



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:05 AM UTC

PDB ID : 7SG7 / pdb_00007sg7
EMDB ID : EMD-25106
Title : In situ cryo-EM structure of bacteriophage Sf6 gp8:gp14N complex at 2.8 Å resolution
Authors : Li, F.; Cingolani, G.; Hou, C.
Deposited on : 2021-10-05
Resolution : 2.83 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
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

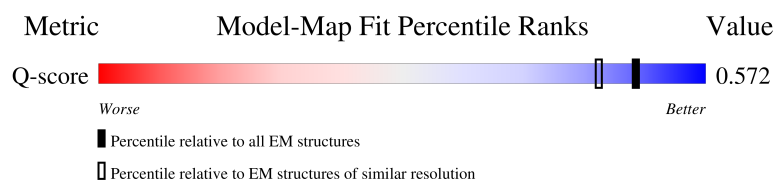
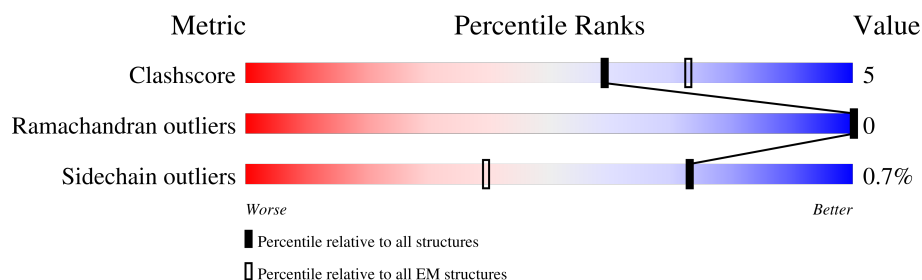
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



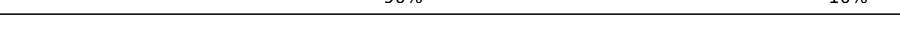
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	623	
1	B	623	
1	C	623	
1	D	623	

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Mol	Chain	Length	Quality of chain
1	E	623	 16% . 81%
1	F	623	 16% . 81%
1	G	623	 17% . 81%
1	H	623	 16% . 81%
1	I	623	 17% . 81%
1	J	623	 17% . 81%
1	K	623	 17% . 81%
1	L	623	 16% . 81%
1	M	623	 17% . 81%
1	N	623	 16% . 81%
1	O	623	 17% . 81%
1	P	623	 17% . 81%
1	Q	623	 17% . 81%
1	R	623	 17% . 81%
2	S	472	 90% 10%
2	T	472	 87% 12% .
2	U	472	 89% 10%
2	V	472	 87% 13%
2	W	472	 88% 12%
2	X	472	 88% 12%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 38802 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 Gene 14 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	B	117	Total	C	N	O	S	0	0
			915	587	148	177	3		
1	C	121	Total	C	N	O	S	0	0
			947	608	153	183	3		
1	D	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	I	117	Total	C	N	O	S	0	0
			915	587	148	177	3		
1	N	121	Total	C	N	O	S	0	0
			947	608	153	183	3		
1	E	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	J	117	Total	C	N	O	S	0	0
			915	587	148	177	3		
1	O	121	Total	C	N	O	S	0	0
			947	608	153	183	3		
1	F	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	K	117	Total	C	N	O	S	0	0
			915	587	148	177	3		
1	P	121	Total	C	N	O	S	0	0
			947	608	153	183	3		
1	G	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	L	117	Total	C	N	O	S	0	0
			915	587	148	177	3		
1	Q	121	Total	C	N	O	S	0	0
			947	608	153	183	3		
1	H	120	Total	C	N	O	S	0	0
			938	603	151	181	3		
1	M	117	Total	C	N	O	S	0	0
			915	587	148	177	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	121	Total	C	N	O	S	0	0
			947	608	153	183	3		

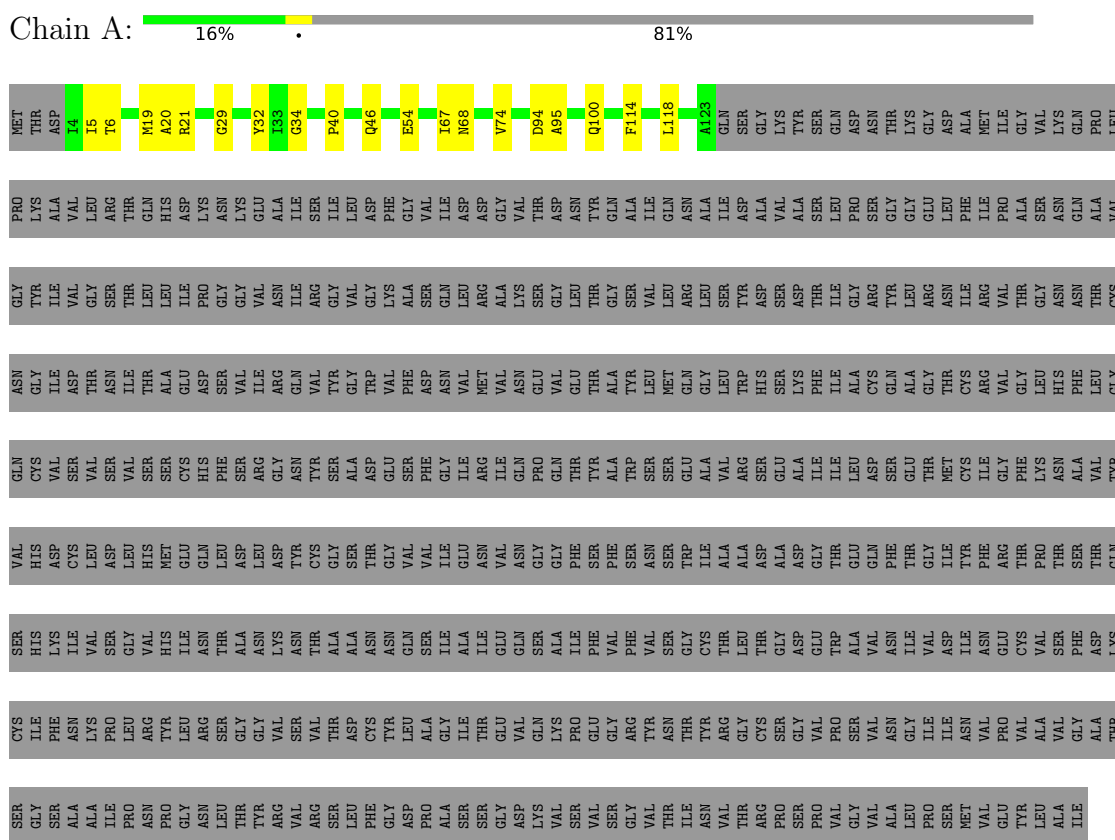
- Molecule 2 is a protein called Gene 8 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		
2	S	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		
2	U	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		
2	V	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		
2	W	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		
2	X	471	Total	C	N	O	S	0	0
			3667	2318	629	707	13		

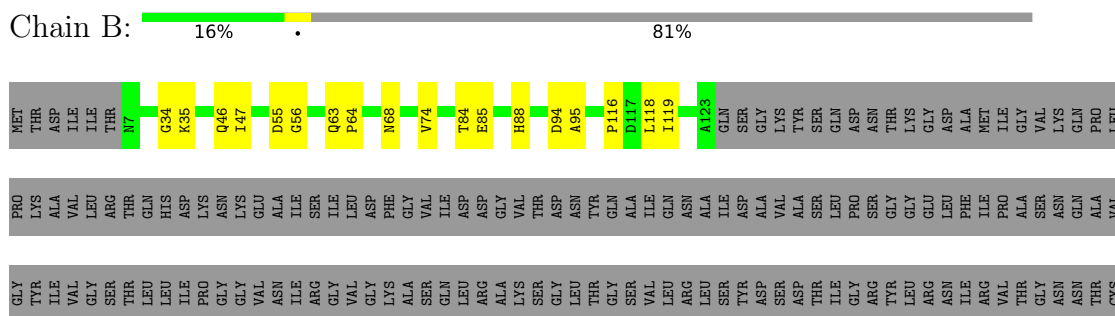
3 Residue-property plots

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

• Molecule 1: Gene 14 protein



• Molecule 1: Gene 14 protein



- Molecule 1: Gene 14 protein

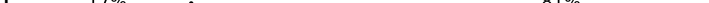
[illegible]

- Molecule 1: Gene 14 protein

[illegible]

ser	gly	cys	ser	asn	gly	asn	gly	tyr
gly	ile	ile	his	his	cys	gly	tyr	asn
ser	phe	asn	lys	asp	asp	ile	tyr	gly
ala	asn	ile	ile	cys	ser	val	asn	asp
ile	lys	val	val	val	val	asn	ser	gly
pro	pro	leu	asp	leu	val	ile	thr	thr
asn	arg	leu	val	his	ser	thr	leu	leu
pro	tyr	tyr	his	met	ser	ala	ala	ile
gly	leu	ile	glu	glu	cys	asn	leu	ile
asn	asn	asn	glu	asn	his	asn	asn	asn
leu	ser	thr	thr	leu	phe	ser	ser	gly
thr	gly	ala	asp	asp	ser	val	gly	gly
tyr	val	gly	asn	leu	arg	ile	val	val
arg	arg	val	lys	asp	gly	asn	asn	asn
val	ser	val	asn	tyr	asn	glu	ile	ile
arg	val	val	cys	cys	tyr	val	arg	val
ser	thr	thr	ala	gly	ser	tyr	gly	gly
leu	asp	ala	ala	ser	ala	asn	gly	val
phe	cys	asn	thr	thr	asn	trp	trp	asn
gly	leu	asn	asn	asn	glu	val	asn	asn
asn	tyr	leu	glu	val	glu	phe	asn	asn
pro	pro	ala	ser	val	asn	asn	asn	asn
ala	gly	gly	ile	val	ile	gly	asn	asn
ser	ile	ile	ala	glu	ile	val	leu	leu
ser	thr	thr	ile	ile	asn	arg	arg	arg
gly	thr	glu	glu	val	ile	val	met	arg
lys	val	asn	glu	asn	glu	asn	asn	lys
val	lys	gly	asn	asn	pro	glu	ser	ser
val	asn	lys	asn	asn	glu	val	gly	gly
ser	pro	pro	ile	phe	thr	glu	thr	thr
val	glu	glu	asn	thr	thr	leu	leu	leu
gly	arg	arg	phe	phe	ser	trp	trp	trp
val	tyr	tyr	val	asn	ser	leu	leu	leu
thr	asn	asn	ser	ser	ser	met	arg	arg
ile	thr	thr	gly	thr	asp	glu	tyr	tyr
pro	ser	ser	gly	thr	asn	ser	asn	asn
ser	gly	gly	asn	asp	asn	lys	asp	asn
pro	val	val	glu	glu	ile	phe	thr	thr
val	pro	pro	trp	trp	ile	ile	gly	gly
gly	ser	ser	ala	glu	leu	leu	ile	ile
val	val	val	val	glu	asn	asn	cys	arg
ala	asn	asn	asn	phe	thr	glu	glu	tyr
leu	leu	gly	ile	thr	ile	ala	ala	leu
pro	pro	ile	val	asn	asn	glu	gly	arg
pro	ser	ile	asn	asp	met	thr	thr	asn
ser	ser	asn	asn	ile	cys	cys	cys	ile
val	val	val	asn	phe	thr	arg	arg	arg
glu	glu	pro	glu	arg	gly	val	val	val
tyr	tyr	val	cys	thr	phe	gly	gly	thr
leu	leu	ala	val	val	lys	leu	leu	asn
ile	ala	gly	thr	ser	ala	phe	asn	asn
ile	ile	gly	asn	thr	val	thr	thr	cys
			lys	asn	tyr	leu	asn	asn

