



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:01 am GMT

PDB ID : 7AEF
EMDB ID : EMD-11745
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the baseplate complex in extended state applied 3-fold symmetry.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.80 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:

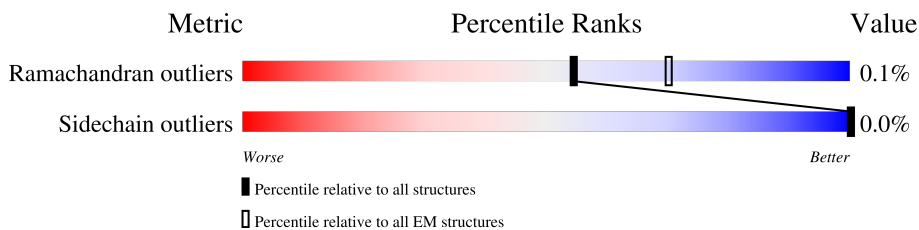
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.80 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	A	933	 10% 58% 41%
1	B	933	 11% 58% 41%
1	C	933	 10% 58% 41%
1	D	933	 12% 58% 41%
1	E	933	 9% 58% 41%
1	F	933	 12% 58% 41%
2	G	1050	 12% 93%
2	H	1050	 12% 94%
2	I	1050	 15% 93%

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Mol	Chain	Length	Quality of chain
2	J	1050	15% 93%
2	K	1050	14% 93%
2	L	1050	14% 94%
3	M	228	99%
3	N	228	98%
3	O	228	99%
3	P	228	98%
3	Q	228	99%
3	R	228	99%
4	S	137	96%
4	T	137	96%
4	U	137	96%
4	V	137	96%
4	W	137	96%
4	X	137	96%
5	Y	147	96%
5	Z	147	96%
5	a	147	95%
5	b	147	96%
5	c	147	96%
5	d	147	96%
6	e	692	27% 93% 5%
6	f	692	27% 93% 5%
6	g	692	26% 93% 5%
6	h	692	27% 93% 5%

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Mol	Chain	Length	Quality of chain
6	i	692	 27% 93% 5%
6	j	692	 27% 93% 5%
7	k	142	 26% 98%
7	l	142	 27% 98%
7	m	142	 27% 98%
7	n	142	 27% 98%
7	o	142	 27% 98%
7	p	142	 27% 98%
8	t	52	 77% 23%
8	u	52	 77% 23%
8	v	52	 77% 23%
9	q	581	 98%
9	r	581	 98%
9	s	581	 98%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 149535 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 baseplate protein (Algo12).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	549	4447	2845	730	858	14	0	0
1	B	549	4447	2845	730	858	14	0	0
1	C	549	4447	2845	730	858	14	0	0
1	D	549	4447	2845	730	858	14	0	0
1	E	549	4447	2845	730	858	14	0	0
1	F	549	4447	2845	730	858	14	0	0

- Molecule 2 is a protein called Baseplate_J domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	1011	7762	4951	1284	1512	15	0	0
2	H	1011	7762	4951	1284	1512	15	0	0
2	I	1011	7762	4951	1284	1512	15	0	0
2	J	1011	7762	4951	1284	1512	15	0	0
2	K	1011	7762	4951	1284	1512	15	0	0
2	L	1011	7762	4951	1284	1512	15	0	0

- Molecule 3 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	225	1849	1185	304	355	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	O	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	P	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	Q	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	R	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		

- Molecule 4 is a protein called Putative tail lysozyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	T	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	U	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	V	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	W	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	X	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		

- Molecule 5 is a protein called Phospholipid/glycerol acyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	Z	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	a	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	b	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	c	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	d	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		

- Molecule 6 is a protein called Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	f	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	g	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	h	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	i	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	j	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		

- Molecule 7 is a protein called Phage tail protein.

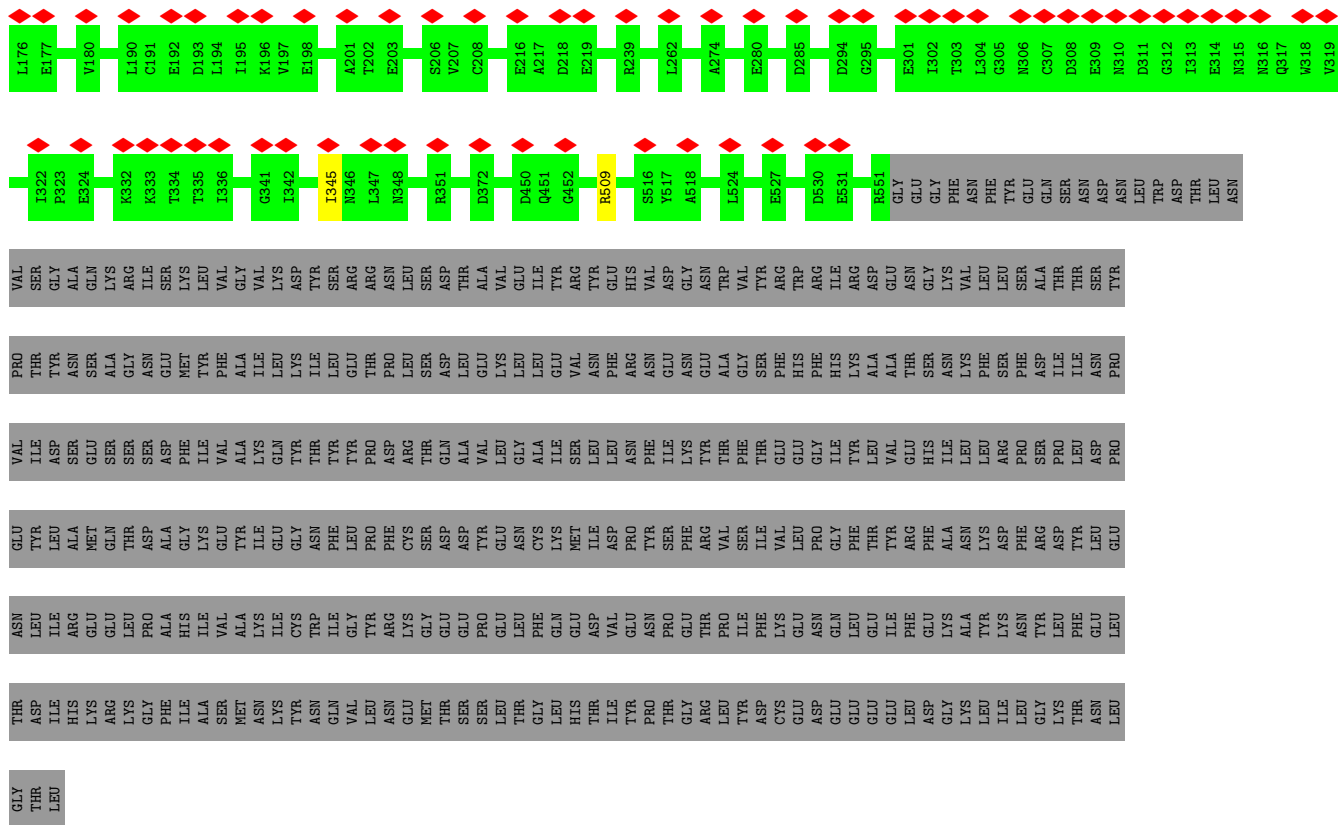
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	l	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	m	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	n	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	o	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	p	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		

- Molecule 8 is a protein called inner protein (Algo6).

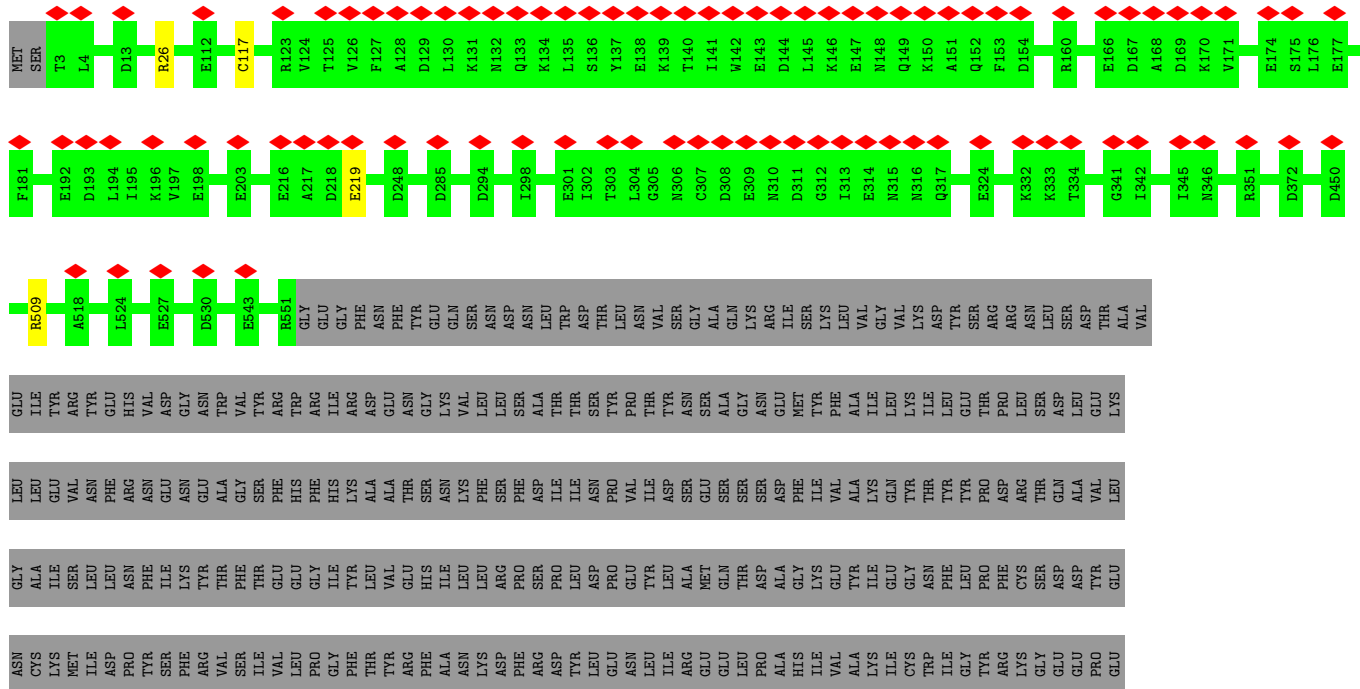
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	t	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	u	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	v	40	Total	C	N	O	S	0	0
			324	202	55	66	1		

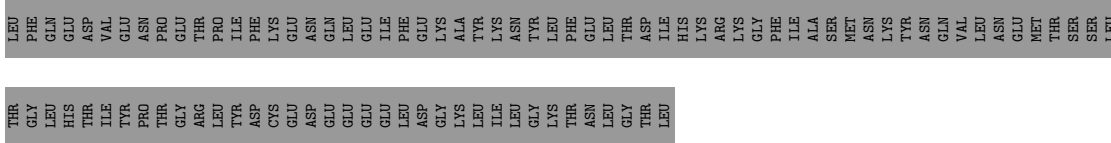
- Molecule 9 is a protein called Phosphoserine phosphatase SerB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	q	580	4469	2771	765	920	13	0	0
9	r	580	4469	2771	765	920	13	0	0
9	s	580	4469	2771	765	920	13	0	0

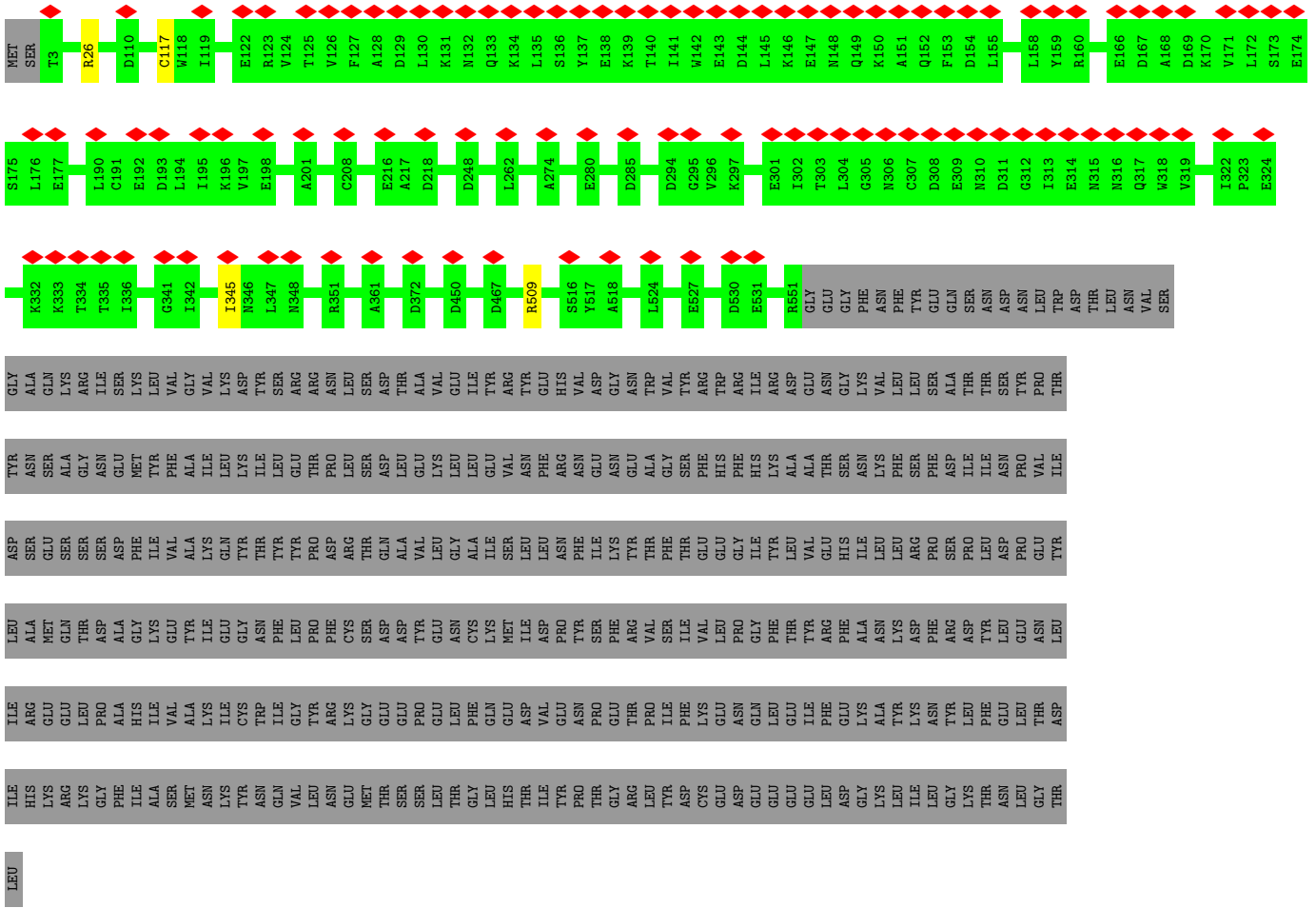


• Molecule 1: baseplate protein (Algo12)

