



Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 06:00 PM JST

PDB ID : 8I4M
EMDB ID : EMD-35175
Title : Portal-tail complex structure of the Cyanophage P-SCSP1u
Authors : Liu, H.; Dang, S.
Deposited on : 2023-01-19
Resolution : 3.81 Å (reported)
Based on initial model : ?

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:

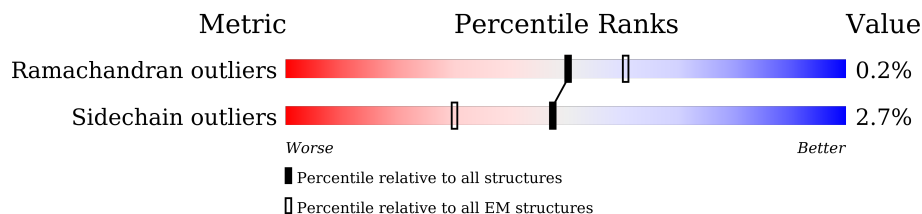
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.81 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	S	565	 14% 97% .
1	T	565	 14% 97% .
1	U	565	 14% 96% .
1	V	565	 14% 96% .
1	W	565	 14% 96% .
1	X	565	 14% 97% .
1	Y	565	 14% 97% .
1	Z	565	 14% 95% .
1	a	565	 13% 96% .

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Mol	Chain	Length	Quality of chain
1	b	565	14% 96%
1	c	565	14% 96%
1	d	565	14% 97%
2	A	806	98%
2	B	806	98%
2	C	806	98%
2	D	806	98%
2	E	806	98%
2	F	806	98%
3	G	200	96%
3	H	200	95%
3	I	200	96%
3	J	200	96%
3	K	200	97%
3	L	200	98%
3	q	200	97%
3	r	200	96%
3	s	200	98%
3	t	200	96%
3	u	200	97%
3	v	200	96%
4	M	1079	17% 82%
4	N	1079	18% 82%
4	O	1079	18% 82%
4	P	1079	17% 82%

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Mol	Chain	Length	Quality of chain
4	Q	1079	 18% 82%
4	R	1079	 18% 82%
4	e	1079	 17% 82%
4	f	1079	 18% 82%
4	g	1079	 17% 82%
4	h	1079	 17% 82%
4	i	1079	 17% 82%
4	j	1079	 18% 82%
4	k	1079	 18% 82%
4	l	1079	 17% 82%
4	m	1079	 18% 82%
4	n	1079	 17% 82%
4	o	1079	 18% 82%
4	p	1079	 18% 82%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 134400 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 Portal protein(gp 16) of the cyanophage P-SCSP1u.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	564	4368	2714	769	864	21	0	0
1	T	564	4368	2714	769	864	21	0	0
1	U	564	4368	2714	769	864	21	0	0
1	V	564	4368	2714	769	864	21	0	0
1	W	564	4368	2714	769	864	21	0	0
1	X	564	4368	2714	769	864	21	0	0
1	Y	564	4368	2714	769	864	21	0	0
1	Z	564	4368	2714	769	864	21	0	0
1	a	564	4368	2714	769	864	21	0	0
1	b	564	4368	2714	769	864	21	0	0
1	c	564	4368	2714	769	864	21	0	0
1	d	564	4368	2714	769	864	21	0	0

- Molecule 2 is a protein called Nozzle protein(gp 23) of the cyanophage P-SCSP1u.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	806	6159	3899	1022	1220	18	0	0
2	B	806	6159	3899	1022	1220	18	0	0
2	C	806	6159	3899	1022	1220	18	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	806	Total	C	N	O	S	0	0
			6159	3899	1022	1220	18		
2	E	806	Total	C	N	O	S	0	0
			6159	3899	1022	1220	18		
2	F	806	Total	C	N	O	S	0	0
			6159	3899	1022	1220	18		

- Molecule 3 is a protein called Adaptor protein(gp22) of the cyanophage P-SCSP1u.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	H	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	I	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	J	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	K	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	L	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	q	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	r	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	s	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	t	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	u	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		
3	v	198	Total	C	N	O	S	0	0
			1582	980	279	320	3		

- Molecule 4 is a protein called Fiber protein(gp 28) of the cyanophage P-SCSP1u.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	192	Total	C	N	O	S	0	0
			1447	898	244	304	1		
4	f	192	Total	C	N	O	S	0	0
			1447	898	244	304	1		

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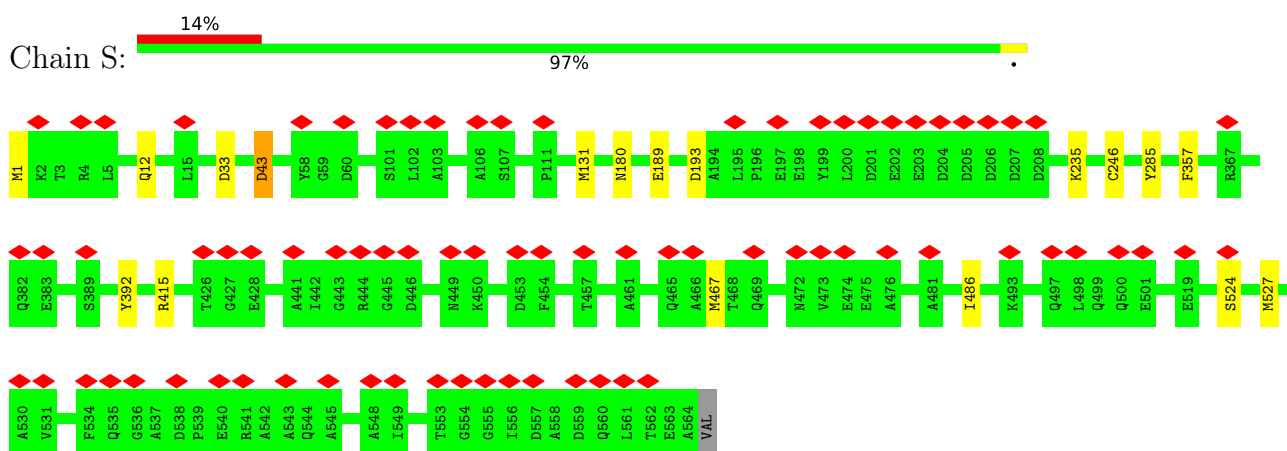
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	g	192	1447	898	244	304	1	0	0
4	h	192	1447	898	244	304	1	0	0
4	j	192	1447	898	244	304	1	0	0
4	l	192	1447	898	244	304	1	0	0
4	i	192	1447	898	244	304	1	0	0
4	k	192	1447	898	244	304	1	0	0
4	m	192	1447	898	244	304	1	0	0
4	n	192	1447	898	244	304	1	0	0
4	o	192	1447	898	244	304	1	0	0
4	p	192	1447	898	244	304	1	0	0
4	M	192	1447	898	244	304	1	0	0
4	N	192	1447	898	244	304	1	0	0
4	O	192	1447	898	244	304	1	0	0
4	P	192	1447	898	244	304	1	0	0
4	Q	192	1447	898	244	304	1	0	0
4	R	192	1447	898	244	304	1	0	0

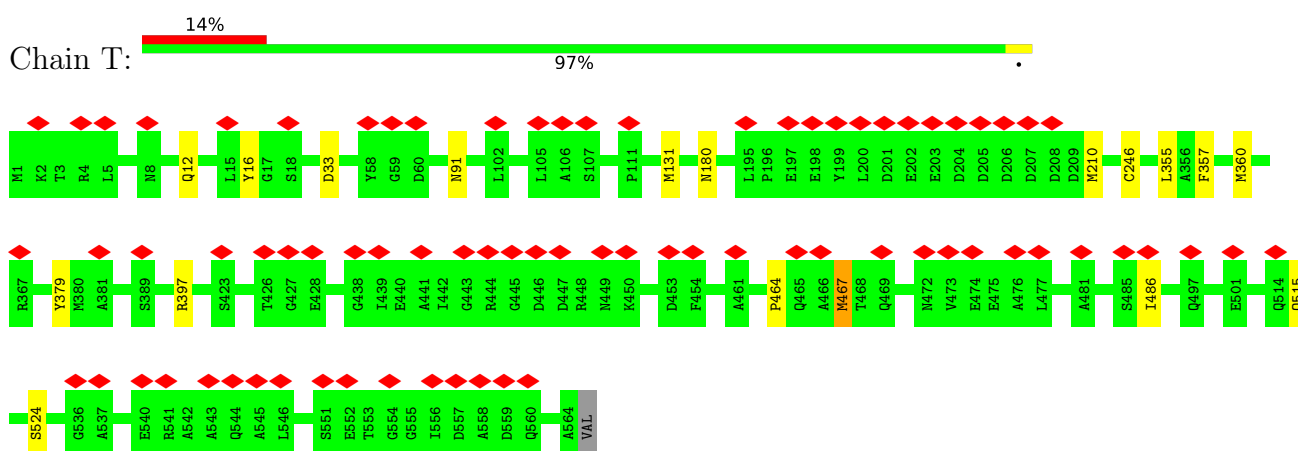
3 Residue-property plots

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.

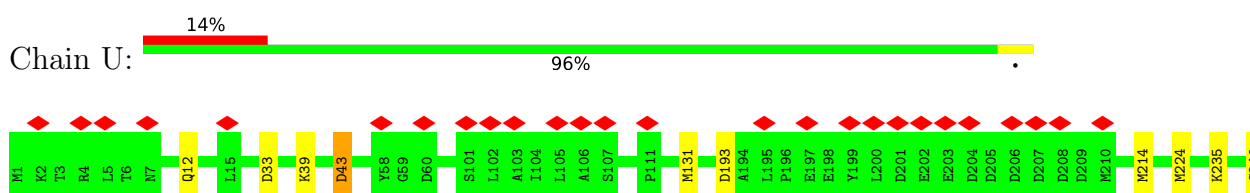
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u

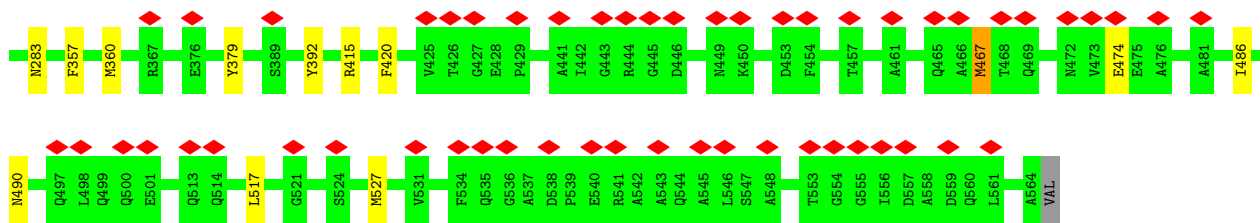


- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



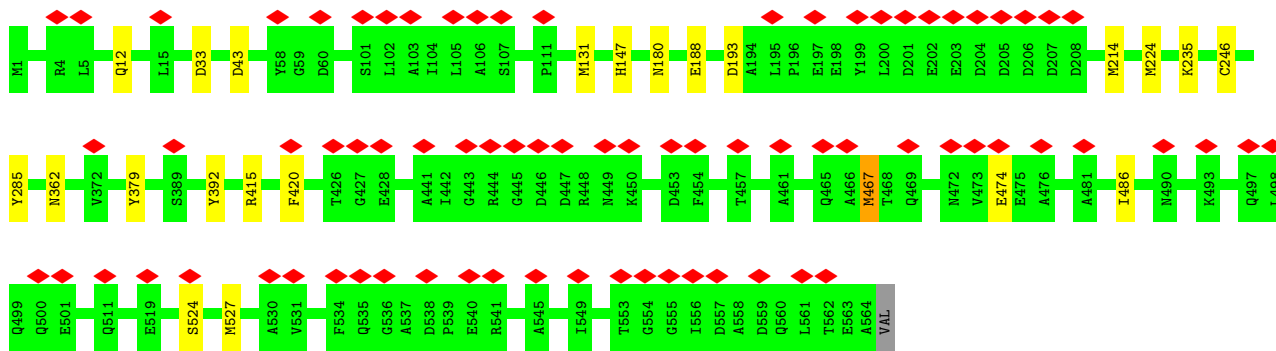
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u





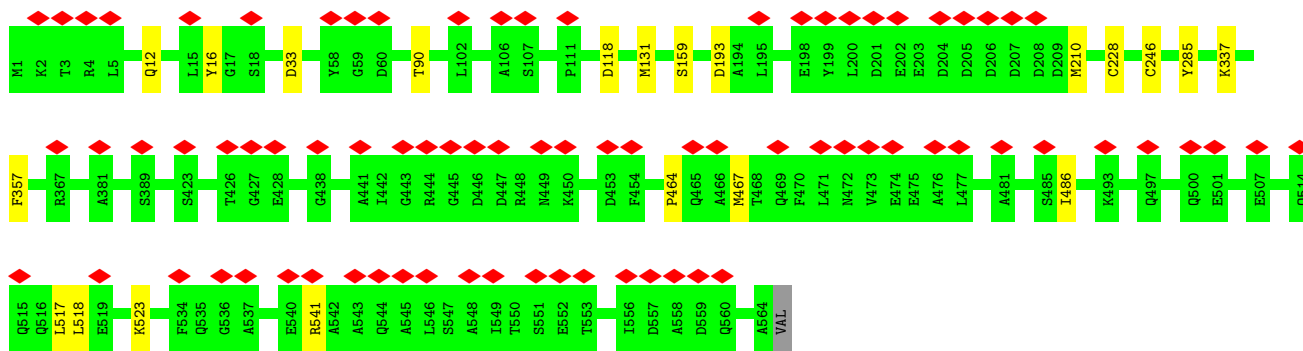
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u