- Molecule 1: Gene 14 protein

Chain I:  17% 81%

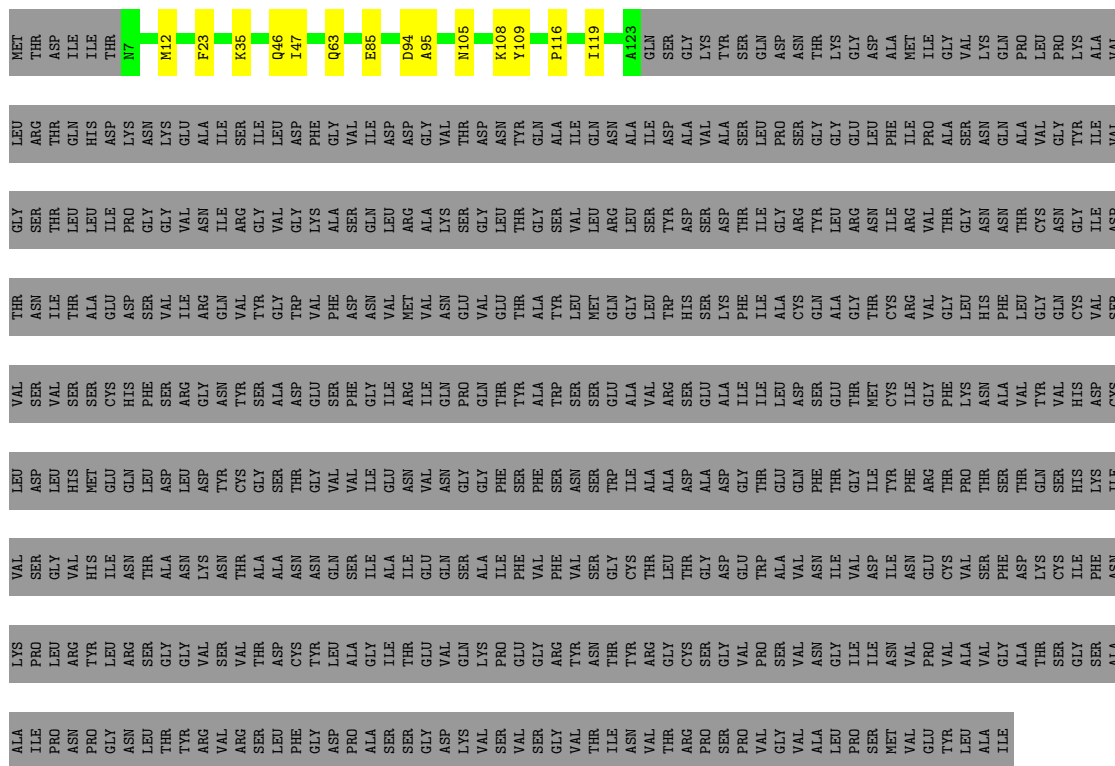
[illegible]

- Molecule 1: Gene 14 protein

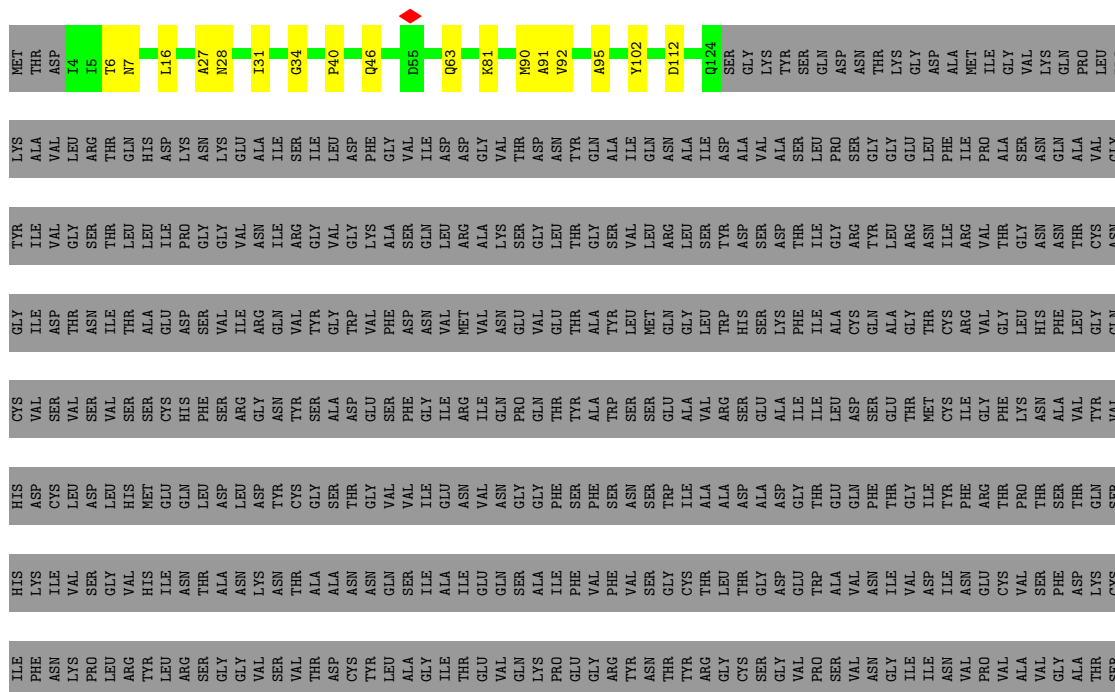
Chain N: 16% 81%

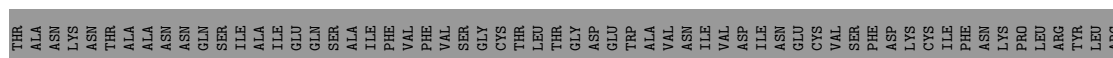
MET	THR	ASP	THR	I4	I5	I6	I7	I8	V8		M19		K24		A27	N28		Q46		D55		Q63		K81		A91		D94	A95		Q99		Y102	F103	Q104		D112		D117		E120		Q124		GLY	GLY	LVS	LVS	TYR	TYR	SER	SER	GLN	ASP	ASN	THR	THR	LYS	GLY	ASP	ALA	ALA	MET	MET	ILE	ILE	GLY	VAL
-----	-----	-----	-----	----	----	----	----	----	----	--	-----	--	-----	--	-----	-----	--	-----	--	-----	--	-----	--	-----	--	-----	--	-----	-----	--	-----	--	------	------	------	--	------	--	------	--	------	--	------	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain J: 17% . 81%



Chain O: 17% . 81%





[illegible]

- Molecule 1: Gene 14 protein



ALA	ILE	VAL	SER	THR	ASN	HIS	ASN	ASN	LYS	MET
GLY	ALA	GLY	PHE	SER	ALA	PHE	ASN	GLN	GLN	THR
ALA	THR	THR	ASP	THR	VAL	GLY	THR	ALA	PRO	ASP
SER	SER	SER	CYS	GLN	THR	GLN	CYS	VAL	LEU	I4
GLY	GLY	ILE	ILE	HIS	HIS	CYS	GLY	THR	LYS	I5
SER	SER	SER	PHE	LYS	ASP	VAL	ILE	ILE	ALA	L16
ALA	ALA	ALA	ASN	ILE	CYS	SER	ASP	VAL	VAL	M19
ALA	ALA	ILE	PRO	VAL	LEU	VAL	THR	GLY	LEU	
ASN	ASN	ASN	ARG	VAL	GLY	VAL	ILE	THR	THR	V26
PRO	PRO	PRO	THR	HIS	MET	SER	ALA	LEU	HIS	A27
GLY	ASN	GLY	ARG	ILE	GLN	CYS	GLU	ILE	ASP	N28
ASN	ASN	ASN	ARG	THR	GLN	HIS	ASP	PRO	LYS	I31
THR	THR	THR	GLY	ALA	LEU	PHE	SER	GLY	LYS	
ARG	ARG	TYR	GLY	ASN	LEU	ARG	ILE	VAL	ASN	K35
VAL	VAL	VAL	VAL	LYS	ASP	GLY	ARG	ASN	ALA	T38
ARG	ARG	THR	VAL	THR	CYS	TYR	GLN	ARG	SER	Q46
SER	SER	SER	THR	ALA	GLY	SER	TYR	GLY	ILE	
LEU	LEU	LEU	CYS	ALA	SER	ALA	ASP	VAL	LEU	D85
PHE	PHE	PHE	CYS	ASN	THR	ASP	TRP	GLY	ASP	
GLY	GLY	GLY	THR	ASN	GLY	GLU	VAL	LYS	PHE	Q63
ASP	ASP	ASP	LEU	GLN	VAL	GLU	PHE	ALA	GLY	
PRO	PRO	PRO	ALA	SER	VAL	PHE	ASP	SER	VAL	K81
ALA	ALA	ALA	ILE	ILE	ILE	GLY	ASN	GLN	ILE	
SER	SER	SER	ILE	ALA	GLU	ILE	VAL	LEU	ASP	M90
SER	SER	SER	THR	ILE	ASN	ARG	MET	ARG	ASP	A91
GLY	GLY	GLY	GLU	GLU	VAL	ILE	VAL	ALA	GLY	V92
ASP	ASP	VAL	VAL	GLN	ASN	GLN	ASN	LYS	VAL	
LYS	LYS	LYS	GLN	SER	GLY	PRO	GLU	SER	THR	A95
SER	SER	SER	ILE	PHE	PHE	THR	GLU	GLY	ASN	Q99
VAL	VAL	VAL	GLU	THR	THR	TYR	THR	THR	TYR	
SER	SER	SER	GLY	PHE	PHE	ALA	ALA	GLY	GLN	Y102
VAL	VAL	VAL	ARG	SER	SER	TRP	TYR	SER	ALA	
THR	THR	THR	ASN	SER	ASN	SER	LEU	VAL	ILE	D112
ILE	ILE	ILE	THR	GLY	TRP	GLU	MET	GLN	ASN	
ASN	ASN	ASN	THR	CYS	ILE	ALA	GLY	ARG	ALA	D117
VAL	VAL	VAL	ARG	THR	ALA	VAL	LEU	LEU	ILE	
THR	THR	THR	GLY	LEU	ALA	ARG	TRP	TYR	ASP	Q124
ARG	ARG	CYS	CYS	THR	ASP	SER	HIS	ASP	ALA	
PRO	PRO	PRO	SER	GLY	ALA	GLU	SER	SER	VAL	LYS
SER	SER	SER	GLY	ASP	ASP	ALA	PHE	THR	ALA	THR
VAL	VAL	VAL	VAL	GLU	GLY	ILE	ILE	ILE	SER	SER
GLY	GLY	GLY	SER	THR	THR	ILE	ILE	GLY	LEU	GLN
ALA	ALA	ALA	ASN	PHE	GLN	SER	CYS	ARG	PRO	ASN
LEU	LEU	LEU	GLY	THR	THR	GLU	ALA	LEU	GLY	THR
PRO	PRO	PRO	ILE	VAL	GLY	THR	GLY	ARG	GLU	LYS
SER	SER	SER	ILE	ASP	ILE	MET	THR	ASN	LEU	GLY
MET	MET	MET	ASN	ILE	TYR	CYS	CYS	ILE	PHE	ASP
VAL	VAL	VAL	PRO	ASN	PHE	ILE	ARG	VAL	ILE	ALA
GLU	GLU	GLU	VAL	ARG	THR	GLY	VAL	VAL	PRO	MET
TYR	TYR	TYR	VAL	THR	PRO	PHE	GLY	THR	ILE	GLY
ILE	ILE	ILE	ALA	ASN	PRO	THR	THR	GLY	ALA	GLY

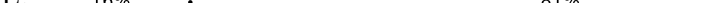
- Molecule 1: Gene 14 protein



VAL	THR	GLY	LEU	MET
SER	ASN	SER	ARG	THR
VAL	ILE	THR	THR	ASP
SER	THR	LEU	GLN	I4
SER	ALA	LEU	HIS	I5
CYS	GLU	ILE	ASP	T6
ASP	ASP	PRO	LYS	
PHE	SER	GLY	ASN	M19
ARG	ILE	GLY	LYS	G29
VAL	VAL	VAL	GLU	
ASN	ASN	ASN	ALA	
GLN	ILE	ILE	ILE	G34
VAL	ARG	ARG	SER	
THR	GLY	GLY	ILE	D39
ALA	VAL	VAL	LEU	P40
ASP	TRP	GLY	ASP	V41
GLU	VAL	LYS	PHE	
SER	PHE	ALA	GLY	Q46
PHE	ASP	SER	VAL	
GLY	ASN	GLN	ILE	E52
ILE	VAL	LEU	ASP	
ARG	MET	ARG	ASP	H68
ILE	VAL	ALA	GLY	
GLN	ASN	LYS	VAL	I67
PRO	GLU	SER	THR	N68
THR	VAL	GLY	ASP	
THR	GLU	LEU	ASN	V74
TYR	THR	THR	GLN	
ALA	ALA	GLY	GLN	D94
TRP	TYR	SER	ALA	A95
SER	LEU	VAL	ILE	
SER	MET	LEU	GLN	
GLU	GLY	LEU	ASN	Q100
ALA	GLN	ARG	ALA	
VAL	LEU	SER	ILE	A123
ARG	TRP	TYR	ASP	GLN
SER	HIS	ASP	ASP	GLY
GLU	SER	SER	VAL	LYS
ALA	LYS	ASP	ALA	TYR
ILE	PHE	THR	LEU	SER
ILE	ILE	ILE	SER	GLN
LEU	ALA	GLY	PRO	ASP
ASP	CYS	ARG	SER	ASN
SER	GLN	TYR	GLY	THR
GLU	ALA	LEU	GLY	GLY
THR	GLY	ARG	GLU	LYS
MET	THR	ASN	LEU	ASP
CYS	CYS	ILE	PHE	ALA
ILE	ARG	ARG	ILE	MET
GLY	VAL	VAL	PRO	GLY
PHE	GLY	THR	ALA	GLY
LYS	LEU	GLY	SER	VAL
ASN	HIS	ASN	ASN	LYS
ALA	PHE	ASN	GLN	GLN
VAL	LEU	THR	ALA	PRO
TYR	GLY	CYS	VAL	LEU
VAL	GLN	ASN	GLY	PRO
VAL	CYS	GLY	TYR	LYS
HIS	VAL	ILE	THR	VAL
ASP	SER	ASP	VAL	ALA