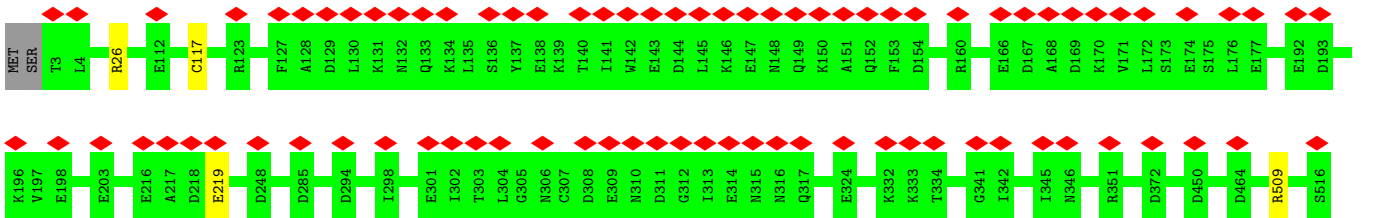




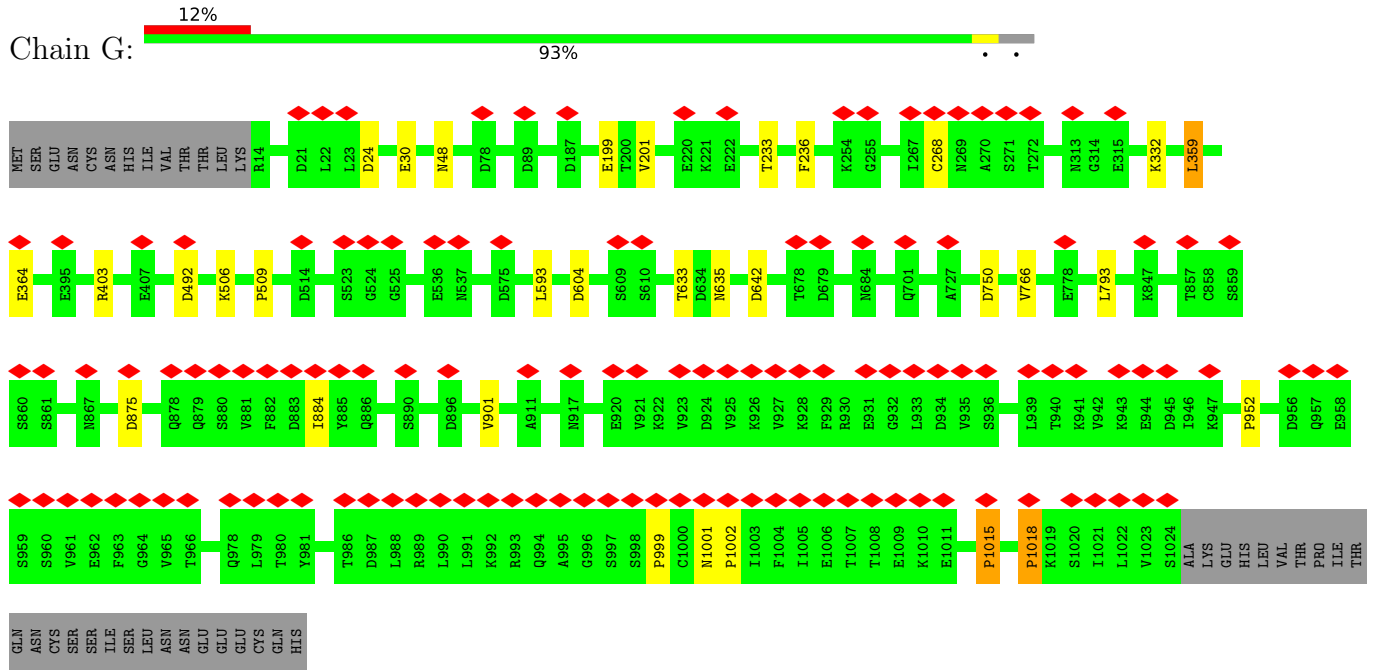
● Molecule 1: baseplate protein (Algo12)



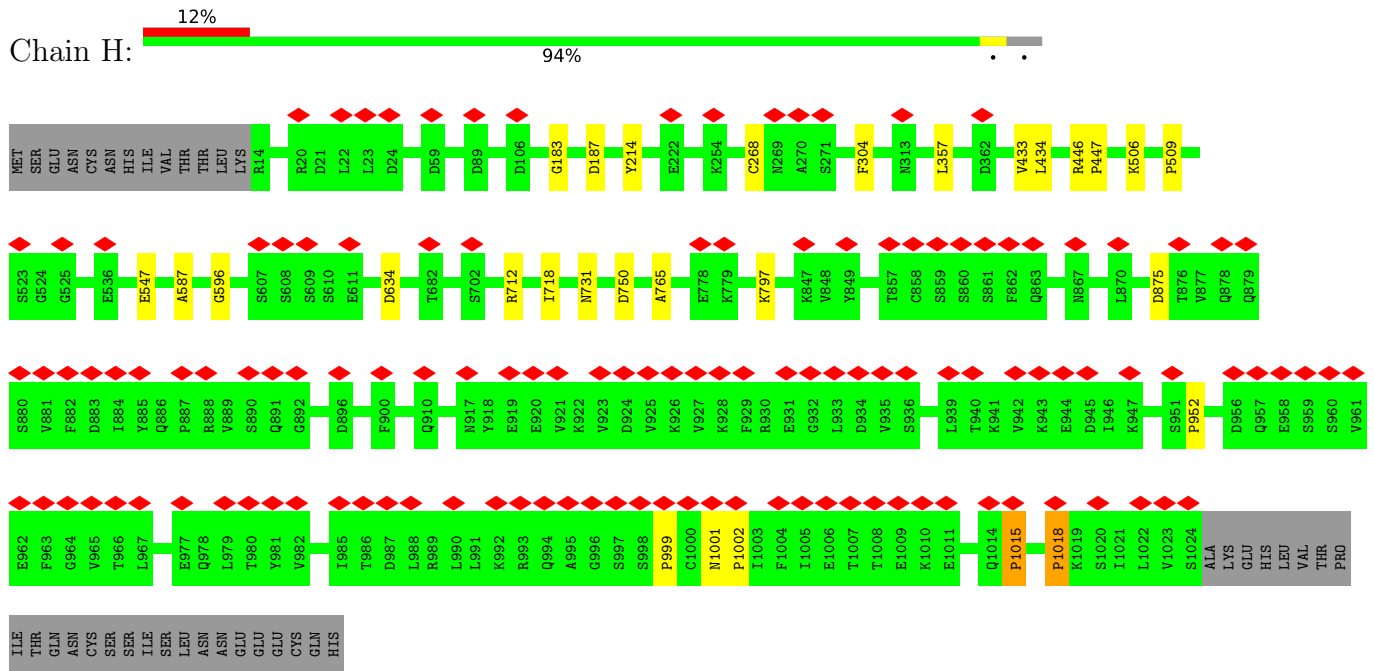
● Molecule 1: baseplate protein (Algo12)



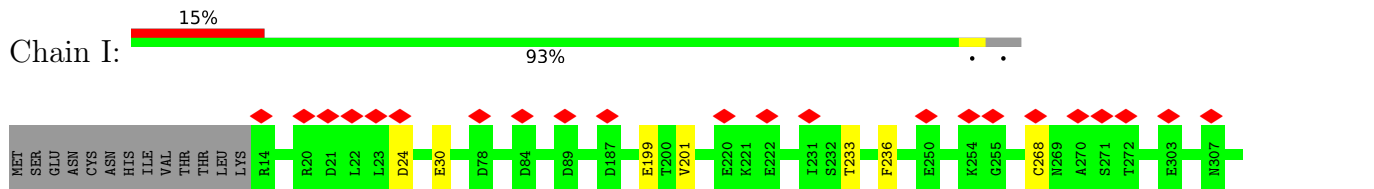
• Molecule 2: Baseplate_J domain-containing protein

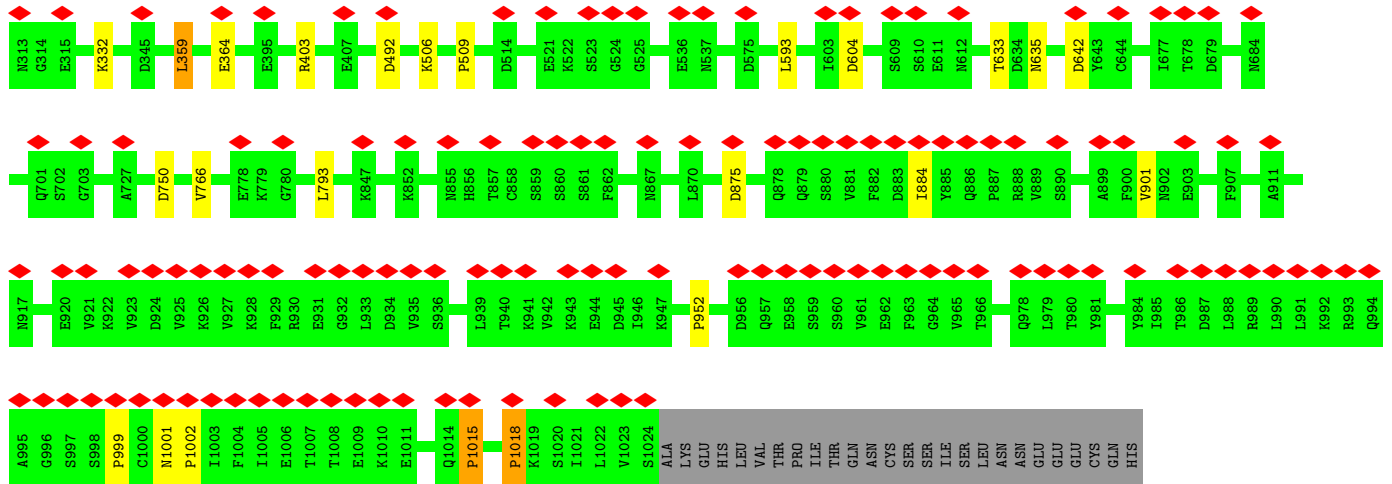


• Molecule 2: Baseplate_J domain-containing protein

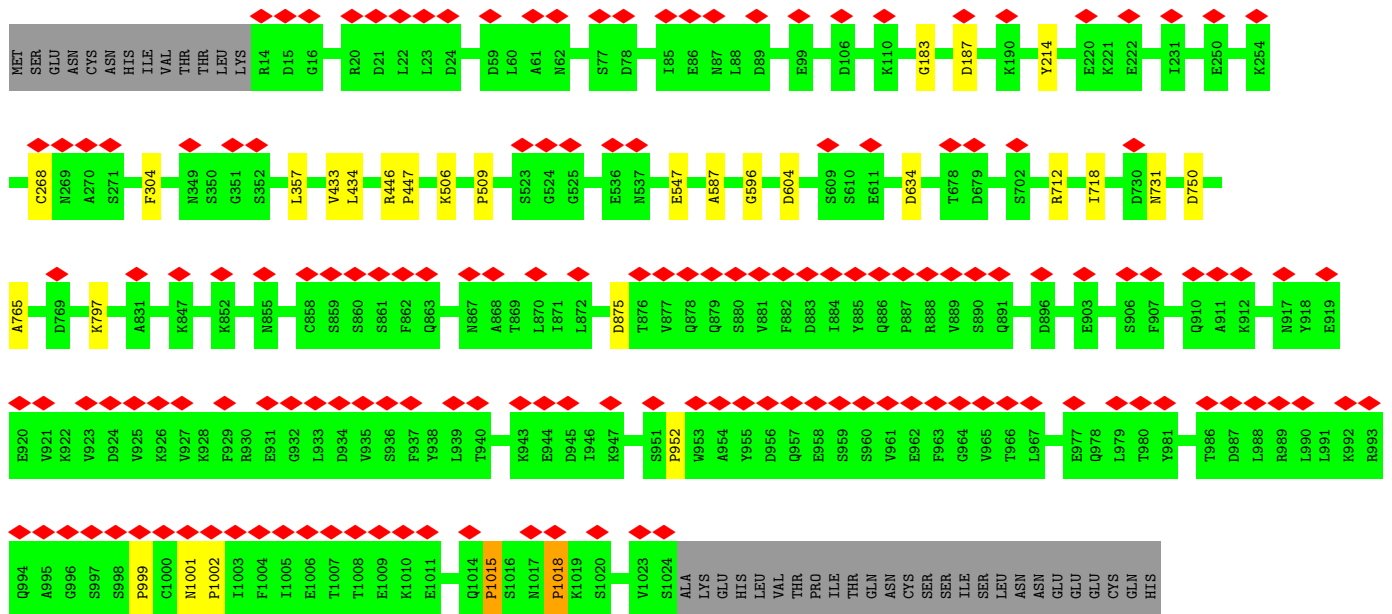


• Molecule 2: Baseplate_J domain-containing protein

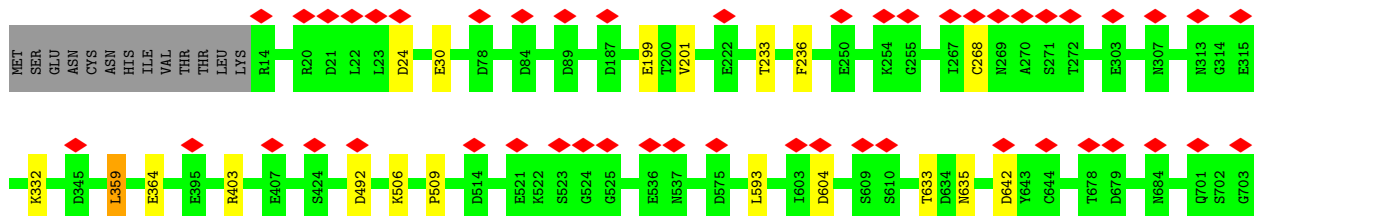
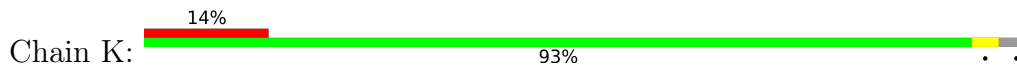


