



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 10:07 am GMT

PDB ID : 7ADZ
EMDB ID : EMD-11734
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the cap portion in extended state.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.50 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

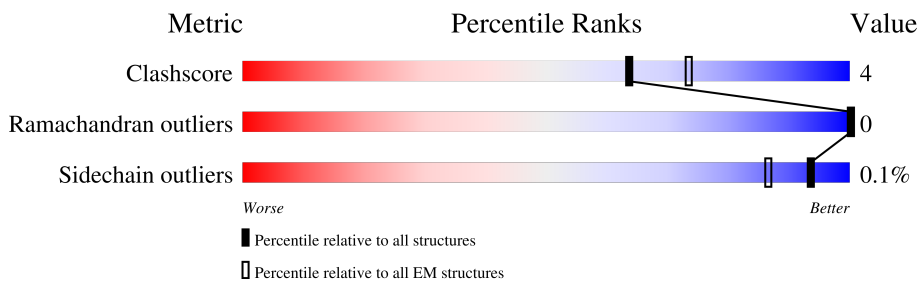
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



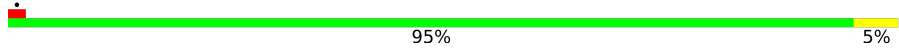
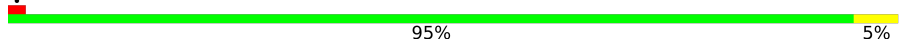
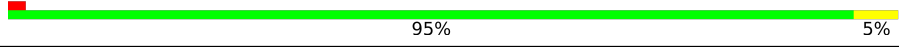
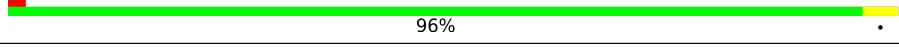
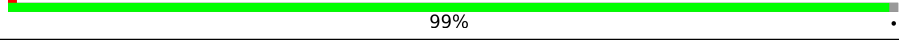
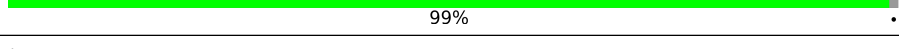
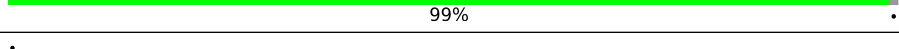
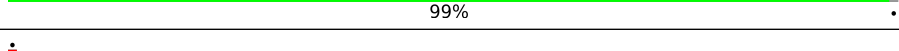
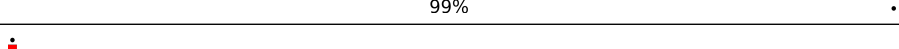
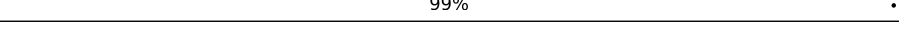
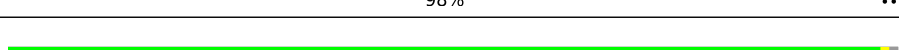
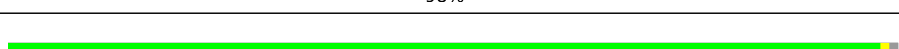
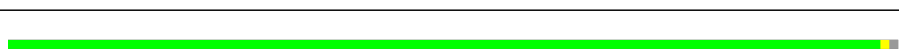
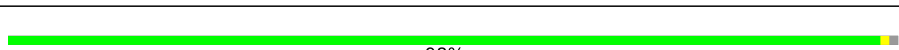
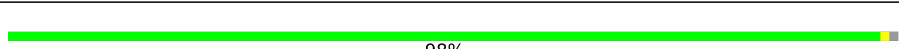





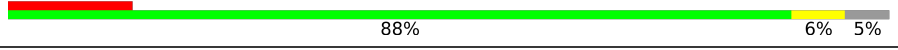

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	0A	197	
1	0B	197	
1	0C	197	
1	0D	197	
1	0E	197	
1	0F	197	
2	1A	284	
2	1B	284	

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Mol	Chain	Length	Quality of chain
2	1C	284	 95% 5%
2	1D	284	 95% 5%
2	1E	284	 95% 5%
2	1F	284	 96% .
3	1a	142	 99% .
3	1b	142	 99% .
3	1c	142	 99% .
3	1d	142	 99% .
3	1e	142	 99% .
3	1f	142	 99% .
3	2a	142	 98% ..
3	2b	142	 98% ..
3	2c	142	 98% ..
3	2d	142	 98% ..
3	2e	142	 98% ..
3	2f	142	 98% ..
4	2A	692	 14% 88% 6% 5%
4	2B	692	 14% 88% 6% 5%
4	2C	692	 14% 89% 6% 5%
4	2D	692	 14% 88% 6% 5%
4	2E	692	 14% 88% 6% 5%
4	2F	692	 14% 88% 6% 5%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 67794 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 cap protein (Algo1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0A	197	Total 1615	C 1030	N 265	O 313	S 7	0	0
1	0B	197	Total 1615	C 1030	N 265	O 313	S 7	0	0
1	0C	197	Total 1615	C 1030	N 265	O 313	S 7	0	0
1	0D	197	Total 1615	C 1030	N 265	O 313	S 7	0	0
1	0E	197	Total 1615	C 1030	N 265	O 313	S 7	0	0
1	0F	197	Total 1615	C 1030	N 265	O 313	S 7	0	0

- Molecule 2 is a protein called cap adaptor protein (Algo2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1A	284	Total 2337	C 1512	N 373	O 446	S 6	0	0
2	1B	284	Total 2337	C 1512	N 373	O 446	S 6	0	0
2	1C	284	Total 2337	C 1512	N 373	O 446	S 6	0	0
2	1D	284	Total 2337	C 1512	N 373	O 446	S 6	0	0
2	1E	284	Total 2337	C 1512	N 373	O 446	S 6	0	0
2	1F	284	Total 2337	C 1512	N 373	O 446	S 6	0	0

- Molecule 3 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1a	141	Total 1145	C 731	N 190	O 221	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1b	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	1c	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	1d	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	1e	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	1f	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2a	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2b	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2c	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2d	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2e	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
3	2f	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		

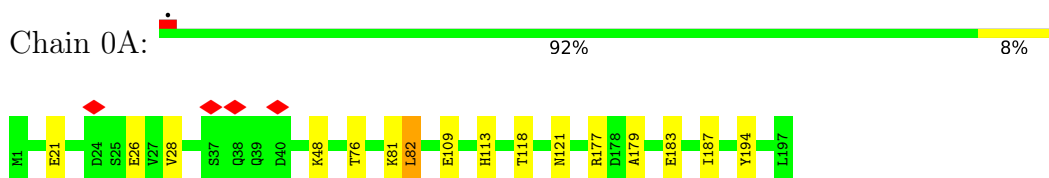
- Molecule 4 is a protein called Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2A	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
4	2B	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
4	2C	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
4	2D	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
4	2E	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
4	2F	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		

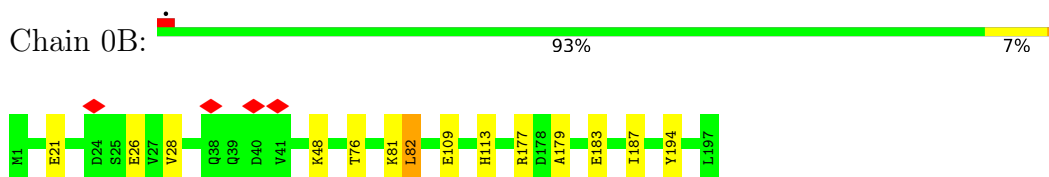
3 Residue-property plots [\(i\)](#)

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

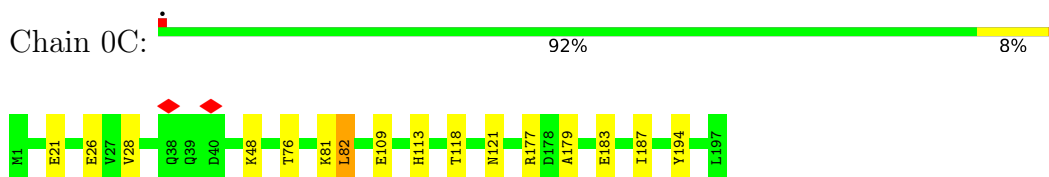
- Molecule 1: cap protein (Algo1)



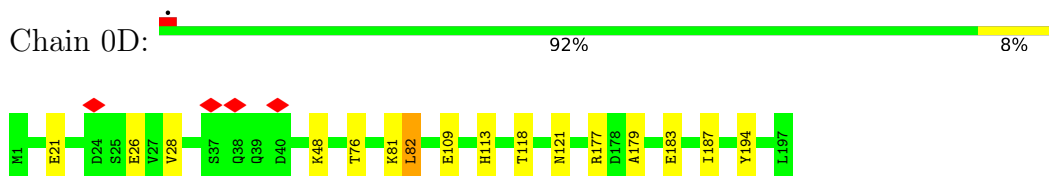
- Molecule 1: cap protein (Algo1)