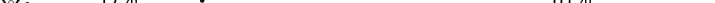
[illegible]

- Molecule 1: Gene 14 protein

Chain L:  16% • 81%

[illegible]

- Molecule 1: Gene 14 protein

Chain Q:  17% . 81%

[illegible]

[illegible]

[illegible]

- Molecule 1: Gene 14 protein

Chain R: 17% 81%

[illegible]

- Molecule 2: Gene 8 protein

Chain T: 87% 12%

MET
P2
M29
K34
E36
I36
L37
S40
L79
V86
D118
W127
P128
T129
D130
L138
D143
R148
M153
S154
K155
T158
F162
S170
A177
P185
D186
I191
G192
T193
I198
S203
S204
T216
A219
Q231
C232
C233



- Molecule 2: Gene 8 protein

Chain S: 90% 10%



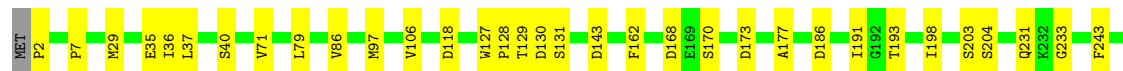
- Molecule 2: Gene 8 protein

Chain U: 89% 10%



- Molecule 2: Gene 8 protein

Chain V: 87% 13%



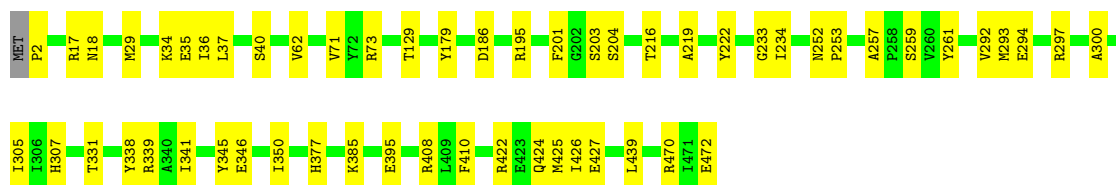
- Molecule 2: Gene 8 protein

Chain W: 88% 12%



- Molecule 2: Gene 8 protein

Chain X: 88% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	574.464, 574.464, 574.464	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	Depositor

5 Model quality

5.1 Standard geometry

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	0.13	0/961	0.29	0/1310
1	B	0.13	0/938	0.34	0/1278
1	C	0.14	0/970	0.39	0/1322
1	D	0.14	0/961	0.33	0/1310
1	E	0.13	0/961	0.30	0/1310
1	F	0.14	0/961	0.32	0/1310
1	G	0.22	0/961	0.39	0/1310
1	H	0.14	0/961	0.32	0/1310
1	I	0.12	0/938	0.32	0/1278
1	J	0.13	0/938	0.32	0/1278
1	K	0.12	0/938	0.32	0/1278
1	L	0.13	0/938	0.36	0/1278
1	M	0.13	0/938	0.34	0/1278
1	N	0.14	0/970	0.39	0/1322
1	O	0.15	0/970	0.43	0/1322
1	P	0.27	0/970	0.44	0/1322
1	Q	0.27	0/970	0.45	0/1322
1	R	0.15	0/970	0.43	1/1322 (0.1%)
2	S	0.23	0/3746	0.41	0/5077
2	T	0.35	0/3746	0.54	5/5077 (0.1%)
2	U	0.18	0/3746	0.36	0/5077
2	V	0.21	0/3746	0.41	2/5077 (0.0%)
2	W	0.21	0/3746	0.40	0/5077
2	X	0.20	0/3746	0.40	0/5077
All	All	0.21	0/39690	0.40	8/53922 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	130	ASP	N-CA-C	-7.21	104.21	113.16
1	R	7	ASN	CB-CA-C	-5.44	109.83	117.23
2	T	372	GLY	CA-C-N	-5.33	115.21	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	372	GLY	C-N-CA	-5.33	115.21	122.93
2	T	426	ILE	CA-C-N	5.10	133.93	122.19
2	T	426	ILE	C-N-CA	5.10	133.93	122.19
2	V	426	ILE	CA-C-N	5.06	133.84	122.19
2	V	426	ILE	C-N-CA	5.06	133.84	122.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	938	0	906	12	0
1	B	915	0	877	12	0
1	C	947	0	914	9	0
1	D	938	0	906	13	0
1	E	938	0	906	13	0
1	F	938	0	906	11	0
1	G	938	0	906	8	0
1	H	938	0	906	12	0
1	I	915	0	877	8	0
1	J	915	0	877	10	0
1	K	915	0	877	6	0
1	L	915	0	877	10	0
1	M	915	0	877	7	0
1	N	947	0	914	13	0
1	O	947	0	914	12	0
1	P	947	0	914	10	0
1	Q	947	0	914	9	0
1	R	947	0	914	10	0
2	S	3667	0	3588	29	0
2	T	3667	0	3588	37	0
2	U	3667	0	3588	31	0
2	V	3667	0	3588	39	0
2	W	3667	0	3588	34	0
2	X	3667	0	3588	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	38802	0	37710	354	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 5.

