



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID : 6CP7 / pdb_00006cp7
EMDB ID : EMD-7549
Title : Monomer yeast ATP synthase Fo reconstituted in nanodisc generated from masked refinement.
Authors : Srivastava, A.P.; Luo, M.; Symersky, J.; Liao, M.F.; Mueller, D.M.
Deposited on : 2018-03-13
Resolution : 4.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

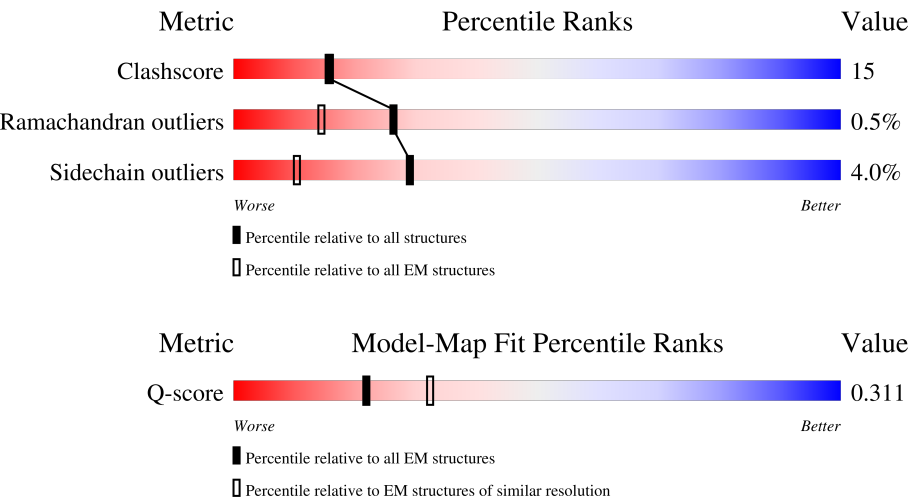
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	K	76	49% 64% 30% ..
1	L	76	39% 49% 42% 7% .
1	M	76	39% 59% 37% ..
1	N	76	16% 75% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	O	76	
1	P	76	
1	Q	76	
1	R	76	
1	S	76	
1	T	76	
2	8	48	
3	X	249	
4	Z	209	
5	7	173	
6	U	95	
7	J	37	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9164 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 ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	74	Total	C	N	O	S	0	0
			534	358	82	90	4		
1	L	74	Total	C	N	O	S	0	0
			529	353	82	91	3		
1	M	75	Total	C	N	O	S	0	0
			535	358	83	91	3		
1	N	74	Total	C	N	O	S	0	0
			532	356	82	91	3		
1	O	74	Total	C	N	O	S	0	0
			533	357	82	91	3		
1	P	74	Total	C	N	O	S	0	0
			529	352	82	91	4		
1	Q	74	Total	C	N	O	S	0	0
			522	347	82	90	3		
1	R	75	Total	C	N	O	S	0	0
			534	356	83	92	3		
1	S	74	Total	C	N	O	S	0	0
			532	356	82	91	3		
1	T	74	Total	C	N	O	S	0	0
			533	357	82	91	3		

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	42	Total	C	N	O	S	0	0
			364	256	52	53	3		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	224	Total	C	N	O	S	0	0
			1760	1198	265	287	10		

- Molecule 4 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	54	Total	C	N	O	S	0	0
			393	253	64	75	1		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	67	Total	C	N	O	S	0	0
			520	329	86	103	2		

- Molecule 6 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	68	Total	C	N	O	S	0	0
			522	346	89	86	1		

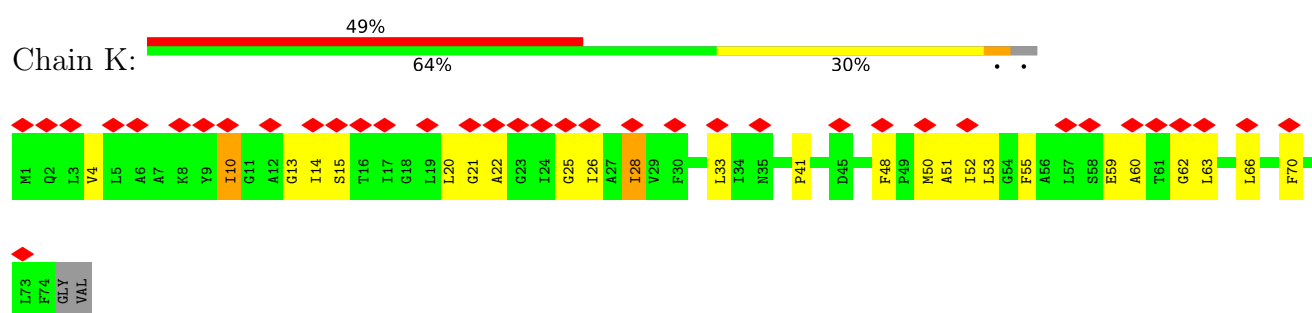
- Molecule 7 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			292	197	45	48	2		

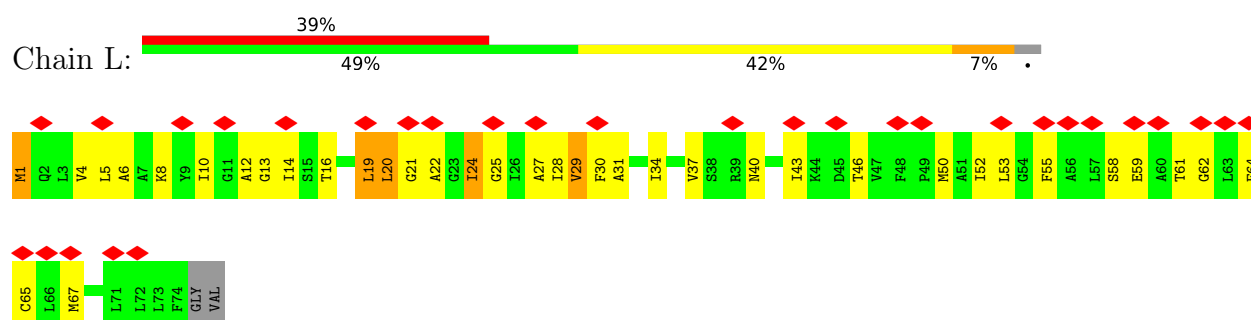
3 Residue-property plots [i](#)

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.

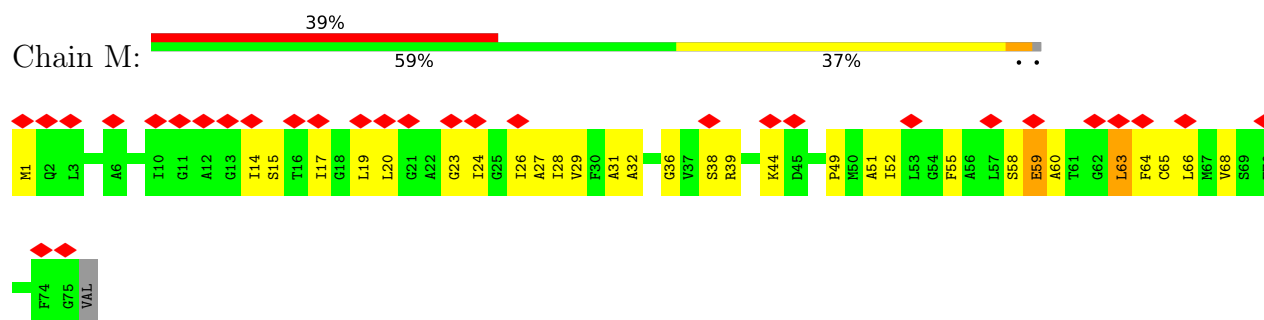
- Molecule 1: ATP synthase subunit 9, mitochondrial



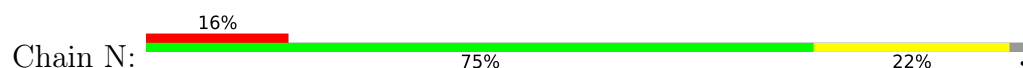
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

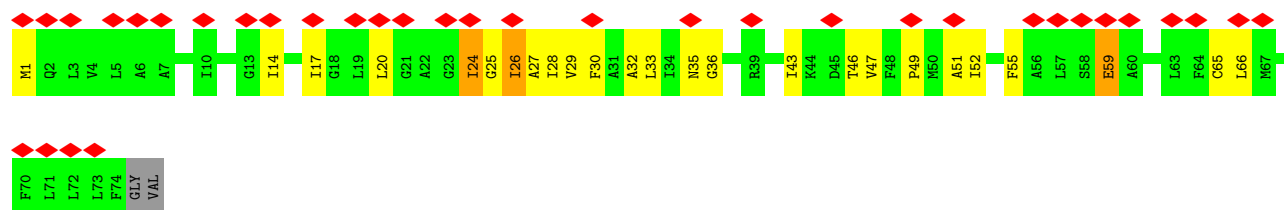


- Molecule 1: ATP synthase subunit 9, mitochondrial

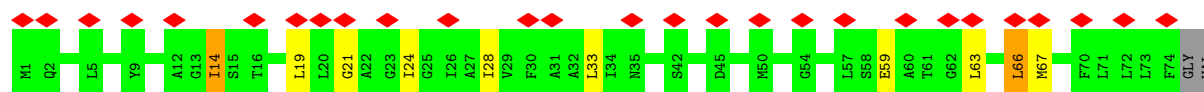
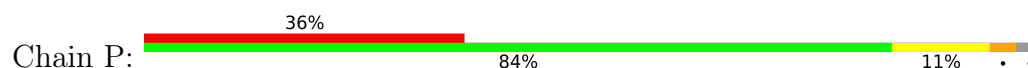




