



Full wwPDB EM Validation Report ⓘ

Jul 16, 2026 – 04:25 PM EDT

PDB ID : 9YAQ / pdb_00009yaq
EMDB ID : EMD-72734
Title : The structure of the cardiac native cross bridge in the rigor state, myosin heads bound to actin molecules 5 and 6.
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2025-09-16
Resolution : 4.63 Å (reported)
Based on initial models : 6SFA, 8DD0, 5H53, 7JH7, 7KO5

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:

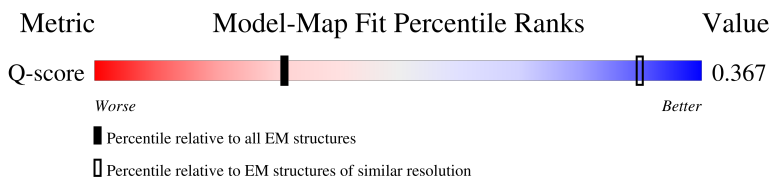
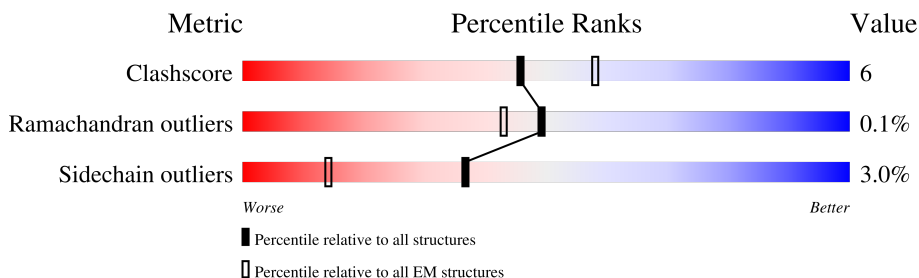
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 4.63 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.



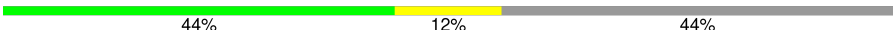
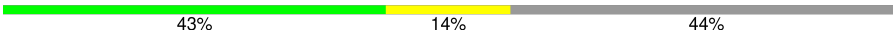
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2068 (4.13 - 5.13)

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	377	
1	B	377	
1	C	377	
1	D	377	

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Mol	Chain	Length	Quality of chain
2	E	284	
2	F	284	
2	G	284	
2	H	284	
3	I	285	
3	P	285	
4	J	1935	
4	K	1935	
5	L	196	
5	M	196	
6	N	161	
7	O	211	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 33966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		
1	B	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		
1	C	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		
1	D	375	Total	C	N	O	S	0	0
			2932	1854	493	565	20		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	160	Total	C	N	O	S	0	0
			1304	802	218	280	4		
2	F	160	Total	C	N	O	S	0	0
			1304	802	218	280	4		
2	G	35	Total	C	N	O	S	0	0
			278	168	51	56	3		
2	H	35	Total	C	N	O	S	0	0
			278	168	51	56	3		

- Molecule 3 is a protein called Troponin T2, cardiac type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	68	Total	C	N	O	S	0	0
			595	359	121	114	1		
3	P	74	Total	C	N	O		0	0
			643	401	123	119			

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	802	Total	C	N	O	S	0	0
			6461	4119	1111	1199	32		
4	K	805	Total	C	N	O	S	0	0
			6475	4127	1114	1202	32		

- Molecule 5 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	153	Total	C	N	O	S	0	0
			1217	766	202	238	11		
5	M	153	Total	C	N	O	S	0	0
			1217	766	202	238	11		

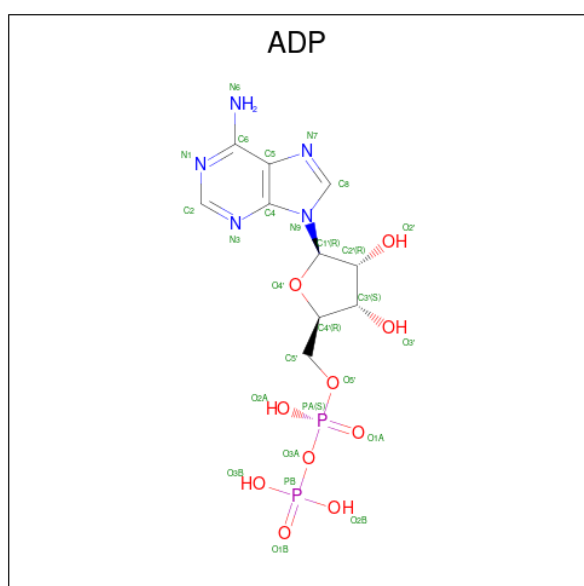
- Molecule 6 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	160	Total	C	N	O	S	0	0
			1274	789	195	278	12		

- Molecule 7 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	134	Total	C	N	O	S	0	0
			1077	667	208	197	5		

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



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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

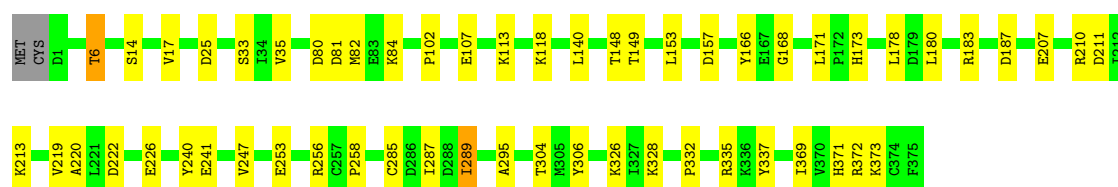
Mol	Chain	Residues	Atoms		AltConf
10	N	3	Total	Ca	0
			3	3	

3 Residue-property plots [i](#)

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

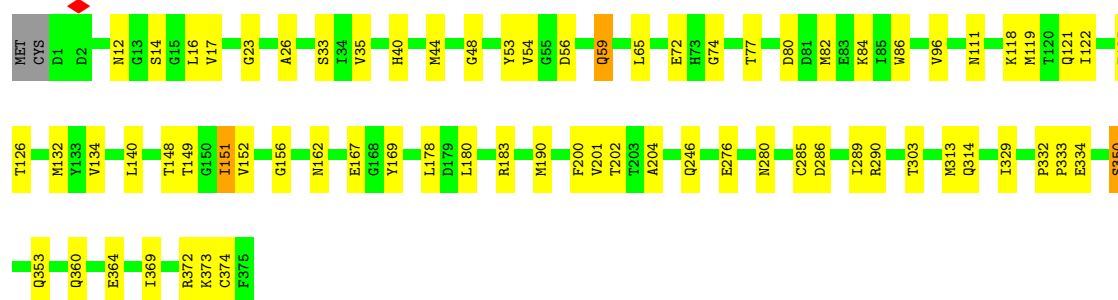
- Molecule 1: Actin, alpha cardiac muscle 1

Chain A: 



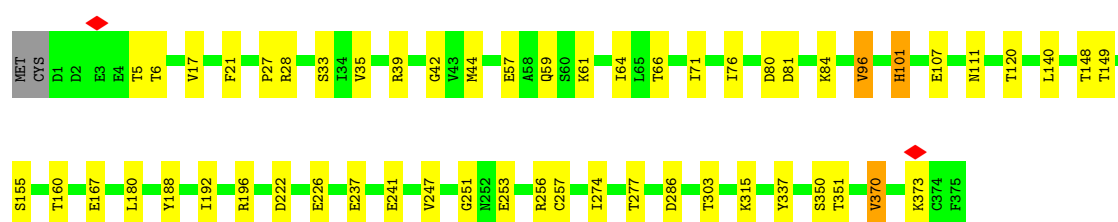
- Molecule 1: Actin, alpha cardiac muscle 1

Chain B: 



- Molecule 1: Actin, alpha cardiac muscle 1

Chain C: 



- Molecule 1: Actin, alpha cardiac muscle 1

D179	L186	R210 D211	E214	V219 A220	L221	D222	M225 E226	Y240	C257 P258	A272	E276	I282	L293	S300	T303 T304	B335	I369	R372 K373	C374	F375																
MET	CYS	D2	E3	V17	S33	T34	R39	G46	T66	L67	I76	K82	S83	X84	H87	P98	Tl06	P109	M123	F124	V129	M132	Q137	L140	Tl48	Tl49	G150	I151	V152	L153	G156	D157	G158	V159	E167	R177

Chain E:

[illegible]

Chain F: 43% 14% 44%

K264	ASP	SER	MET
L265	GLU	GLU	ASP
K266	SER	ALA	ILE
Y267	GLU	PRO	LYS
K268	R125	ASP	LYS
		ALA	LYS
L274	T130	GLN	MET
L278	R133	GLU	GLN
N279	A134	LYS	MET
D280	K135	LEU	LEU
K281	K136	GLU	LYS
T282	D137	LEU	LEU
S283		ALA	ASP
I284	K140	GLU	LYS
		LYS	GLU
	K152	ASN	ASN
	E156	ALA	ALA
		THR	LEU
	K161	ASP	ASP
		ALA	ARG
	V165	GLU	ALA
		ALA	GLU
	S174	ASP	GLN
D175		VAL	ALA
L176	D175	ALA	GLU
E177	L176	SER	GLU
R178	E177	LEU	ALA
A179	R178	ASN	ASP
E180	A179	ASN	LYS
		ARG	LYS
	L204	ILE	ALA
		GLN	ALA
	E208	LEU	GLU
		VAL	ASP
	E212	GLU	ARG
Q216		GLU	LYS
K217	Q216	LEU	ARG
E218	K217	LEU	ARG
		ASP	GLU
	K231	ALA	GLU
		GLN	LEU
	A242	GLU	VAL
E243	A242	GLU	LEU
R244	E243	ARG	SER
S245	R244	LEU	LEU
V246	S245	ALA	GLN
T247	V246	THR	LYS
K248	T247	ALA	LYS
L249	K248	LEU	LYS
		GLN	LEU
	L253	LYS	ALA
		LEU	THR
	L256	GLU	GLU
		ALA	GLU
	L260	LYS	ASP
		LYS	LEU
	O263	ALA	TYR

Chain G: 9% 1% 88%

THR	GLU	THR	M1
ASP	LYS	ASP	D2
ALA	MET	ALA	A3
GLU	ILE	GLU	I4
ILE	GLN	ALA	K5
ASP	GLU	ASP	K6
VAL	GLU	VAL	K7
ALA	ILE	ALA	M8
GLN	GLN	SER	Q9
SER	LEU	LEU	
LYS	LYS	ASN	R21
ARG	GLU	ARG	
ALA	ALA	ARG	E26
LYS	LYS	ILE	
HIS	HIS	GLN	K30
ILE	ILE	LEU	
ALA	ALA	VAL	R35
GLU	GLU	GLU	SER
ASP	ASP	GLU	LYS
ALA	ALA	GLU	ARG
ASP	ASP	LEU	LEU
ARG	ARG	ASP	GLU
TYR	TYR	ALA	ASP
GLU	GLU	GLN	GLU
GLU	GLU	GLU	LEU
VAL	VAL	ARG	VAL
ALA	ALA	LEU	SER
ARG	ALA	LEU	LEU
LYS	LYS	THR	GLN
LEU	LEU	ALA	LYS
VAL	VAL	LEU	LEU
ILE	ILE	GLN	LYS
ILE	ILE	LYS	ALA
SER	SER	LEU	THR
ASP	ASP	GLU	GLU
LEU	LEU	GLU	ASP
ARG	ARG	ALA	GLU
ALA	ALA	LYS	LEU
GLU	GLU	ALA	ASP
ARG	ARG	ALA	LYS
ALA	ALA	THR	TYR
GLU	GLU	MET	ASP
GLY	GLY	LYS	GLN
CYS	CYS	ILE	GLU
ALA	ALA	GLU	LEU
GLU	GLU	SER	GLU
LEU	LEU	ARG	LEU
GLU	GLU	ALA	ALA
GLU	GLU	GLN	GLU
LYS	LYS	LYS	LYS
LYS	LYS	ASP	LYS
LYS	LYS	GLU	ALA

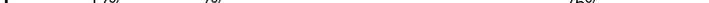
[illegible]

- Molecule 2: Tropomyosin alpha-1 chain

Chain H: 8% . 88%

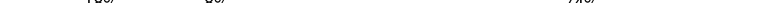
ASP	ASP	GLU	GLU	GLN	ALA
LEU	LEU	GLU	GLN	GLU	GLU
GLU	GLU	LEU	ASP	LYS	LYS
GLU	ASP	LYS	GLU	ALA	ALA
LEU	THR	THR	GLU	LYS	THR
LEU	THR	VAL	GLU	ASP	ASP
TYR	TYR	ASN	MET	ALA	ALA
ALA	ALA	THR	GLU	GLU	GLU
GLN	GLN	ASN	ILE	GLN	ALA
LYS	LYS	LEU	GLN	GLU	ASP
LEU	LEU	LYS	ILE	ALA	VAL
TYR	TYR	SER	ILE	ALA	VAL
LYS	LYS	GLU	GLN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

