



Full wwPDB EM Validation Report ⓘ

Jul 16, 2026 – 04:27 PM EDT

PDB ID : 9YK9 / pdb_00009yk9
EMDB ID : EMD-73042
Title : The structure of the cardiac native crossbridge in the rigor state, myosin heads bound to actin molecules 1 and 2
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2025-10-06
Resolution : 4.50 Å (reported)
Based on initial models : 5H53, 7JH7, 6SFA, 8DD0, 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

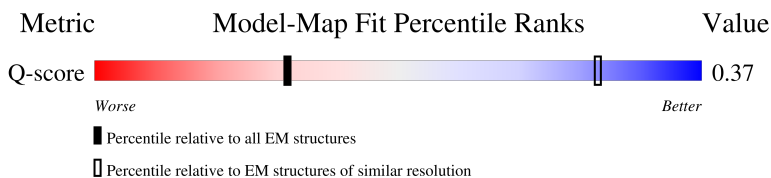
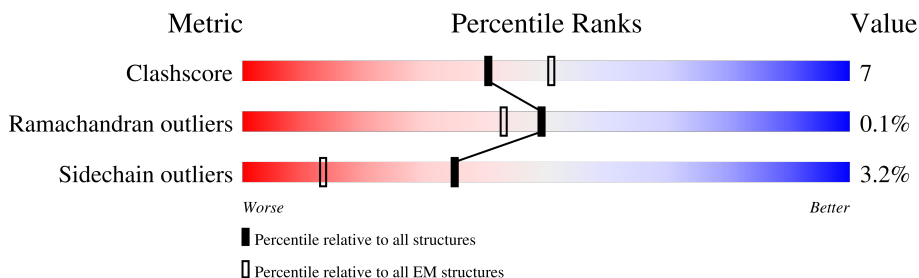
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	284	8% 88%
2	F	284	7%5% 88%
2	G	284	38%16% 45%
2	H	284	40%14% 45%
3	I	285	14% 84%
4	J	1935	35%6% 58%
4	K	1935	39% 58%
5	L	196	63%15% 22%
5	M	196	61%17% 22%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30678 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	35	Total	C	N	O	S	0	0
			285	177	43	64	1		
2	F	35	Total	C	N	O	S	0	0
			285	177	43	64	1		
2	G	155	Total	C	N	O	S	0	0
			1238	753	219	261	5		
2	H	155	Total	C	N	O	S	0	0
			1238	753	219	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	47	Total	C	N	O	S	0	0
			408	251	78	78	1		

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	805	Total	C	N	O	S	0	0
			6475	4127	1114	1202	32		

Continued on next page...

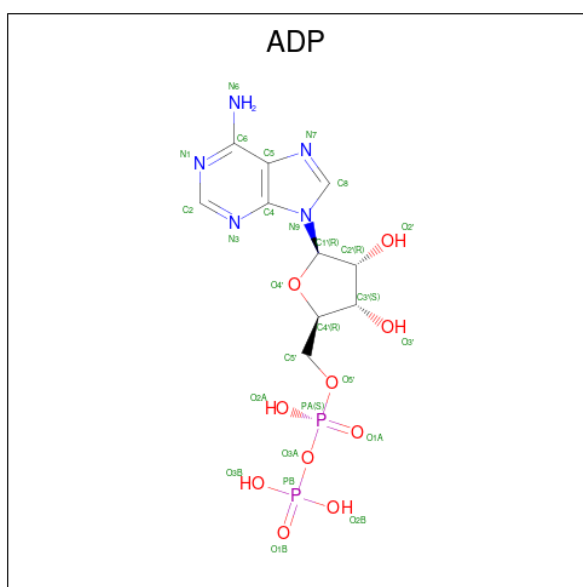
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

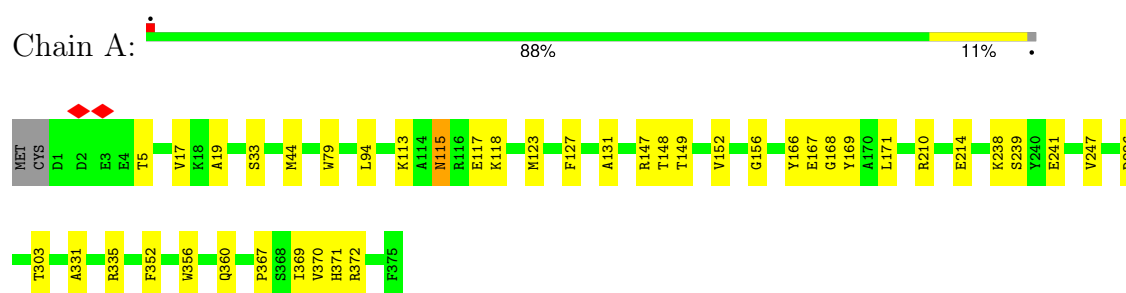
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

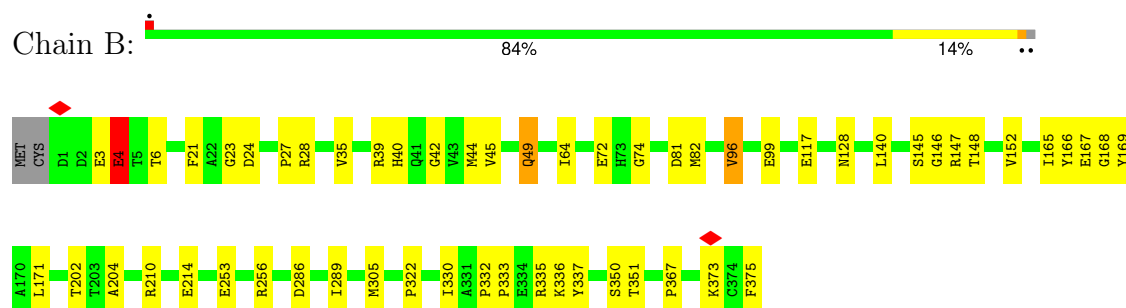
3 Residue-property plots [i](#)

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

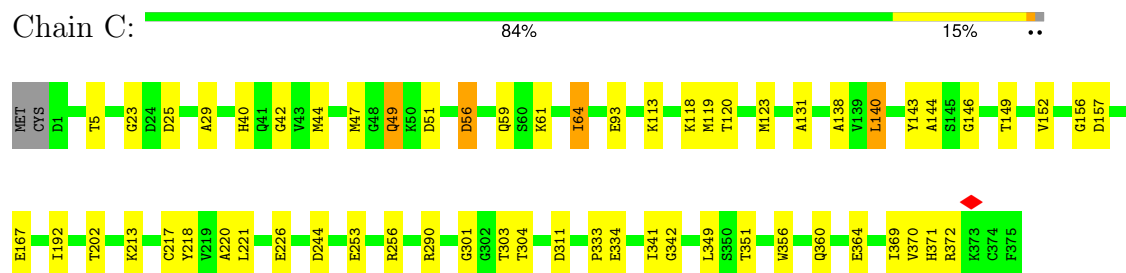
- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1





Chain E: 8% 88%



Chain F: 7% 5% 88%



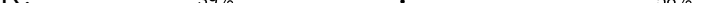
Chain G: 38% 16% 46%





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

- Molecule 4: Myosin-7

Chain K:  39% . 58%

NET	VAL	ASP
A4		
R17		
D32		
V37		
K43		
E44		
E62		
E68		
D89		
N90		
T116		
S156		
T201		
G202		
D203		
R204		
S205		
K206		
E208		
Q209		
T210		
E217		
N305		
A326		
L339		
E344		
K365		
Q368		
D376		
H401		
P402		
R403		
V404		
K405		
V406		
T412		
G412		

G414
Y422
L447
F470
N471
S472
E536
F540
P541
K551
D587
E603
V606
A627
V631
E632
K633
G634
K635
G636
K637
A638
K639
F644
E700
R703
R723
R787
I788
Q789
R793
G794
S797
R798
R808
ASP
SER
LEU
LEU
ILE

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

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

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

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

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

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

[illegible]

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

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

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

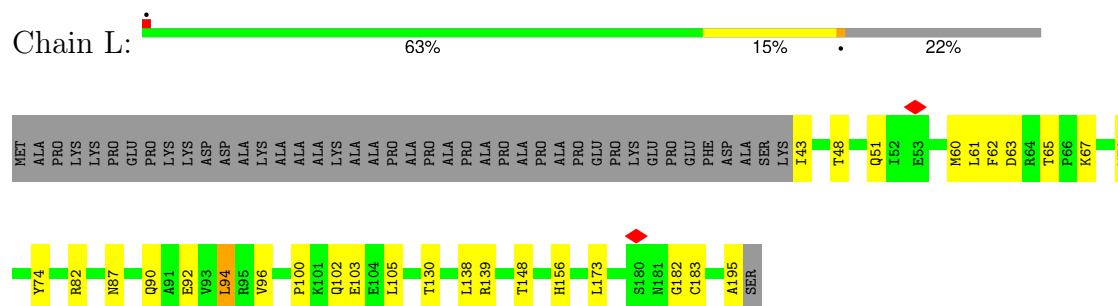
GLU
LYS
THR
LYS
HIS
ARG
LEU
GLN
ASN
GLU
ILE
GLU
ASP
LEU
MET
VAL
ASP
VAL
GLU
ARG
SER
ASN
ALA
ALA
ALA
LEU
ASP
LYS
GLN
LYN
ARG
ASN
PHE
ASP
LYS
ILE
LEU
LEU
ALA
GLU
TRP
LYS
GLN
LYS
TYR
GLU
GLU
SER
GLN
SER
LEU
GLU
GLU
SER
LYS
GLN
GLU
ALA

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

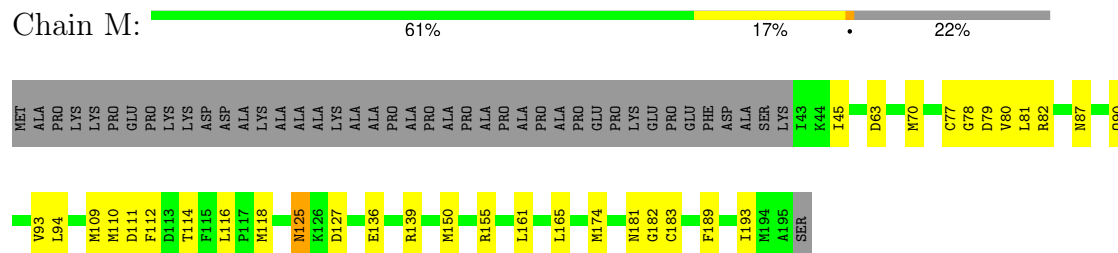
[illegible]

[illegible]

- Molecule 5: Myosin light chain 3



- Molecule 5: Myosin light chain 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54451	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	11.410	Depositor
Minimum map value	-5.567	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.178	Depositor
Recommended contour level	1.05	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: 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	0.15	0/2995	0.34	0/4057
1	B	0.17	0/2995	0.39	0/4057
1	C	0.17	0/2995	0.37	0/4057
1	D	0.15	0/2995	0.33	0/4057
2	E	0.16	0/287	0.29	0/383
2	F	0.18	0/287	0.28	0/383
2	G	0.26	0/1240	0.43	0/1647
2	H	0.24	0/1240	0.39	0/1647
3	I	0.16	0/411	0.23	0/544
4	J	0.12	0/6609	0.33	0/8899
4	K	0.82	0/6609	1.33	8/8899 (0.1%)
5	L	0.16	0/1236	0.43	2/1658 (0.1%)
5	M	0.15	0/1236	0.44	2/1658 (0.1%)
All	All	0.41	0/31135	0.69	12/41946 (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	B	0	1
4	K	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	182	GLY	CA-C-N	7.78	135.71	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	182	GLY	C-N-CA	7.78	135.71	121.70
5	L	182	GLY	CA-C-N	7.29	134.82	121.70
5	L	182	GLY	C-N-CA	7.29	134.82	121.70
4	K	401	HIS	CA-C-N	6.18	127.04	120.11
4	K	401	HIS	C-N-CA	6.18	127.04	120.11
4	K	368	GLN	N-CA-C	5.58	118.08	111.33
4	K	88	GLU	N-CA-C	5.35	117.19	111.36
4	K	637	LYS	N-CA-C	5.34	117.18	110.24
4	K	326	ALA	N-CA-C	5.23	116.67	111.07
4	K	472	SER	CA-C-N	5.10	127.11	120.28
4	K	472	SER	C-N-CA	5.10	127.11	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	GLU	Peptide
4	K	422	TYR	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	2932	0	2894	25	0
1	B	2932	0	2894	71	0
1	C	2932	0	2894	81	0
1	D	2932	0	2894	23	0
2	E	285	0	274	13	0
2	F	285	0	274	31	0
2	G	1238	0	1265	78	0
2	H	1238	0	1265	66	0
3	I	408	0	412	13	0
4	J	6475	0	6475	99	0
4	K	6475	0	6475	67	0
5	L	1217	0	1199	25	0
5	M	1217	0	1199	22	0
6	A	27	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	27	0	12	1	0
6	C	27	0	12	1	0
6	D	27	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	30678	0	30462	425	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 7.