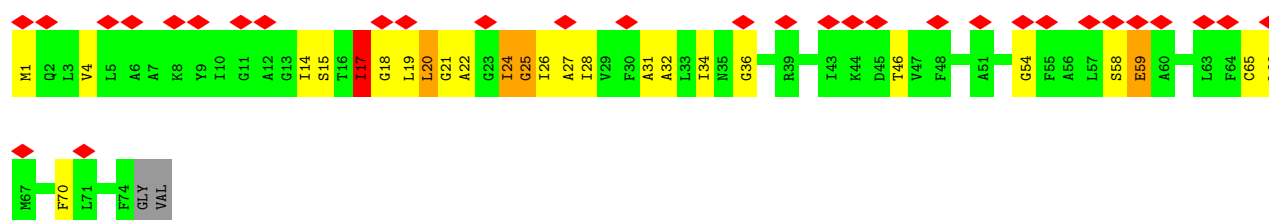
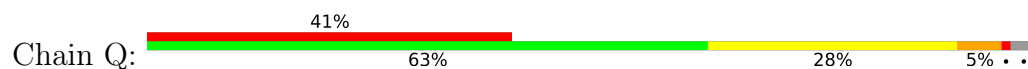
- Molecule 1: ATP synthase subunit 9, mitochondrial



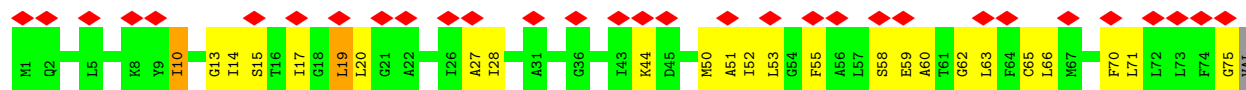
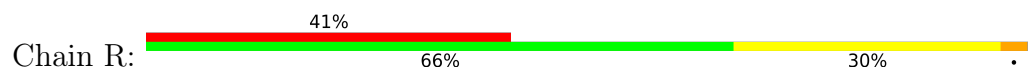
- Molecule 1: ATP synthase subunit 9, mitochondrial



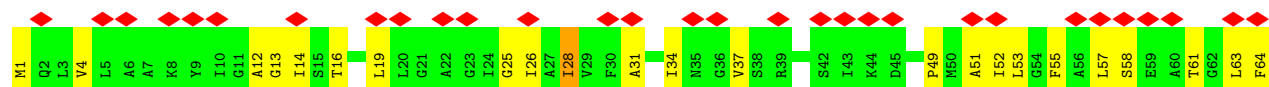
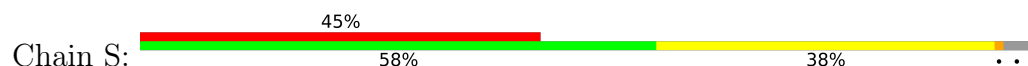
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

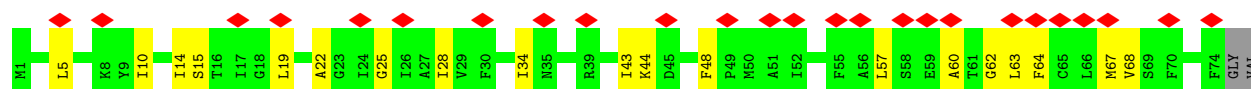
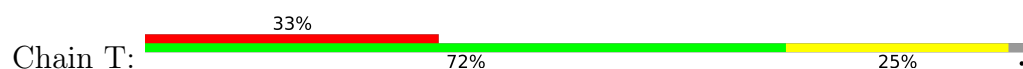


- Molecule 1: ATP synthase subunit 9, mitochondrial

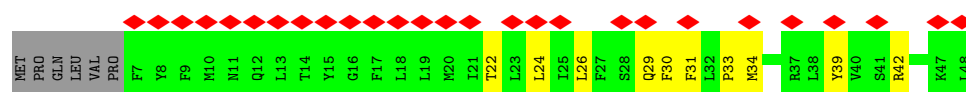




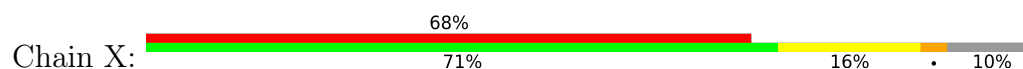
- Molecule 1: ATP synthase subunit 9, mitochondrial



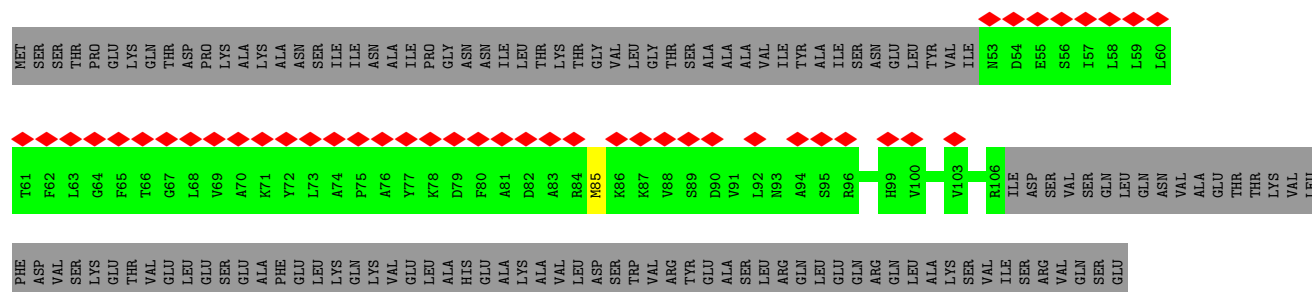
- Molecule 2: ATP synthase protein 8



- Molecule 3: ATP synthase subunit a



- Molecule 4: ATP synthase subunit 4, mitochondrial



LEU
GLY
ASN
PRO
LYS
PHE
GLN
GLU
VAL
LEU
GLN
SER
SER
SER
ILE
GLU
GLN
LEU
SER
LEU
LYS

• Molecule 5: ATP synthase subunit d, mitochondrial



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

VAL
LEU
LYS
ASN
THR
SER
VAL
ILE
ASP
LYS
ILE
GLU
SER
GLU
TYR
VAL
LYS
ILE
TYR
LYS
PRO
VAL
ILE
LYS
ILE
ALA
SER
LYS
GLN
LEU
VAL
ILE
GLY
SER
THR
ALA
SER
LYS
GLN
GLN
VAL
ILE
GLU
SER
PHE
GLU
LYS
HIS
ALA
MET
THR
ASN
ALA
LYS
GLU
THR
E107
V110
S111
K112
E113
L114
K115
D116
L117
Q118
S119
T120
L121

D122
N123
I124
Q125
S126
A127
R128
P129
F130
D131
T134
D136
D137
L138
T139
K140
I141
E144
I145
E151
M152
V153
K154
K157
W158
D159
G162
Y163
K164
D165
R166
F167
G168
M169
L170
M171
V172
M173

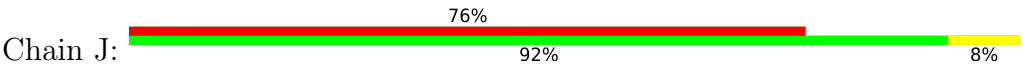
• Molecule 6: ATP synthase subunit f, mitochondrial



VAL
SER
THR
LEU
ILE
PRO
PRO
LYS
VAL
VAL
SER
SER
LYS
ASN
ILE
GLY
SER
ALA
P19
I24
Y27
F30
Y31
K32
S33
L34
P35
Q36
G37
P38
A39
P40
A41
I42
K43
A44
M45
T46
R47
L48
A49
R50
Y51
K52
A53
K54
Y55
F56
D57
G58
D59
N60
A61
S62
G63
K64
P65

L66
W67
H68
F69
A70
L71
G72
I73
I74
A75
F76
G77
Y78
S79
M80
E81
Y82
Y83
F84
H85
L86
ARG
HIS
HIS
HIS
LYS
GLY
ALA
GLU
GLU
HIS

• Molecule 7: ATP synthase subunit J, mitochondrial



M1
L2
K3
R4
F5
P6
T7
F8
I9
L10
K11
V12
Y13
W14
P15
F16
A19
G20
A21
A22
V23
Y24
Y25
G26
M27
S28
K29
A30
A31
D32
L33
S34
S35
N36
T37

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.101	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0475	Depositor
Map size ($\text{\AA}$)	393.6, 393.6, 393.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.23, 1.23, 1.23	Depositor

5 Model quality

5.1 Standard geometry

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

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	K	0.42	0/532	0.85	0/721
1	L	0.39	0/530	0.94	0/718
1	M	0.40	0/535	0.88	0/724
1	N	0.37	0/533	0.87	0/722
1	O	0.39	0/533	0.86	1/722 (0.1%)
1	P	0.37	0/527	0.83	0/714
1	Q	0.37	0/523	0.81	0/709
1	R	0.41	0/534	0.80	0/723
1	S	0.43	0/533	0.85	1/722 (0.1%)
1	T	0.45	0/533	0.78	1/722 (0.1%)
2	8	0.40	0/374	0.77	0/503
3	X	0.33	0/1807	0.75	1/2466 (0.0%)
4	Z	0.23	0/398	0.60	0/538
5	7	0.26	0/527	0.60	0/709
6	U	0.29	0/540	0.69	0/731
7	J	0.28	0/302	0.57	0/410
All	All	0.36	0/9261	0.79	4/12554 (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	R	0	1
6	U	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	59	GLU	N-CA-C	-5.55	105.23	112.23
3	X	155	VAL	O-C-N	5.50	123.94	120.42
1	S	25	GLY	N-CA-C	5.29	118.90	112.49
1	T	25	GLY	N-CA-C	5.15	118.72	112.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	19	LEU	Peptide
6	U	75	ALA	Peptide

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	K	534	0	575	31	0
1	L	529	0	562	49	0
1	M	535	0	571	29	0
1	N	532	0	571	14	0
1	O	533	0	573	24	0
1	P	529	0	560	9	0
1	Q	522	0	541	33	0
1	R	534	0	567	33	0
1	S	532	0	571	35	0
1	T	533	0	573	18	0
2	8	364	0	390	9	0
3	X	1760	0	1847	50	0
4	Z	393	0	377	1	0
5	7	520	0	511	8	0
6	U	522	0	483	14	0
7	J	292	0	298	3	0
All	All	9164	0	9570	272	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 15.