- Molecule 3: Troponin T2, cardiac type

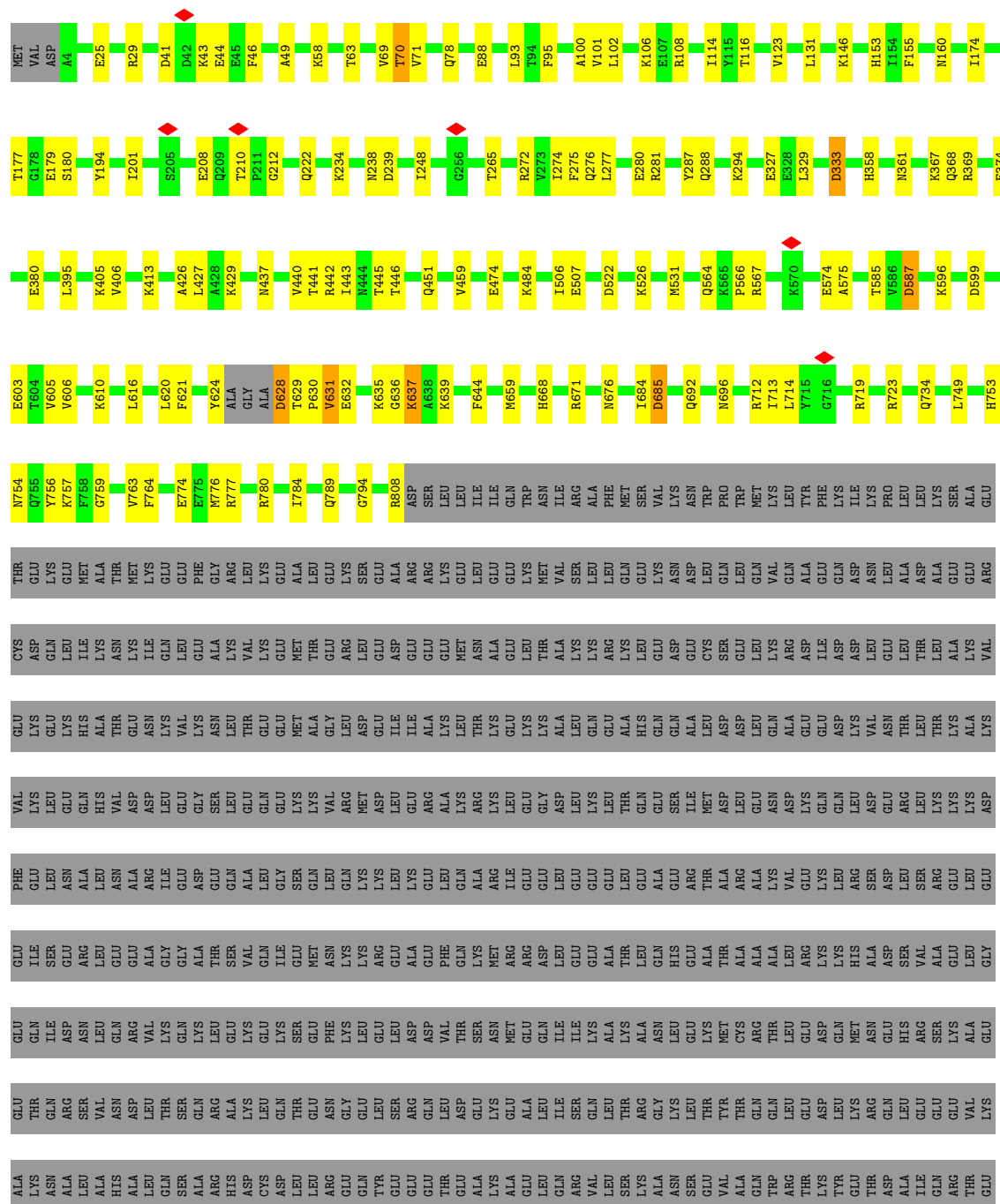
Chain I:  17% 7% 76%

[illegible]

- Molecule 3: Troponin T2, cardiac type

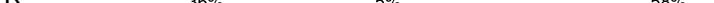
Chain P:  18% 8% 74%

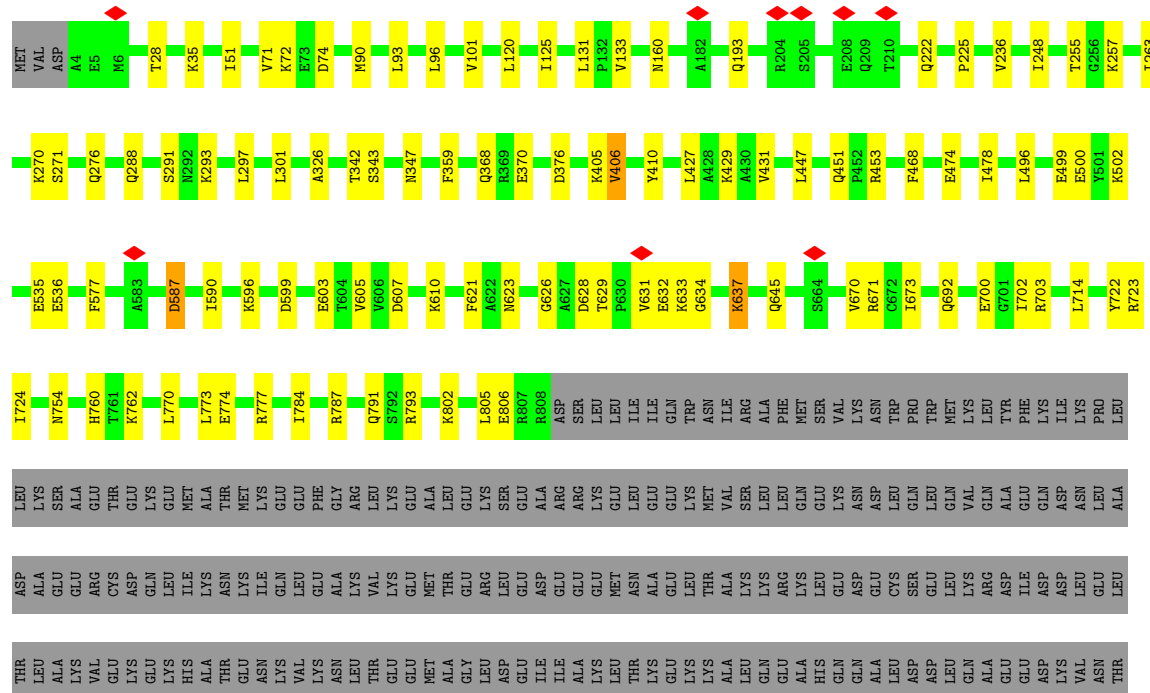
[illegible]



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

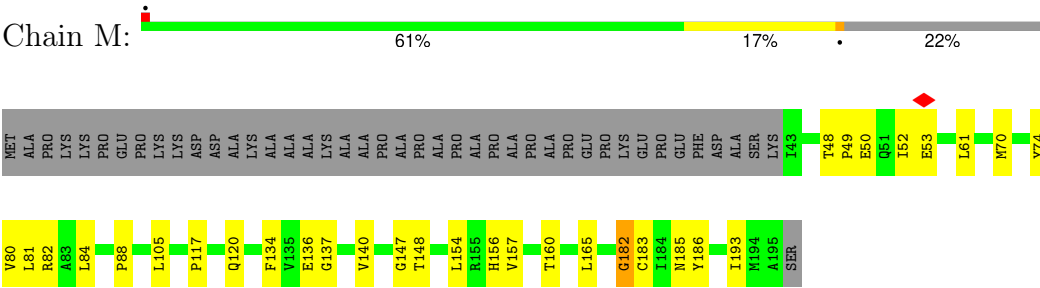
- Molecule 4: Myosin-7

Chain K:  36% 5% 58%

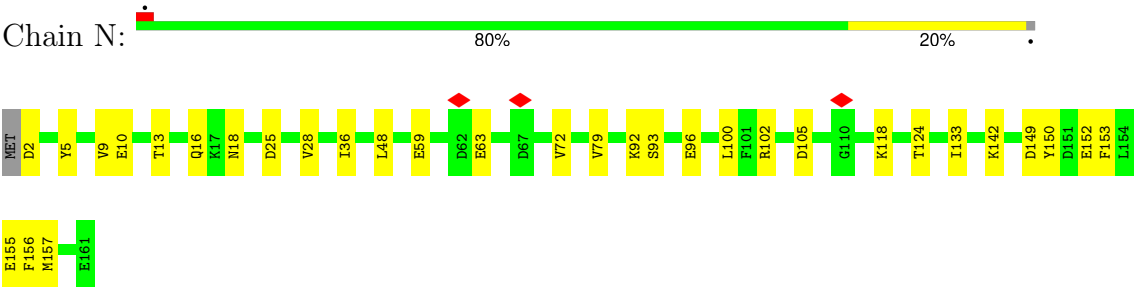




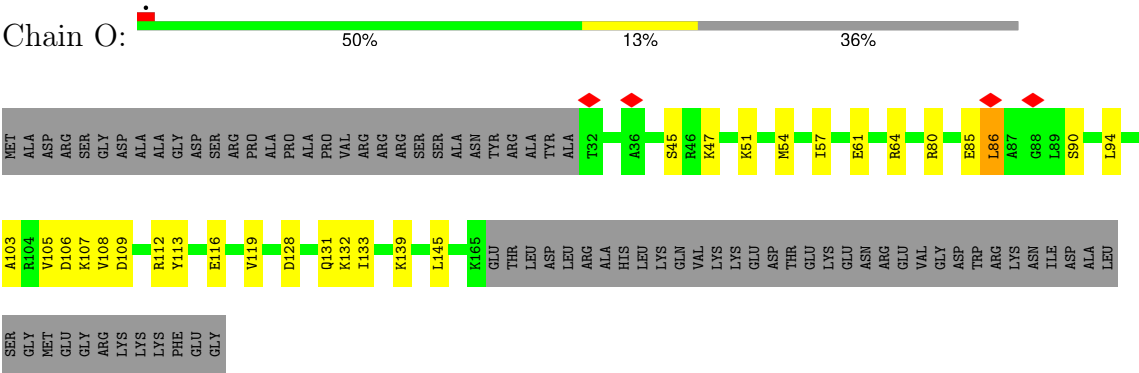
• Molecule 5: Myosin light chain 3



• Molecule 6: Troponin C, slow skeletal and cardiac muscles



• Molecule 7: Troponin I, cardiac muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55229	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 ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.125	Depositor
Minimum map value	-6.174	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.213	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	536.97595, 536.97595, 536.97595	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3559998, 1.3559998, 1.3559998	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/2995	0.30	0/4057
1	B	0.10	0/2995	0.29	0/4057
1	C	0.10	0/2995	0.31	0/4057
1	D	0.10	0/2995	0.29	0/4057
2	E	0.13	0/1311	0.27	0/1746
2	F	0.14	0/1311	0.26	0/1746
2	G	0.09	0/277	0.22	0/363
2	H	0.09	0/277	0.23	0/363
3	I	0.10	0/598	0.28	0/791
3	P	0.11	0/649	0.27	0/861
4	J	0.12	0/6594	0.33	0/8877
4	K	0.11	0/6609	0.32	0/8899
5	L	0.11	0/1236	0.40	2/1658 (0.1%)
5	M	0.11	0/1236	0.39	2/1658 (0.1%)
6	N	0.10	0/1287	0.29	0/1720
7	O	0.10	0/1085	0.25	0/1445
All	All	0.11	0/34450	0.31	4/46355 (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
4	J	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	182	GLY	CA-C-N	7.44	135.09	121.70
5	M	182	GLY	C-N-CA	7.44	135.09	121.70
5	L	182	GLY	CA-C-N	7.07	134.43	121.70
5	L	182	GLY	C-N-CA	7.07	134.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	J	628	ASP	Peptide

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	2932	0	2894	32	0
1	B	2932	0	2894	48	0
1	C	2932	0	2894	31	0
1	D	2932	0	2894	29	0
2	E	1304	0	1301	32	0
2	F	1304	0	1301	39	0
2	G	278	0	291	11	0
2	H	278	0	291	10	0
3	I	595	0	603	16	0
3	P	643	0	663	24	0
4	J	6461	0	6461	101	0
4	K	6475	0	6475	55	0
5	L	1217	0	1199	19	0
5	M	1217	0	1199	19	0
6	N	1274	0	1203	16	0
7	O	1077	0	1143	23	0
8	A	27	0	12	1	0
8	B	27	0	12	1	0
8	C	27	0	12	0	0
8	D	27	0	12	2	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
10	N	3	0	0	0	0
All	All	33966	0	33754	420	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 6.