Chain V: 14% 96%



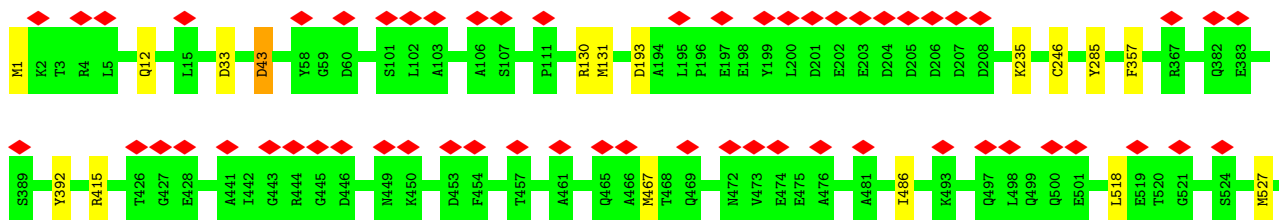
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u

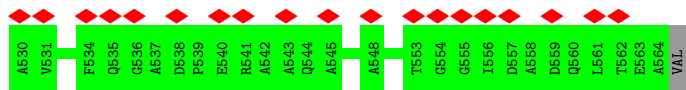
Chain W: 14% 96%



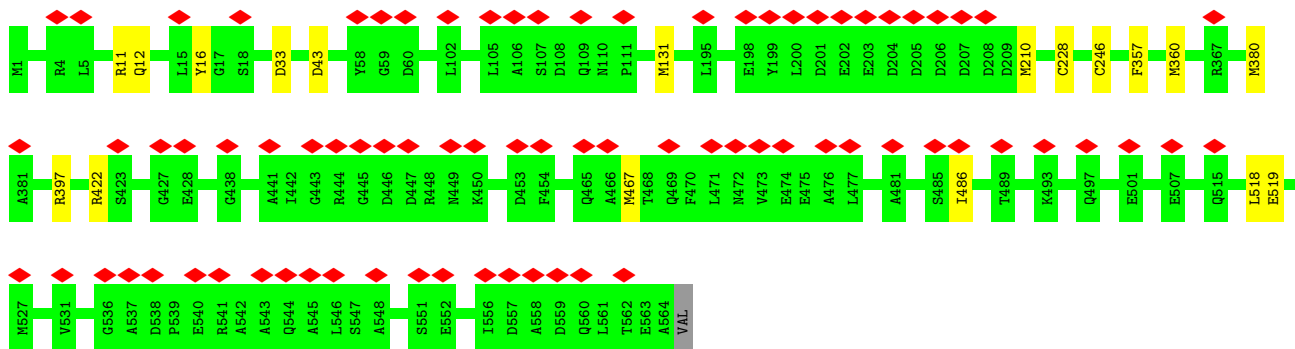
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u

Chain X: 14% 97%

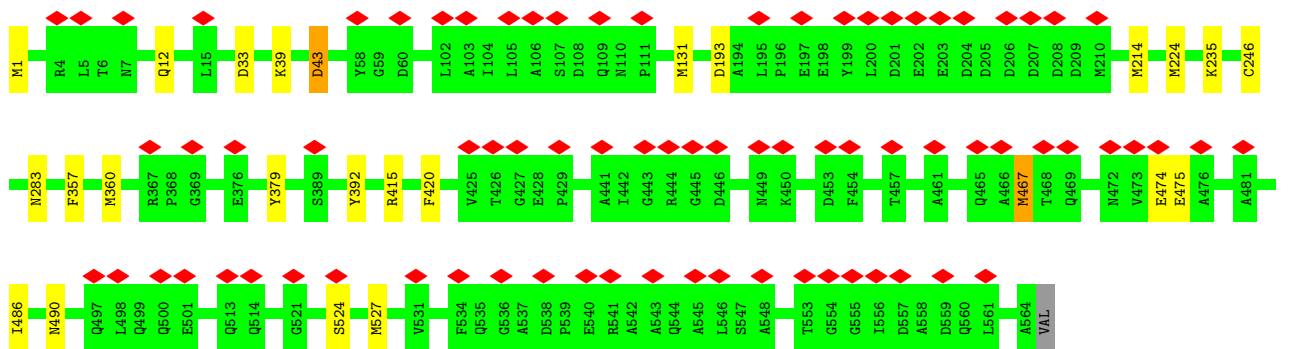




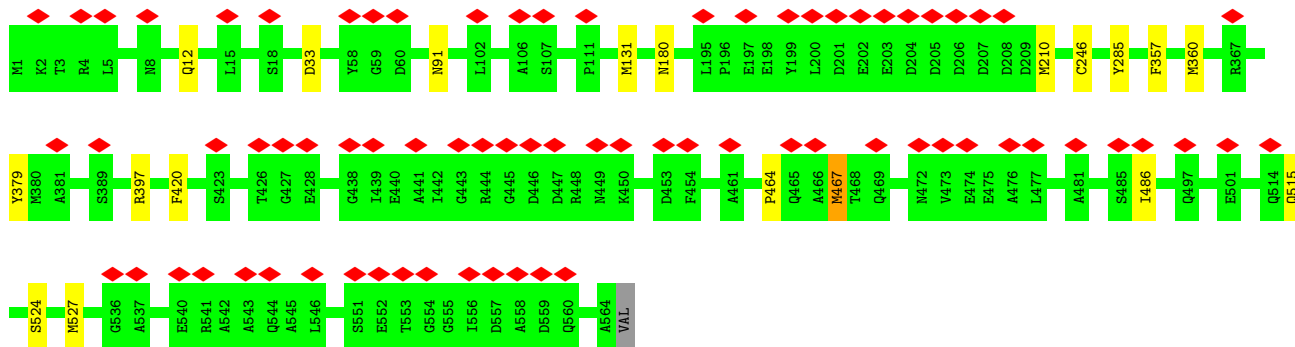
• Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



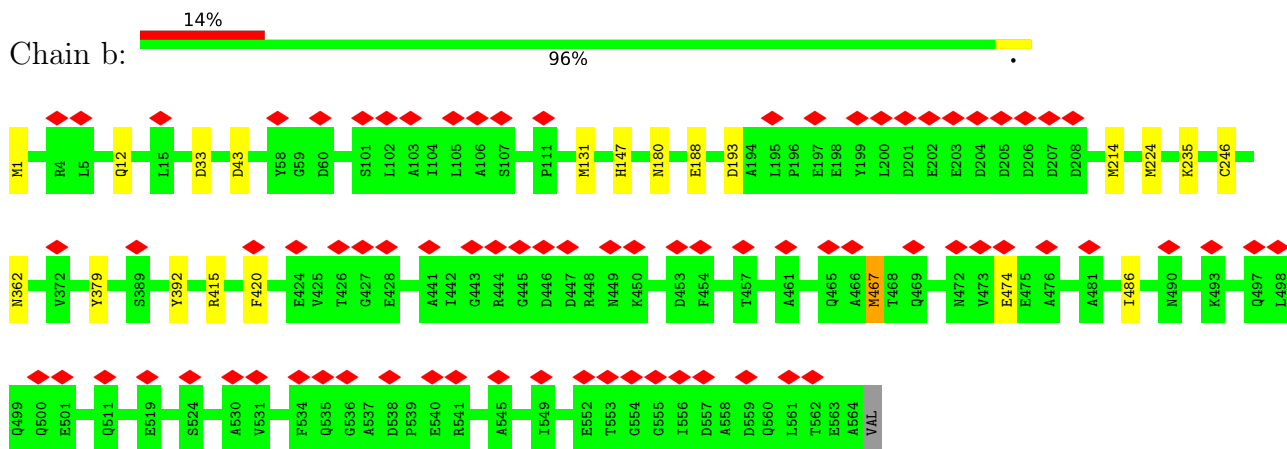
• Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



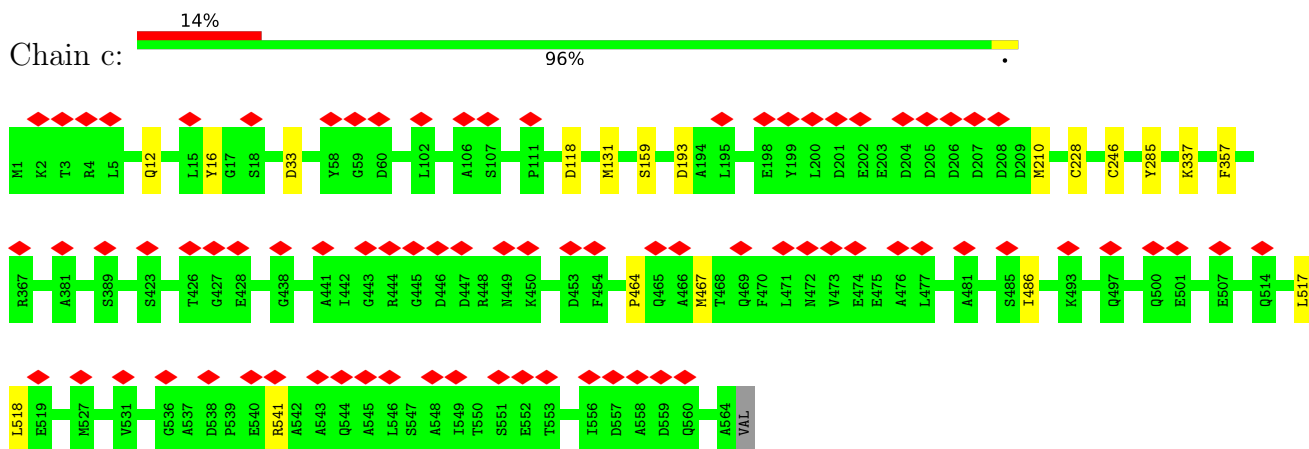
• Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



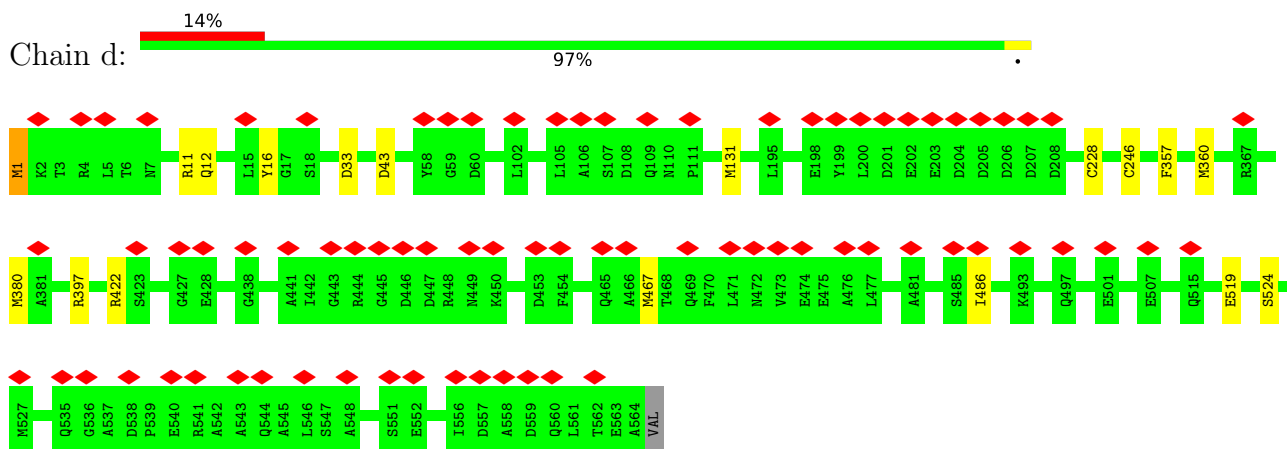
• Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



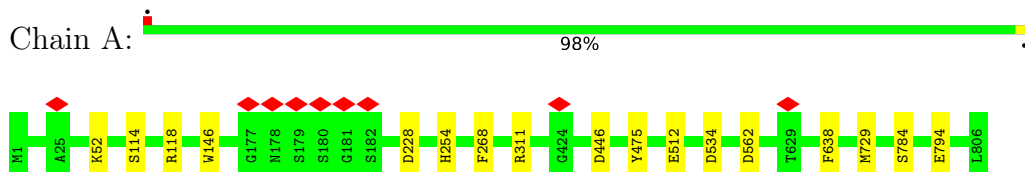
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



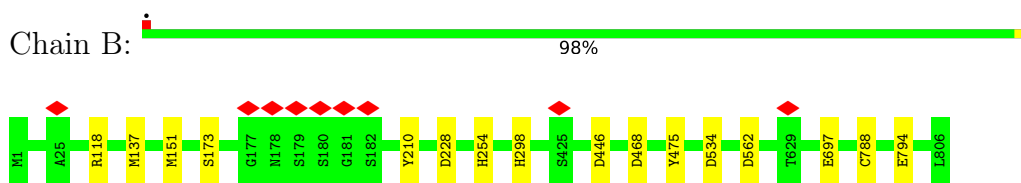
- Molecule 1: Portal protein(gp 16) of the cyanophage P-SCSP1u



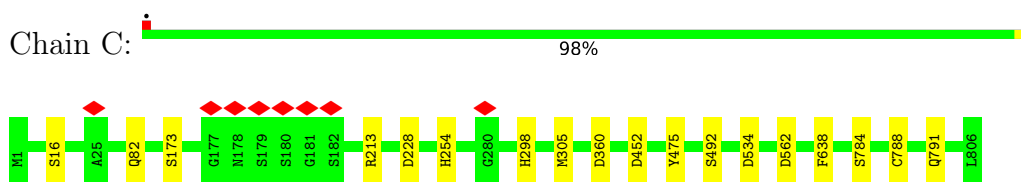
- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