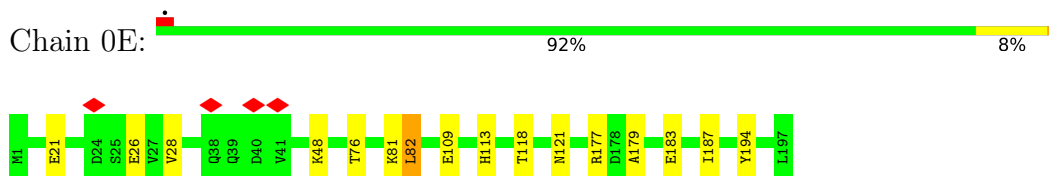
- Molecule 1: cap protein (Algo1)



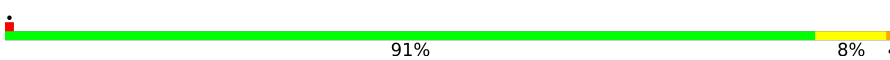
- Molecule 1: cap protein (Algo1)



- Molecule 1: cap protein (Algo1)



- Molecule 1: cap protein (Algo1)

Chain 0F:  91% 8%



- Molecule 2: cap adaptor protein (Algo2)

Chain 1A:  96%



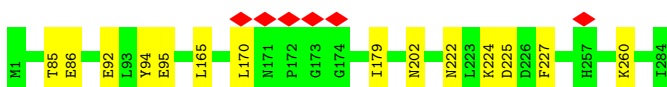
- Molecule 2: cap adaptor protein (Algo2)

Chain 1B:  95% 5%



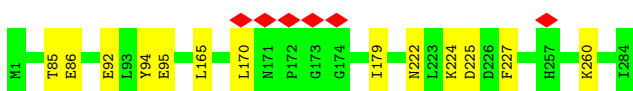
- Molecule 2: cap adaptor protein (Algo2)

Chain 1C:  95% 5%



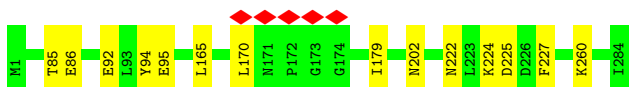
- Molecule 2: cap adaptor protein (Algo2)

Chain 1D:  95% 5%



- Molecule 2: cap adaptor protein (Algo2)

Chain 1E:  95% 5%

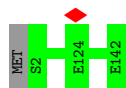


- Molecule 2: cap adaptor protein (Algo2)

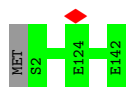
Chain 1F:  96%



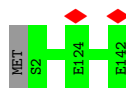
• Molecule 3: Phage tail protein



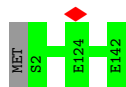
• Molecule 3: Phage tail protein



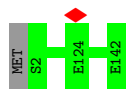
• Molecule 3: Phage tail protein



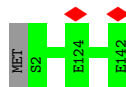
• Molecule 3: Phage tail protein



• Molecule 3: Phage tail protein



• Molecule 3: Phage tail protein



• Molecule 3: Phage tail protein

Chain 2a:  98% ..



● Molecule 3: Phage tail protein

Chain 2b:  98% ..



● Molecule 3: Phage tail protein

Chain 2c:  98% ..



● Molecule 3: Phage tail protein

Chain 2d:  98% ..



● Molecule 3: Phage tail protein

Chain 2e:  98% ..




● Molecule 3: Phage tail protein

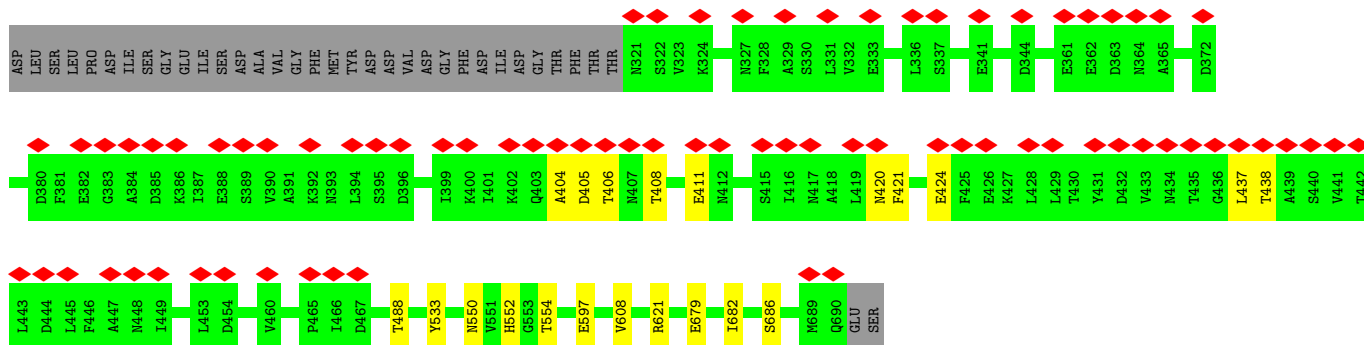
Chain 2f:  98% ..



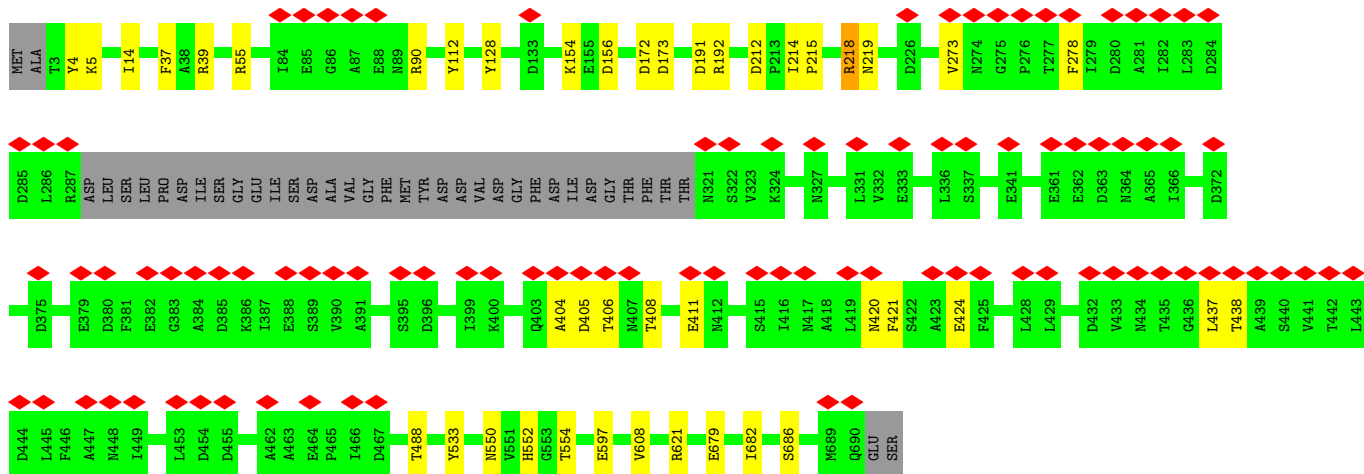
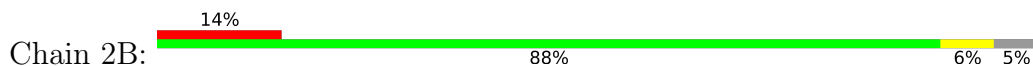
● Molecule 4: Putative phage tail sheath protein FI

Chain 2A:  14% 88% 6% 5%

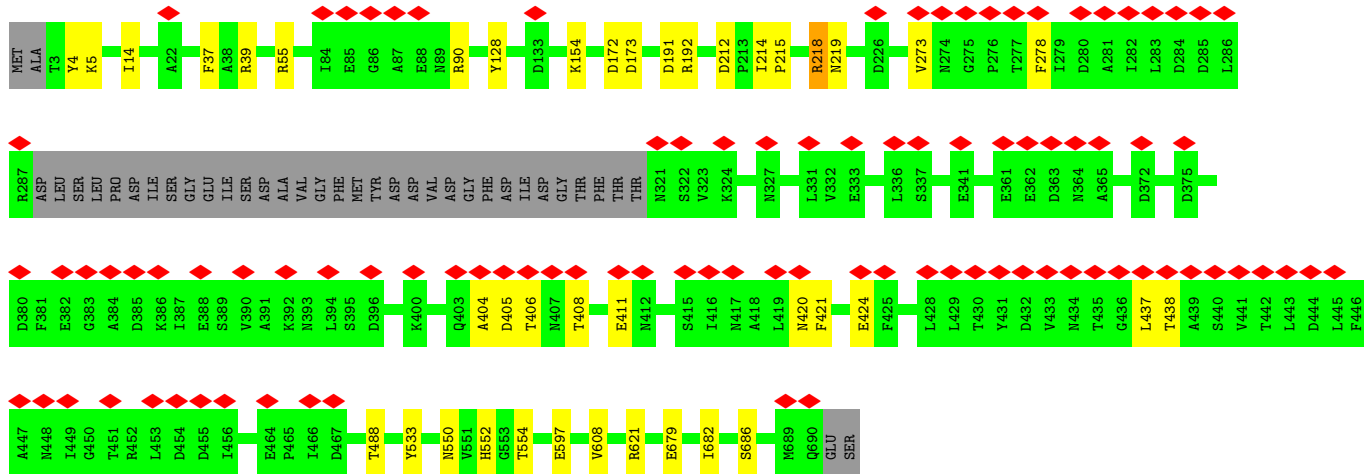
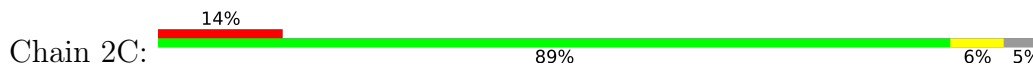