All (420) 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)
4:J:628:ASP:HB2	4:J:630:PRO:CD	1.71	1.19
4:J:603:GLU:HG2	4:J:628:ASP:CG	1.82	1.05
4:J:628:ASP:HB2	4:J:630:PRO:HD3	1.07	1.05
4:J:603:GLU:HB3	4:J:628:ASP:OD1	1.57	1.04
4:J:628:ASP:HB3	4:J:630:PRO:N	1.75	1.02
4:J:628:ASP:CB	4:J:630:PRO:CD	2.40	1.00
4:J:603:GLU:HG2	4:J:628:ASP:OD1	1.70	0.92
4:J:603:GLU:CG	4:J:628:ASP:OD1	2.18	0.92
4:J:603:GLU:CB	4:J:628:ASP:OD1	2.19	0.91
4:J:628:ASP:CB	4:J:630:PRO:HD3	1.98	0.86
4:J:628:ASP:CB	4:J:630:PRO:N	2.40	0.84
4:J:628:ASP:CG	4:J:630:PRO:HG3	2.04	0.83
4:J:610:LYS:NZ	4:J:624:TYR:O	2.11	0.83
1:B:149:THR:HG22	1:B:167:GLU:H	1.48	0.78
4:J:603:GLU:HG2	4:J:628:ASP:OD2	1.83	0.78
4:K:293:LYS:HD3	4:K:326:ALA:HB1	1.66	0.76
1:B:122:ILE:HG12	3:P:198:ARG:HG2	1.69	0.75
1:D:149:THR:HG22	1:D:167:GLU:H	1.53	0.73
2:F:268:LYS:HE2	3:I:118:VAL:HG23	1.72	0.71
4:J:610:LYS:NZ	4:J:621:PHE:O	2.22	0.71
2:G:6:LYS:HD3	3:I:99:GLU:HB3	1.73	0.70
2:F:268:LYS:HE3	3:I:114:GLU:HB3	1.72	0.70
7:O:86:LEU:HD13	7:O:94:LEU:HD22	1.75	0.68
5:M:148:THR:HA	5:M:185:ASN:HA	1.76	0.67
3:P:199:GLN:HE22	3:P:202:ARG:HD2	1.59	0.67
2:G:3:ALA:HA	3:I:103:LEU:HD22	1.76	0.67
2:F:212:GLU:O	2:F:216:GLN:NE2	2.28	0.67
7:O:108:VAL:HG21	3:P:237:ILE:HG13	1.77	0.67
1:D:109:PRO:O	1:D:177:ARG:NH1	2.28	0.66
2:G:1:MET:HB2	3:I:107:HIS:HE1	1.59	0.66
1:B:169:TYR:HA	1:C:42:GLY:HA2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:SER:OG	4:K:536:GLU:OE2	2.11	0.66
2:E:214:TYR:OH	4:J:368:GLN:OE1	2.09	0.66
4:J:628:ASP:HB3	4:J:629:THR:C	2.19	0.66
6:N:156:PHE:O	7:O:51:LYS:NZ	2.30	0.65
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.78	0.65
6:N:150:TYR:HB3	3:P:264:ARG:HD3	1.79	0.64
4:J:179:GLU:HB3	4:J:238:ASN:HD21	1.63	0.64
6:N:13:THR:OG1	6:N:16:GLN:NE2	2.31	0.64
1:C:222:ASP:OD1	1:C:315:LYS:NZ	2.31	0.64
4:J:606:VAL:HG12	4:J:610:LYS:HE2	1.79	0.63
4:J:712:ARG:HG2	4:J:764:PHE:HD1	1.64	0.63
4:J:628:ASP:HB3	4:J:630:PRO:CA	2.29	0.63
1:C:149:THR:HG22	1:C:167:GLU:H	1.65	0.62
2:E:278:LEU:HD21	2:H:3:ALA:HB3	1.80	0.62
2:F:245:SER:HA	2:F:248:LYS:HE2	1.82	0.62
2:H:17:ASN:OD1	2:H:21:ARG:NH2	2.32	0.62
4:J:628:ASP:CB	4:J:630:PRO:CG	2.77	0.62
1:D:148:THR:HG23	1:D:149:THR:HG23	1.81	0.61
4:J:361:ASN:HB3	4:J:380:GLU:HG3	1.81	0.61
4:K:90:MET:HA	4:K:93:LEU:HD13	1.83	0.60
2:G:21:ARG:NH1	2:H:23:GLU:OE2	2.34	0.60
1:D:156:GLY:O	1:D:303:THR:OG1	2.19	0.60
3:P:211:GLU:O	3:P:214:LYS:NZ	2.34	0.60
1:B:276:GLU:O	1:B:280:ASN:ND2	2.32	0.59
1:C:237:GLU:HG2	1:C:251:GLY:HA2	1.84	0.59
1:A:25:ASP:HA	7:O:145:LEU:HB3	1.85	0.59
4:J:234:LYS:HB3	4:J:281:ARG:H	1.68	0.59
1:A:168:GLY:HA2	1:B:44:MET:HG3	1.85	0.59
2:E:253:ILE:HD11	2:F:256:LEU:HD12	1.83	0.59
4:J:367:LYS:NZ	4:J:374:GLU:OE2	2.28	0.59
2:F:208:GLU:OE2	4:J:367:LYS:NZ	2.35	0.59
1:B:350:SER:HA	1:B:353:GLN:HB2	1.84	0.58
2:F:274:LEU:O	2:F:278:LEU:HG	2.04	0.58
1:C:253:GLU:HA	1:C:256:ARG:HB2	1.85	0.58
1:C:17:VAL:HG23	1:C:33:SER:HB3	1.86	0.58
5:L:81:LEU:HD21	5:L:122:ILE:HG13	1.86	0.58
3:P:235:GLN:O	3:P:239:ASN:ND2	2.36	0.58
1:B:80:ASP:OD2	1:B:84:LYS:NZ	2.36	0.58
1:C:57:GLU:OE1	1:C:61:LYS:NZ	2.37	0.57
2:F:279:ASN:O	2:F:282:THR:OG1	2.19	0.57
1:A:304:THR:O	1:A:335:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:451:GLN:H	4:K:453:ARG:HH12	1.52	0.57
4:K:700:GLU:OE2	4:K:703:ARG:NH2	2.37	0.57
1:C:80:ASP:OD2	1:C:84:LYS:NZ	2.37	0.57
1:A:14:SER:HB3	1:A:157:ASP:HB3	1.86	0.57
1:B:122:ILE:HG23	3:P:198:ARG:HH21	1.68	0.57
1:B:286:ASP:OD2	1:C:39:ARG:NH2	2.37	0.57
1:B:26:ALA:HB1	4:J:406:VAL:HG22	1.88	0.56
1:B:118:LYS:O	1:B:122:ILE:HG13	2.05	0.56
5:L:111:ASP:HB2	5:L:114:THR:HG22	1.87	0.56
4:J:507:GLU:OE2	4:J:757:LYS:NZ	2.38	0.56
4:J:628:ASP:CB	4:J:630:PRO:HG3	2.35	0.56
6:N:142:LYS:NZ	6:N:155:GLU:OE1	2.32	0.56
4:K:714:LEU:HD23	4:K:762:LYS:HG3	1.87	0.56
2:E:232:LEU:HD11	2:F:231:LYS:HZ2	1.69	0.56
4:K:587:ASP:OD1	4:K:587:ASP:N	2.38	0.56
1:B:14:SER:OG	1:B:183:ARG:NH2	2.39	0.56
1:C:196:ARG:NH2	1:C:237:GLU:OE2	2.39	0.56
1:D:17:VAL:HG23	1:D:33:SER:HB3	1.88	0.56
2:E:182:ARG:HH22	2:F:180:GLU:HG3	1.70	0.56
2:F:264:LYS:HE3	3:I:121:LYS:HE3	1.87	0.56
4:J:587:ASP:OD1	4:J:587:ASP:N	2.27	0.56
1:B:23:GLY:HA2	4:J:644:PHE:HZ	1.71	0.55
1:B:35:VAL:HG22	1:B:54:VAL:HG12	1.88	0.55
1:D:282:ILE:HG12	1:D:293:LEU:HD23	1.89	0.55
4:J:106:LYS:HE3	4:J:684:ILE:HB	1.88	0.55
1:B:369:ILE:HD12	1:B:372:ARG:HD3	1.89	0.55
4:K:499:GLU:HA	4:K:502:LYS:HE3	1.88	0.55
1:D:220:ALA:HB1	1:D:226:GLU:HG3	1.89	0.55
1:A:369:ILE:HD12	1:A:372:ARG:HD3	1.87	0.55
1:B:148:THR:HA	1:C:44:MET:HE1	1.89	0.54
2:E:281:MET:HE2	2:H:7:LYS:HB3	1.88	0.54
4:K:784:ILE:HD13	5:M:137:GLY:HA3	1.89	0.54
1:A:17:VAL:HG23	1:A:33:SER:HB3	1.88	0.54
1:A:178:LEU:HG	1:A:180:LEU:H	1.72	0.54
3:I:135:GLN:OE1	3:I:138:ARG:NH2	2.36	0.54
1:D:153:LEU:O	1:D:300:SER:N	2.41	0.54
2:E:259:GLU:OE1	3:I:121:LYS:NZ	2.40	0.54
1:B:86:TRP:HH2	1:B:119:MET:HG3	1.73	0.54
1:A:222:ASP:O	1:A:226:GLU:HG2	2.08	0.54
2:E:133:ARG:HH21	2:F:134:ALA:HB1	1.74	0.53
4:J:628:ASP:HB2	4:J:630:PRO:CG	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:102:ARG:NH1	6:N:105:ASP:O	2.42	0.53
4:J:685:ASP:N	4:J:685:ASP:OD1	2.42	0.52
6:N:25:ASP:HA	6:N:28:VAL:HG22	1.91	0.52
2:G:3:ALA:HB2	3:I:103:LEU:HD13	1.91	0.52
4:J:272:ARG:O	4:J:276:GLN:NE2	2.42	0.52
4:K:343:SER:O	4:K:347:ASN:ND2	2.40	0.52
1:B:334:GLU:OE2	4:J:413:LYS:NZ	2.38	0.52
4:J:713:ILE:HG12	4:J:714:LEU:H	1.75	0.52
1:A:148:THR:HG23	1:A:149:THR:HG23	1.90	0.52
2:E:174:SER:O	2:E:178:ARG:HG2	2.10	0.52
2:F:249:LEU:O	2:F:253:ILE:HG12	2.10	0.52
2:F:264:LYS:O	2:F:268:LYS:HD3	2.08	0.52
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.91	0.52
4:K:724:ILE:HG13	5:M:136:GLU:HG3	1.92	0.52
1:C:6:THR:OG1	1:C:101:HIS:ND1	2.22	0.52
2:E:152:LYS:O	2:E:156:GLU:HG2	2.10	0.52
4:J:671:ARG:NH2	4:J:696:ASN:O	2.43	0.52
4:K:101:VAL:HG21	4:K:702:ILE:HD13	1.92	0.52
3:P:227:ARG:HH12	3:P:231:LYS:HE3	1.73	0.52
1:A:25:ASP:OD1	1:A:25:ASP:N	2.43	0.51
1:D:98:PRO:HB2	1:D:129:VAL:HG12	1.92	0.51
1:D:159:VAL:HG23	1:D:179:ASP:HA	1.92	0.51
4:J:208:GLU:OE1	4:J:451:GLN:NE2	2.44	0.51
4:K:784:ILE:HD11	5:M:134:PHE:HA	1.92	0.51
2:F:130:ILE:HG23	2:F:133:ARG:HH21	1.74	0.51
4:J:358:HIS:ND1	4:J:380:GLU:OE1	2.43	0.51
1:B:121:GLN:NE2	3:P:199:GLN:OE1	2.42	0.51
1:D:369:ILE:HD12	1:D:372:ARG:HD3	1.91	0.51
4:J:234:LYS:HB2	4:J:281:ARG:HB2	1.92	0.51
1:B:202:THR:HG22	1:B:204:ALA:H	1.76	0.51
2:E:163:GLU:O	2:E:167:ARG:HG2	2.10	0.51
4:K:255:THR:HG23	4:K:257:LYS:H	1.75	0.51
4:K:722:TYR:CE1	4:K:773:LEU:HB3	2.46	0.51
5:M:74:TYR:HB3	5:M:105:LEU:HA	1.93	0.51
5:M:117:PRO:O	5:M:120:GLN:HG3	2.11	0.51
2:F:133:ARG:HA	2:F:136:LYS:HE3	1.93	0.51
6:N:36:ILE:HD11	6:N:72:VAL:HB	1.93	0.51
7:O:119:VAL:HG12	3:P:251:PHE:HD1	1.74	0.51
1:A:253:GLU:HA	1:A:256:ARG:HB2	1.93	0.51
4:J:443:ILE:O	4:J:446:THR:OG1	2.26	0.51
4:K:607:ASP:HA	4:K:610:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:THR:HG21	1:D:46:GLY:HA2	1.93	0.50
5:M:81:LEU:HD23	5:M:84:LEU:HD12	1.93	0.50
1:D:157:ASP:OD2	8:D:401:ADP:O3'	2.29	0.50
2:E:270:ILE:HG13	2:F:267:TYR:HE1	1.76	0.50
2:F:281:MET:HE3	2:G:7:LYS:HG3	1.93	0.50
4:J:368:GLN:O	4:J:369:ARG:HG3	2.11	0.50
4:K:368:GLN:C	4:K:370:GLU:H	2.20	0.50
4:J:265:THR:HG23	4:J:440:VAL:HG21	1.94	0.50
4:J:723:ARG:NH1	5:L:136:GLU:OE1	2.45	0.50
5:M:147:GLY:HA2	5:M:186:TYR:CZ	2.47	0.50
6:N:124:THR:HG22	7:O:57:ILE:HG21	1.93	0.50
1:B:122:ILE:HG12	3:P:198:ARG:CG	2.41	0.50
4:J:426:ALA:HA	4:J:429:LYS:HE3	1.94	0.50
1:B:125:GLU:OE1	3:P:202:ARG:NE	2.45	0.50
1:B:156:GLY:O	1:B:303:THR:OG1	2.27	0.50
4:J:58:LYS:HG3	4:J:70:THR:HG22	1.94	0.50
1:B:74:GLY:O	1:B:111:ASN:ND2	2.43	0.50
7:O:105:VAL:HG22	3:P:237:ILE:HB	1.93	0.50
1:A:157:ASP:OD1	8:A:401:ADP:O3'	2.30	0.49
2:E:278:LEU:HD13	2:H:4:ILE:HG12	1.94	0.49
4:J:274:ILE:HG23	4:J:275:PHE:CD2	2.47	0.49
4:J:566:PRO:HG3	4:J:575:ALA:O	2.12	0.49
1:C:28:ARG:HH22	4:K:631:VAL:HG11	1.77	0.49
1:A:211:ASP:OD2	1:A:240:TYR:OH	2.20	0.49
1:D:222:ASP:O	1:D:225:ASN:ND2	2.45	0.49
4:J:248:ILE:HG13	4:J:459:VAL:HB	1.93	0.49
5:M:48:THR:HG22	5:M:50:GLU:H	1.77	0.49
5:M:154:LEU:HA	5:M:157:VAL:HG22	1.95	0.49
1:B:56:ASP:HA	1:B:59:GLN:HB2	1.95	0.49
1:A:113:LYS:HB3	1:A:371:HIS:CE1	2.47	0.49
4:J:281:ARG:HG2	4:J:287:TYR:CZ	2.48	0.49
5:L:74:TYR:HA	5:L:77:CYS:HB3	1.95	0.49
5:M:82:ARG:HG2	5:M:88:PRO:HD2	1.95	0.49
1:B:48:GLY:O	7:O:131:GLN:NE2	2.45	0.49
7:O:116:GLU:HA	7:O:119:VAL:HG22	1.94	0.49
1:B:17:VAL:HG23	1:B:33:SER:HB3	1.95	0.49
2:F:278:LEU:O	2:F:282:THR:HG23	2.13	0.48
4:J:753:HIS:HA	4:J:756:TYR:CZ	2.48	0.48
2:E:218:GLU:HG3	2:F:218:GLU:HG3	1.95	0.48
2:E:263:GLN:HG3	2:F:263:GLN:HB3	1.95	0.48
3:I:137:ILE:HG13	3:I:141:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:200:THR:O	3:P:204:LYS:HB2	2.12	0.48
1:D:304:THR:O	1:D:335:ARG:NH1	2.40	0.48
4:J:794:GLY:HA2	5:L:82:ARG:HB3	1.94	0.48
7:O:54:MET:HA	7:O:57:ILE:HG12	1.95	0.48
4:K:692:GLN:HE21	4:K:692:GLN:HA	1.79	0.48
7:O:103:ALA:O	7:O:107:LYS:HG2	2.12	0.48
1:C:27:PRO:HG2	4:K:406:VAL:HG23	1.95	0.48
1:C:71:ILE:HG12	1:C:76:ILE:HG12	1.95	0.48
1:D:272:ALA:HB1	1:D:276:GLU:HB3	1.95	0.48
2:F:281:MET:HE1	2:G:4:ILE:HD13	1.95	0.48
4:J:288:GLN:HB3	4:J:329:LEU:HB2	1.96	0.48
6:N:118:LYS:HG2	6:N:133:ILE:HD13	1.96	0.48
3:P:200:THR:HA	3:P:203:GLU:HG2	1.95	0.48
7:O:128:ASP:O	7:O:132:LYS:HD3	2.14	0.48
1:B:132:MET:HE1	1:B:134:VAL:HG23	1.96	0.48
4:K:599:ASP:OD2	4:K:645:GLN:NE2	2.47	0.48
7:O:85:GLU:OE1	3:P:227:ARG:NH2	2.46	0.48
7:O:90:SER:O	7:O:94:LEU:HG	2.14	0.48
1:B:122:ILE:HG23	3:P:198:ARG:HE	1.78	0.47
2:E:270:ILE:O	2:E:273:GLU:HG3	2.14	0.47
2:F:174:SER:O	2:F:178:ARG:HG2	2.14	0.47
1:B:53:TYR:HD2	1:B:65:LEU:HD11	1.79	0.47
1:D:211:ASP:OD2	1:D:240:TYR:OH	2.24	0.47
4:K:723:ARG:HG3	5:M:136:GLU:HG2	1.95	0.47
2:F:267:TYR:CD2	2:F:268:LYS:HD2	2.49	0.47
4:K:805:LEU:HD13	5:M:61:LEU:HD13	1.96	0.47
6:N:96:GLU:O	6:N:100:LEU:HG	2.14	0.47
5:L:86:GLN:HG3	5:L:126:LYS:HE2	1.97	0.47
4:J:484:LYS:HG3	4:J:659:MET:HE3	1.97	0.47
4:K:787:ARG:O	4:K:791:GLN:HG2	2.14	0.47
5:L:154:LEU:HA	5:L:157:VAL:HG22	1.97	0.47
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.46	0.47
1:C:148:THR:HG23	1:C:149:THR:HG23	1.96	0.47
4:K:802:LYS:NZ	4:K:806:GLU:OE1	2.48	0.47