All (425) 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)
2:G:91:ARG:HH21	2:H:92:ILE:CD1	1.22	1.52
2:G:91:ARG:NH2	2:H:92:ILE:HD13	1.39	1.38
1:C:334:GLU:CB	4:K:413:LYS:HE2	1.54	1.36
1:C:341:ILE:HD11	4:K:413:LYS:NZ	1.56	1.20
2:G:105:ARG:HH21	2:H:106:LEU:CD2	1.58	1.14
4:J:794:GLY:HA2	5:L:82:ARG:HB3	1.28	1.12
1:C:334:GLU:HB2	4:K:413:LYS:HE2	1.20	1.09
2:G:90:ARG:O	2:G:93:GLN:HG2	1.55	1.07
1:C:341:ILE:HD11	4:K:413:LYS:HZ1	1.03	1.06
2:G:91:ARG:NH2	2:H:92:ILE:CD1	2.07	1.05
2:G:51:LYS:O	2:G:54:GLU:HG3	1.58	1.03
1:B:168:GLY:N	1:C:47:MET:HE1	1.73	1.01
1:C:334:GLU:HB3	4:K:413:LYS:HE2	1.39	1.01
2:G:105:ARG:HE	2:H:106:LEU:HD21	1.27	0.99
1:B:146:GLY:C	4:J:541:PRO:HB3	1.87	0.98
2:G:105:ARG:HH21	2:H:106:LEU:HD21	1.25	0.98
1:C:341:ILE:CD1	4:K:413:LYS:NZ	2.25	0.98
1:B:305:MET:CE	1:B:336:LYS:HD2	1.93	0.97
1:C:334:GLU:CB	4:K:413:LYS:CE	2.43	0.96
2:G:105:ARG:NH2	2:H:106:LEU:HD21	1.81	0.96
1:B:305:MET:HE1	1:B:336:LYS:HD2	1.45	0.94
2:G:112:LYS:O	2:G:115:GLU:HG2	1.67	0.94
1:B:168:GLY:CA	1:C:47:MET:HE1	1.99	0.93
2:G:105:ARG:NE	2:H:106:LEU:HD21	1.84	0.92
1:B:337:TYR:CZ	4:J:406:VAL:HG21	2.07	0.90
2:G:105:ARG:HH21	2:H:106:LEU:HD23	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:91:ARG:HH21	2:H:92:ILE:HD12	1.36	0.88
2:G:90:ARG:HG3	2:G:93:GLN:NE2	1.89	0.88
4:K:403:ARG:HG2	4:K:412:THR:HG22	1.53	0.87
4:J:805:LEU:HD13	5:L:61:LEU:HD11	1.57	0.86
4:K:403:ARG:CG	4:K:412:THR:HG22	2.03	0.86
4:K:794:GLY:HA2	5:M:82:ARG:HB3	1.57	0.86
2:G:90:ARG:HA	2:G:93:GLN:NE2	1.90	0.86
2:G:90:ARG:HA	2:G:93:GLN:HE21	1.41	0.86
1:C:334:GLU:HB3	4:K:413:LYS:HG2	1.58	0.86
1:C:334:GLU:HB3	4:K:413:LYS:CE	2.05	0.85
1:B:148:THR:OG1	1:C:47:MET:HE2	1.77	0.85
2:G:91:ARG:HH21	2:H:92:ILE:HD13	0.68	0.85
2:G:91:ARG:CZ	2:H:92:ILE:HD13	2.05	0.85
2:G:106:LEU:HD21	2:H:105:ARG:HD2	1.58	0.85
4:J:574:GLU:H	4:K:633:LYS:HZ1	1.24	0.84
1:D:46:GLY:O	4:K:551:LYS:NZ	2.11	0.83
2:G:105:ARG:CZ	2:H:106:LEU:HD21	2.10	0.82
1:C:25:ASP:OD2	4:K:404:VAL:HG11	1.79	0.81
1:C:29:ALA:CB	1:C:93:GLU:HG2	2.12	0.80
1:B:167:GLU:O	1:C:47:MET:SD	2.39	0.80
1:B:21:PHE:CG	4:J:638:ALA:HB2	2.17	0.80
4:J:794:GLY:CA	5:L:82:ARG:HB3	2.11	0.80
4:K:365:LYS:HE2	4:K:376:ASP:OD1	1.83	0.78
2:H:62:GLU:OE1	2:H:62:GLU:HA	1.82	0.77
1:C:221:LEU:HD22	2:H:90:ARG:HG3	1.65	0.77
2:G:96:GLU:OE2	4:K:368:GLN:NE2	2.18	0.77
4:J:805:LEU:HD13	5:L:61:LEU:CD1	2.15	0.76
2:G:90:ARG:HG3	2:G:93:GLN:HE21	1.51	0.76
1:A:286:ASP:OD2	1:B:39:ARG:NH2	2.19	0.75
1:B:351:THR:N	4:J:536:GLU:OE2	2.19	0.75
1:C:149:THR:HG22	1:C:167:GLU:H	1.50	0.75
4:J:540:PHE:HB3	4:J:543:ALA:HB2	1.67	0.75
1:C:29:ALA:HB1	1:C:93:GLU:HG2	1.66	0.75
1:C:29:ALA:CB	1:C:93:GLU:CG	2.64	0.74
1:B:167:GLU:O	1:B:167:GLU:HG3	1.86	0.74
1:B:169:TYR:OH	1:C:49:GLN:NE2	2.20	0.74
1:B:168:GLY:CA	1:C:47:MET:CE	2.65	0.74
2:G:35:ARG:O	2:G:38:ARG:HG2	1.87	0.74
2:F:282:THR:HG22	3:I:100:LEU:HD11	1.68	0.73
1:C:23:GLY:HA2	4:K:644:PHE:HZ	1.53	0.73
2:G:90:ARG:CA	2:G:93:GLN:HE21	2.01	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:ALA:HA	2:H:66:ASP:OD2	1.89	0.73
1:B:305:MET:SD	1:B:336:LYS:HG2	2.29	0.72
2:G:6:LYS:HZ1	3:I:100:LEU:HD13	1.53	0.72
1:C:334:GLU:HB3	4:K:413:LYS:CG	2.19	0.72
1:B:21:PHE:CD2	4:J:638:ALA:HB2	2.24	0.72
1:C:349:LEU:HD22	4:K:536:GLU:HG3	1.70	0.72
1:C:341:ILE:CD1	4:K:413:LYS:HZ1	1.89	0.71
1:C:341:ILE:CD1	4:K:413:LYS:HZ3	2.00	0.71
5:L:65:THR:HG22	5:L:67:LYS:H	1.55	0.71
2:G:96:GLU:CD	4:K:368:GLN:NE2	2.49	0.70
2:G:90:ARG:CG	2:G:93:GLN:HE21	2.04	0.70
1:C:351:THR:N	4:K:536:GLU:OE1	2.24	0.70
4:K:365:LYS:HG3	4:K:376:ASP:HA	1.74	0.69
4:J:794:GLY:N	5:L:82:ARG:HD2	2.07	0.69
2:G:105:ARG:NH2	2:H:106:LEU:CD2	2.39	0.69
4:J:794:GLY:HA2	5:L:82:ARG:CB	2.17	0.69
1:B:168:GLY:HA3	1:C:47:MET:CE	2.23	0.68
1:C:334:GLU:HB3	4:K:413:LYS:CD	2.23	0.68
1:A:148:THR:HA	1:B:44:MET:HE1	1.76	0.68
4:K:797:SER:OG	5:M:79:ASP:O	2.06	0.68
1:B:21:PHE:CG	4:J:638:ALA:CB	2.77	0.68
2:F:281:MET:O	2:G:7:LYS:NZ	2.24	0.68
2:G:26:GLU:OE2	2:H:21:ARG:NH1	2.25	0.68
1:D:47:MET:HE3	4:K:540:PHE:HE2	1.57	0.67
4:J:792:SER:HB3	5:L:173:LEU:HD13	1.75	0.67
1:C:23:GLY:HA2	4:K:644:PHE:CZ	2.29	0.67
2:G:91:ARG:NH2	2:H:92:ILE:HG21	2.10	0.67
1:B:305:MET:SD	1:B:336:LYS:CG	2.82	0.67
4:J:574:GLU:N	4:K:633:LYS:HZ1	1.91	0.67
2:H:133:ARG:HA	2:H:136:LYS:HE3	1.77	0.67
2:E:281:MET:HG2	2:H:7:LYS:HG2	1.75	0.67
2:G:35:ARG:NH2	2:H:40:GLU:OE2	2.25	0.67
1:B:148:THR:OG1	1:C:47:MET:CE	2.43	0.67
1:B:286:ASP:OD1	1:B:289:ILE:CD1	2.43	0.66
2:H:63:ALA:O	2:H:66:ASP:CG	2.39	0.66
1:B:147:ARG:N	4:J:541:PRO:HB3	2.10	0.65
2:G:105:ARG:HE	2:H:106:LEU:CD2	2.06	0.65
4:J:403:ARG:H	4:J:604:THR:HG21	1.62	0.65
1:D:222:ASP:O	1:D:225:ASN:ND2	2.30	0.64
2:E:259:GLU:OE1	3:I:121:LYS:NZ	2.29	0.64
4:J:467:ILE:HD12	4:J:586:VAL:HG22	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:GLU:O	2:G:101:ARG:HG2	1.97	0.63
2:H:63:ALA:O	2:H:66:ASP:OD2	2.17	0.63
1:B:167:GLU:C	1:C:47:MET:HE1	2.24	0.63
1:C:334:GLU:CD	4:K:413:LYS:HD3	2.24	0.63
5:M:93:VAL:HG13	5:M:94:LEU:HG	1.81	0.62
1:C:56:ASP:OD1	1:C:56:ASP:N	2.23	0.62
1:C:351:THR:H	4:K:536:GLU:CD	2.08	0.62
2:G:106:LEU:HD21	2:H:105:ARG:CD	2.29	0.62
5:L:48:THR:OG1	5:L:51:GLN:OE1	2.17	0.62
1:B:337:TYR:CE1	4:J:406:VAL:HG21	2.35	0.61
2:F:275:ASP:HA	2:F:278:LEU:HD12	1.81	0.61
1:C:333:PRO:HB2	4:K:412:THR:O	2.00	0.61
2:G:91:ARG:NE	2:H:92:ILE:HD13	2.15	0.61
1:C:351:THR:HB	4:K:536:GLU:OE2	2.00	0.61
2:H:130:ILE:HG12	2:H:133:ARG:HH22	1.64	0.61
4:K:723:ARG:NH1	5:M:136:GLU:OE1	2.34	0.60
1:A:352:PHE:HD1	1:B:45:VAL:HG11	1.67	0.60
2:G:96:GLU:HG3	4:K:368:GLN:CG	2.31	0.60
1:B:24:ASP:OD1	4:J:639:LYS:O	2.19	0.60
2:F:275:ASP:OD2	3:I:111:ARG:NE	2.33	0.60
1:C:143:TYR:CD1	4:K:541:PRO:HG2	2.37	0.60
1:B:202:THR:HG22	1:B:204:ALA:H	1.67	0.59
2:F:271:SER:OG	3:I:114:GLU:OE2	2.17	0.59
2:G:70:LYS:HD3	2:H:71:LEU:HD21	1.83	0.59
4:J:448:GLU:OE1	4:J:453:ARG:NH2	2.35	0.59
4:J:801:PHE:HE1	5:L:62:PHE:HB2	1.67	0.59
1:A:168:GLY:HA2	1:B:44:MET:SD	2.42	0.59
2:E:263:GLN:HB2	2:F:264:LYS:HZ3	1.68	0.59
2:E:274:LEU:HD13	2:F:274:LEU:HD11	1.84	0.59
1:C:29:ALA:HB2	1:C:93:GLU:CG	2.33	0.58
4:J:367:LYS:HE2	4:J:372:GLN:HB3	1.85	0.58
2:G:91:ARG:NH2	2:H:92:ILE:HD12	2.04	0.58
1:C:120:THR:HG21	1:C:370:VAL:HG21	1.86	0.57
2:G:90:ARG:O	2:G:93:GLN:CG	2.43	0.57
1:B:99:GLU:OE2	1:B:128:ASN:ND2	2.37	0.57
1:C:156:GLY:O	1:C:303:THR:OG1	2.21	0.57
2:H:137:ASP:HA	2:H:140:LYS:HE3	1.85	0.57
1:C:146:GLY:C	4:K:541:PRO:HB3	2.28	0.57
1:D:17:VAL:HG23	1:D:33:SER:HB3	1.86	0.57
2:G:54:GLU:OE2	2:G:55:ASP:HB2	2.05	0.57
2:G:54:GLU:CD	2:G:55:ASP:N	2.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:HG21	1:B:81:ASP:HB3	1.87	0.57
1:C:290:ARG:HD2	1:D:244:ASP:HB2	1.87	0.57
2:G:93:GLN:HG3	2:G:94:LEU:N	2.18	0.57
1:B:96:VAL:HG13	4:J:636:GLY:HA3	1.85	0.57
4:J:793:ARG:NH2	5:L:90:GLN:HG3	2.20	0.57
2:F:268:LYS:HZ2	3:I:114:GLU:HA	1.69	0.56
2:G:96:GLU:C	2:G:96:GLU:OE1	2.49	0.56
5:L:148:THR:OG1	5:L:183:CYS:SG	2.62	0.56
1:A:352:PHE:CD1	1:B:45:VAL:HG11	2.41	0.56
1:D:47:MET:HG2	4:K:540:PHE:CZ	2.40	0.56
2:G:106:LEU:HD13	2:H:106:LEU:HA	1.87	0.56
1:B:333:PRO:HB2	4:J:412:THR:O	2.06	0.56
5:L:94:LEU:HD12	5:L:100:PRO:HD2	1.86	0.56
2:H:90:ARG:HA	2:H:93:GLN:HE21	1.72	0.55
1:C:143:TYR:HD1	4:K:541:PRO:HG2	1.70	0.55
2:E:253:ILE:HD13	2:F:253:ILE:HG23	1.87	0.55
4:K:43:LYS:NZ	4:K:43:LYS:HB3	2.21	0.55
2:H:93:GLN:HG2	2:H:94:LEU:HD22	1.89	0.55
2:G:115:GLU:HG3	2:G:116:ALA:N	2.20	0.55
2:F:264:LYS:O	2:F:268:LYS:HG2	2.06	0.55
4:J:565:LYS:O	4:J:567:ARG:NH1	2.40	0.55
1:D:47:MET:HG2	4:K:540:PHE:HZ	1.72	0.54
2:F:278:LEU:HD13	3:I:107:HIS:NE2	2.22	0.54
1:B:167:GLU:C	1:C:47:MET:SD	2.91	0.54
2:G:51:LYS:O	2:G:54:GLU:CG	2.46	0.54
4:K:798:ARG:NH1	5:M:87:ASN:HD21	2.06	0.54
1:C:360:GLN:O	1:C:364:GLU:N	2.40	0.54
1:D:211:ASP:OD2	1:D:240:TYR:OH	2.22	0.54
4:K:43:LYS:HB3	4:K:43:LYS:HZ3	1.71	0.54
4:J:794:GLY:CA	5:L:82:ARG:HD2	2.37	0.54
1:B:23:GLY:HA2	4:J:644:PHE:CZ	2.43	0.54
4:J:272:ARG:O	4:J:276:GLN:NE2	2.37	0.53
2:E:253:ILE:HD11	2:F:256:LEU:HD12	1.89	0.53
4:K:43:LYS:HD2	4:K:43:LYS:C	2.33	0.53
4:K:403:ARG:CD	4:K:412:THR:HG22	2.39	0.53
1:C:220:ALA:HB1	1:C:226:GLU:HG3	1.91	0.53
4:J:343:SER:HA	4:J:346:LYS:HE2	1.91	0.53
1:C:334:GLU:CG	4:K:413:LYS:HE2	2.33	0.53
2:G:54:GLU:OE2	2:G:55:ASP:N	2.42	0.53
5:L:74:TYR:HB2	5:L:105:LEU:HA	1.89	0.53
1:C:29:ALA:HB1	1:C:93:GLU:CG	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:470:PHE:HZ	4:J:589:ASN:HD22	1.57	0.53
2:F:281:MET:HG3	2:G:7:LYS:HG3	1.91	0.52
2:E:282:THR:HA	2:H:7:LYS:HE3	1.91	0.52
1:B:350:SER:OG	4:J:536:GLU:OE2	2.21	0.52
2:H:19:LEU:O	2:H:23:GLU:HG2	2.09	0.52
1:C:369:ILE:HD12	1:C:372:ARG:HD2	1.91	0.52
4:J:352:LEU:HD23	4:J:435:MET:HG3	1.91	0.52
1:B:332:PRO:O	1:B:335:ARG:NE	2.32	0.52
4:J:614:LEU:O	4:J:616:LEU:N	2.42	0.52
4:J:239:ASP:O	4:J:241:SER:N	2.39	0.52
1:A:156:GLY:O	1:A:303:THR:OG1	2.27	0.52
4:J:808:ARG:NH2	5:L:63:ASP:O	2.43	0.52
5:L:92:GLU:O	5:L:96:VAL:HG22	2.10	0.52
1:C:29:ALA:HB2	1:C:93:GLU:HG3	1.91	0.52
1:C:47:MET:HA	4:J:540:PHE:CZ	2.46	0.51
4:J:268:LEU:HD21	4:J:436:PHE:HB3	1.91	0.51
2:F:278:LEU:O	2:F:282:THR:HG23	2.10	0.51
1:B:253:GLU:H	1:B:253:GLU:CD	2.18	0.51
1:A:241:GLU:HA	1:A:247:VAL:HG12	1.92	0.51
1:D:148:THR:HG23	1:D:149:THR:HG23	1.93	0.51
2:H:90:ARG:O	2:H:94:LEU:HD23	2.10	0.51
4:J:530:ILE:HD13	4:J:552:LEU:HD11	1.93	0.51
1:B:21:PHE:CD1	4:J:638:ALA:HB2	2.45	0.50
1:B:351:THR:OG1	4:J:536:GLU:OE1	2.30	0.50
2:F:278:LEU:HD23	2:G:4:ILE:HG13	1.92	0.50
1:C:143:TYR:CE2	1:D:44:MET:HB2	2.47	0.50
1:C:301:GLY:O	1:C:304:THR:OG1	2.29	0.50
4:K:627:ALA:HB2	4:K:639:LYS:HD2	1.94	0.50
1:B:169:TYR:HA	1:C:42:GLY:HA2	1.93	0.50
5:M:45:ILE:HD13	5:M:116:LEU:HG	1.93	0.50
2:H:54:GLU:OE2	4:J:367:LYS:HB2	2.12	0.50