All (272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:58:SER:HB3	1:S:26:ILE:CD1	1.39	1.51
1:Q:18:GLY:HA3	1:Q:65:CYS:SG	1.56	1.43
1:R:58:SER:CB	1:S:26:ILE:HD11	1.54	1.35
3:X:164:LEU:O	3:X:168:ALA:N	1.58	1.34
3:X:164:LEU:O	3:X:168:ALA:CB	1.88	1.22
1:R:58:SER:CB	1:S:26:ILE:CD1	2.15	1.15
1:Q:24:ILE:CG2	1:Q:25:GLY:H	1.56	1.10
1:Q:24:ILE:HG22	1:Q:25:GLY:N	1.37	1.09
1:R:58:SER:HB3	1:S:26:ILE:HD12	1.29	1.07
1:Q:24:ILE:CG2	1:Q:25:GLY:N	2.13	1.03
1:Q:18:GLY:CA	1:Q:65:CYS:SG	2.48	1.02
3:X:164:LEU:O	3:X:168:ALA:CA	2.07	1.02
1:Q:54:GLY:O	1:Q:58:SER:CB	2.08	1.01
1:Q:24:ILE:O	1:Q:26:ILE:N	1.95	1.00
1:R:58:SER:HB2	1:S:26:ILE:HD11	1.44	0.97
1:Q:24:ILE:HG22	1:Q:25:GLY:H	0.80	0.94
1:L:28:ILE:HG13	1:L:29:VAL:N	1.86	0.91
1:L:19:LEU:HD21	1:L:62:GLY:C	1.95	0.90
1:M:58:SER:O	1:M:60:ALA:N	2.04	0.90
1:L:19:LEU:HD21	1:L:62:GLY:O	1.74	0.88
1:L:28:ILE:O	1:L:31:ALA:N	2.06	0.88
3:X:164:LEU:O	3:X:168:ALA:HB3	1.72	0.87
1:M:58:SER:C	1:M:60:ALA:H	1.81	0.86
1:R:58:SER:HB3	1:S:26:ILE:CG1	2.05	0.86
3:X:164:LEU:C	3:X:168:ALA:CB	2.48	0.85
3:X:164:LEU:C	3:X:168:ALA:HB3	2.02	0.85
1:L:19:LEU:CD2	1:L:62:GLY:O	2.25	0.84
1:R:52:ILE:HA	1:R:55:PHE:HB3	1.61	0.81
1:Q:17:ILE:HG12	1:R:17:ILE:HG21	1.63	0.81
3:X:158:LEU:HD12	3:X:158:LEU:O	1.82	0.79
1:K:20:LEU:HD23	1:L:20:LEU:HD22	1.65	0.78
3:X:164:LEU:O	3:X:168:ALA:HB2	1.82	0.78
3:X:115:LEU:O	3:X:119:ILE:HB	1.84	0.78
1:Q:19:LEU:O	1:Q:22:ALA:HB3	1.84	0.76
1:T:64:PHE:CZ	3:X:164:LEU:CB	2.68	0.76
3:X:165:SER:O	3:X:169:ARG:CB	2.35	0.75
3:X:147:PRO:HD2	3:X:158:LEU:HD23	1.69	0.74
1:P:21:GLY:HA3	1:Q:20:LEU:O	1.87	0.73
1:L:28:ILE:O	1:L:29:VAL:C	2.29	0.72
1:L:20:LEU:HD12	1:L:20:LEU:O	1.90	0.71
1:M:65:CYS:O	1:M:68:VAL:HB	1.90	0.71
1:Q:20:LEU:C	1:Q:20:LEU:HD12	2.14	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:CYS:HB2	1:N:19:LEU:HD11	1.73	0.70
1:Q:17:ILE:HG12	1:R:17:ILE:CG2	2.20	0.70
1:K:14:ILE:HG23	1:T:14:ILE:HD12	1.74	0.70
1:K:28:ILE:HG23	1:T:28:ILE:HD12	1.74	0.69
1:L:28:ILE:HG13	1:L:29:VAL:H	1.55	0.69
1:M:58:SER:C	1:M:60:ALA:N	2.45	0.69
1:M:63:LEU:C	1:M:63:LEU:HD22	2.17	0.69
3:X:165:SER:O	3:X:169:ARG:HB2	1.93	0.69
1:K:15:SER:HB3	1:L:13:GLY:HA2	1.73	0.68
1:M:63:LEU:HD22	1:M:63:LEU:O	1.94	0.67
1:Q:20:LEU:O	1:Q:20:LEU:HD12	1.94	0.67
6:U:68:HIS:O	6:U:71:LEU:HB3	1.94	0.67
1:O:17:ILE:O	1:O:20:LEU:HB3	1.94	0.66
3:X:159:VAL:O	3:X:163:THR:HG23	1.95	0.66
1:R:50:MET:O	1:R:53:LEU:HB3	1.95	0.66
3:X:147:PRO:HD2	3:X:158:LEU:CD2	2.27	0.65
1:R:58:SER:CA	1:S:26:ILE:HD11	2.26	0.65
1:Q:20:LEU:HG	1:R:20:LEU:HD13	1.78	0.65
1:R:58:SER:CB	1:S:26:ILE:CG1	2.71	0.64
1:T:64:PHE:CE1	3:X:164:LEU:CB	2.81	0.64
1:Q:25:GLY:HA2	1:Q:28:ILE:HD12	1.80	0.64
1:M:14:ILE:HD12	1:N:14:ILE:HG23	1.80	0.63
1:S:14:ILE:HD12	1:T:14:ILE:HG23	1.80	0.63
1:K:52:ILE:HA	1:K:55:PHE:HB3	1.80	0.63
3:X:164:LEU:C	3:X:168:ALA:HB2	2.24	0.63
1:Q:14:ILE:HD12	1:R:14:ILE:HG23	1.81	0.62
1:N:24:ILE:HG21	1:O:24:ILE:HG13	1.80	0.62
1:L:61:THR:O	1:L:64:PHE:HB2	2.00	0.62
1:L:20:LEU:HD12	1:L:20:LEU:C	2.25	0.62
1:Q:65:CYS:HB2	1:R:19:LEU:HD11	1.82	0.61
1:R:65:CYS:HB2	1:S:19:LEU:HD11	1.81	0.61
1:S:69:SER:O	1:S:73:LEU:N	2.33	0.61
3:X:55:GLY:HA2	3:X:59:LEU:HD23	1.81	0.61
1:S:65:CYS:HB3	1:T:19:LEU:HD11	1.82	0.61
1:Q:24:ILE:O	1:Q:25:GLY:C	2.43	0.60
1:K:21:GLY:HA3	1:L:20:LEU:HD12	1.82	0.60
1:K:50:MET:O	1:K:53:LEU:HB3	2.01	0.60
1:R:62:GLY:O	1:R:65:CYS:HB3	2.02	0.60
1:Q:32:ALA:O	1:Q:36:GLY:N	2.35	0.59
1:K:25:GLY:O	1:L:27:ALA:HB1	2.03	0.59
1:L:40:ASN:ND2	1:M:38:SER:O	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:52:ILE:O	1:S:55:PHE:HB3	2.03	0.59
1:L:25:GLY:HA3	1:M:23:GLY:O	2.03	0.59
1:S:49:PRO:HA	1:S:52:ILE:HG22	1.84	0.59
1:L:19:LEU:HD23	1:L:62:GLY:O	2.01	0.58
1:N:39:ARG:NH2	1:O:35:ASN:OD1	2.37	0.58
1:L:28:ILE:CG1	1:L:29:VAL:N	2.61	0.58
1:O:24:ILE:HG12	1:O:24:ILE:O	2.03	0.58
1:L:14:ILE:HD12	1:M:14:ILE:HG23	1.87	0.57
1:R:14:ILE:HD12	1:S:14:ILE:HG23	1.85	0.57
1:N:14:ILE:HB	1:O:14:ILE:HG23	1.87	0.57
1:Q:24:ILE:O	1:Q:27:ALA:N	2.36	0.57
1:S:63:LEU:HD13	1:S:66:LEU:HD21	1.86	0.56
2:8:26:LEU:O	2:8:30:PHE:HB2	2.06	0.56
1:M:32:ALA:O	1:M:36:GLY:N	2.38	0.56
1:O:65:CYS:HB2	1:P:19:LEU:HD11	1.88	0.56
5:7:112:LYS:HA	5:7:115:LYS:HE3	1.88	0.56
1:L:28:ILE:O	1:L:30:PHE:N	2.39	0.55
1:L:19:LEU:CD2	1:L:62:GLY:C	2.72	0.55
1:M:64:PHE:O	1:M:68:VAL:HG23	2.06	0.55
1:O:14:ILE:HB	1:P:14:ILE:HG23	1.89	0.55
1:O:32:ALA:O	1:O:36:GLY:N	2.39	0.55
1:Q:54:GLY:O	1:Q:58:SER:N	2.39	0.55
1:S:66:LEU:O	1:S:69:SER:HB3	2.07	0.55
1:L:28:ILE:CG1	1:L:29:VAL:H	2.20	0.55
1:N:28:ILE:HG21	1:O:28:ILE:HG22	1.89	0.54
6:U:64:LYS:O	6:U:67:TRP:HB3	2.06	0.54
1:K:51:ALA:O	1:K:55:PHE:N	2.36	0.54
3:X:147:PRO:CD	3:X:158:LEU:CD2	2.85	0.54
3:X:49:ASN:ND2	3:X:56:SER:OG	2.41	0.54
1:M:17:ILE:O	1:M:20:LEU:HB3	2.08	0.54
3:X:88:MET:HA	3:X:91:THR:HG22	1.90	0.54
6:U:51:TYR:O	6:U:55:TYR:HB2	2.08	0.53
1:S:65:CYS:SG	1:S:66:LEU:N	2.80	0.53
1:R:58:SER:CB	1:S:26:ILE:HG13	2.38	0.53
3:X:165:SER:HA	3:X:168:ALA:HB3	1.90	0.53
1:K:14:ILE:HD12	1:L:14:ILE:HG23	1.91	0.53
1:L:50:MET:O	1:L:53:LEU:HB3	2.07	0.53
1:K:25:GLY:C	1:L:27:ALA:HB1	2.33	0.53
1:M:20:LEU:HG	1:N:20:LEU:HD13	1.91	0.53
1:M:51:ALA:O	1:M:55:PHE:N	2.41	0.53
1:L:50:MET:HE1	1:M:44:LYS:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:165:SER:O	3:X:169:ARG:HB3	2.07	0.52
1:K:4:VAL:HG12	1:L:6:ALA:HB2	1.90	0.52
5:7:120:THR:HG21	6:U:27:VAL:HG12	1.90	0.52
1:R:51:ALA:O	1:R:55:PHE:N	2.43	0.52
1:T:44:LYS:O	1:T:48:PHE:HB2	2.09	0.52
1:L:25:GLY:O	1:L:28:ILE:HG12	2.09	0.52
1:L:65:CYS:HB2	1:M:19:LEU:HD11	1.91	0.52
1:T:22:ALA:HB2	1:T:62:GLY:HA3	1.91	0.52
1:T:57:LEU:HD11	3:X:162:GLU:HB3	1.92	0.52
1:O:28:ILE:HD11	1:P:28:ILE:HG22	1.92	0.51
2:8:39:TYR:OH	3:X:67:ASP:OD1	2.28	0.51
1:N:24:ILE:CG2	1:O:24:ILE:HG13	2.40	0.51
1:N:24:ILE:O	1:N:27:ALA:HB3	2.10	0.51
3:X:147:PRO:CD	3:X:158:LEU:HD21	2.41	0.51
1:K:21:GLY:N	1:L:20:LEU:HD13	2.26	0.51
1:K:26:ILE:HG21	1:K:59:GLU:HB2	1.92	0.51
1:L:43:ILE:O	1:L:46:THR:HB	2.11	0.51
5:7:123:ASN:O	5:7:127:ALA:N	2.43	0.51
1:M:15:SER:HB3	1:N:13:GLY:HA2	1.93	0.51
1:R:58:SER:HB3	1:S:26:ILE:HG13	1.88	0.51
1:O:17:ILE:O	1:O:20:LEU:CB	2.57	0.50
3:X:155:VAL:HB	3:X:156:PRO:HD3	1.94	0.50
1:O:49:PRO:HA	1:O:52:ILE:HG22	1.93	0.50
1:K:21:GLY:HA3	1:L:20:LEU:O	2.11	0.50