All (354) 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:X:426:ILE:HG13	2:X:427:GLU:H	1.38	0.87
1:N:94:ASP:OD1	1:N:95:ALA:N	2.09	0.84
1:Q:27:ALA:O	1:Q:28:ASN:ND2	2.12	0.82
1:K:94:ASP:OD1	1:K:95:ALA:N	2.14	0.81
1:L:94:ASP:OD1	1:L:95:ALA:N	2.13	0.81
1:J:94:ASP:OD2	1:J:95:ALA:N	2.14	0.80
1:B:94:ASP:OD1	1:B:95:ALA:N	2.17	0.78
2:W:331:THR:HG21	2:W:339:ARG:HG3	1.67	0.76
1:R:94:ASP:OD1	1:R:95:ALA:N	2.17	0.76
1:O:27:ALA:O	1:O:28:ASN:ND2	2.17	0.75
1:A:114:PHE:HB2	1:C:7:ASN:HD22	1.53	0.73
1:D:114:PHE:HB2	1:N:7:ASN:HD22	1.56	0.71
2:T:185:PRO:O	2:W:101:ARG:NH2	2.18	0.70
2:V:292:VAL:HG21	2:V:341:ILE:HD11	1.74	0.70
2:T:422:ARG:NH2	2:T:424:GLN:OE1	2.26	0.69
1:E:34:GLY:HA2	1:E:46:GLN:HA	1.74	0.69
2:U:426:ILE:O	2:U:427:GLU:HG3	1.93	0.69
2:V:422:ARG:NH2	2:V:424:GLN:OE1	2.26	0.69
1:G:34:GLY:HA2	1:G:46:GLN:HA	1.73	0.69
1:F:34:GLY:HA2	1:F:46:GLN:HA	1.75	0.68
2:S:331:THR:HG21	2:S:339:ARG:HG3	1.75	0.68
1:A:34:GLY:HA2	1:A:46:GLN:HA	1.74	0.67
2:W:426:ILE:O	2:W:427:GLU:HG3	1.93	0.67
1:M:84:THR:HG21	1:M:88:HIS:HD2	1.61	0.66
2:T:426:ILE:O	2:T:427:GLU:HG3	1.94	0.66
2:U:422:ARG:NH2	2:U:424:GLN:OE1	2.28	0.66
1:C:81:LYS:NZ	1:C:112:ASP:OD2	2.29	0.66
2:W:292:VAL:HG21	2:W:341:ILE:HD11	1.78	0.66
2:W:422:ARG:NH2	2:W:424:GLN:OE1	2.28	0.66
2:X:426:ILE:O	2:X:427:GLU:HG3	1.97	0.65
1:H:19:MET:O	1:H:100:GLN:NE2	2.30	0.65
2:V:426:ILE:O	2:V:427:GLU:HG3	1.96	0.64
1:G:52:GLU:HG2	1:G:58:HIS:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:19:MET:SD	1:R:24:LYS:NZ	2.69	0.64
1:G:19:MET:O	1:G:100:GLN:NE2	2.31	0.64
2:X:29:MET:HE3	2:X:377:HIS:HB3	1.80	0.64
2:W:294:GLU:OE2	2:W:307:HIS:NE2	2.31	0.64
1:E:52:GLU:HG2	1:E:58:HIS:CE1	2.32	0.63
2:W:186:ASP:OD2	2:W:203:SER:OG	2.13	0.63
1:D:34:GLY:HA2	1:D:46:GLN:HA	1.79	0.63
1:Q:19:MET:SD	1:Q:24:LYS:NZ	2.70	0.63
1:H:34:GLY:HA2	1:H:46:GLN:HA	1.80	0.63
2:T:37:LEU:HD22	2:S:385:LYS:HB2	1.81	0.63
2:V:29:MET:HE3	2:V:377:HIS:HB3	1.81	0.62
1:O:81:LYS:NZ	1:O:112:ASP:OD2	2.32	0.62
2:V:127:TRP:HE3	2:V:128:PRO:HD2	1.62	0.62
1:I:94:ASP:OD1	1:I:95:ALA:N	2.32	0.62
2:U:36:ILE:HG13	2:U:37:LEU:H	1.63	0.62
2:V:37:LEU:HD22	2:X:385:LYS:HB2	1.81	0.62
1:N:81:LYS:NZ	1:N:112:ASP:OD2	2.32	0.62
2:T:331:THR:HG21	2:T:339:ARG:HG3	1.81	0.62
2:W:36:ILE:HG13	2:W:37:LEU:H	1.63	0.61
2:W:108:VAL:HG23	2:W:109:ASN:H	1.65	0.61
1:M:84:THR:HG21	1:M:88:HIS:CD2	2.35	0.61
1:G:94:ASP:OD1	1:G:95:ALA:N	2.33	0.61
2:W:146:ARG:HH21	2:W:149:GLY:HA2	1.66	0.61
1:M:94:ASP:OD1	1:M:95:ALA:N	2.32	0.61
2:T:143:ASP:HB3	2:T:191:ILE:HG22	1.81	0.60
1:N:19:MET:SD	1:N:24:LYS:NZ	2.69	0.60
1:E:19:MET:O	1:E:100:GLN:NE2	2.33	0.60
2:V:297:ARG:NH2	2:X:257:ALA:O	2.34	0.60
2:X:422:ARG:NH2	2:X:424:GLN:OE1	2.34	0.60
2:T:297:ARG:NH2	2:S:257:ALA:O	2.35	0.60
2:X:292:VAL:HG21	2:X:341:ILE:HD11	1.84	0.60
1:A:94:ASP:OD1	1:A:95:ALA:N	2.33	0.59
1:E:29:GLY:HA3	1:E:67:ILE:HD12	1.85	0.59
2:U:331:THR:HG21	2:U:339:ARG:HG3	1.84	0.59
1:R:81:LYS:NZ	1:R:112:ASP:OD2	2.35	0.59
2:T:277:GLU:OE1	2:W:297:ARG:NH1	2.35	0.59
2:W:36:ILE:HG13	2:W:37:LEU:N	2.18	0.58
1:G:29:GLY:HA3	1:G:67:ILE:HD12	1.84	0.58
2:T:36:ILE:HG13	2:T:37:LEU:H	1.68	0.58
1:G:39:ASP:OD2	1:G:41:VAL:HG12	2.02	0.58
2:T:36:ILE:HG13	2:T:37:LEU:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ASP:OD2	1:E:41:VAL:HG12	2.03	0.58
2:U:146:ARG:HH21	2:U:149:GLY:HA2	1.66	0.58
1:E:5:ILE:HG13	1:E:6:THR:H	1.69	0.58
1:F:94:ASP:OD1	1:F:95:ALA:N	2.33	0.58
2:V:36:ILE:HG13	2:V:37:LEU:N	2.19	0.58
2:S:36:ILE:HG13	2:S:37:LEU:H	1.69	0.57
2:U:36:ILE:HG13	2:U:37:LEU:N	2.18	0.57
2:U:297:ARG:NH1	2:V:277:GLU:OE1	2.37	0.57
1:A:19:MET:O	1:A:100:GLN:NE2	2.37	0.57
2:S:292:VAL:HG21	2:S:341:ILE:HD11	1.86	0.57
1:E:94:ASP:OD1	1:E:95:ALA:N	2.33	0.57
1:F:19:MET:O	1:F:100:GLN:NE2	2.37	0.57
1:H:94:ASP:OD1	1:H:95:ALA:N	2.33	0.57
2:V:36:ILE:HG13	2:V:37:LEU:H	1.68	0.57
2:U:393:ASP:OD2	2:U:470:ARG:NH1	2.38	0.57
2:X:426:ILE:HG13	2:X:427:GLU:N	2.16	0.57
2:W:393:ASP:OD2	2:W:470:ARG:NH1	2.38	0.57
1:F:68:ASN:OD1	1:F:69:ALA:N	2.38	0.56
2:X:36:ILE:HG13	2:X:37:LEU:H	1.69	0.56
1:C:104:GLN:NE2	2:T:423:GLU:OE1	2.39	0.56
1:N:99:GLN:NE2	2:S:423:GLU:O	2.37	0.56
2:W:385:LYS:HB2	2:X:37:LEU:HD22	1.88	0.56
2:T:331:THR:HG23	2:T:338:TYR:HA	1.88	0.55
1:F:44:GLU:CD	1:F:45:ASN:H	2.14	0.55
2:S:216:THR:HB	2:S:219:ALA:HB2	1.87	0.55
2:S:37:LEU:HD22	2:U:385:LYS:HB2	1.87	0.55
2:X:216:THR:HB	2:X:219:ALA:HB2	1.87	0.55
1:O:27:ALA:C	1:O:28:ASN:HD22	2.10	0.55
1:H:68:ASN:OD1	1:H:69:ALA:N	2.38	0.55
2:U:194:TRP:O	2:V:231:GLN:NE2	2.40	0.55
2:U:130:ASP:OD1	2:U:131:SER:N	2.40	0.54
1:A:54:GLU:OE1	2:T:453:LYS:NZ	2.39	0.54
2:V:331:THR:HG23	2:V:338:TYR:HA	1.89	0.54
2:V:71:VAL:HG21	2:V:346:GLU:HG2	1.90	0.54
1:O:31:ILE:HG12	1:O:92:VAL:HG23	1.89	0.54
2:X:331:THR:HG21	2:X:339:ARG:HG3	1.89	0.54
1:L:35:LYS:HG2	1:L:47:ILE:HD11	1.90	0.53
2:T:231:GLN:NE2	2:W:194:TRP:O	2.41	0.53
1:H:29:GLY:HA3	1:H:67:ILE:HD12	1.91	0.53
1:B:84:THR:HG21	1:B:88:HIS:ND1	2.23	0.53
2:T:29:MET:HE3	2:T:377:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:LYS:HG2	1:J:47:ILE:HD11	1.91	0.52
1:A:5:ILE:HG13	1:A:6:THR:H	1.74	0.52
2:S:428:GLN:HA	2:S:438:VAL:HG21	1.90	0.52
1:L:84:THR:HG21	1:L:88:HIS:ND1	2.25	0.52
2:S:297:ARG:HH12	2:S:300:ALA:H	1.57	0.52
1:P:81:LYS:NZ	1:P:112:ASP:OD2	2.42	0.52
1:C:28:ASN:HB2	1:C:95:ALA:HB2	1.92	0.52
1:L:85:GLU:HG3	1:Q:5:ILE:O	2.09	0.52
2:X:297:ARG:HH12	2:X:300:ALA:H	1.57	0.52
1:D:5:ILE:HG13	1:D:6:THR:H	1.75	0.52
1:D:68:ASN:OD1	1:D:69:ALA:N	2.42	0.52
1:D:5:ILE:HG13	1:D:6:THR:N	2.25	0.51
2:S:297:ARG:NH1	2:U:277:GLU:OE1	2.44	0.51
2:U:204:SER:H	2:U:233:GLY:HA3	1.75	0.51
2:S:331:THR:HG23	2:S:338:TYR:HA	1.93	0.51
1:Q:99:GLN:HE21	1:Q:102:TYR:HB2	1.75	0.51
1:Q:31:ILE:HG12	1:Q:92:VAL:HG23	1.93	0.51
2:T:127:TRP:HE3	2:T:128:PRO:HD2	1.75	0.51
1:P:28:ASN:HB2	1:P:95:ALA:HB2	1.92	0.51
1:A:68:ASN:HB2	1:A:74:VAL:HG21	1.93	0.51
1:N:27:ALA:C	1:N:28:ASN:HD22	2.18	0.51
2:W:277:GLU:OE1	2:X:297:ARG:NH1	2.44	0.50
2:U:331:THR:HG23	2:U:338:TYR:HA	1.93	0.50
1:D:29:GLY:HA3	1:D:67:ILE:HD12	1.94	0.50
1:F:5:ILE:HG13	1:F:6:THR:H	1.77	0.49
2:X:331:THR:HG23	2:X:338:TYR:HA	1.94	0.49
1:K:85:GLU:HG2	1:K:85:GLU:O	2.10	0.49
2:X:40:SER:O	2:X:40:SER:OG	2.26	0.49
1:D:52:GLU:HG2	1:D:58:HIS:CE1	2.47	0.49
2:V:427:GLU:OE1	2:V:436:LYS:NZ	2.30	0.49
1:B:68:ASN:HB3	1:B:74:VAL:HG21	1.93	0.49
1:E:112:ASP:OD1	1:J:109:TYR:OH	2.28	0.49
1:R:27:ALA:C	1:R:28:ASN:HD22	2.21	0.49
1:B:35:LYS:HG2	1:B:47:ILE:HD11	1.95	0.48
2:U:2:PRO:HD2	2:U:472:GLU:HB3	1.95	0.48
2:W:2:PRO:HD2	2:W:472:GLU:HB3	1.95	0.48
2:T:2:PRO:HD2	2:T:472:GLU:HB3	1.96	0.48
2:W:108:VAL:HG23	2:W:109:ASN:N	2.28	0.48
2:V:2:PRO:HD2	2:V:472:GLU:HB3	1.95	0.48
1:I:85:GLU:HA	1:N:6:THR:O	2.14	0.48
1:P:31:ILE:HG12	1:P:92:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:99:GLN:HE21	1:P:102:TYR:HB2	1.78	0.48
2:X:410:PHE:HE2	2:X:425:MET:HE2	1.78	0.48
1:F:54:GLU:OE1	2:V:453:LYS:NZ	2.39	0.48
2:U:193:THR:HG22	2:U:198:ILE:HD13	1.96	0.48
1:K:68:ASN:HB3	1:K:74:VAL:HG21	1.95	0.48
2:T:186:ASP:OD2	2:T:203:SER:HB3	2.14	0.47
1:F:68:ASN:HB2	1:F:74:VAL:HG21	1.95	0.47
1:Q:117:ASP:OD1	1:Q:118:LEU:N	2.47	0.47
2:U:146:ARG:HD2	2:U:150:ARG:O	2.15	0.47
2:T:79:LEU:HD23	2:T:86:VAL:HG23	1.97	0.47
2:U:216:THR:HB	2:U:219:ALA:HB2	1.94	0.47
1:K:84:THR:HG21	1:K:88:HIS:CE1	2.50	0.47
2:V:168:ASP:OD1	2:V:170:SER:OG	2.29	0.47
1:M:116:PRO:HA	1:M:119:ILE:HG12	1.96	0.47
2:V:250:ILE:HG13	2:V:293:MET:HE1	1.97	0.47
1:M:85:GLU:O	1:M:85:GLU:HG2	2.13	0.47
2:S:294:GLU:OE2	2:S:307:HIS:NE2	2.39	0.47
1:I:68:ASN:HB3	1:I:74:VAL:HG21	1.96	0.47
2:V:331:THR:HG21	2:V:339:ARG:HG2	1.95	0.47
2:V:79:LEU:HD23	2:V:86:VAL:HG23	1.96	0.46
2:W:146:ARG:HD2	2:W:150:ARG:O	2.14	0.46
2:W:297:ARG:HH12	2:W:300:ALA:H	1.62	0.46
2:V:173:ASP:HB3	2:V:177:ALA:HB2	1.97	0.46
1:N:91:ALA:HB2	1:N:102:TYR:HD1	1.80	0.46
1:D:68:ASN:HB2	1:D:74:VAL:HG21	1.98	0.46
2:X:294:GLU:OE2	2:X:307:HIS:NE2	2.41	0.46
2:T:29:MET:CE	2:T:377:HIS:HB3	2.45	0.46
2:V:297:ARG:HG3	2:V:301:HIS:O	2.15	0.46
2:X:71:VAL:HG21	2:X:346:GLU:HG2	1.96	0.46
1:F:29:GLY:HA3	1:F:67:ILE:HD12	1.97	0.46
2:T:216:THR:HB	2:T:219:ALA:HB2	1.97	0.46
1:L:23:PHE:HE1	1:Q:16:LEU:HD21	1.81	0.46
1:A:29:GLY:HA3	1:A:67:ILE:HD12	1.98	0.46
2:T:290:ASP:OD1	2:T:290:ASP:N	2.48	0.46
2:T:297:ARG:HG3	2:T:301:HIS:O	2.15	0.46
1:D:15:GLN:HE22	1:I:14:SER:HB3	1.80	0.46
1:I:116:PRO:HA	1:I:119:ILE:HG12	1.96	0.46
1:M:68:ASN:HB3	1:M:74:VAL:HG21	1.98	0.46
1:A:118:LEU:HD11	1:B:118:LEU:HD23	1.97	0.45
1:P:117:ASP:OD2	1:P:117:ASP:N	2.47	0.45
1:G:68:ASN:HB2	1:G:74:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:TYR:HB3	1:F:40:PRO:HB2	1.98	0.45
1:B:55:ASP:OD2	1:B:56:GLY:N	2.50	0.45
1:K:46:GLN:CD	1:K:63:GLN:HG2	2.42	0.45
2:X:62:VAL:HG23	2:X:73:ARG:HG2	1.99	0.45
2:V:342:ASP:O	2:V:352:CYS:HA	2.17	0.45
2:W:35:GLU:HA	2:W:40:SER:HA	1.99	0.45
1:R:92:VAL:HG12	1:R:101:PHE:HB2	1.99	0.45