1:B:148:THR:HG23	1:B:149:THR:HG23	1.96	0.47
4:J:789:GLN:HG2	5:L:165:LEU:HD12	1.97	0.47
1:B:126:THR:HG21	3:P:198:ARG:HH12	1.80	0.47
1:C:241:GLU:HG2	1:C:247:VAL:HG12	1.97	0.47
4:J:574:GLU:OE2	4:K:633:LYS:HG2	2.15	0.47
2:E:172:ILE:HG23	2:F:176:LEU:HD22	1.96	0.46
4:J:442:ARG:O	4:J:446:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:692:GLN:N	4:J:692:GLN:OE1	2.48	0.46
4:K:632:GLU:O	4:K:634:GLY:N	2.48	0.46
4:K:670:VAL:C	4:K:671:ARG:HE	2.22	0.46
1:B:314:GLN:HB2	1:B:329:ILE:HD12	1.98	0.46
2:E:261:TYR:O	2:E:264:LYS:HG3	2.15	0.46
3:I:110:ASN:O	3:I:114:GLU:HG2	2.16	0.46
2:F:256:LEU:HD23	2:F:256:LEU:HA	1.76	0.46
4:K:270:LYS:HD2	4:K:429:LYS:HB3	1.97	0.46
6:N:10:GLU:OE1	7:O:45:SER:N	2.48	0.46
2:E:266:LYS:HD3	2:F:267:TYR:CZ	2.50	0.46
2:G:6:LYS:HA	2:G:9:GLN:HG2	1.98	0.46
4:J:610:LYS:NZ	4:J:621:PHE:HB3	2.30	0.46
5:L:118:MET:O	5:L:122:ILE:HG12	2.15	0.46
1:B:151:ILE:HD11	1:B:162:ASN:HD21	1.80	0.46
1:C:107:GLU:OE1	1:C:111:ASN:ND2	2.49	0.46
2:E:177:GLU:OE1	2:E:178:ARG:NH2	2.43	0.46
2:E:263:GLN:HE21	2:F:264:LYS:NZ	2.14	0.46
4:J:635:LYS:NZ	3:P:266:ASN:HD21	2.13	0.46
4:K:431:VAL:HG12	4:K:621:PHE:HZ	1.80	0.45
5:M:49:PRO:HA	5:M:52:ILE:HB	1.97	0.45
1:A:241:GLU:HA	1:A:247:VAL:HG12	1.98	0.45
4:J:395:LEU:HD12	4:J:605:VAL:HG12	1.97	0.45
4:J:749:LEU:HD11	4:J:776:MET:HE1	1.99	0.45
4:J:774:GLU:HA	4:J:777:ARG:HG2	1.98	0.45
4:J:808:ARG:NH2	5:L:68:CYS:SG	2.89	0.45
7:O:106:ASP:OD2	3:P:213:ARG:NH1	2.49	0.45
2:F:152:LYS:O	2:F:156:GLU:HG2	2.17	0.45
4:J:88:GLU:HG2	4:J:108:ARG:NH1	2.31	0.45
4:K:405:LYS:HB3	4:K:410:TYR:CZ	2.50	0.45
4:K:577:PHE:CE1	4:K:590:ILE:HD11	2.51	0.45
4:K:603:GLU:OE1	4:K:603:GLU:N	2.44	0.45
2:E:249:LEU:HD12	2:F:253:ILE:HG13	1.98	0.45
2:E:263:GLN:HB2	2:F:264:LYS:HZ3	1.81	0.45
7:O:47:LYS:O	7:O:51:LYS:HG2	2.16	0.45
4:J:179:GLU:HB3	4:J:238:ASN:ND2	2.31	0.45
5:L:189:PHE:O	5:L:193:ILE:HG12	2.17	0.45
5:M:182:GLY:N	5:M:183:CYS:HB3	2.31	0.45
2:G:7:LYS:HB3	2:H:8:MET:HE1	1.98	0.45
4:J:427:LEU:HD11	4:J:605:VAL:HG21	1.98	0.45
6:N:2:ASP:HA	6:N:5:TYR:HD2	1.81	0.45
1:A:213:LYS:NZ	1:A:306:TYR:OH	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:294:LYS:NZ	4:J:333:ASP:OD2	2.43	0.45
4:J:506:ILE:HD13	4:J:759:GLY:HA2	1.99	0.45
1:B:12:ASN:OD1	1:B:86:TRP:NE1	2.40	0.45
4:J:610:LYS:HZ1	4:J:621:PHE:HB3	1.82	0.45
4:K:777:ARG:HH12	5:M:140:VAL:HG21	1.81	0.45
6:N:149:ASP:H	6:N:152:GLU:HB2	1.82	0.45
7:O:139:LYS:HE3	7:O:139:LYS:HB2	1.83	0.45
2:E:168:LYS:O	2:E:172:ILE:HG12	2.17	0.44
1:A:171:LEU:HD23	1:A:285:CYS:SG	2.57	0.44
1:C:21:PHE:HE1	1:C:96:VAL:HG11	1.83	0.44
3:P:234:TRP:O	3:P:237:ILE:HG22	2.17	0.44
1:C:120:THR:HG21	1:C:370:VAL:HG21	1.99	0.44
4:K:271:SER:HB2	4:K:596:LYS:HE2	1.99	0.44
1:A:6:THR:O	1:A:102:PRO:HD2	2.18	0.44
1:B:72:GLU:O	1:B:74:GLY:N	2.50	0.44
1:D:123:MET:HE3	1:D:129:VAL:HG11	2.00	0.44
4:J:754:ASN:OD1	4:J:754:ASN:N	2.44	0.44
1:D:214:GLU:HG2	8:D:401:ADP:C2	2.53	0.44
4:J:155:PHE:HB3	4:J:194:TYR:CE2	2.52	0.44
2:E:229:SER:O	2:E:233:LYS:HD3	2.18	0.44
4:J:506:ILE:HD12	4:J:506:ILE:HA	1.87	0.44
1:A:157:ASP:OD2	1:A:183:ARG:NH2	2.42	0.44
1:C:155:SER:HB2	1:C:160:THR:HG23	1.99	0.44
7:O:109:ASP:O	7:O:112:ARG:HG3	2.18	0.44
1:D:3:GLU:O	1:D:4:GLU:HB2	2.17	0.44
1:D:210:ARG:O	1:D:214:GLU:HG3	2.18	0.44
4:K:131:LEU:HB3	4:K:133:VAL:HG23	1.99	0.44
1:C:28:ARG:NH2	4:K:631:VAL:HG11	2.33	0.43
3:I:136:ARG:HA	3:I:136:ARG:HD3	1.84	0.43
4:J:146:LYS:HA	4:J:160:ASN:HD21	1.83	0.43
4:J:210:THR:O	4:J:212:GLY:N	2.50	0.43
4:K:248:ILE:HG22	4:K:263:ILE:HG22	1.99	0.43
1:D:219:VAL:HG22	1:D:258:PRO:HB2	2.00	0.43
4:J:275:PHE:CD2	4:J:596:LYS:HG2	2.53	0.43
4:J:639:LYS:HE2	4:J:639:LYS:HA	2.01	0.43
7:O:80:ARG:HH12	3:P:244:LYS:HD2	1.83	0.43
2:F:260:LEU:O	2:F:264:LYS:HG2	2.17	0.43
4:K:96:LEU:HD23	4:K:96:LEU:HA	1.87	0.43
4:K:793:ARG:HD3	5:M:165:LEU:HD11	2.00	0.43
2:E:253:ILE:HD13	2:F:253:ILE:HD12	2.00	0.43
2:F:161:LYS:O	2:F:165:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:LYS:O	2:H:16:GLU:HG2	2.17	0.43
4:J:41:ASP:HB2	4:J:44:GLU:H	1.83	0.43
5:L:151:GLY:O	5:L:155:ARG:NH2	2.50	0.43
1:A:326:LYS:HE3	1:A:326:LYS:HB2	1.86	0.43
1:B:96:VAL:HG12	4:J:636:GLY:HA2	2.00	0.43
3:I:92:LYS:HD2	3:I:92:LYS:HA	1.82	0.43
4:J:93:LEU:HD21	4:J:100:ALA:HB1	2.00	0.43
4:J:776:MET:O	4:J:780:ARG:HG2	2.18	0.43
1:A:207:GLU:OE1	1:A:210:ARG:NH2	2.43	0.43
1:C:337:TYR:CZ	4:K:406:VAL:HG21	2.52	0.43
2:F:242:ALA:O	2:F:246:VAL:HG13	2.19	0.43
4:J:327:GLU:OE1	4:J:327:GLU:N	2.46	0.43
4:K:626:GLY:O	4:K:628:ASP:N	2.52	0.43
1:A:171:LEU:HD13	1:B:40:HIS:CG	2.54	0.43
1:D:76:ILE:HD13	1:D:82:MET:HG2	2.00	0.43
4:K:222:GLN:O	4:K:225:PRO:HD2	2.19	0.43
5:L:182:GLY:HA2	5:L:183:CYS:HB2	1.99	0.43
2:E:267:TYR:CZ	2:F:266:LYS:HE2	2.54	0.43
2:F:278:LEU:HD22	2:G:3:ALA:HB3	2.01	0.43
4:J:474:GLU:H	4:J:474:GLU:CD	2.27	0.43
4:J:784:ILE:HG21	5:L:137:GLY:HA3	2.01	0.43
4:K:35:LYS:HA	4:K:51:ILE:HB	2.00	0.43
5:M:76:GLN:O	5:M:80:VAL:HG22	2.18	0.43
5:L:113:ASP:OD1	5:L:113:ASP:N	2.52	0.43
6:N:9:VAL:HG21	6:N:79:VAL:HG22	2.01	0.43
1:C:35:VAL:HG21	1:C:81:ASP:HB3	2.01	0.42
5:L:65:THR:HG22	5:L:67:LYS:H	1.84	0.42
4:J:405:LYS:NZ	4:J:632:GLU:OE1	2.52	0.42
4:K:770:LEU:O	4:K:774:GLU:HG2	2.19	0.42
1:B:360:GLN:O	1:B:364:GLU:HG2	2.19	0.42
4:J:88:GLU:HG2	4:J:108:ARG:HH12	1.84	0.42
1:C:160:THR:OG1	1:C:180:LEU:O	2.28	0.42
1:D:185:LEU:HD21	1:D:257:CYS:O	2.20	0.42
1:D:34:ILE:HD12	1:D:67:LEU:HD22	2.02	0.42
3:I:119:SER:O	3:I:123:ARG:HG2	2.19	0.42
7:O:61:GLU:HA	7:O:64:ARG:HG2	2.01	0.42
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.00	0.42
2:E:139:GLU:O	2:E:143:ILE:HG12	2.19	0.42
2:E:263:GLN:HE22	2:E:266:LYS:HD2	1.85	0.42
4:J:616:LEU:O	4:J:620:LEU:HG	2.20	0.42
7:O:113:TYR:CE1	3:P:208:ILE:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLY:HA2	4:J:644:PHE:CZ	2.53	0.42
4:J:174:ILE:HD13	4:J:668:HIS:HB2	2.00	0.42
4:K:120:LEU:HD11	4:K:496:LEU:HD13	2.01	0.42
4:K:474:GLU:O	4:K:478:ILE:HG12	2.20	0.42
1:A:118:LYS:HE3	1:A:118:LYS:HB3	1.88	0.42
1:A:369:ILE:HA	1:A:372:ARG:HD3	2.02	0.42
4:J:239:ASP:OD1	4:J:239:ASP:N	2.52	0.42
2:E:226:LYS:HE3	2:E:226:LYS:HB3	1.85	0.41
4:J:25:GLU:O	4:J:29:ARG:HG3	2.20	0.41
4:J:49:ALA:HB2	4:J:63:THR:HG22	2.01	0.41
4:J:631:VAL:HG21	4:J:637:LYS:HE3	2.02	0.41
1:B:178:LEU:HG	1:B:180:LEU:H	1.85	0.41
4:K:427:LEU:HD11	4:K:605:VAL:HG21	2.02	0.41
5:L:63:ASP:OD2	5:L:70:MET:N	2.53	0.41
6:N:59:GLU:O	6:N:63:GLU:HG3	2.21	0.41
1:B:16:LEU:HD13	8:B:401:ADP:H5'1	2.02	0.41
1:B:313:MET:HE3	1:B:313:MET:HB2	1.98	0.41
1:C:286:ASP:OD2	1:D:39:ARG:NH2	2.54	0.41
1:D:3:GLU:HG2	1:D:4:GLU:H	1.84	0.41
2:E:253:ILE:HD12	2:E:256:LEU:HB2	2.02	0.41
2:G:26:GLU:O	2:G:30:LYS:HG2	2.20	0.41
4:J:114:ILE:HD13	4:J:131:LEU:HD12	2.03	0.41
1:B:190:MET:HG3	1:B:200:PHE:HB2	2.02	0.41
2:H:10:MET:HE2	2:H:10:MET:HB2	2.00	0.41
4:J:222:GLN:HE21	4:J:222:GLN:HB2	1.68	0.41
5:L:43:ILE:HD12	5:L:43:ILE:HA	1.95	0.41
1:B:332:PRO:HA	1:B:333:PRO:HD3	1.94	0.41
2:H:19:LEU:O	2:H:23:GLU:HG2	2.20	0.41
3:I:106:ALA:O	3:I:109:GLU:HG3	2.20	0.41
4:J:437:ASN:O	4:J:440:VAL:HG12	2.20	0.41
1:C:274:ILE:HA	1:C:277:THR:HG22	2.03	0.41
1:D:106:THR:HB	1:D:137:GLN:HG2	2.03	0.41
2:E:152:LYS:HE3	2:E:152:LYS:HB2	1.84	0.41
3:I:122:ASP:O	3:I:126:LYS:HG2	2.20	0.41
4:J:277:LEU:HD12	4:J:280:GLU:HG3	2.03	0.41
4:K:236:VAL:HB	4:K:468:PHE:HE2	1.85	0.41
5:M:156:HIS:O	5:M:160:THR:OG1	2.33	0.41
2:H:18:ALA:O	2:H:21:ARG:HG2	2.21	0.41
4:J:522:ASP:HA	4:J:526:LYS:HG2	2.03	0.41
4:K:125:ILE:HD13	4:K:673:ILE:HB	2.02	0.41
5:L:77:CYS:SG	5:L:78:GLY:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:153:PHE:O	6:N:157:MET:HG2	2.21	0.41
1:A:295:ALA:HA	1:A:328:LYS:HB2	2.03	0.40
1:B:285:CYS:HB3	1:B:289:ILE:HD11	2.03	0.40
3:P:249:GLU:HA	3:P:252:LYS:HE3	2.02	0.40
1:C:226:GLU:OE2	2:F:244:ARG:NH1	2.32	0.40
2:F:137:ASP:HA	2:F:140:LYS:HE3	2.02	0.40
4:J:441:THR:O	4:J:445:THR:HG23	2.21	0.40
1:A:287:ILE:HD11	1:B:246:GLN:NE2	2.36	0.40
1:D:132:MET:HE2	1:D:132:MET:HB2	1.85	0.40
4:J:367:LYS:HG2	4:J:368:GLN:H	1.86	0.40
4:K:72:LYS:HE2	4:K:72:LYS:HB3	1.94	0.40
4:K:90:MET:O	4:K:96:LEU:HD21	2.22	0.40
4:K:288:GLN:O	4:K:291:SER:OG	2.34	0.40
4:K:637:LYS:H	4:K:637:LYS:HD2	1.86	0.40
7:O:107:LYS:HA	7:O:107:LYS:HD3	1.96	0.40
1:A:166:TYR:CD1	1:A:289:ILE:HB	2.57	0.40
1:A:332:PRO:O	1:A:335:ARG:HG3	2.22	0.40
4:K:297:LEU:O	4:K:301:LEU:HB2	2.22	0.40
1:B:285:CYS:O	1:B:290:ARG:NH2	2.50	0.40
1:C:188:TYR:HE1	1:C:257:CYS:HA	1.85	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	373/377 (99%)	357 (96%)	16 (4%)	0	100	100
1	B	373/377 (99%)	359 (96%)	14 (4%)	0	100	100
1	C	373/377 (99%)	353 (95%)	20 (5%)	0	100	100
1	D	373/377 (99%)	359 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	158/284 (56%)	158 (100%)	0	0	100	100
2	F	158/284 (56%)	158 (100%)	0	0	100	100
2	G	33/284 (12%)	33 (100%)	0	0	100	100
2	H	33/284 (12%)	33 (100%)	0	0	100	100
3	I	66/285 (23%)	66 (100%)	0	0	100	100
3	P	72/285 (25%)	70 (97%)	2 (3%)	0	100	100
4	J	798/1935 (41%)	762 (96%)	34 (4%)	2 (0%)	36	71
4	K	803/1935 (42%)	766 (95%)	37 (5%)	0	100	100
5	L	151/196 (77%)	143 (95%)	8 (5%)	0	100	100
5	M	151/196 (77%)	147 (97%)	4 (3%)	0	100	100
6	N	158/161 (98%)	148 (94%)	9 (6%)	1 (1%)	21	58
7	O	132/211 (63%)	131 (99%)	1 (1%)	0	100	100
All	All	4205/7848 (54%)	4043 (96%)	159 (4%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	93	SER
4	J	46	PHE
4	J	180	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/320 (99%)	308 (97%)	10 (3%)	35	56
1	B	318/320 (99%)	308 (97%)	10 (3%)	35	56
1	C	318/320 (99%)	307 (96%)	11 (4%)	32	53
1	D	318/320 (99%)	308 (97%)	10 (3%)	35	56
2	E	142/245 (58%)	138 (97%)	4 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	142/245 (58%)	141 (99%)	1 (1%)	76	79
2	G	28/245 (11%)	28 (100%)	0	100	100
2	H	28/245 (11%)	28 (100%)	0	100	100
3	I	64/249 (26%)	64 (100%)	0	100	100
3	P	69/249 (28%)	67 (97%)	2 (3%)	37	57
4	J	695/1697 (41%)	668 (96%)	27 (4%)	28	49
4	K	695/1697 (41%)	676 (97%)	19 (3%)	39	59
5	L	133/163 (82%)	125 (94%)	8 (6%)	17	39
5	M	133/163 (82%)	129 (97%)	4 (3%)	36	56
6	N	141/142 (99%)	138 (98%)	3 (2%)	47	65
7	O	115/176 (65%)	113 (98%)	2 (2%)	53	67
All	All	3657/6796 (54%)	3546 (97%)	111 (3%)	37	56