3:X:211:VAL:HG23	3:X:212:PRO:HD3	1.93	0.50
1:Q:24:ILE:HG22	1:Q:25:GLY:CA	2.32	0.50
1:R:28:ILE:HD12	1:S:28:ILE:HG23	1.93	0.50
1:T:63:LEU:HD23	3:X:168:ALA:HB1	1.93	0.50
3:X:53:ILE:HG12	5:7:135:VAL:HG13	1.92	0.50
1:K:21:GLY:HA2	1:L:24:ILE:HD11	1.94	0.49
1:K:33:LEU:HD21	1:K:48:PHE:HD1	1.78	0.49
1:R:15:SER:HB3	1:S:13:GLY:HA2	1.93	0.49
1:R:63:LEU:HD23	1:R:66:LEU:HD21	1.94	0.49
1:Q:24:ILE:C	1:Q:26:ILE:N	2.70	0.49
1:M:63:LEU:C	1:M:63:LEU:CD2	2.85	0.49
1:O:43:ILE:HG13	1:O:46:THR:HB	1.94	0.49
6:U:66:LEU:O	6:U:70:ALA:N	2.36	0.49
3:X:174:GLY:HA2	3:X:234:TRP:HZ3	1.78	0.48
3:X:57:ARG:HD2	6:U:61:ALA:HB3	1.95	0.48
6:U:71:LEU:O	6:U:74:ILE:HB	2.13	0.48
1:R:66:LEU:O	1:R:70:PHE:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:21:GLY:O	1:Q:24:ILE:N	2.47	0.48
6:U:75:ALA:O	6:U:78:TYR:HB3	2.14	0.48
1:M:52:ILE:O	1:M:55:PHE:HB3	2.14	0.47
6:U:65:PRO:O	6:U:69:PHE:N	2.38	0.47
1:K:50:MET:HE1	1:L:37:VAL:HG11	1.96	0.47
1:L:19:LEU:HD22	1:L:19:LEU:HA	1.66	0.47
1:P:63:LEU:HA	1:P:66:LEU:HD23	1.96	0.47
1:S:64:PHE:O	1:S:67:MET:HG3	2.15	0.47
3:X:93:PHE:O	3:X:97:PHE:N	2.47	0.47
3:X:158:LEU:HD12	3:X:158:LEU:C	2.36	0.47
1:T:60:ALA:HB2	3:X:165:SER:HB2	1.97	0.47
3:X:56:SER:HA	4:Z:85:MET:HE1	1.97	0.47
1:R:71:LEU:O	1:R:75:GLY:N	2.45	0.46
1:O:24:ILE:HG23	1:P:24:ILE:HG12	1.97	0.46
2:8:42:ARG:NH2	3:X:53:ILE:O	2.39	0.46
1:K:22:ALA:HB2	1:K:62:GLY:HA3	1.96	0.46
5:7:134:THR:HG22	5:7:136:ASP:H	1.80	0.46
1:K:25:GLY:HA3	1:L:27:ALA:CB	2.46	0.46
1:L:21:GLY:HA3	1:M:20:LEU:HD12	1.97	0.46
2:8:31:PHE:HA	2:8:34:MET:HG2	1.98	0.46
1:S:4:VAL:HG21	1:T:5:LEU:HG	1.97	0.46
6:U:64:LYS:O	6:U:68:HIS:N	2.40	0.46
1:O:25:GLY:O	1:O:26:ILE:C	2.57	0.46
1:Q:59:GLU:OE1	1:Q:59:GLU:HA	2.15	0.46
1:P:33:LEU:HA	1:Q:34:ILE:HG21	1.97	0.46
1:M:28:ILE:O	1:M:31:ALA:HB3	2.16	0.46
1:Q:46:THR:HG22	1:R:44:LYS:HE3	1.97	0.45
1:O:25:GLY:O	1:O:27:ALA:N	2.48	0.45
1:R:71:LEU:HD11	1:S:73:LEU:HD21	1.98	0.45
1:L:58:SER:HA	1:M:26:ILE:HD11	1.97	0.45
1:S:34:ILE:HA	1:S:37:VAL:HG12	1.97	0.45
1:S:28:ILE:HA	1:S:31:ALA:HB3	1.99	0.45
1:S:49:PRO:HG2	5:7:173:MET:HG2	1.99	0.45
3:X:122:SER:OG	3:X:170:ALA:O	2.31	0.45
1:K:66:LEU:HD13	1:T:64:PHE:HB3	1.99	0.45
3:X:223:GLU:HA	3:X:226:ILE:HG22	1.98	0.45
5:7:165:ASP:N	5:7:165:ASP:OD1	2.50	0.45
1:O:26:ILE:HD12	1:O:55:PHE:HE1	1.81	0.45
2:8:22:THR:O	2:8:26:LEU:CB	2.64	0.45
3:X:165:SER:CA	3:X:168:ALA:HB3	2.47	0.45
1:S:51:ALA:HA	1:T:34:ILE:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:67:MET:HE3	1:T:68:VAL:HG23	1.99	0.45
3:X:216:ILE:HA	3:X:219:ILE:HB	1.99	0.45
1:M:49:PRO:HA	1:M:52:ILE:HG22	1.99	0.44
1:O:25:GLY:O	1:O:28:ILE:N	2.46	0.44
2:8:22:THR:O	2:8:26:LEU:HB3	2.17	0.44
1:K:33:LEU:HA	1:L:34:ILE:HG21	1.98	0.44
1:Q:28:ILE:O	1:Q:31:ALA:HB3	2.17	0.44
1:K:13:GLY:HA2	1:T:15:SER:HB3	1.98	0.44
1:N:34:ILE:HA	1:N:37:VAL:HG12	2.00	0.44
6:U:71:LEU:HA	6:U:74:ILE:HD12	2.00	0.44
1:K:66:LEU:O	1:K:70:PHE:N	2.50	0.44
3:X:171:ILE:O	3:X:175:LEU:HB2	2.18	0.44
1:N:21:GLY:O	1:N:25:GLY:N	2.49	0.44
6:U:78:TYR:O	6:U:81:GLU:HB3	2.18	0.44
6:U:24:ILE:HA	6:U:27:VAL:HG22	1.98	0.43
1:M:24:ILE:O	1:M:27:ALA:HB3	2.19	0.43
2:8:24:LEU:HD21	7:J:13:TYR:HD2	1.83	0.43
1:R:52:ILE:HA	1:R:55:PHE:CB	2.40	0.43
1:S:58:SER:O	1:S:61:THR:OG1	2.33	0.43
1:K:21:GLY:CA	1:L:20:LEU:CD1	2.97	0.43
1:O:25:GLY:C	1:O:27:ALA:N	2.77	0.43
1:L:5:LEU:HA	1:L:8:LYS:HD3	2.00	0.43
2:8:29:GLN:HG2	7:J:7:THR:H	1.83	0.42
1:O:14:ILE:HD12	1:P:14:ILE:HD13	2.01	0.42
1:K:60:ALA:HA	1:K:63:LEU:HB2	2.01	0.42
1:N:50:MET:HE3	1:N:50:MET:HB2	1.85	0.42
1:R:60:ALA:O	1:R:63:LEU:HB2	2.19	0.42
3:X:165:SER:N	3:X:168:ALA:HB3	2.33	0.42
1:K:21:GLY:HA3	1:L:20:LEU:CD1	2.49	0.42
3:X:163:THR:O	3:X:167:PHE:CD1	2.73	0.42
1:O:26:ILE:O	1:O:29:VAL:HB	2.20	0.42
3:X:160:ILE:HA	3:X:163:THR:HG23	2.02	0.42
3:X:176:ARG:O	3:X:180:ASN:ND2	2.52	0.42
1:L:52:ILE:O	1:L:55:PHE:HB3	2.18	0.42
1:K:25:GLY:CA	1:L:27:ALA:CB	2.98	0.42
1:M:26:ILE:O	1:M:29:VAL:HB	2.19	0.42
1:S:12:ALA:O	1:S:16:THR:OG1	2.38	0.42
1:T:57:LEU:HD11	3:X:162:GLU:CB	2.49	0.42
1:L:1:FME:O1	1:L:4:VAL:N	2.53	0.42
1:L:19:LEU:HD22	1:L:22:ALA:CB	2.50	0.42
1:M:14:ILE:H	1:M:14:ILE:HG12	1.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:PHE:HA	1:O:33:LEU:HB3	2.02	0.42
1:Q:15:SER:HB3	1:R:13:GLY:HA2	2.02	0.42
1:S:57:LEU:HD23	1:S:57:LEU:HA	1.84	0.42
1:L:28:ILE:C	1:L:30:PHE:N	2.78	0.41
1:P:67:MET:HE1	1:Q:70:PHE:HZ	1.85	0.41
1:S:70:PHE:O	1:S:74:PHE:N	2.54	0.41
5:7:128:ARG:HG2	5:7:130:PHE:HB3	2.02	0.41
6:U:65:PRO:HA	6:U:68:HIS:HB2	2.02	0.41
1:K:10:ILE:O	1:K:14:ILE:HG12	2.21	0.41
1:K:41:PRO:HG3	1:T:43:ILE:HD12	2.03	0.41
1:S:14:ILE:H	1:S:14:ILE:HG12	1.71	0.41
1:L:64:PHE:O	1:L:67:MET:HG3	2.20	0.41
1:K:26:ILE:HD13	1:K:55:PHE:HE1	1.86	0.41
1:L:12:ALA:O	1:L:16:THR:OG1	2.39	0.41
3:X:187:LEU:HD12	3:X:191:LEU:HD13	2.02	0.41
1:Q:21:GLY:O	1:Q:22:ALA:C	2.64	0.41
3:X:86:PHE:HA	3:X:89:ILE:HG22	2.02	0.41
1:M:63:LEU:HD13	1:M:64:PHE:HD1	1.85	0.40
1:Q:25:GLY:O	1:R:27:ALA:HB1	2.21	0.40
1:R:10:ILE:O	1:R:14:ILE:HG12	2.21	0.40
1:S:28:ILE:H	1:S:28:ILE:HG13	1.67	0.40
1:O:47:VAL:O	1:O:51:ALA:N	2.49	0.40
2:8:33:PRO:HB2	7:J:5:PHE:HD2	1.86	0.40
1:N:63:LEU:HD23	1:N:66:LEU:HD21	2.03	0.40
3:X:115:LEU:HB3	3:X:119:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	K	72/76 (95%)	66 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	72/76 (95%)	67 (93%)	4 (6%)	1 (1%)	9	39
1	M	73/76 (96%)	65 (89%)	7 (10%)	1 (1%)	9	39
1	N	72/76 (95%)	68 (94%)	4 (6%)	0	100	100
1	O	72/76 (95%)	65 (90%)	6 (8%)	1 (1%)	9	39
1	P	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	Q	72/76 (95%)	68 (94%)	1 (1%)	3 (4%)	2	20
1	R	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
1	S	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
1	T	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
2	8	40/48 (83%)	38 (95%)	2 (5%)	0	100	100
3	X	222/249 (89%)	204 (92%)	18 (8%)	0	100	100
4	Z	52/209 (25%)	52 (100%)	0	0	100	100
5	7	65/173 (38%)	63 (97%)	2 (3%)	0	100	100
6	U	66/95 (70%)	57 (86%)	9 (14%)	0	100	100
7	J	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
All	All	1202/1571 (76%)	1117 (93%)	79 (7%)	6 (0%)	26	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	59	GLU
1	Q	25	GLY
1	Q	24	ILE
1	L	29	VAL
1	Q	17	ILE
1	O	26	ILE