1:A:68:ASN:HB2	1:A:74:VAL:CG2	2.47	0.45
2:W:342:ASP:O	2:W:352:CYS:HA	2.17	0.45
1:C:99:GLN:HE21	1:C:102:TYR:HB2	1.81	0.45
2:S:62:VAL:HG23	2:S:73:ARG:HG2	1.99	0.45
1:Q:46:GLN:CD	1:Q:63:GLN:HG2	2.41	0.45
1:J:85:GLU:O	1:J:85:GLU:HG2	2.16	0.45
1:H:20:ALA:C	1:H:21:ARG:HD2	2.41	0.45
1:O:46:GLN:CD	1:O:63:GLN:HG2	2.42	0.45
1:L:46:GLN:CD	1:L:63:GLN:HG2	2.42	0.45
1:J:116:PRO:HA	1:J:119:ILE:HG12	1.98	0.44
2:U:379:LEU:HD12	2:U:379:LEU:HA	1.74	0.44
2:X:186:ASP:OD2	2:X:203:SER:HB3	2.17	0.44
1:J:23:PHE:HE1	1:O:16:LEU:HD21	1.83	0.44
1:O:28:ASN:HB2	1:O:95:ALA:HB2	1.99	0.44
2:V:29:MET:CE	2:V:377:HIS:HB3	2.46	0.44
1:H:68:ASN:HB2	1:H:74:VAL:HG21	1.98	0.44
2:X:35:GLU:HA	2:X:40:SER:HA	1.99	0.44
2:W:331:THR:HG23	2:W:338:TYR:HA	1.98	0.44
1:I:46:GLN:CD	1:I:63:GLN:HG2	2.43	0.44
1:J:46:GLN:CD	1:J:63:GLN:HG2	2.43	0.44
2:U:186:ASP:OD2	2:U:203:SER:HB3	2.18	0.44
1:H:88:HIS:NE2	1:H:90:MET:HE3	2.31	0.44
1:L:116:PRO:HA	1:L:119:ILE:HG12	1.99	0.44
2:X:2:PRO:HD2	2:X:472:GLU:HB3	2.00	0.44
2:X:345:TYR:HD1	2:X:350:ILE:HG13	1.82	0.44
1:F:68:ASN:HB2	1:F:74:VAL:CG2	2.48	0.44
2:W:252:ASN:OD1	2:W:253:PRO:HD2	2.18	0.44
1:M:46:GLN:CD	1:M:63:GLN:HG2	2.42	0.44
2:X:34:LYS:HA	2:X:34:LYS:HD2	1.78	0.44
2:T:204:SER:H	2:T:233:GLY:HA3	1.82	0.44
2:S:173:ASP:HB3	2:S:177:ALA:HB2	2.00	0.44
2:X:410:PHE:CE2	2:X:425:MET:HE2	2.53	0.44
2:U:35:GLU:HA	2:U:40:SER:HA	1.99	0.44
1:O:91:ALA:HB2	1:O:102:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:216:THR:HB	2:W:219:ALA:HB2	2.00	0.43
2:S:2:PRO:HD2	2:S:472:GLU:HB3	2.00	0.43
2:V:143:ASP:HB3	2:V:191:ILE:HG22	1.99	0.43
1:C:117:ASP:HA	1:C:120:GLU:HG3	1.99	0.43
2:U:118:ASP:OD1	2:U:118:ASP:N	2.51	0.43
2:V:118:ASP:OD1	2:V:118:ASP:N	2.51	0.43
2:W:118:ASP:OD1	2:W:118:ASP:N	2.51	0.43
1:J:105:ASN:ND2	1:J:108:LYS:O	2.51	0.43
2:T:193:THR:HG22	2:T:198:ILE:HD13	1.99	0.43
2:T:292:VAL:HG21	2:T:341:ILE:HD11	1.99	0.43
1:N:46:GLN:CD	1:N:63:GLN:HG2	2.44	0.43
2:S:342:ASP:O	2:S:352:CYS:HA	2.19	0.43
2:V:186:ASP:OD2	2:V:203:SER:HB3	2.19	0.43
1:E:11:GLY:O	1:O:90:MET:HE1	2.19	0.43
2:S:35:GLU:HA	2:S:40:SER:HA	2.00	0.43
1:J:12:MET:HE3	1:J:12:MET:HB3	1.90	0.43
1:B:85:GLU:HA	1:C:6:THR:O	2.19	0.43
2:U:252:ASN:OD1	2:U:253:PRO:HD2	2.19	0.43
2:V:35:GLU:HA	2:V:40:SER:HA	2.01	0.43
2:V:193:THR:HG22	2:V:198:ILE:HD13	2.00	0.43
2:X:408:ARG:HA	2:X:427:GLU:HA	2.01	0.43
1:B:116:PRO:HA	1:B:119:ILE:HG12	2.00	0.42
2:T:118:ASP:OD1	2:T:118:ASP:N	2.51	0.42
1:N:117:ASP:O	1:N:120:GLU:HG3	2.18	0.42
1:R:46:GLN:CD	1:R:63:GLN:HG2	2.43	0.42
1:D:68:ASN:HB2	1:D:74:VAL:CG2	2.50	0.42
1:D:88:HIS:NE2	1:D:90:MET:HE3	2.34	0.42
2:X:36:ILE:HG13	2:X:37:LEU:N	2.34	0.42
2:T:162:PHE:HA	2:T:177:ALA:O	2.20	0.42
2:W:193:THR:HG22	2:W:198:ILE:HD13	2.00	0.42
1:A:20:ALA:C	1:A:21:ARG:HD2	2.44	0.42
1:D:94:ASP:OD1	1:D:98:SER:N	2.49	0.42
2:S:168:ASP:OD1	2:S:170:SER:OG	2.32	0.42
2:V:162:PHE:HA	2:V:177:ALA:O	2.20	0.42
2:W:204:SER:H	2:W:233:GLY:HA3	1.85	0.42
1:R:117:ASP:O	1:R:120:GLU:HG3	2.19	0.42
2:T:35:GLU:HA	2:T:40:SER:HA	2.01	0.42
2:U:174:ARG:H	2:U:174:ARG:HG2	1.69	0.42
1:P:46:GLN:CD	1:P:63:GLN:HG2	2.44	0.42
1:C:46:GLN:CD	1:C:63:GLN:HG2	2.44	0.42
1:E:68:ASN:HB2	1:E:74:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:7:PRO:O	2:V:382:PRO:HD2	2.20	0.42
2:W:95:VAL:HG12	2:W:108:VAL:HG12	2.02	0.42
1:H:6:THR:HA	1:R:85:GLU:HB3	2.02	0.42
2:X:293:MET:HA	2:X:305:ILE:O	2.20	0.42
2:V:379:LEU:HD12	2:V:379:LEU:HA	1.84	0.42
2:S:252:ASN:OD1	2:S:253:PRO:HD2	2.20	0.42
1:P:35:LYS:HB2	1:P:38:THR:OG1	2.19	0.42
1:B:46:GLN:CD	1:B:63:GLN:HG2	2.45	0.42
2:T:250:ILE:HG13	2:T:293:MET:HE1	2.02	0.42
2:V:204:SER:H	2:V:233:GLY:HA3	1.85	0.42
1:B:34:GLY:HA2	1:B:46:GLN:HA	2.01	0.41
2:U:179:TYR:OH	2:U:220:ALA:O	2.30	0.41
2:W:183:SER:HB2	2:W:207:GLU:OE2	2.20	0.41
1:H:79:ILE:HD13	1:R:101:PHE:HE1	1.85	0.41
2:X:252:ASN:OD1	2:X:253:PRO:HD2	2.20	0.41
1:A:32:TYR:HB3	1:A:40:PRO:HB2	2.02	0.41
1:B:63:GLN:HB3	1:B:64:PRO:HD3	2.01	0.41
1:N:104:GLN:NE2	2:S:423:GLU:OE1	2.53	0.41
1:P:19:MET:HG3	1:P:26:VAL:HG22	2.02	0.41
2:V:243:PHE:CE2	2:V:304:LEU:HB2	2.55	0.41
2:X:179:TYR:CE1	2:X:222:TYR:HB2	2.55	0.41
2:X:201:PHE:HB3	2:X:234:ILE:HD13	2.02	0.41
2:T:153:TRP:CD1	2:T:153:TRP:N	2.89	0.41
2:S:293:MET:HA	2:S:305:ILE:O	2.20	0.41
2:U:297:ARG:HH12	2:U:300:ALA:H	1.69	0.41
1:R:84:THR:HG21	1:R:88:HIS:CE1	2.56	0.41
2:X:204:SER:H	2:X:233:GLY:HA3	1.86	0.41
1:C:19:MET:HG3	1:C:26:VAL:HG22	2.01	0.41
2:T:302:GLU:HB2	2:T:317:ALA:HB3	2.02	0.41
2:S:470:ARG:HE	2:S:472:GLU:HG2	1.86	0.41
1:G:68:ASN:HB2	1:G:74:VAL:CG2	2.51	0.41
2:W:259:SER:HB3	2:W:261:TYR:CE2	2.56	0.41
2:T:155:LYS:HB3	2:T:158:THR:OG1	2.20	0.41
2:S:195:ARG:O	2:U:229:MET:HE1	2.21	0.41
1:Q:112:ASP:C	1:Q:113:GLN:HG2	2.46	0.41
2:W:229:MET:HE1	2:X:195:ARG:O	2.21	0.41
2:T:243:PHE:CE2	2:T:304:LEU:HB2	2.56	0.41
1:I:88:HIS:CE1	1:N:8:VAL:HG11	2.55	0.41
2:S:36:ILE:HG13	2:S:37:LEU:N	2.34	0.41
2:S:395:GLU:HG3	2:S:439:LEU:HB3	2.03	0.41
1:J:85:GLU:HA	1:O:6:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:162:PHE:HA	2:U:177:ALA:O	2.21	0.41
2:U:183:SER:HB2	2:U:207:GLU:OE2	2.20	0.41
2:U:259:SER:HB3	2:U:261:TYR:CE2	2.56	0.41
1:L:108:LYS:HA	1:L:108:LYS:HD3	1.92	0.41
2:X:470:ARG:HE	2:X:472:GLU:HG2	1.86	0.41
1:B:46:GLN:HB3	1:B:63:GLN:HE21	1.85	0.41
1:I:88:HIS:HE1	1:N:8:VAL:HG11	1.85	0.41
2:W:162:PHE:HA	2:W:177:ALA:O	2.21	0.41
2:T:243:PHE:HE2	2:T:304:LEU:HB2	1.86	0.40
2:S:179:TYR:CE1	2:S:222:TYR:HB2	2.56	0.40
2:V:97:MET:HG2	2:V:106:VAL:HG22	2.03	0.40
1:L:33:ILE:HG23	1:L:88:HIS:CD2	2.57	0.40
2:T:435:ASP:OD1	2:T:435:ASP:N	2.54	0.40
2:S:259:SER:HB3	2:S:261:TYR:CE2	2.57	0.40
2:V:127:TRP:CE3	2:V:128:PRO:HD2	2.50	0.40
2:V:186:ASP:OD1	2:V:186:ASP:N	2.54	0.40
1:E:68:ASN:HB2	1:E:74:VAL:CG2	2.51	0.40
1:E:114:PHE:HB2	1:O:7:ASN:OD1	2.21	0.40
1:O:34:GLY:HA3	1:O:40:PRO:HB3	2.03	0.40
1:P:90:MET:HG2	1:P:92:VAL:HG23	2.02	0.40
2:U:437:ARG:HG2	2:U:439:LEU:HD23	2.02	0.40
2:V:259:SER:HB3	2:V:261:TYR:CE2	2.57	0.40
2:V:302:GLU:HB2	2:V:317:ALA:HB3	2.04	0.40
1:H:52:GLU:HG2	1:H:58:HIS:CE1	2.56	0.40
2:T:34:LYS:HA	2:T:34:LYS:HD2	1.82	0.40
1:D:44:GLU:O	1:D:45:ASN:HB2	2.21	0.40
2:S:127:TRP:HE3	2:S:128:PRO:HD2	1.86	0.40
1:E:63:GLN:HB3	1:E:64:PRO:HD3	2.04	0.40
1:K:23:PHE:HE1	1:P:16:LEU:HD21	1.86	0.40
1:L:105:ASN:ND2	1:L:108:LYS:O	2.54	0.40
2:W:437:ARG:HG2	2:W:439:LEU:HD23	2.02	0.40
1:H:68:ASN:HB2	1:H:74:VAL:CG2	2.51	0.40
2:X:259:SER:HB3	2:X:261:TYR:CE2	2.57	0.40
2:X:395:GLU:HG3	2:X:439:LEU:HB3	2.02	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	A	118/623 (19%)	110 (93%)	8 (7%)	0	100	100
1	B	115/623 (18%)	110 (96%)	5 (4%)	0	100	100
1	C	119/623 (19%)	102 (86%)	17 (14%)	0	100	100
1	D	118/623 (19%)	108 (92%)	10 (8%)	0	100	100
1	E	118/623 (19%)	111 (94%)	7 (6%)	0	100	100
1	F	118/623 (19%)	112 (95%)	6 (5%)	0	100	100
1	G	118/623 (19%)	109 (92%)	9 (8%)	0	100	100
1	H	118/623 (19%)	110 (93%)	8 (7%)	0	100	100
1	I	115/623 (18%)	103 (90%)	12 (10%)	0	100	100
1	J	115/623 (18%)	104 (90%)	11 (10%)	0	100	100
1	K	115/623 (18%)	100 (87%)	15 (13%)	0	100	100
1	L	115/623 (18%)	104 (90%)	11 (10%)	0	100	100
1	M	115/623 (18%)	102 (89%)	13 (11%)	0	100	100
1	N	119/623 (19%)	106 (89%)	13 (11%)	0	100	100
1	O	119/623 (19%)	106 (89%)	13 (11%)	0	100	100
1	P	119/623 (19%)	105 (88%)	14 (12%)	0	100	100
1	Q	119/623 (19%)	102 (86%)	17 (14%)	0	100	100
1	R	119/623 (19%)	106 (89%)	13 (11%)	0	100	100
2	S	469/472 (99%)	429 (92%)	40 (8%)	0	100	100
2	T	469/472 (99%)	430 (92%)	39 (8%)	0	100	100
2	U	469/472 (99%)	428 (91%)	41 (9%)	0	100	100
2	V	469/472 (99%)	429 (92%)	40 (8%)	0	100	100
2	W	469/472 (99%)	426 (91%)	43 (9%)	0	100	100
2	X	469/472 (99%)	427 (91%)	42 (9%)	0	100	100
All	All	4926/14046 (35%)	4479 (91%)	447 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	102/519 (20%)	102 (100%)	0	100	100
1	B	99/519 (19%)	99 (100%)	0	100	100
1	C	103/519 (20%)	103 (100%)	0	100	100
1	D	102/519 (20%)	102 (100%)	0	100	100
1	E	102/519 (20%)	102 (100%)	0	100	100
1	F	102/519 (20%)	102 (100%)	0	100	100
1	G	102/519 (20%)	99 (97%)	3 (3%)	37	61
1	H	102/519 (20%)	102 (100%)	0	100	100
1	I	99/519 (19%)	99 (100%)	0	100	100
1	J	99/519 (19%)	99 (100%)	0	100	100
1	K	99/519 (19%)	99 (100%)	0	100	100
1	L	99/519 (19%)	99 (100%)	0	100	100
1	M	99/519 (19%)	99 (100%)	0	100	100
1	N	103/519 (20%)	103 (100%)	0	100	100
1	O	103/519 (20%)	103 (100%)	0	100	100
1	P	103/519 (20%)	102 (99%)	1 (1%)	68	83
1	Q	103/519 (20%)	102 (99%)	1 (1%)	68	83
1	R	103/519 (20%)	103 (100%)	0	100	100
2	S	392/393 (100%)	389 (99%)	3 (1%)	73	86
2	T	392/393 (100%)	384 (98%)	8 (2%)	48	72
2	U	392/393 (100%)	390 (100%)	2 (0%)	81	90
2	V	392/393 (100%)	388 (99%)	4 (1%)	68	83
2	W	392/393 (100%)	388 (99%)	4 (1%)	68	83
2	X	392/393 (100%)	389 (99%)	3 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4176/11700 (36%)	4147 (99%)	29 (1%)	73	88

