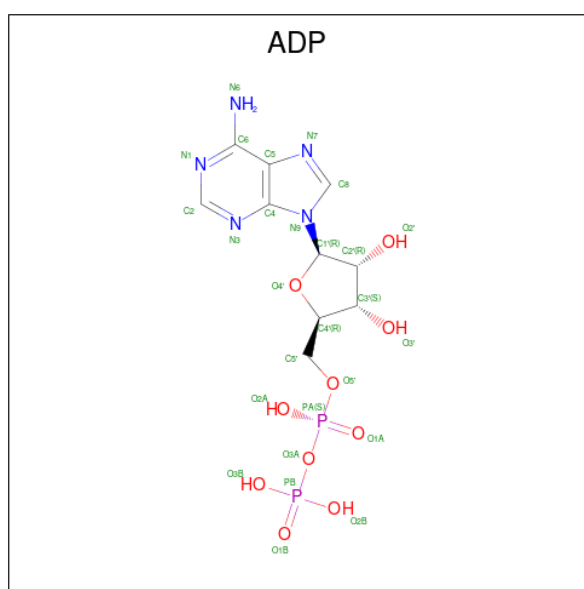
- Molecule 2 is a protein called Myosin light chain 1/3, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	152	Total	C	N	O	S	0	0
			1188	743	198	239	8		
2	D	152	Total	C	N	O	S	0	0
			1188	743	198	239	8		

- Molecule 3 is a protein called Myosin regulatory light chain 11.

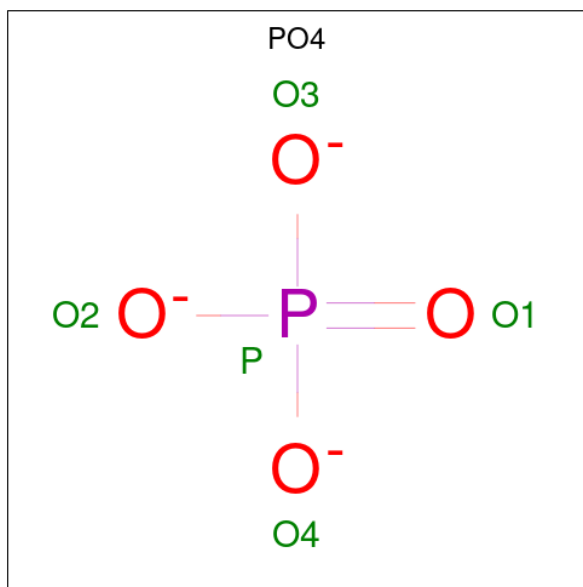
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	142	Total	C	N	O	S	0	0
			1127	715	183	222	7		
3	F	142	Total	C	N	O	S	0	0
			1127	715	183	222	7		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

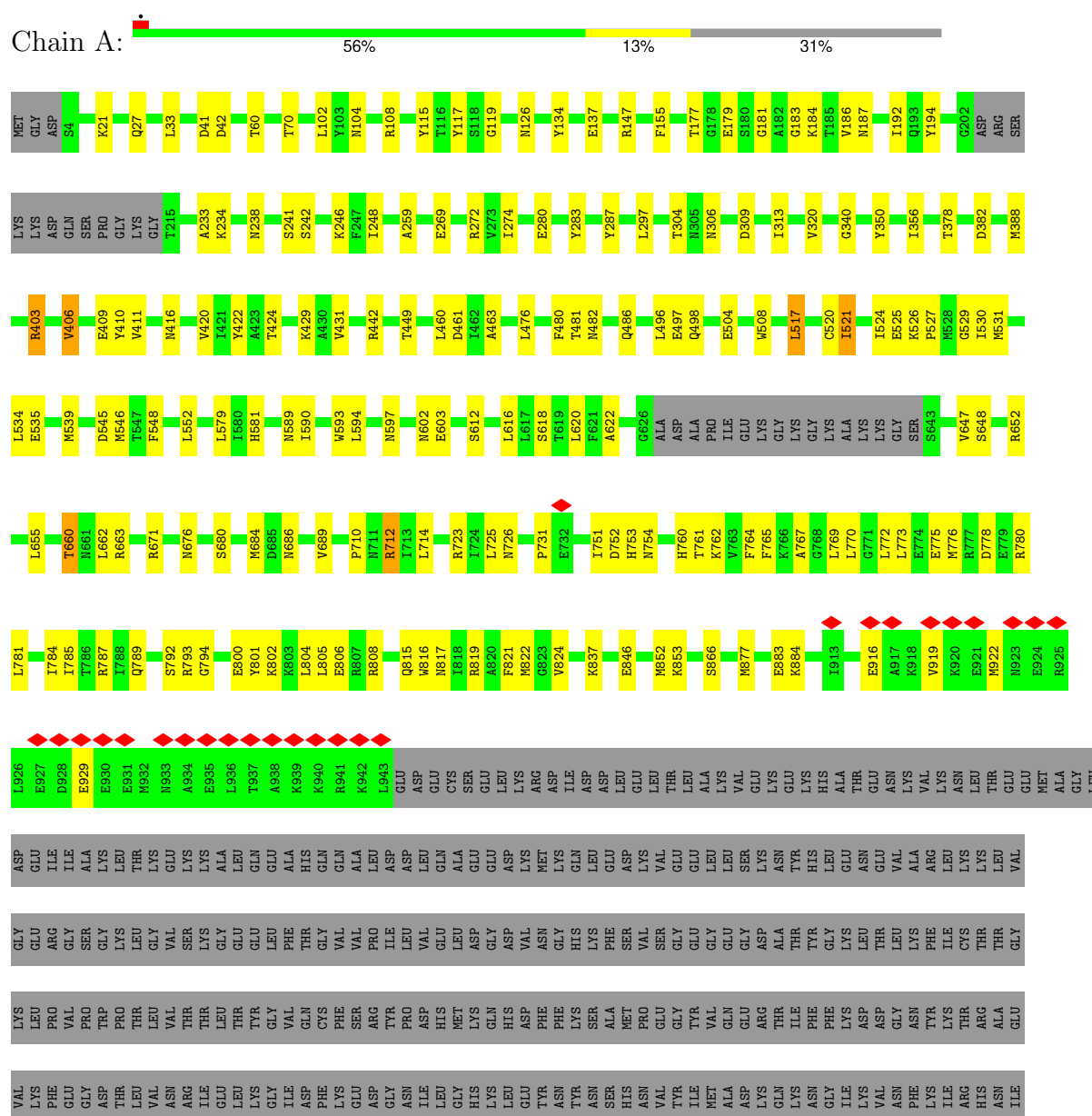


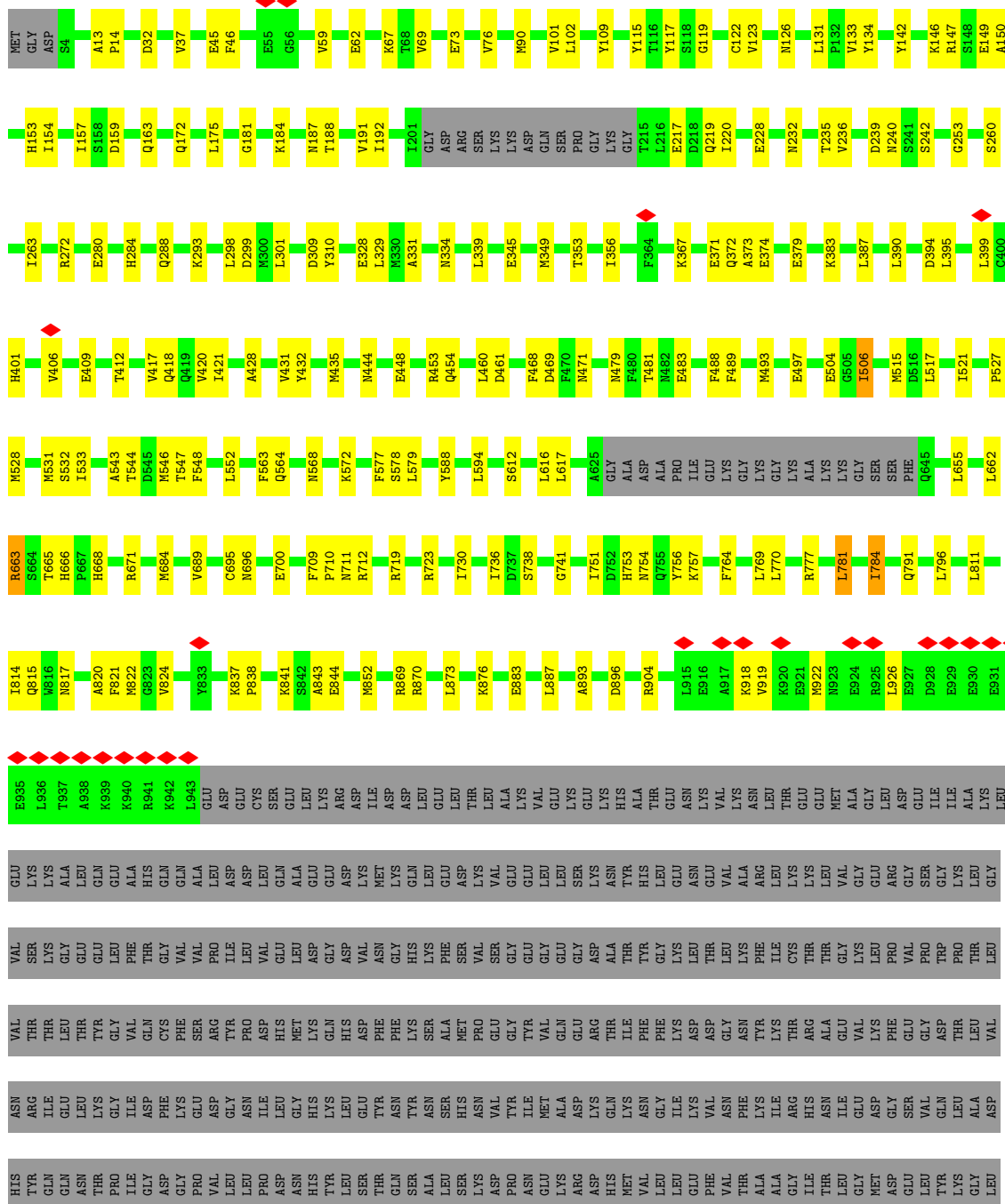
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	P	0
			5	4	1	
5	B	1	Total	O	P	0
			5	4	1	

3 Residue-property plots

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

- Molecule 1: Myosin-7,General control transcription factor GCN4,Enhanced Green fluorescent protein





ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
LYS
ILE
TRP
GLU
HIS
GLU
ASP
TYR
PRO
ASP
ASP
ASP
LYS

- Molecule 2: Myosin light chain 1/3, skeletal muscle isoform

Chain C:



MET
ALA
PRO
LYS
LYS
VAL
LYS
LYS
PRO
ALA
ALA
ALA
PRO
ALA
ALA
PRO
PRO
PRO
ALA
ALA
PRO
LYS
PRO
LYS
GLU
GLU
LYS
ILE
ASP
LEU
SER
A36
I37
K38
I39
S42
K43
E44
E51
L55
L66
V69
L73
R74
T78
K86
L89

N94
F107
L108
P109
M110
G121
E124
D125
F126
V127
E128
G129
V132
L150
L153
G154
E155
K156
M157
L165
Q169
Y178
V182
M186
S187
VAL

- Molecule 2: Myosin light chain 1/3, skeletal muscle isoform

Chain D:



MET
ALA
PRO
LYS
LYS
VAL
ASP
VAL
LYS
LYS
PRO
ALA
ALA
ALA
PRO
ALA
ALA
PRO
PRO
PRO
LYS
PRO
LYS
GLU
GLU
LYS
ILE
ASP
LEU
SER
A36
I37
A52
F53
F56
V72
G90
N91
M97
F104
F107
L108
P109
F126
V132

M142
V149
L153
K156
M157
K158
E159
E160
L165
D171
C175
F181
I185
M186
S187
VAL

- Molecule 3: Myosin regulatory light chain 11

Chain E:



MET
ALA
PRO
LYS
LYS
ALA
ARG
ARG
ALA
GLY
ALA
ALA
GLY
SER
SER
ASN
VAL
PHE
SER
MET
F22
D23
Q24
E32
A33
F34
T35
V36
Q39
M40
R41
M57
G58
A74
I78
N79
F80
T81
V82
F83
L84
T85
M86
E89
K90
L91
A94
D95
P96
E97
I100

N138
M139
W140
D146
Y153
K154
N155
I156
C157
Y158
T161
H162
G163
ASP
ALA
ALA
LYS
ASP
GLN
GLU

- Molecule 3: Myosin regulatory light chain 11

Chain F:



MET
ALA
PRO
LYS
LYS
ALA
ARG
ARG
ALA
GLY
ALA
GLY
GLY
SER
SER
ASN
VAL
PHE
SER
MET
F22
D23
E29
A33
F34
T44
I45
D46
D49
A56
M57
G58
R59
E65
D68
A69
I78
N79
M85
F87
D95
I100
L107
E121
L124

I136
M139
W140
D146
Y153
C157
I160
G163
ASP
ALA
ALA
LYS
ASP
GLN
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.059	Depositor
Minimum map value	-0.633	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PO4

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	0.45	2/7530 (0.0%)	0.62	3/10129 (0.0%)
1	B	0.40	0/7504	0.57	0/10095
2	C	0.15	0/1203	0.32	0/1611
2	D	0.20	0/1203	0.38	0/1611
3	E	0.25	0/1147	0.36	0/1544
3	F	0.20	0/1147	0.41	0/1544
All	All	0.39	2/19734 (0.0%)	0.55	3/26534 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	LEU	C-N	10.09	1.46	1.33
1	A	497	GLU	C-N	-7.82	1.23	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	LEU	O-C-N	7.89	130.49	122.12
1	A	521	ILE	N-CA-C	-5.71	106.23	112.80
1	A	520	CYS	N-CA-C	-5.37	107.38	114.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	ARG	Sidechain
1	A	712	ARG	Sidechain
1	B	663	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7387	0	7416	143	0
1	B	7362	0	7396	148	0
2	C	1188	0	1164	30	0
2	D	1188	0	1164	16	0
3	E	1127	0	1098	22	0
3	F	1127	0	1098	21	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
All	All	19443	0	19360	342	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.