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	K	53/55 (96%)	51 (96%)	2 (4%)	29	51
1	L	53/55 (96%)	48 (91%)	5 (9%)	8	28
1	M	53/55 (96%)	49 (92%)	4 (8%)	12	35
1	N	54/55 (98%)	53 (98%)	1 (2%)	50	67
1	O	54/55 (98%)	51 (94%)	3 (6%)	19	43
1	P	52/55 (94%)	49 (94%)	3 (6%)	18	42
1	Q	50/55 (91%)	45 (90%)	5 (10%)	7	26
1	R	53/55 (96%)	51 (96%)	2 (4%)	29	51
1	S	54/55 (98%)	52 (96%)	2 (4%)	30	52
1	T	54/55 (98%)	53 (98%)	1 (2%)	50	67
2	8	41/47 (87%)	41 (100%)	0	100	100
3	X	190/217 (88%)	181 (95%)	9 (5%)	23	47
4	Z	37/182 (20%)	37 (100%)	0	100	100
5	7	56/158 (35%)	56 (100%)	0	100	100
6	U	45/76 (59%)	45 (100%)	0	100	100
7	J	30/30 (100%)	30 (100%)	0	100	100
All	All	929/1260 (74%)	892 (96%)	37 (4%)	29	50

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	10	ILE
1	K	28	ILE
1	L	10	ILE
1	L	19	LEU
1	L	20	LEU
1	L	24	ILE
1	L	59	GLU
1	M	39	ARG
1	M	59	GLU
1	M	63	LEU
1	M	66	LEU
1	N	57	LEU
1	O	24	ILE
1	O	59	GLU
1	O	66	LEU
1	P	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	59	GLU
1	P	66	LEU
1	Q	4	VAL
1	Q	17	ILE
1	Q	20	LEU
1	Q	59	GLU
1	Q	66	LEU
1	R	10	ILE
1	R	59	GLU
1	S	28	ILE
1	S	53	LEU
1	T	10	ILE
3	X	46	LEU
3	X	154	LEU
3	X	159	VAL
3	X	160	ILE
3	X	162	GLU
3	X	163	THR
3	X	165	SER
3	X	166	TYR
3	X	211	VAL

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

Mol	Chain	Res	Type
1	N	2	GLN
3	X	71	ASN
3	X	185	HIS
3	X	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	O	1	1	6,7,10	0.98	0	7,7,11	1.18	1 (14%)
1	FME	L	1	1	5,6,10	1.29	1 (20%)	4,6,11	1.40	1 (25%)
1	FME	T	1	1	6,7,10	1.01	0	7,7,11	1.14	0
1	FME	S	1	1	5,6,10	1.49	1 (20%)	4,6,11	1.50	1 (25%)
1	FME	R	1	1	6,7,10	1.05	0	7,7,11	1.13	0
1	FME	P	1	1	8,9,10	0.95	0	8,9,11	0.90	0
1	FME	Q	1	1	5,6,10	1.32	1 (20%)	4,6,11	1.27	1 (25%)
1	FME	N	1	1	5,6,10	1.40	1 (20%)	4,6,11	1.56	1 (25%)
1	FME	M	1	1	6,7,10	1.01	0	7,7,11	1.27	1 (14%)
1	FME	K	1	1	8,9,10	0.98	0	8,9,11	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	O	1	1	-	3/5/7/11	-
1	FME	L	1	1	-	1/3/5/11	-
1	FME	T	1	1	-	3/5/7/11	-
1	FME	S	1	1	-	1/3/5/11	-
1	FME	R	1	1	-	1/5/7/11	-
1	FME	P	1	1	-	4/7/9/11	-
1	FME	Q	1	1	-	1/3/5/11	-
1	FME	N	1	1	-	0/3/5/11	-
1	FME	M	1	1	-	3/5/7/11	-
1	FME	K	1	1	-	6/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	1	FME	CA-N	-2.66	1.43	1.46
1	N	1	FME	CA-N	-2.41	1.44	1.46
1	Q	1	FME	CA-N	-2.04	1.44	1.46
1	L	1	FME	CA-N	-2.01	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	1	FME	CB-CA-N	2.86	112.91	109.68
1	N	1	FME	CB-CA-N	2.86	112.90	109.68
1	L	1	FME	CB-CA-N	2.44	112.43	109.68
1	Q	1	FME	CB-CA-N	2.33	112.31	109.68
1	M	1	FME	CB-CA-C	-2.24	107.21	112.62
1	O	1	FME	CB-CA-C	-2.15	107.42	112.62

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	1	FME	O-C-CA-CB
1	L	1	FME	O-C-CA-CB
1	O	1	FME	CB-CA-N-CN
1	O	1	FME	C-CA-CB-CG
1	P	1	FME	N-CA-CB-CG
1	P	1	FME	O-C-CA-CB
1	Q	1	FME	O-C-CA-CB
1	S	1	FME	O-C-CA-CB
1	T	1	FME	N-CA-CB-CG
1	K	1	FME	CA-CB-CG-SD
1	K	1	FME	N-CA-CB-CG
1	P	1	FME	CA-CB-CG-SD
1	K	1	FME	C-CA-CB-CG
1	O	1	FME	N-CA-CB-CG
1	K	1	FME	CB-CG-SD-CE
1	M	1	FME	C-CA-CB-CG
1	R	1	FME	C-CA-CB-CG
1	T	1	FME	C-CA-CB-CG
1	P	1	FME	C-CA-CB-CG
1	T	1	FME	CB-CA-N-CN
1	M	1	FME	N-CA-CB-CG
1	K	1	FME	CB-CA-N-CN
1	M	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

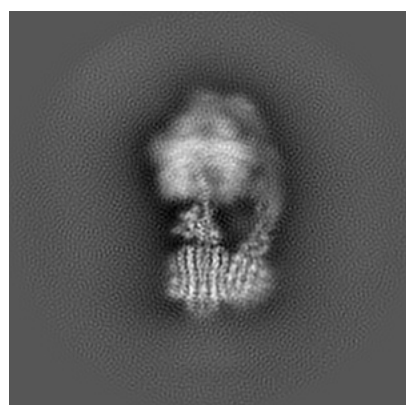
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7549. These allow visual inspection of the internal detail of the map and identification of artifacts.