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	129	THR
2	T	138	LEU
2	T	148	ARG
2	T	153	TRP
2	T	154	SER
2	T	155	LYS
2	T	170	SER
2	T	381	THR
2	S	22	ILE
2	S	427	GLU
2	S	430	GLU
2	U	379	LEU
2	U	381	THR
1	P	5	ILE
2	V	129	THR
2	V	130	ASP
2	V	131	SER
2	V	381	THR
1	G	4	ILE
1	G	5	ILE
1	G	6	THR
1	Q	5	ILE
2	W	346	GLU
2	W	348	ASN
2	W	379	LEU
2	W	381	THR
2	X	17	ARG
2	X	18	ASN
2	X	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	B	58	HIS
1	C	7	ASN

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Mol	Chain	Res	Type
1	C	15	GLN
2	T	225	GLN
2	T	449	ASN
1	D	48	GLN
1	D	58	HIS
1	D	104	GLN
1	D	105	ASN
1	I	48	GLN
1	I	76	ASN
1	I	88	HIS
1	N	7	ASN
1	N	15	GLN
2	S	18	ASN
2	S	225	GLN
1	E	48	GLN
1	E	105	ASN
1	J	48	GLN
1	J	121	GLN
2	U	178	GLN
2	U	322	ASN
1	F	15	GLN
1	F	48	GLN
1	K	48	GLN
1	K	88	HIS
1	P	7	ASN
1	P	15	GLN
1	P	121	GLN
2	V	225	GLN
2	V	449	ASN
1	G	15	GLN
1	G	100	GLN
1	G	105	ASN
1	L	15	GLN
1	L	48	GLN
1	Q	7	ASN
1	Q	121	GLN
2	W	225	GLN
2	W	348	ASN
1	H	48	GLN
1	H	105	ASN
1	M	15	GLN
1	M	48	GLN

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Mol	Chain	Res	Type
1	M	88	HIS
1	R	58	HIS
1	R	121	GLN
2	X	178	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](#)

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.

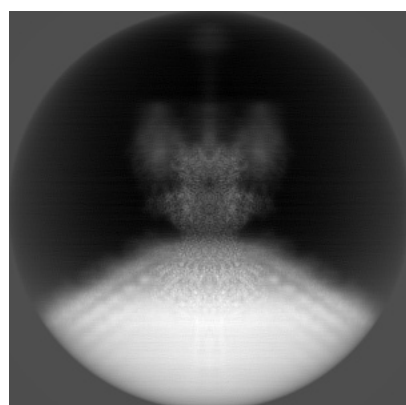
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25106. These allow visual inspection of the internal detail of the map and identification of artifacts.

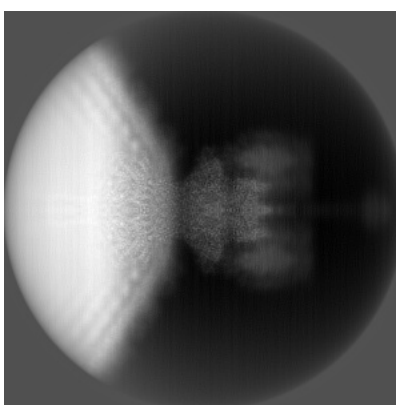
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

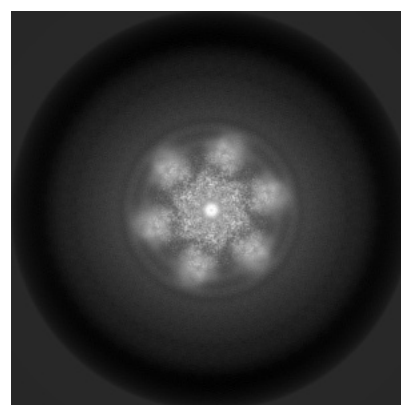
6.1.1 Primary map



X



Y

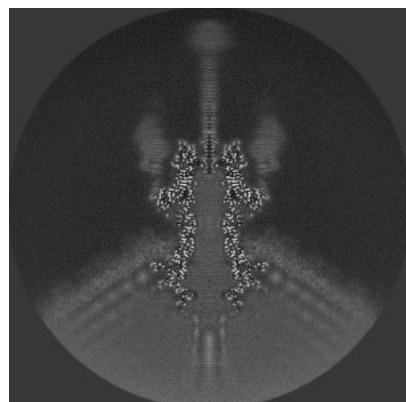


Z

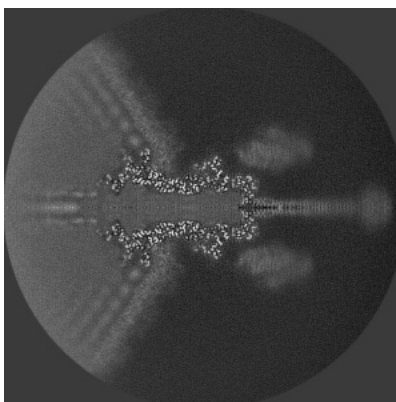
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

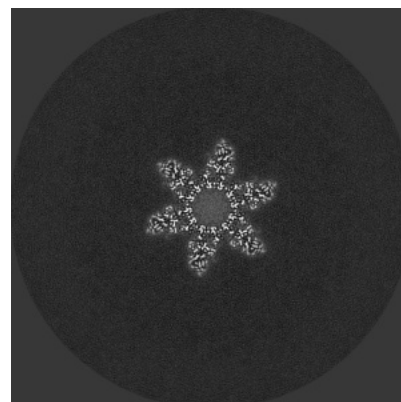
6.2.1 Primary map



X Index: 256



Y Index: 256

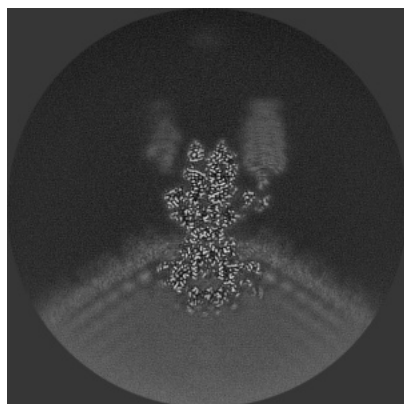


Z Index: 256

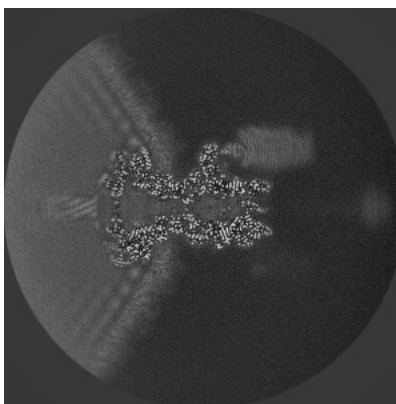
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

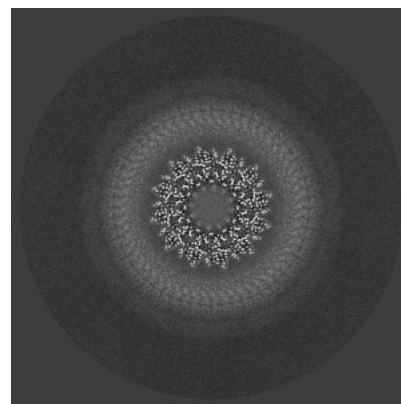
6.3.1 Primary map



X Index: 285



Y Index: 272

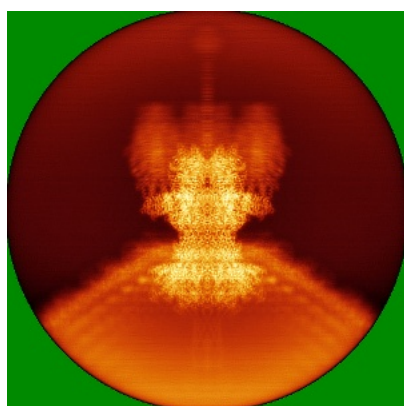


Z Index: 178

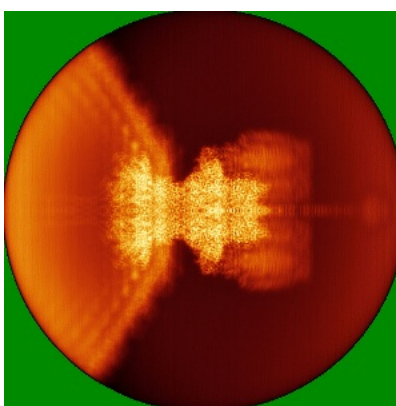
The images above show the largest variance slices of the map in three orthogonal directions.