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	82	MET
1	A	107	GLU
1	A	140	LEU
1	A	153	LEU
1	A	173	HIS
1	A	187	ASP
1	A	289	ILE
1	A	337	TYR
1	A	373	LYS
1	B	59	GLN
1	B	77	THR
1	B	82	MET
1	B	140	LEU
1	B	151	ILE
1	B	152	VAL
1	B	201	VAL
1	B	350	SER
1	B	373	LYS
1	B	374	CYS
1	C	5	THR
1	C	59	GLN

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Mol	Chain	Res	Type
1	C	64	ILE
1	C	66	THR
1	C	96	VAL
1	C	101	HIS
1	C	140	LEU
1	C	192	ILE
1	C	303	THR
1	C	370	VAL
1	C	373	LYS
1	D	1	ASP
1	D	66	THR
1	D	84	LYS
1	D	87	HIS
1	D	124	PHE
1	D	140	LEU
1	D	151	ILE
1	D	185	LEU
1	D	225	ASN
1	D	374	CYS
2	E	131	GLU
2	E	142	GLU
2	E	148	LEU
2	E	218	GLU
2	F	204	LEU
4	J	43	LYS
4	J	69	VAL
4	J	70	THR
4	J	71	VAL
4	J	78	GLN
4	J	95	PHE
4	J	101	VAL
4	J	102	LEU
4	J	116	THR
4	J	123	VAL
4	J	153	HIS
4	J	177	THR
4	J	201	ILE
4	J	333	ASP
4	J	531	MET
4	J	564	GLN
4	J	567	ARG
4	J	585	THR

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Mol	Chain	Res	Type
4	J	587	ASP
4	J	599	ASP
4	J	631	VAL
4	J	637	LYS
4	J	676	ASN
4	J	685	ASP
4	J	719	ARG
4	J	734	GLN
4	J	763	VAL
4	K	28	THR
4	K	71	VAL
4	K	74	ASP
4	K	160	ASN
4	K	193	GLN
4	K	276	GLN
4	K	342	THR
4	K	359	PHE
4	K	376	ASP
4	K	406	VAL
4	K	447	LEU
4	K	500	GLU
4	K	535	GLU
4	K	587	ASP
4	K	623	ASN
4	K	629	THR
4	K	637	LYS
4	K	754	ASN
4	K	760	HIS
5	L	45	ILE
5	L	67	LYS
5	L	126	LYS
5	L	154	LEU
5	L	165	LEU
5	L	169	GLU
5	L	177	GLN
5	L	184	ILE
5	M	53	GLU
5	M	70	MET
5	M	77	CYS
5	M	193	ILE
6	N	18	ASN
6	N	48	LEU

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Mol	Chain	Res	Type
6	N	92	LYS
7	O	86	LEU
7	O	133	ILE
3	P	202	ARG
3	P	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	92	ASN
1	B	87	HIS
1	B	371	HIS
1	C	41	GLN
1	C	49	GLN
1	C	88	HIS
1	C	92	ASN
1	C	297	ASN
1	D	92	ASN
1	D	225	ASN
1	D	275	HIS
2	E	135	GLN
2	E	144	GLN
2	E	202	ASN
2	E	263	GLN
2	F	263	GLN
3	I	107	HIS
4	J	75	GLN
4	J	78	GLN
4	J	153	HIS
4	J	160	ASN
4	J	171	ASN
4	J	222	GLN
4	J	238	ASN
4	J	292	ASN
4	J	334	ASN
4	J	391	ASN
4	J	451	GLN
4	J	454	GLN
4	J	482	ASN
4	J	711	ASN
4	K	27	GLN

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Mol	Chain	Res	Type
4	K	163	GLN
4	K	172	GLN
4	K	437	ASN
4	K	451	GLN
4	K	486	GLN
4	K	555	ASN
4	K	602	ASN
4	K	692	GLN
4	K	734	GLN
4	K	789	GLN
5	L	76	GLN
5	L	90	GLN
5	L	102	GLN
6	N	16	GLN
6	N	18	ASN
6	N	50	GLN
6	N	144	ASN
7	O	56	GLN
7	O	82	GLN
7	O	122	ASN
7	O	131	GLN
7	O	157	GLN
3	P	225	GLN
3	P	248	GLN
3	P	254	GLN
3	P	266	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 7 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
8	ADP	C	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
8	ADP	B	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
8	ADP	D	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
8	ADP	A	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	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
8	ADP	C	401	-	-	4/16/32/32	0/3/3/3
8	ADP	B	401	-	-	4/16/32/32	0/3/3/3
8	ADP	D	401	-	-	4/16/32/32	0/3/3/3
8	ADP	A	401	-	-	3/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	ADP	C5-C4	4.77	1.47	1.39
8	C	401	ADP	C5-C4	4.76	1.47	1.39
8	A	401	ADP	C5-C4	4.68	1.47	1.39
8	B	401	ADP	C5-C4	4.67	1.47	1.39
8	C	401	ADP	C5-C6	2.70	1.48	1.41
8	D	401	ADP	C5-C6	2.70	1.48	1.41
8	A	401	ADP	C5-C6	2.67	1.48	1.41
8	B	401	ADP	C5-C6	2.66	1.48	1.41
8	B	401	ADP	C5-N7	-2.35	1.34	1.39
8	C	401	ADP	C5-N7	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	401	ADP	C5-N7	-2.29	1.34	1.39
8	D	401	ADP	C5-N7	-2.28	1.34	1.39
8	A	401	ADP	C8-N7	2.27	1.36	1.31
8	C	401	ADP	C8-N7	2.26	1.36	1.31
8	B	401	ADP	C8-N7	2.24	1.36	1.31
8	D	401	ADP	C8-N7	2.23	1.36	1.31

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	ADP	C5-C4-N3	-5.94	118.54	126.72
8	C	401	ADP	C5-C4-N3	-5.88	118.62	126.72
8	B	401	ADP	C5-C4-N3	-5.84	118.67	126.72
8	A	401	ADP	C5-C4-N3	-5.78	118.75	126.72
8	B	401	ADP	N3-C4-N9	4.72	135.19	127.17
8	D	401	ADP	N3-C4-N9	4.71	135.19	127.17
8	C	401	ADP	N3-C4-N9	4.67	135.11	127.17
8	A	401	ADP	N3-C4-N9	4.66	135.09	127.17
8	C	401	ADP	C2-N3-C4	3.68	120.81	111.83
8	D	401	ADP	C2-N3-C4	3.65	120.73	111.83
8	A	401	ADP	C2-N3-C4	3.64	120.73	111.83
8	B	401	ADP	C2-N3-C4	3.63	120.70	111.83
8	D	401	ADP	C4-C5-N7	-3.47	106.61	110.58
8	C	401	ADP	C4-C5-N7	-3.45	106.63	110.58
8	B	401	ADP	C4-C5-N7	-3.29	106.82	110.58
8	A	401	ADP	C4-C5-N7	-3.27	106.85	110.58
8	A	401	ADP	N3-C2-N1	-3.17	123.78	128.58
8	C	401	ADP	N3-C2-N1	-3.16	123.79	128.58
8	B	401	ADP	N3-C2-N1	-3.13	123.84	128.58
8	D	401	ADP	N3-C2-N1	-3.01	124.02	128.58
8	A	401	ADP	C4-N9-C8	2.65	108.52	105.74
8	B	401	ADP	C4-N9-C8	2.62	108.48	105.74
8	C	401	ADP	C4-N9-C8	2.58	108.45	105.74
8	D	401	ADP	C4-N9-C8	2.53	108.39	105.74
8	D	401	ADP	C5-N7-C8	2.49	107.37	103.45
8	C	401	ADP	C5-N7-C8	2.49	107.36	103.45
8	C	401	ADP	C2'-C1'-N9	-2.42	107.30	113.30
8	B	401	ADP	C5-N7-C8	2.40	107.22	103.45
8	A	401	ADP	C5-N7-C8	2.36	107.16	103.45
8	D	401	ADP	C3'-C2'-C1'	2.35	105.91	101.46
8	B	401	ADP	C2'-C1'-N9	-2.22	107.80	113.30
8	C	401	ADP	C3'-C2'-C1'	2.21	105.64	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	401	ADP	C2'-C1'-N9	-2.20	107.83	113.30
8	D	401	ADP	C2'-C1'-N9	-2.19	107.86	113.30
8	A	401	ADP	C3'-C2'-C1'	2.18	105.58	101.46
8	B	401	ADP	C3'-C2'-C1'	2.06	105.35	101.46
8	C	401	ADP	C6-C5-N7	2.03	135.99	132.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	401	ADP	C5'-O5'-PA-O1A
8	A	401	ADP	C5'-O5'-PA-O2A
8	A	401	ADP	C5'-O5'-PA-O3A
8	B	401	ADP	C5'-O5'-PA-O3A
8	C	401	ADP	C5'-O5'-PA-O3A
8	D	401	ADP	C5'-O5'-PA-O3A
8	C	401	ADP	C3'-C4'-C5'-O5'
8	B	401	ADP	C3'-C4'-C5'-O5'
8	C	401	ADP	O4'-C4'-C5'-O5'
8	D	401	ADP	C3'-C4'-C5'-O5'
8	B	401	ADP	C5'-O5'-PA-O1A
8	C	401	ADP	C5'-O5'-PA-O1A
8	D	401	ADP	C5'-O5'-PA-O1A
8	B	401	ADP	O4'-C4'-C5'-O5'
8	D	401	ADP	O4'-C4'-C5'-O5'

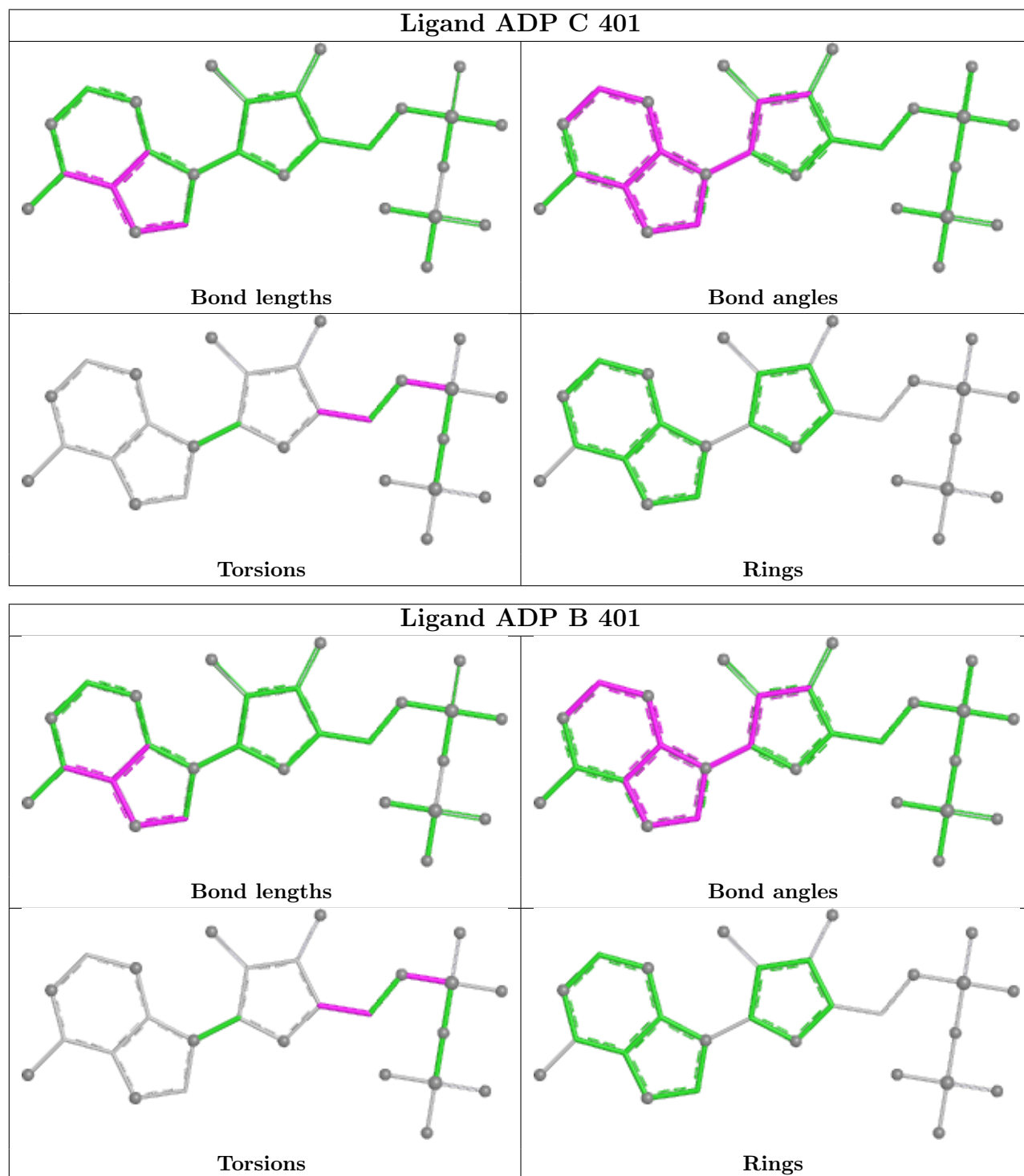
There are no ring outliers.