All (342) 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:726:ASN:H	1:A:780:ARG:NH1	1.69	0.91
2:C:73:LEU:O	2:C:78:THR:OG1	1.94	0.86
1:A:179:GLU:O	1:A:184:LYS:NZ	2.13	0.81
3:F:65:GLU:N	3:F:65:GLU:OE2	2.13	0.80
1:B:837:LYS:NZ	3:F:33:ALA:O	2.15	0.79
1:A:751:ILE:HD13	1:A:773:LEU:HD11	1.64	0.78
1:B:272:ARG:NH2	1:B:280:GLU:OE2	2.15	0.78
1:A:726:ASN:H	1:A:780:ARG:HH11	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:N	5:A:1402:PO4:O3	2.18	0.77
1:B:481:THR:HG23	1:B:655:LEU:HD21	1.67	0.76
1:A:33:LEU:HD12	1:A:33:LEU:O	1.86	0.75
1:B:671:ARG:NH2	1:B:696:ASN:OD1	2.20	0.75
1:B:700:GLU:N	1:B:700:GLU:OE1	2.19	0.75
1:A:41:ASP:OD1	1:A:42:ASP:N	2.22	0.73
2:C:51:GLU:O	2:C:55:LEU:HD23	1.90	0.72
2:C:69:VAL:HG11	2:C:89:LEU:HD21	1.70	0.71
1:A:785:ILE:HG13	2:C:153:LEU:HD23	1.72	0.71
1:B:784:ILE:HD11	2:D:126:PHE:HA	1.71	0.71
1:A:297:LEU:HD11	1:A:350:TYR:CD2	2.26	0.70
1:A:663:ARG:NH2	1:B:896:ASP:OD2	2.23	0.70
1:A:108:ARG:NH1	1:A:115:TYR:O	2.25	0.70
1:B:232:ASN:O	1:B:284:HIS:ND1	2.26	0.68
1:A:846:GLU:N	1:A:846:GLU:OE1	2.27	0.68
1:A:137:GLU:N	1:A:137:GLU:OE1	2.28	0.67
1:A:603:GLU:N	1:A:603:GLU:OE2	2.26	0.67
1:A:787:ARG:HH21	2:C:121:GLY:HA2	1.60	0.67
1:A:406:VAL:HG22	1:A:411:VAL:HG21	1.77	0.67
1:A:922:MET:HG2	1:B:922:MET:SD	2.36	0.65
1:B:811:LEU:HD23	1:B:814:ILE:HD11	1.79	0.64
1:B:820:ALA:O	1:B:824:VAL:HG22	1.97	0.64
1:B:479:ASN:OD1	1:B:588:TYR:OH	2.16	0.64
1:B:719:ARG:HH21	1:B:741:GLY:HA3	1.61	0.63
1:B:506:ILE:HD11	1:B:757:LYS:HG3	1.81	0.63
1:A:676:ASN:ND2	1:A:680:SER:OG	2.31	0.63
3:E:155:ASN:OD1	3:E:156:ILE:N	2.32	0.62
1:B:533:ILE:HG21	1:B:552:LEU:HD23	1.81	0.62
1:B:852:MET:HE3	1:B:852:MET:O	1.99	0.62
1:A:545:ASP:OD1	1:A:546:MET:N	2.32	0.62
1:B:298:LEU:HD12	1:B:299:ASP:N	2.15	0.61
1:A:486:GLN:OE1	1:A:671:ARG:NH2	2.34	0.61
1:A:287:TYR:OH	1:A:313:ILE:O	2.18	0.60
1:A:919:VAL:HG23	1:A:922:MET:HE3	1.83	0.60
1:A:378:THR:HG22	1:A:382:ASP:OD1	2.02	0.60
1:A:238:ASN:ND2	4:A:1401:ADP:O3B	2.35	0.60
1:B:777:ARG:HH21	2:D:132:VAL:HG22	1.66	0.60
1:B:460:LEU:HD23	1:B:461:ASP:N	2.18	0.59
1:B:497:GLU:CD	1:B:712:ARG:HH22	2.10	0.59
1:B:684:MET:HG2	1:B:689:VAL:HG21	1.85	0.59
1:A:524:ILE:O	1:A:531:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:LEU:HD21	2:C:132:VAL:HG21	1.83	0.59
2:C:89:LEU:HD23	2:C:110:MET:HE1	1.84	0.59
1:A:27:GLN:OE1	1:A:27:GLN:N	2.36	0.58
1:B:117:TYR:CE2	1:B:147:ARG:HG3	2.38	0.58
1:B:260:SER:OG	1:B:453:ARG:HD3	2.03	0.58
1:B:515:MET:HE2	1:B:515:MET:HA	1.85	0.58
1:B:544:THR:O	1:B:547:THR:OG1	2.19	0.58
1:B:841:LYS:NZ	3:F:29:GLU:O	2.36	0.58
3:E:138:ASN:OD1	3:E:139:MET:N	2.37	0.57
1:A:822:MET:HE2	1:A:822:MET:N	2.19	0.57
1:B:751:ILE:HA	1:B:753:HIS:CE1	2.39	0.57
1:B:791:GLN:HG2	2:D:185:ILE:HG22	1.87	0.57
1:A:126:ASN:ND2	1:A:181:GLY:O	2.38	0.56
1:A:821:PHE:HA	1:A:824:VAL:HG22	1.86	0.56
1:B:367:LYS:NZ	1:B:374:GLU:O	2.29	0.56
1:A:246:LYS:NZ	1:A:461:ASP:OD2	2.26	0.56
1:B:301:LEU:HD21	1:B:310:TYR:OH	2.05	0.56
1:A:463:ALA:O	1:A:482:ASN:ND2	2.32	0.56
1:A:723:ARG:NH2	1:A:731:PRO:O	2.39	0.56
1:A:726:ASN:N	1:A:780:ARG:NH1	2.48	0.56
1:A:852:MET:C	1:A:852:MET:HE3	2.30	0.56
1:B:417:VAL:HG13	1:B:418:GLN:OE1	2.05	0.56
1:B:239:ASP:OD1	1:B:240:ASN:ND2	2.36	0.56
3:E:89:GLU:N	3:E:89:GLU:OE1	2.39	0.56
1:B:379:GLU:N	1:B:379:GLU:OE1	2.38	0.55
1:A:817:ASN:OD1	3:E:100:ILE:HD11	2.06	0.55
1:B:253:GLY:HA2	1:B:454:GLN:HG2	1.87	0.55
1:B:796:LEU:HG	2:D:165:LEU:HD11	1.88	0.55
1:A:525:GLU:HG2	1:A:526:LYS:H	1.72	0.55
1:A:801:TYR:CZ	1:A:805:LEU:HD21	2.41	0.55
3:E:23:ASP:OD1	3:E:24:GLN:N	2.40	0.55
1:A:597:ASN:HA	1:A:647:VAL:HG22	1.87	0.55
1:B:723:ARG:NH1	1:B:730:ILE:O	2.40	0.55
1:A:792:SER:OG	2:C:165:LEU:HD22	2.07	0.55
1:B:172:GLN:HG2	1:B:668:HIS:HE1	1.70	0.55
1:A:356:ILE:HD11	1:A:431:VAL:HG13	1.89	0.55
2:C:186:MET:O	2:C:187:SER:C	2.50	0.54
1:B:543:ALA:HB1	1:B:594:LEU:HD13	1.89	0.54
1:A:751:ILE:O	1:A:753:HIS:ND1	2.40	0.54
1:B:260:SER:HB3	1:B:448:GLU:HA	1.88	0.54
1:A:527:PRO:HB2	1:B:904:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:O	1:B:399:LEU:HD13	2.07	0.54
2:C:129:GLY:O	2:C:132:VAL:HG22	2.08	0.54
1:A:808:ARG:HD3	2:C:55:LEU:HD11	1.90	0.54
1:B:293:LYS:HB3	1:B:329:LEU:HD23	1.90	0.54
1:A:801:TYR:CE2	1:A:805:LEU:HD11	2.43	0.54
1:A:183:GLY:O	1:A:187:ASN:ND2	2.41	0.54
1:A:919:VAL:HG23	1:A:922:MET:CE	2.38	0.54
1:A:752:ASP:OD1	1:A:752:ASP:N	2.39	0.53
3:F:46:ASP:N	3:F:49:ASP:OD2	2.41	0.53
1:B:469:ASP:HB2	1:B:572:LYS:HD3	1.89	0.53
3:E:85:THR:OG1	3:E:86:MET:HE2	2.09	0.53
1:A:785:ILE:O	1:A:789:GLN:HG3	2.08	0.53
1:B:515:MET:HE3	1:B:700:GLU:OE2	2.09	0.53
1:A:416:ASN:O	1:A:420:VAL:HG23	2.08	0.53
1:B:460:LEU:HD12	1:B:662:LEU:HD21	1.91	0.53
1:A:725:LEU:HD11	1:A:776:MET:HB3	1.91	0.53
1:A:480:PHE:HE1	1:A:521:ILE:HG23	1.74	0.52
1:A:531:MET:HG3	1:A:652:ARG:HD3	1.91	0.52
1:B:142:TYR:HE1	1:B:150:ALA:HB1	1.74	0.52
1:A:297:LEU:HD11	1:A:350:TYR:HD2	1.69	0.52
1:A:481:THR:HA	1:A:655:LEU:HD21	1.92	0.52
2:D:149:VAL:HG23	2:D:153:LEU:HG	1.91	0.52
1:A:789:GLN:NE2	2:C:150:LEU:O	2.43	0.52
1:B:822:MET:HE1	3:F:139:MET:HB3	1.91	0.52
1:B:219:GLN:NE2	1:B:339:LEU:O	2.43	0.52
2:D:56:PHE:HE2	2:D:72:VAL:HG22	1.75	0.52
1:A:866:SER:HA	1:B:870:ARG:HH22	1.75	0.51
1:B:489:PHE:CE1	1:B:493:MET:HG3	2.45	0.51
2:C:66:LEU:O	2:C:69:VAL:HG12	2.11	0.51
1:B:517:LEU:HD12	1:B:517:LEU:O	2.10	0.51
1:A:800:GLU:C	1:A:800:GLU:OE1	2.54	0.51
1:B:869:ARG:HG3	1:B:873:LEU:HD23	1.92	0.51
1:B:131:LEU:O	1:B:133:VAL:N	2.39	0.50
1:B:235:THR:HG22	1:B:236:VAL:H	1.76	0.50
1:A:119:GLY:O	1:A:147:ARG:NH2	2.45	0.50
1:A:403:ARG:HH11	1:A:410:TYR:HB3	1.75	0.50
1:A:922:MET:CG	1:B:922:MET:SD	2.99	0.50
1:A:714:LEU:HA	1:A:762:LYS:HB3	1.93	0.50
1:A:409:GLU:HB3	1:B:453:ARG:HH21	1.77	0.50
1:B:751:ILE:HA	1:B:753:HIS:HE1	1.77	0.50
1:B:126:ASN:ND2	1:B:181:GLY:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:HD11	1:B:612:SER:HA	1.94	0.50
1:A:117:TYR:HB3	1:A:147:ARG:NH2	2.26	0.50
2:C:127:VAL:HG12	2:C:182:VAL:HG11	1.93	0.50
2:C:169:GLN:N	2:C:169:GLN:OE1	2.44	0.50
3:F:121:GLU:OE2	3:F:136:ILE:HG23	2.11	0.50
1:A:816:TRP:HA	1:A:819:ARG:HE	1.77	0.49
1:B:45:GLU:O	1:B:46:PHE:CG	2.65	0.49
1:B:578:SER:O	1:B:578:SER:OG	2.28	0.49
1:B:394:ASP:OD1	1:B:395:LEU:N	2.45	0.49
1:B:187:ASN:O	1:B:191:VAL:HG23	2.12	0.49
3:E:82:VAL:HG13	3:E:86:MET:HE3	1.94	0.49
3:F:57:MET:HE3	3:F:57:MET:N	2.27	0.49
1:A:808:ARG:CD	2:C:55:LEU:HD11	2.42	0.49
1:A:916:GLU:O	1:A:919:VAL:HG12	2.13	0.49
1:B:844:GLU:OE1	1:B:844:GLU:N	2.45	0.49
1:B:32:ASP:N	1:B:32:ASP:OD1	2.44	0.49
1:B:504:GLU:HG3	1:B:764:PHE:CZ	2.47	0.48
1:A:234:LYS:CD	1:A:320:VAL:HG11	2.44	0.48
1:B:172:GLN:CG	1:B:668:HIS:HE1	2.26	0.48
3:F:79:ASN:OD1	3:F:79:ASN:C	2.56	0.48
1:A:804:LEU:HD23	1:A:804:LEU:C	2.38	0.48
1:A:590:ILE:O	1:A:590:ILE:HG22	2.12	0.48
1:B:546:MET:HA	1:B:546:MET:HE2	1.94	0.48
1:A:460:LEU:HD22	1:A:662:LEU:HD11	1.96	0.48
1:A:660:THR:HG21	1:B:893:ALA:HB2	1.95	0.48
2:C:42:SER:OG	2:C:44:GLU:OE2	2.21	0.48
3:E:81:THR:O	3:E:84:LEU:HD12	2.14	0.48
3:F:86:MET:SD	3:F:87:PHE:N	2.86	0.48
1:A:274:ILE:HD13	1:A:429:LYS:CD	2.43	0.48
2:D:158:LYS:NZ	2:D:160:GLU:OE1	2.46	0.48
1:A:712:ARG:HD3	1:A:764:PHE:CE2	2.49	0.48
1:B:59:VAL:HG23	1:B:73:GLU:HG2	1.95	0.48
1:B:142:TYR:CE1	1:B:150:ALA:HB1	2.49	0.48
1:A:765:PHE:CD1	1:A:769:LEU:HD23	2.49	0.47
3:F:68:ASP:OD1	3:F:69:ALA:N	2.46	0.47
1:B:159:ASP:O	1:B:163:GLN:HG2	2.13	0.47
1:B:756:TYR:HD2	1:B:769:LEU:HD21	1.79	0.47
1:B:62:GLU:OE2	1:B:67:LYS:N	2.47	0.47
1:A:602:ASN:OD1	1:A:602:ASN:O	2.32	0.47
1:B:564:GLN:OE1	1:B:564:GLN:N	2.48	0.47
3:E:36:VAL:O	3:E:39:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ARG:HH12	1:B:738:SER:HA	1.80	0.47
1:B:883:GLU:O	1:B:887:LEU:HD23	2.14	0.47