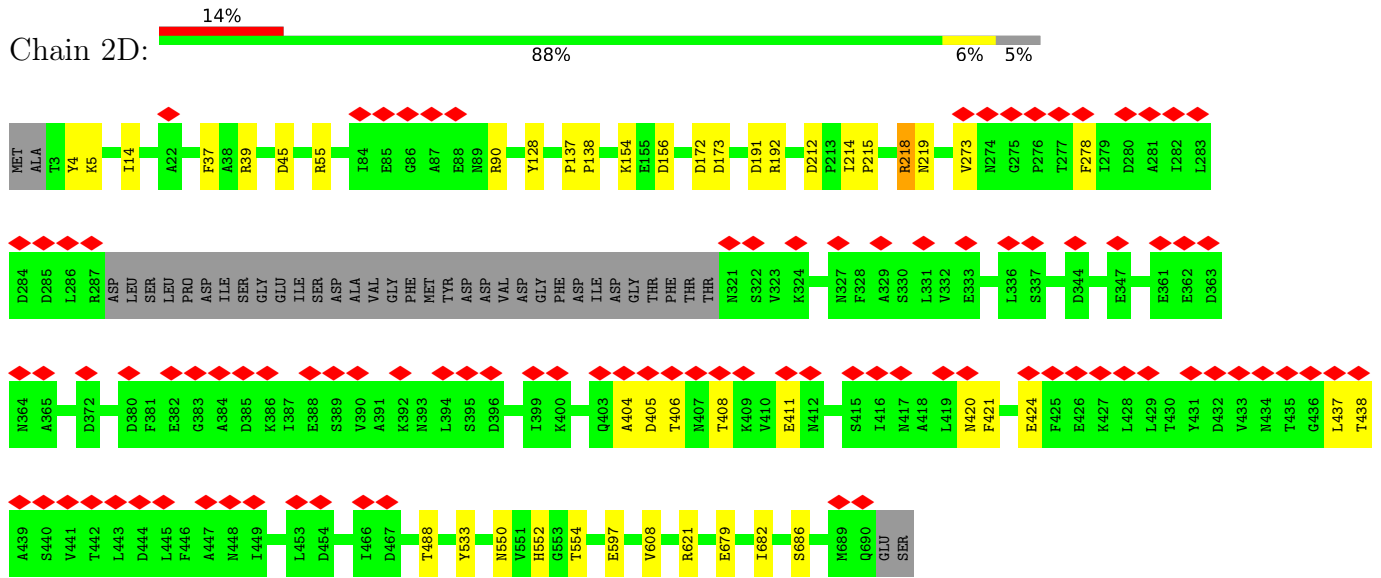
• Molecule 4: Putative phage tail sheath protein FI



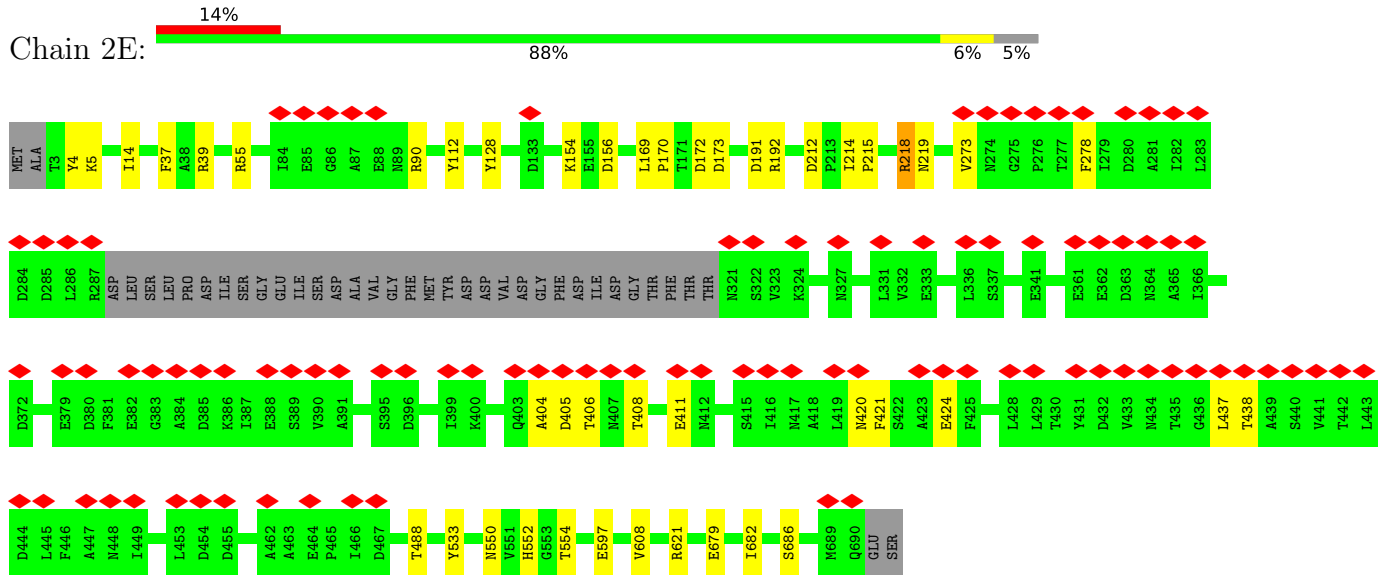
• Molecule 4: Putative phage tail sheath protein FI



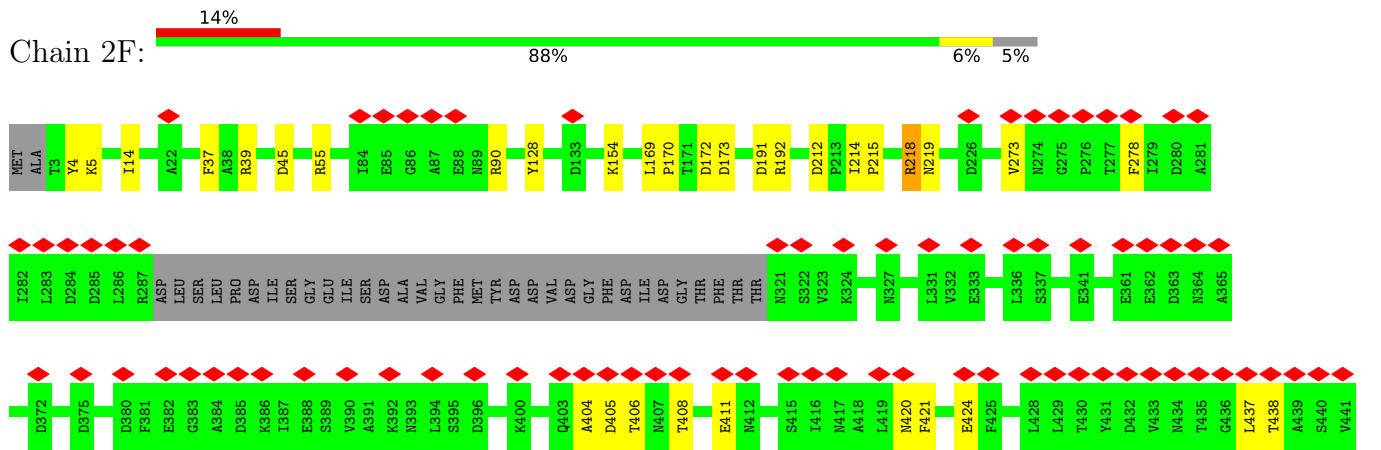
• Molecule 4: Putative phage tail sheath protein FI