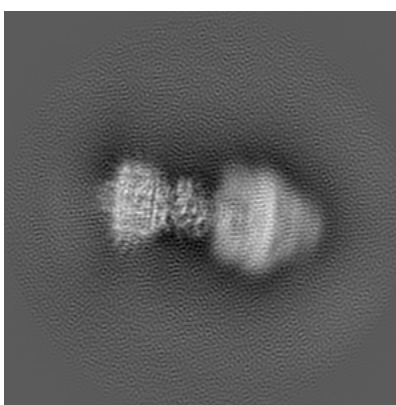
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

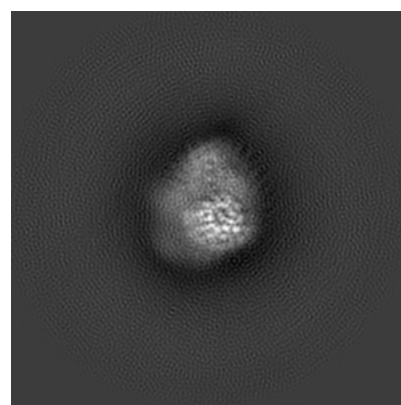
6.1.1 Primary map



X



Y

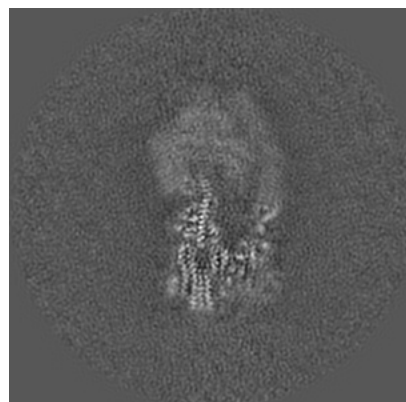


Z

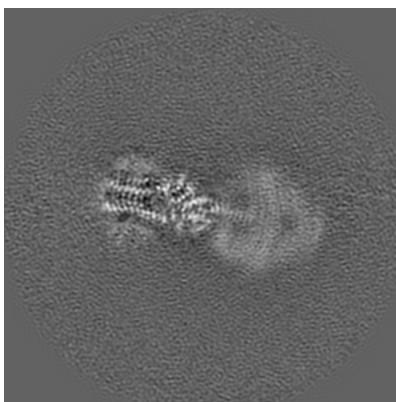
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

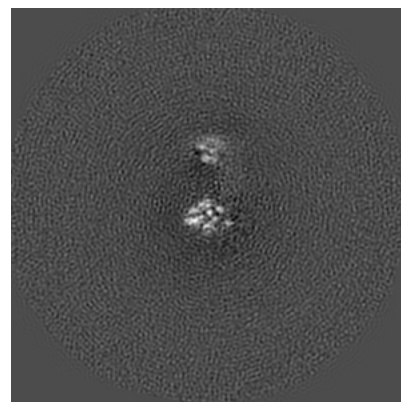
6.2.1 Primary map



X Index: 160



Y Index: 160

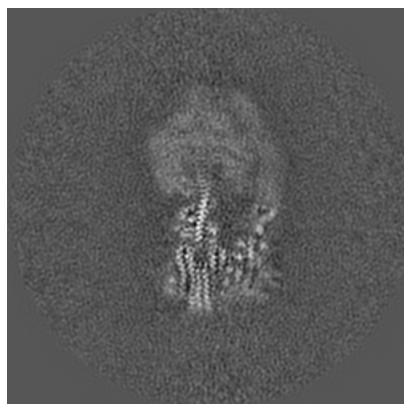


Z Index: 160

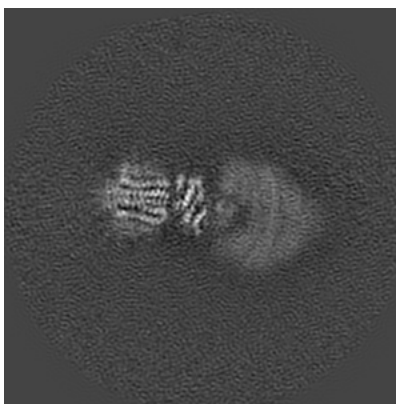
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

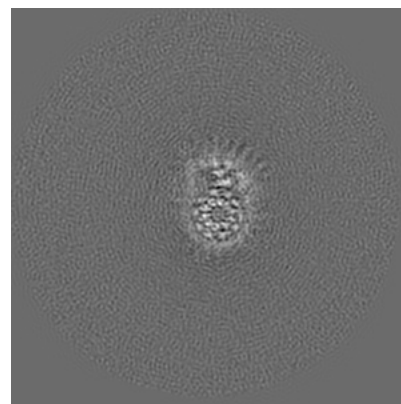
6.3.1 Primary map



X Index: 159



Y Index: 145

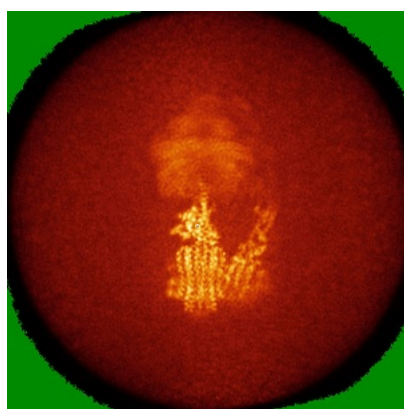


Z Index: 115

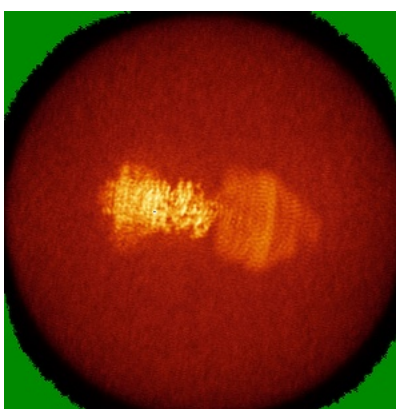
The images above show the largest variance slices of the map in three orthogonal directions.

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

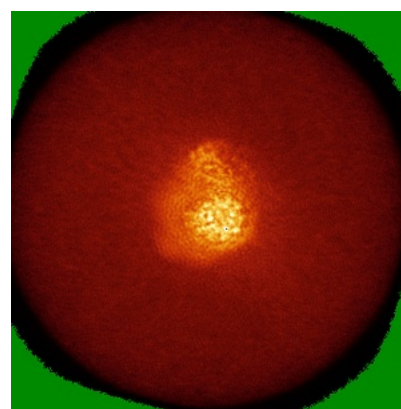
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0475. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

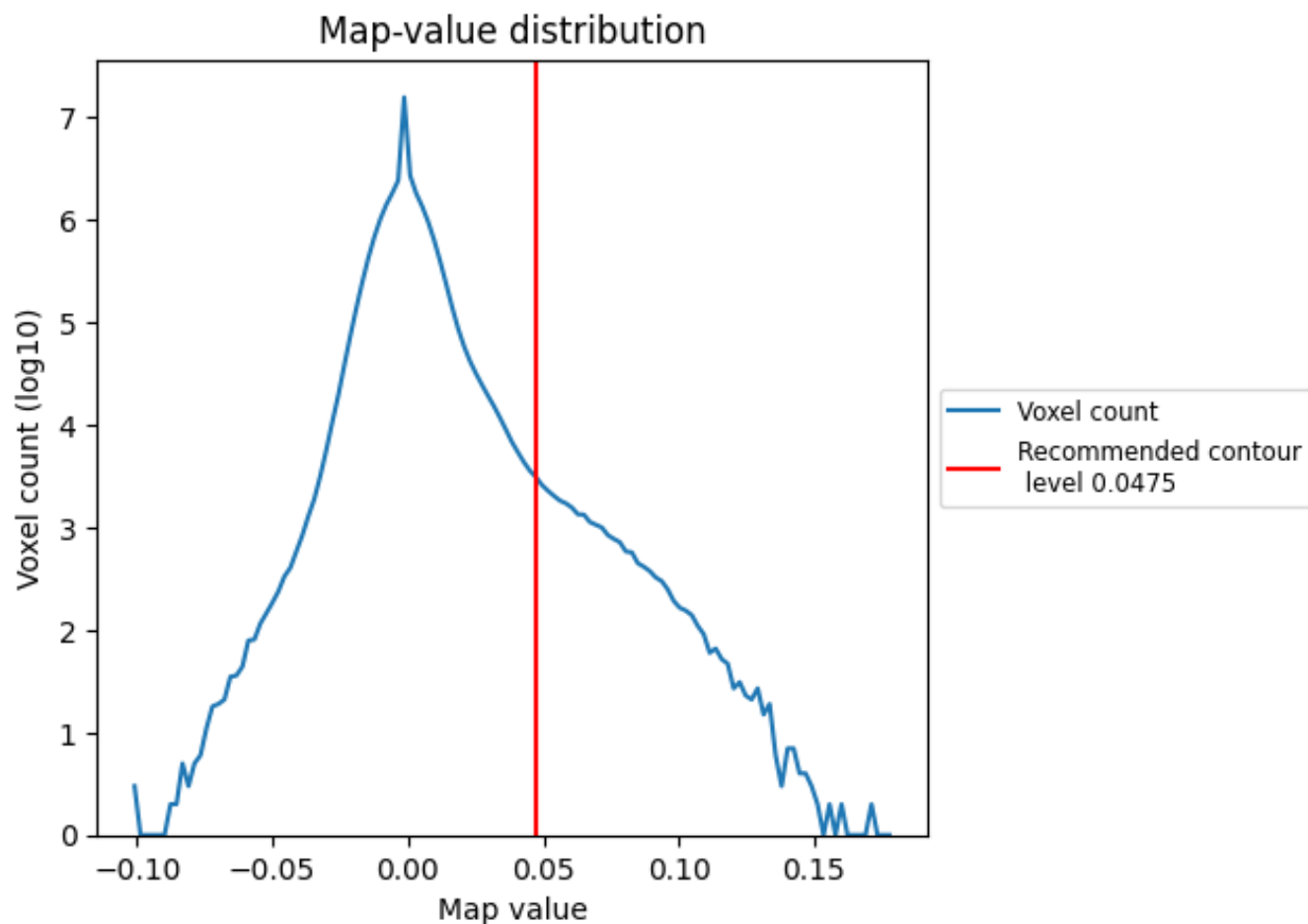
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