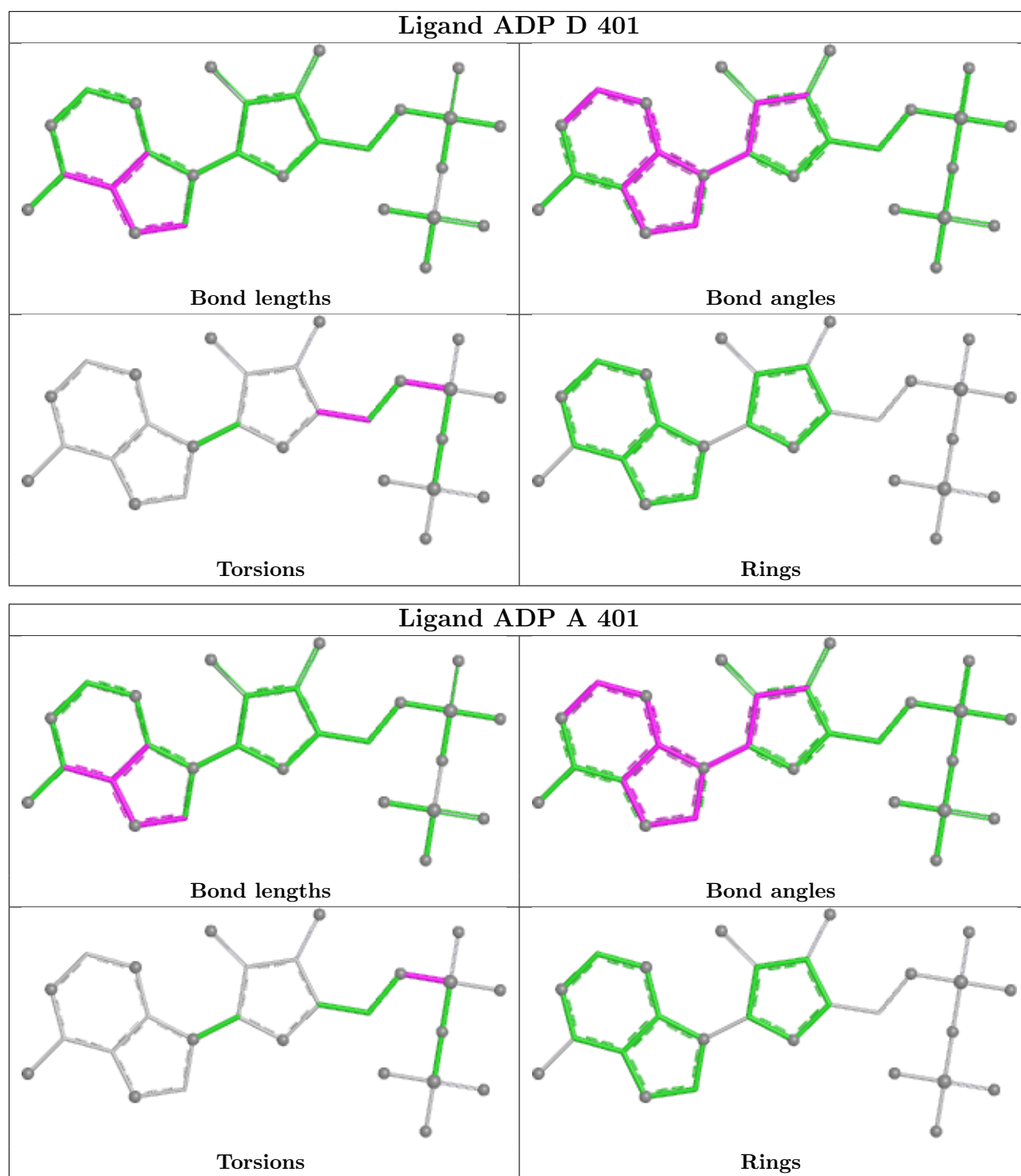
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	401	ADP	1	0
8	D	401	ADP	2	0
8	A	401	ADP	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

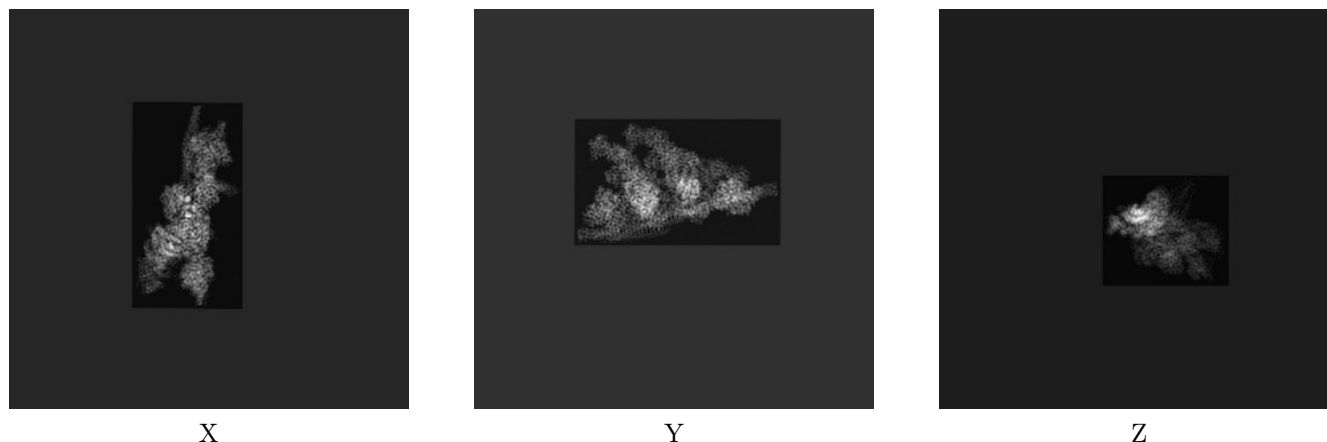
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72734. These allow visual inspection of the internal detail of the map and identification of artifacts.

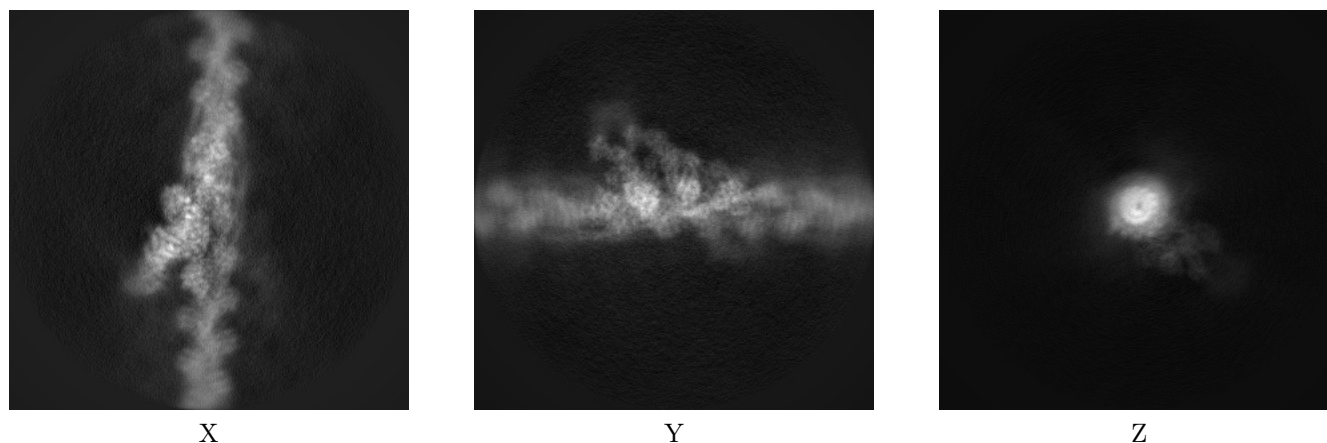
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



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

6.2 Central slices [i](#)

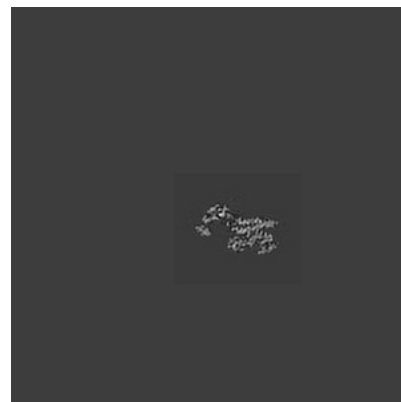
6.2.1 Primary map



X Index: 198

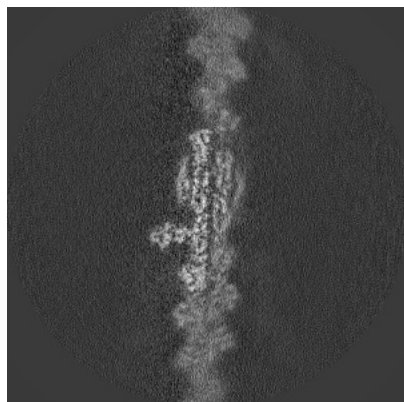


Y Index: 198

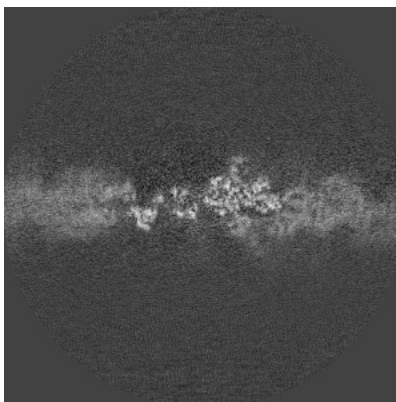


Z Index: 198

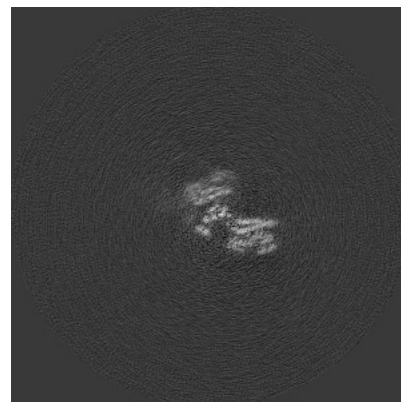
6.2.2 Raw map



X Index: 198



Y Index: 198



Z Index: 198

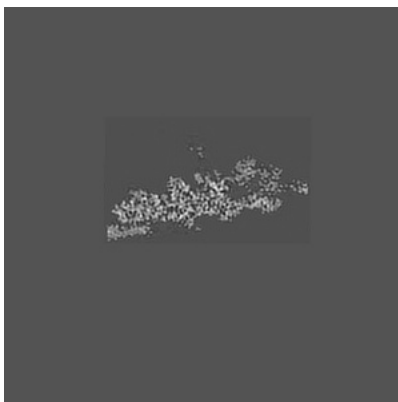
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 208

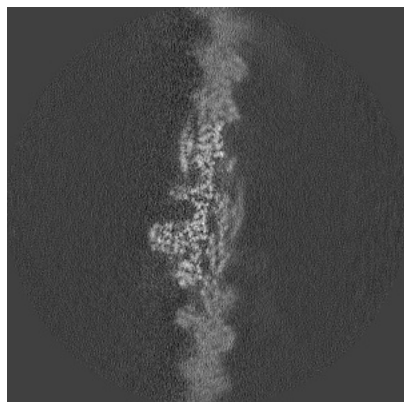


Y Index: 188

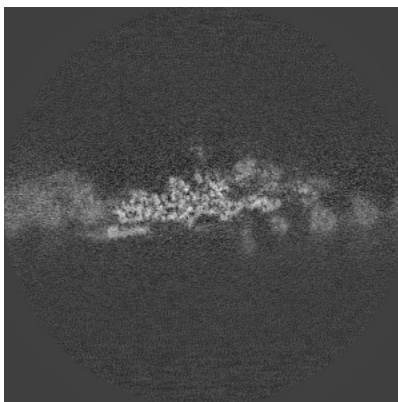


Z Index: 166

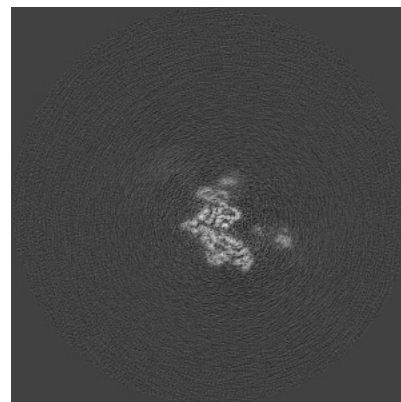
6.3.2 Raw map



X Index: 207



Y Index: 188

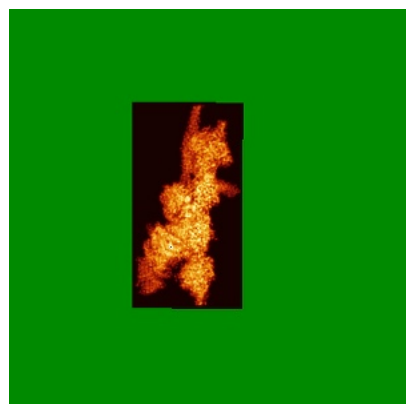


Z Index: 167

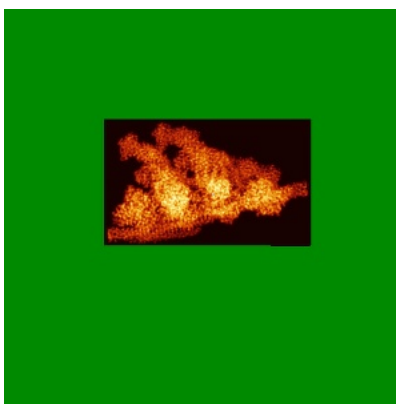
The images above show the largest variance slices of the map in three orthogonal directions.