• Molecule 4: Putative phage tail sheath protein FI



• Molecule 4: Putative phage tail sheath protein FI





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65059	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	0.213	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0A	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
1	0B	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
1	0C	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
1	0D	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
1	0E	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
1	0F	0.36	2/1642 (0.1%)	0.69	5/2219 (0.2%)
2	1A	0.89	1/2398 (0.0%)	0.77	0/3235
2	1B	0.89	1/2398 (0.0%)	0.77	0/3235
2	1C	0.89	1/2398 (0.0%)	0.77	0/3235
2	1D	0.89	1/2398 (0.0%)	0.77	0/3235
2	1E	0.89	1/2398 (0.0%)	0.77	0/3235
2	1F	0.89	1/2398 (0.0%)	0.77	0/3235
3	1a	0.32	0/1172	0.56	0/1584
3	1b	0.32	0/1172	0.56	0/1584
3	1c	0.32	0/1172	0.56	0/1584
3	1d	0.32	0/1172	0.56	0/1584
3	1e	0.32	0/1172	0.56	0/1584
3	1f	0.32	0/1172	0.56	0/1584
3	2a	0.99	0/1172	0.84	2/1584 (0.1%)
3	2b	0.99	0/1172	0.84	2/1584 (0.1%)
3	2c	0.99	0/1172	0.84	2/1584 (0.1%)
3	2d	0.99	0/1172	0.85	2/1584 (0.1%)
3	2e	0.99	0/1172	0.84	2/1584 (0.1%)
3	2f	0.99	0/1172	0.84	2/1584 (0.1%)
4	2A	0.91	4/5155 (0.1%)	0.87	8/7021 (0.1%)
4	2B	0.91	4/5155 (0.1%)	0.87	9/7021 (0.1%)
4	2C	0.91	4/5155 (0.1%)	0.87	8/7021 (0.1%)
4	2D	0.91	4/5155 (0.1%)	0.87	8/7021 (0.1%)
4	2E	0.91	4/5155 (0.1%)	0.87	9/7021 (0.1%)
4	2F	0.91	4/5155 (0.1%)	0.87	8/7021 (0.1%)
All	All	0.82	42/69234 (0.1%)	0.80	92/93858 (0.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0F	82	LEU	C-N	-7.32	1.17	1.34
1	0B	82	LEU	C-N	-7.29	1.17	1.34
1	0E	82	LEU	C-N	-7.29	1.17	1.34
1	0A	82	LEU	C-N	-7.27	1.17	1.34
1	0D	82	LEU	C-N	-7.27	1.17	1.34
1	0C	82	LEU	C-N	-7.26	1.17	1.34
1	0E	81	LYS	C-N	-5.79	1.20	1.34
1	0C	81	LYS	C-N	-5.79	1.20	1.34
4	2E	128	TYR	CD2-CE2	-5.79	1.30	1.39
1	0F	81	LYS	C-N	-5.78	1.20	1.34
1	0B	81	LYS	C-N	-5.77	1.20	1.34
1	0A	81	LYS	C-N	-5.76	1.20	1.34
4	2A	128	TYR	CD2-CE2	-5.75	1.30	1.39
1	0D	81	LYS	C-N	-5.75	1.20	1.34
4	2D	128	TYR	CD2-CE2	-5.75	1.30	1.39
4	2B	128	TYR	CD2-CE2	-5.73	1.30	1.39
4	2C	128	TYR	CD2-CE2	-5.73	1.30	1.39
4	2F	128	TYR	CD2-CE2	-5.73	1.30	1.39
4	2C	679	GLU	CD-OE1	-5.65	1.19	1.25
4	2A	679	GLU	CD-OE1	-5.63	1.19	1.25
4	2D	679	GLU	CD-OE1	-5.63	1.19	1.25
4	2F	679	GLU	CD-OE1	-5.63	1.19	1.25
4	2B	679	GLU	CD-OE1	-5.62	1.19	1.25
4	2E	679	GLU	CD-OE1	-5.62	1.19	1.25
4	2E	424	GLU	CD-OE1	-5.54	1.19	1.25
4	2A	424	GLU	CD-OE1	-5.51	1.19	1.25
4	2B	424	GLU	CD-OE1	-5.51	1.19	1.25
4	2C	424	GLU	CD-OE1	-5.51	1.19	1.25
4	2F	424	GLU	CD-OE1	-5.51	1.19	1.25
4	2D	128	TYR	CE2-CZ	-5.49	1.31	1.38
4	2C	128	TYR	CE2-CZ	-5.46	1.31	1.38
4	2F	128	TYR	CE2-CZ	-5.45	1.31	1.38
4	2A	128	TYR	CE2-CZ	-5.44	1.31	1.38
4	2B	128	TYR	CE2-CZ	-5.43	1.31	1.38
4	2E	128	TYR	CE2-CZ	-5.43	1.31	1.38
4	2D	424	GLU	CD-OE1	-5.39	1.19	1.25
2	1D	95	GLU	CD-OE2	-5.35	1.19	1.25
2	1B	95	GLU	CD-OE2	-5.32	1.19	1.25
2	1C	95	GLU	CD-OE2	-5.28	1.19	1.25
2	1A	95	GLU	CD-OE2	-5.23	1.19	1.25
2	1E	95	GLU	CD-OE2	-5.21	1.20	1.25
2	1F	95	GLU	CD-OE2	-5.21	1.20	1.25