2:C:125:ASP:OD1	2:C:126:PHE:N	2.48	0.47
1:A:802:LYS:O	1:A:806:GLU:HG2	2.14	0.47
1:A:531:MET:SD	1:A:648:SER:OG	2.73	0.47
1:B:468:PHE:HB2	1:B:471:ASN:OD1	2.15	0.47
1:B:37:VAL:HG11	1:B:76:VAL:HG13	1.97	0.46
1:B:616:LEU:C	1:B:616:LEU:HD23	2.39	0.46
1:A:304:THR:HG23	1:A:306:ASN:H	1.80	0.46
1:B:188:THR:O	1:B:192:ILE:HG13	2.15	0.46
2:D:142:MET:SD	2:D:142:MET:N	2.88	0.46
1:B:184:LYS:N	4:B:1401:ADP:O1B	2.35	0.46
3:F:153:TYR:HH	3:F:157:CYS:HG	1.64	0.46
1:B:528:MET:O	1:B:528:MET:SD	2.74	0.46
1:A:772:LEU:O	1:A:775:GLU:HG2	2.16	0.46
1:A:804:LEU:HD23	1:A:804:LEU:O	2.16	0.46
1:B:263:ILE:O	1:B:444:ASN:ND2	2.48	0.46
1:B:353:THR:O	1:B:356:ILE:HG13	2.15	0.46
1:B:814:ILE:HD13	3:F:107:LEU:HD22	1.98	0.46
1:B:371:GLU:OE1	1:B:371:GLU:HA	2.15	0.46
1:B:548:PHE:O	1:B:552:LEU:HG	2.15	0.46
1:B:531:MET:SD	1:B:532:SER:N	2.88	0.46
3:E:153:TYR:HA	3:E:156:ILE:HG12	1.98	0.46
1:A:837:LYS:NZ	3:E:161:THR:O	2.49	0.45
1:B:345:GLU:O	1:B:349:MET:HG3	2.16	0.45
2:C:89:LEU:HD23	2:C:110:MET:CE	2.45	0.45
1:A:134:TYR:OH	4:A:1401:ADP:N6	2.41	0.45
1:A:761:THR:O	1:A:761:THR:HG22	2.16	0.45
1:B:488:PHE:HE1	1:B:663:ARG:HG2	1.80	0.45
1:B:331:ALA:HA	1:B:334:ASN:HD21	1.82	0.45
1:B:260:SER:HB3	1:B:448:GLU:HG2	1.98	0.45
1:A:778:ASP:HA	2:C:153:LEU:HD11	1.99	0.45
1:A:877:MET:HG3	1:B:876:LYS:HZ3	1.80	0.45
1:B:309:ASP:N	1:B:309:ASP:OD1	2.50	0.45
2:C:124:GLU:O	2:C:127:VAL:HG22	2.16	0.45
1:A:60:THR:HG22	1:A:70:THR:HG22	1.99	0.45
1:A:784:ILE:HG12	2:C:129:GLY:HA3	1.98	0.45
1:A:877:MET:HG3	1:B:876:LYS:NZ	2.32	0.45
1:A:272:ARG:NH2	1:A:280:GLU:OE1	2.43	0.45
1:A:422:TYR:CD1	1:A:422:TYR:C	2.95	0.45
1:A:498:GLN:HG2	1:A:508:TRP:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:O	1:A:521:ILE:HG13	2.17	0.45
1:A:754:ASN:N	1:A:754:ASN:OD1	2.50	0.45
3:E:97:GLU:CG	3:E:161:THR:HG21	2.47	0.45
1:A:725:LEU:HA	1:A:780:ARG:NH1	2.32	0.45
1:A:793:ARG:HG2	2:C:157:MET:HE3	1.99	0.45
2:D:171:ASP:N	2:D:175:CYS:O	2.48	0.45
1:A:710:PRO:HG3	1:A:767:ALA:HA	1.99	0.44
1:A:916:GLU:HA	1:A:919:VAL:HG12	1.97	0.44
1:A:929:GLU:HG3	1:B:926:LEU:HD11	1.99	0.44
1:B:115:TYR:CG	1:B:153:HIS:HA	2.52	0.44
1:B:154:ILE:HA	1:B:157:ILE:HD12	1.99	0.44
1:A:530:ILE:HG23	1:A:552:LEU:HD21	1.99	0.44
1:A:794:GLY:HA2	2:C:74:ARG:HB3	1.98	0.44
1:B:781:LEU:HA	1:B:784:ILE:HG22	2.00	0.44
2:D:97:MET:SD	2:D:97:MET:C	3.00	0.44
1:B:172:GLN:HG3	1:B:666:HIS:HB3	1.99	0.44
1:B:568:ASN:OD1	1:B:568:ASN:N	2.50	0.44
1:B:730:ILE:HG23	1:B:736:ILE:HG21	1.99	0.44
3:E:158:TYR:O	3:E:162:HIS:N	2.51	0.44
3:E:139:MET:HE1	3:E:140:TRP:CE3	2.53	0.44
1:A:233:ALA:O	1:A:241:SER:OG	2.20	0.44
1:A:269:GLU:O	1:A:283:TYR:OH	2.31	0.44
1:A:805:LEU:O	1:A:808:ARG:HG2	2.18	0.44
1:B:417:VAL:HA	1:B:420:VAL:HG22	1.99	0.44
3:E:95:ASP:OD1	3:E:95:ASP:N	2.49	0.44
1:B:401:HIS:CE1	1:B:412:THR:HG23	2.53	0.44
1:B:504:GLU:HG3	1:B:764:PHE:HZ	1.83	0.44
1:A:388:MET:O	1:A:612:SER:OG	2.36	0.44
1:A:684:MET:HE3	1:A:689:VAL:HG11	1.99	0.43
1:B:821:PHE:CE1	3:F:160:ILE:HA	2.53	0.43
1:A:117:TYR:CE2	1:A:147:ARG:HG3	2.52	0.43
1:B:122:CYS:SG	1:B:123:VAL:N	2.92	0.43
1:B:418:GLN:O	1:B:421:ILE:HG22	2.18	0.43
1:A:527:PRO:HD2	1:B:904:ARG:HH11	1.83	0.43
3:E:34:PHE:CD1	3:E:34:PHE:C	2.96	0.43
1:A:529:GLY:O	1:A:530:ILE:C	2.62	0.43
1:A:548:PHE:CE2	1:A:590:ILE:HD12	2.52	0.43
1:B:217:GLU:O	1:B:220:ILE:HG22	2.19	0.43
2:C:107:PHE:O	2:C:110:MET:HG2	2.18	0.43
3:E:41:ARG:HE	3:F:44:ILE:HG21	1.83	0.43
1:B:527:PRO:O	1:B:528:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:LEU:HD12	3:E:91:LEU:O	2.18	0.43
1:A:177:THR:HG21	1:A:671:ARG:NH1	2.34	0.43
1:B:90:MET:SD	1:B:101:VAL:HG13	2.59	0.43
1:B:242:SER:O	1:B:242:SER:OG	2.36	0.43
1:B:684:MET:CG	1:B:689:VAL:HG21	2.48	0.43
1:A:274:ILE:HD13	1:A:429:LYS:HD2	2.01	0.43
1:B:146:LYS:HB3	1:B:149:GLU:HG3	2.00	0.43
1:B:919:VAL:O	1:B:922:MET:HB3	2.19	0.43
1:A:476:LEU:HD22	1:A:593:TRP:CH2	2.54	0.43
1:A:789:GLN:NE2	2:C:155:GLU:O	2.52	0.43
1:A:104:ASN:O	1:A:108:ARG:HB3	2.18	0.42
1:B:109:TYR:CD2	1:B:684:MET:HE3	2.54	0.42
1:B:119:GLY:O	1:B:147:ARG:NH1	2.52	0.42
2:C:38:LYS:HD3	2:C:108:LEU:HD23	2.01	0.42
1:A:751:ILE:HG22	1:A:772:LEU:HD23	2.00	0.42
1:A:883:GLU:OE2	1:A:884:LYS:N	2.53	0.42
1:B:115:TYR:CD2	1:B:153:HIS:HA	2.54	0.42
1:B:372:GLN:OE1	1:B:373:ALA:N	2.52	0.42
1:B:383:LYS:O	1:B:387:LEU:HG	2.19	0.42
1:B:406:VAL:HG22	1:B:409:GLU:HB2	2.01	0.42
1:B:753:HIS:C	1:B:754:ASN:OD1	2.62	0.42
1:B:838:PRO:O	1:B:843:ALA:HB2	2.19	0.42
2:D:104:PHE:O	2:D:107:PHE:N	2.49	0.42
1:B:131:LEU:O	1:B:134:TYR:CE1	2.72	0.42
1:B:235:THR:HG22	1:B:236:VAL:N	2.34	0.42
2:C:86:LYS:HE2	2:C:86:LYS:HA	2.01	0.42
3:E:32:GLU:O	3:E:36:VAL:HG12	2.19	0.42
1:A:676:ASN:N	1:A:676:ASN:OD1	2.52	0.42
1:A:769:LEU:O	1:A:770:LEU:C	2.61	0.42
1:A:922:MET:HE1	1:B:918:LYS:HE3	2.00	0.42
1:B:102:LEU:HD23	1:B:102:LEU:C	2.44	0.42
3:F:34:PHE:N	3:F:34:PHE:CD1	2.87	0.42
1:A:234:LYS:HD2	1:A:320:VAL:HG11	2.02	0.42
1:A:618:SER:O	1:A:622:ALA:N	2.52	0.42
1:B:175:LEU:N	1:B:175:LEU:HD12	2.34	0.42
1:B:579:LEU:HD12	1:B:579:LEU:HA	1.96	0.42
1:B:695:CYS:SG	1:B:696:ASN:N	2.92	0.42
2:D:53:PHE:CZ	2:D:72:VAL:HG21	2.54	0.42
1:A:192:ILE:HD11	1:A:248:ILE:HD12	2.01	0.42
1:B:817:ASN:ND2	3:F:100:ILE:HD12	2.34	0.42
1:A:815:GLN:O	1:A:819:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:PHE:O	2:D:185:ILE:HG12	2.20	0.42
1:A:534:LEU:HD12	1:A:594:LEU:HD13	2.02	0.42
1:B:67:LYS:HZ3	1:B:69:VAL:HG22	1.84	0.42
1:A:504:GLU:O	1:A:760:HIS:ND1	2.53	0.42
2:D:52:ALA:HB1	2:D:56:PHE:CZ	2.54	0.42
1:A:259:ALA:O	1:A:449:THR:OG1	2.34	0.41
3:E:79:ASN:O	3:E:83:PHE:N	2.45	0.41
1:A:524:ILE:CD1	1:A:581:HIS:HE1	2.32	0.41
1:A:616:LEU:O	1:A:620:LEU:HG	2.20	0.41
1:A:21:LYS:O	1:A:21:LYS:HD3	2.20	0.41
1:B:483:GLU:HB3	1:B:521:ILE:HD11	2.01	0.41
1:B:719:ARG:HH22	1:B:738:SER:HA	1.85	0.41
1:A:340:GLY:O	1:A:442:ARG:NH2	2.52	0.41
1:A:461:ASP:OD1	1:A:461:ASP:C	2.63	0.41
1:B:432:TYR:HA	1:B:435:MET:HG2	2.02	0.41
1:A:530:ILE:HD12	1:A:579:LEU:HD11	2.02	0.41
1:A:726:ASN:H	1:A:780:ARG:HH12	1.62	0.41
3:F:146:ASP:OD1	3:F:146:ASP:N	2.53	0.41
1:B:288:GLN:HG2	1:B:328:GLU:HB2	2.03	0.41
1:A:155:PHE:CD1	1:A:194:TYR:HB2	2.55	0.41
1:A:486:GLN:HG3	1:A:517:LEU:HD11	2.03	0.41
1:A:852:MET:HE3	1:A:853:LYS:N	2.34	0.41
1:B:815:GLN:NE2	3:F:124:LEU:O	2.54	0.41
2:D:90:GLY:O	2:D:91:ASN:OD1	2.39	0.41
3:F:95:ASP:OD1	3:F:95:ASP:C	2.64	0.41
1:B:13:ALA:N	1:B:14:PRO:HD2	2.35	0.41
1:B:612:SER:OG	1:B:617:LEU:HD23	2.20	0.41
1:B:709:PHE:HB2	1:B:764:PHE:HD2	1.86	0.41
2:C:94:ASN:OD1	2:C:94:ASN:C	2.63	0.41
3:E:74:ALA:HB1	3:E:78:ILE:HD12	2.03	0.41
3:F:22:PHE:O	3:F:23:ASP:OD1	2.39	0.41
1:B:228:GLU:O	1:B:232:ASN:N	2.53	0.41
1:B:242:SER:OG	5:B:1402:PO4:O4	2.33	0.41
3:F:86:MET:SD	3:F:86:MET:C	3.04	0.41
1:A:801:TYR:HE2	1:A:805:LEU:HD11	1.84	0.40
3:E:57:MET:SD	3:E:58:GLY:N	2.94	0.40
1:A:535:GLU:O	1:A:539:MET:HG2	2.22	0.40
1:A:589:ASN:O	1:A:593:TRP:NE1	2.54	0.40
1:B:102:LEU:HD23	1:B:102:LEU:O	2.21	0.40
1:B:239:ASP:OD1	1:B:239:ASP:C	2.64	0.40
1:B:711:ASN:HB3	1:B:770:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG21	1:A:309:ASP:OD2	2.21	0.40
2:C:178:TYR:O	2:C:182:VAL:HG12	2.22	0.40
2:D:108:LEU:N	2:D:109:PRO:CD	2.85	0.40
1:A:102:LEU:HD21	1:A:686:ASN:HD22	1.85	0.40
1:A:186:VAL:HG23	4:A:1401:ADP:O1A	2.22	0.40
1:B:428:ALA:O	1:B:431:VAL:HG12	2.21	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	906/1315 (69%)	880 (97%)	26 (3%)	0	100	100
1	B	902/1315 (69%)	862 (96%)	39 (4%)	1 (0%)	48	79
2	C	150/188 (80%)	148 (99%)	2 (1%)	0	100	100
2	D	150/188 (80%)	144 (96%)	6 (4%)	0	100	100
3	E	140/169 (83%)	134 (96%)	6 (4%)	0	100	100
3	F	140/169 (83%)	134 (96%)	6 (4%)	0	100	100
All	All	2388/3344 (71%)	2302 (96%)	85 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	710	PRO