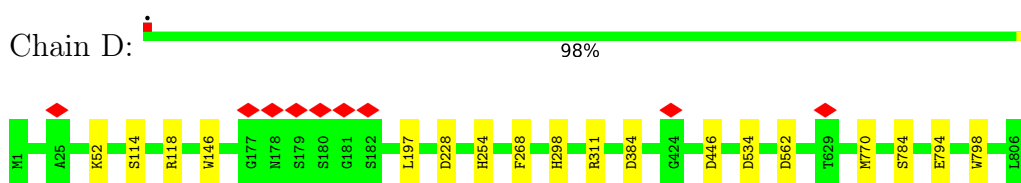
- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



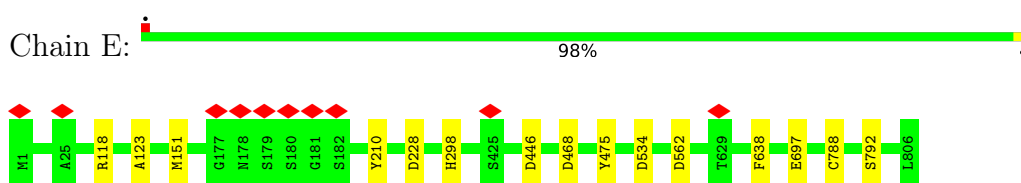
- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



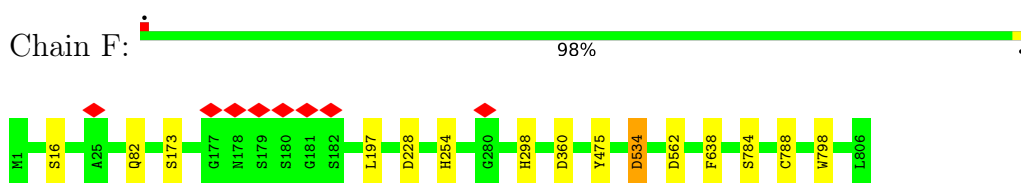
- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



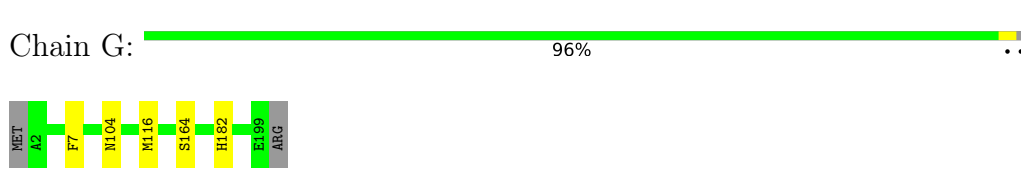
- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



- Molecule 2: Nozzle protein(gp 23) of the cyanophage P-SCSP1u



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u





- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

Chain I: 96%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

Chain J: 96%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

Chain K: 97%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

Chain L: 98%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

Chain q: 97%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

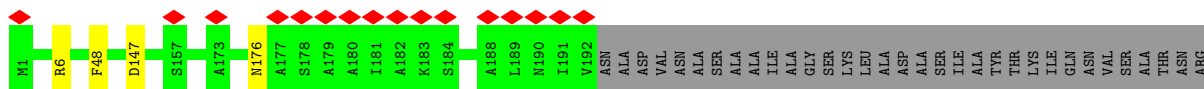
Chain r: 96%



- Molecule 3: Adaptor protein(gp22) of the cyanophage P-SCSP1u

PHE
LEU
ILE
ASN
LYS
ARG
THR
SER
LYS
TYR
LYS
PHE
ASN
LEU
THR
GLU
VAL
SER

• Molecule 4: Fiber protein(gp 28) of the cyanophage P-SCSP1u



ILE
LEU
GLY
ARG
ASP
SER
GLY
ALA
VAL
VAL
ILE
GLY
GLU
ILE

ASN
ALA
ILE
GLU
VAL
SER
THR
THR
VAL
VAL
ASN
VAL
VAL
ILE

THR
SER
GLN
PRO
LEU
ASP
SER
GLU
ASP
SER
ALA
GLY
MET
THR
SER
THR

VAL
VAL
ASN
PHE
ASP
VAL
ALA
VAL
ASN
GLN
ILE
PRO
ALA
VAL
GLY
ILE

SER
ASP
ASN
VAL
THR
ILE
LYS
ASN
PHE
PRO
ALA
SER
ARG
ASN
ASN
THR

TYR
ARG
VAL
GLU
ASN
THR
LEU
PRO
ALA
ASN
ALA
SER
SER
ASN
HIS
SER

ALA
PHE
GLY
SER
LEU
GLN
ASP
PHE
THR
ILE
ASN
ALA
PRO
ASN
THR

ASP
TYR
PHE
ALA
ILE
VAL
ASN
ILE
GLY
PRO
THR
SER
ASN
ASN
THR

GLY
ASP
GLY
SER
ASP
GLY
TYR
LEU
GLN
LEU
ASN
CYS
SER
SER
GLN
ILE

VAL
THR
ASP
VAL
ASN
THR
SER
PRO
GLN
LEU
GLY
GLY
ASN
ASN
THR

ASP
LEU
HIS
LEU
ARG
LEU
ASN
GLY
SER
VAL
ILE
VAL
VAL
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ALA
GLN
LEU
HIS
GLY
ASN
HIS
GLN
TYR

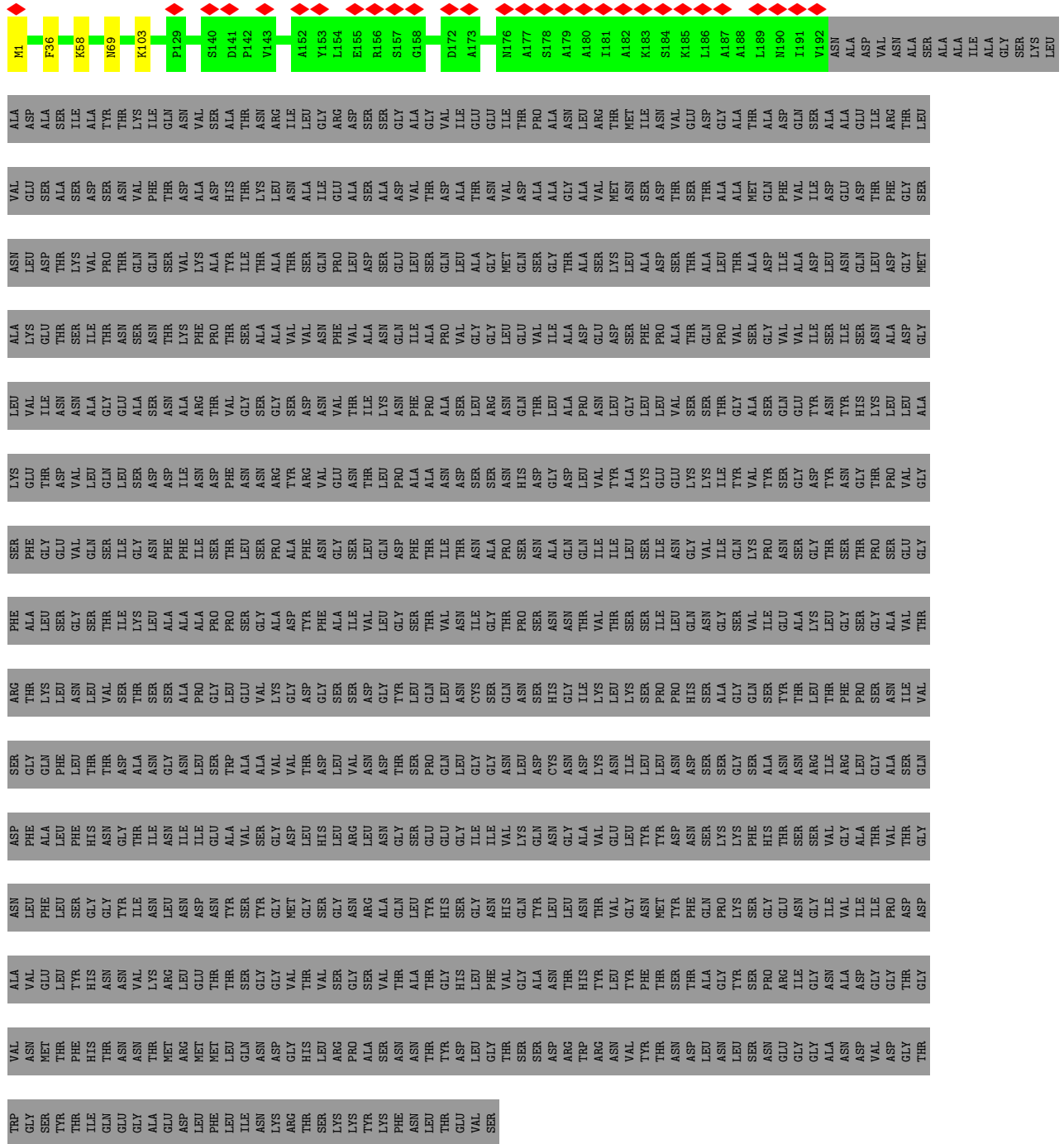
VAL
THR
VAL
SER
GLY
SER
VAL
THR
HIS
HIS
PHE
THR
HIS
THR

GLY
HIS
LEU
ARG
PRO
ALA
SER
ASN
ASN
TYR
TYR
ASP
LEU
GLY
THR

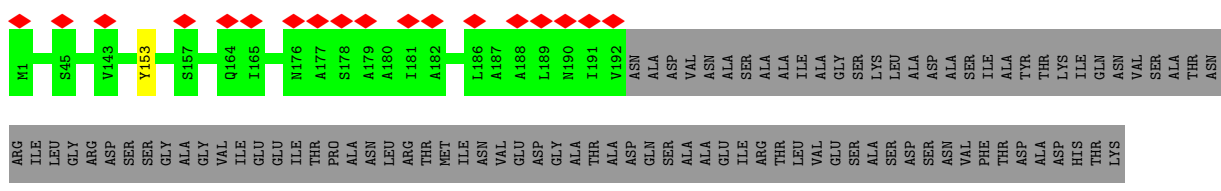
ARG
THR
SER
LYS
TYR
LYS
PHE
ASN
ASN
LEU
THR
GLU
VAL
SER

• Molecule 4: Fiber protein(gp 28) of the cyanophage P-SCSP1u





• Molecule 4: Fiber protein(gp 28) of the cyanophage P-SCSP1u



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	S	0.26	0/4428	0.56	2/5983 (0.0%)
1	T	0.27	0/4428	0.57	3/5983 (0.1%)
1	U	0.26	0/4428	0.57	4/5983 (0.1%)
1	V	0.27	0/4428	0.57	2/5983 (0.0%)
1	W	0.27	0/4428	0.57	3/5983 (0.1%)
1	X	0.26	0/4428	0.55	2/5983 (0.0%)
1	Y	0.26	0/4428	0.54	1/5983 (0.0%)
1	Z	0.26	0/4428	0.56	4/5983 (0.1%)
1	a	0.27	0/4428	0.57	3/5983 (0.1%)
1	b	0.27	0/4428	0.57	2/5983 (0.0%)
1	c	0.27	0/4428	0.58	3/5983 (0.1%)
1	d	0.26	0/4428	0.55	2/5983 (0.0%)
2	A	0.27	0/6293	0.52	1/8571 (0.0%)
2	B	0.27	0/6293	0.52	1/8571 (0.0%)
2	C	0.27	0/6293	0.52	0/8571
2	D	0.27	0/6293	0.53	1/8571 (0.0%)
2	E	0.27	0/6293	0.53	1/8571 (0.0%)
2	F	0.27	0/6293	0.53	1/8571 (0.0%)
3	G	0.27	0/1603	0.51	0/2171
3	H	0.29	0/1603	0.51	0/2171
3	I	0.27	0/1603	0.54	1/2171 (0.0%)
3	J	0.27	0/1603	0.51	0/2171
3	K	0.27	0/1603	0.52	0/2171
3	L	0.27	0/1603	0.51	0/2171
3	q	0.27	0/1603	0.51	0/2171
3	r	0.28	0/1603	0.51	0/2171
3	s	0.27	0/1603	0.53	1/2171 (0.0%)
3	t	0.28	0/1603	0.52	0/2171
3	u	0.27	0/1603	0.53	0/2171
3	v	0.27	0/1603	0.51	0/2171
4	M	0.26	0/1462	0.50	0/1985
4	N	0.26	0/1462	0.48	0/1985
4	O	0.26	0/1462	0.49	0/1985
4	P	0.27	0/1462	0.52	0/1985

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Q	0.26	0/1462	0.48	0/1985
4	R	0.27	0/1462	0.51	0/1985
4	e	0.27	0/1462	0.50	0/1985
4	f	0.26	0/1462	0.48	0/1985
4	g	0.28	0/1462	0.50	0/1985
4	h	0.26	0/1462	0.49	0/1985
4	i	0.27	0/1462	0.51	0/1985
4	j	0.26	0/1462	0.50	0/1985
4	k	0.26	0/1462	0.49	0/1985
4	l	0.26	0/1462	0.49	0/1985
4	m	0.27	0/1462	0.51	0/1985
4	n	0.26	0/1462	0.50	0/1985
4	o	0.26	0/1462	0.48	0/1985
4	p	0.27	0/1462	0.50	0/1985
All	All	0.27	0/136446	0.53	38/185004 (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	U	0	1
1	V	0	1
1	Z	0	1
1	b	0	1
All	All	0	4