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0B	82	LEU	O-C-N	-13.82	100.59	122.70
1	0E	82	LEU	O-C-N	-13.81	100.61	122.70
1	0F	82	LEU	O-C-N	-13.80	100.62	122.70
1	0A	82	LEU	O-C-N	-13.79	100.64	122.70
1	0D	82	LEU	O-C-N	-13.79	100.64	122.70
1	0C	82	LEU	O-C-N	-13.77	100.66	122.70
1	0E	82	LEU	CA-C-N	9.92	139.01	117.20
1	0F	82	LEU	CA-C-N	9.92	139.01	117.20
1	0B	82	LEU	CA-C-N	9.90	138.99	117.20
1	0D	82	LEU	CA-C-N	9.89	138.96	117.20
1	0C	82	LEU	CA-C-N	9.88	138.94	117.20
1	0A	82	LEU	CA-C-N	9.88	138.93	117.20
4	2C	192	ARG	NE-CZ-NH1	8.38	124.49	120.30
4	2B	39	ARG	NE-CZ-NH2	-8.37	116.11	120.30
4	2C	39	ARG	NE-CZ-NH2	-8.36	116.12	120.30
4	2F	192	ARG	NE-CZ-NH1	8.35	124.48	120.30
4	2A	39	ARG	NE-CZ-NH2	-8.32	116.14	120.30
4	2D	39	ARG	NE-CZ-NH2	-8.32	116.14	120.30
4	2D	192	ARG	NE-CZ-NH1	8.32	124.46	120.30
4	2F	39	ARG	NE-CZ-NH2	-8.32	116.14	120.30
4	2B	192	ARG	NE-CZ-NH1	8.29	124.45	120.30
4	2E	39	ARG	NE-CZ-NH2	-8.30	116.15	120.30
4	2E	192	ARG	NE-CZ-NH1	8.29	124.45	120.30
4	2A	192	ARG	NE-CZ-NH1	8.29	124.44	120.30
4	2C	55	ARG	NE-CZ-NH2	-7.64	116.48	120.30
4	2A	55	ARG	NE-CZ-NH2	-7.58	116.51	120.30
4	2F	55	ARG	NE-CZ-NH2	-7.58	116.51	120.30
4	2B	55	ARG	NE-CZ-NH2	-7.58	116.51	120.30
4	2E	55	ARG	NE-CZ-NH2	-7.52	116.54	120.30
4	2D	55	ARG	NE-CZ-NH2	-7.50	116.55	120.30
4	2B	621	ARG	NE-CZ-NH2	-7.19	116.71	120.30
4	2E	621	ARG	NE-CZ-NH2	-7.16	116.72	120.30
4	2C	621	ARG	NE-CZ-NH2	-7.11	116.74	120.30
4	2F	621	ARG	NE-CZ-NH2	-7.11	116.74	120.30
4	2D	621	ARG	NE-CZ-NH2	-7.07	116.76	120.30
4	2A	621	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	0B	81	LYS	C-N-CA	6.86	138.86	121.70
1	0F	81	LYS	C-N-CA	6.86	138.84	121.70
1	0E	81	LYS	C-N-CA	6.85	138.81	121.70
1	0C	81	LYS	C-N-CA	6.84	138.81	121.70
1	0D	81	LYS	C-N-CA	6.82	138.76	121.70
1	0A	81	LYS	C-N-CA	6.81	138.74	121.70
4	2E	218	ARG	NE-CZ-NH2	-6.80	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2D	533	TYR	CB-CG-CD2	-6.76	116.94	121.00
4	2C	533	TYR	CB-CG-CD2	-6.73	116.96	121.00
3	2e	62	ARG	NE-CZ-NH2	-6.73	116.94	120.30
4	2B	218	ARG	NE-CZ-NH2	-6.70	116.95	120.30
4	2A	533	TYR	CB-CG-CD2	-6.70	116.98	121.00
4	2C	218	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	2c	62	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	2f	62	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	2d	62	ARG	NE-CZ-NH2	-6.67	116.97	120.30
4	2E	533	TYR	CB-CG-CD2	-6.66	117.00	121.00
4	2A	218	ARG	NE-CZ-NH2	-6.66	116.97	120.30
3	2b	62	ARG	NE-CZ-NH2	-6.66	116.97	120.30
4	2F	533	TYR	CB-CG-CD2	-6.65	117.01	121.00
4	2D	218	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	2a	62	ARG	NE-CZ-NH2	-6.63	116.99	120.30
4	2B	533	TYR	CB-CG-CD2	-6.62	117.03	121.00
4	2F	218	ARG	NE-CZ-NH2	-6.52	117.04	120.30
4	2E	37	PHE	CB-CG-CD1	-6.14	116.50	120.80
4	2C	37	PHE	CB-CG-CD1	-6.13	116.51	120.80
4	2A	37	PHE	CB-CG-CD1	-6.07	116.55	120.80
4	2D	37	PHE	CB-CG-CD1	-6.07	116.55	120.80
4	2B	37	PHE	CB-CG-CD1	-6.06	116.56	120.80
4	2F	37	PHE	CB-CG-CD1	-6.05	116.56	120.80
1	0B	82	LEU	C-N-CA	5.84	136.31	121.70
1	0E	82	LEU	C-N-CA	5.83	136.28	121.70
1	0F	82	LEU	C-N-CA	5.83	136.28	121.70
1	0A	82	LEU	C-N-CA	5.82	136.24	121.70
1	0D	82	LEU	C-N-CA	5.82	136.24	121.70
1	0C	82	LEU	C-N-CA	5.81	136.21	121.70
3	2a	86	ARG	NE-CZ-NH2	-5.75	117.42	120.30
3	2d	86	ARG	NE-CZ-NH2	-5.73	117.43	120.30
3	2e	86	ARG	NE-CZ-NH2	-5.70	117.45	120.30
3	2c	86	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	2f	86	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	2b	86	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	0B	81	LYS	O-C-N	-5.51	113.89	122.70
1	0F	81	LYS	O-C-N	-5.48	113.93	122.70
1	0E	81	LYS	O-C-N	-5.46	113.96	122.70
1	0C	81	LYS	O-C-N	-5.46	113.96	122.70
1	0D	81	LYS	O-C-N	-5.45	113.99	122.70
1	0A	81	LYS	O-C-N	-5.44	113.99	122.70
4	2D	173	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2F	173	ASP	CB-CG-OD2	5.23	123.00	118.30
4	2B	173	ASP	CB-CG-OD2	5.21	122.99	118.30
4	2A	173	ASP	CB-CG-OD2	5.20	122.97	118.30
4	2C	173	ASP	CB-CG-OD2	5.20	122.97	118.30
4	2E	173	ASP	CB-CG-OD2	5.15	122.93	118.30
4	2B	112	TYR	CB-CG-CD2	-5.01	118.00	121.00
4	2E	112	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0A	1615	0	1603	13	0
1	0B	1615	0	1603	12	0
1	0C	1615	0	1603	13	0
1	0D	1615	0	1603	13	0
1	0E	1615	0	1603	13	0
1	0F	1615	0	1603	14	0
2	1A	2337	0	2288	15	0
2	1B	2337	0	2288	17	0
2	1C	2337	0	2288	18	0
2	1D	2337	0	2288	17	0
2	1E	2337	0	2288	18	0
2	1F	2337	0	2288	16	0
3	1a	1145	0	1118	0	0
3	1b	1145	0	1118	0	0
3	1c	1145	0	1118	0	0
3	1d	1145	0	1118	0	0
3	1e	1145	0	1118	0	0
3	1f	1145	0	1118	0	0
3	2a	1145	0	1117	0	0
3	2b	1145	0	1117	0	0
3	2c	1145	0	1117	0	0
3	2d	1145	0	1117	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2e	1145	0	1117	0	0
3	2f	1145	0	1117	0	0
4	2A	5057	0	4910	73	0
4	2B	5057	0	4910	72	0
4	2C	5057	0	4910	71	0
4	2D	5057	0	4910	75	0
4	2E	5057	0	4910	74	0
4	2F	5057	0	4910	74	0
All	All	67794	0	66216	391	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2D:406:THR:HG21	4:2E:554:THR:CG2	1.26	1.61
4:2E:406:THR:HG21	4:2F:554:THR:CG2	1.24	1.60
4:2A:554:THR:CG2	4:2F:406:THR:HG21	1.22	1.60
4:2B:406:THR:HG21	4:2C:554:THR:CG2	1.24	1.59
4:2C:406:THR:HG21	4:2D:554:THR:CG2	1.23	1.57
4:2A:406:THR:HG21	4:2B:554:THR:CG2	1.22	1.54
4:2D:406:THR:CG2	4:2E:554:THR:HG21	1.03	1.51
4:2D:406:THR:CG2	4:2E:554:THR:CG2	1.82	1.50
4:2E:406:THR:CG2	4:2F:554:THR:HG21	1.02	1.50