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	797/1145 (70%)	793 (100%)	4 (0%)	81	85
1	B	795/1145 (69%)	789 (99%)	6 (1%)	73	82
2	C	128/154 (83%)	128 (100%)	0	100	100
2	D	128/154 (83%)	128 (100%)	0	100	100
3	E	122/142 (86%)	122 (100%)	0	100	100
3	F	122/142 (86%)	122 (100%)	0	100	100
All	All	2092/2882 (73%)	2082 (100%)	10 (0%)	78	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	VAL
1	A	424	THR
1	A	517	LEU
1	A	660	THR
1	B	506	ILE
1	B	563	PHE
1	B	577	PHE
1	B	665	THR
1	B	781	LEU
1	B	784	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	288	GLN
1	A	305	ASN
1	A	358	HIS
1	A	491	HIS
1	A	581	HIS
1	A	676	ASN
1	A	696	ASN
1	A	914	GLN
1	B	224	ASN
1	B	315	GLN

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Mol	Chain	Res	Type
1	B	347	ASN
1	B	401	HIS
1	B	416	ASN
1	B	589	ASN
1	B	826	ASN
1	B	907	GLN
1	B	911	ASN
2	C	68	GLN
3	E	61	ASN
3	E	150	ASN
3	F	26	GLN
3	F	61	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	B	1401	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	9 (20%)
5	PO4	B	1402	-	4,4,4	1.02	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	A	1402	-	4,4,4	1.14	0	6,6,6	0.42	0
4	ADP	A	1401	-	28,29,29	1.39	4 (14%)	43,45,45	1.85	9 (20%)

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	B	1401	-	-	8/16/32/32	0/3/3/3
4	ADP	A	1401	-	-	6/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1401	ADP	C5-C4	4.71	1.47	1.39
4	A	1401	ADP	C5-C4	4.65	1.47	1.39
4	B	1401	ADP	C5-C6	2.77	1.48	1.41
4	A	1401	ADP	C5-C6	2.75	1.48	1.41
4	B	1401	ADP	C8-N7	2.31	1.36	1.31
4	A	1401	ADP	C8-N7	2.26	1.36	1.31
4	B	1401	ADP	C5-N7	-2.25	1.35	1.39
4	A	1401	ADP	C5-N7	-2.24	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1401	ADP	C5-C4-N3	-5.91	118.57	126.72
4	A	1401	ADP	C5-C4-N3	-5.83	118.68	126.72
4	B	1401	ADP	N3-C4-N9	4.64	135.06	127.17
4	A	1401	ADP	N3-C4-N9	4.58	134.96	127.17
4	B	1401	ADP	C2-N3-C4	3.73	120.94	111.83
4	A	1401	ADP	C2-N3-C4	3.70	120.88	111.83
4	B	1401	ADP	C4-C5-N7	-3.63	106.44	110.58
4	A	1401	ADP	C4-C5-N7	-3.61	106.45	110.58
4	A	1401	ADP	N3-C2-N1	-3.18	123.76	128.58
4	B	1401	ADP	N3-C2-N1	-3.18	123.77	128.58
4	A	1401	ADP	C4-N9-C8	2.66	108.53	105.74
4	B	1401	ADP	C5-N7-C8	2.63	107.59	103.45
4	B	1401	ADP	C4-N9-C8	2.62	108.49	105.74
4	A	1401	ADP	C5-N7-C8	2.61	107.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1401	ADP	C3'-C2'-C1'	2.49	106.17	101.46
4	A	1401	ADP	C3'-C2'-C1'	2.42	106.05	101.46
4	A	1401	ADP	C6-C5-N7	2.16	136.25	132.09
4	B	1401	ADP	C6-C5-N7	2.13	136.20	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1401	ADP	C5'-O5'-PA-O1A
4	A	1401	ADP	C5'-O5'-PA-O2A
4	A	1401	ADP	C5'-O5'-PA-O3A
4	B	1401	ADP	PA-O3A-PB-O3B
4	B	1401	ADP	C5'-O5'-PA-O1A
4	B	1401	ADP	C5'-O5'-PA-O2A
4	B	1401	ADP	C5'-O5'-PA-O3A
4	B	1401	ADP	O4'-C4'-C5'-O5'
4	B	1401	ADP	C3'-C4'-C5'-O5'
4	A	1401	ADP	O4'-C4'-C5'-O5'
4	A	1401	ADP	C3'-C4'-C5'-O5'
4	B	1401	ADP	PA-O3A-PB-O1B
4	B	1401	ADP	PA-O3A-PB-O2B
4	A	1401	ADP	PB-O3A-PA-O1A

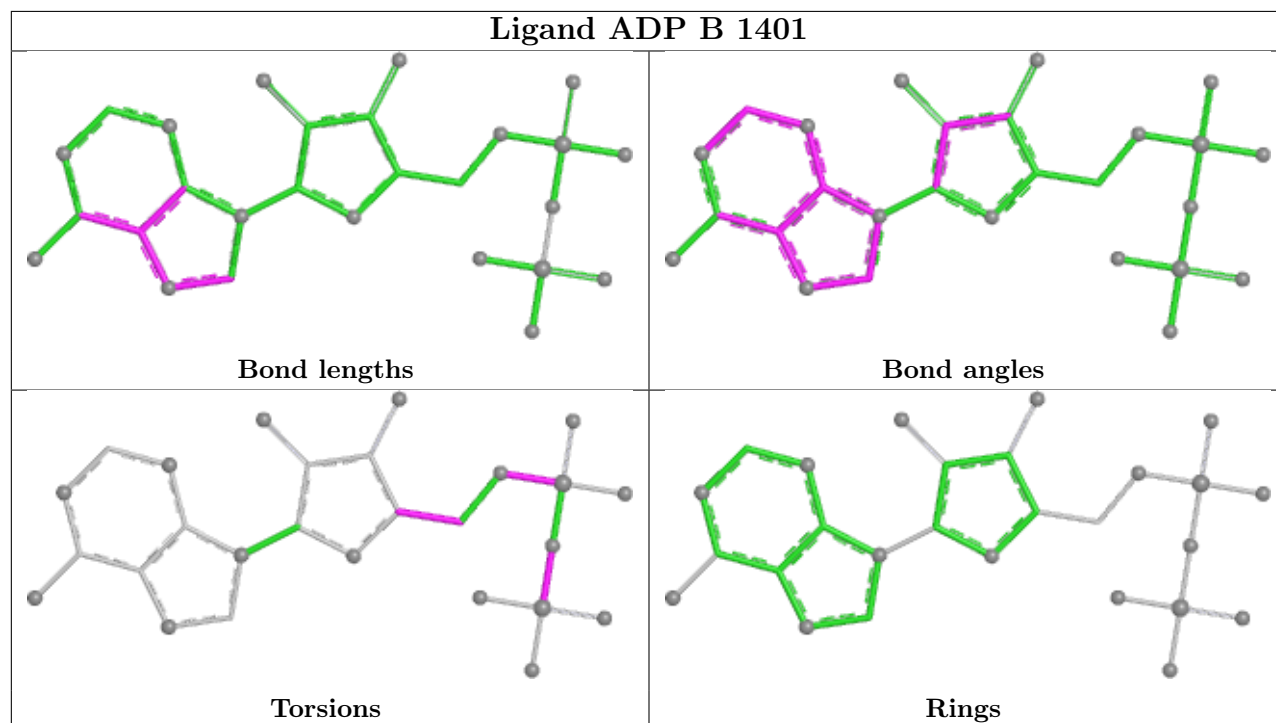
There are no ring outliers.

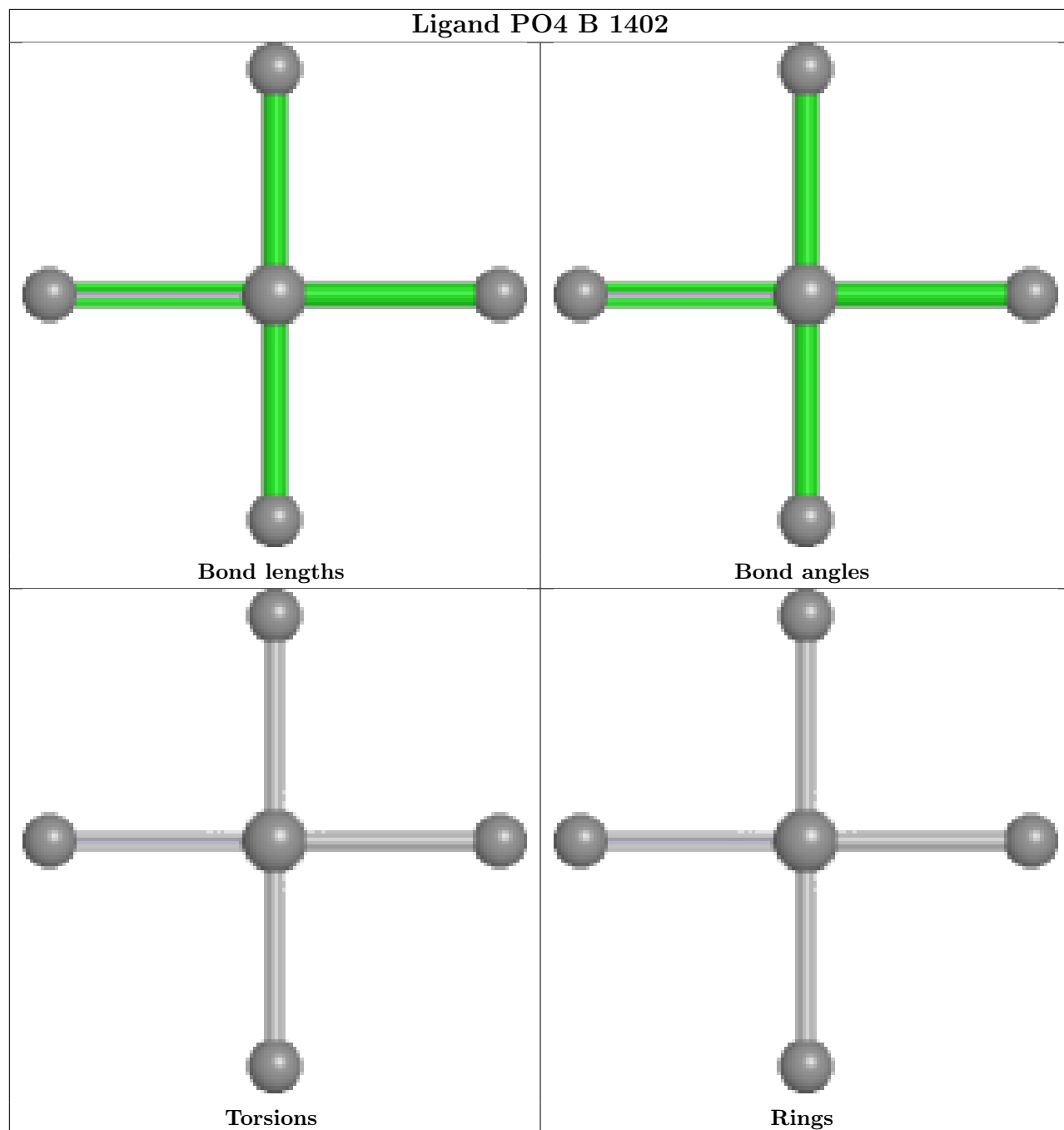
4 monomers are involved in 6 short contacts:

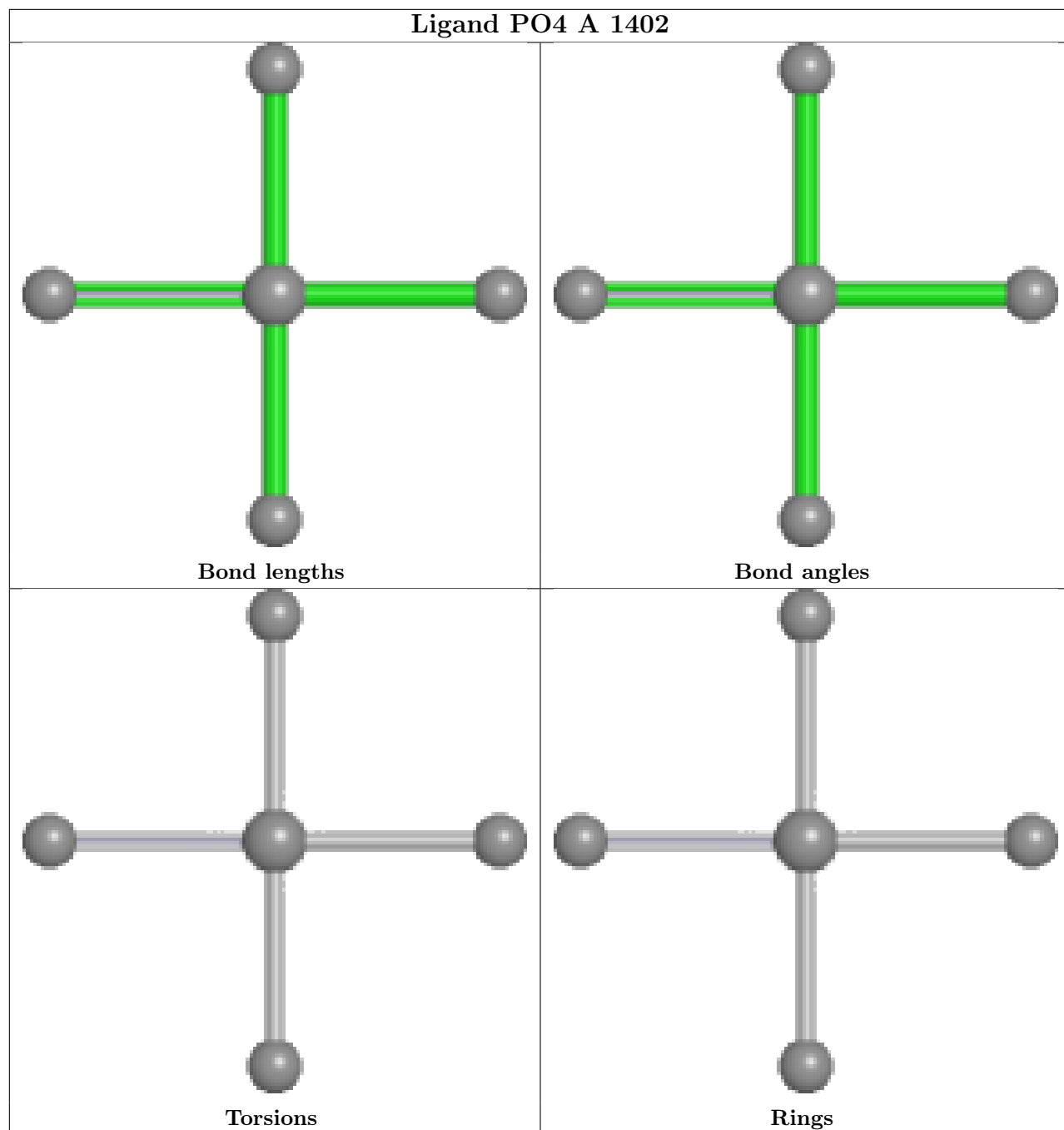
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1401	ADP	1	0
5	B	1402	PO4	1	0
5	A	1402	PO4	1	0
4	A	1401	ADP	3	0

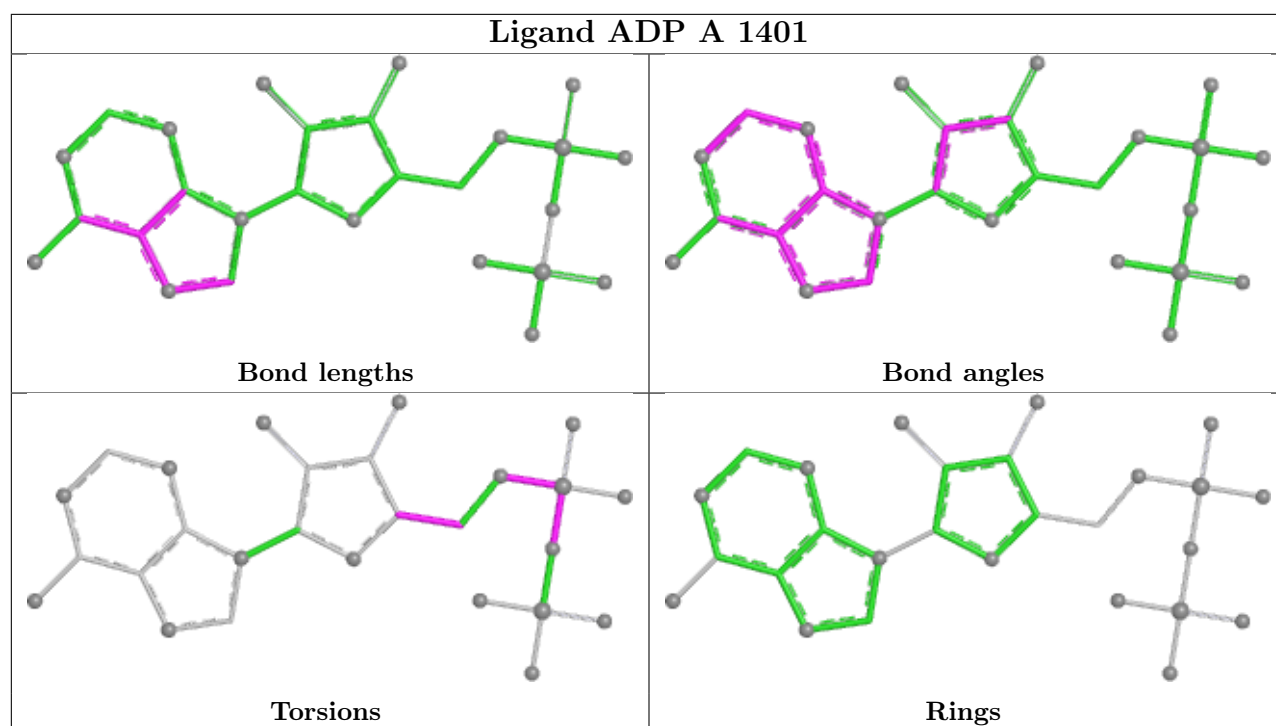
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

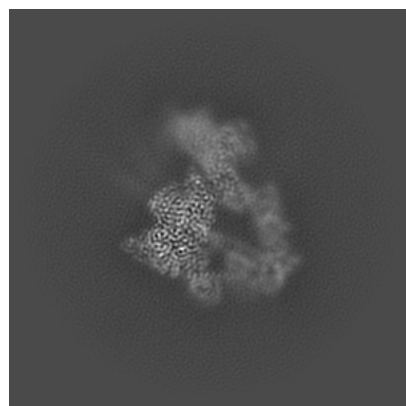
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73367. These allow visual inspection of the internal detail of the map and identification of artifacts.

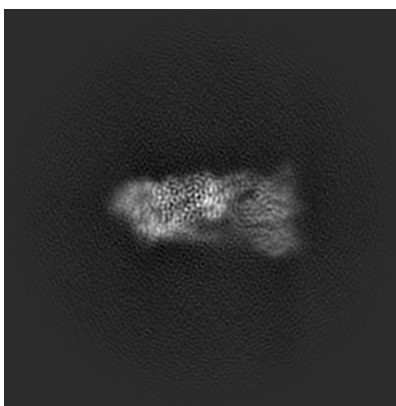
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

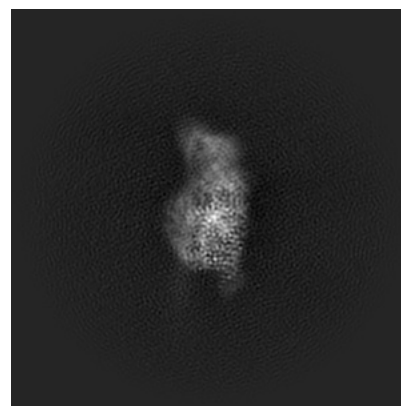
6.1.1 Primary map



X

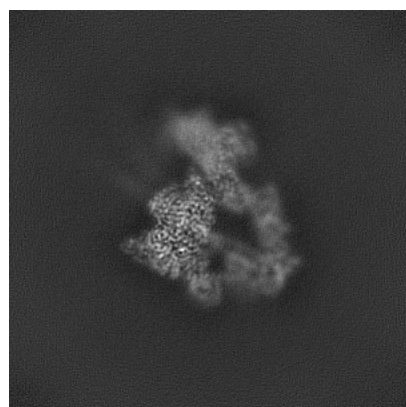


Y

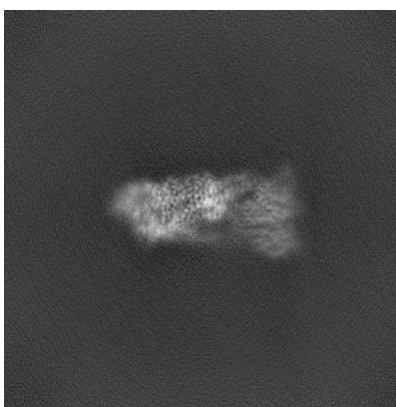


Z

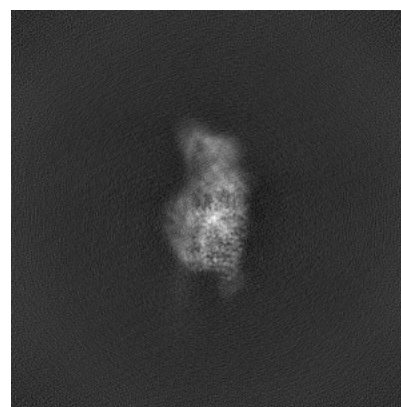
6.1.2 Raw map



X



Y

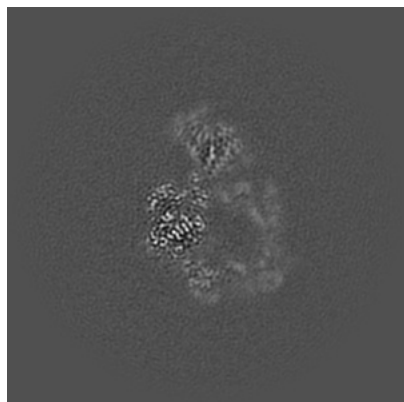


Z

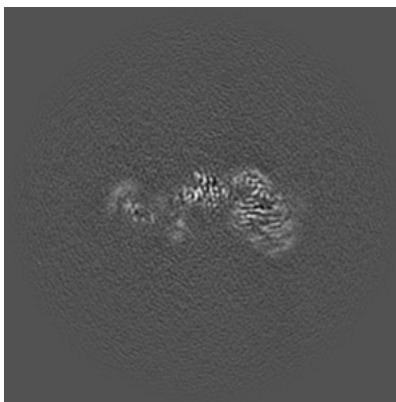
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