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

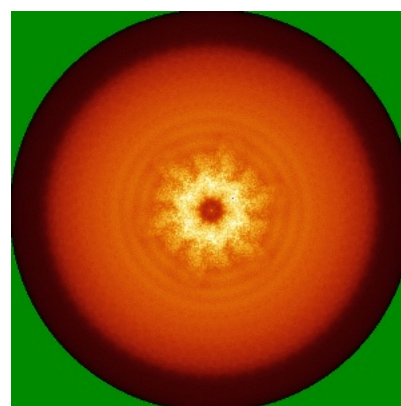
6.4.1 Primary map



X



Y

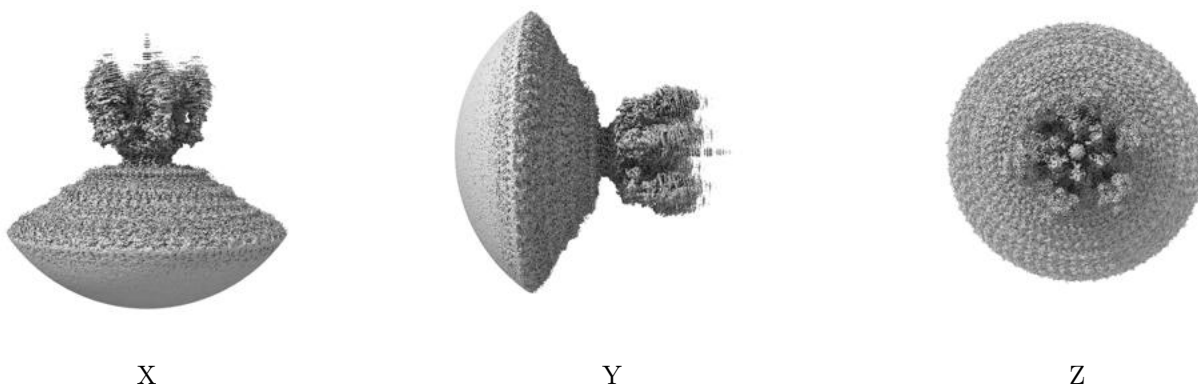


Z

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

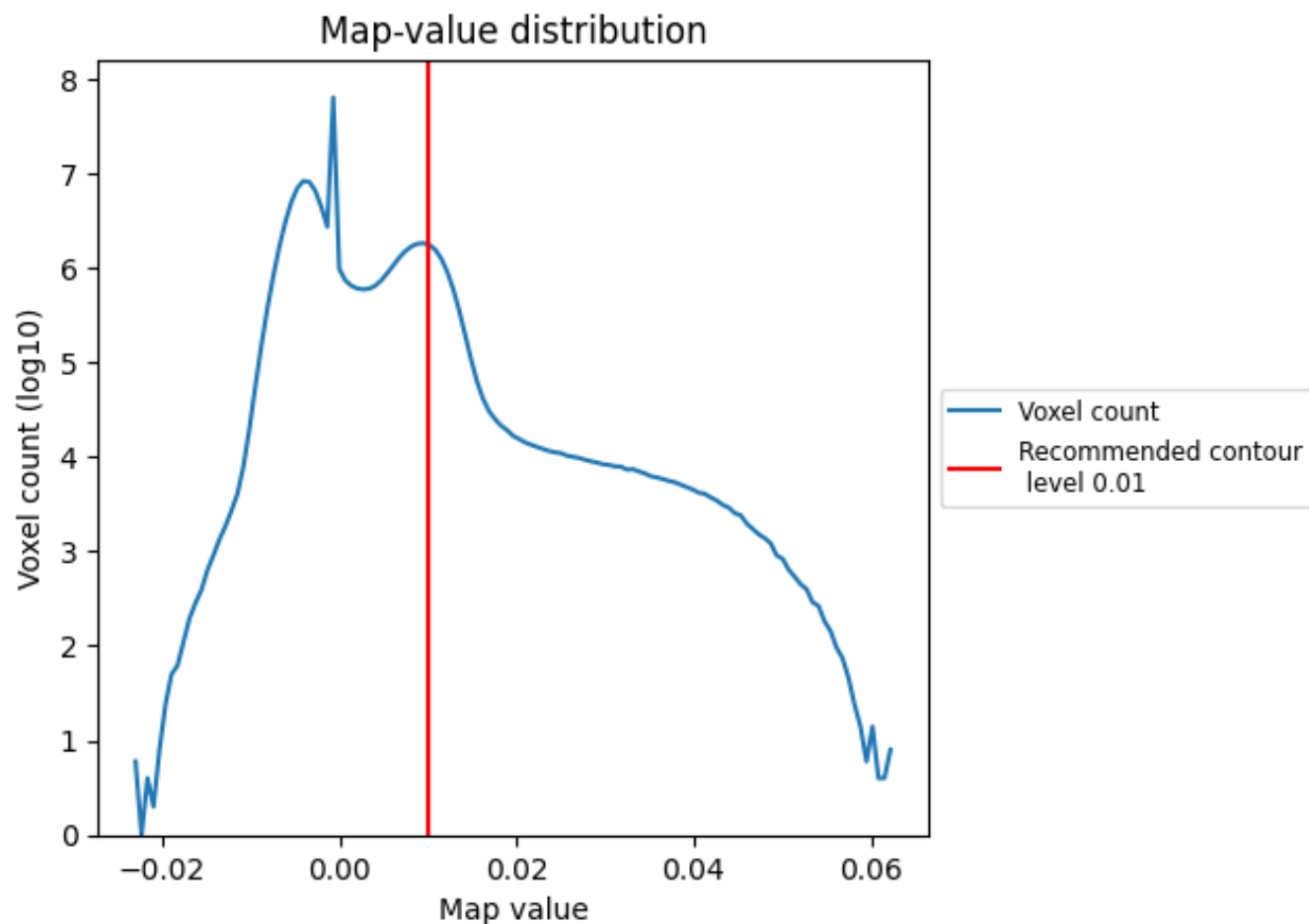
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

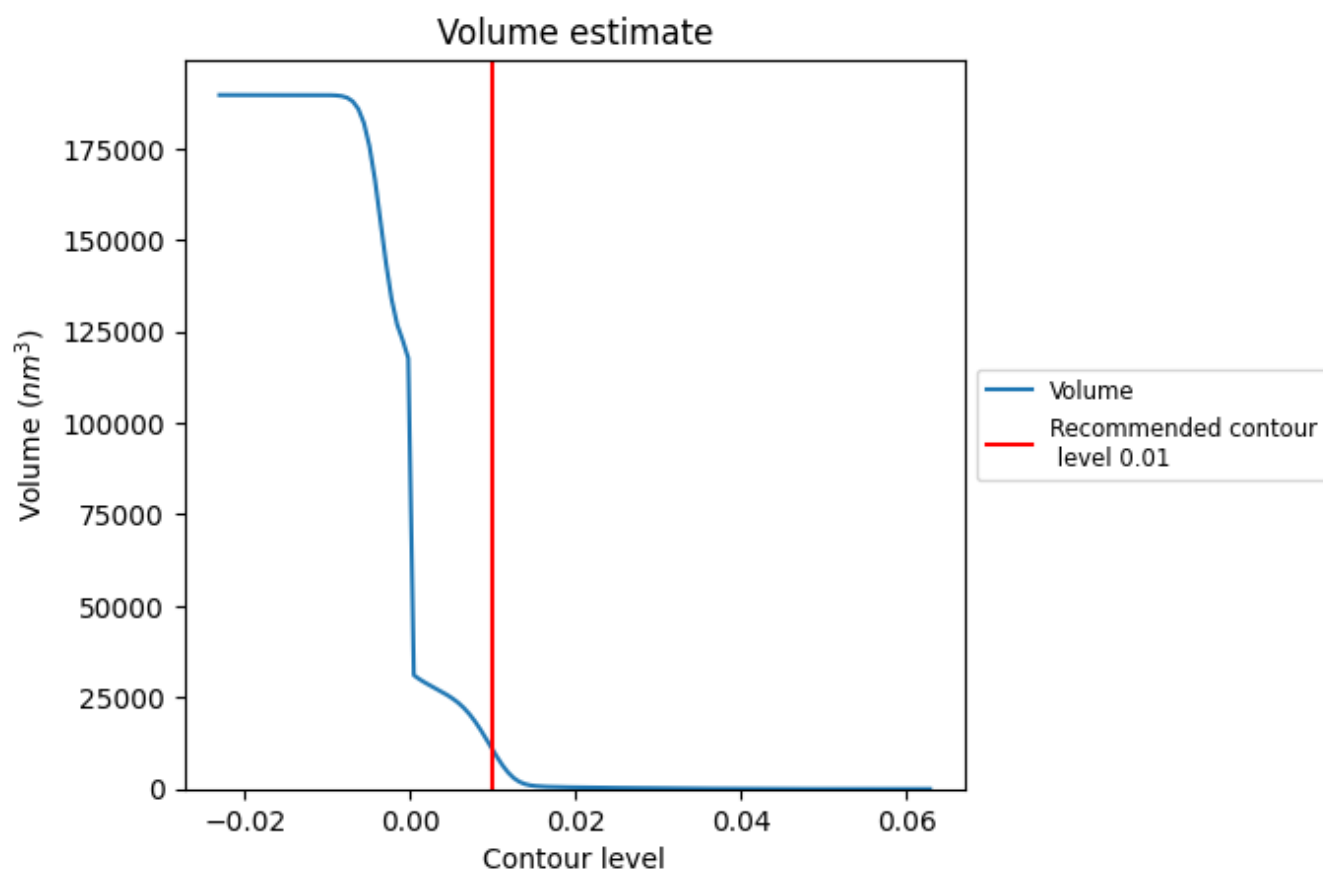
This section contains the results of statistical analysis of the map.

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.

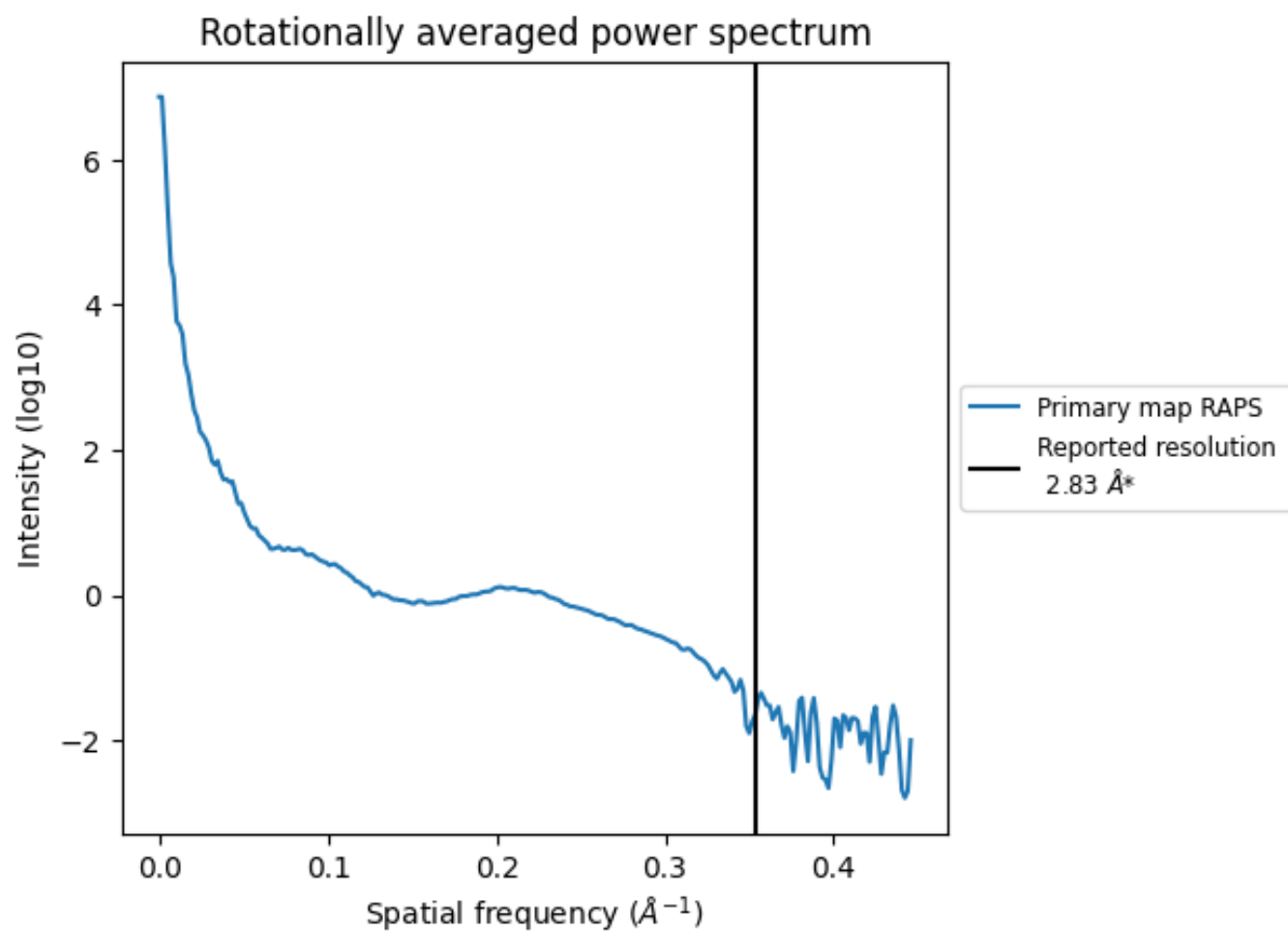
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10656 nm^3 ; this corresponds to an approximate mass of 9626 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 ⓘ