4:2A:554:THR:CG2	4:2F:406:THR:CG2	1.79	1.49
4:2C:406:THR:CG2	4:2D:554:THR:HG21	1.01	1.48
4:2A:554:THR:HG21	4:2F:406:THR:CG2	1.00	1.47
4:2B:406:THR:CG2	4:2C:554:THR:HG21	1.02	1.46
4:2A:406:THR:CG2	4:2B:554:THR:HG21	1.00	1.45
4:2C:406:THR:CG2	4:2D:554:THR:CG2	1.80	1.40
4:2E:406:THR:CG2	4:2F:554:THR:CG2	1.80	1.40
4:2A:406:THR:CG2	4:2B:554:THR:CG2	1.79	1.38
4:2B:406:THR:CG2	4:2C:554:THR:CG2	1.80	1.35
4:2A:406:THR:HG21	4:2B:554:THR:CB	1.72	1.18
4:2C:406:THR:HG21	4:2D:554:THR:CB	1.73	1.18
4:2A:554:THR:CB	4:2F:406:THR:HG21	1.73	1.17
4:2E:406:THR:HG21	4:2F:554:THR:CB	1.72	1.17
4:2B:406:THR:HG21	4:2C:554:THR:CB	1.74	1.16
2:1C:94:TYR:CE1	4:2C:154:LYS:NZ	2.14	1.16
2:1D:94:TYR:CE1	4:2D:154:LYS:NZ	2.14	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2D:406:THR:HG21	4:2E:554:THR:CB	1.73	1.15
2:1F:94:TYR:CE1	4:2F:154:LYS:NZ	2.13	1.13
2:1B:94:TYR:CE1	4:2B:154:LYS:NZ	2.15	1.13
4:2D:406:THR:OG1	4:2E:552:HIS:HE1	1.32	1.13
4:2E:406:THR:OG1	4:2F:552:HIS:HE1	1.31	1.13
2:1E:94:TYR:CE1	4:2E:154:LYS:NZ	2.16	1.13
1:0C:194:TYR:OH	4:2E:597:GLU:OE1	1.68	1.12
2:1A:94:TYR:CE1	4:2A:154:LYS:NZ	2.14	1.12
1:0E:194:TYR:OH	4:2C:597:GLU:OE1	1.68	1.12
4:2E:406:THR:CB	4:2F:554:THR:HG21	1.80	1.12
4:2A:552:HIS:HE1	4:2F:406:THR:OG1	1.32	1.11
4:2C:406:THR:OG1	4:2D:552:HIS:HE1	1.32	1.11
1:0D:194:TYR:OH	4:2D:597:GLU:OE1	1.69	1.11
4:2B:406:THR:OG1	4:2C:552:HIS:HE1	1.32	1.11
4:2A:406:THR:CB	4:2B:554:THR:HG21	1.81	1.10
4:2A:406:THR:OG1	4:2B:552:HIS:HE1	1.32	1.09
4:2D:406:THR:CB	4:2E:554:THR:HG21	1.82	1.09
4:2A:554:THR:HG21	4:2F:406:THR:CB	1.83	1.09
4:2C:406:THR:CB	4:2D:554:THR:HG21	1.82	1.08
1:0F:194:TYR:OH	4:2B:597:GLU:OE1	1.70	1.08
4:2B:406:THR:CB	4:2C:554:THR:HG21	1.83	1.08
1:0B:194:TYR:OH	4:2F:597:GLU:OE1	1.71	1.07
1:0A:194:TYR:OH	4:2A:597:GLU:OE1	1.69	1.06
2:1A:222:ASN:ND2	2:1A:227:PHE:HE2	1.57	1.03
4:2A:554:THR:HG23	4:2F:406:THR:HG21	1.39	1.03
2:1E:222:ASN:ND2	2:1E:227:PHE:HE2	1.57	1.02
4:2C:406:THR:HG21	4:2D:554:THR:HG23	1.41	1.02
2:1C:222:ASN:ND2	2:1C:227:PHE:HE2	1.57	1.01
2:1F:222:ASN:ND2	2:1F:227:PHE:HE2	1.57	1.01
2:1B:222:ASN:ND2	2:1B:227:PHE:HE2	1.57	1.01
2:1D:222:ASN:ND2	2:1D:227:PHE:HE2	1.57	1.01
4:2A:406:THR:HG21	4:2B:554:THR:HG23	1.40	1.01
4:2D:406:THR:HG22	4:2E:554:THR:HG21	1.01	1.00
2:1D:222:ASN:ND2	2:1D:227:PHE:CE2	2.30	1.00
2:1E:222:ASN:ND2	2:1E:227:PHE:CE2	2.30	1.00
4:2D:406:THR:OG1	4:2E:552:HIS:CE1	2.14	1.00
4:2B:406:THR:HG21	4:2C:554:THR:HG23	1.41	1.00
2:1A:222:ASN:ND2	2:1A:227:PHE:CE2	2.30	0.99
4:2E:406:THR:HG21	4:2F:554:THR:HG23	1.43	0.99
4:2C:406:THR:HG22	4:2D:554:THR:HG21	1.00	0.99
4:2E:406:THR:OG1	4:2F:552:HIS:CE1	2.14	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:406:THR:HG22	4:2F:554:THR:HG21	1.01	0.99
2:1F:222:ASN:ND2	2:1F:227:PHE:CE2	2.30	0.99
4:2B:406:THR:OG1	4:2C:552:HIS:CE1	2.15	0.99
4:2D:406:THR:HG21	4:2E:554:THR:HG23	1.43	0.99
2:1B:222:ASN:ND2	2:1B:227:PHE:CE2	2.30	0.99
2:1C:222:ASN:ND2	2:1C:227:PHE:CE2	2.30	0.99
4:2A:552:HIS:CE1	4:2F:406:THR:OG1	2.16	0.99
4:2B:406:THR:HG22	4:2C:554:THR:HG21	0.99	0.98
4:2A:406:THR:OG1	4:2B:552:HIS:CE1	2.16	0.98
4:2C:406:THR:OG1	4:2D:552:HIS:CE1	2.15	0.98
4:2A:406:THR:HG22	4:2B:554:THR:HG21	0.99	0.97
4:2C:408:THR:HG23	4:2C:411:GLU:HG2	1.47	0.96
1:0D:21:GLU:OE2	2:1D:260:LYS:NZ	1.97	0.96
1:0A:21:GLU:OE2	2:1A:260:LYS:NZ	1.99	0.96
4:2A:554:THR:HG21	4:2F:406:THR:HG22	0.99	0.96
4:2B:408:THR:HG23	4:2B:411:GLU:HG2	1.47	0.96
1:0B:21:GLU:OE2	2:1F:260:LYS:NZ	2.00	0.95
4:2E:408:THR:HG23	4:2E:411:GLU:HG2	1.47	0.94
4:2F:408:THR:HG23	4:2F:411:GLU:HG2	1.47	0.94
4:2A:408:THR:HG23	4:2A:411:GLU:HG2	1.47	0.94
4:2D:408:THR:HG23	4:2D:411:GLU:HG2	1.47	0.94
1:0E:194:TYR:CZ	4:2C:597:GLU:OE1	2.20	0.93
1:0C:194:TYR:CZ	4:2E:597:GLU:OE1	2.20	0.93
1:0C:21:GLU:OE2	2:1E:260:LYS:NZ	2.01	0.93
1:0F:194:TYR:CZ	4:2B:597:GLU:OE1	2.21	0.93
1:0A:194:TYR:CZ	4:2A:597:GLU:OE1	2.21	0.93
1:0B:194:TYR:CZ	4:2F:597:GLU:OE1	2.22	0.92
4:2A:406:THR:CB	4:2B:554:THR:CG2	2.45	0.92
1:0D:194:TYR:CZ	4:2D:597:GLU:OE1	2.21	0.92
1:0E:21:GLU:OE2	2:1C:260:LYS:NZ	2.00	0.92
2:1D:94:TYR:HE1	4:2D:154:LYS:NZ	1.57	0.92
1:0F:21:GLU:OE2	2:1B:260:LYS:NZ	2.02	0.91
4:2A:554:THR:CG2	4:2F:406:THR:CB	2.46	0.91
2:1C:94:TYR:HE1	4:2C:154:LYS:NZ	1.57	0.90
2:1E:94:TYR:HE1	4:2E:154:LYS:NZ	1.58	0.90
4:2E:406:THR:CB	4:2F:554:THR:CG2	2.44	0.89
2:1F:94:TYR:HE1	4:2F:154:LYS:NZ	1.56	0.88
2:1B:94:TYR:HE1	4:2B:154:LYS:NZ	1.57	0.88
4:2C:406:THR:CB	4:2D:554:THR:CG2	2.45	0.88
4:2E:408:THR:CG2	4:2E:411:GLU:HG2	2.06	0.86
4:2E:406:THR:HG21	4:2F:554:THR:OG1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1A:94:TYR:HE1	4:2A:154:LYS:NZ	1.57	0.86
4:2D:406:THR:CB	4:2E:554:THR:CG2	2.46	0.86
4:2D:408:THR:CG2	4:2D:411:GLU:HG2	2.06	0.86
4:2F:408:THR:CG2	4:2F:411:GLU:HG2	2.06	0.86
4:2C:408:THR:CG2	4:2C:411:GLU:HG2	2.06	0.85
4:2D:406:THR:HG21	4:2E:554:THR:OG1	1.77	0.85
4:2E:405:ASP:O	4:2F:219:ASN:OD1	1.95	0.85
4:2A:408:THR:CG2	4:2A:411:GLU:HG2	2.06	0.85
4:2B:408:THR:CG2	4:2B:411:GLU:HG2	2.06	0.84
4:2D:405:ASP:O	4:2E:219:ASN:OD1	1.96	0.83
4:2C:406:THR:HG21	4:2D:554:THR:OG1	1.78	0.83
4:2A:405:ASP:O	4:2B:219:ASN:OD1	1.96	0.83
4:2C:405:ASP:O	4:2D:219:ASN:OD1	1.97	0.82
4:2A:219:ASN:OD1	4:2F:405:ASP:O	1.98	0.82
4:2B:406:THR:CB	4:2C:554:THR:CG2	2.46	0.82
4:2A:406:THR:HG21	4:2B:554:THR:OG1	1.78	0.82
4:2B:406:THR:HG21	4:2C:554:THR:OG1	1.79	0.81
4:2A:554:THR:OG1	4:2F:406:THR:HG21	1.80	0.81