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	464	PRO	CA-N-CD	-10.90	96.24	111.50
1	c	464	PRO	CA-N-CD	-10.90	96.24	111.50
1	a	464	PRO	CA-N-CD	-7.46	101.05	111.50
1	T	464	PRO	CA-N-CD	-7.43	101.10	111.50
1	Y	360	MET	CA-CB-CG	6.34	124.07	113.30
1	T	467	MET	CA-CB-CG	6.09	123.66	113.30
2	D	197	LEU	CA-CB-CG	5.73	128.48	115.30
2	F	197	LEU	CA-CB-CG	5.70	128.41	115.30
1	U	467	MET	CA-CB-CG	5.69	122.97	113.30
1	W	467	MET	CA-CB-CG	5.67	122.94	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	467	MET	CA-CB-CG	5.66	122.91	113.30
1	c	467	MET	CA-CB-CG	5.65	122.91	113.30
1	b	467	MET	CA-CB-CG	5.61	122.84	113.30
1	V	467	MET	CA-CB-CG	5.59	122.81	113.30
1	a	467	MET	CA-CB-CG	5.52	122.68	113.30
1	V	33	ASP	CB-CG-OD1	5.35	123.11	118.30
2	A	512	GLU	CA-CB-CG	5.33	125.13	113.40
1	b	33	ASP	CB-CG-OD1	5.32	123.09	118.30
1	U	33	ASP	CB-CG-OD1	5.29	123.06	118.30
2	E	468	ASP	CB-CG-OD2	5.29	123.06	118.30
1	Z	33	ASP	CB-CG-OD1	5.28	123.05	118.30
1	a	360	MET	CA-CB-CG	5.26	122.25	113.30
1	T	360	MET	CA-CB-CG	5.25	122.22	113.30
1	Z	43	ASP	CB-CG-OD1	5.22	123.00	118.30
1	d	1	MET	CB-CG-SD	5.21	128.01	112.40
1	U	43	ASP	CB-CG-OD1	5.20	122.98	118.30
1	U	360	MET	CA-CB-CG	5.19	122.12	113.30
3	s	123	ASP	CB-CG-OD2	5.16	122.94	118.30
1	Z	360	MET	CA-CB-CG	5.14	122.03	113.30
2	B	468	ASP	CB-CG-OD2	5.13	122.92	118.30
1	W	464	PRO	N-CD-CG	-5.11	95.53	103.20
1	c	464	PRO	N-CD-CG	-5.08	95.58	103.20
3	I	123	ASP	CB-CG-OD2	5.08	122.87	118.30
1	S	43	ASP	CB-CG-OD1	5.07	122.86	118.30
1	X	43	ASP	CB-CG-OD1	5.07	122.86	118.30
1	d	360	MET	CA-CB-CG	5.03	121.85	113.30
1	S	33	ASP	CB-CG-OD2	5.02	122.82	118.30
1	X	33	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	474	GLU	Peptide
1	V	474	GLU	Peptide
1	Z	474	GLU	Peptide
1	b	474	GLU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	S	562/565 (100%)	525 (93%)	35 (6%)	2 (0%)	34	70
1	T	562/565 (100%)	527 (94%)	33 (6%)	2 (0%)	34	70
1	U	562/565 (100%)	528 (94%)	30 (5%)	4 (1%)	22	59
1	V	562/565 (100%)	530 (94%)	30 (5%)	2 (0%)	34	70
1	W	562/565 (100%)	529 (94%)	30 (5%)	3 (0%)	29	66
1	X	562/565 (100%)	525 (93%)	34 (6%)	3 (0%)	29	66
1	Y	562/565 (100%)	526 (94%)	33 (6%)	3 (0%)	29	66
1	Z	562/565 (100%)	528 (94%)	30 (5%)	4 (1%)	22	59
1	a	562/565 (100%)	527 (94%)	33 (6%)	2 (0%)	34	70
1	b	562/565 (100%)	529 (94%)	31 (6%)	2 (0%)	34	70
1	c	562/565 (100%)	526 (94%)	33 (6%)	3 (0%)	29	66
1	d	562/565 (100%)	520 (92%)	40 (7%)	2 (0%)	34	70
2	A	804/806 (100%)	764 (95%)	39 (5%)	1 (0%)	51	83
2	B	804/806 (100%)	764 (95%)	39 (5%)	1 (0%)	51	83
2	C	804/806 (100%)	771 (96%)	33 (4%)	0	100	100
2	D	804/806 (100%)	763 (95%)	40 (5%)	1 (0%)	51	83
2	E	804/806 (100%)	765 (95%)	37 (5%)	2 (0%)	47	78
2	F	804/806 (100%)	768 (96%)	35 (4%)	1 (0%)	51	83
3	G	196/200 (98%)	189 (96%)	7 (4%)	0	100	100
3	H	196/200 (98%)	187 (95%)	9 (5%)	0	100	100
3	I	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
3	J	196/200 (98%)	186 (95%)	10 (5%)	0	100	100
3	K	196/200 (98%)	192 (98%)	4 (2%)	0	100	100
3	L	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
3	q	196/200 (98%)	192 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	r	196/200 (98%)	187 (95%)	9 (5%)	0	100	100
3	s	196/200 (98%)	186 (95%)	10 (5%)	0	100	100
3	t	196/200 (98%)	185 (94%)	11 (6%)	0	100	100
3	u	196/200 (98%)	189 (96%)	7 (4%)	0	100	100
3	v	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
4	M	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
4	N	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
4	O	190/1079 (18%)	182 (96%)	8 (4%)	0	100	100
4	P	190/1079 (18%)	180 (95%)	10 (5%)	0	100	100
4	Q	190/1079 (18%)	183 (96%)	7 (4%)	0	100	100
4	R	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
4	e	190/1079 (18%)	177 (93%)	13 (7%)	0	100	100
4	f	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
4	g	190/1079 (18%)	180 (95%)	10 (5%)	0	100	100
4	h	190/1079 (18%)	178 (94%)	12 (6%)	0	100	100
4	i	190/1079 (18%)	179 (94%)	11 (6%)	0	100	100
4	j	190/1079 (18%)	179 (94%)	11 (6%)	0	100	100
4	k	190/1079 (18%)	182 (96%)	8 (4%)	0	100	100
4	l	190/1079 (18%)	184 (97%)	6 (3%)	0	100	100
4	m	190/1079 (18%)	184 (97%)	6 (3%)	0	100	100
4	n	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
4	o	190/1079 (18%)	182 (96%)	8 (4%)	0	100	100
4	p	190/1079 (18%)	181 (95%)	9 (5%)	0	100	100
All	All	17340/33438 (52%)	16430 (95%)	872 (5%)	38 (0%)	50	78

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	486	ILE
1	U	486	ILE
1	V	486	ILE
1	W	486	ILE
1	Y	486	ILE
1	Z	486	ILE

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Mol	Chain	Res	Type
1	a	486	ILE
1	b	486	ILE
1	c	486	ILE
1	d	486	ILE
1	S	467	MET
1	S	486	ILE
1	V	467	MET
1	W	517	LEU
1	X	467	MET
1	X	486	ILE
1	b	467	MET
1	d	467	MET
1	Y	467	MET
1	c	517	LEU
1	W	518	LEU
1	X	518	LEU
1	c	518	LEU
1	U	467	MET
1	Z	467	MET
2	E	123	ALA
1	T	467	MET
1	U	490	ASN
1	U	517	LEU
1	Y	518	LEU
1	Z	475	GLU
1	Z	490	ASN
1	a	467	MET
2	A	534	ASP
2	B	534	ASP
2	D	534	ASP
2	E	534	ASP
2	F	534	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	466/467 (100%)	451 (97%)	15 (3%)	39	65
1	T	466/467 (100%)	452 (97%)	14 (3%)	41	66
1	U	466/467 (100%)	450 (97%)	16 (3%)	37	64
1	V	466/467 (100%)	447 (96%)	19 (4%)	30	59
1	W	466/467 (100%)	450 (97%)	16 (3%)	37	64
1	X	466/467 (100%)	453 (97%)	13 (3%)	43	67
1	Y	466/467 (100%)	452 (97%)	14 (3%)	41	66
1	Z	466/467 (100%)	448 (96%)	18 (4%)	32	60
1	a	466/467 (100%)	451 (97%)	15 (3%)	39	65
1	b	466/467 (100%)	449 (96%)	17 (4%)	35	63
1	c	466/467 (100%)	452 (97%)	14 (3%)	41	66
1	d	466/467 (100%)	451 (97%)	15 (3%)	39	65
2	A	686/686 (100%)	671 (98%)	15 (2%)	52	72
2	B	686/686 (100%)	672 (98%)	14 (2%)	55	75
2	C	686/686 (100%)	668 (97%)	18 (3%)	46	69
2	D	686/686 (100%)	670 (98%)	16 (2%)	50	71
2	E	686/686 (100%)	674 (98%)	12 (2%)	60	78
2	F	686/686 (100%)	672 (98%)	14 (2%)	55	75
3	G	177/179 (99%)	172 (97%)	5 (3%)	43	67
3	H	177/179 (99%)	169 (96%)	8 (4%)	27	57
3	I	177/179 (99%)	172 (97%)	5 (3%)	43	67
3	J	177/179 (99%)	171 (97%)	6 (3%)	37	64
3	K	177/179 (99%)	173 (98%)	4 (2%)	50	71
3	L	177/179 (99%)	175 (99%)	2 (1%)	73	85
3	q	177/179 (99%)	173 (98%)	4 (2%)	50	71
3	r	177/179 (99%)	172 (97%)	5 (3%)	43	67
3	s	177/179 (99%)	175 (99%)	2 (1%)	73	85
3	t	177/179 (99%)	170 (96%)	7 (4%)	31	59
3	u	177/179 (99%)	173 (98%)	4 (2%)	50	71
3	v	177/179 (99%)	172 (97%)	5 (3%)	43	67
4	M	163/886 (18%)	157 (96%)	6 (4%)	34	61
4	N	163/886 (18%)	160 (98%)	3 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	163/886 (18%)	160 (98%)	3 (2%)	59	77
4	P	163/886 (18%)	157 (96%)	6 (4%)	34	61
4	Q	163/886 (18%)	160 (98%)	3 (2%)	59	77
4	R	163/886 (18%)	160 (98%)	3 (2%)	59	77
4	e	163/886 (18%)	159 (98%)	4 (2%)	47	70
4	f	163/886 (18%)	161 (99%)	2 (1%)	71	84
4	g	163/886 (18%)	158 (97%)	5 (3%)	40	65
4	h	163/886 (18%)	156 (96%)	7 (4%)	29	58
4	i	163/886 (18%)	158 (97%)	5 (3%)	40	65
4	j	163/886 (18%)	161 (99%)	2 (1%)	71	84
4	k	163/886 (18%)	162 (99%)	1 (1%)	86	92
4	l	163/886 (18%)	159 (98%)	4 (2%)	47	70
4	m	163/886 (18%)	160 (98%)	3 (2%)	59	77
4	n	163/886 (18%)	158 (97%)	5 (3%)	40	65
4	o	163/886 (18%)	162 (99%)	1 (1%)	86	92
4	p	163/886 (18%)	162 (99%)	1 (1%)	86	92
All	All	14766/27816 (53%)	14370 (97%)	396 (3%)	48	68

All (396) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	1	MET
1	S	12	GLN
1	S	43	ASP
1	S	131	MET
1	S	180	ASN
1	S	189	GLU
1	S	193	ASP
1	S	235	LYS
1	S	246	CYS
1	S	285	TYR
1	S	357	PHE
1	S	392	TYR
1	S	415	ARG
1	S	524	SER
1	S	527	MET

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Mol	Chain	Res	Type
1	T	12	GLN
1	T	16	TYR
1	T	33	ASP
1	T	91	ASN
1	T	131	MET
1	T	180	ASN
1	T	210	MET
1	T	246	CYS
1	T	355	LEU
1	T	357	PHE
1	T	379	TYR
1	T	397	ARG
1	T	515	GLN
1	T	524	SER
1	U	12	GLN
1	U	39	LYS
1	U	43	ASP
1	U	131	MET
1	U	193	ASP
1	U	214	MET
1	U	224	MET
1	U	235	LYS
1	U	246	CYS
1	U	283	ASN
1	U	357	PHE
1	U	379	TYR
1	U	392	TYR
1	U	415	ARG
1	U	420	PHE
1	U	527	MET
1	V	12	GLN
1	V	43	ASP
1	V	131	MET
1	V	147	HIS
1	V	180	ASN
1	V	188	GLU
1	V	193	ASP
1	V	214	MET
1	V	224	MET
1	V	235	LYS
1	V	246	CYS
1	V	285	TYR

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Mol	Chain	Res	Type
1	V	362	ASN
1	V	379	TYR
1	V	392	TYR
1	V	415	ARG
1	V	420	PHE
1	V	524	SER
1	V	527	MET
1	W	12	GLN
1	W	16	TYR
1	W	33	ASP
1	W	90	THR
1	W	118	ASP
1	W	131	MET
1	W	159	SER
1	W	193	ASP
1	W	210	MET
1	W	228	CYS
1	W	246	CYS
1	W	285	TYR
1	W	337	LYS
1	W	357	PHE
1	W	523	LYS
1	W	541	ARG
1	X	1	MET
1	X	12	GLN
1	X	43	ASP
1	X	130	ARG
1	X	131	MET
1	X	193	ASP
1	X	235	LYS
1	X	246	CYS
1	X	285	TYR
1	X	357	PHE
1	X	392	TYR
1	X	415	ARG
1	X	527	MET
1	Y	11	ARG
1	Y	12	GLN
1	Y	16	TYR
1	Y	33	ASP
1	Y	43	ASP
1	Y	131	MET