4:J:114:ILE:HD11	4:J:133:VAL:HG11	1.94	0.50
2:G:93:GLN:CG	2:G:94:LEU:N	2.75	0.49
1:B:147:ARG:HH22	4:J:371:GLU:CD	2.19	0.49
4:J:801:PHE:CE1	5:L:62:PHE:HB2	2.46	0.49
2:F:284:ILE:HD13	2:H:12:LYS:HE2	1.95	0.49
4:J:798:ARG:HH12	5:L:195:ALA:C	2.20	0.49
1:B:3:GLU:O	1:B:4:GLU:HB2	2.13	0.49
2:F:279:ASN:O	2:F:282:THR:OG1	2.18	0.49
1:D:3:GLU:HG2	1:D:4:GLU:H	1.77	0.49
2:F:267:TYR:O	2:F:271:SER:OG	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:280:ASP:OD1	2:F:281:MET:N	2.46	0.49
4:J:508:TRP:CZ2	4:J:510:PHE:HB2	2.48	0.49
4:K:787:ARG:NH1	5:M:127:ASP:OD1	2.34	0.49
1:D:308:GLY:HA2	2:G:125:ARG:NH1	2.28	0.49
2:G:91:ARG:HE	2:H:92:ILE:HD13	1.75	0.48
4:J:248:ILE:HG23	4:J:263:ILE:HG22	1.95	0.48
4:J:808:ARG:NH2	5:L:61:LEU:O	2.45	0.48
1:B:305:MET:CE	1:B:336:LYS:CD	2.80	0.48
2:G:106:LEU:CD2	2:H:105:ARG:HD2	2.36	0.48
2:H:93:GLN:CG	2:H:94:LEU:HD22	2.43	0.48
5:M:125:ASN:OD1	5:M:125:ASN:N	2.43	0.48
4:J:196:ALA:HA	4:J:258:LEU:HD21	1.96	0.48
5:L:60:MET:HB2	5:L:70:MET:HE1	1.95	0.48
1:D:220:ALA:HB1	1:D:226:GLU:HG3	1.95	0.48
3:I:100:LEU:HD12	3:I:103:LEU:HD11	1.95	0.48
2:G:57:LEU:HA	2:H:57:LEU:HD13	1.95	0.48
4:J:657:LYS:O	4:J:660:THR:HG22	2.14	0.48
2:E:270:ILE:O	2:E:273:GLU:HG3	2.14	0.48
4:K:43:LYS:HD2	4:K:44:GLU:HG3	1.95	0.48
1:B:72:GLU:O	1:B:74:GLY:N	2.45	0.47
1:D:314:GLN:O	1:D:318:THR:OG1	2.31	0.47
4:J:42:ASP:OD1	4:J:43:LYS:N	2.46	0.47
4:J:174:ILE:HG22	4:J:459:VAL:HA	1.94	0.47
5:M:150:MET:HA	5:M:183:CYS:H	1.79	0.47
2:F:284:ILE:HD12	2:G:7:LYS:HZ1	1.79	0.47
2:G:15:LYS:HD2	2:H:14:ASP:HB3	1.95	0.47
1:C:351:THR:CB	4:K:536:GLU:OE2	2.62	0.47
4:J:796:LEU:HB2	5:L:173:LEU:HD21	1.97	0.47
1:D:138:ALA:HB1	1:D:152:VAL:HG11	1.97	0.47
2:G:55:ASP:OD1	2:G:55:ASP:O	2.33	0.47
1:B:305:MET:SD	1:B:336:LYS:HD2	2.55	0.47
1:B:330:ILE:HG12	4:J:371:GLU:OE1	2.15	0.47
2:E:263:GLN:HE21	2:F:264:LYS:NZ	2.13	0.47
1:C:138:ALA:HB1	1:C:152:VAL:HG11	1.97	0.46
5:M:155:ARG:HG2	5:M:174:MET:HG3	1.97	0.46
2:G:38:ARG:HG3	2:G:39:LEU:N	2.29	0.46
1:C:253:GLU:CD	1:C:253:GLU:H	2.23	0.46
4:J:16:LEU:HA	4:J:113:MET:HE3	1.96	0.46
4:J:88:GLU:HA	4:J:108:ARG:HH12	1.80	0.46
4:J:239:ASP:OD1	4:J:239:ASP:N	2.45	0.46
5:M:77:CYS:HA	5:M:80:VAL:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:O	1:C:342:GLY:HA3	2.16	0.46
2:H:8:MET:HE3	2:H:8:MET:HB2	1.80	0.46
4:J:172:GLN:HB2	4:J:457:ILE:HG12	1.98	0.46
4:J:318:THR:HG22	4:J:319:THR:H	1.79	0.46
1:B:286:ASP:OD1	1:B:289:ILE:HD13	2.15	0.46
4:J:204:ARG:HA	4:J:204:ARG:NE	2.31	0.45
4:J:730:ILE:HD13	4:J:732:GLU:HA	1.97	0.45
5:M:110:MET:HG3	5:M:114:THR:HB	1.97	0.45
1:A:210:ARG:O	1:A:214:GLU:HG3	2.17	0.45
1:B:145:SER:O	1:B:147:ARG:NE	2.49	0.45
2:E:261:TYR:O	2:E:264:LYS:HG3	2.17	0.45
1:B:117:GLU:HB3	1:B:367:PRO:HB2	1.99	0.45
3:I:121:LYS:HD3	3:I:121:LYS:HA	1.74	0.45
1:B:333:PRO:HD2	4:J:414:GLY:H	1.82	0.45
2:F:278:LEU:HD11	2:G:1:MET:HG3	1.97	0.45
2:G:55:ASP:OD1	2:G:55:ASP:C	2.59	0.45
1:C:334:GLU:CG	4:K:413:LYS:CE	2.92	0.45
4:J:262:ASP:HB2	4:J:444:ASN:HD21	1.82	0.45
4:J:396:LEU:O	4:J:400:CYS:HB2	2.17	0.45
4:K:344:GLU:CD	4:K:344:GLU:H	2.25	0.45
1:B:168:GLY:HA2	1:C:44:MET:HE3	1.99	0.45
2:G:39:LEU:HD21	2:H:40:GLU:HG3	1.99	0.45
4:J:128:TYR:OH	4:J:676:ASN:O	2.27	0.45
1:A:169:TYR:CD2	1:B:42:GLY:HA2	2.52	0.45
1:C:143:TYR:HE2	1:D:44:MET:HB2	1.81	0.45
1:B:23:GLY:O	4:J:644:PHE:CD2	2.70	0.45
1:A:166:TYR:HD2	1:B:64:ILE:HD13	1.80	0.45
1:A:171:LEU:HG	1:B:40:HIS:NE2	2.32	0.45
2:E:250:GLU:O	2:E:253:ILE:HG22	2.17	0.45
2:G:91:ARG:CZ	2:H:92:ILE:HG21	2.47	0.45
4:K:789:GLN:NE2	5:M:161:LEU:O	2.50	0.45
1:D:44:MET:N	1:D:44:MET:SD	2.81	0.44
4:J:96:LEU:HB3	4:J:702:ILE:HG23	1.98	0.44
1:A:149:THR:HG22	1:A:167:GLU:H	1.82	0.44
2:F:277:ALA:HA	2:F:280:ASP:OD2	2.17	0.44
4:K:798:ARG:HH12	5:M:87:ASN:HD21	1.65	0.44
2:F:275:ASP:HB3	3:I:111:ARG:NH2	2.32	0.44
2:G:112:LYS:O	2:G:115:GLU:CG	2.52	0.44
1:C:113:LYS:HE2	1:C:371:HIS:CE1	2.52	0.44
4:J:364:PHE:HA	4:J:375:PRO:HA	2.00	0.44
1:B:210:ARG:O	1:B:214:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ILE:HD12	1:D:79:TRP:CZ3	2.52	0.44
1:D:312:ARG:O	1:D:316:GLU:HG2	2.17	0.44
1:A:113:LYS:HE2	1:A:371:HIS:CE1	2.53	0.44
1:B:166:TYR:CD1	1:C:64:ILE:HD12	2.53	0.44
4:J:35:LYS:HE2	4:J:35:LYS:HB2	1.78	0.44
4:K:90:MET:HE2	4:K:116:THR:HG21	2.00	0.44
4:J:186:VAL:O	4:J:190:ARG:HG3	2.17	0.44
2:H:90:ARG:NH2	2:H:91:ARG:HB2	2.33	0.44
2:G:150:GLU:O	2:G:154:ILE:HG12	2.18	0.43
2:H:94:LEU:HD13	2:H:94:LEU:HA	1.78	0.43
2:G:99:LEU:HD13	2:H:99:LEU:HA	1.99	0.43
2:G:115:GLU:CG	2:G:116:ALA:N	2.79	0.43
1:B:214:GLU:HG2	6:B:401:ADP:C2	2.53	0.43
4:J:538:CYS:HB2	4:J:598:LYS:HE2	1.99	0.43
4:K:789:GLN:HB3	5:M:165:LEU:HD11	2.01	0.43
5:M:63:ASP:CG	5:M:70:MET:H	2.26	0.43
2:F:274:LEU:HA	2:H:1:MET:SD	2.59	0.43
4:J:32:ASP:HB3	4:J:35:LYS:HB3	2.00	0.43
4:J:114:ILE:HG13	4:J:115:TYR:HD2	1.83	0.43
5:M:81:LEU:HD11	5:M:118:MET:HE1	1.99	0.43
1:C:157:ASP:OD1	6:C:401:ADP:O3'	2.27	0.43
1:D:253:GLU:H	1:D:253:GLU:CD	2.27	0.43
2:F:277:ALA:HB1	2:H:5:LYS:HE3	2.01	0.43
4:J:21:LYS:HA	4:J:21:LYS:HD3	1.65	0.43
1:B:167:GLU:C	1:C:47:MET:CE	2.92	0.43
1:C:131:ALA:HB1	1:C:356:TRP:HB3	2.01	0.43
5:M:118:MET:HE3	5:M:118:MET:HB3	1.97	0.43
2:F:260:LEU:O	2:F:264:LYS:HG2	2.19	0.43
1:A:19:ALA:HB1	1:A:94:LEU:HD11	1.99	0.43
1:A:331:ALA:HB1	1:A:335:ARG:HE	1.83	0.43
2:E:281:MET:SD	2:H:4:ILE:HG23	2.59	0.42
2:F:268:LYS:HE3	3:I:118:VAL:HG23	2.01	0.42
2:G:50:LEU:HA	2:H:50:LEU:HD13	2.00	0.42
1:A:117:GLU:HB3	1:A:367:PRO:HB2	2.01	0.42
1:B:322:PRO:HG2	1:C:244:ASP:O	2.19	0.42
1:C:61:LYS:HD2	1:C:61:LYS:N	2.34	0.42
1:A:115:ASN:O	1:A:115:ASN:ND2	2.52	0.42
1:A:169:TYR:OH	1:B:49:GLN:HB2	2.20	0.42
1:B:28:ARG:NH1	4:J:637:LYS:O	2.52	0.42
1:C:144:ALA:HB2	1:C:342:GLY:N	2.33	0.42
1:C:146:GLY:HA2	4:K:541:PRO:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:278:LEU:HB3	2:G:3:ALA:HB3	2.01	0.42
1:A:369:ILE:HD12	1:A:372:ARG:HD3	2.00	0.42
1:B:171:LEU:HD22	1:C:40:HIS:CD2	2.54	0.42
2:E:281:MET:HE3	2:G:8:MET:HB2	2.00	0.42
2:H:90:ARG:HH22	2:H:91:ARG:HB2	1.84	0.42
2:F:256:LEU:HD23	2:F:256:LEU:HA	1.88	0.42
4:J:568:ASN:HD21	4:K:635:LYS:HE2	1.84	0.42
2:G:148:LEU:HD12	2:H:148:LEU:HA	2.02	0.42
4:J:771:GLY:O	4:J:775:GLU:HG2	2.20	0.42
1:C:333:PRO:HD2	4:K:414:GLY:H	1.84	0.42
2:G:54:GLU:CD	2:G:54:GLU:C	2.87	0.42
4:J:238:ASN:HD22	4:J:238:ASN:HA	1.61	0.42
4:K:43:LYS:NZ	4:K:43:LYS:CB	2.81	0.42
5:M:189:PHE:O	5:M:193:ILE:HG12	2.20	0.42
1:A:123:MET:HA	1:A:127:PHE:HB2	2.02	0.42
1:D:222:ASP:O	1:D:226:GLU:HG2	2.20	0.42
4:K:700:GLU:CD	4:K:703:ARG:HE	2.27	0.42
1:B:337:TYR:CE2	4:J:406:VAL:HG11	2.54	0.42
1:D:189:LEU:HD12	1:D:192:ILE:HD11	2.02	0.42
2:G:47:GLN:HB3	2:G:51:LYS:NZ	2.35	0.42
2:H:145:GLU:HG2	2:H:149:LYS:HZ3	1.85	0.42
3:I:126:LYS:HE3	3:I:126:LYS:HB3	1.80	0.42
1:C:119:MET:O	1:C:123:MET:HG2	2.20	0.42
1:C:351:THR:HG1	4:K:536:GLU:CD	2.27	0.42
2:H:145:GLU:HG2	2:H:149:LYS:NZ	2.34	0.42
4:J:730:ILE:HG12	4:J:731:PRO:N	2.35	0.42
5:M:78:GLY:O	5:M:82:ARG:HG3	2.20	0.42
1:A:214:GLU:OE1	6:A:401:ADP:N6	2.53	0.41
1:C:118:LYS:HE3	1:C:118:LYS:HB3	1.88	0.41
4:J:390:LEU:HD13	4:J:395:LEU:HD13	2.01	0.41
1:A:238:LYS:HG3	1:A:239:SER:H	1.85	0.41
1:C:213:LYS:HA	1:C:217:CYS:SG	2.60	0.41
1:C:23:GLY:O	4:K:644:PHE:CE1	2.73	0.41
2:G:11:LEU:HD21	2:H:12:LYS:HG3	2.03	0.41
4:J:93:LEU:HG	4:J:95:PHE:H	1.85	0.41
4:J:284:HIS:HD1	4:J:288:GLN:HE21	1.66	0.41
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.03	0.41
1:B:23:GLY:HA2	4:J:644:PHE:CE1	2.55	0.41
1:C:311:ASP:OD2	2:H:90:ARG:NH2	2.53	0.41
2:G:33:GLU:O	2:G:37:LYS:HG2	2.21	0.41
2:H:62:GLU:OE1	2:H:62:GLU:CA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:537:GLU:OE2	4:J:551:LYS:HG3	2.21	0.41
4:J:798:ARG:NH1	5:L:195:ALA:O	2.35	0.41
4:K:793:ARG:NH1	5:M:90:GLN:OE1	2.47	0.41
1:C:253:GLU:HA	1:C:256:ARG:HB2	2.01	0.41
1:D:226:GLU:HG2	1:D:226:GLU:H	1.74	0.41
4:K:217:GLU:CD	4:K:217:GLU:H	2.28	0.41
5:M:111:ASP:OD1	5:M:112:PHE:N	2.40	0.41
1:B:27:PRO:HG2	4:J:406:VAL:HG23	2.02	0.41
2:F:268:LYS:HD2	3:I:114:GLU:HB3	2.02	0.41
2:G:111:GLN:OE1	2:G:111:GLN:HA	2.21	0.41
2:H:20:ASP:OD1	2:H:21:ARG:N	2.53	0.41
2:H:47:GLN:HE21	2:H:47:GLN:HB2	1.57	0.41
2:H:93:GLN:HG2	2:H:94:LEU:CD2	2.49	0.41
2:H:150:GLU:O	2:H:154:ILE:HG13	2.21	0.41
4:J:194:TYR:O	4:J:198:ILE:HG12	2.21	0.41
4:J:538:CYS:O	4:J:598:LYS:NZ	2.48	0.41
4:J:545:ASP:N	4:J:545:ASP:OD1	2.53	0.41
4:J:791:GLN:HA	5:L:87:ASN:ND2	2.36	0.41
1:A:79:TRP:CH2	1:A:118:LYS:HB2	2.56	0.41
2:G:126:GLY:O	2:G:130:ILE:HG13	2.21	0.40
4:J:28:THR:HG21	5:L:156:HIS:HE1	1.86	0.40
1:A:17:VAL:HG23	1:A:33:SER:HB3	2.04	0.40
2:G:96:GLU:CD	2:G:96:GLU:C	2.90	0.40
1:B:253:GLU:HA	1:B:256:ARG:HG3	2.02	0.40
1:B:350:SER:C	4:J:536:GLU:OE2	2.64	0.40
4:J:670:VAL:O	4:J:671:ARG:NH1	2.51	0.40
4:J:129:LYS:HG2	4:J:130:TRP:H	1.87	0.40
4:K:603:GLU:HA	4:K:606:VAL:HG12	2.04	0.40
1:B:4:GLU:O	1:B:6:THR:HG23	2.22	0.40
1:C:47:MET:HA	4:J:540:PHE:CE1	2.57	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%)	352 (94%)	21 (6%)	0	100	100
1	B	373/377 (99%)	357 (96%)	15 (4%)	1 (0%)	36	71
1	C	373/377 (99%)	348 (93%)	25 (7%)	0	100	100
1	D	373/377 (99%)	355 (95%)	18 (5%)	0	100	100
2	E	33/284 (12%)	33 (100%)	0	0	100	100
2	F	33/284 (12%)	33 (100%)	0	0	100	100
2	G	153/284 (54%)	153 (100%)	0	0	100	100
2	H	153/284 (54%)	153 (100%)	0	0	100	100
3	I	45/285 (16%)	45 (100%)	0	0	100	100
4	J	803/1935 (42%)	763 (95%)	38 (5%)	2 (0%)	43	77
4	K	803/1935 (42%)	747 (93%)	55 (7%)	1 (0%)	48	83
5	L	151/196 (77%)	141 (93%)	9 (6%)	1 (1%)	18	55
5	M	151/196 (77%)	145 (96%)	6 (4%)	0	100	100
All	All	3817/7191 (53%)	3625 (95%)	187 (5%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLU
4	J	615	LYS
5	L	102	GLN
4	K	638	ALA
4	J	46	PHE