4:2B:405:ASP:O	4:2C:219:ASN:OD1	1.98	0.81
1:0B:187:ILE:O	4:2F:608:VAL:O	2.05	0.74
1:0E:187:ILE:O	4:2C:608:VAL:O	2.04	0.74
1:0C:187:ILE:O	4:2E:608:VAL:O	2.06	0.74
1:0A:187:ILE:O	4:2A:608:VAL:O	2.04	0.74
4:2B:406:THR:CG2	4:2C:554:THR:CB	2.50	0.74
1:0F:187:ILE:O	4:2B:608:VAL:O	2.05	0.73
1:0D:187:ILE:O	4:2D:608:VAL:O	2.06	0.73
4:2D:406:THR:CG2	4:2E:554:THR:CB	2.50	0.73
2:1D:94:TYR:CD1	4:2D:154:LYS:NZ	2.58	0.71
2:1F:94:TYR:CD1	4:2F:154:LYS:NZ	2.58	0.71
2:1C:94:TYR:CD1	4:2C:154:LYS:NZ	2.58	0.71
4:2E:406:THR:HB	4:2F:554:THR:CG2	2.21	0.71
2:1E:222:ASN:HD22	2:1E:227:PHE:HE2	1.20	0.70
4:2D:4:TYR:CE1	4:2E:682:ILE:HD11	2.26	0.70
2:1B:94:TYR:CD1	4:2B:154:LYS:NZ	2.59	0.70
2:1E:94:TYR:CD1	4:2E:154:LYS:NZ	2.60	0.70
4:2C:4:TYR:CE1	4:2D:682:ILE:HD11	2.27	0.69
2:1A:94:TYR:CD1	4:2A:154:LYS:NZ	2.59	0.69
4:2E:4:TYR:CE1	4:2F:682:ILE:HD11	2.26	0.69
2:1C:94:TYR:HE1	4:2C:154:LYS:HZ2	0.73	0.69
4:2E:406:THR:CG2	4:2F:554:THR:CB	2.49	0.69
4:2B:4:TYR:CE1	4:2C:682:ILE:HD11	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:4:TYR:CE1	4:2B:682:ILE:HD11	2.28	0.68
4:2D:406:THR:HB	4:2E:554:THR:CG2	2.22	0.68
4:2D:406:THR:CG2	4:2E:554:THR:HG23	2.11	0.67
4:2A:406:THR:HB	4:2B:554:THR:CG2	2.23	0.67
4:2B:406:THR:HG23	4:2C:218:ARG:HD3	1.76	0.67
4:2C:406:THR:HB	4:2D:554:THR:CG2	2.23	0.67
4:2A:554:THR:CG2	4:2F:406:THR:HB	2.24	0.67
4:2D:406:THR:HG23	4:2E:218:ARG:HD3	1.74	0.67
4:2E:406:THR:HG23	4:2F:218:ARG:HD3	1.75	0.67
4:2A:682:ILE:HD11	4:2F:4:TYR:CE1	2.30	0.67
4:2B:406:THR:HB	4:2C:554:THR:CG2	2.24	0.67
4:2A:554:THR:CB	4:2F:406:THR:CG2	2.50	0.66
4:2C:406:THR:HG23	4:2D:218:ARG:HD3	1.77	0.66
2:1D:94:TYR:HE1	4:2D:154:LYS:HZ2	0.72	0.66
4:2C:406:THR:CG2	4:2D:554:THR:CB	2.50	0.66
2:1D:222:ASN:HD22	2:1D:227:PHE:HE2	1.20	0.66
4:2A:406:THR:HG23	4:2B:218:ARG:HD3	1.78	0.66
4:2E:406:THR:CG2	4:2F:554:THR:HG23	2.10	0.65
4:2A:218:ARG:HD3	4:2F:406:THR:HG23	1.78	0.65
2:1A:94:TYR:HE1	4:2A:154:LYS:HZ2	0.69	0.64
2:1C:222:ASN:HD22	2:1C:227:PHE:HE2	1.20	0.64
4:2A:406:THR:CG2	4:2B:554:THR:CB	2.49	0.64
4:2A:554:THR:HG23	4:2F:406:THR:CG2	2.08	0.63
4:2A:14:ILE:O	4:2B:686:SER:HB3	2.01	0.61
4:2D:14:ILE:O	4:2E:686:SER:HB3	1.99	0.61
4:2E:14:ILE:O	4:2F:686:SER:HB3	2.00	0.61
4:2C:406:THR:CG2	4:2D:554:THR:OG1	2.49	0.60
4:2E:406:THR:CG2	4:2F:554:THR:OG1	2.47	0.60
4:2D:406:THR:CG2	4:2E:554:THR:OG1	2.48	0.60
2:1E:94:TYR:HE1	4:2E:154:LYS:HZ2	0.75	0.60
4:2C:14:ILE:O	4:2D:686:SER:HB3	2.00	0.60
4:2A:406:THR:CG2	4:2B:554:THR:OG1	2.49	0.59
4:2B:14:ILE:O	4:2C:686:SER:HB3	2.02	0.59
4:2A:686:SER:HB3	4:2F:14:ILE:O	2.03	0.59
4:2A:554:THR:CG2	4:2F:406:THR:HG22	1.89	0.58
2:1B:94:TYR:HE1	4:2B:154:LYS:HZ2	0.73	0.58
4:2C:406:THR:HB	4:2D:554:THR:HG21	1.82	0.57
1:0F:194:TYR:CE2	4:2B:597:GLU:OE1	2.58	0.57
4:2B:406:THR:CB	4:2C:554:THR:HG23	2.34	0.57
1:0E:194:TYR:CE2	4:2C:597:GLU:OE1	2.56	0.57
4:2A:554:THR:OG1	4:2F:406:THR:CG2	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2C:406:THR:HG21	4:2D:554:THR:HG1	1.70	0.57
1:0D:194:TYR:CE2	4:2D:597:GLU:OE1	2.58	0.56
4:2B:406:THR:CG2	4:2C:554:THR:OG1	2.49	0.56
4:2E:406:THR:HG22	4:2F:554:THR:CG2	1.91	0.56
4:2D:406:THR:CB	4:2E:554:THR:HG23	2.34	0.56
1:0A:194:TYR:CE2	4:2A:597:GLU:OE1	2.58	0.56
1:0C:194:TYR:CE2	4:2E:597:GLU:OE1	2.57	0.56
1:0B:194:TYR:CE2	4:2F:597:GLU:OE1	2.59	0.55
4:2D:172:ASP:N	4:2D:172:ASP:OD1	2.38	0.55
1:0F:76:THR:HG22	1:0F:183:GLU:HG2	1.89	0.55
4:2E:5:LYS:O	4:2F:550:ASN:ND2	2.38	0.55
4:2E:406:THR:HG21	4:2F:554:THR:HG1	1.71	0.55
1:0E:76:THR:HG22	1:0E:183:GLU:HG2	1.89	0.55
4:2C:172:ASP:N	4:2C:172:ASP:OD1	2.38	0.55
4:2A:554:THR:HG23	4:2F:406:THR:CB	2.33	0.55
4:2D:406:THR:HG21	4:2E:554:THR:HG1	1.72	0.55
1:0D:76:THR:HG22	1:0D:183:GLU:HG2	1.89	0.54
2:1F:94:TYR:HE1	4:2F:154:LYS:HZ2	0.70	0.54
4:2D:406:THR:HG22	4:2E:554:THR:CG2	1.91	0.54
4:2A:406:THR:CB	4:2B:554:THR:HG23	2.33	0.54
1:0A:76:THR:HG22	1:0A:183:GLU:HG2	1.89	0.54
1:0C:76:THR:HG22	1:0C:183:GLU:HG2	1.89	0.54
4:2A:212:ASP:OD1	4:2A:215:PRO:HD2	2.08	0.54
4:2C:406:THR:CB	4:2D:554:THR:HG23	2.33	0.53
4:2E:212:ASP:OD1	4:2E:215:PRO:HD2	2.08	0.53
4:2F:172:ASP:OD1	4:2F:172:ASP:N	2.38	0.53
4:2A:5:LYS:O	4:2B:550:ASN:ND2	2.38	0.53
4:2C:212:ASP:OD1	4:2C:215:PRO:HD2	2.08	0.53
4:2B:212:ASP:OD1	4:2B:215:PRO:HD2	2.08	0.53
4:2D:212:ASP:OD1	4:2D:215:PRO:HD2	2.08	0.53
4:2C:90:ARG:NH1	4:2C:488:THR:OG1	2.42	0.53
1:0B:76:THR:HG22	1:0B:183:GLU:HG2	1.89	0.53
4:2B:90:ARG:NH1	4:2B:488:THR:OG1	2.42	0.53
4:2B:172:ASP:OD1	4:2B:172:ASP:N	2.38	0.53
4:2C:5:LYS:O	4:2D:550:ASN:ND2	2.38	0.53
4:2A:554:THR:HG21	4:2F:406:THR:HB	1.84	0.53
4:2A:550:ASN:ND2	4:2F:5:LYS:O	2.40	0.52
4:2F:212:ASP:OD1	4:2F:215:PRO:HD2	2.08	0.52
2:1E:224:LYS:HG3	2:1E:225:ASP:OD1	2.10	0.52
4:2D:90:ARG:NH1	4:2D:488:THR:OG1	2.42	0.52
4:2E:90:ARG:NH1	4:2E:488:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:90:ARG:NH1	4:2A:488:THR:OG1	2.42	0.52
4:2E:406:THR:CB	4:2F:554:THR:HG23	2.33	0.52
4:2F:90:ARG:NH1	4:2F:488:THR:OG1	2.42	0.52
4:2A:406:THR:HG22	4:2B:554:THR:CG2	1.89	0.52
2:1D:224:LYS:HG3	2:1D:225:ASP:OD1	2.10	0.52
4:2D:5:LYS:O	4:2E:550:ASN:ND2	2.38	0.52
2:1B:224:LYS:HG3	2:1B:225:ASP:OD1	2.10	0.52
2:1F:224:LYS:HG3	2:1F:225:ASP:OD1	2.10	0.52
4:2B:5:LYS:O	4:2C:550:ASN:ND2	2.40	0.51
2:1C:92:GLU:O	4:2C:154:LYS:HE2	2.11	0.51
2:1A:224:LYS:HG3	2:1A:225:ASP:OD1	2.10	0.51
2:1F:92:GLU:O	4:2F:154:LYS:HE2	2.10	0.51
2:1C:224:LYS:HG3	2:1C:225:ASP:OD1	2.10	0.51