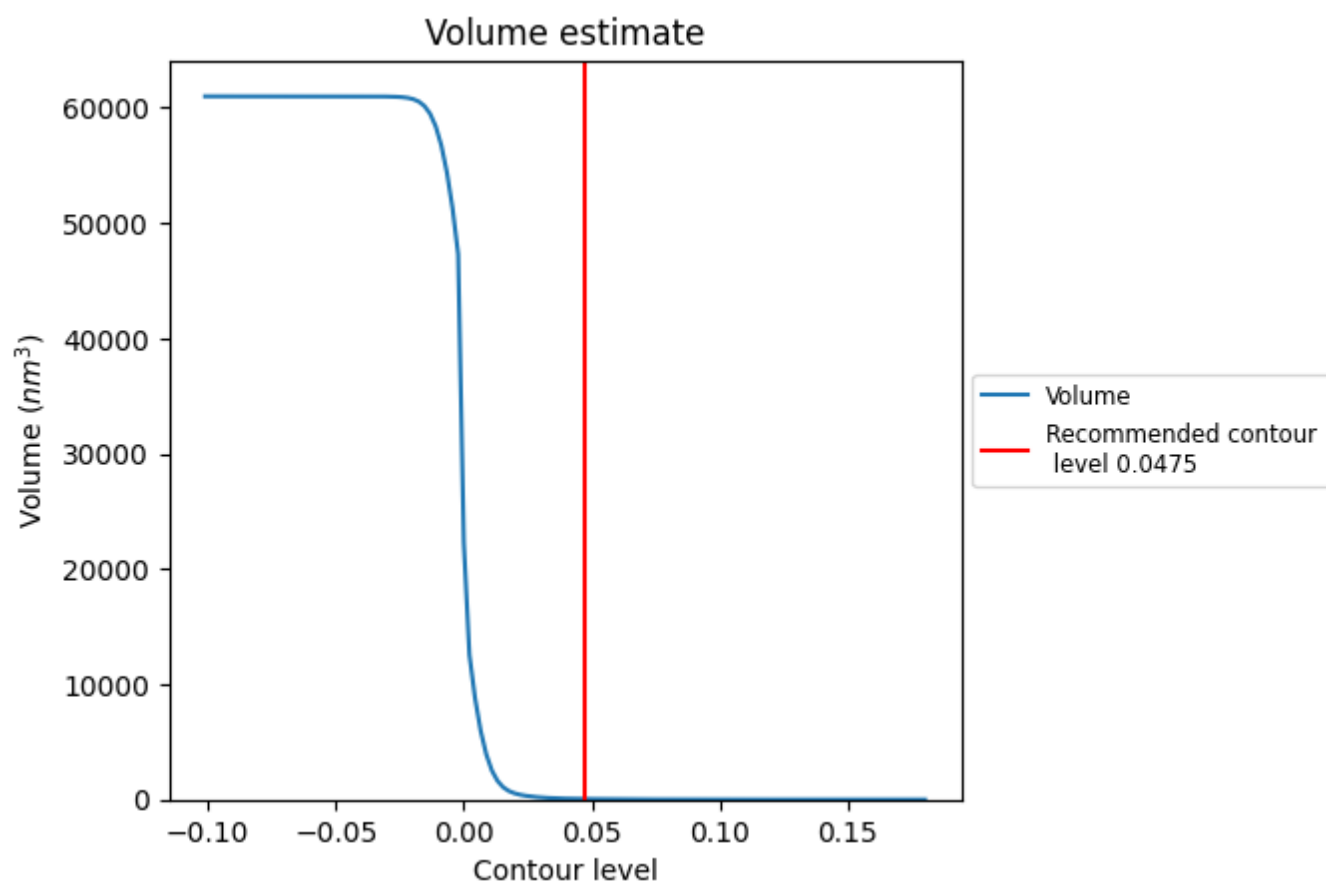
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

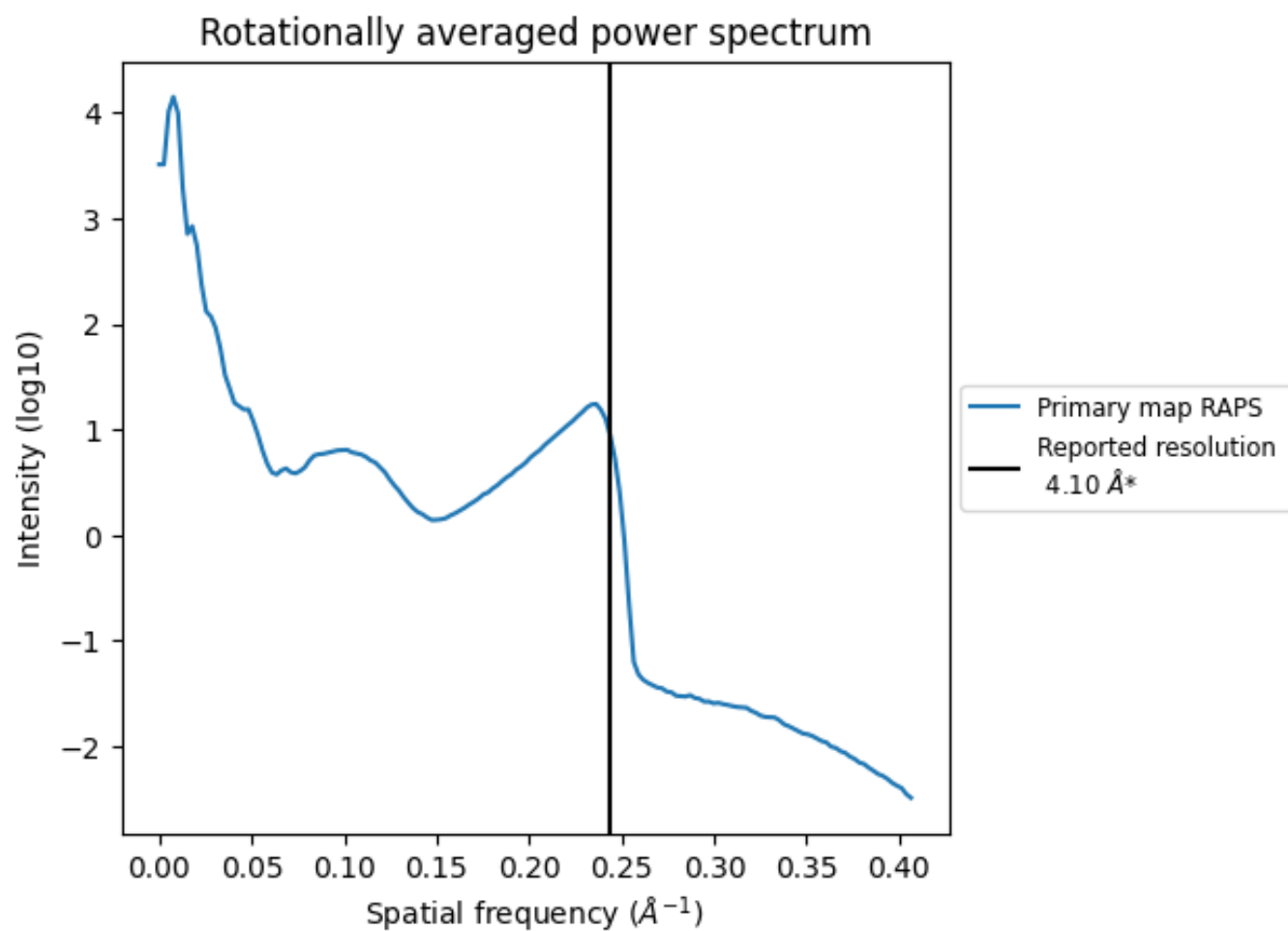
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm³; this corresponds to an approximate mass of 47 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 ⓘ