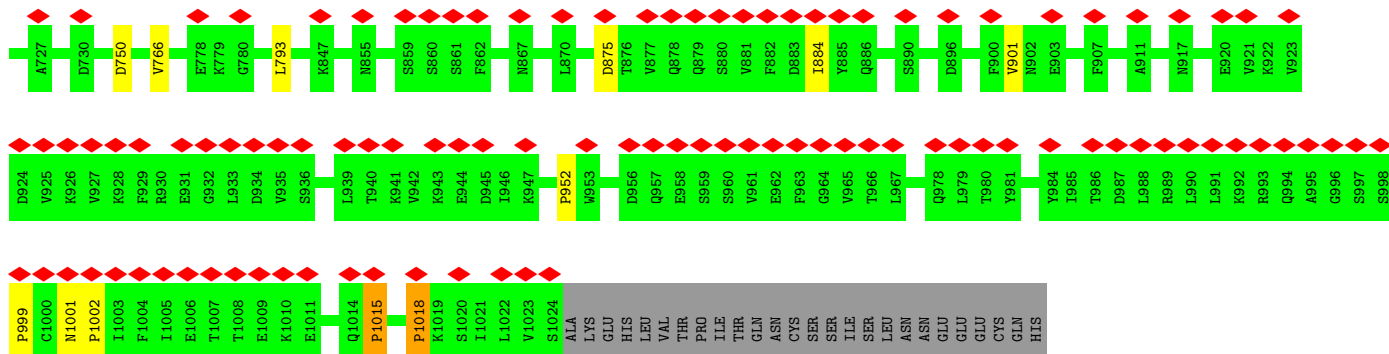


• Molecule 2: Baseplate_J domain-containing protein

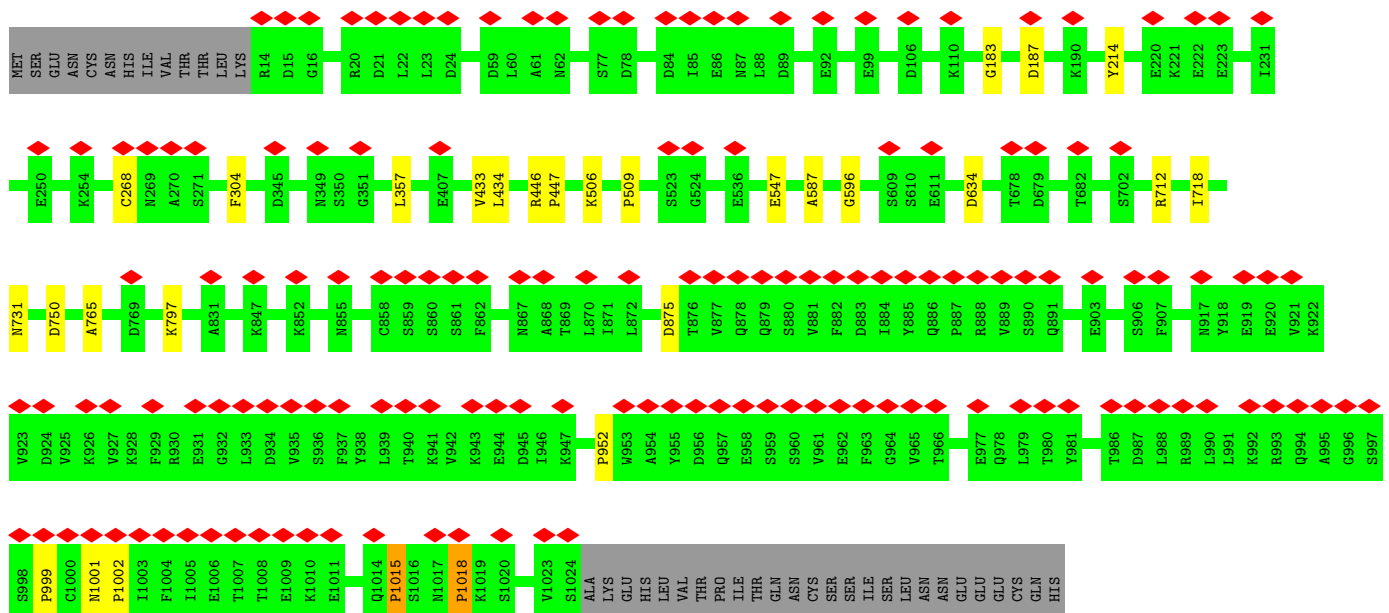


• Molecule 2: Baseplate_J domain-containing protein

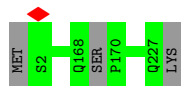




• Molecule 2: Baseplate_J domain-containing protein



• Molecule 3: LysM domain-containing protein

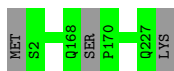


• Molecule 3: LysM domain-containing protein



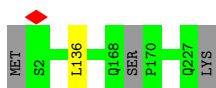
• Molecule 3: LysM domain-containing protein

Chain O:  99%



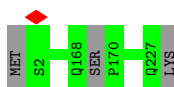
- Molecule 3: LysM domain-containing protein

Chain P:  98%



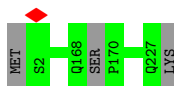
- Molecule 3: LysM domain-containing protein

Chain Q:  99%



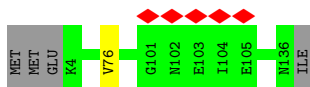
- Molecule 3: LysM domain-containing protein

Chain R:  99%



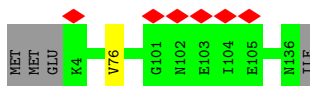
- Molecule 4: Putative tail lysozyme

Chain S:  96%



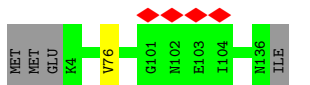
- Molecule 4: Putative tail lysozyme

Chain T:  96%

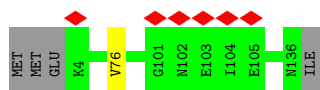


- Molecule 4: Putative tail lysozyme

Chain U:  96%



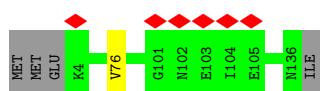
- Molecule 4: Putative tail lysozyme



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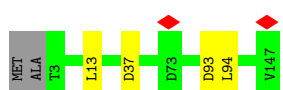
- Molecule 4: Putative tail lysozyme



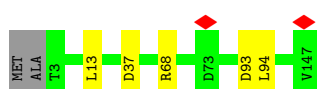
- Molecule 5: Phospholipid/glycerol acyltransferase



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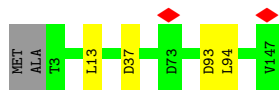


- Molecule 5: Phospholipid/glycerol acyltransferase

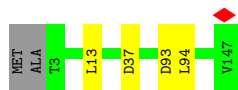




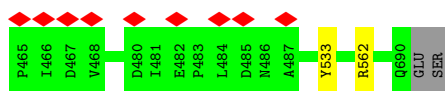
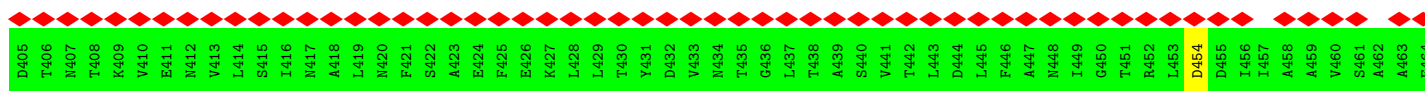
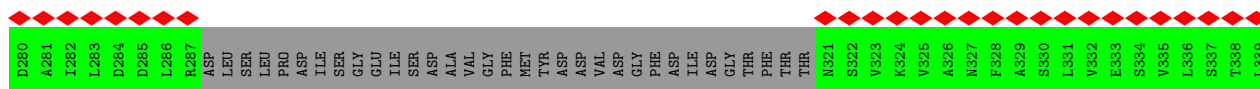
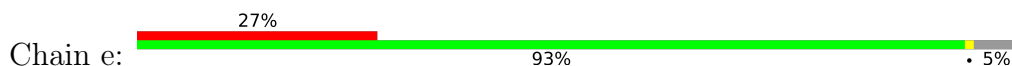
• Molecule 5: Phospholipid/glycerol acyltransferase



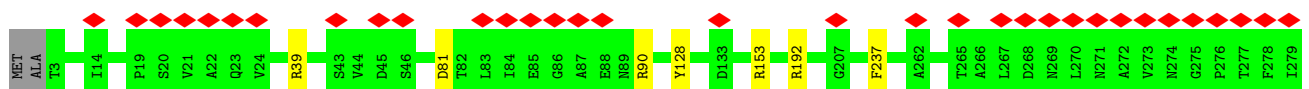
• Molecule 5: Phospholipid/glycerol acyltransferase

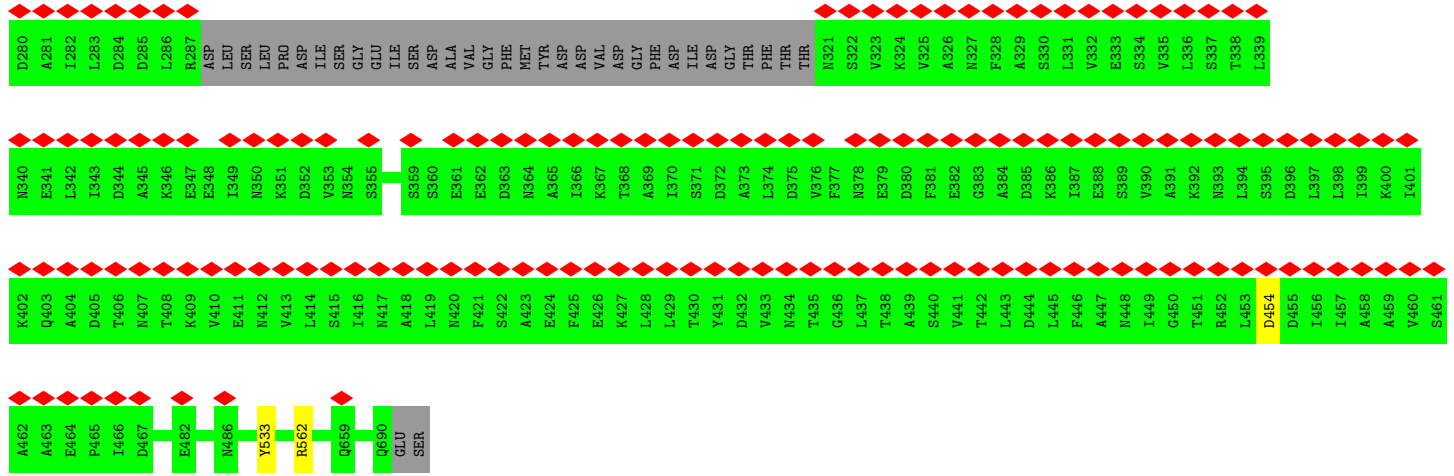


• Molecule 6: Putative phage tail sheath protein FI

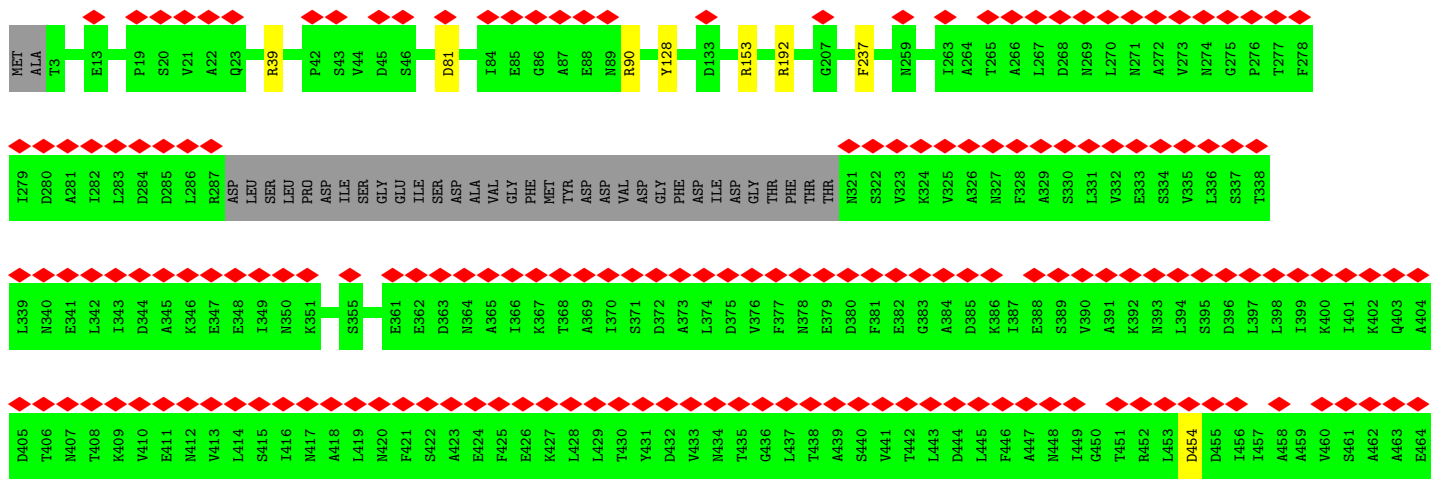
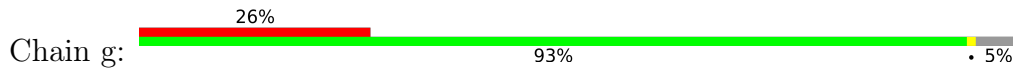


• Molecule 6: Putative phage tail sheath protein FI

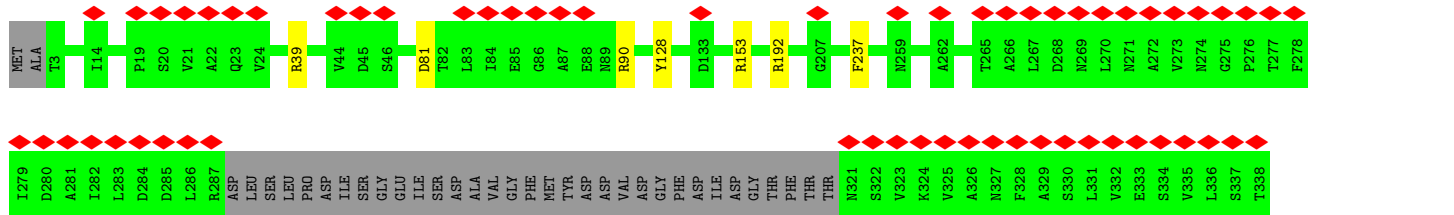
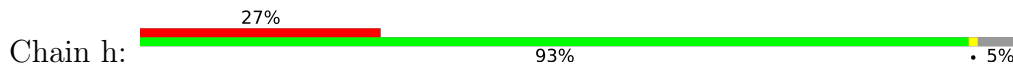