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Mol	Chain	Res	Type
1	Y	210	MET
1	Y	228	CYS
1	Y	246	CYS
1	Y	357	PHE
1	Y	380	MET
1	Y	397	ARG
1	Y	422	ARG
1	Y	519	GLU
1	Z	1	MET
1	Z	12	GLN
1	Z	39	LYS
1	Z	43	ASP
1	Z	131	MET
1	Z	193	ASP
1	Z	214	MET
1	Z	224	MET
1	Z	235	LYS
1	Z	246	CYS
1	Z	283	ASN
1	Z	357	PHE
1	Z	379	TYR
1	Z	392	TYR
1	Z	415	ARG
1	Z	420	PHE
1	Z	524	SER
1	Z	527	MET
1	a	12	GLN
1	a	33	ASP
1	a	91	ASN
1	a	131	MET
1	a	180	ASN
1	a	210	MET
1	a	246	CYS
1	a	285	TYR
1	a	357	PHE
1	a	379	TYR
1	a	397	ARG
1	a	420	PHE
1	a	515	GLN
1	a	524	SER
1	a	527	MET
1	b	1	MET

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Mol	Chain	Res	Type
1	b	12	GLN
1	b	43	ASP
1	b	131	MET
1	b	147	HIS
1	b	180	ASN
1	b	188	GLU
1	b	193	ASP
1	b	214	MET
1	b	224	MET
1	b	235	LYS
1	b	246	CYS
1	b	362	ASN
1	b	379	TYR
1	b	392	TYR
1	b	415	ARG
1	b	420	PHE
1	c	12	GLN
1	c	16	TYR
1	c	33	ASP
1	c	118	ASP
1	c	131	MET
1	c	159	SER
1	c	193	ASP
1	c	210	MET
1	c	228	CYS
1	c	246	CYS
1	c	285	TYR
1	c	337	LYS
1	c	357	PHE
1	c	541	ARG
1	d	1	MET
1	d	11	ARG
1	d	12	GLN
1	d	16	TYR
1	d	33	ASP
1	d	43	ASP
1	d	131	MET
1	d	228	CYS
1	d	246	CYS
1	d	357	PHE
1	d	380	MET
1	d	397	ARG

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Mol	Chain	Res	Type
1	d	422	ARG
1	d	519	GLU
1	d	524	SER
2	A	52	LYS
2	A	114	SER
2	A	118	ARG
2	A	146	TRP
2	A	228	ASP
2	A	254	HIS
2	A	268	PHE
2	A	311	ARG
2	A	446	ASP
2	A	475	TYR
2	A	562	ASP
2	A	638	PHE
2	A	729	MET
2	A	784	SER
2	A	794	GLU
2	B	118	ARG
2	B	137	MET
2	B	151	MET
2	B	173	SER
2	B	210	TYR
2	B	228	ASP
2	B	254	HIS
2	B	298	HIS
2	B	446	ASP
2	B	475	TYR
2	B	562	ASP
2	B	697	GLU
2	B	788	CYS
2	B	794	GLU
2	C	16	SER
2	C	82	GLN
2	C	173	SER
2	C	213	ARG
2	C	228	ASP
2	C	254	HIS
2	C	298	HIS
2	C	305	MET
2	C	360	ASP
2	C	452	ASP

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Mol	Chain	Res	Type
2	C	475	TYR
2	C	492	SER
2	C	534	ASP
2	C	562	ASP
2	C	638	PHE
2	C	784	SER
2	C	788	CYS
2	C	791	GLN
2	D	52	LYS
2	D	114	SER
2	D	118	ARG
2	D	146	TRP
2	D	228	ASP
2	D	254	HIS
2	D	268	PHE
2	D	298	HIS
2	D	311	ARG
2	D	384	ASP
2	D	446	ASP
2	D	562	ASP
2	D	770	MET
2	D	784	SER
2	D	794	GLU
2	D	798	TRP
2	E	118	ARG
2	E	151	MET
2	E	210	TYR
2	E	228	ASP
2	E	298	HIS
2	E	446	ASP
2	E	475	TYR
2	E	562	ASP
2	E	638	PHE
2	E	697	GLU
2	E	788	CYS
2	E	792	SER
2	F	16	SER
2	F	82	GLN
2	F	173	SER
2	F	228	ASP
2	F	254	HIS
2	F	298	HIS

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Mol	Chain	Res	Type
2	F	360	ASP
2	F	475	TYR
2	F	534	ASP
2	F	562	ASP
2	F	638	PHE
2	F	784	SER
2	F	788	CYS
2	F	798	TRP
3	G	7	PHE
3	G	104	ASN
3	G	116	MET
3	G	164	SER
3	G	182	HIS
3	H	57	ASP
3	H	59	GLU
3	H	109	ASP
3	H	136	LYS
3	H	139	ARG
3	H	159	GLU
3	H	180	ARG
3	H	192	TYR
3	I	78	ARG
3	I	104	ASN
3	I	111	ASP
3	I	143	GLU
3	I	192	TYR
3	J	17	MET
3	J	116	MET
3	J	136	LYS
3	J	153	LYS
3	J	180	ARG
3	J	190	ASN
3	K	57	ASP
3	K	96	ASP
3	K	104	ASN
3	K	115	ASP
3	L	136	LYS
3	L	184	ASN
3	q	7	PHE
3	q	104	ASN
3	q	116	MET
3	q	164	SER

Continued on next page...

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Mol	Chain	Res	Type
3	r	57	ASP
3	r	59	GLU
3	r	109	ASP
3	r	136	LYS
3	r	180	ARG
3	s	104	ASN
3	s	115	ASP
3	t	17	MET
3	t	97	LYS
3	t	116	MET
3	t	136	LYS
3	t	153	LYS
3	t	180	ARG
3	t	190	ASN
3	u	57	ASP
3	u	88	ASP
3	u	104	ASN
3	u	115	ASP
3	v	35	GLN
3	v	77	SER
3	v	136	LYS
3	v	139	ARG
3	v	182	HIS
4	e	1	MET
4	e	36	PHE
4	e	48	PHE
4	e	69	ASN
4	f	140	SER
4	f	167	ASN
4	g	1	MET
4	g	6	ARG
4	g	48	PHE
4	g	147	ASP
4	g	167	ASN
4	h	1	MET
4	h	31	LYS
4	h	36	PHE
4	h	48	PHE
4	h	66	SER
4	h	71	ARG
4	h	73	GLU
4	j	48	PHE

Continued on next page...

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Mol	Chain	Res	Type
4	j	58	LYS
4	l	6	ARG
4	l	48	PHE
4	l	147	ASP
4	l	176	ASN
4	i	1	MET
4	i	36	PHE
4	i	58	LYS
4	i	69	ASN
4	i	103	LYS
4	k	153	TYR
4	m	1	MET
4	m	6	ARG
4	m	156	ARG
4	n	1	MET
4	n	31	LYS
4	n	48	PHE
4	n	58	LYS
4	n	71	ARG
4	o	140	SER
4	p	6	ARG
4	M	1	MET
4	M	31	LYS
4	M	36	PHE
4	M	48	PHE
4	M	66	SER
4	M	75	ARG
4	N	48	PHE
4	N	58	LYS
4	N	153	TYR
4	O	6	ARG
4	O	39	LYS
4	O	48	PHE
4	P	1	MET
4	P	36	PHE
4	P	46	ASN
4	P	58	LYS
4	P	103	LYS
4	P	123	ASP
4	Q	6	ARG
4	Q	11	ASN
4	Q	48	PHE

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Mol	Chain	Res	Type
4	R	1	MET
4	R	6	ARG
4	R	156	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	8	ASN
1	S	243	HIS
1	U	243	HIS
1	U	516	GLN
1	X	8	ASN
1	X	243	HIS
1	Z	243	HIS
1	b	180	ASN
1	b	529	GLN
1	b	533	ASN
2	A	791	GLN
2	C	196	GLN
2	C	791	GLN
2	D	791	GLN
2	E	261	GLN
3	G	176	HIS
3	I	176	HIS
3	J	48	GLN
3	L	176	HIS
3	L	182	HIS
3	q	176	HIS
3	v	176	HIS
3	v	182	HIS
4	e	138	ASN
4	f	146	GLN
4	f	167	ASN
4	h	35	ASN
4	h	167	ASN
4	l	167	ASN
4	i	35	ASN
4	n	167	ASN
4	M	35	ASN
4	M	167	ASN
4	N	146	GLN
4	P	35	ASN

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Mol	Chain	Res	Type
4	Q	146	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 monosaccharides 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.

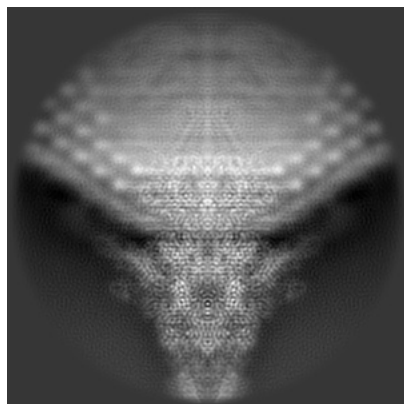
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35175. These allow visual inspection of the internal detail of the map and identification of artifacts.

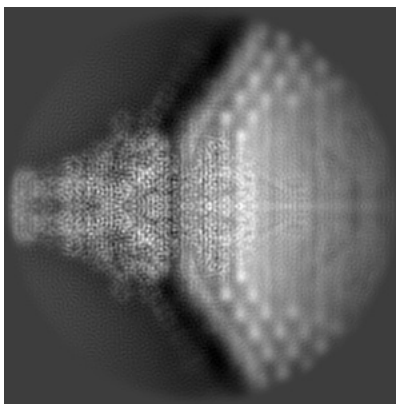
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

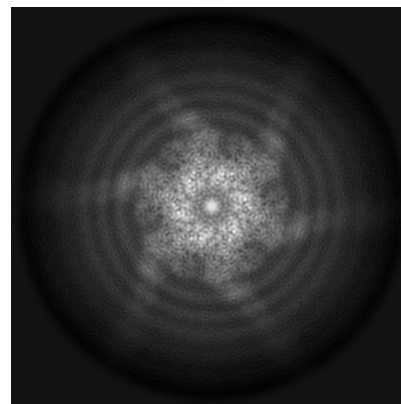
6.1.1 Primary map



X

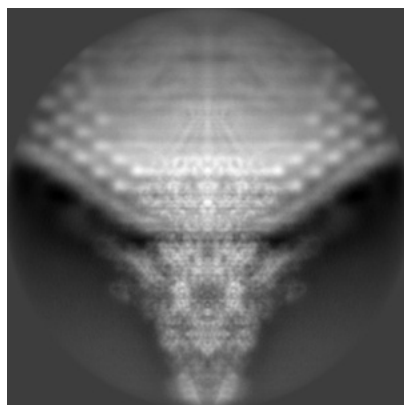


Y

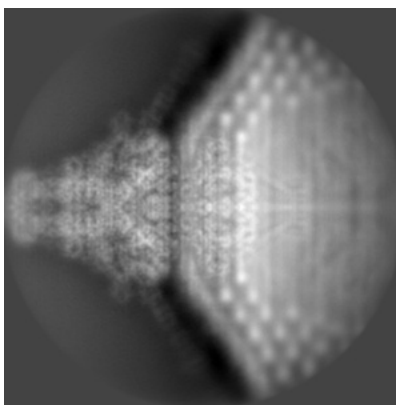


Z

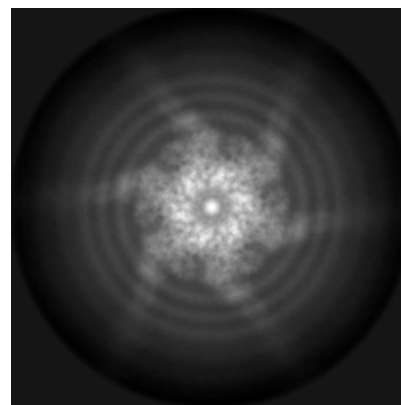
6.1.2 Raw map



X



Y

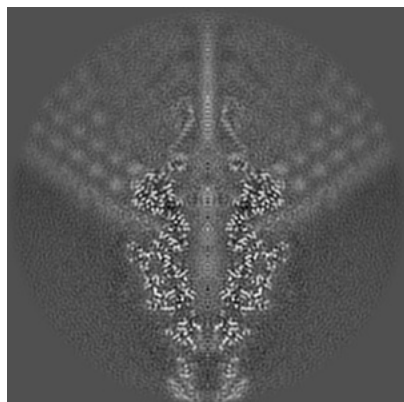


Z

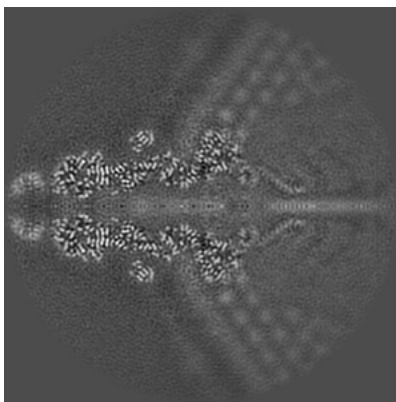
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