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%)	311 (98%)	7 (2%)	45	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	318/320 (99%)	310 (98%)	8 (2%)	42	62
1	C	318/320 (99%)	308 (97%)	10 (3%)	35	56
1	D	318/320 (99%)	305 (96%)	13 (4%)	27	49
2	E	32/245 (13%)	30 (94%)	2 (6%)	16	38
2	F	32/245 (13%)	29 (91%)	3 (9%)	8	26
2	G	130/245 (53%)	124 (95%)	6 (5%)	24	46
2	H	130/245 (53%)	127 (98%)	3 (2%)	44	63
3	I	45/249 (18%)	44 (98%)	1 (2%)	45	64
4	J	695/1697 (41%)	667 (96%)	28 (4%)	28	49
4	K	695/1697 (41%)	680 (98%)	15 (2%)	45	64
5	L	133/163 (82%)	127 (96%)	6 (4%)	24	46
5	M	133/163 (82%)	129 (97%)	4 (3%)	36	57
All	All	3297/6229 (53%)	3191 (97%)	106 (3%)	35	55

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	44	MET
1	A	115	ASN
1	A	147	ARG
1	A	152	VAL
1	A	360	GLN
1	A	370	VAL
1	B	49	GLN
1	B	82	MET
1	B	96	VAL
1	B	140	LEU
1	B	152	VAL
1	B	165	ILE
1	B	373	LYS
1	B	375	PHE
1	C	5	THR
1	C	49	GLN
1	C	51	ASP
1	C	56	ASP
1	C	59	GLN
1	C	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	140	LEU
1	C	192	ILE
1	C	202	THR
1	C	218	TYR
1	D	44	MET
1	D	47	MET
1	D	59	GLN
1	D	80	ASP
1	D	140	LEU
1	D	152	VAL
1	D	183	ARG
1	D	185	LEU
1	D	194	THR
1	D	218	TYR
1	D	225	ASN
1	D	306	TYR
1	D	318	THR
2	E	253	ILE
2	E	284	ILE
2	F	253	ILE
2	F	274	LEU
2	F	284	ILE
2	G	1	MET
2	G	9	GLN
2	G	24	GLN
2	G	60	TYR
2	G	113	LEU
2	G	141	MET
2	H	47	GLN
2	H	60	TYR
2	H	88	LEU
3	I	107	HIS
4	J	63	THR
4	J	67	LYS
4	J	83	LYS
4	J	101	VAL
4	J	184	LYS
4	J	265	THR
4	J	284	HIS
4	J	304	THR
4	J	318	THR
4	J	344	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	369	ARG
4	J	378	THR
4	J	406	VAL
4	J	412	THR
4	J	437	ASN
4	J	448	GLU
4	J	453	ARG
4	J	509	GLU
4	J	587	ASP
4	J	602	ASN
4	J	603	GLU
4	J	615	LYS
4	J	631	VAL
4	J	660	THR
4	J	678	THR
4	J	704	ILE
4	J	730	ILE
4	J	752	ASP
4	K	17	ARG
4	K	32	ASP
4	K	37	VAL
4	K	43	LYS
4	K	62	GLU
4	K	88	GLU
4	K	156	SER
4	K	205	SER
4	K	305	ASN
4	K	339	LEU
4	K	406	VAL
4	K	447	LEU
4	K	470	PHE
4	K	587	ASP
4	K	633	LYS
5	L	43	ILE
5	L	94	LEU
5	L	103	GLU
5	L	130	THR
5	L	138	LEU
5	L	139	ARG
5	M	109	MET
5	M	125	ASN
5	M	139	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	181	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	59	GLN
1	A	92	ASN
1	A	275	HIS
1	B	49	GLN
1	B	275	HIS
1	B	297	ASN
1	B	314	GLN
1	C	40	HIS
1	C	101	HIS
1	D	40	HIS
1	D	128	ASN
1	D	137	GLN
2	E	263	GLN
2	G	9	GLN
2	G	17	ASN
2	G	24	GLN
2	G	68	GLN
2	G	93	GLN
2	G	144	GLN
2	G	147	GLN
2	H	9	GLN
2	H	47	GLN
2	H	93	GLN
2	H	153	HIS
3	I	98	ASN
4	J	163	GLN
4	J	171	ASN
4	J	238	ASN
4	J	288	GLN
4	J	358	HIS
4	J	555	ASN
4	J	581	HIS
4	J	623	ASN
4	J	711	ASN
4	J	791	GLN
4	K	126	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	224	ASN
4	K	276	GLN
4	K	358	HIS
4	K	368	GLN
4	K	372	GLN
4	K	482	ASN
4	K	492	HIS
4	K	562	ASN
4	K	619	ASN
4	K	696	ASN
5	L	87	ASN
5	L	121	HIS
5	L	156	HIS
5	L	177	GLN