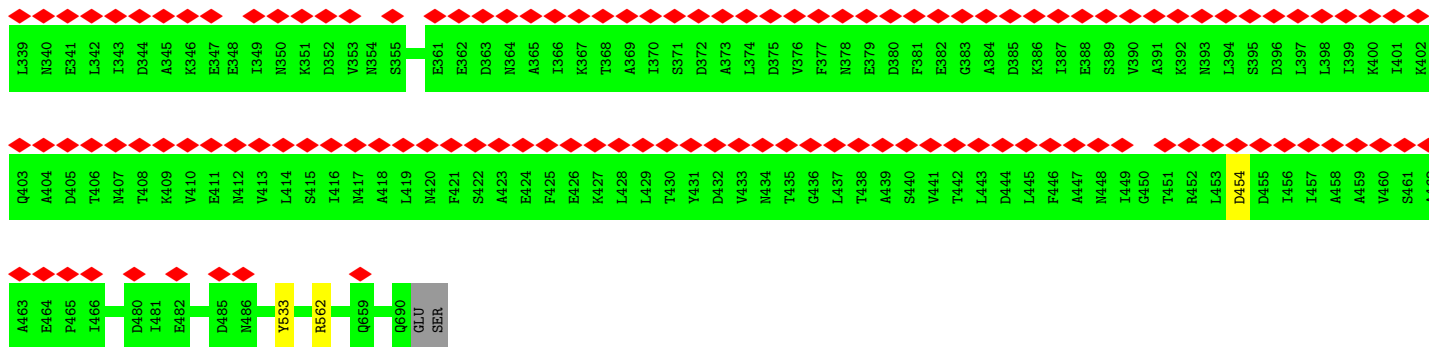


• Molecule 6: Putative phage tail sheath protein FI



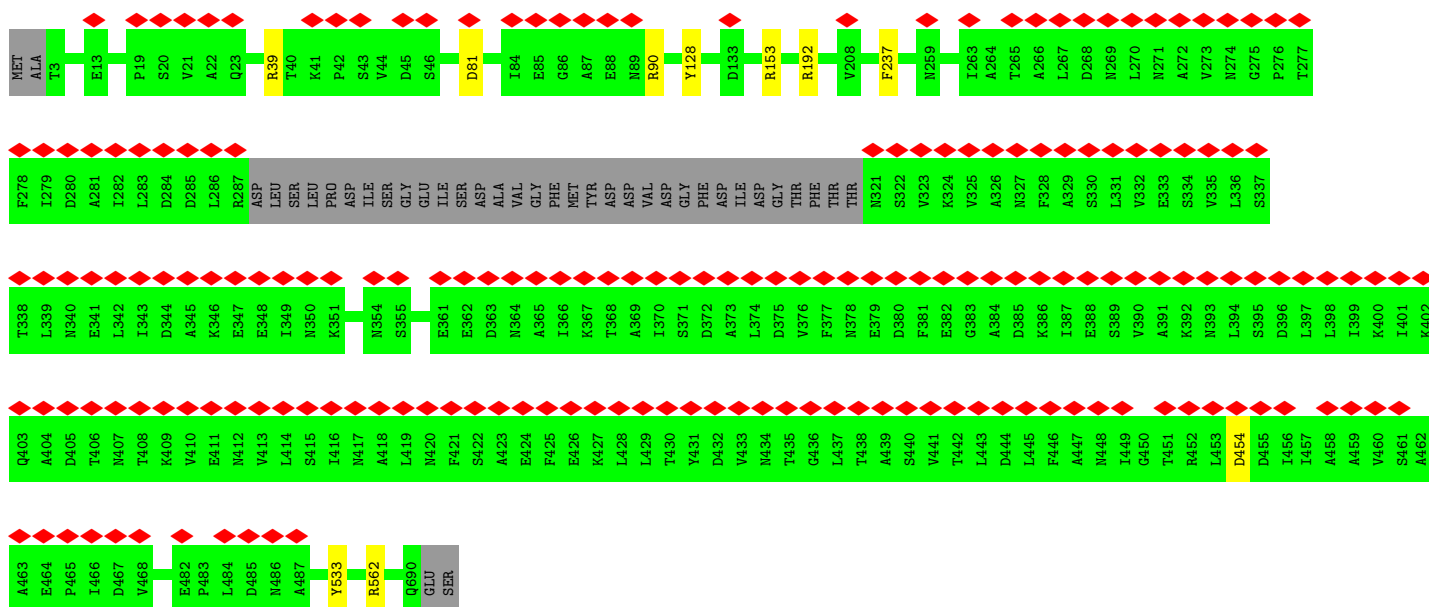
• Molecule 6: Putative phage tail sheath protein FI





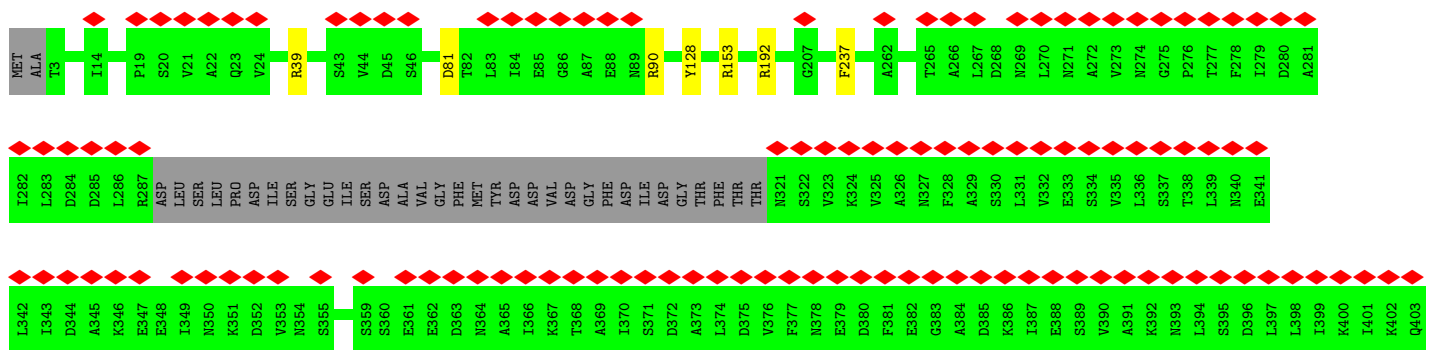
• Molecule 6: Putative phage tail sheath protein FI

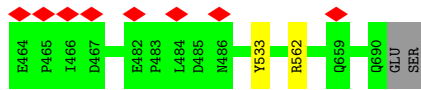
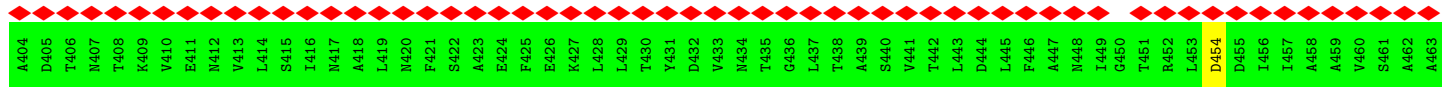
Chain i: 27% 93% 5%



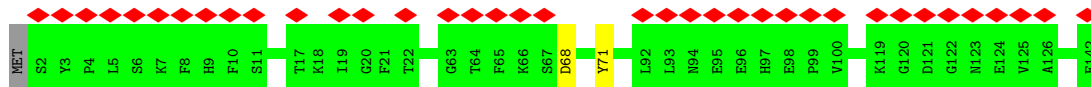
• Molecule 6: Putative phage tail sheath protein FI

Chain j: 27% 93% 5%

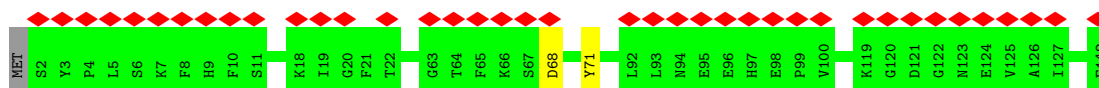




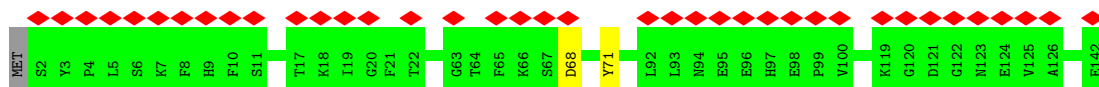
• Molecule 7: Phage tail protein



• Molecule 7: Phage tail protein



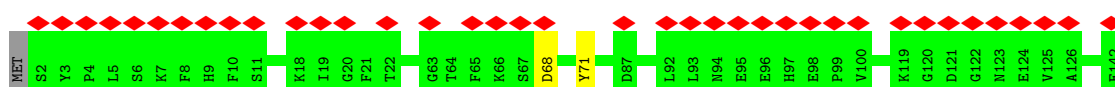
• Molecule 7: Phage tail protein



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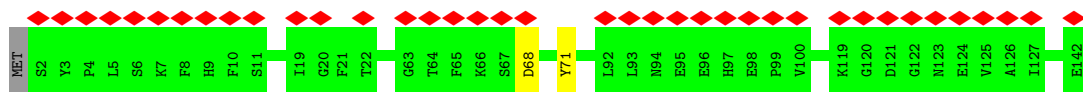


• Molecule 7: Phage tail protein

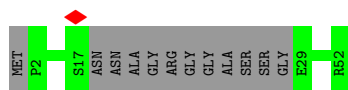
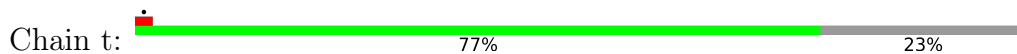


• Molecule 7: Phage tail protein

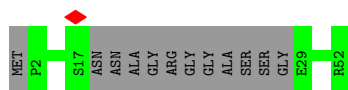
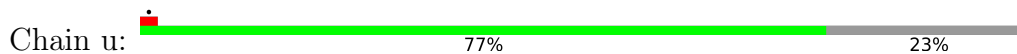




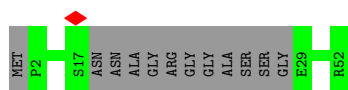
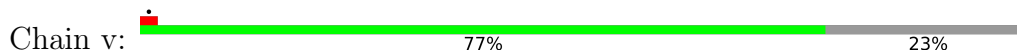
• Molecule 8: inner protein (Algo6)



• Molecule 8: inner protein (Algo6)



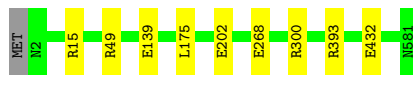
• Molecule 8: inner protein (Algo6)



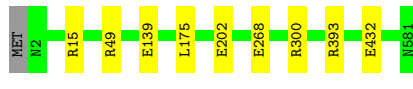
• Molecule 9: Phosphoserine phosphatase SerB



• Molecule 9: Phosphoserine phosphatase SerB



• Molecule 9: Phosphoserine phosphatase SerB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	82969	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	A	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	B	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
1	C	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	D	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
1	E	0.76	2/4531 (0.0%)	0.77	2/6117 (0.0%)
1	F	0.75	1/4531 (0.0%)	0.78	3/6117 (0.0%)
2	G	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	H	0.80	12/7935 (0.2%)	0.87	26/10781 (0.2%)
2	I	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	J	0.80	12/7935 (0.2%)	0.87	27/10781 (0.3%)
2	K	0.69	11/7935 (0.1%)	0.90	29/10781 (0.3%)
2	L	0.80	12/7935 (0.2%)	0.87	26/10781 (0.2%)
3	M	0.41	0/1889	0.58	0/2544
3	N	0.43	0/1889	0.57	1/2544 (0.0%)
3	O	0.41	0/1889	0.58	0/2544
3	P	0.43	0/1889	0.57	1/2544 (0.0%)
3	Q	0.41	0/1889	0.58	0/2544
3	R	0.43	0/1889	0.57	0/2544
4	S	0.68	1/1096 (0.1%)	0.80	0/1483
4	T	0.70	1/1096 (0.1%)	0.80	0/1483
4	U	0.69	1/1096 (0.1%)	0.80	0/1483
4	V	0.70	1/1096 (0.1%)	0.80	0/1483
4	W	0.69	1/1096 (0.1%)	0.80	0/1483
4	X	0.70	1/1096 (0.1%)	0.79	0/1483
5	Y	0.73	0/1226	0.89	5/1664 (0.3%)
5	Z	0.73	0/1226	0.89	5/1664 (0.3%)
5	a	0.73	0/1226	0.89	6/1664 (0.4%)
5	b	0.73	0/1226	0.89	5/1664 (0.3%)
5	c	0.73	0/1226	0.89	5/1664 (0.3%)
5	d	0.73	0/1226	0.89	5/1664 (0.3%)
6	e	0.78	0/5155	0.83	10/7021 (0.1%)
6	f	0.78	0/5155	0.83	10/7021 (0.1%)
6	g	0.78	0/5155	0.83	10/7021 (0.1%)
6	h	0.78	0/5155	0.83	10/7021 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	i	0.78	0/5155	0.83	10/7021 (0.1%)
6	j	0.79	0/5155	0.83	10/7021 (0.1%)
7	k	0.97	0/1172	0.85	2/1584 (0.1%)
7	l	0.97	0/1172	0.85	2/1584 (0.1%)
7	m	0.97	0/1172	0.85	2/1584 (0.1%)
7	n	0.97	0/1172	0.85	2/1584 (0.1%)
7	o	0.97	0/1172	0.85	2/1584 (0.1%)
7	p	0.97	0/1172	0.85	2/1584 (0.1%)
8	t	0.32	0/324	0.47	0/432
8	u	0.32	0/324	0.47	0/432
8	v	0.32	0/324	0.47	0/432
9	q	0.96	3/4536 (0.1%)	0.86	6/6145 (0.1%)
9	r	0.96	4/4536 (0.1%)	0.86	6/6145 (0.1%)
9	s	0.96	4/4536 (0.1%)	0.86	6/6145 (0.1%)
All	All	0.76	95/152604 (0.1%)	0.83	304/206895 (0.1%)

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
2	G	0	5
2	H	0	2
2	I	0	4
2	J	0	2
2	K	0	4
2	L	0	2
All	All	0	19