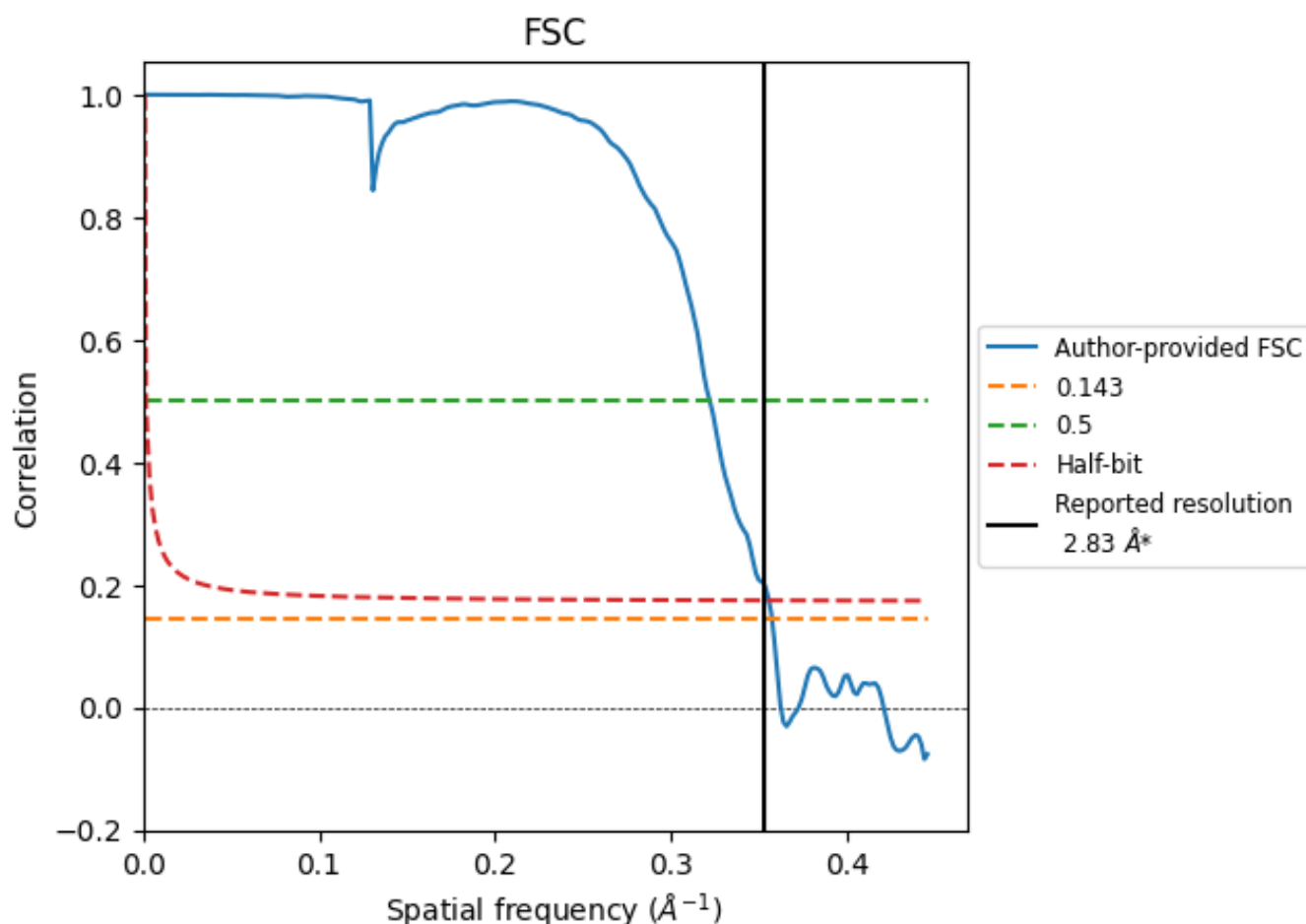


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

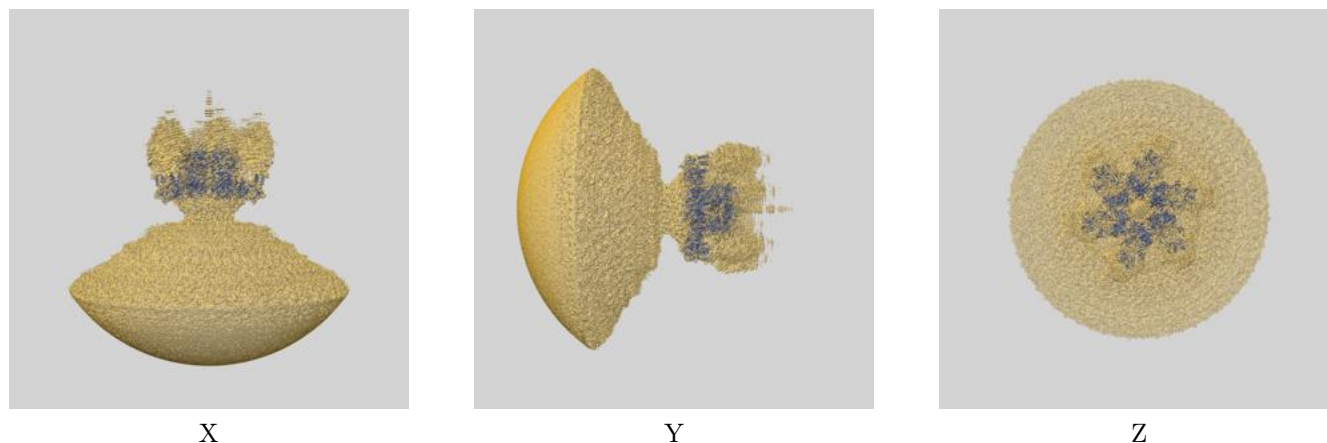
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.80	3.11	2.81
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

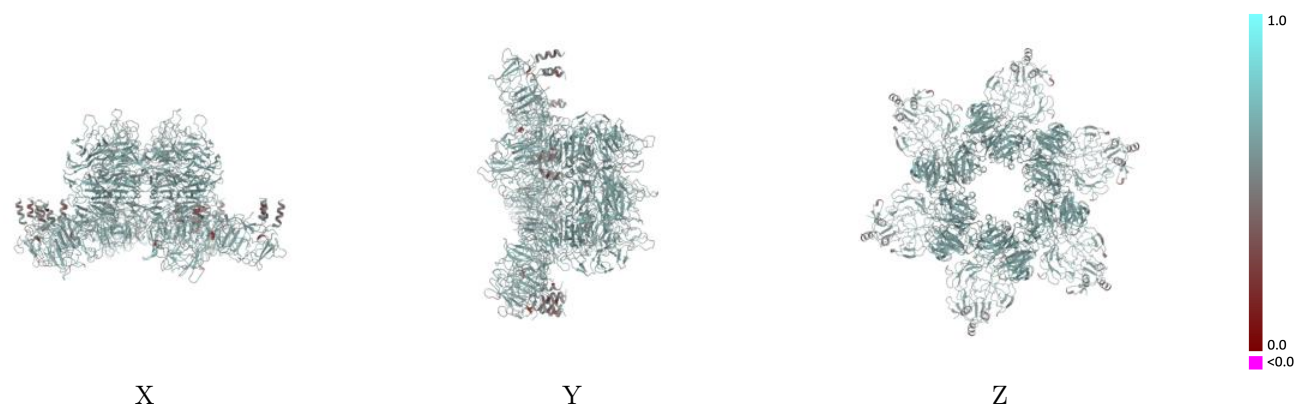
This section contains information regarding the fit between EMDB map EMD-25106 and PDB model 7SG7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



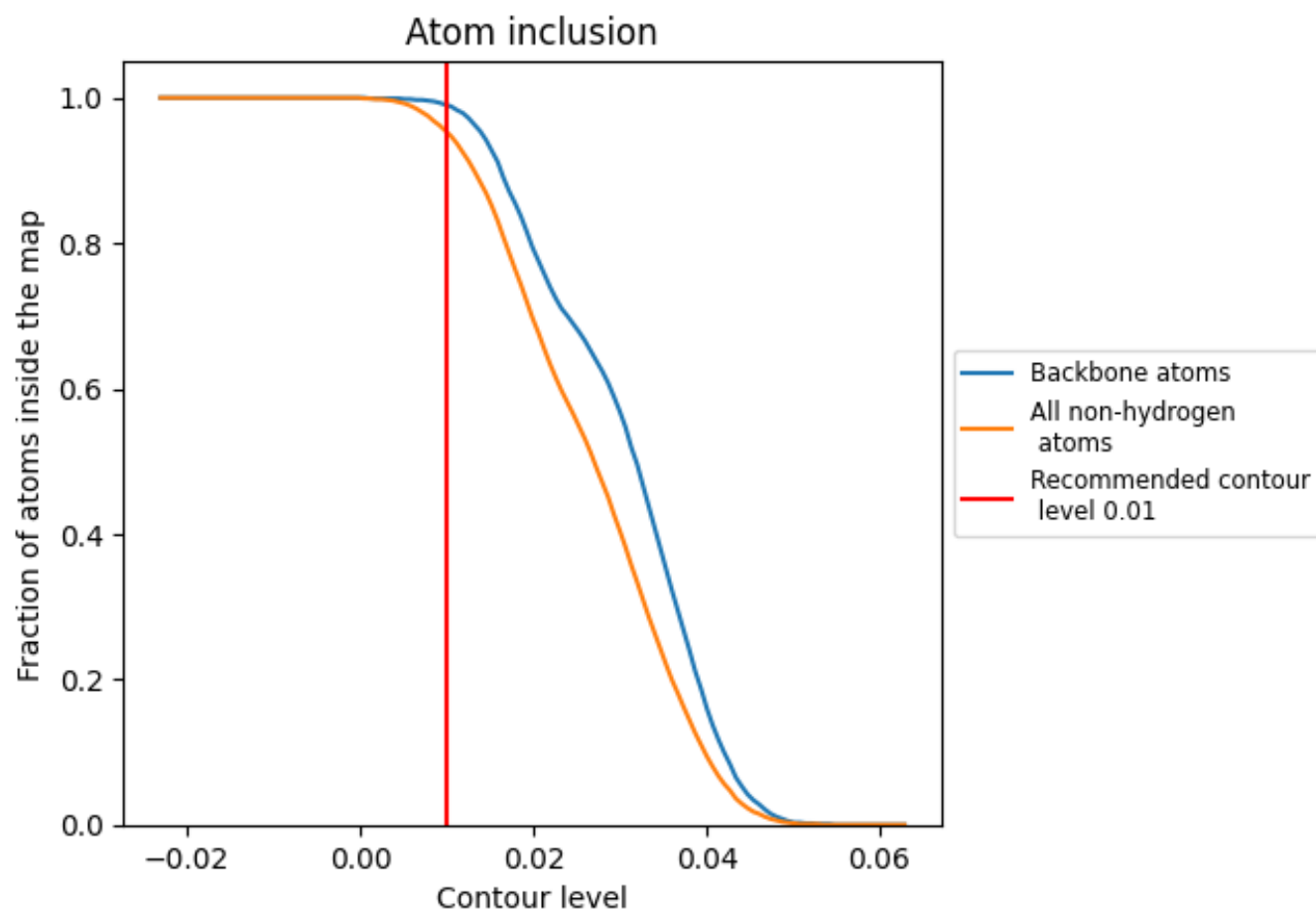
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.5720
A	 0.9550	 0.5710
B	 0.9310	 0.5490
C	 0.9420	 0.5530
D	 0.9590	 0.5690
E	 0.9570	 0.5680
F	 0.9550	 0.5710
G	 0.9550	 0.5690
H	 0.9550	 0.5670
I	 0.9370	 0.5380
J	 0.9310	 0.5390
K	 0.9290	 0.5390
L	 0.9370	 0.5380
M	 0.9360	 0.5360
N	 0.9430	 0.5550
O	 0.9510	 0.5570
P	 0.9480	 0.5570
Q	 0.9510	 0.5590
R	 0.9510	 0.5560
S	 0.9580	 0.5850
T	 0.9580	 0.5850
U	 0.9590	 0.5860
V	 0.9580	 0.5860
W	 0.9570	 0.5840
X	 0.9570	 0.5840