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	B	401	7	28,29,29	1.38	4 (14%)	43,45,45	1.81	7 (16%)
6	ADP	A	401	7	28,29,29	1.39	5 (17%)	43,45,45	1.78	9 (20%)
6	ADP	D	401	7	28,29,29	1.37	4 (14%)	43,45,45	1.75	7 (16%)
6	ADP	C	401	7	28,29,29	1.38	4 (14%)	43,45,45	1.81	7 (16%)

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
6	ADP	B	401	7	-	3/16/32/32	0/3/3/3
6	ADP	A	401	7	-	4/16/32/32	0/3/3/3
6	ADP	D	401	7	-	3/16/32/32	0/3/3/3
6	ADP	C	401	7	-	2/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	ADP	C5-C4	4.59	1.47	1.39
6	B	401	ADP	C5-C4	4.53	1.47	1.39
6	D	401	ADP	C5-C4	4.46	1.47	1.39
6	A	401	ADP	C5-C4	4.35	1.46	1.39
6	A	401	ADP	C5-C6	2.69	1.48	1.41
6	B	401	ADP	C5-C6	2.67	1.48	1.41
6	C	401	ADP	C5-C6	2.64	1.48	1.41
6	D	401	ADP	C5-C6	2.61	1.48	1.41
6	D	401	ADP	C5-N7	-2.46	1.34	1.39
6	C	401	ADP	C5-N7	-2.45	1.34	1.39
6	B	401	ADP	C5-N7	-2.41	1.34	1.39
6	A	401	ADP	C5-N7	-2.37	1.34	1.39
6	B	401	ADP	C8-N7	2.27	1.36	1.31
6	A	401	ADP	C8-N7	2.24	1.36	1.31
6	C	401	ADP	C8-N7	2.12	1.35	1.31
6	D	401	ADP	C8-N7	2.12	1.35	1.31
6	A	401	ADP	C4-N9	-2.09	1.33	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	401	ADP	C5-C4-N3	-6.04	118.40	126.72
6	C	401	ADP	C5-C4-N3	-6.01	118.44	126.72
6	D	401	ADP	C5-C4-N3	-5.89	118.61	126.72
6	A	401	ADP	C5-C4-N3	-5.55	119.07	126.72
6	C	401	ADP	N3-C4-N9	4.75	135.24	127.17
6	B	401	ADP	N3-C4-N9	4.72	135.20	127.17
6	D	401	ADP	N3-C4-N9	4.66	135.09	127.17
6	A	401	ADP	N3-C4-N9	4.43	134.69	127.17
6	C	401	ADP	C2-N3-C4	3.70	120.88	111.83
6	B	401	ADP	C2-N3-C4	3.68	120.82	111.83
6	D	401	ADP	C2-N3-C4	3.68	120.81	111.83
6	A	401	ADP	C2-N3-C4	3.63	120.71	111.83
6	C	401	ADP	C4-C5-N7	-3.50	106.58	110.58
6	B	401	ADP	C4-C5-N7	-3.50	106.58	110.58
6	A	401	ADP	C4-C5-N7	-3.47	106.62	110.58
6	D	401	ADP	C4-C5-N7	-3.22	106.90	110.58
6	A	401	ADP	N3-C2-N1	-3.20	123.73	128.58
6	D	401	ADP	N3-C2-N1	-3.11	123.87	128.58
6	C	401	ADP	N3-C2-N1	-3.10	123.89	128.58
6	A	401	ADP	C4-N9-C8	3.04	108.93	105.74
6	B	401	ADP	N3-C2-N1	-2.98	124.07	128.58
6	A	401	ADP	C5-N7-C8	2.70	107.69	103.45
6	C	401	ADP	C5-N7-C8	2.58	107.50	103.45
6	B	401	ADP	C5-N7-C8	2.55	107.47	103.45
6	B	401	ADP	C4-N9-C8	2.44	108.30	105.74
6	C	401	ADP	C4-N9-C8	2.42	108.28	105.74
6	A	401	ADP	N9-C8-N7	-2.40	110.53	113.94
6	D	401	ADP	C4-N9-C8	2.38	108.24	105.74
6	D	401	ADP	C5-N7-C8	2.31	107.08	103.45
6	A	401	ADP	C6-C5-N7	2.29	136.50	132.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

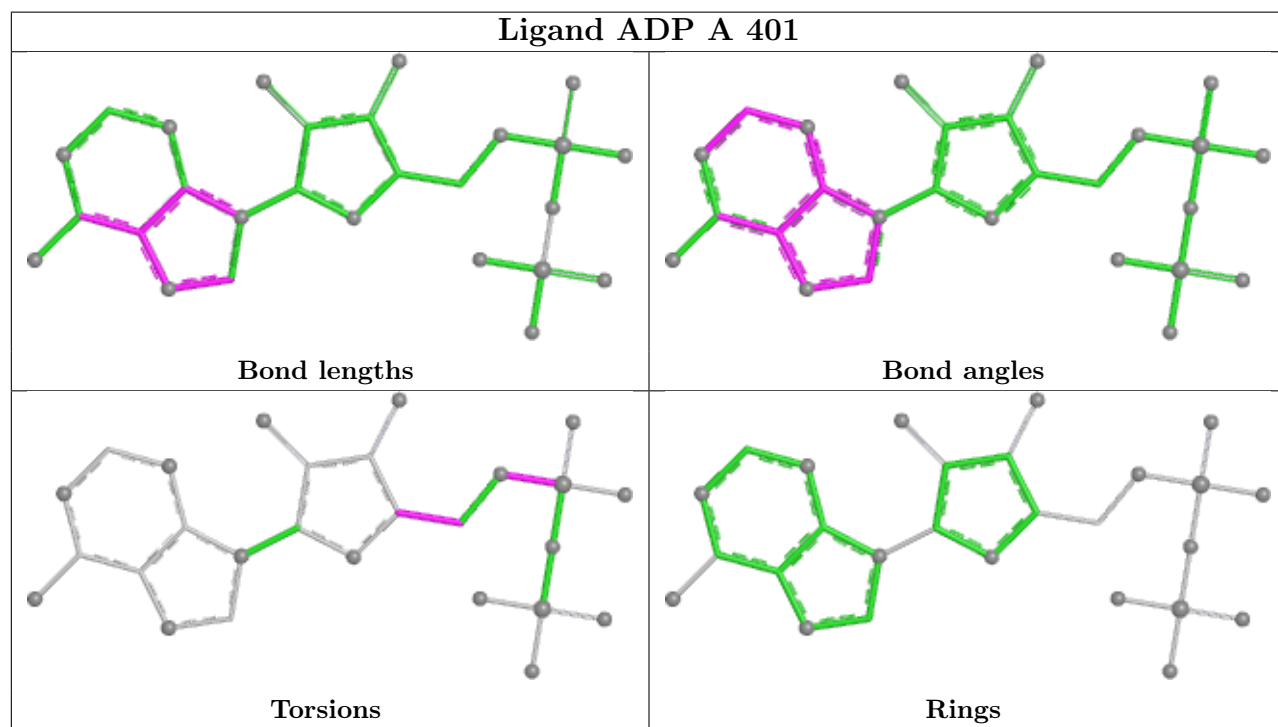
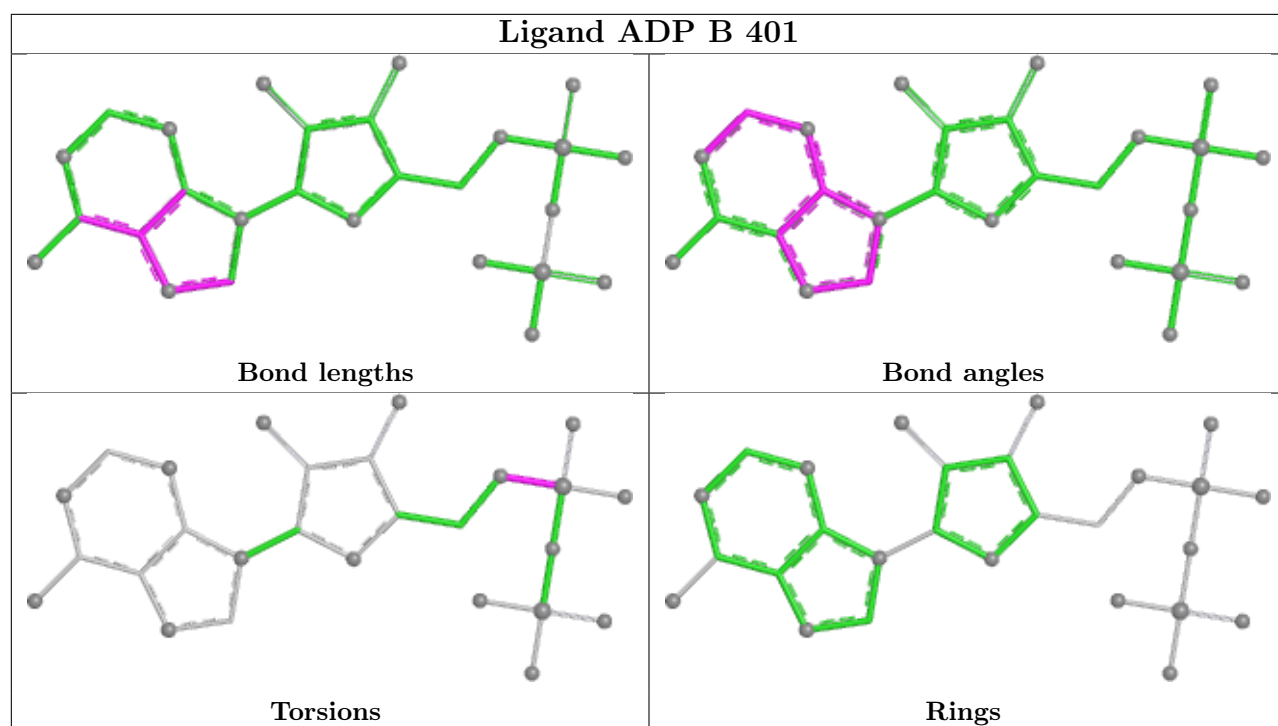
Mol	Chain	Res	Type	Atoms
6	D	401	ADP	C3'-C4'-C5'-O5'
6	B	401	ADP	C5'-O5'-PA-O1A
6	C	401	ADP	C5'-O5'-PA-O1A
6	D	401	ADP	C5'-O5'-PA-O1A

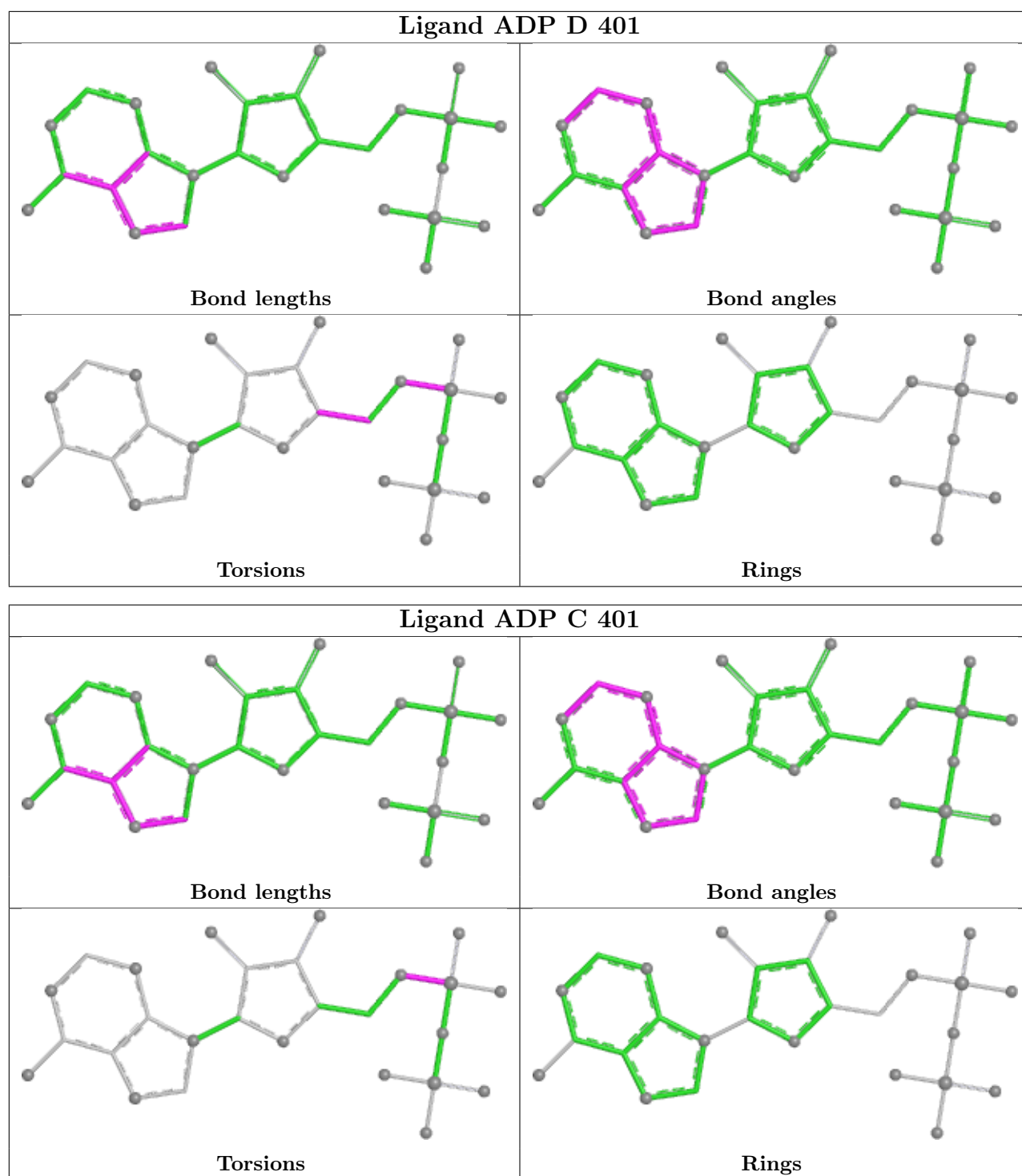
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	401	ADP	1	0
6	A	401	ADP	1	0
6	C	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-73042. These allow visual inspection of the internal detail of the map and identification of artifacts.