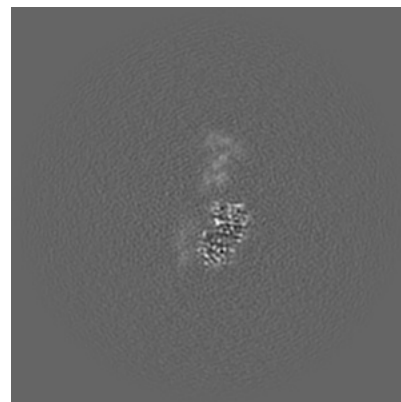
6.2.1 Primary map



X Index: 200

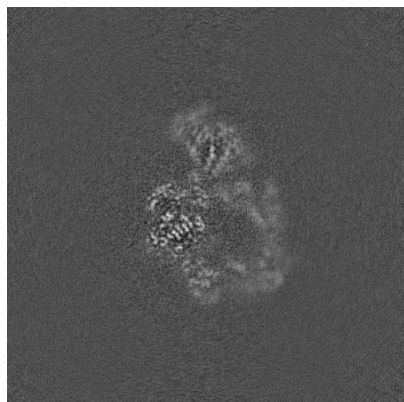


Y Index: 200

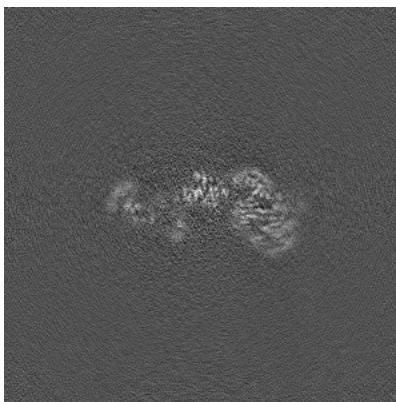


Z Index: 200

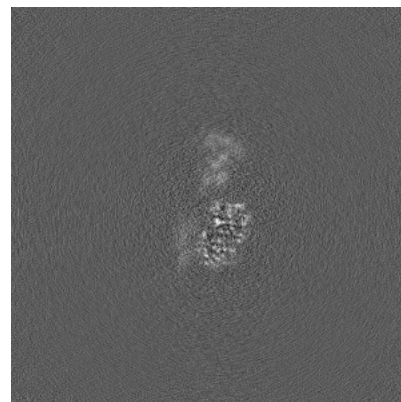
6.2.2 Raw map



X Index: 200



Y Index: 200

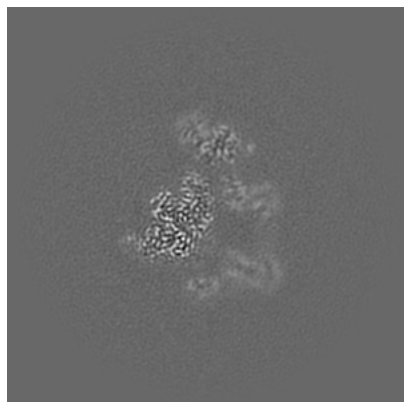


Z Index: 200

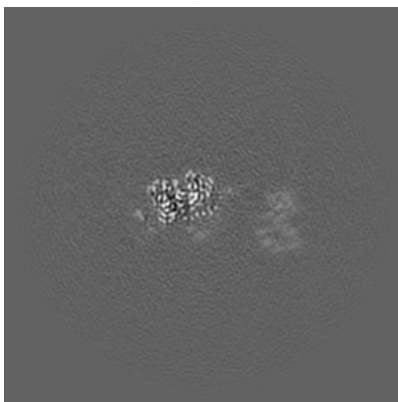
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

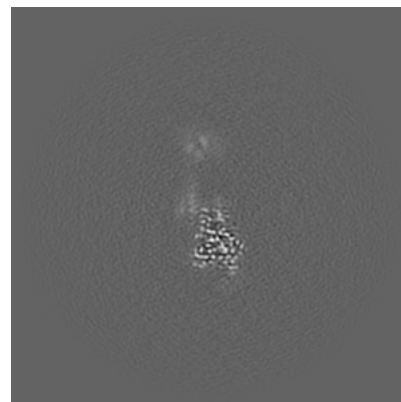
6.3.1 Primary map



X Index: 210

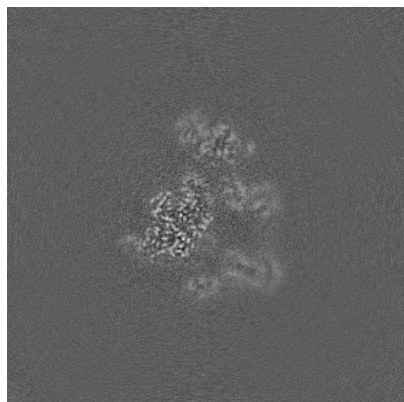


Y Index: 173

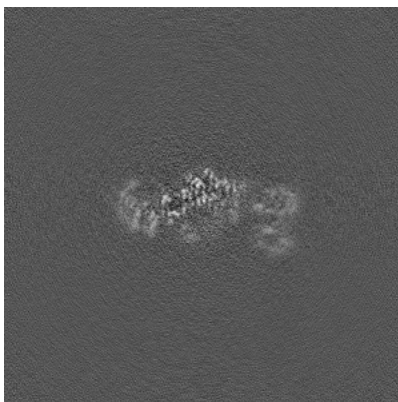


Z Index: 174

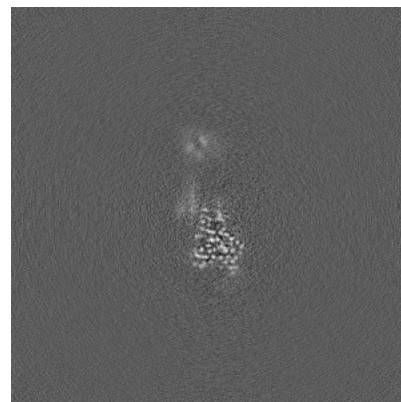
6.3.2 Raw map



X Index: 210



Y Index: 185

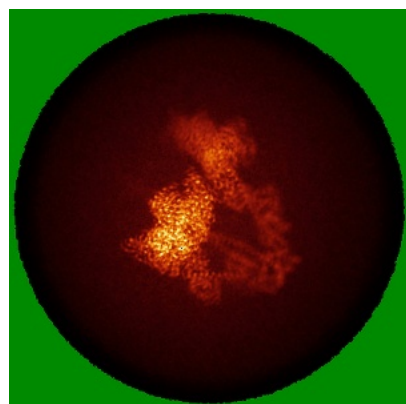


Z Index: 174

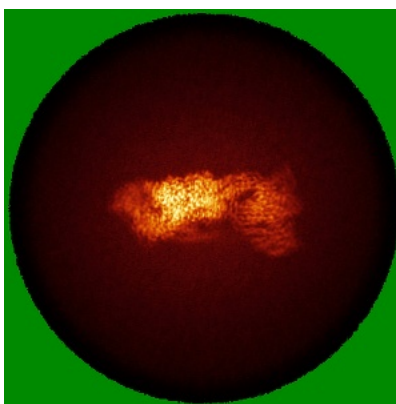
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

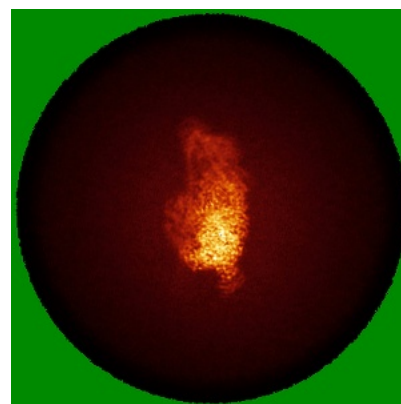
6.4.1 Primary map



X

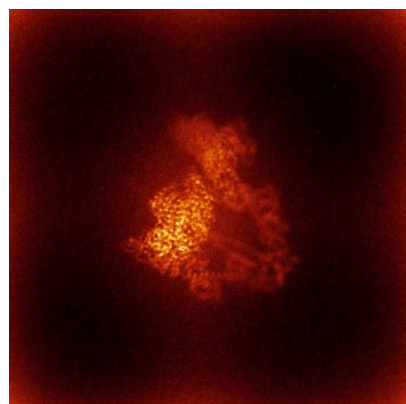


Y

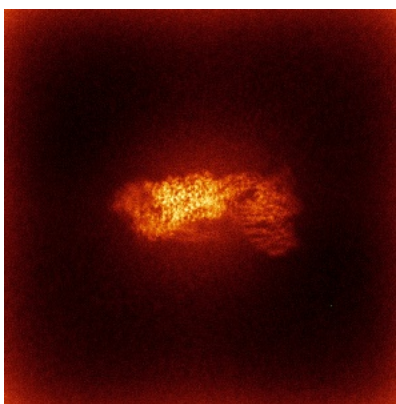


Z

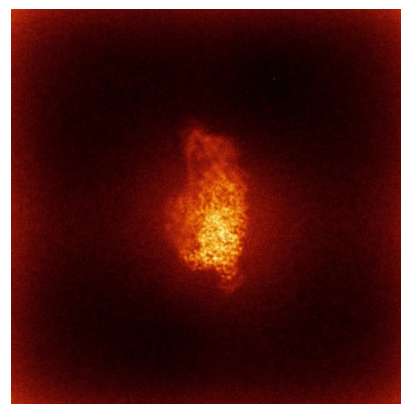
6.4.2 Raw map



X



Y

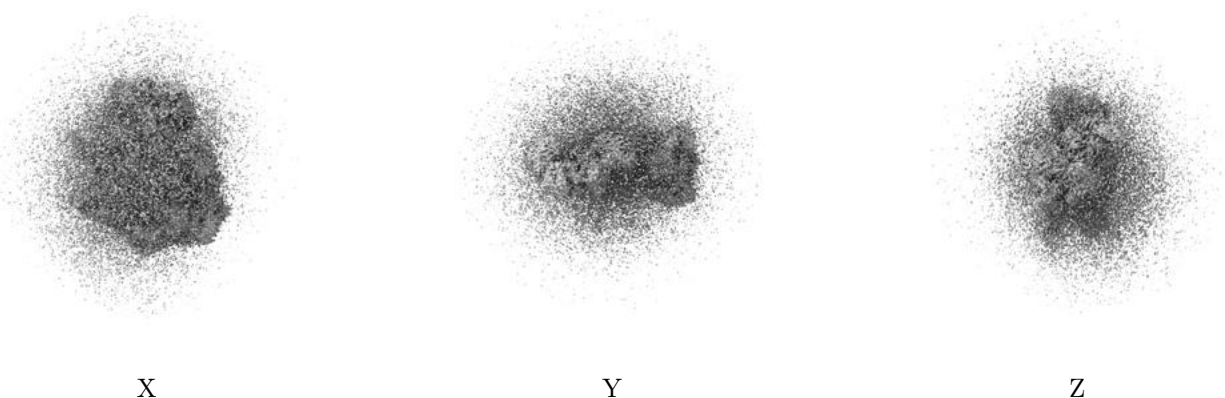


Z

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.

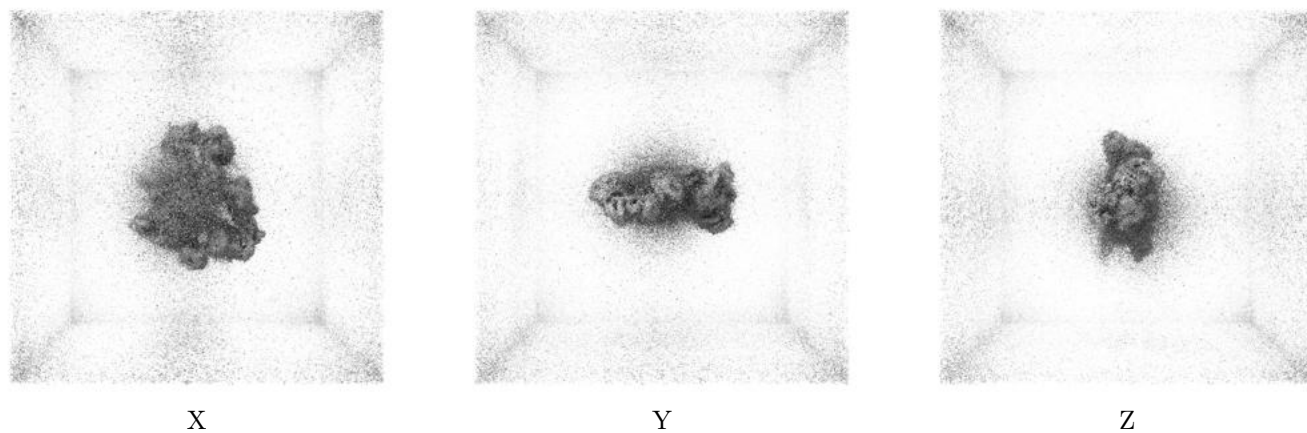
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



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.