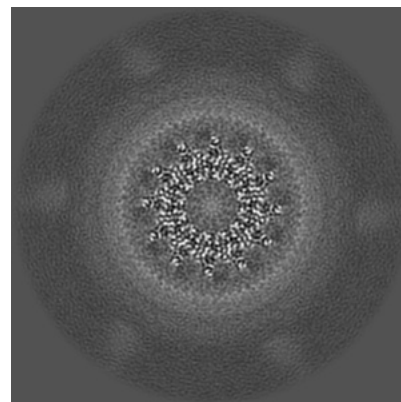
6.2.1 Primary map



X Index: 128

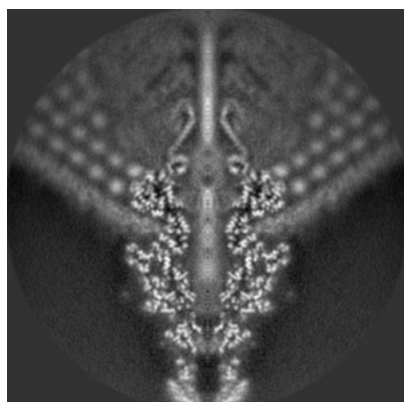


Y Index: 128

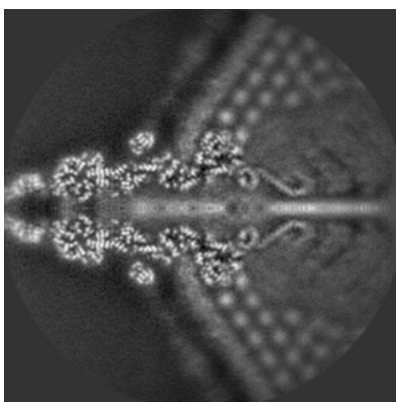


Z Index: 128

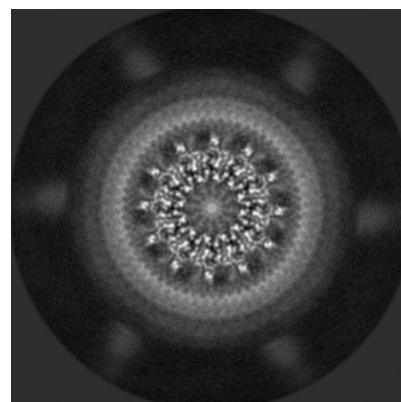
6.2.2 Raw map



X Index: 128



Y Index: 128

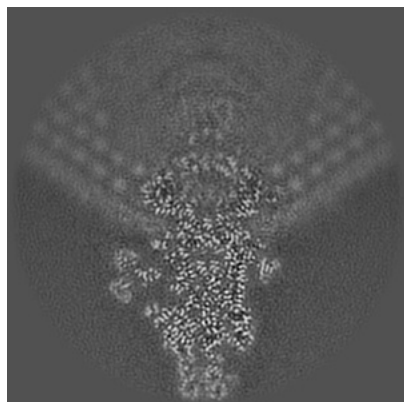


Z Index: 128

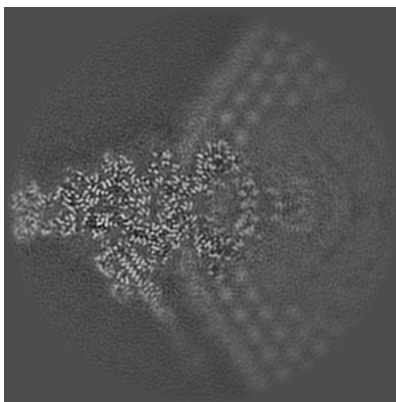
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

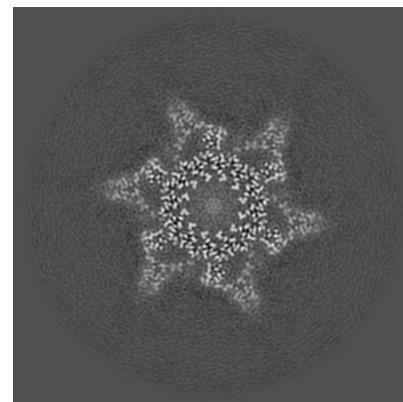
6.3.1 Primary map



X Index: 143

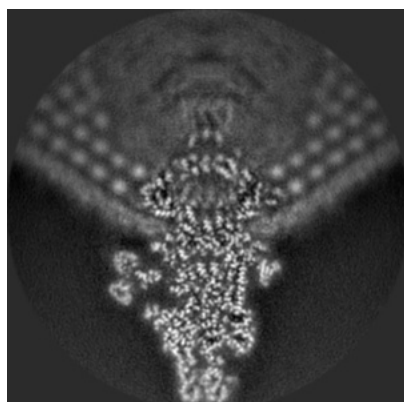


Y Index: 143

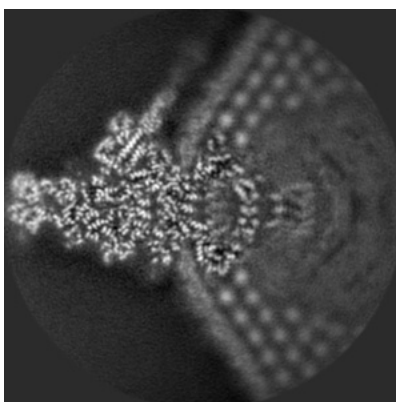


Z Index: 95

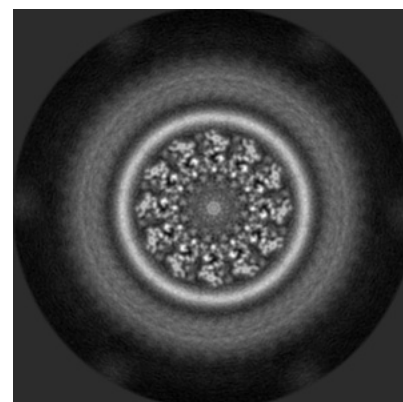
6.3.2 Raw map



X Index: 143



Y Index: 113

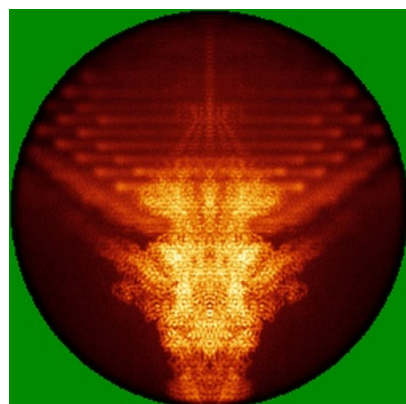


Z Index: 141

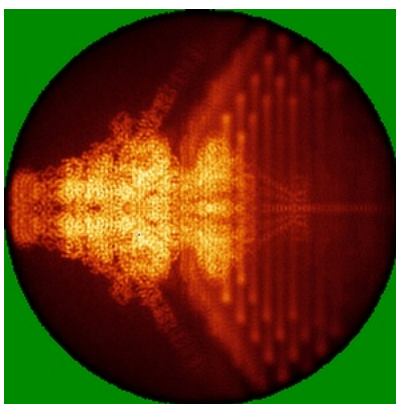
The images above show the largest variance slices of the map in three orthogonal directions.

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

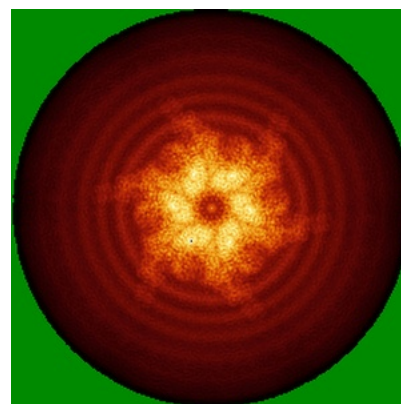
6.4.1 Primary map



X

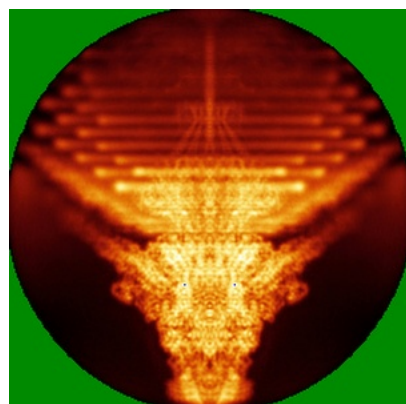


Y

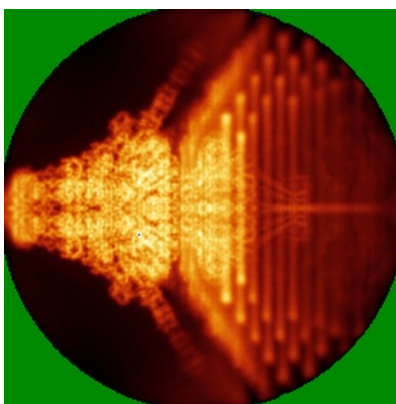


Z

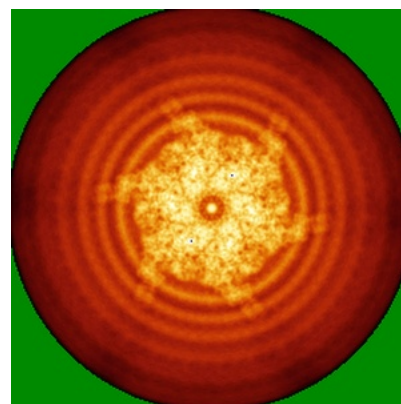
6.4.2 Raw map



X



Y

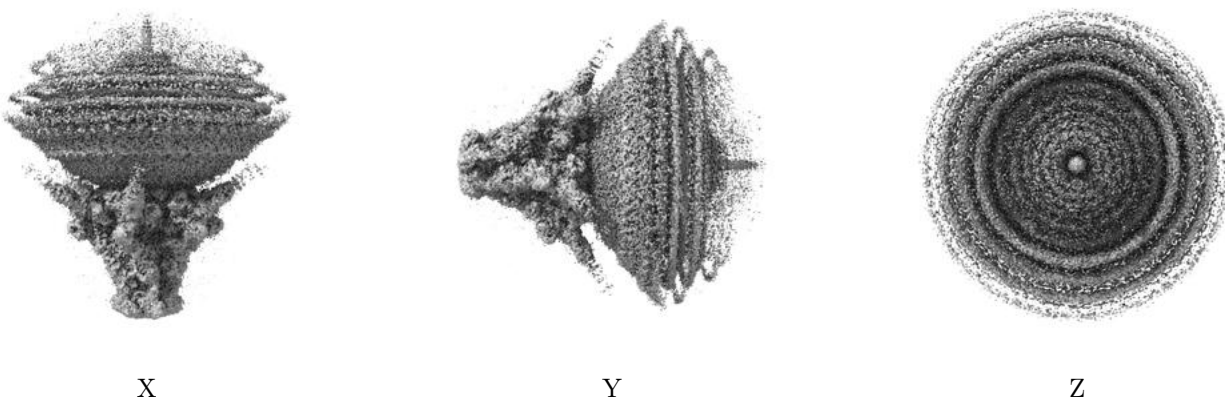


Z

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

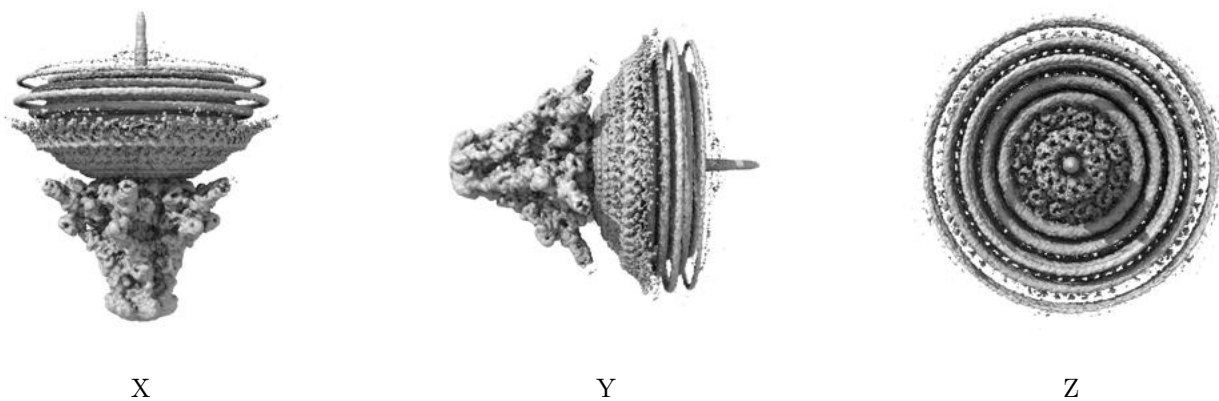
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

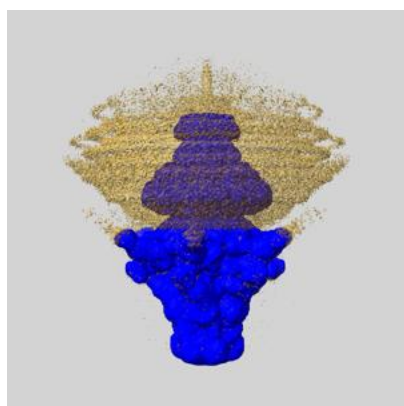
6.6 Mask visualisation [i](#)

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

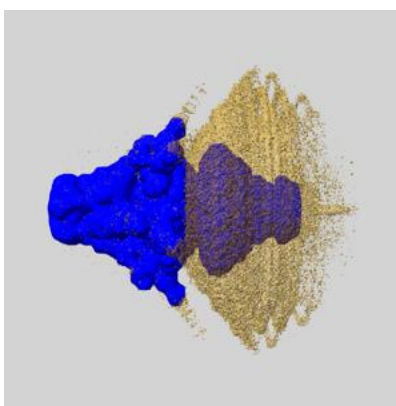
A mask typically either:

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

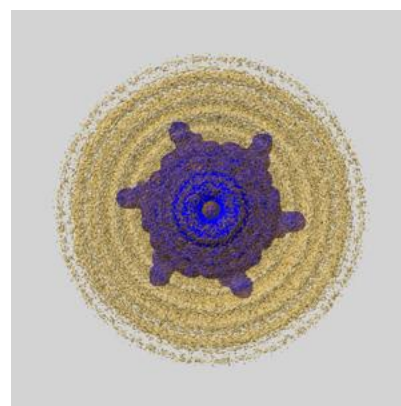
6.6.1 emd_35175_msk_1.map [i](#)



X



Y

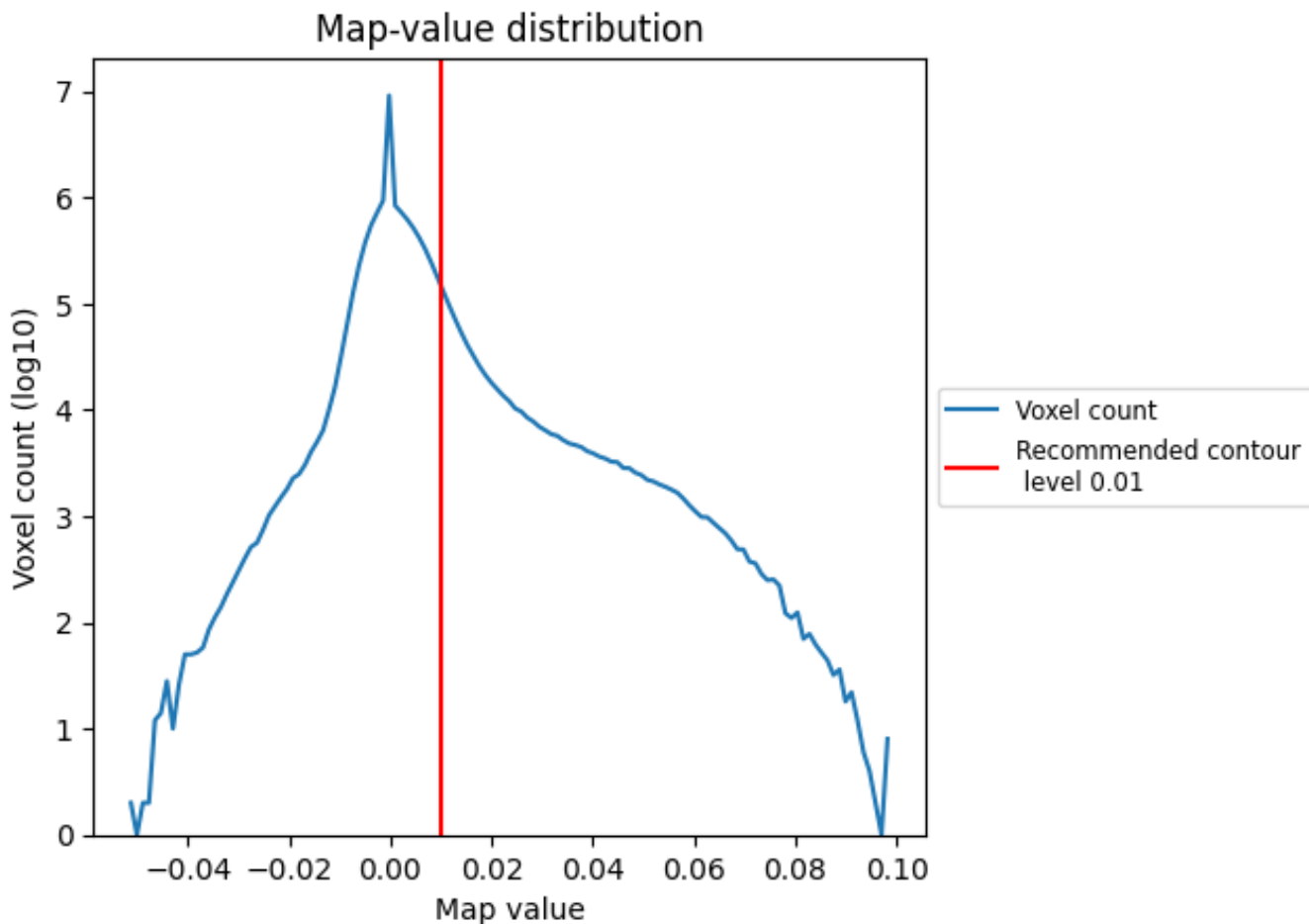


Z

7 Map analysis [i](#)

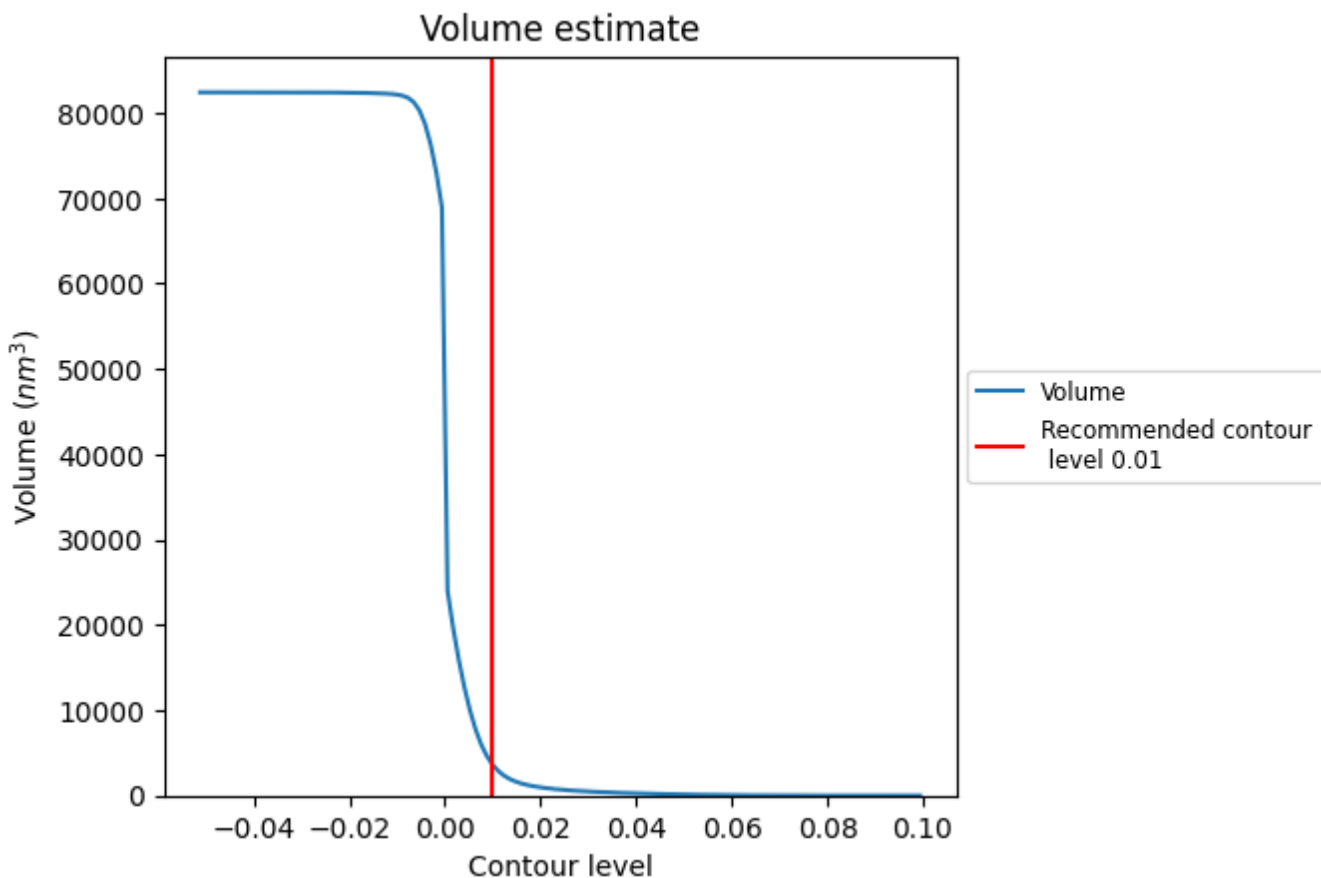
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

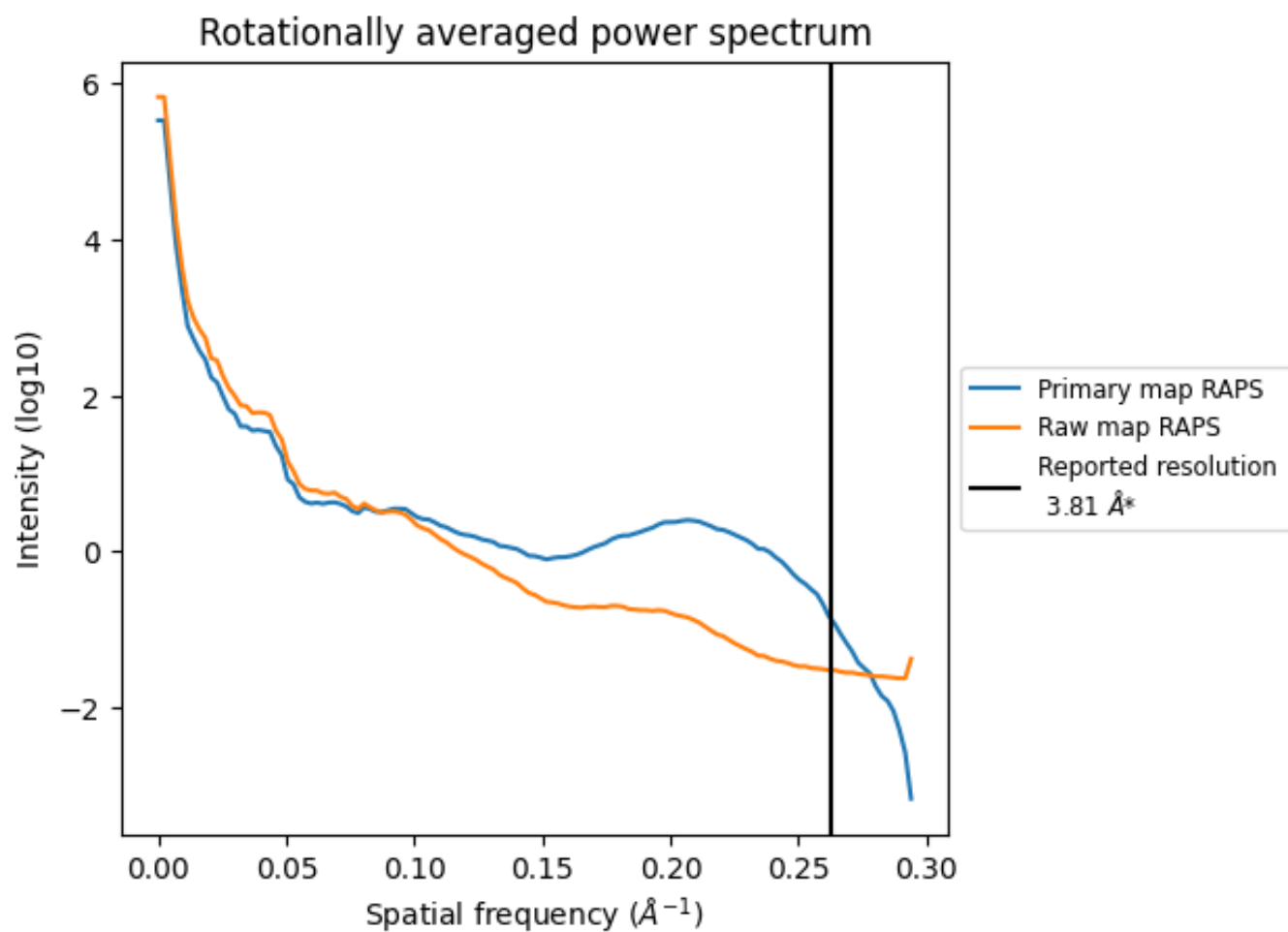
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3611 nm³; this corresponds to an approximate mass of 3262 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 i