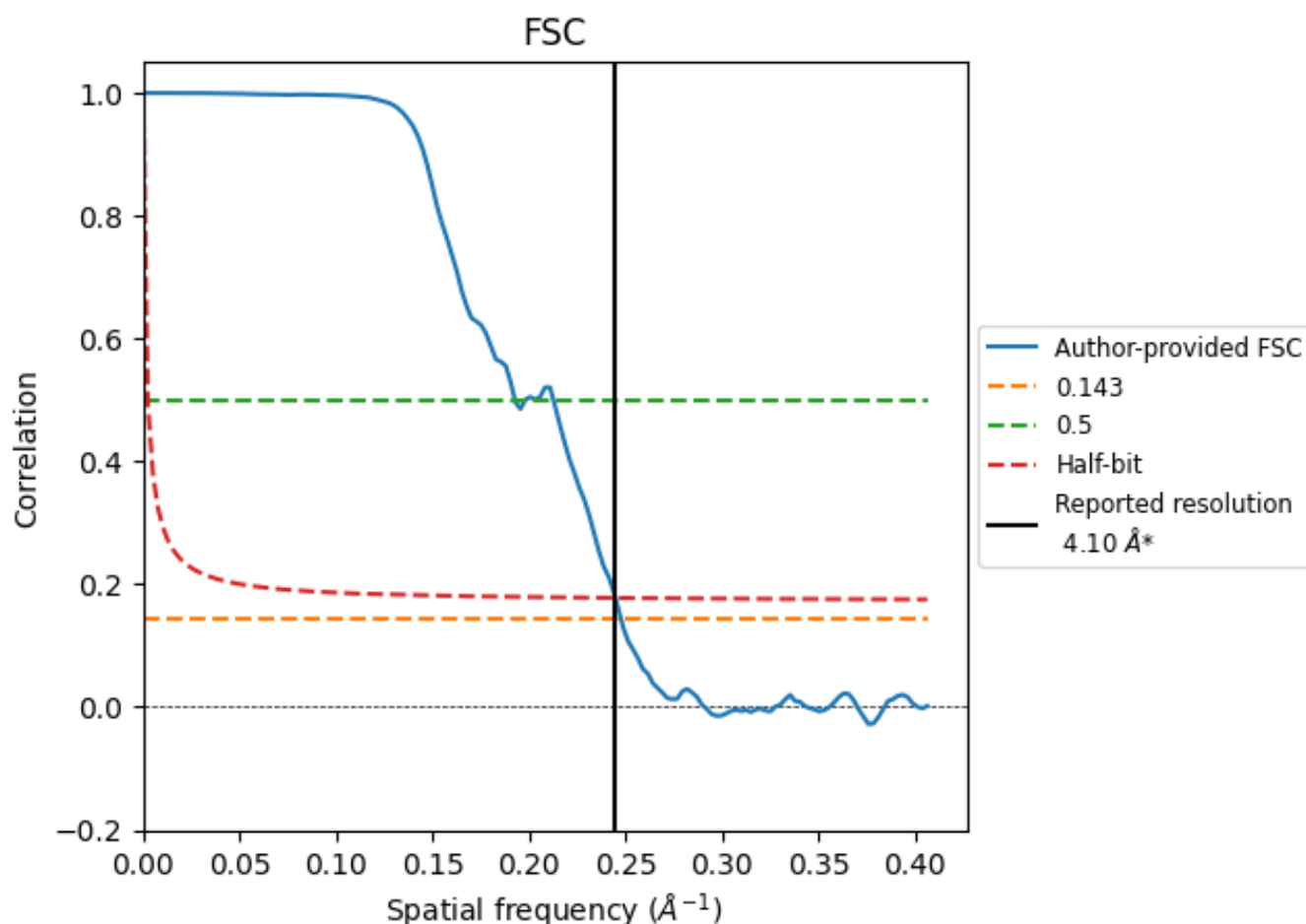


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.04	5.19	4.08
Unmasked-calculated*	-	-	-

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

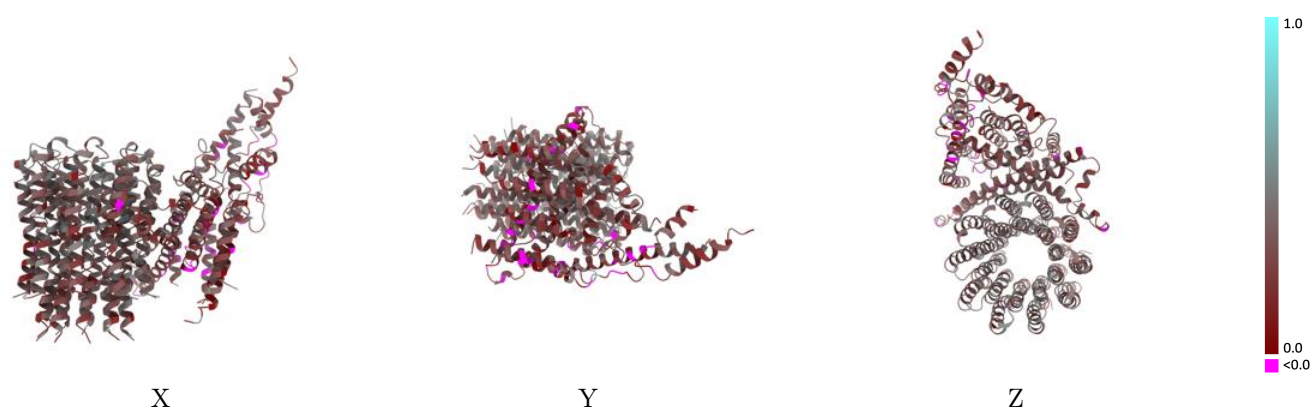
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7549 and PDB model 6CP7. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

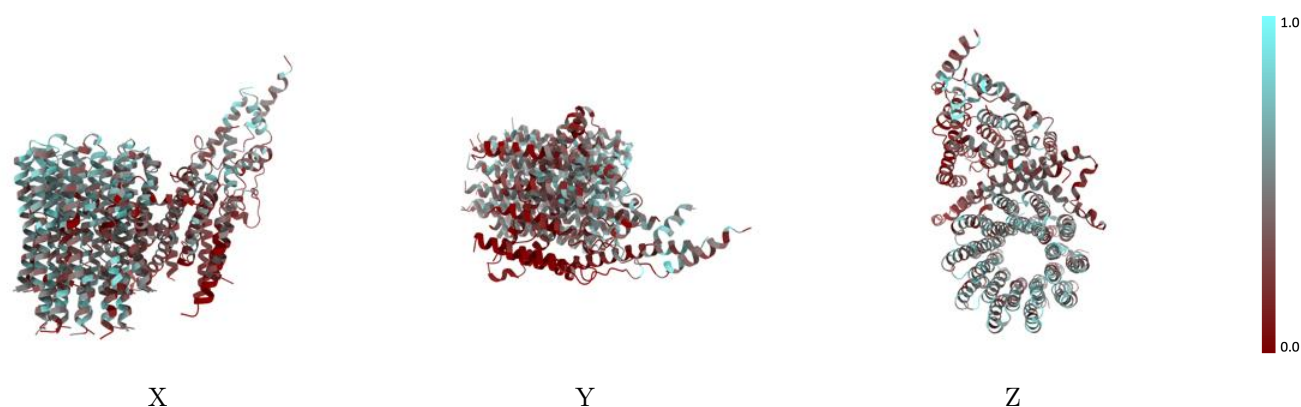
This section was not generated.

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



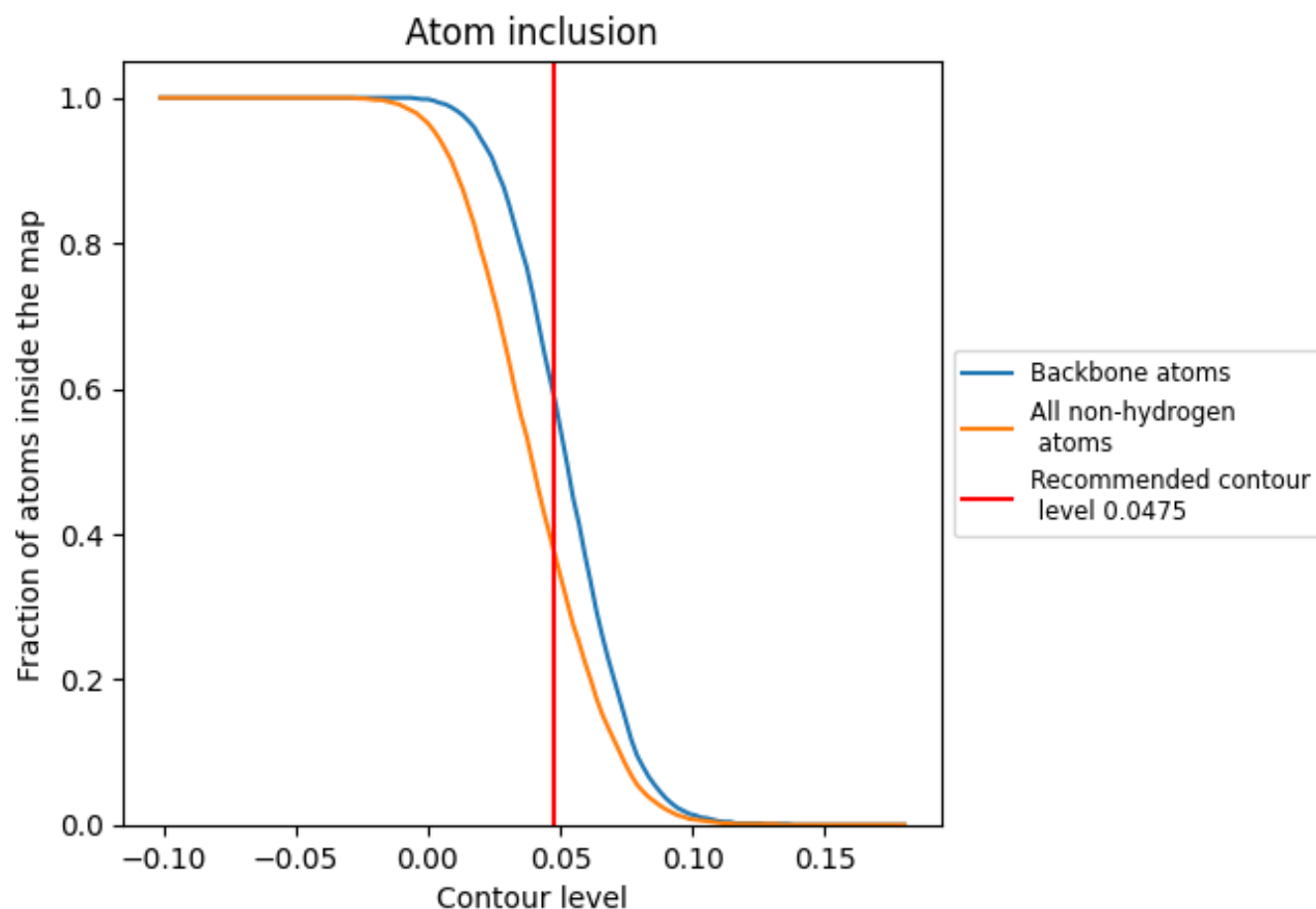
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0475).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3780	 0.3110
7	 0.3770	 0.2710
8	 0.3470	 0.2800
J	 0.2200	 0.2830
K	 0.4140	 0.3190
L	 0.4730	 0.3450
M	 0.4760	 0.3540
N	 0.5730	 0.3570
O	 0.4320	 0.3360
P	 0.4870	 0.3450
Q	 0.4610	 0.3410
R	 0.4440	 0.3530
S	 0.4330	 0.3700
T	 0.4940	 0.3820
U	 0.1470	 0.2320
X	 0.2440	 0.2540
Z	 0.2010	 0.2410