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

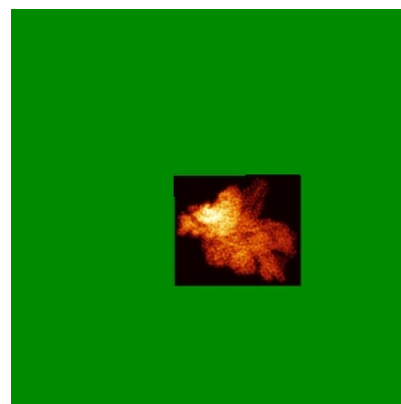
6.4.1 Primary map



X

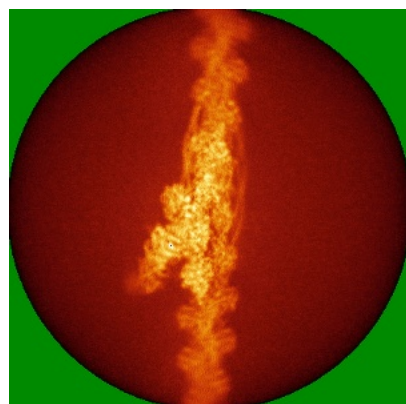


Y

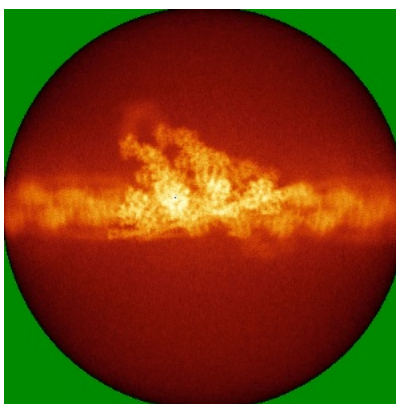


Z

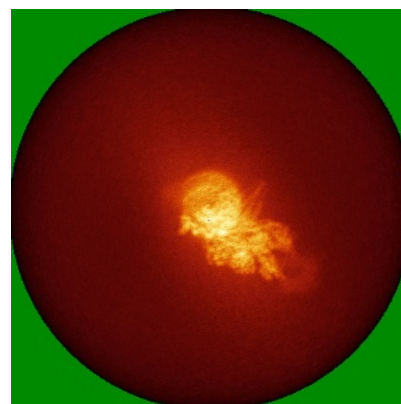
6.4.2 Raw map



X



Y

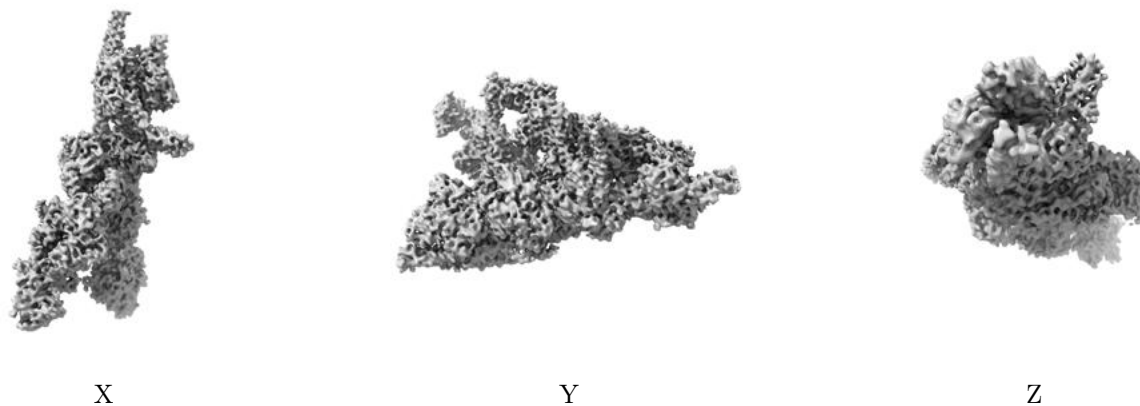


Z

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 1.35. 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.

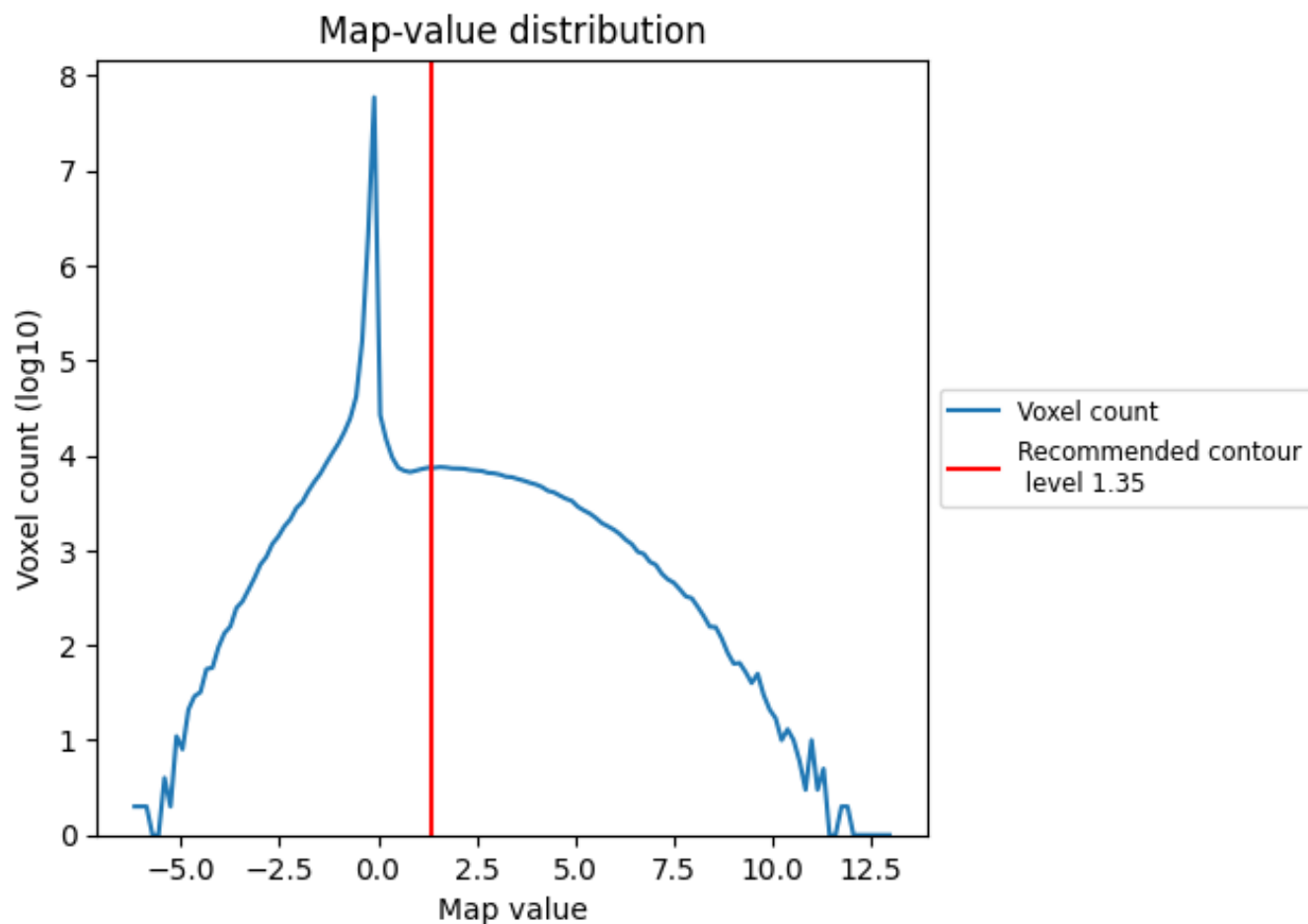
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

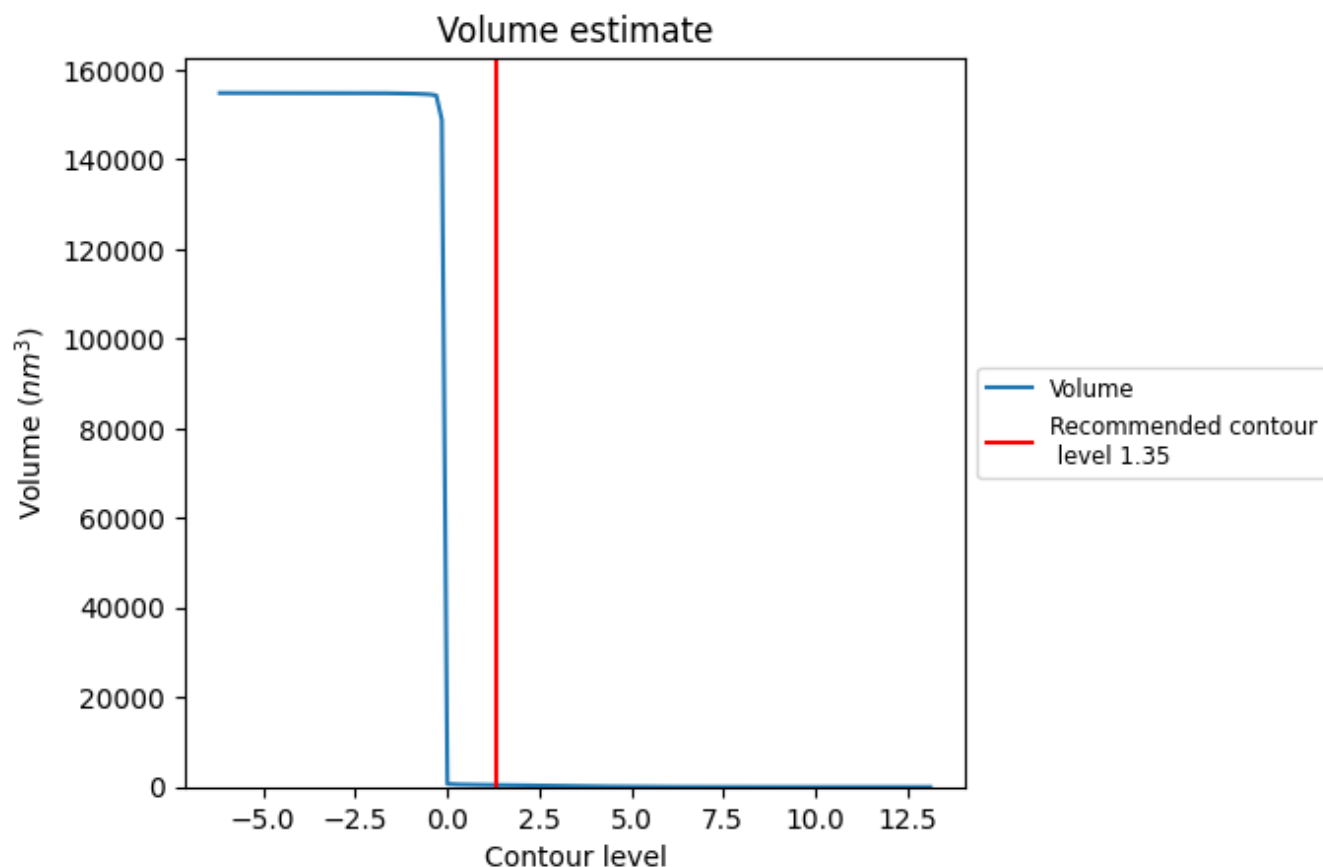
This section contains the results of statistical analysis of the map.

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.

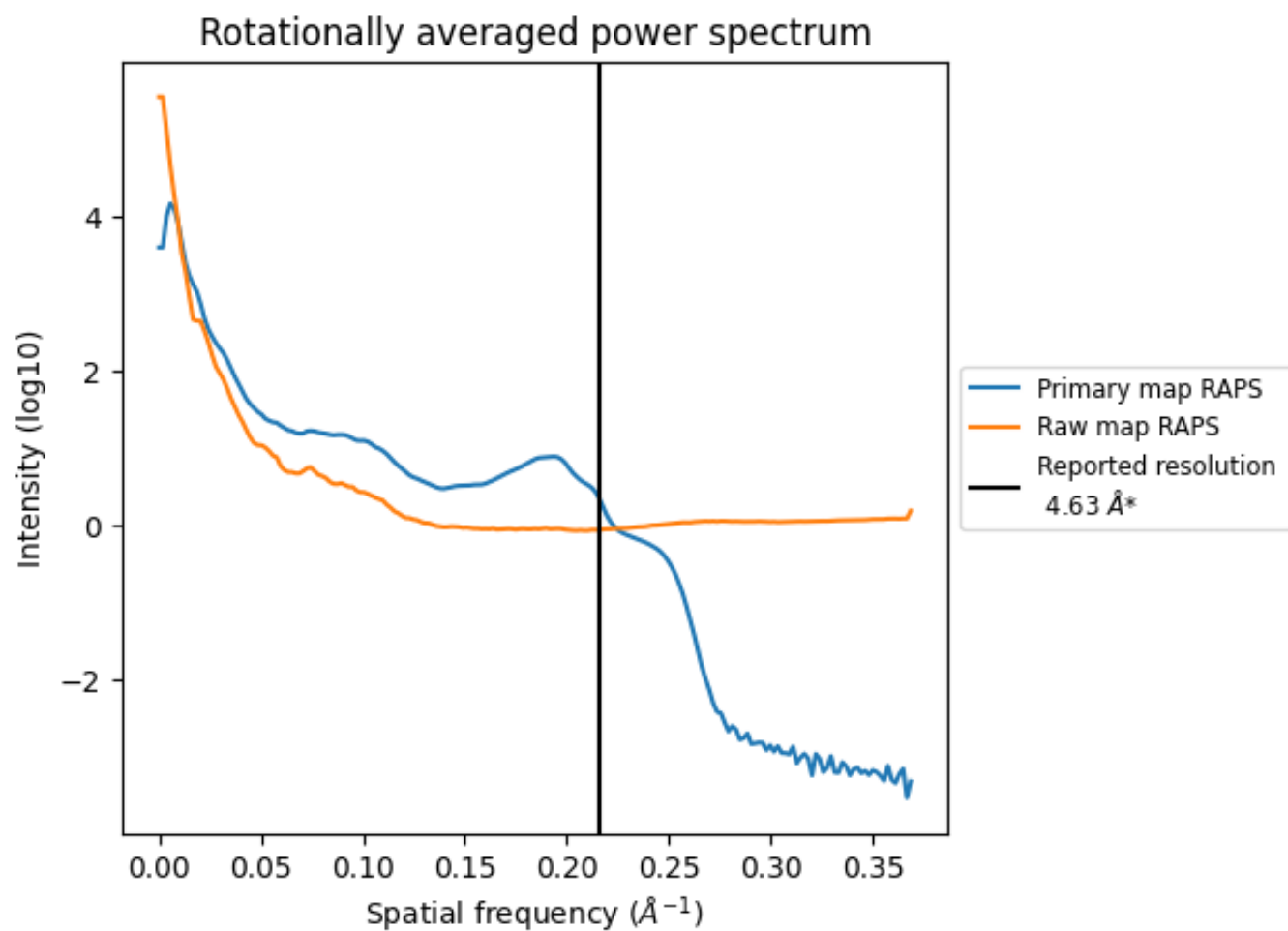
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 427 nm^3 ; this corresponds to an approximate mass of 386 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 ⓘ