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	509	PRO	C-N	15.90	1.70	1.34
2	I	509	PRO	C-N	15.90	1.70	1.34
2	G	509	PRO	C-N	15.89	1.70	1.34
2	L	506	LYS	C-N	14.66	1.67	1.34
2	H	506	LYS	C-N	14.61	1.67	1.34
2	J	506	LYS	C-N	14.61	1.67	1.34
2	I	233	THR	CB-CG2	-12.94	1.09	1.52
2	G	233	THR	CB-CG2	-12.93	1.09	1.52
2	K	233	THR	CB-CG2	-12.93	1.09	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	446	ARG	C-N	12.50	1.57	1.34
2	H	446	ARG	C-N	12.50	1.57	1.34
2	J	446	ARG	C-N	12.47	1.57	1.34
2	J	731	ASN	C-N	12.03	1.61	1.34
2	H	731	ASN	C-N	12.02	1.61	1.34
2	L	731	ASN	C-N	12.02	1.61	1.34
2	H	433	VAL	C-N	11.94	1.61	1.34
2	J	433	VAL	C-N	11.93	1.61	1.34
2	L	433	VAL	C-N	11.93	1.61	1.34
2	H	587	ALA	C-N	11.85	1.56	1.34
2	J	587	ALA	C-N	11.84	1.56	1.34
2	L	587	ALA	C-N	11.76	1.56	1.34
2	L	304	PHE	C-N	11.27	1.59	1.34
2	H	304	PHE	C-N	11.25	1.59	1.34
2	J	304	PHE	C-N	11.23	1.59	1.34
2	K	403	ARG	CZ-NH1	-11.13	1.18	1.33
2	I	403	ARG	CZ-NH1	-11.10	1.18	1.33
2	G	403	ARG	CZ-NH1	-11.09	1.18	1.33
2	J	357	LEU	C-N	11.03	1.59	1.34
2	H	357	LEU	C-N	11.03	1.59	1.34
2	L	357	LEU	C-N	11.01	1.59	1.34
2	L	547	GLU	C-N	7.71	1.51	1.34
2	H	547	GLU	C-N	7.70	1.51	1.34
2	J	547	GLU	C-N	7.69	1.51	1.34
2	J	214	TYR	C-N	7.65	1.51	1.34
2	L	214	TYR	C-N	7.63	1.51	1.34
2	H	214	TYR	C-N	7.62	1.51	1.34
2	I	506	LYS	C-N	7.43	1.51	1.34
2	K	506	LYS	C-N	7.41	1.51	1.34
2	G	506	LYS	C-N	7.40	1.51	1.34
2	G	201	VAL	CB-CG2	-6.80	1.38	1.52
2	K	201	VAL	CB-CG2	-6.77	1.38	1.52
2	I	201	VAL	CB-CG2	-6.73	1.38	1.52
1	D	117	CYS	CB-SG	-5.86	1.72	1.81
2	H	268	CYS	CB-SG	-5.83	1.72	1.81
2	J	268	CYS	CB-SG	-5.82	1.72	1.81
2	K	236	PHE	CG-CD1	-5.82	1.30	1.38
1	B	117	CYS	CB-SG	-5.78	1.72	1.81
2	G	236	PHE	CG-CD1	-5.78	1.30	1.38
1	F	117	CYS	CB-SG	-5.78	1.72	1.81
2	I	236	PHE	CG-CD1	-5.78	1.30	1.38
2	L	268	CYS	CB-SG	-5.74	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	CYS	CB-SG	-5.74	1.72	1.81
1	E	117	CYS	CB-SG	-5.73	1.72	1.81
2	K	268	CYS	CB-SG	-5.72	1.72	1.81
9	s	268	GLU	CD-OE1	-5.70	1.19	1.25
2	G	268	CYS	CB-SG	-5.69	1.72	1.81
1	A	117	CYS	CB-SG	-5.69	1.72	1.81
2	I	268	CYS	CB-SG	-5.68	1.72	1.81
2	J	765	ALA	C-N	5.68	1.47	1.34
2	H	765	ALA	C-N	5.66	1.47	1.34
1	E	219	GLU	CD-OE1	-5.64	1.19	1.25
2	L	765	ALA	C-N	5.63	1.47	1.34
9	q	268	GLU	CD-OE1	-5.62	1.19	1.25
9	r	268	GLU	CD-OE1	-5.62	1.19	1.25
1	A	219	GLU	CD-OE1	-5.60	1.19	1.25
2	I	201	VAL	CB-CG1	-5.60	1.41	1.52
1	C	219	GLU	CD-OE1	-5.56	1.19	1.25
2	K	201	VAL	CB-CG1	-5.53	1.41	1.52
2	G	201	VAL	CB-CG1	-5.53	1.41	1.52
2	K	766	VAL	C-N	-5.29	1.21	1.34
2	G	199	GLU	CD-OE2	-5.28	1.19	1.25
2	H	447	PRO	N-CA	5.27	1.56	1.47
2	I	766	VAL	C-N	-5.27	1.22	1.34
2	G	766	VAL	C-N	-5.27	1.22	1.34
2	I	199	GLU	CD-OE2	-5.26	1.19	1.25
2	K	199	GLU	CD-OE2	-5.25	1.19	1.25
2	L	447	PRO	N-CA	5.25	1.56	1.47
2	J	447	PRO	N-CA	5.24	1.56	1.47
4	U	76	VAL	CB-CG2	-5.23	1.41	1.52
2	K	901	VAL	CB-CG1	-5.20	1.42	1.52
2	G	901	VAL	CB-CG1	-5.19	1.42	1.52
4	W	76	VAL	CB-CG2	-5.18	1.42	1.52
2	I	901	VAL	CB-CG1	-5.17	1.42	1.52
4	S	76	VAL	CB-CG2	-5.17	1.42	1.52
4	X	76	VAL	CB-CG2	-5.14	1.42	1.52
9	r	139	GLU	CD-OE1	-5.14	1.20	1.25
9	r	432	GLU	CD-OE2	-5.12	1.20	1.25
4	V	76	VAL	CB-CG2	-5.12	1.42	1.52
4	T	76	VAL	CB-CG2	-5.10	1.42	1.52
9	q	432	GLU	CD-OE2	-5.09	1.20	1.25
9	s	139	GLU	CD-OE1	-5.08	1.20	1.25
9	q	139	GLU	CD-OE1	-5.07	1.20	1.25
9	s	202	GLU	CD-OE2	-5.05	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	432	GLU	CD-OE2	-5.03	1.20	1.25
9	r	202	GLU	CD-OE2	-5.01	1.20	1.25

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	175	LEU	CA-CB-CG	10.64	139.77	115.30
9	s	175	LEU	CA-CB-CG	10.63	139.76	115.30
9	q	175	LEU	CA-CB-CG	10.62	139.73	115.30
2	K	506	LYS	O-C-N	-10.34	106.15	122.70
2	G	506	LYS	O-C-N	-10.34	106.16	122.70
2	I	506	LYS	O-C-N	-10.31	106.21	122.70
2	L	1018	PRO	N-CA-CB	9.65	114.89	103.30
2	J	1018	PRO	N-CA-CB	9.63	114.85	103.30
2	H	1018	PRO	N-CA-CB	9.59	114.81	103.30
2	G	403	ARG	NE-CZ-NH2	9.59	125.09	120.30
2	I	403	ARG	NE-CZ-NH2	9.59	125.09	120.30
2	K	403	ARG	NE-CZ-NH2	9.51	125.06	120.30
9	r	300	ARG	NE-CZ-NH1	9.43	125.02	120.30
9	q	300	ARG	NE-CZ-NH1	9.40	125.00	120.30
9	s	300	ARG	NE-CZ-NH1	9.37	124.99	120.30
2	G	1018	PRO	N-CA-CB	9.33	114.49	103.30
2	I	1018	PRO	N-CA-CB	9.30	114.46	103.30
2	K	1018	PRO	N-CA-CB	9.28	114.43	103.30
2	L	434	LEU	O-C-N	9.16	137.36	122.70
2	L	434	LEU	CA-C-N	-9.14	97.09	117.20
2	H	434	LEU	O-C-N	9.12	137.29	122.70
2	J	434	LEU	CA-C-N	-9.11	97.17	117.20
2	H	434	LEU	CA-C-N	-9.10	97.18	117.20
2	J	434	LEU	O-C-N	9.08	137.23	122.70
2	J	750	ASP	CB-CG-OD1	-8.80	110.38	118.30
2	L	750	ASP	CB-CG-OD1	-8.78	110.40	118.30
2	H	750	ASP	CB-CG-OD1	-8.76	110.42	118.30
5	c	94	LEU	CA-CB-CG	8.43	134.68	115.30
5	Y	94	LEU	CA-CB-CG	8.40	134.62	115.30
5	Z	94	LEU	CA-CB-CG	8.39	134.61	115.30
5	d	94	LEU	CA-CB-CG	8.39	134.60	115.30
5	b	94	LEU	CA-CB-CG	8.39	134.59	115.30
5	a	94	LEU	CA-CB-CG	8.38	134.57	115.30
6	f	192	ARG	NE-CZ-NH2	-7.83	116.38	120.30
6	h	192	ARG	NE-CZ-NH2	-7.77	116.41	120.30
6	e	192	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	192	ARG	NE-CZ-NH2	-7.76	116.42	120.30
6	g	192	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	G	506	LYS	CA-C-N	7.72	134.19	117.20
2	K	506	LYS	CA-C-N	7.71	134.17	117.20
2	I	506	LYS	CA-C-N	7.71	134.16	117.20
5	Z	37	ASP	CB-CG-OD2	7.68	125.22	118.30
5	Y	37	ASP	CB-CG-OD2	7.68	125.21	118.30
5	a	37	ASP	CB-CG-OD2	7.65	125.19	118.30
5	d	37	ASP	CB-CG-OD2	7.64	125.17	118.30
6	j	192	ARG	NE-CZ-NH2	-7.63	116.48	120.30
5	c	37	ASP	CB-CG-OD2	7.61	125.15	118.30
5	b	37	ASP	CB-CG-OD2	7.59	125.13	118.30
2	K	750	ASP	CB-CG-OD1	-7.41	111.63	118.30
2	G	750	ASP	CB-CG-OD1	-7.41	111.64	118.30
2	I	750	ASP	CB-CG-OD1	-7.36	111.68	118.30
2	K	268	CYS	CA-CB-SG	-7.34	100.79	114.00
2	G	268	CYS	CA-CB-SG	-7.32	100.82	114.00
2	I	268	CYS	CA-CB-SG	-7.32	100.83	114.00
2	K	403	ARG	NH1-CZ-NH2	-7.21	111.47	119.40
2	G	403	ARG	NH1-CZ-NH2	-7.18	111.51	119.40
6	f	90	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	I	403	ARG	NH1-CZ-NH2	-7.15	111.53	119.40
6	i	90	ARG	NE-CZ-NH2	-7.14	116.73	120.30
6	e	90	ARG	NE-CZ-NH2	-7.14	116.73	120.30
6	g	90	ARG	NE-CZ-NH2	-7.13	116.73	120.30
6	j	90	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	L	434	LEU	C-N-CA	-7.09	103.98	121.70
2	H	434	LEU	C-N-CA	-7.05	104.07	121.70
2	J	434	LEU	C-N-CA	-7.04	104.10	121.70
6	h	90	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	I	793	LEU	CB-CG-CD1	-6.96	99.17	111.00
2	G	793	LEU	CB-CG-CD1	-6.95	99.18	111.00
2	K	793	LEU	CB-CG-CD1	-6.93	99.22	111.00
2	I	199	GLU	OE1-CD-OE2	-6.78	115.17	123.30
2	G	199	GLU	OE1-CD-OE2	-6.76	115.19	123.30
2	K	199	GLU	OE1-CD-OE2	-6.76	115.19	123.30
6	j	39	ARG	NE-CZ-NH2	-6.73	116.93	120.30
6	g	39	ARG	NE-CZ-NH2	-6.73	116.94	120.30
6	i	39	ARG	NE-CZ-NH2	-6.67	116.96	120.30
2	L	509	PRO	N-CA-C	-6.66	94.78	112.10
2	H	509	PRO	N-CA-C	-6.65	94.81	112.10
2	J	509	PRO	N-CA-C	-6.65	94.81	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	39	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	G	875	ASP	CB-CG-OD1	-6.61	112.35	118.30
7	n	71	TYR	CB-CG-CD1	-6.61	117.03	121.00
2	K	875	ASP	CB-CG-OD1	-6.60	112.36	118.30
7	k	71	TYR	CB-CG-CD1	-6.60	117.04	121.00
5	b	13	LEU	CA-CB-CG	6.59	130.45	115.30
2	I	875	ASP	CB-CG-OD1	-6.58	112.37	118.30
6	h	39	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	26	ARG	NE-CZ-NH2	-6.58	117.01	120.30
5	a	13	LEU	CA-CB-CG	6.58	130.43	115.30
5	d	13	LEU	CA-CB-CG	6.58	130.43	115.30
6	e	39	ARG	NE-CZ-NH2	-6.58	117.01	120.30
5	c	13	LEU	CA-CB-CG	6.57	130.41	115.30
1	C	26	ARG	NE-CZ-NH2	-6.57	117.02	120.30
7	o	71	TYR	CB-CG-CD1	-6.57	117.06	121.00
2	H	433	VAL	C-N-CA	6.56	138.09	121.70
2	L	433	VAL	C-N-CA	6.56	138.09	121.70
9	s	393	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	J	433	VAL	C-N-CA	6.55	138.07	121.70
1	B	26	ARG	NE-CZ-NH2	-6.55	117.03	120.30
5	Y	13	LEU	CA-CB-CG	6.55	130.36	115.30
5	Z	13	LEU	CA-CB-CG	6.55	130.36	115.30
7	p	71	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	A	26	ARG	NE-CZ-NH2	-6.52	117.04	120.30
6	i	533	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	E	26	ARG	NE-CZ-NH2	-6.51	117.04	120.30
6	f	533	TYR	CB-CG-CD2	-6.51	117.09	121.00
7	m	71	TYR	CB-CG-CD1	-6.51	117.09	121.00
9	r	393	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	F	26	ARG	NE-CZ-NH2	-6.50	117.05	120.30
7	l	71	TYR	CB-CG-CD1	-6.49	117.11	121.00
6	e	533	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	K	793	LEU	CA-CB-CG	6.47	130.18	115.30
2	L	797	LYS	C-N-CA	-6.47	105.54	121.70
2	H	797	LYS	C-N-CA	-6.46	105.54	121.70
2	J	797	LYS	C-N-CA	-6.46	105.54	121.70
2	G	793	LEU	CA-CB-CG	6.45	130.14	115.30
6	h	533	TYR	CB-CG-CD2	-6.45	117.13	121.00
9	q	393	ARG	NE-CZ-NH2	-6.44	117.08	120.30
6	j	533	TYR	CB-CG-CD2	-6.43	117.14	121.00
2	I	793	LEU	CA-CB-CG	6.42	130.06	115.30
6	g	533	TYR	CB-CG-CD2	-6.37	117.18	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	s	15	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	G	359	LEU	CA-CB-CG	6.21	129.59	115.30
2	K	359	LEU	CA-CB-CG	6.21	129.57	115.30
2	I	359	LEU	CA-CB-CG	6.21	129.57	115.30
9	q	15	ARG	NE-CZ-NH1	6.15	123.38	120.30
9	r	15	ARG	NE-CZ-NH1	6.15	123.37	120.30
6	f	153	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	J	750	ASP	CB-CG-OD2	6.08	123.77	118.30
2	G	952	PRO	N-CA-CB	6.07	110.59	103.30
6	j	153	ARG	NE-CZ-NH1	6.06	123.33	120.30
6	g	153	ARG	NE-CZ-NH1	6.06	123.33	120.30
6	h	153	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	I	952	PRO	N-CA-CB	6.05	110.56	103.30
6	i	153	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	H	750	ASP	CB-CG-OD2	6.04	123.73	118.30
2	K	952	PRO	N-CA-CB	6.04	110.54	103.30
2	L	750	ASP	CB-CG-OD2	6.03	123.72	118.30
2	G	1002	PRO	N-CA-CB	5.97	110.47	103.30
6	e	153	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	J	446	ARG	CA-C-N	5.95	133.76	117.10
2	H	446	ARG	CA-C-N	5.94	133.73	117.10
2	L	446	ARG	CA-C-N	5.94	133.73	117.10
2	K	1002	PRO	N-CA-CB	5.94	110.43	103.30
2	I	1015	PRO	N-CA-CB	5.93	110.41	103.30
2	G	236	PHE	CB-CG-CD1	5.92	124.95	120.80
2	I	1002	PRO	N-CA-CB	5.92	110.41	103.30
2	K	1015	PRO	N-CA-CB	5.92	110.40	103.30
2	H	183	GLY	N-CA-C	5.89	127.84	113.10
2	K	236	PHE	CB-CG-CD1	5.89	124.92	120.80
2	L	183	GLY	N-CA-C	5.89	127.81	113.10
2	I	236	PHE	CB-CG-CD1	5.88	124.92	120.80
2	J	183	GLY	N-CA-C	5.87	127.77	113.10
2	G	1015	PRO	N-CA-CB	5.87	110.34	103.30
2	J	1002	PRO	N-CA-CB	5.86	110.33	103.30
2	G	604	ASP	CB-CG-OD1	5.85	123.57	118.30
2	H	1002	PRO	N-CA-CB	5.85	110.32	103.30
2	L	1002	PRO	N-CA-CB	5.85	110.32	103.30
2	G	509	PRO	C-N-CA	5.85	136.32	121.70
2	K	604	ASP	CB-CG-OD1	5.84	123.56	118.30
2	K	509	PRO	C-N-CA	5.83	136.27	121.70
2	I	509	PRO	C-N-CA	5.83	136.27	121.70
2	I	604	ASP	CB-CG-OD1	5.82	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	952	PRO	N-CA-CB	5.81	110.28	103.30
2	L	446	ARG	C-N-CD	-5.80	107.83	120.60
2	J	952	PRO	N-CA-CB	5.80	110.26	103.30
2	H	952	PRO	N-CA-CB	5.80	110.26	103.30
2	J	446	ARG	C-N-CD	-5.80	107.85	120.60
2	H	446	ARG	C-N-CD	-5.79	107.86	120.60
2	H	1015	PRO	N-CA-CB	5.77	110.22	103.30
2	J	1015	PRO	N-CA-CB	5.77	110.22	103.30
2	L	1015	PRO	N-CA-CB	5.76	110.22	103.30
6	h	562	ARG	NE-CZ-NH1	5.73	123.17	120.30
6	j	562	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	F	509	ARG	NE-CZ-NH2	-5.70	117.45	120.30
6	f	562	ARG	NE-CZ-NH1	5.70	123.15	120.30
6	g	562	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	K	999	PRO	N-CA-CB	5.65	110.08	103.30
6	e	562	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	I	593	LEU	CB-CG-CD1	-5.62	101.44	111.00
2	K	593	LEU	CB-CG-CD1	-5.61	101.46	111.00
2	G	999	PRO	N-CA-CB	5.61	110.03	103.30
2	G	593	LEU	CB-CG-CD1	-5.60	101.48	111.00
2	K	403	ARG	NE-CZ-NH1	5.59	123.10	120.30
6	i	562	ARG	NE-CZ-NH1	5.59	123.09	120.30
9	q	49	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	I	999	PRO	N-CA-CB	5.57	109.99	103.30
9	s	49	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	509	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	509	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	509	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	G	750	ASP	CB-CG-OD2	5.53	123.28	118.30
2	L	433	VAL	CA-C-N	5.53	129.36	117.20
2	J	433	VAL	CA-C-N	5.52	129.35	117.20
2	I	750	ASP	CB-CG-OD2	5.51	123.26	118.30
2	H	433	VAL	CA-C-N	5.51	129.31	117.20
2	K	750	ASP	CB-CG-OD2	5.49	123.24	118.30
2	K	884	ILE	CB-CA-C	-5.47	100.65	111.60
2	J	718	ILE	CA-C-N	-5.47	105.17	117.20
9	r	49	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	L	718	ILE	CA-C-N	-5.47	105.17	117.20
2	I	884	ILE	CB-CA-C	-5.46	100.68	111.60
2	G	884	ILE	CB-CA-C	-5.46	100.68	111.60
2	H	718	ILE	CA-C-N	-5.45	105.20	117.20
2	H	587	ALA	C-N-CD	-5.44	108.63	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	403	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	J	587	ALA	C-N-CD	-5.43	108.65	120.60
2	L	587	ALA	C-N-CD	-5.41	108.70	120.60
1	A	509	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	I	403	ARG	NE-CZ-NH1	5.39	123.00	120.30
9	q	300	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	G	332	LYS	CA-CB-CG	-5.33	101.67	113.40
2	K	332	LYS	CA-CB-CG	-5.33	101.68	113.40
9	r	300	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	E	509	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	I	332	LYS	CA-CB-CG	-5.30	101.75	113.40
7	l	68	ASP	CB-CG-OD1	5.29	123.06	118.30
7	p	68	ASP	CB-CG-OD1	5.29	123.06	118.30
9	s	300	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	K	30	GLU	CB-CA-C	-5.28	99.85	110.40
2	G	30	GLU	CB-CA-C	-5.26	99.88	110.40
2	H	634	ASP	CB-CG-OD1	5.26	123.03	118.30
2	L	634	ASP	CB-CG-OD1	5.25	123.03	118.30
2	L	433	VAL	O-C-N	-5.25	114.30	122.70
2	H	214	TYR	O-C-N	5.25	131.10	122.70
7	m	68	ASP	CB-CG-OD1	5.25	123.02	118.30
6	h	454	ASP	CB-CG-OD1	5.24	123.02	118.30
2	H	433	VAL	O-C-N	-5.24	114.32	122.70
2	I	30	GLU	CB-CA-C	-5.24	99.93	110.40
2	L	214	TYR	O-C-N	5.23	131.07	122.70
2	H	587	ALA	O-C-N	-5.23	111.16	121.10
2	J	433	VAL	O-C-N	-5.23	114.33	122.70
2	L	187	ASP	CB-CG-OD2	5.23	123.00	118.30
2	H	999	PRO	N-CA-CB	5.22	109.57	103.30
2	J	587	ALA	O-C-N	-5.22	111.18	121.10
2	J	999	PRO	N-CA-CB	5.22	109.56	103.30
7	n	68	ASP	CB-CG-OD1	5.22	122.99	118.30
2	J	634	ASP	CB-CG-OD1	5.21	122.99	118.30
2	J	214	TYR	O-C-N	5.21	131.04	122.70
6	i	454	ASP	CB-CG-OD1	5.21	122.99	118.30
2	L	999	PRO	N-CA-CB	5.21	109.55	103.30
7	k	68	ASP	CB-CG-OD1	5.21	122.99	118.30
2	J	187	ASP	CB-CG-OD2	5.21	122.99	118.30
6	j	81	ASP	CB-CG-OD1	5.20	122.98	118.30
7	o	68	ASP	CB-CG-OD1	5.20	122.98	118.30
2	H	187	ASP	CB-CG-OD2	5.19	122.97	118.30
2	L	587	ALA	O-C-N	-5.19	111.24	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	712	ARG	NE-CZ-NH2	-5.18	117.71	120.30
6	g	128	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	D	345	ILE	CG1-CB-CG2	-5.18	100.00	111.40
2	K	359	LEU	CB-CG-CD1	5.18	119.80	111.00
2	I	359	LEU	CB-CG-CD1	5.18	119.80	111.00
2	G	359	LEU	CB-CG-CD1	5.17	119.80	111.00
6	j	454	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	345	ILE	CG1-CB-CG2	-5.17	100.02	111.40
6	f	81	ASP	CB-CG-OD1	5.17	122.95	118.30
6	f	454	ASP	CB-CG-OD1	5.16	122.95	118.30
6	g	454	ASP	CB-CG-OD1	5.16	122.95	118.30
6	e	454	ASP	CB-CG-OD1	5.16	122.94	118.30
1	F	345	ILE	CG1-CB-CG2	-5.16	100.06	111.40
2	H	268	CYS	CA-CB-SG	-5.16	104.72	114.00
6	g	81	ASP	CB-CG-OD1	5.16	122.94	118.30
6	h	237	PHE	CB-CG-CD1	5.15	124.41	120.80
2	J	268	CYS	CA-CB-SG	-5.15	104.73	114.00
2	L	268	CYS	CA-CB-SG	-5.15	104.73	114.00
5	Z	93	ASP	CB-CG-OD1	5.15	122.93	118.30
6	e	81	ASP	CB-CG-OD1	5.14	122.93	118.30
5	b	93	ASP	CB-CG-OD1	5.14	122.93	118.30
5	Y	93	ASP	CB-CG-OD1	5.14	122.93	118.30
6	i	81	ASP	CB-CG-OD1	5.14	122.92	118.30
2	K	24	ASP	CB-CG-OD1	5.13	122.92	118.30
5	a	94	LEU	CB-CG-CD1	-5.13	102.27	111.00
2	I	24	ASP	CB-CG-OD1	5.13	122.91	118.30
2	H	712	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	K	875	ASP	CB-CG-OD2	5.12	122.91	118.30
5	a	93	ASP	CB-CG-OD1	5.12	122.91	118.30
5	b	94	LEU	CB-CG-CD1	-5.12	102.29	111.00
6	f	128	TYR	CB-CG-CD2	-5.12	117.93	121.00
6	i	237	PHE	CB-CG-CD1	5.12	124.38	120.80
5	d	94	LEU	CB-CG-CD1	-5.12	102.30	111.00
6	f	237	PHE	CB-CG-CD1	5.12	124.38	120.80
6	h	81	ASP	CB-CG-OD1	5.11	122.90	118.30
5	c	93	ASP	CB-CG-OD1	5.11	122.90	118.30
2	I	633	THR	CA-CB-CG2	-5.11	105.25	112.40
5	Y	94	LEU	CB-CG-CD1	-5.11	102.32	111.00
5	Z	94	LEU	CB-CG-CD1	-5.10	102.33	111.00
2	L	712	ARG	NE-CZ-NH2	-5.10	117.75	120.30
5	c	94	LEU	CB-CG-CD1	-5.09	102.34	111.00
2	G	24	ASP	CB-CG-OD1	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	e	237	PHE	CB-CG-CD1	5.09	124.36	120.80
2	G	633	THR	CA-CB-CG2	-5.07	105.30	112.40
6	h	128	TYR	CB-CG-CD2	-5.06	117.96	121.00
6	e	128	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	K	633	THR	CA-CB-CG2	-5.06	105.32	112.40
6	j	128	TYR	CB-CG-CD2	-5.06	117.97	121.00
5	d	93	ASP	CB-CG-OD1	5.06	122.85	118.30
6	i	128	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	G	875	ASP	CB-CG-OD2	5.04	122.84	118.30
2	I	875	ASP	CB-CG-OD2	5.04	122.84	118.30
5	a	68	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	j	237	PHE	CB-CG-CD1	5.02	124.31	120.80
6	g	237	PHE	CB-CG-CD1	5.01	124.31	120.80
3	P	136	LEU	CA-CB-CG	5.00	126.81	115.30
2	J	604	ASP	CB-CG-OD1	5.00	122.80	118.30
3	N	136	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	364	GLU	Sidechain
2	G	48	ASN	Sidechain
2	G	492	ASP	Sidechain
2	G	635	ASN	Sidechain
2	G	642	ASP	Sidechain
2	H	596	GLY	Mainchain
2	H	875	ASP	Sidechain
2	I	364	GLU	Sidechain
2	I	492	ASP	Sidechain
2	I	635	ASN	Sidechain
2	I	642	ASP	Sidechain
2	J	596	GLY	Mainchain
2	J	875	ASP	Sidechain
2	K	364	GLU	Sidechain
2	K	492	ASP	Sidechain
2	K	635	ASN	Sidechain
2	K	642	ASP	Sidechain
2	L	596	GLY	Mainchain
2	L	875	ASP	Sidechain