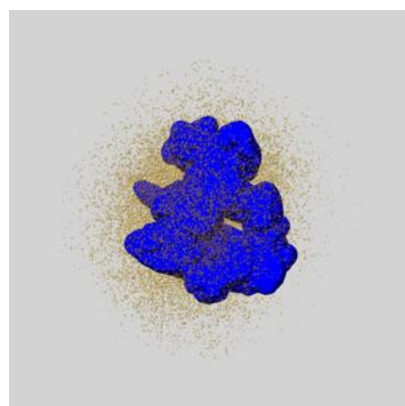
6.6 Mask visualisation [i](#)

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

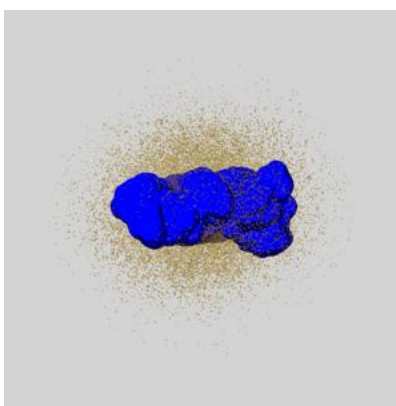
A mask typically either:

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

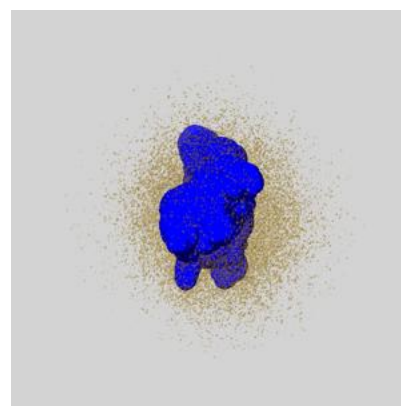
6.6.1 emd_73367_msk_1.map [i](#)



X



Y

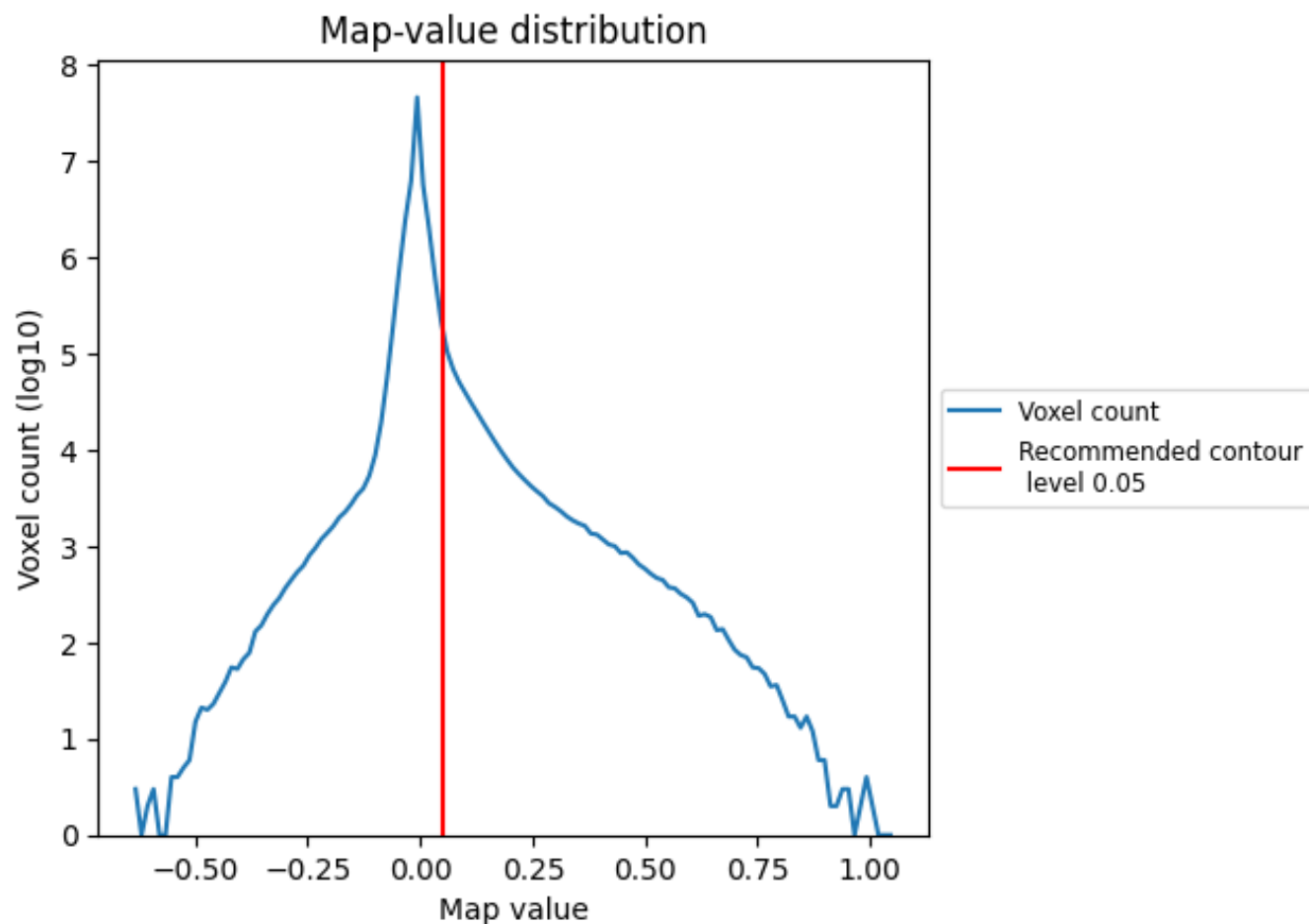


Z

7 Map analysis [i](#)

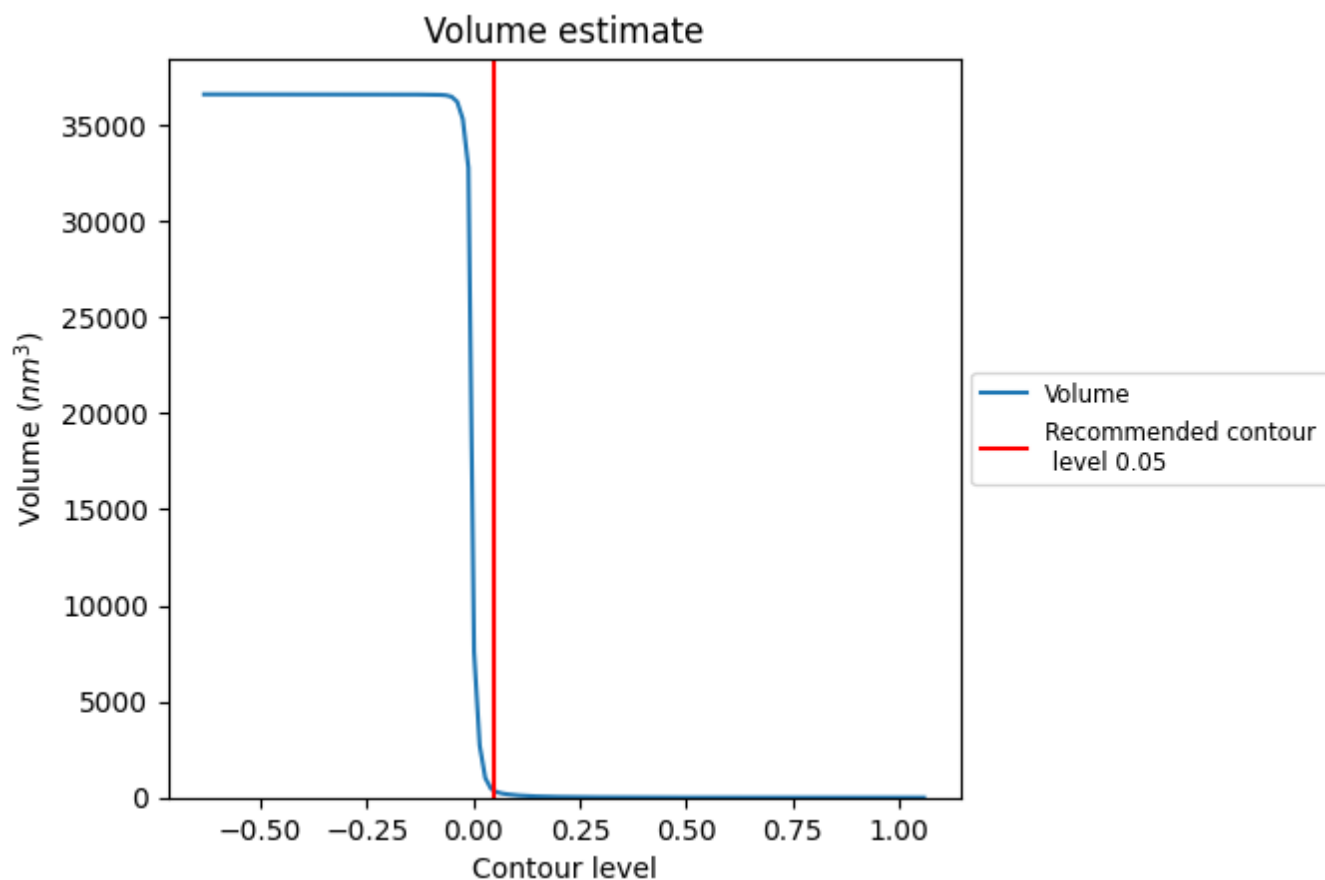
This section contains the results of statistical analysis of the map.

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.

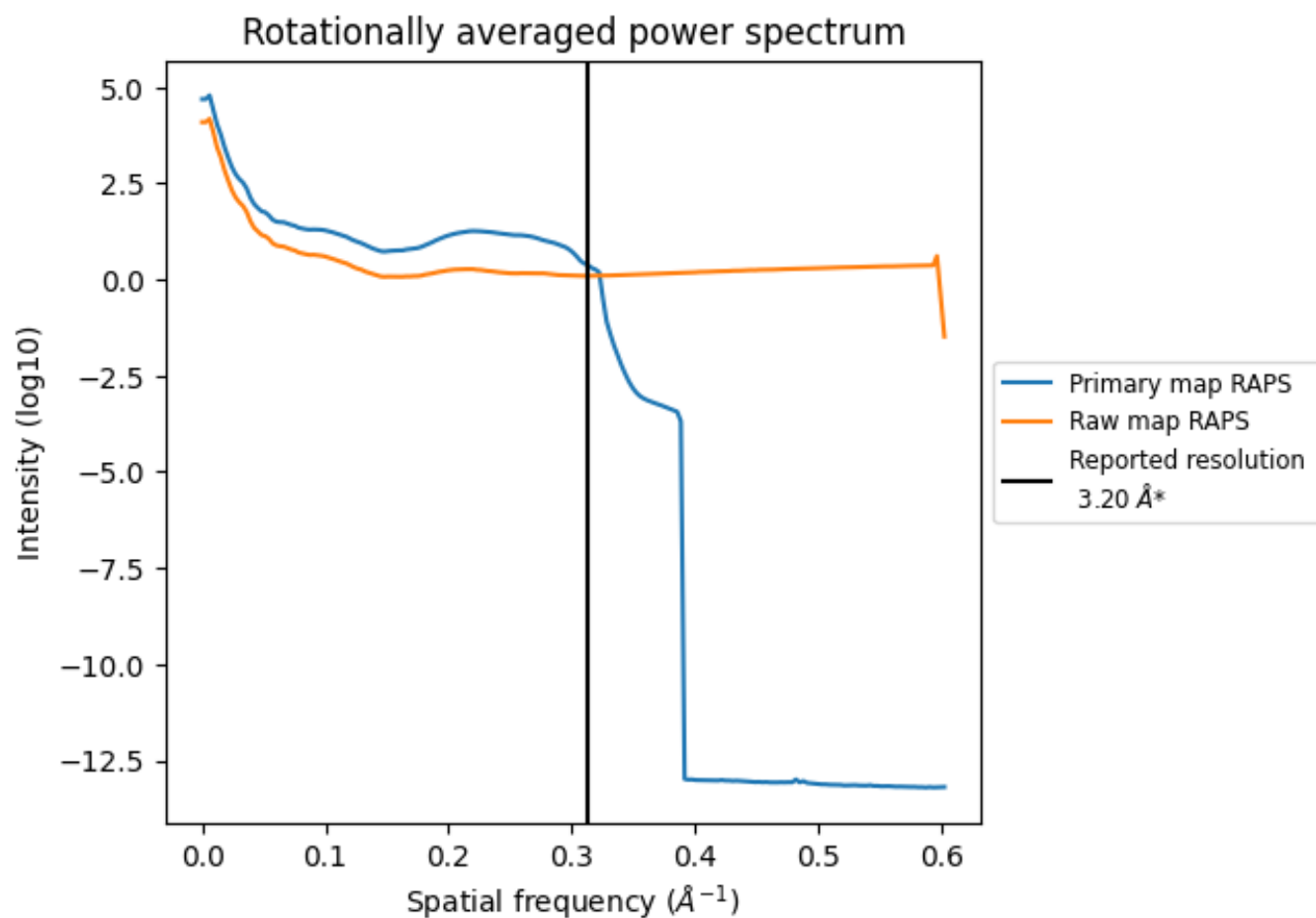
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 314 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 ⓘ