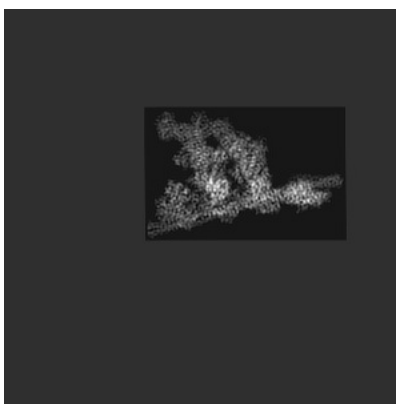
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

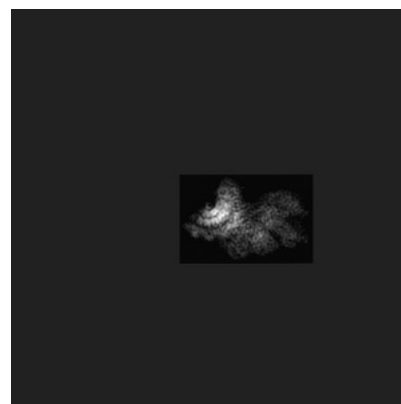
6.1.1 Primary map



X

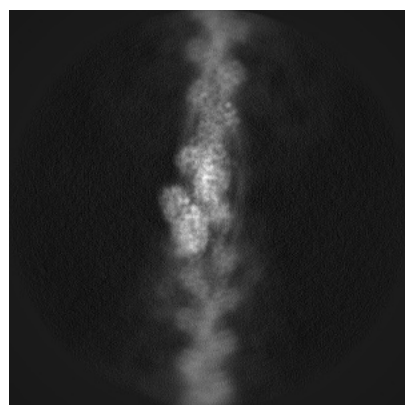


Y

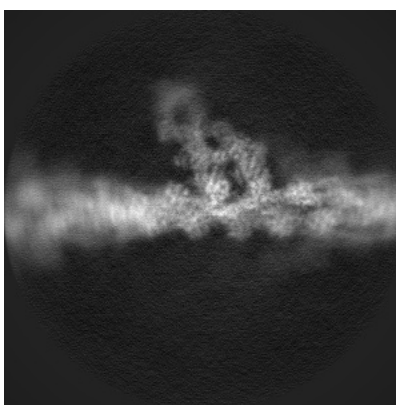


Z

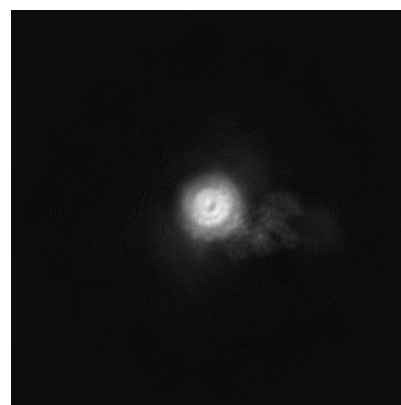
6.1.2 Raw map



X



Y



Z

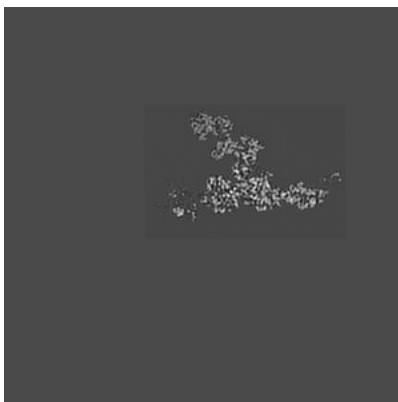
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 198

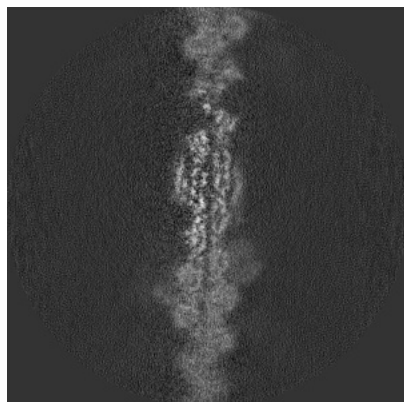


Y Index: 198

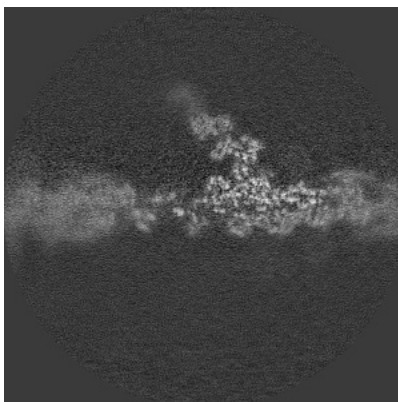


Z Index: 198

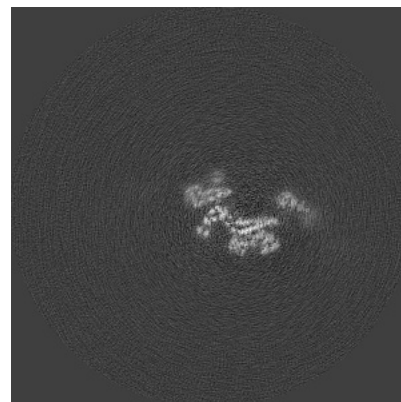
6.2.2 Raw map



X Index: 198



Y Index: 198

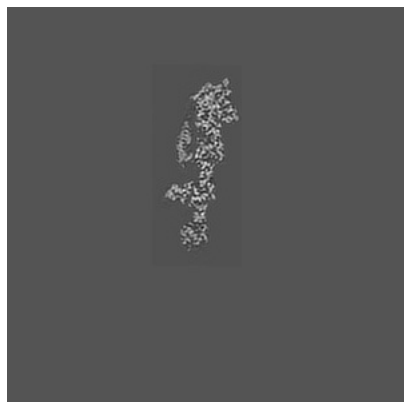


Z Index: 198

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: 211

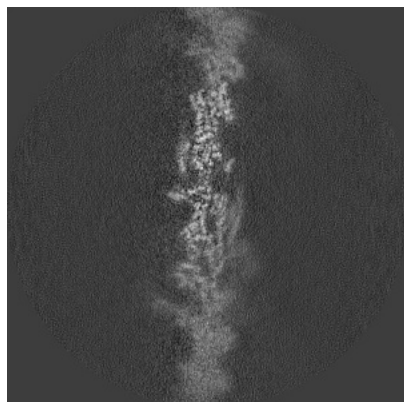


Y Index: 193

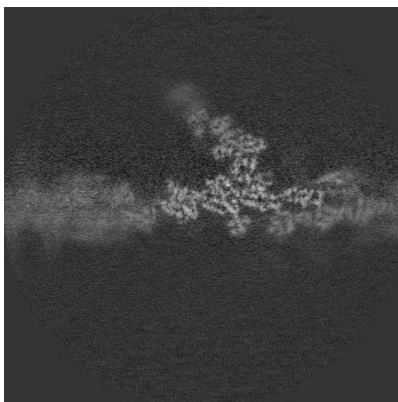


Z Index: 208

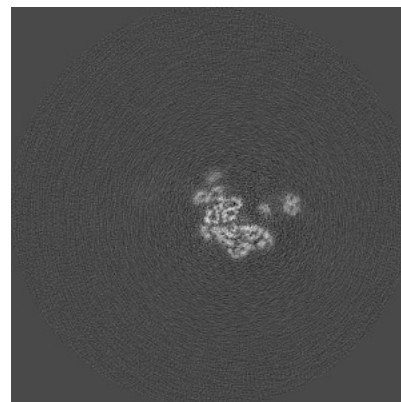
6.3.2 Raw map



X Index: 207



Y Index: 194

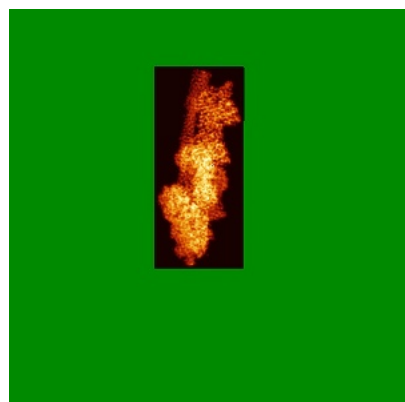


Z Index: 207

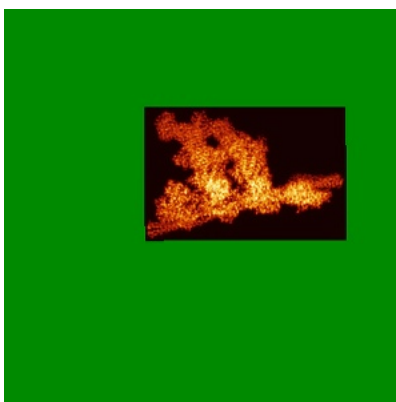
The images above show the largest variance slices of the map in three orthogonal directions.

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

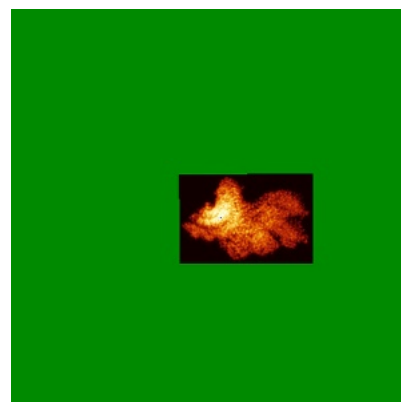
6.4.1 Primary map



X

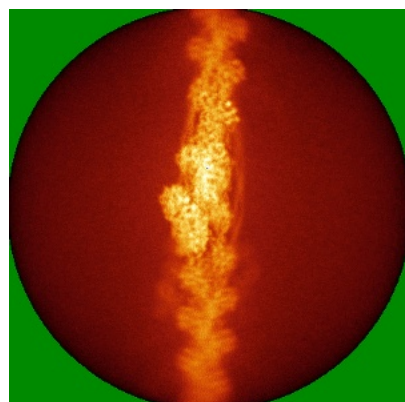


Y

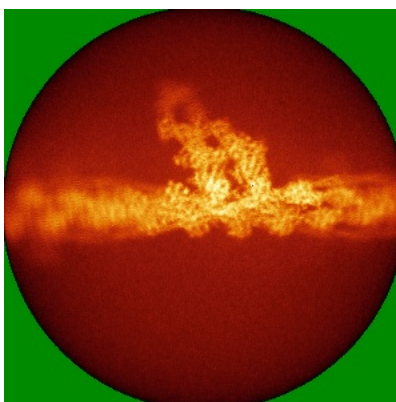


Z

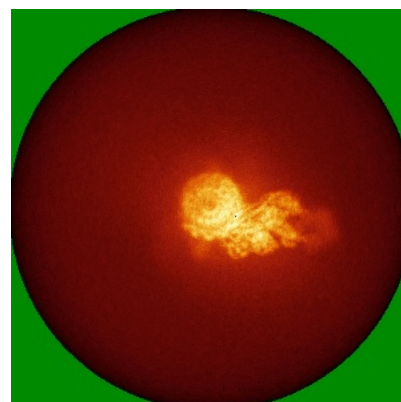
6.4.2 Raw map



X



Y

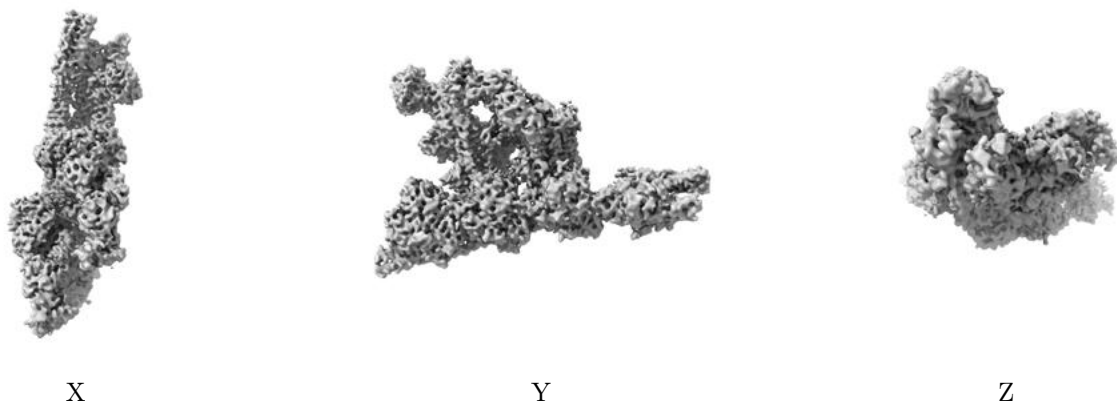


Z

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.