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	B	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	C	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	D	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	E	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	F	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
2	G	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	H	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	I	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	J	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	K	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
2	L	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	41	72
3	M	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	N	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	O	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	P	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	Q	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	R	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
4	S	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	T	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	U	131/137 (96%)	130 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	W	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	X	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
5	Y	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	Z	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	a	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	b	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	c	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	d	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
6	e	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	f	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	g	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	h	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	i	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	j	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
7	k	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	l	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	m	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	n	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	o	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	p	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
8	t	36/52 (69%)	36 (100%)	0	0	100	100
8	u	36/52 (69%)	36 (100%)	0	0	100	100
8	v	36/52 (69%)	36 (100%)	0	0	100	100
9	q	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	r	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	s	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
All	All	18888/21873 (86%)	18397 (97%)	473 (2%)	18 (0%)	54	81

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1001	ASN

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Mol	Chain	Res	Type
2	G	1015	PRO
2	G	1018	PRO
2	H	1001	ASN
2	H	1015	PRO
2	H	1018	PRO
2	I	1001	ASN
2	I	1015	PRO
2	I	1018	PRO
2	J	1001	ASN
2	J	1015	PRO
2	J	1018	PRO
2	K	1001	ASN
2	K	1015	PRO
2	K	1018	PRO
2	L	1001	ASN
2	L	1015	PRO
2	L	1018	PRO

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	A	497/842 (59%)	497 (100%)	0	100	100
1	B	497/842 (59%)	497 (100%)	0	100	100
1	C	497/842 (59%)	497 (100%)	0	100	100
1	D	497/842 (59%)	497 (100%)	0	100	100
1	E	497/842 (59%)	497 (100%)	0	100	100
1	F	497/842 (59%)	497 (100%)	0	100	100
2	G	814/955 (85%)	813 (100%)	1 (0%)	93	98
2	H	814/955 (85%)	814 (100%)	0	100	100
2	I	814/955 (85%)	813 (100%)	1 (0%)	93	98
2	J	814/955 (85%)	814 (100%)	0	100	100
2	K	814/955 (85%)	813 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	814/955 (85%)	814 (100%)	0	100	100
3	M	201/204 (98%)	201 (100%)	0	100	100
3	N	201/204 (98%)	201 (100%)	0	100	100
3	O	201/204 (98%)	201 (100%)	0	100	100
3	P	201/204 (98%)	201 (100%)	0	100	100
3	Q	201/204 (98%)	201 (100%)	0	100	100
3	R	201/204 (98%)	201 (100%)	0	100	100
4	S	121/125 (97%)	121 (100%)	0	100	100
4	T	121/125 (97%)	121 (100%)	0	100	100
4	U	121/125 (97%)	121 (100%)	0	100	100
4	V	121/125 (97%)	121 (100%)	0	100	100
4	W	121/125 (97%)	121 (100%)	0	100	100
4	X	121/125 (97%)	121 (100%)	0	100	100
5	Y	134/135 (99%)	134 (100%)	0	100	100
5	Z	134/135 (99%)	134 (100%)	0	100	100
5	a	134/135 (99%)	134 (100%)	0	100	100
5	b	134/135 (99%)	134 (100%)	0	100	100
5	c	134/135 (99%)	134 (100%)	0	100	100
5	d	134/135 (99%)	134 (100%)	0	100	100
6	e	547/593 (92%)	547 (100%)	0	100	100
6	f	547/593 (92%)	547 (100%)	0	100	100
6	g	547/593 (92%)	547 (100%)	0	100	100
6	h	547/593 (92%)	547 (100%)	0	100	100
6	i	547/593 (92%)	547 (100%)	0	100	100
6	j	547/593 (92%)	547 (100%)	0	100	100
7	k	127/128 (99%)	127 (100%)	0	100	100
7	l	127/128 (99%)	127 (100%)	0	100	100
7	m	127/128 (99%)	127 (100%)	0	100	100
7	n	127/128 (99%)	127 (100%)	0	100	100
7	o	127/128 (99%)	127 (100%)	0	100	100
7	p	127/128 (99%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	t	39/45 (87%)	39 (100%)	0	100	100
8	u	39/45 (87%)	39 (100%)	0	100	100
8	v	39/45 (87%)	39 (100%)	0	100	100
9	q	499/500 (100%)	499 (100%)	0	100	100
9	r	499/500 (100%)	499 (100%)	0	100	100
9	s	499/500 (100%)	499 (100%)	0	100	100
All	All	16260/19527 (83%)	16257 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	359	LEU
2	I	359	LEU
2	K	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	B	316	ASN
1	B	348	ASN
1	C	316	ASN
1	D	316	ASN
1	D	348	ASN
1	E	316	ASN
1	F	316	ASN
1	F	348	ASN
2	G	139	HIS
2	G	437	GLN
2	G	471	GLN
2	G	626	GLN
2	G	667	GLN
2	H	139	HIS
2	H	513	ASN
2	H	667	GLN
2	H	800	GLN
2	I	139	HIS
2	I	437	GLN
2	I	471	GLN