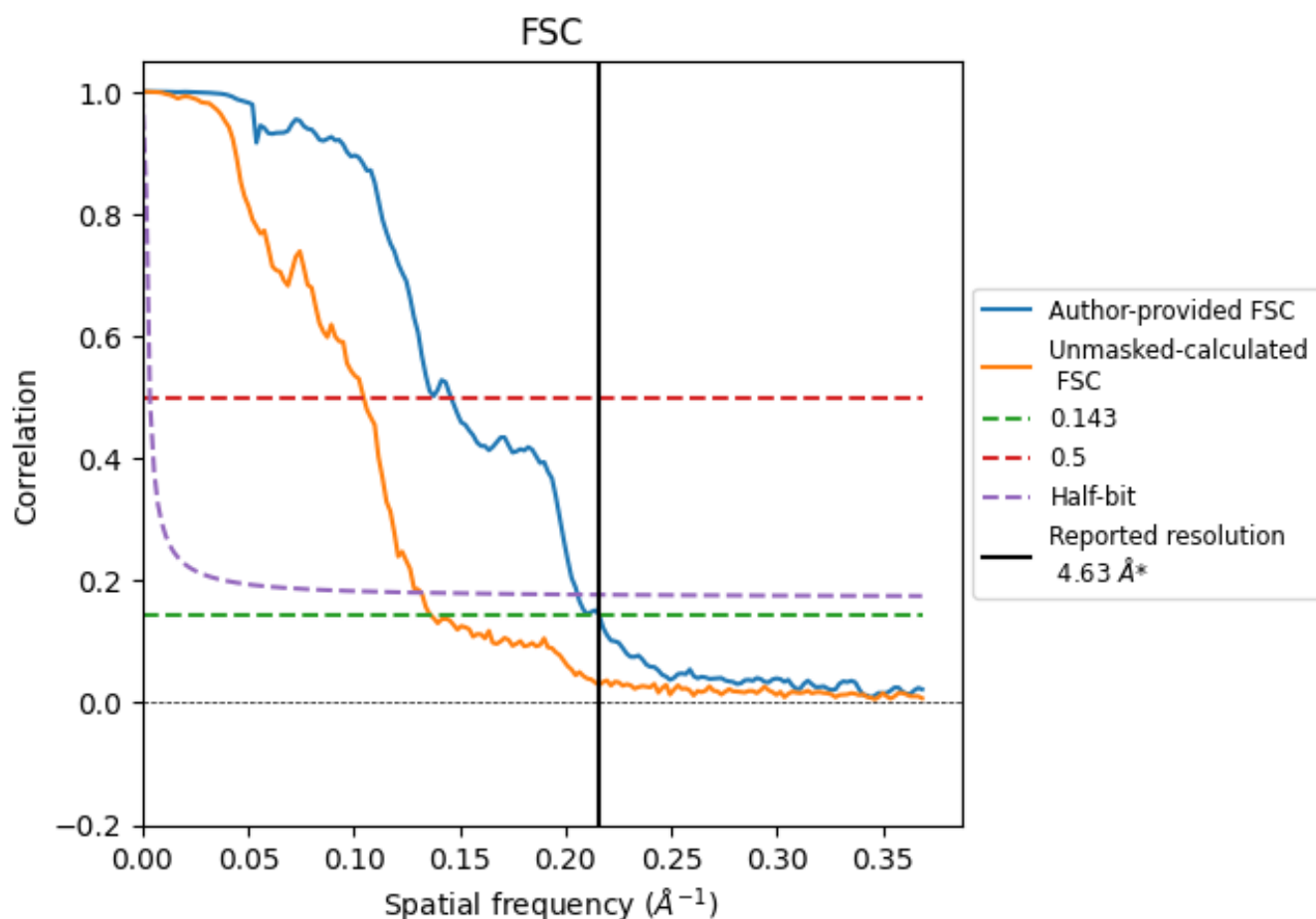


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 0.216 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

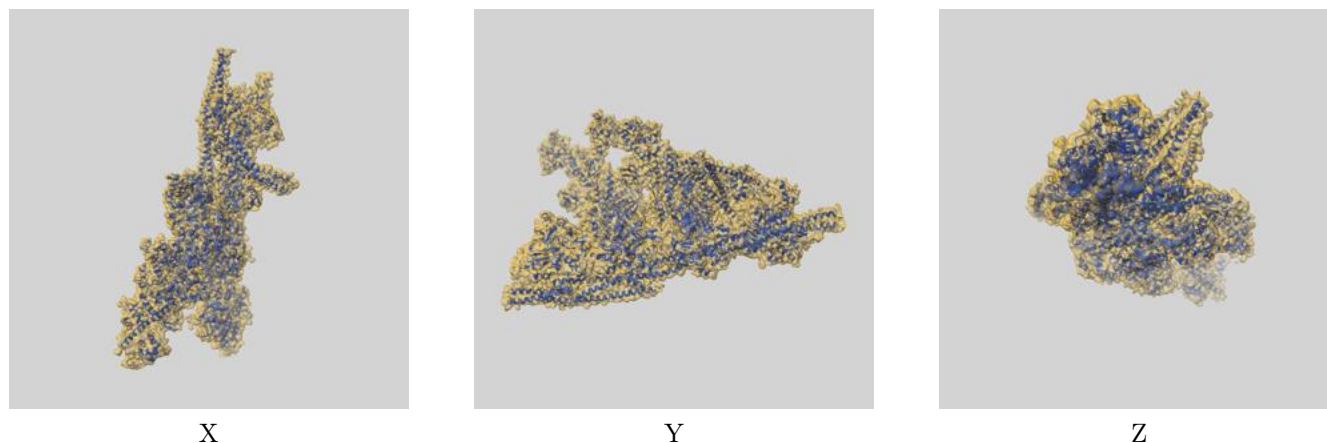
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	6.85	4.86
Unmasked-calculated*	7.33	9.56	7.58

*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 7.33 differs from the reported value 4.63 by more than 10 %

9 Map-model fit [i](#)

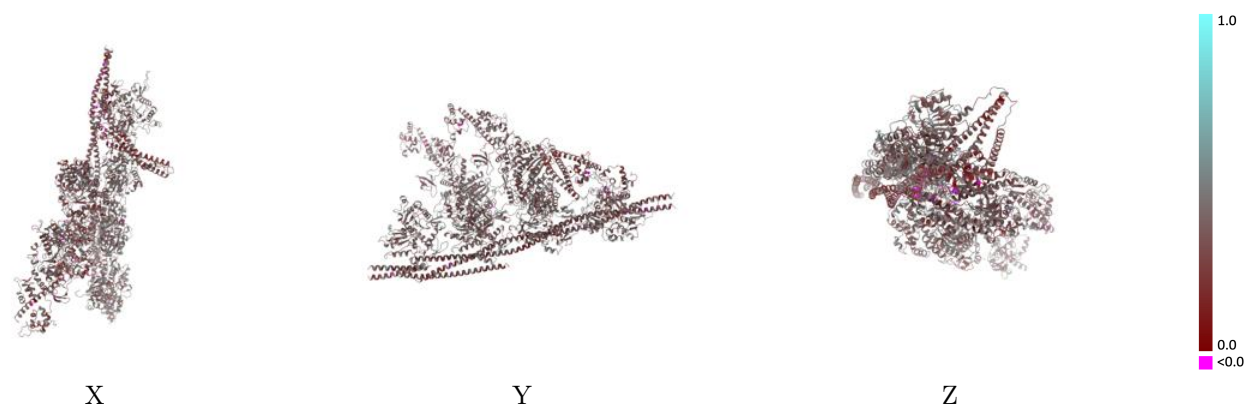
This section contains information regarding the fit between EMDB map EMD-72734 and PDB model 9YAQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



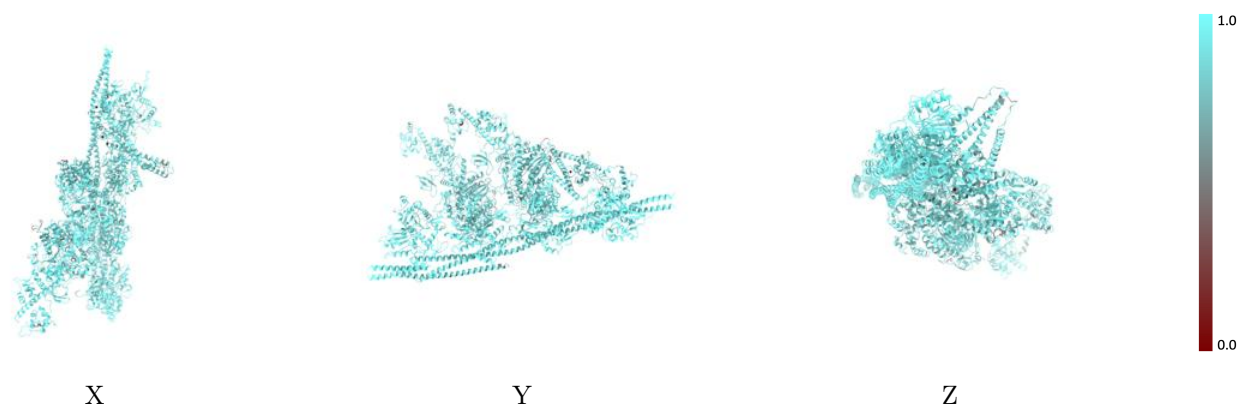
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



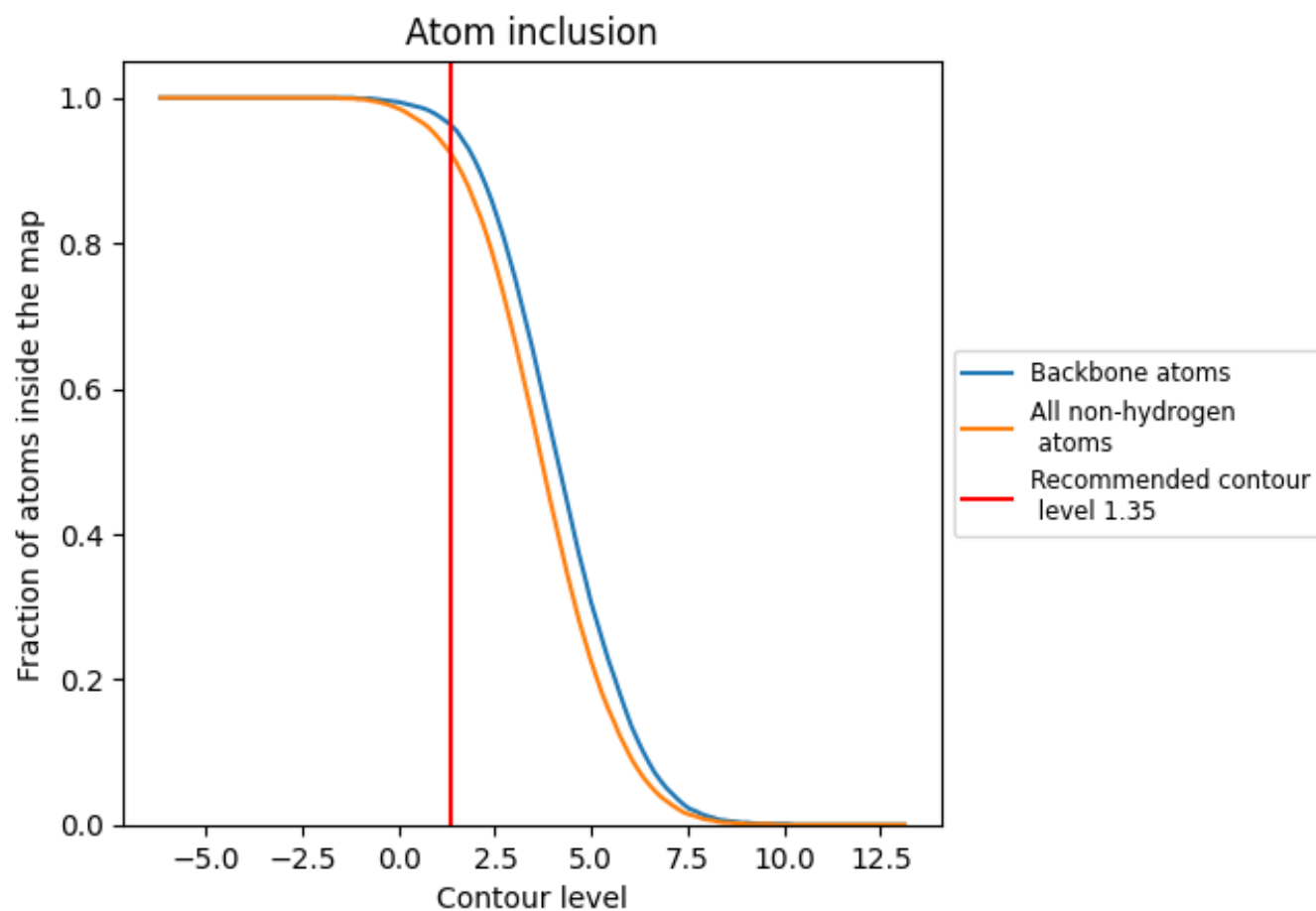
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.3670
A	 0.9630	 0.4000
B	 0.9420	 0.4040
C	 0.9340	 0.3980
D	 0.9590	 0.3980
E	 0.9550	 0.2890
F	 0.9560	 0.3100
G	 0.9930	 0.3270
H	 0.9670	 0.3440
I	 0.8690	 0.3220
J	 0.9060	 0.3670
K	 0.9270	 0.3680
L	 0.8570	 0.3670
M	 0.9220	 0.3630
N	 0.8600	 0.2840
O	 0.8600	 0.3320
P	 0.8500	 0.3110