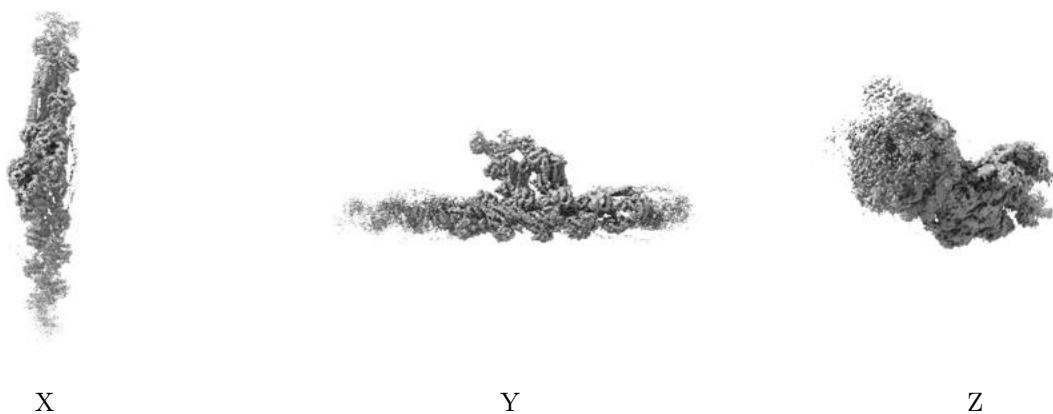
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.05. 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.

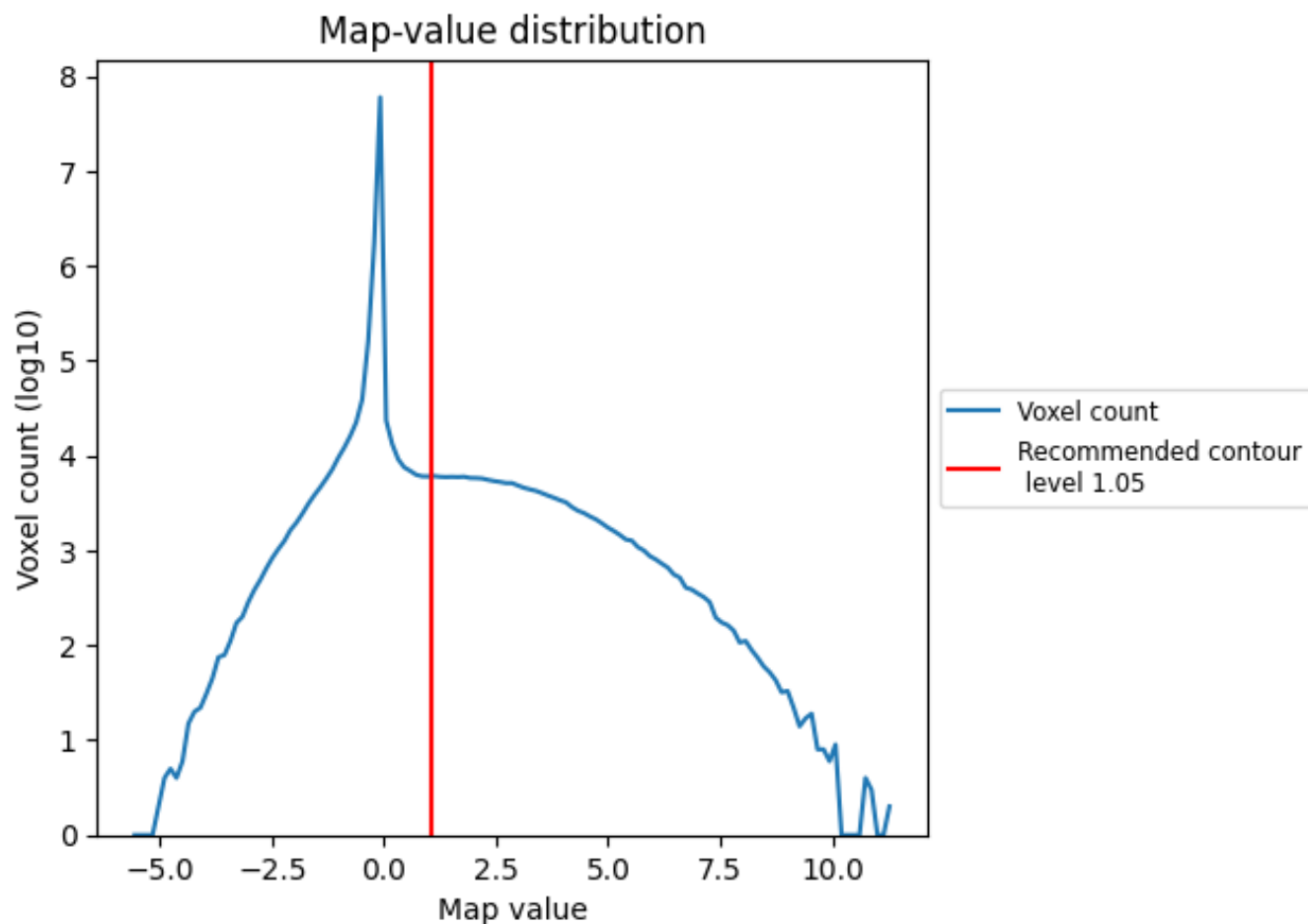
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

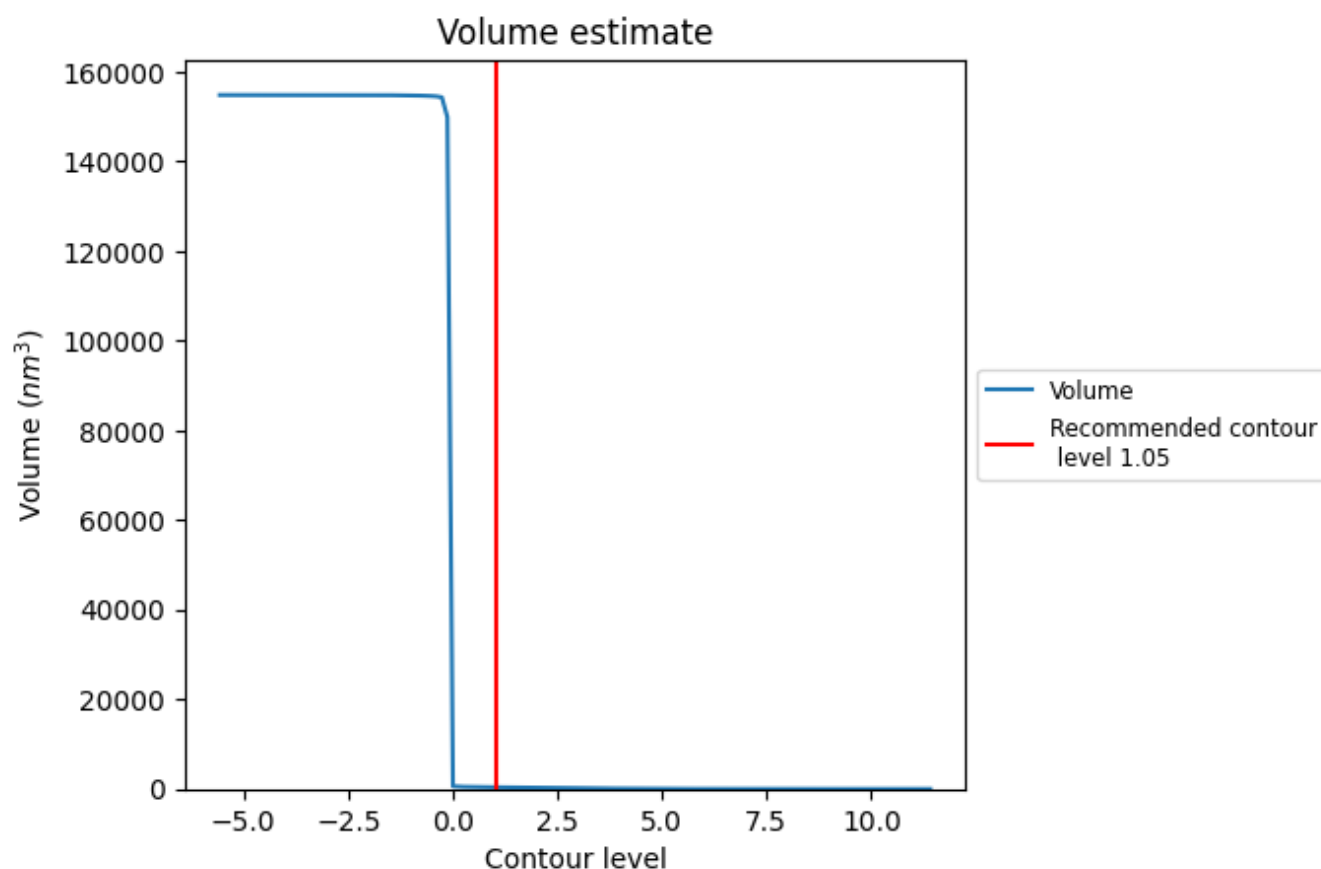
This section contains the results of statistical analysis of the map.

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.

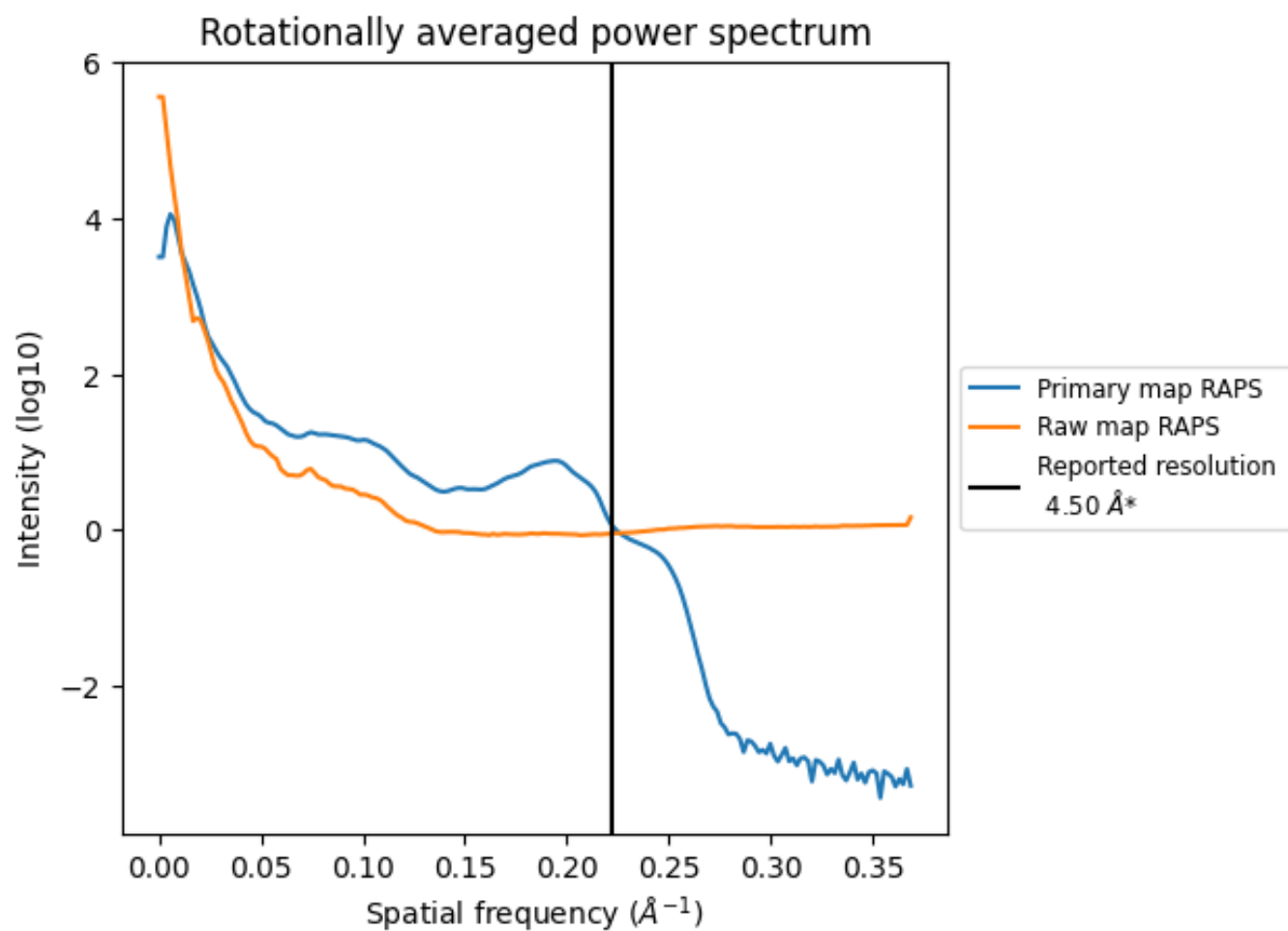
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 374 nm³; this corresponds to an approximate mass of 337 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 ⓘ