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Mol	Chain	Res	Type
2	I	626	GLN
2	I	667	GLN
2	J	35	GLN
2	J	54	HIS
2	J	139	HIS
2	J	172	GLN
2	J	513	ASN
2	J	667	GLN
2	J	800	GLN
2	K	139	HIS
2	K	437	GLN
2	K	471	GLN
2	K	626	GLN
2	K	667	GLN
2	L	35	GLN
2	L	54	HIS
2	L	139	HIS
2	L	172	GLN
2	L	513	ASN
2	L	667	GLN
2	L	800	GLN
3	M	92	ASN
3	M	225	GLN
3	N	92	ASN
3	N	227	GLN
3	O	46	ASN
3	O	92	ASN
3	P	92	ASN
3	P	227	GLN
3	Q	46	ASN
3	R	92	ASN
3	R	227	GLN
4	S	36	GLN
4	S	102	ASN
4	T	36	GLN
4	T	102	ASN
4	U	36	GLN
4	U	102	ASN
4	V	36	GLN
4	V	102	ASN
4	W	36	GLN
4	W	102	ASN

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Mol	Chain	Res	Type
4	X	36	GLN
4	X	102	ASN
8	t	9	HIS
8	u	9	HIS
8	v	9	HIS
9	q	363	HIS
9	q	467	HIS
9	r	363	HIS
9	r	467	HIS
9	s	363	HIS
9	s	467	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	3

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Mol	Chain	Number of breaks
2	J	3
2	L	3
2	G	1
2	I	1
2	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	509:PRO	C	510:LYS	N	1.70
1	I	509:PRO	C	510:LYS	N	1.70
1	K	509:PRO	C	510:LYS	N	1.70
1	H	506:LYS	C	507:SER	N	1.67
1	J	506:LYS	C	507:SER	N	1.67
1	L	506:LYS	C	507:SER	N	1.67
1	H	433:VAL	C	434:LEU	N	1.61
1	H	731:ASN	C	732:THR	N	1.61
1	J	433:VAL	C	434:LEU	N	1.61
1	J	731:ASN	C	732:THR	N	1.61
1	L	433:VAL	C	434:LEU	N	1.61
1	L	731:ASN	C	732:THR	N	1.61

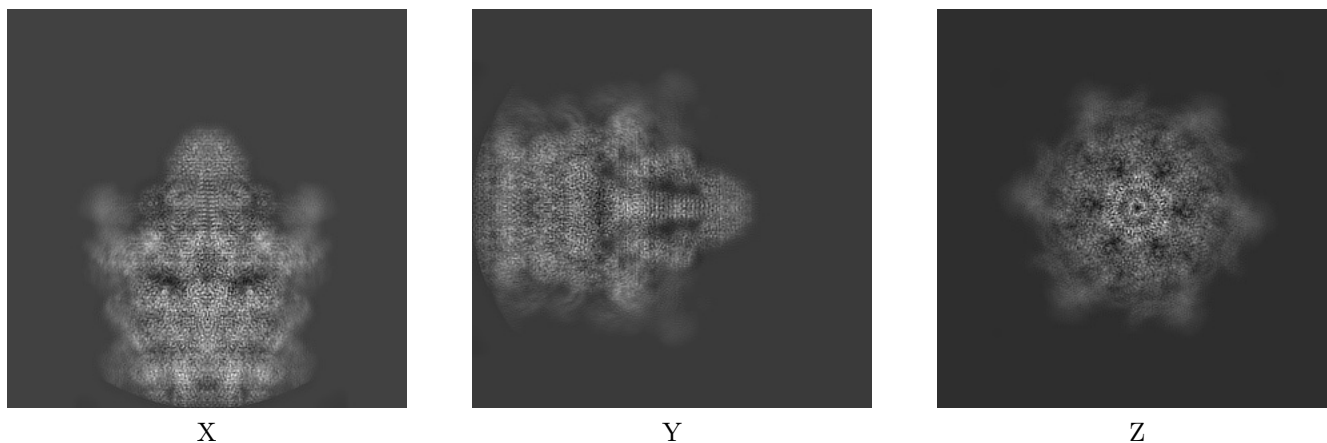
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11745. 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](#)

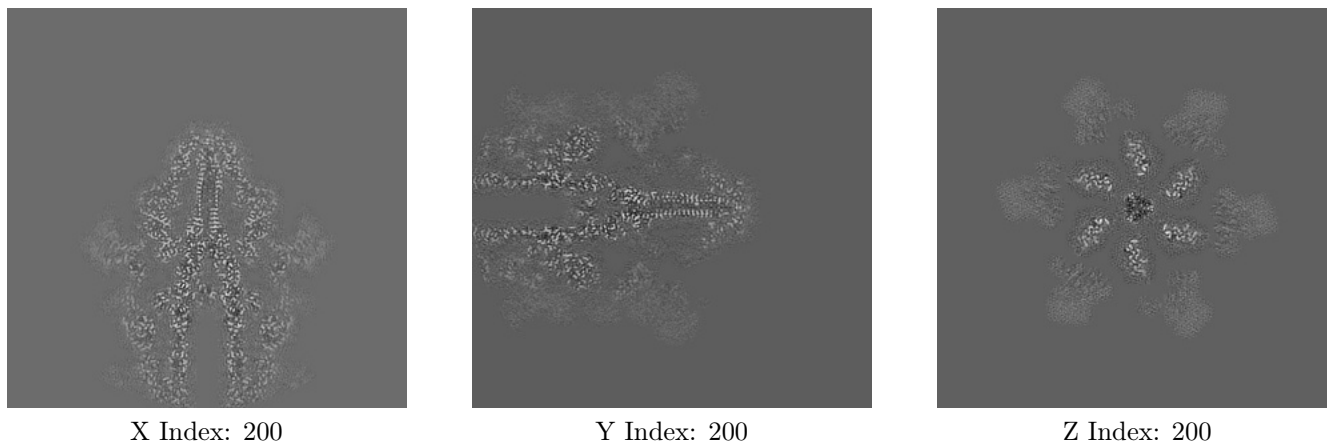
6.1.1 Primary map



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

6.2 Central slices [i](#)

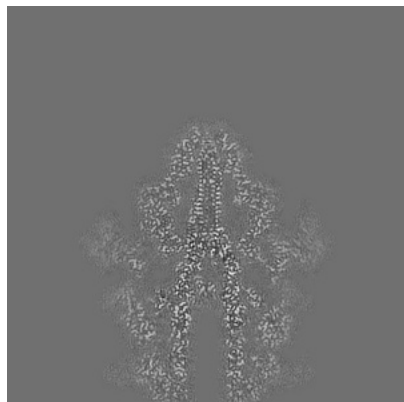
6.2.1 Primary map



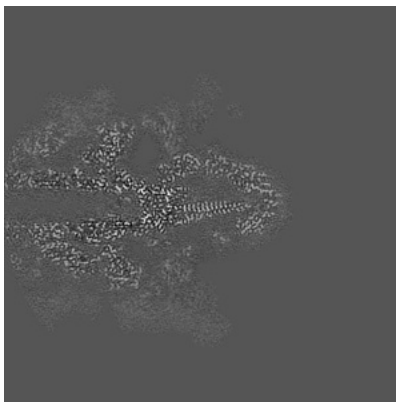
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

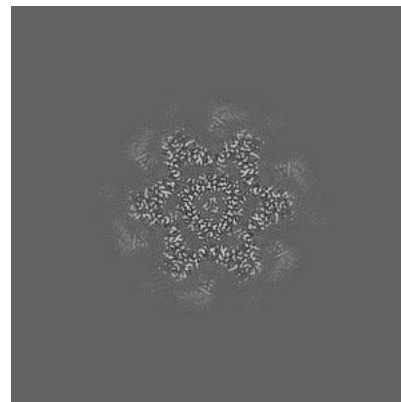
6.3.1 Primary map



X Index: 198



Y Index: 210

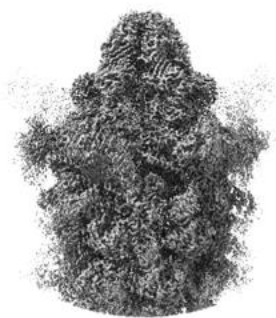


Z Index: 110

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

6.4 Orthogonal surface views [i](#)

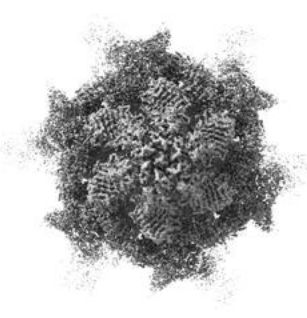
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

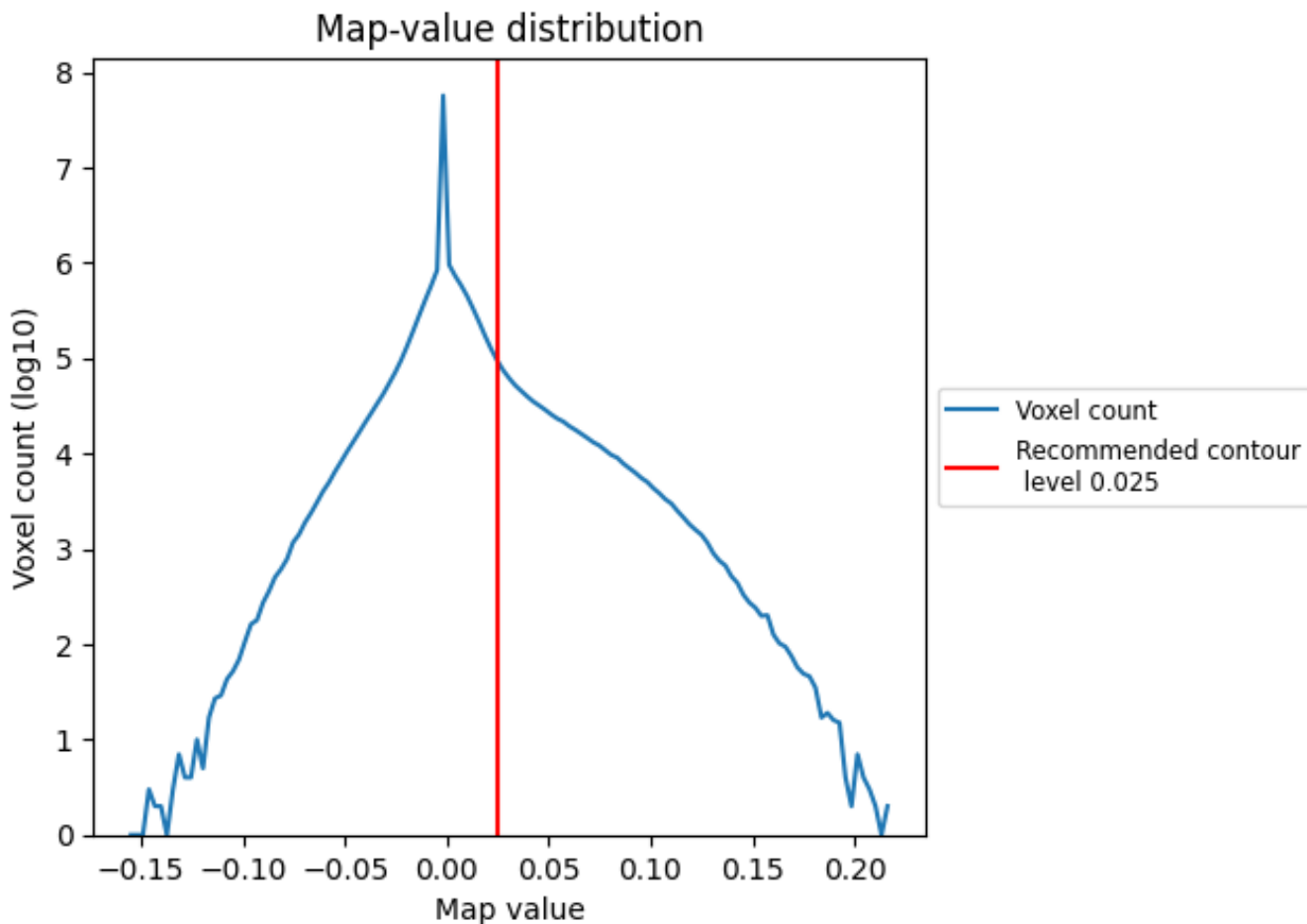
6.5 Mask visualisation

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

7 Map analysis [i](#)

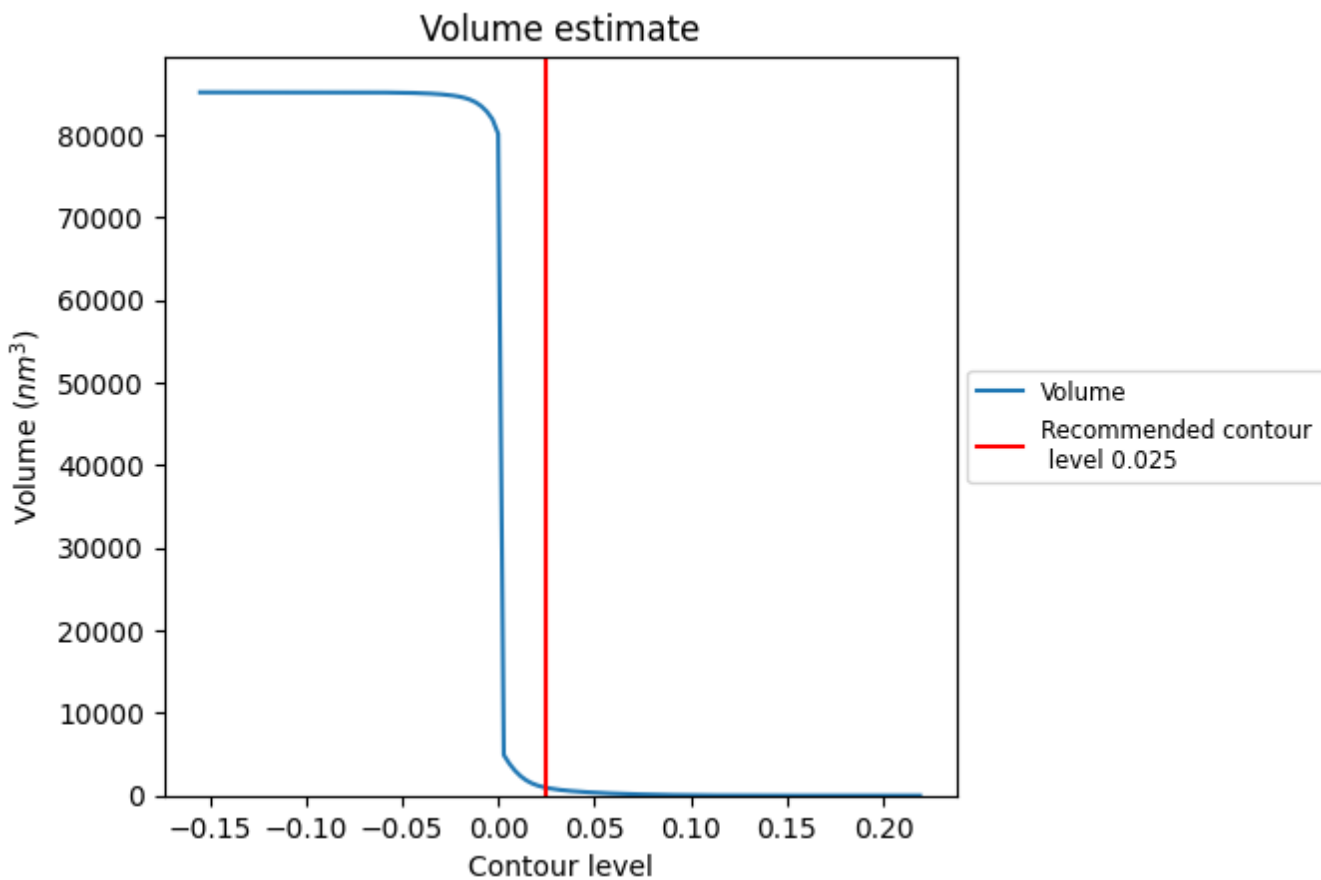
This section contains the results of statistical analysis of the map.