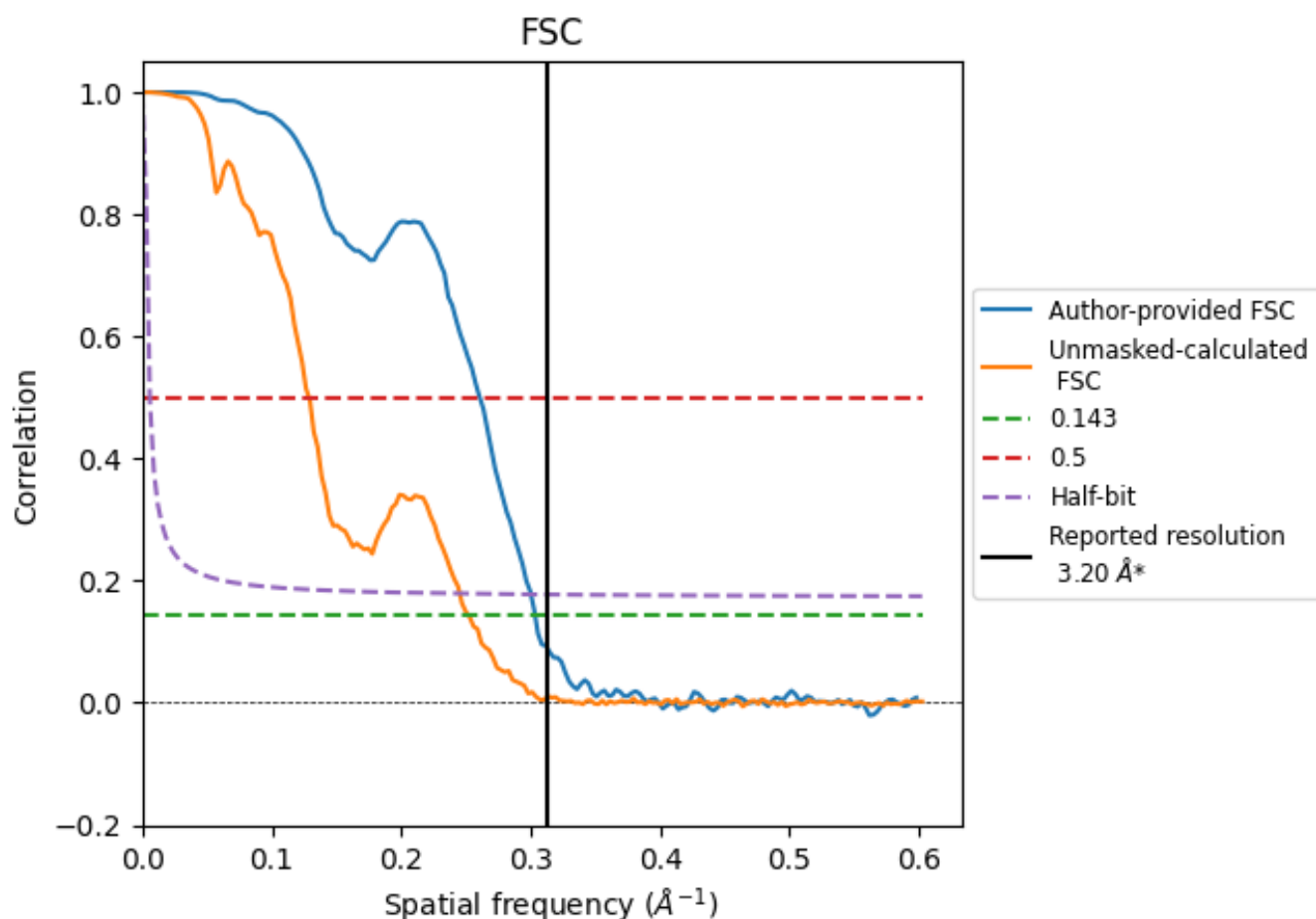


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

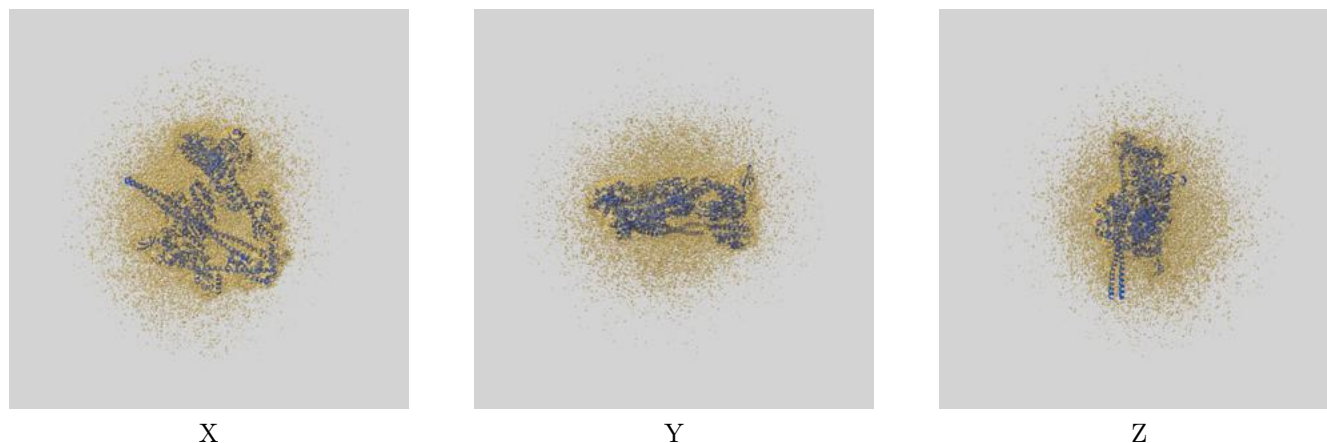
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.29	3.84	3.33
Unmasked-calculated*	3.97	7.76	4.08

*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 3.97 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

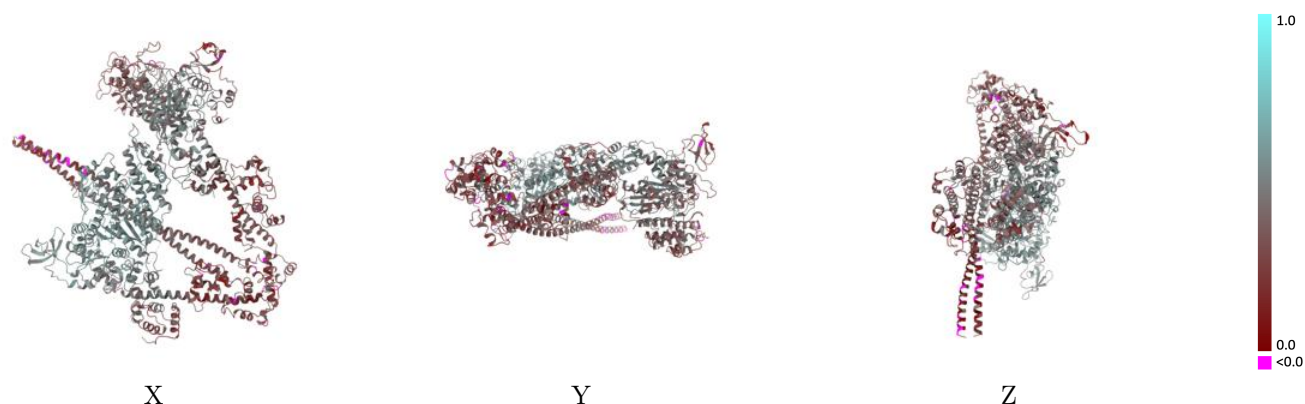
This section contains information regarding the fit between EMDB map EMD-73367 and PDB model 9YRG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



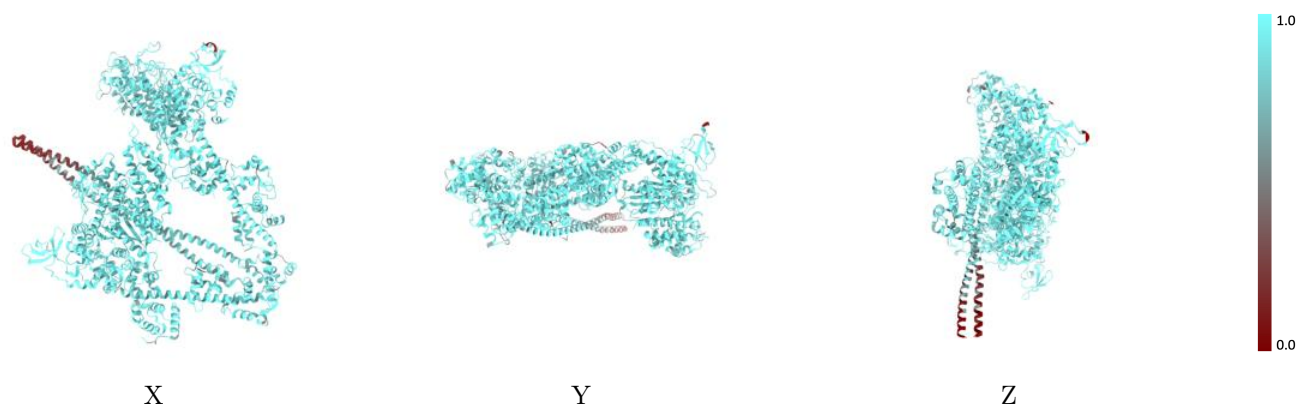
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



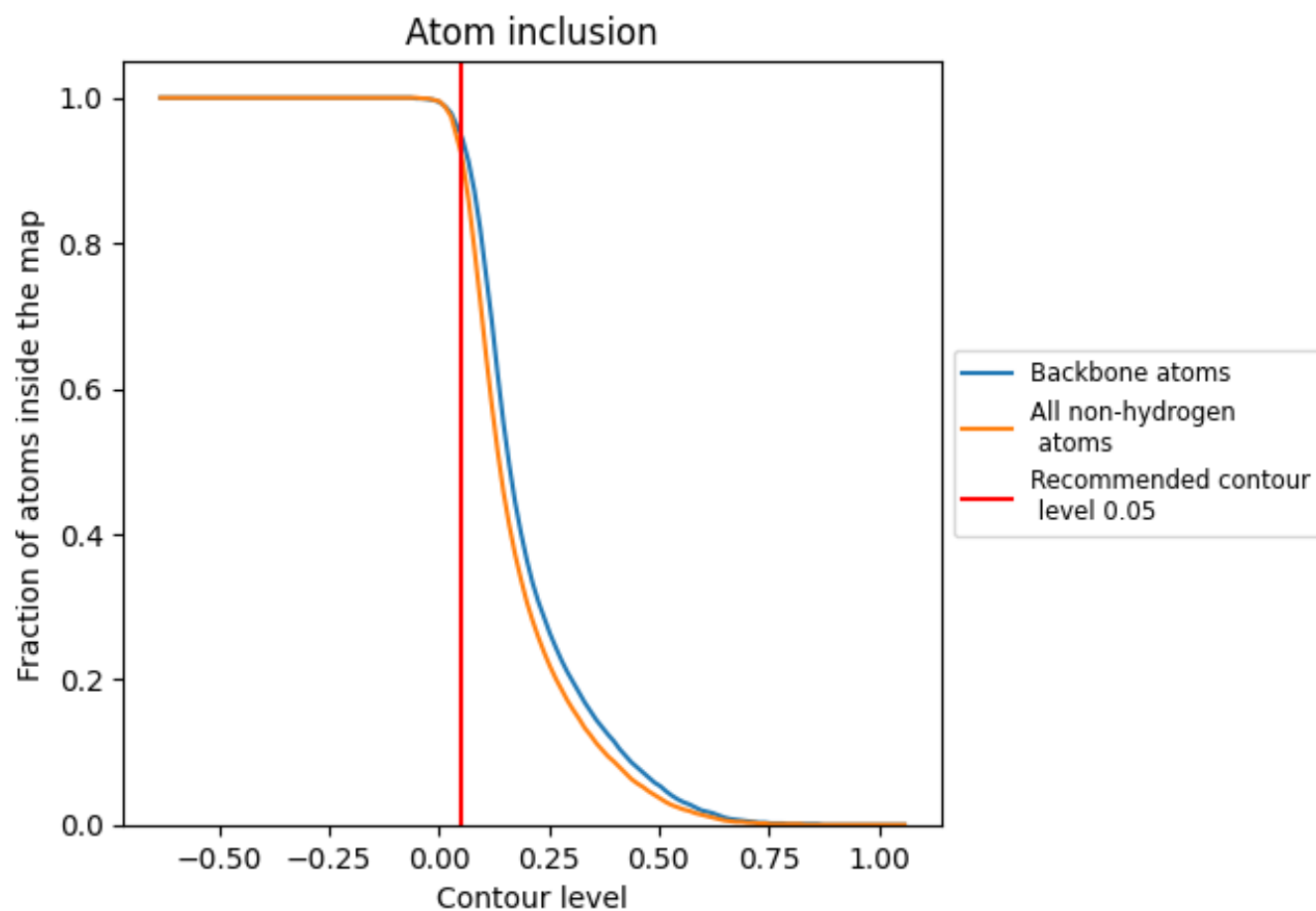
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9250</div>	<div><div></div>0.4090</div>
A	<div><div></div>0.9400</div>	<div><div></div>0.4950</div>
B	<div><div></div>0.9100</div>	<div><div></div>0.3800</div>
C	<div><div></div>0.9530</div>	<div><div></div>0.4040</div>
D	<div><div></div>0.9370</div>	<div><div></div>0.3240</div>
E	<div><div></div>0.9020</div>	<div><div></div>0.2700</div>
F	<div><div></div>0.8980</div>	<div><div></div>0.2620</div>

1.0

0.0

<0.0