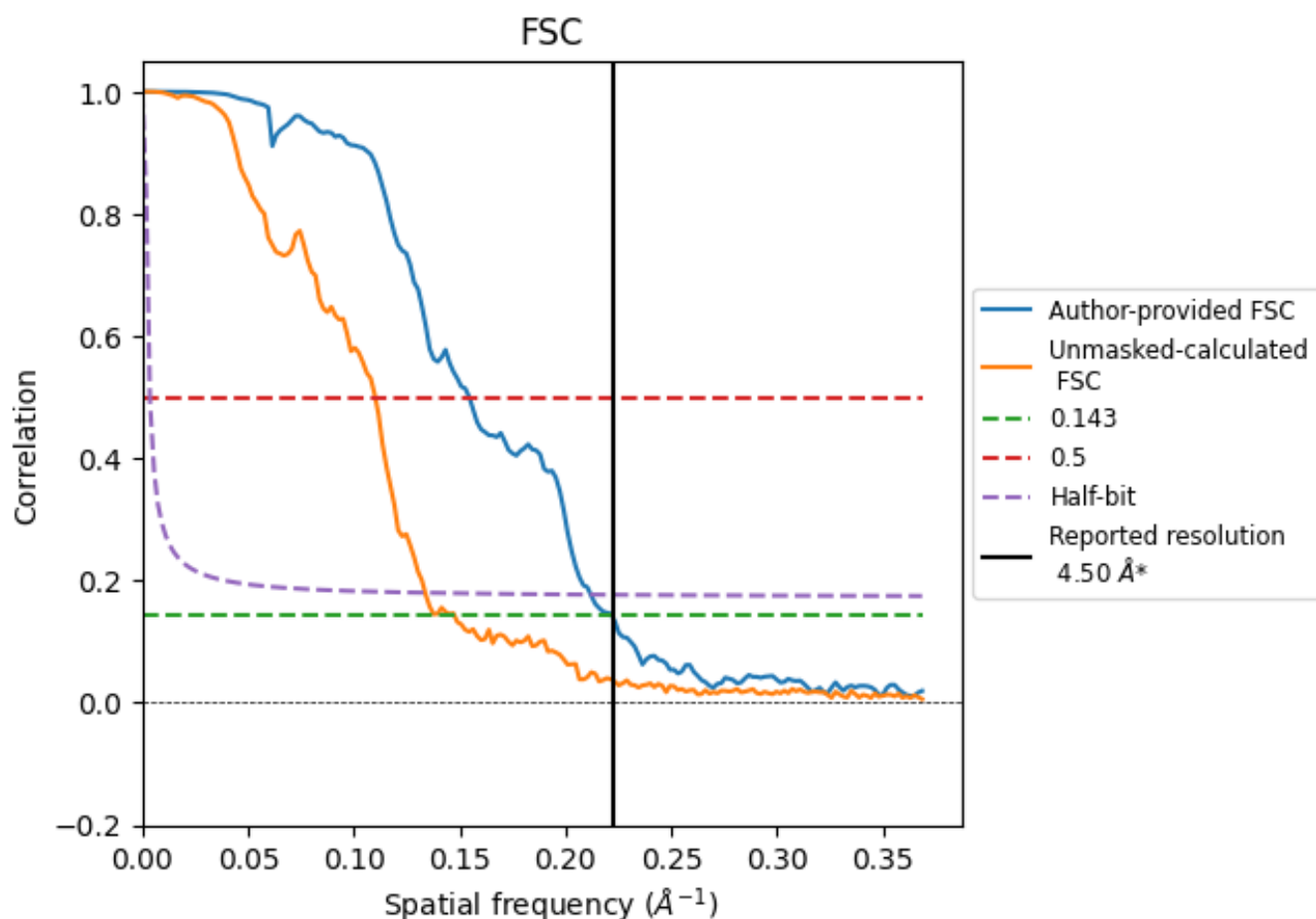


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

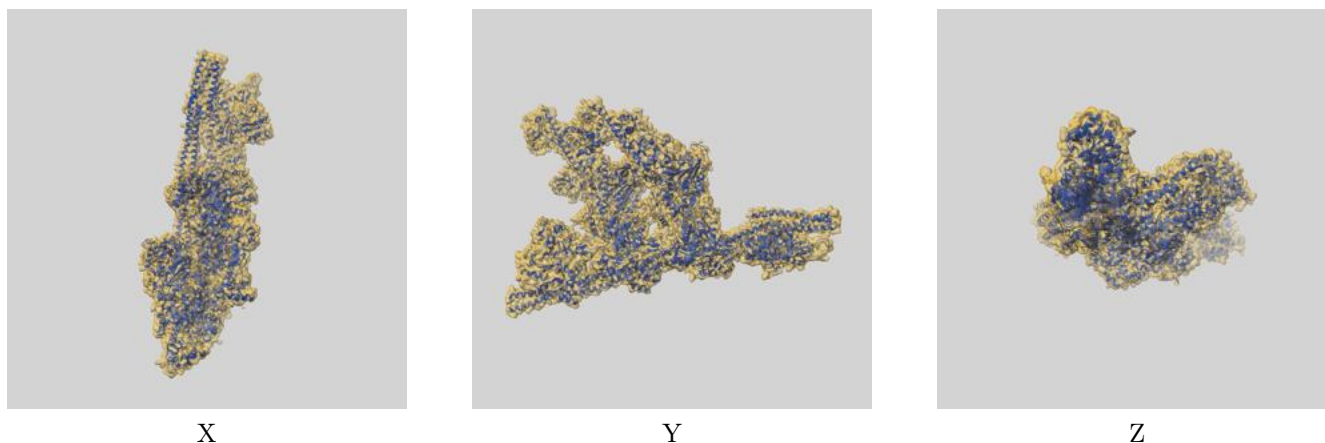
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.47	4.71
Unmasked-calculated*	6.78	9.08	7.47

*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 6.78 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

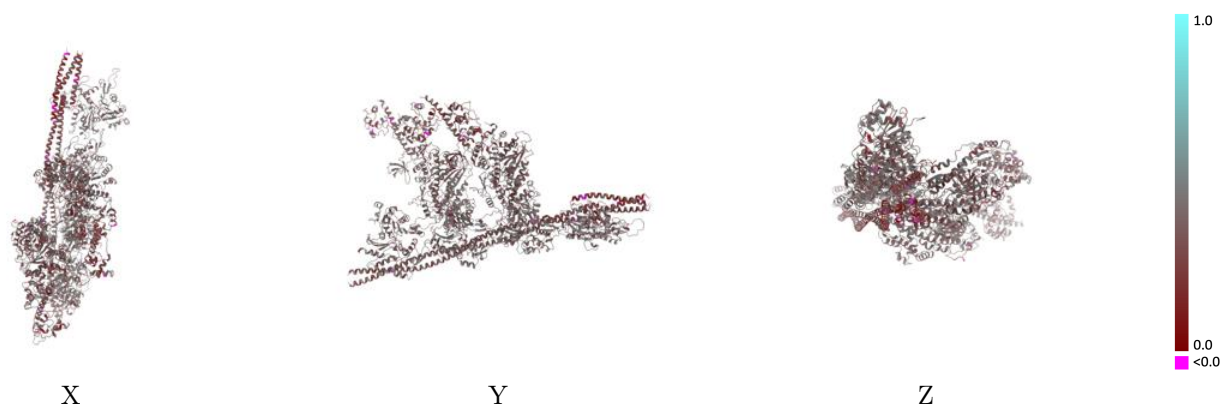
This section contains information regarding the fit between EMDB map EMD-73042 and PDB model 9YK9. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



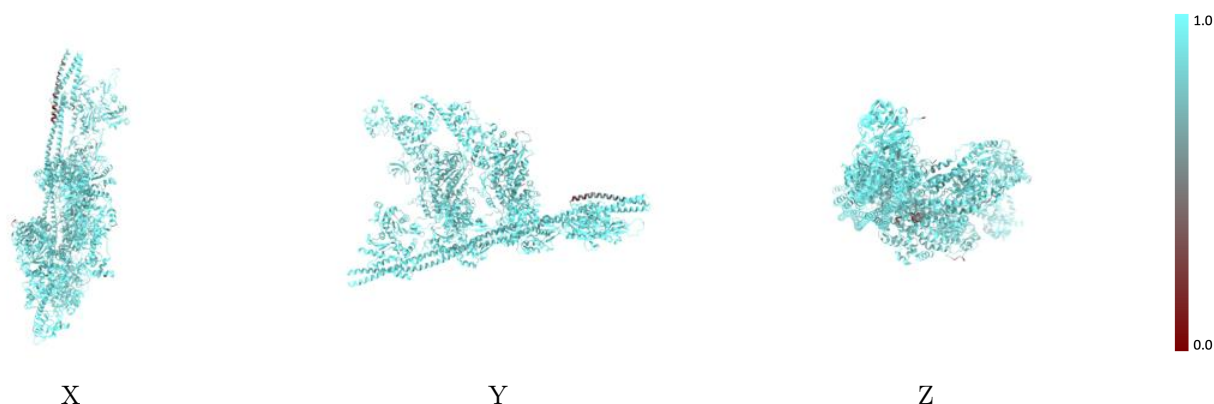
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



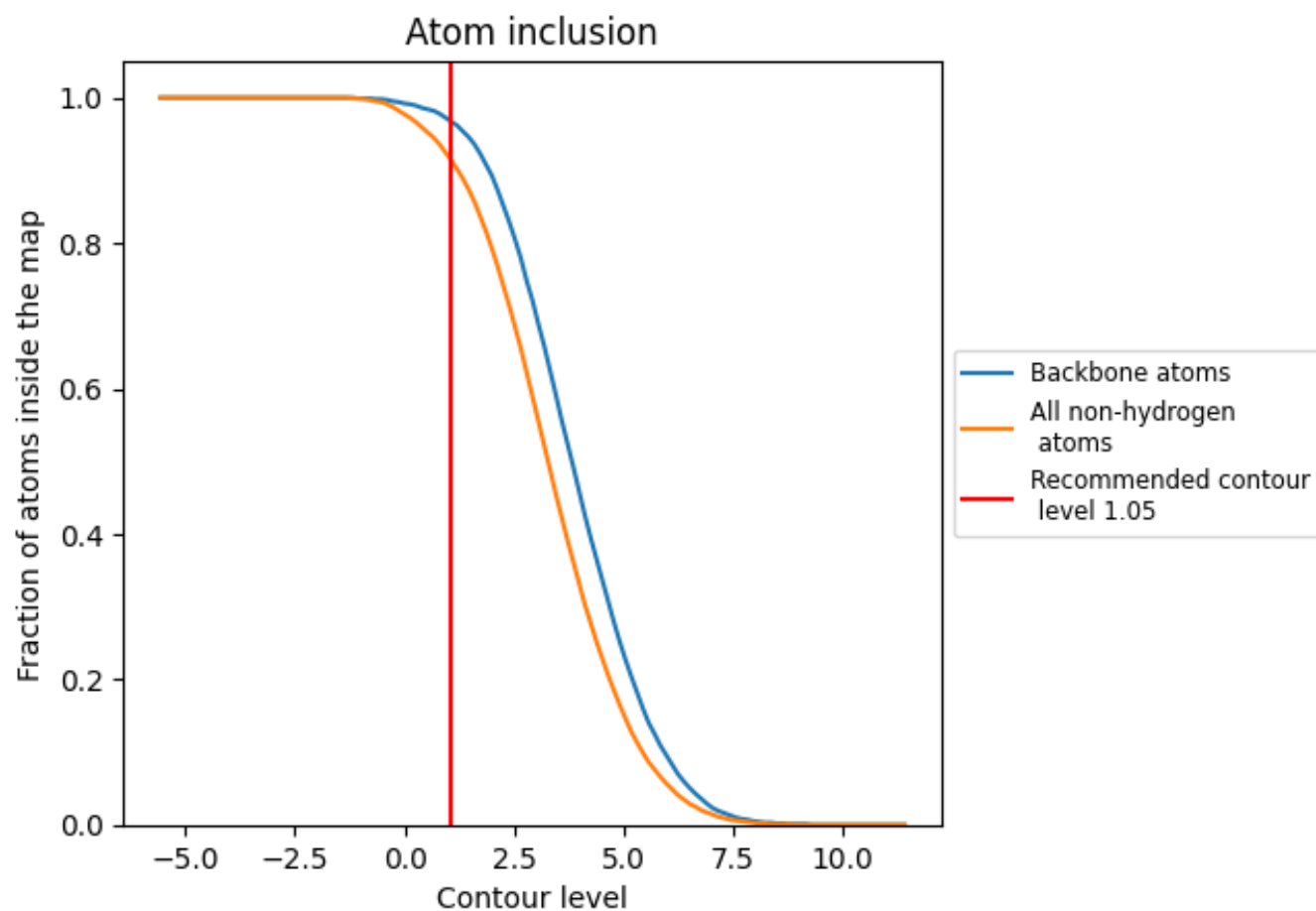
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.3700
A	 0.9460	 0.4050
B	 0.9240	 0.3970
C	 0.9270	 0.4130
D	 0.9390	 0.4020
E	 0.9120	 0.2370
F	 0.8300	 0.2590
G	 0.9230	 0.3120
H	 0.8880	 0.2720
I	 0.5580	 0.1870
J	 0.9090	 0.3680
K	 0.9190	 0.3730
L	 0.8990	 0.3290
M	 0.9220	 0.3440