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.

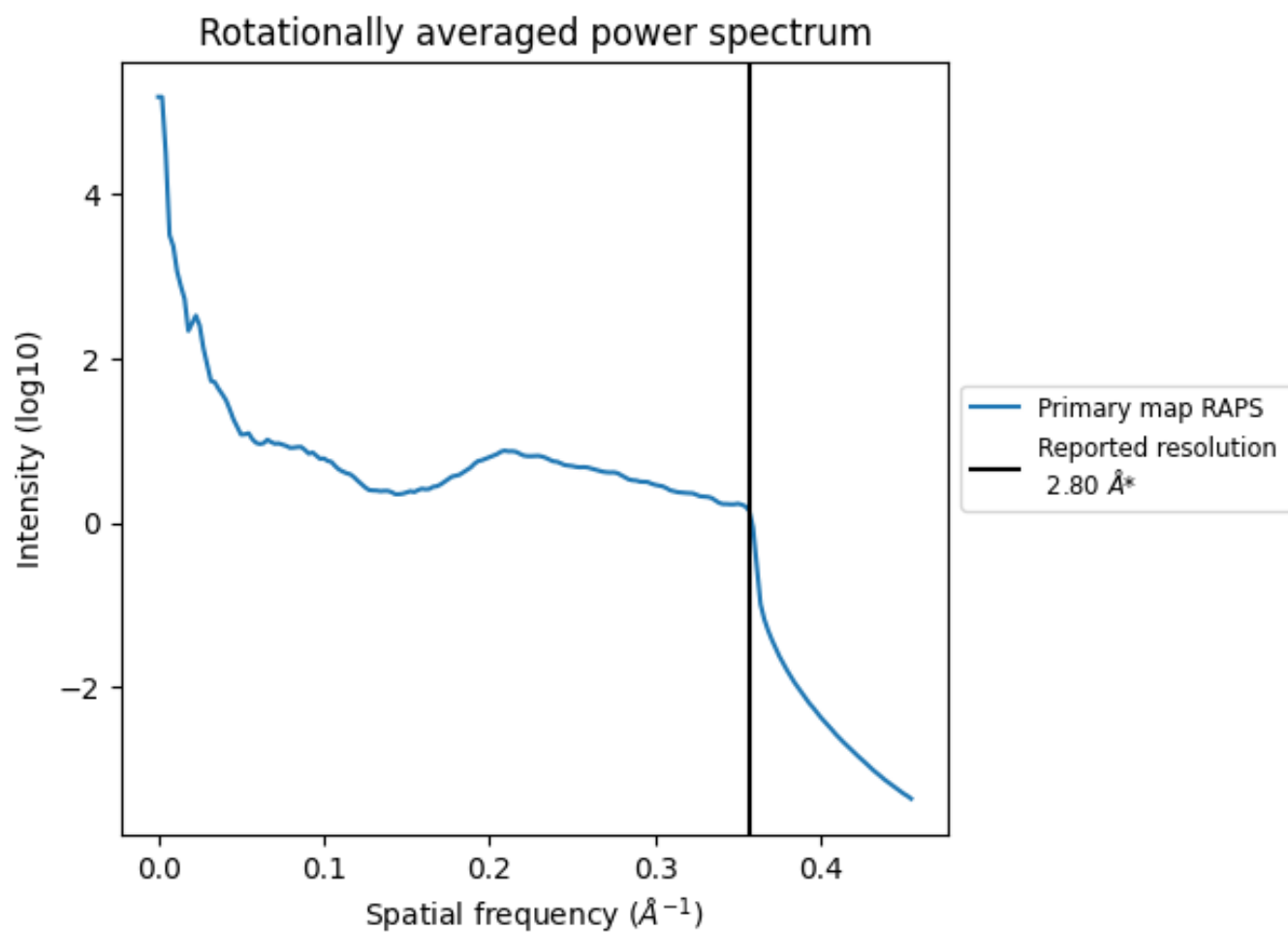
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm³; this corresponds to an approximate mass of 856 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 0.357\AA^{-1}

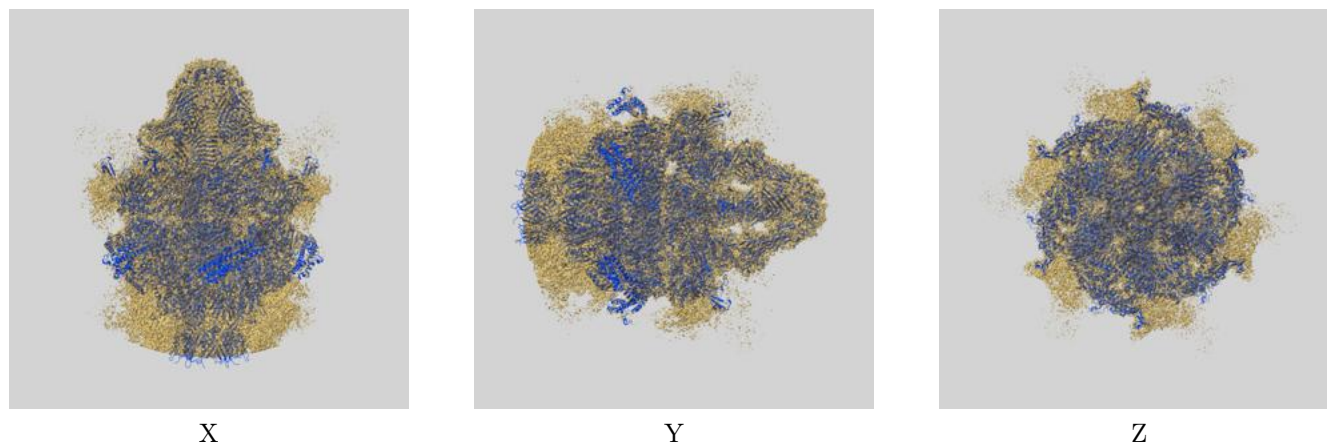
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

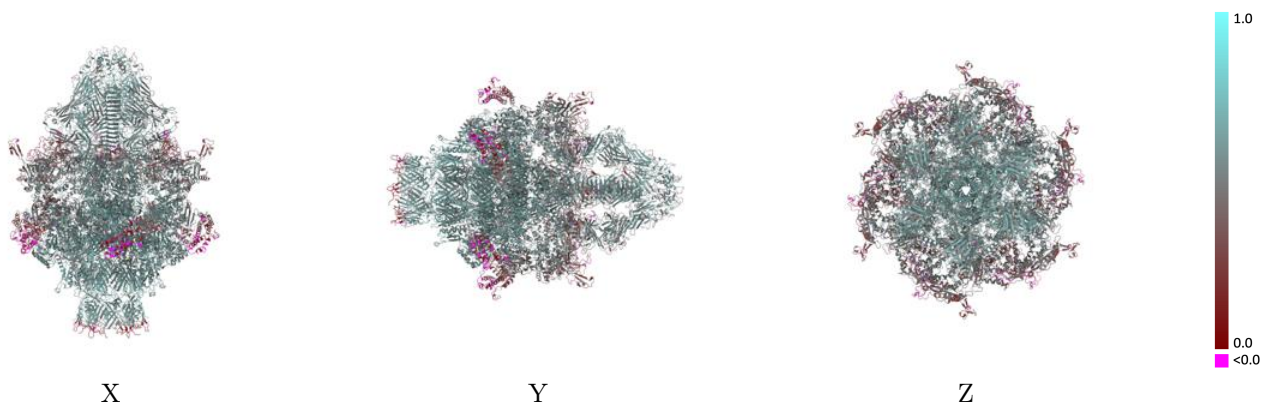
This section contains information regarding the fit between EMDB map EMD-11745 and PDB model 7AEF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



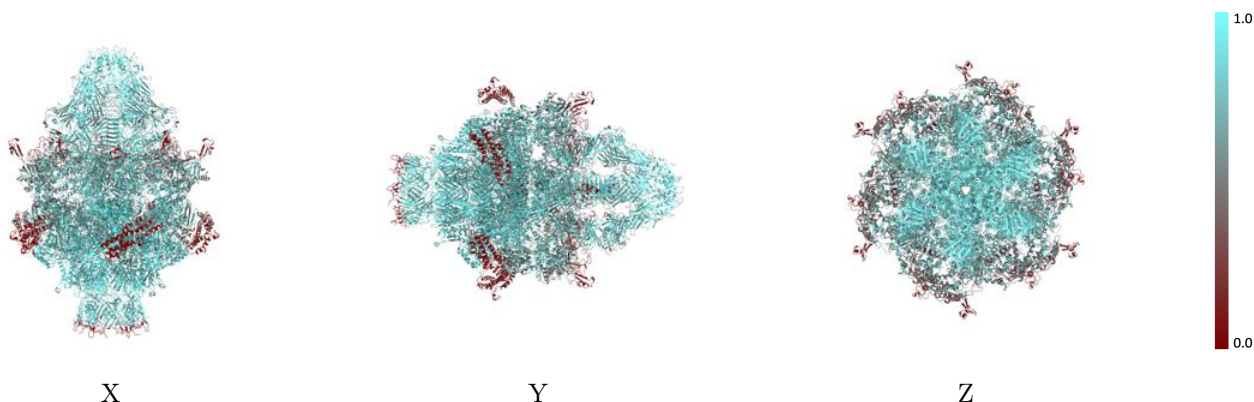
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



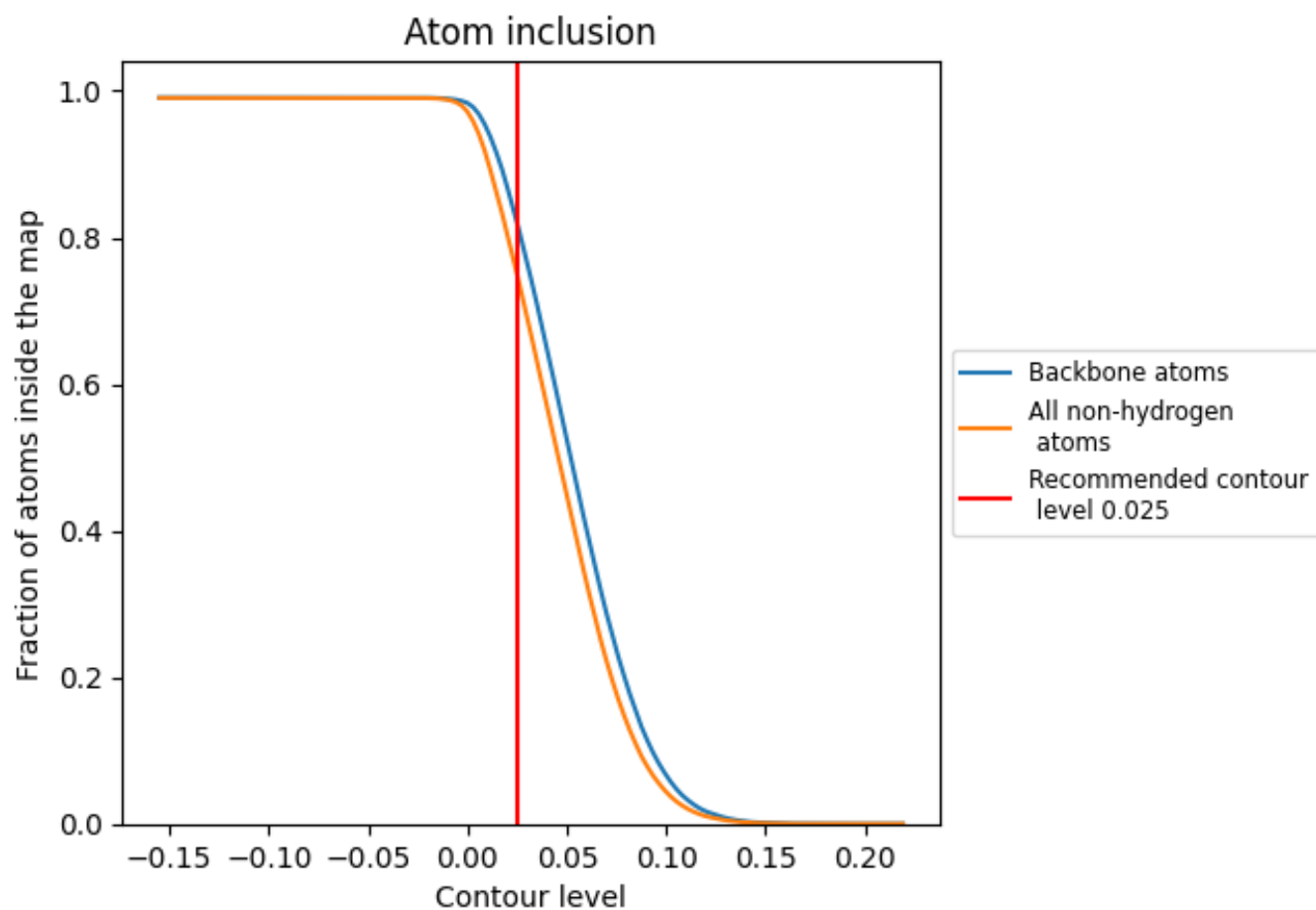
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7503	 0.5290
A	 0.6794	 0.5040
B	 0.6611	 0.5020
C	 0.6773	 0.5040
D	 0.6670	 0.5010
E	 0.6844	 0.5050
F	 0.6666	 0.5000
G	 0.7750	 0.5410
H	 0.7816	 0.5400
I	 0.7501	 0.5140
J	 0.7231	 0.4740
K	 0.7522	 0.5180
L	 0.7214	 0.4740
M	 0.9227	 0.6340
N	 0.9172	 0.6300
O	 0.9233	 0.6320
P	 0.9161	 0.6340
Q	 0.9178	 0.6330
R	 0.9145	 0.6300
S	 0.8742	 0.5930
T	 0.8524	 0.5840
U	 0.8723	 0.5890
V	 0.8543	 0.5850
W	 0.8751	 0.5910
X	 0.8505	 0.5850
Y	 0.8972	 0.6160
Z	 0.9006	 0.6190
a	 0.8904	 0.6150
b	 0.8963	 0.6190
c	 0.8955	 0.6160
d	 0.8997	 0.6210
e	 0.6401	 0.4800
f	 0.6481	 0.4780
g	 0.6437	 0.4810
h	 0.6451	 0.4790



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Chain	Atom inclusion	Q-score
i	 0.6383	 0.4800
j	 0.6435	 0.4780
k	 0.6480	 0.4770
l	 0.6463	 0.4760
m	 0.6427	 0.4710
n	 0.6516	 0.4690
o	 0.6463	 0.4710
p	 0.6463	 0.4780
q	 0.9244	 0.6240
r	 0.9235	 0.6200
s	 0.9228	 0.6240
t	 0.8106	 0.6230
u	 0.8137	 0.6180
v	 0.8075	 0.6160