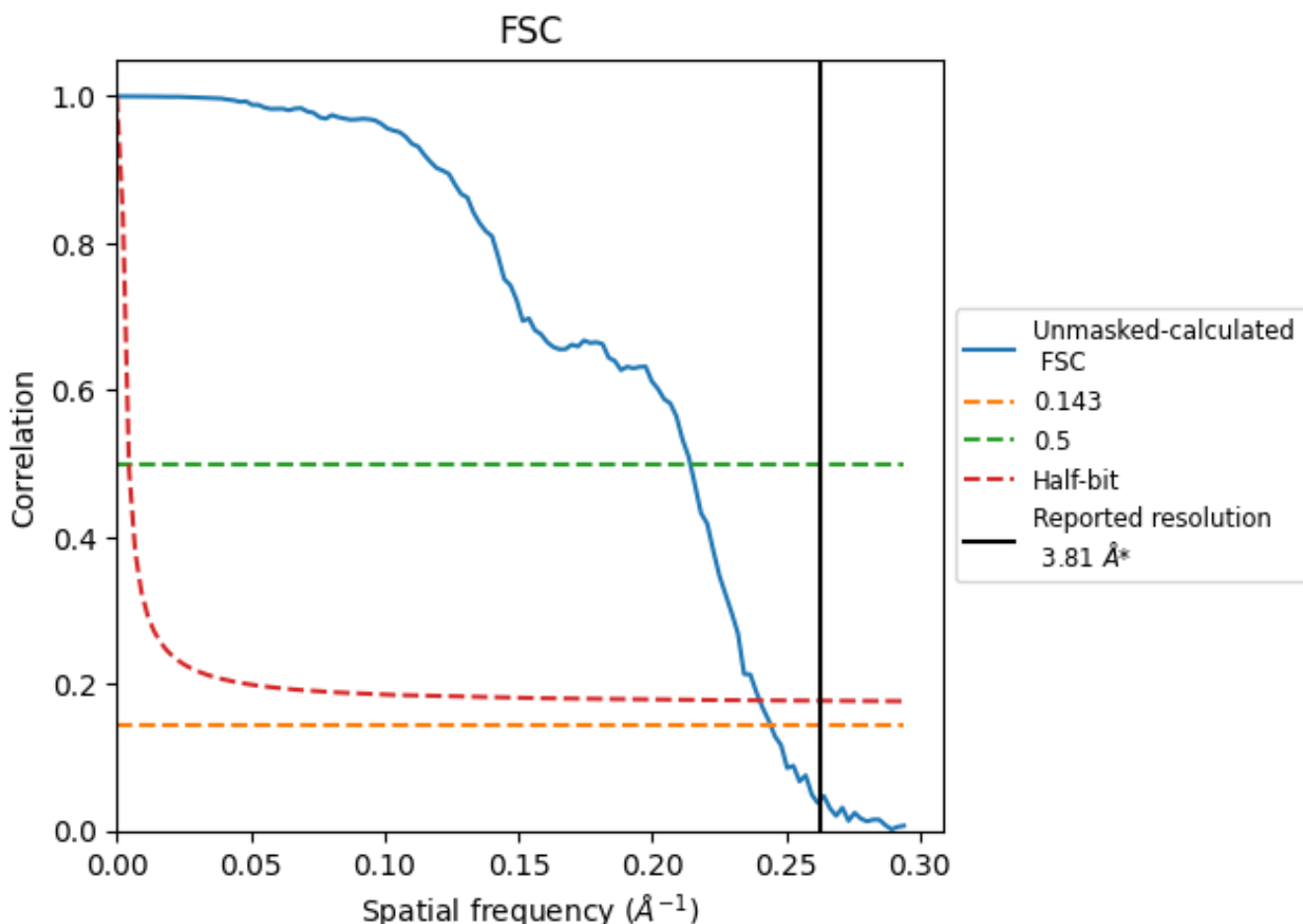


*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

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 0.262 Å⁻¹

8.2 Resolution estimates [i](#)

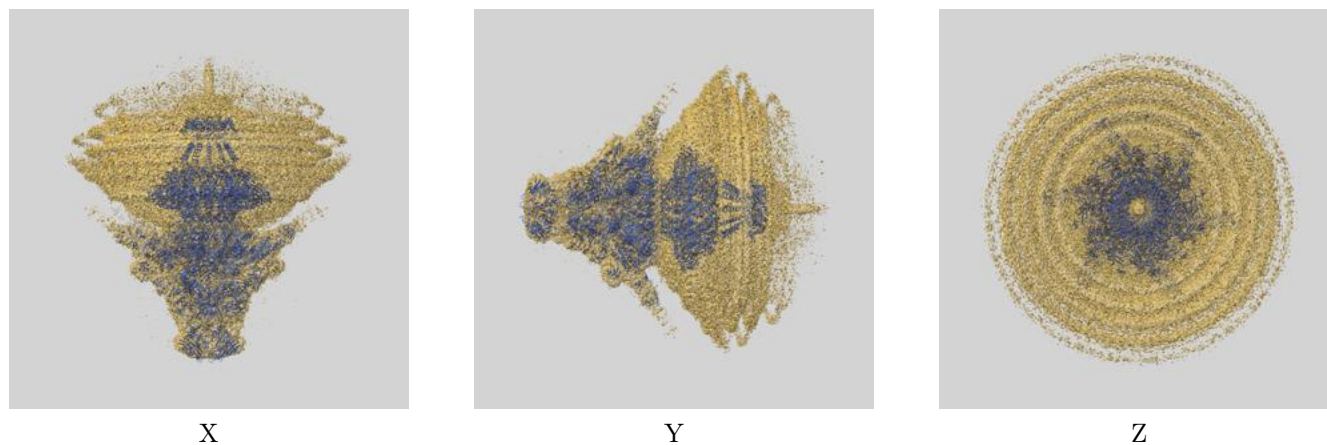
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	4.67	4.16

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

9 Map-model fit [i](#)

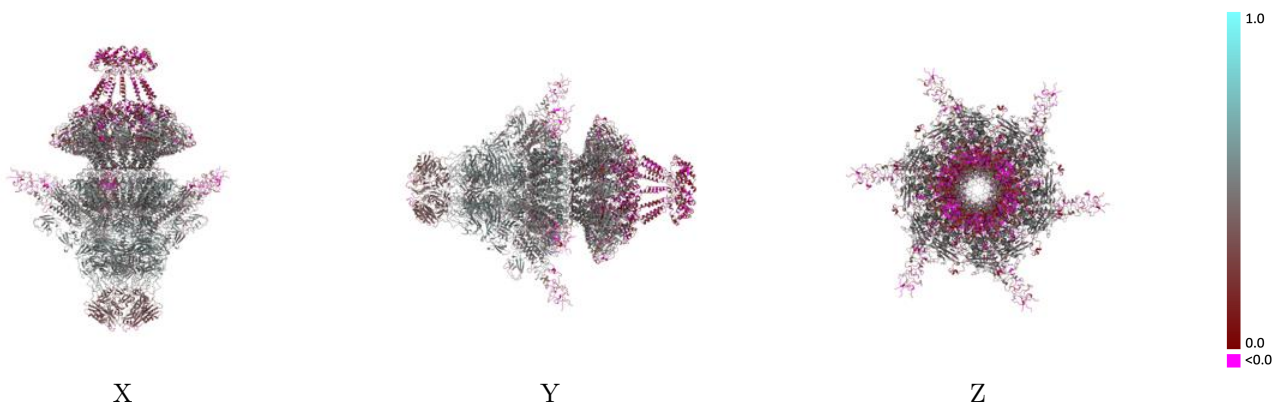
This section contains information regarding the fit between EMDB map EMD-35175 and PDB model 8I4M. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



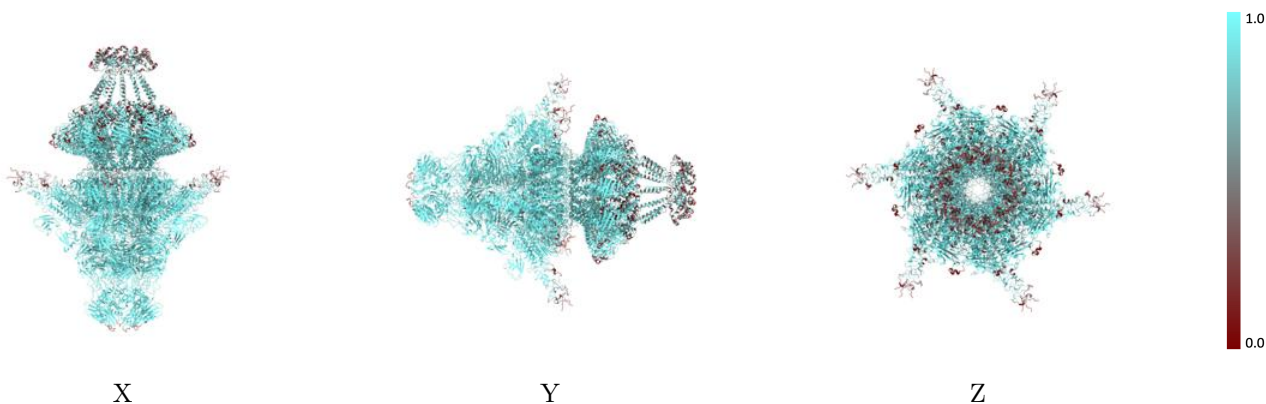
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



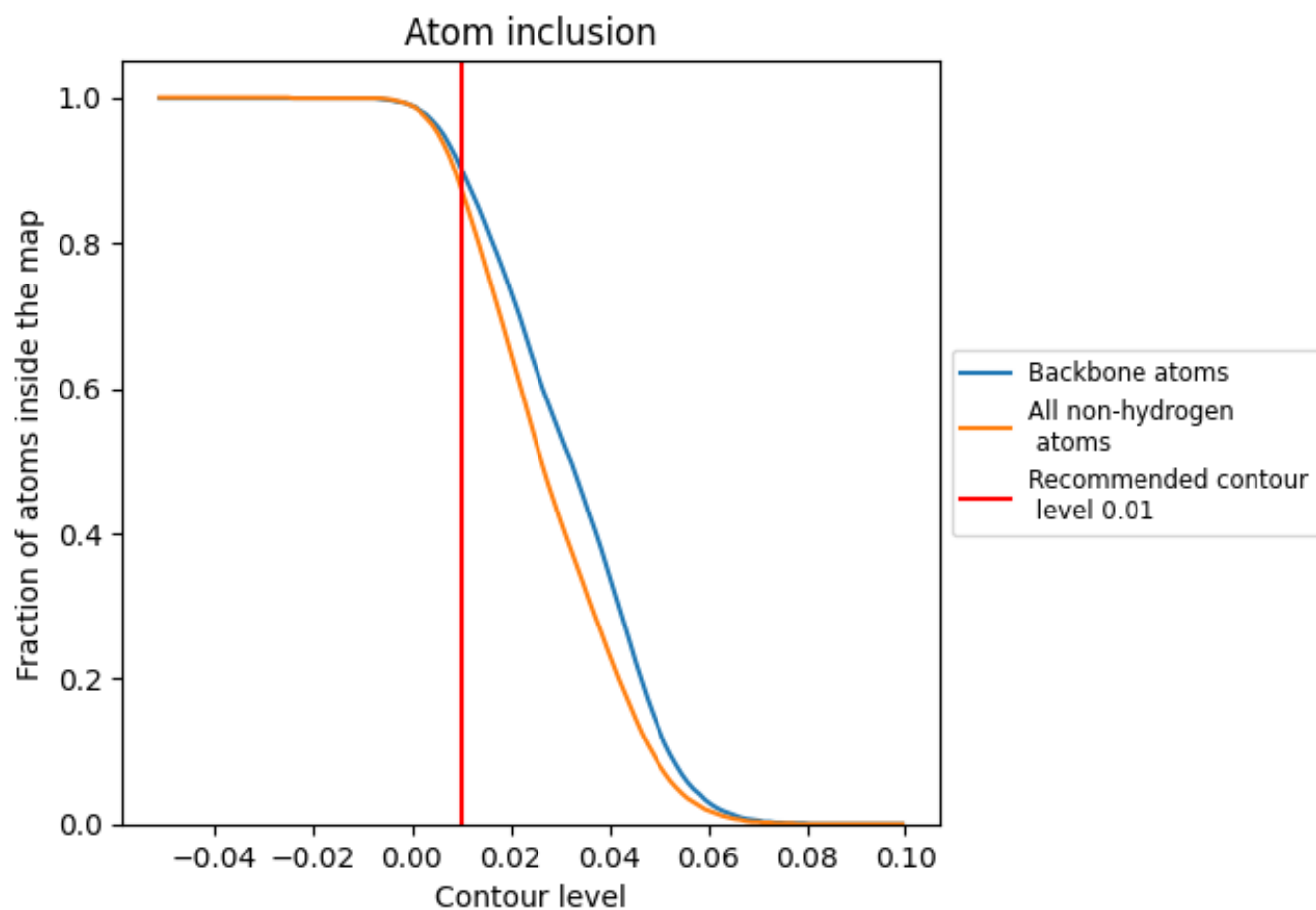
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 87% 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	 0.8740	 0.3940
A	 0.9720	 0.4630
B	 0.9710	 0.4640
C	 0.9700	 0.4640
D	 0.9720	 0.4640
E	 0.9710	 0.4640
F	 0.9700	 0.4630
G	 0.9560	 0.4740
H	 0.9540	 0.4650
I	 0.9580	 0.4770
J	 0.9480	 0.4610
K	 0.9520	 0.4730
L	 0.9540	 0.4650
M	 0.8180	 0.3470
N	 0.8810	 0.3710
O	 0.8900	 0.3970
P	 0.8230	 0.3470
Q	 0.8830	 0.3660
R	 0.8860	 0.3940
S	 0.7810	 0.3280
T	 0.7820	 0.3320
U	 0.7800	 0.3260
V	 0.7800	 0.3220
W	 0.7830	 0.3300
X	 0.7790	 0.3280
Y	 0.7810	 0.3330
Z	 0.7800	 0.3260
a	 0.7810	 0.3330
b	 0.7820	 0.3250
c	 0.7840	 0.3320
d	 0.7810	 0.3340
e	 0.8160	 0.3430
f	 0.8910	 0.3720
g	 0.8990	 0.3960
h	 0.8190	 0.3460



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Chain	Atom inclusion	Q-score
i	 0.8210	 0.3460
j	 0.8810	 0.3650
k	 0.8810	 0.3640
l	 0.8900	 0.4000
m	 0.8870	 0.3940
n	 0.8210	 0.3460
o	 0.8930	 0.3740
p	 0.8970	 0.3990
q	 0.9550	 0.4770
r	 0.9550	 0.4650
s	 0.9560	 0.4770
t	 0.9480	 0.4600
u	 0.9540	 0.4730
v	 0.9550	 0.4650