2:1D:92:GLU:O	4:2D:154:LYS:HE2	2.11	0.51
4:2B:411:GLU:OE1	4:2B:411:GLU:HA	2.11	0.51
4:2E:172:ASP:OD1	4:2E:172:ASP:N	2.38	0.50
4:2A:411:GLU:OE1	4:2A:411:GLU:HA	2.11	0.50
4:2E:4:TYR:CE1	4:2F:682:ILE:CD1	2.95	0.50
4:2E:411:GLU:HA	4:2E:411:GLU:OE1	2.11	0.50
4:2D:411:GLU:HA	4:2D:411:GLU:OE1	2.12	0.50
4:2F:411:GLU:OE1	4:2F:411:GLU:HA	2.11	0.50
4:2C:406:THR:HG22	4:2D:554:THR:CG2	1.90	0.50
4:2C:411:GLU:OE1	4:2C:411:GLU:HA	2.11	0.50
2:1E:92:GLU:O	4:2E:154:LYS:HE2	2.12	0.49
2:1A:92:GLU:O	4:2A:154:LYS:HE2	2.12	0.49
2:1B:92:GLU:O	4:2B:154:LYS:HE2	2.12	0.49
1:0D:28:VAL:HG21	1:0D:48:LYS:HD3	1.94	0.49
2:1C:85:THR:OG1	2:1C:86:GLU:N	2.45	0.49
1:0C:28:VAL:HG21	1:0C:48:LYS:HD3	1.94	0.49
2:1B:85:THR:OG1	2:1B:86:GLU:N	2.45	0.49
2:1D:85:THR:OG1	2:1D:86:GLU:N	2.45	0.49
1:0B:28:VAL:HG21	1:0B:48:LYS:HD3	1.94	0.49
2:1A:85:THR:OG1	2:1A:86:GLU:N	2.45	0.49
2:1F:85:THR:OG1	2:1F:86:GLU:N	2.45	0.49
2:1E:85:THR:OG1	2:1E:86:GLU:N	2.45	0.49
4:2B:406:THR:HG22	4:2C:554:THR:CG2	1.90	0.49
4:2A:172:ASP:OD1	4:2A:172:ASP:N	2.38	0.48
1:0E:28:VAL:HG21	1:0E:48:LYS:HD3	1.94	0.48
4:2A:406:THR:HG21	4:2B:554:THR:HG1	1.78	0.48
1:0B:177:ARG:HD2	1:0C:109:GLU:HG2	1.96	0.48
2:1E:165:LEU:HD22	2:1E:170:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0A:28:VAL:HG21	1:0A:48:LYS:HD3	1.94	0.48
4:2D:4:TYR:CE1	4:2E:682:ILE:CD1	2.95	0.48
2:1A:165:LEU:HD22	2:1A:170:LEU:HD12	1.96	0.48
2:1D:165:LEU:HD22	2:1D:170:LEU:HD12	1.96	0.48
2:1F:222:ASN:HD22	2:1F:227:PHE:HE2	1.20	0.48
1:0C:177:ARG:HD2	1:0D:109:GLU:HG2	1.96	0.47
2:1F:165:LEU:HD22	2:1F:170:LEU:HD12	1.96	0.47
1:0F:28:VAL:HG21	1:0F:48:LYS:HD3	1.94	0.47
2:1B:165:LEU:HD22	2:1B:170:LEU:HD12	1.96	0.47
2:1C:222:ASN:CB	2:1C:227:PHE:CE2	2.98	0.47
1:0A:109:GLU:HG2	1:0F:177:ARG:HD2	1.97	0.47
2:1E:222:ASN:CB	2:1E:227:PHE:CE2	2.98	0.47
1:0A:113:HIS:CD2	1:0F:179:ALA:HB3	2.50	0.47
1:0B:179:ALA:HB3	1:0C:113:HIS:CD2	2.50	0.47
2:1B:222:ASN:CB	2:1B:227:PHE:CE2	2.98	0.47
2:1C:165:LEU:HD22	2:1C:170:LEU:HD12	1.96	0.47
4:2A:4:TYR:CE1	4:2B:682:ILE:CD1	2.97	0.47
4:2A:682:ILE:CD1	4:2F:4:TYR:CE1	2.98	0.47
1:0A:177:ARG:HD2	1:0B:109:GLU:HG2	1.97	0.47
1:0E:177:ARG:HD2	1:0F:109:GLU:HG2	1.97	0.47
4:2C:4:TYR:CE1	4:2D:682:ILE:CD1	2.96	0.46
2:1D:222:ASN:CB	2:1D:227:PHE:CE2	2.98	0.46
2:1F:222:ASN:CB	2:1F:227:PHE:CE2	2.98	0.46
4:2B:4:TYR:CE1	4:2C:682:ILE:CD1	2.97	0.46
4:2B:406:THR:HG21	4:2C:554:THR:HG1	1.79	0.46
2:1A:222:ASN:CB	2:1A:227:PHE:CE2	2.98	0.46
1:0D:177:ARG:HD2	1:0E:109:GLU:HG2	1.98	0.46
1:0C:179:ALA:HB3	1:0D:113:HIS:CD2	2.51	0.46
4:2A:191:ASP:OD1	4:2A:191:ASP:N	2.48	0.46
4:2B:156:ASP:OD1	4:2B:156:ASP:N	2.47	0.46
4:2E:273:VAL:HG13	4:2E:278:PHE:CE2	2.51	0.46
1:0A:179:ALA:HB3	1:0B:113:HIS:CD2	2.51	0.46
2:1A:222:ASN:HD22	2:1A:227:PHE:HE2	1.20	0.45
4:2C:273:VAL:HG13	4:2C:278:PHE:CE2	2.51	0.45
4:2B:191:ASP:OD1	4:2B:191:ASP:N	2.48	0.45
4:2C:191:ASP:N	4:2C:191:ASP:OD1	2.48	0.45
4:2F:273:VAL:HG13	4:2F:278:PHE:CE2	2.51	0.45
1:0E:179:ALA:HB3	1:0F:113:HIS:CD2	2.51	0.45
4:2A:273:VAL:HG13	4:2A:278:PHE:CE2	2.51	0.45
4:2D:273:VAL:HG13	4:2D:278:PHE:CE2	2.51	0.45
4:2A:437:LEU:O	4:2A:438:THR:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:554:THR:HG1	4:2F:406:THR:HG21	1.79	0.45
4:2B:273:VAL:HG13	4:2B:278:PHE:CE2	2.51	0.45
1:0D:179:ALA:HB3	1:0E:113:HIS:CD2	2.51	0.45
4:2B:437:LEU:O	4:2B:438:THR:C	2.55	0.45
4:2F:191:ASP:OD1	4:2F:191:ASP:N	2.48	0.45
4:2D:437:LEU:O	4:2D:438:THR:C	2.55	0.45
4:2D:137:PRO:HA	4:2D:138:PRO:HD3	1.87	0.44
4:2E:191:ASP:OD1	4:2E:191:ASP:N	2.48	0.44
4:2D:156:ASP:OD1	4:2D:156:ASP:N	2.47	0.44
2:1C:92:GLU:O	4:2C:154:LYS:CE	2.66	0.44
4:2C:14:ILE:O	4:2D:686:SER:CB	2.66	0.43
4:2D:14:ILE:O	4:2E:686:SER:CB	2.66	0.43
4:2E:420:ASN:O	4:2E:421:PHE:C	2.57	0.43
4:2A:406:THR:CG2	4:2B:554:THR:HG23	2.09	0.43
4:2F:420:ASN:O	4:2F:421:PHE:C	2.57	0.43
1:0B:26:GLU:OE2	1:0B:48:LYS:NZ	2.52	0.43
2:1C:202:ASN:OD1	2:1C:202:ASN:N	2.50	0.43
4:2E:14:ILE:O	4:2F:686:SER:CB	2.67	0.43
4:2A:169:LEU:HA	4:2A:170:PRO:HD3	1.94	0.43
4:2A:420:ASN:O	4:2A:421:PHE:C	2.57	0.43
1:0A:26:GLU:OE2	1:0A:48:LYS:NZ	2.52	0.43
2:1D:92:GLU:O	4:2D:154:LYS:CE	2.67	0.43
1:0C:26:GLU:OE2	1:0C:48:LYS:NZ	2.52	0.43
4:2D:191:ASP:OD1	4:2D:191:ASP:N	2.48	0.43
4:2E:437:LEU:O	4:2E:438:THR:C	2.55	0.43
2:1F:92:GLU:O	4:2F:154:LYS:CE	2.66	0.43
4:2F:437:LEU:O	4:2F:438:THR:C	2.55	0.43
1:0F:26:GLU:OE2	1:0F:48:LYS:NZ	2.52	0.42
4:2A:404:ALA:HB1	4:2A:411:GLU:HB2	2.01	0.42
1:0E:26:GLU:OE2	1:0E:48:LYS:NZ	2.52	0.42
4:2B:404:ALA:HB1	4:2B:411:GLU:HB2	2.01	0.42
4:2F:404:ALA:HB1	4:2F:411:GLU:HB2	2.01	0.42
4:2D:45:ASP:OD1	4:2D:45:ASP:N	2.49	0.42
1:0D:26:GLU:OE2	1:0D:48:LYS:NZ	2.51	0.42
4:2C:404:ALA:HB1	4:2C:411:GLU:HB2	2.01	0.42
4:2D:404:ALA:HB1	4:2D:411:GLU:HB2	2.01	0.42
4:2E:156:ASP:OD1	4:2E:156:ASP:N	2.47	0.42
4:2E:404:ALA:HB1	4:2E:411:GLU:HB2	2.01	0.42
1:0D:118:THR:H	1:0D:121:ASN:HB2	1.85	0.42
2:1C:165:LEU:CD2	2:1C:170:LEU:HD12	2.50	0.42
2:1E:165:LEU:CD2	2:1E:170:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2C:420:ASN:O	4:2C:421:PHE:C	2.57	0.42
2:1F:222:ASN:HB3	2:1F:227:PHE:CE2	2.55	0.42
2:1D:222:ASN:HB3	2:1D:227:PHE:CE2	2.55	0.41
4:2B:420:ASN:O	4:2B:421:PHE:C	2.57	0.41
2:1A:222:ASN:HB3	2:1A:227:PHE:CE2	2.55	0.41
2:1B:145:ASN:OD1	2:1B:145:ASN:N	2.51	0.41
2:1B:165:LEU:CD2	2:1B:170:LEU:HD12	2.50	0.41
2:1C:222:ASN:HB3	2:1C:227:PHE:CE2	2.55	0.41
1:0E:118:THR:H	1:0E:121:ASN:HB2	1.85	0.41
2:1B:92:GLU:O	4:2B:154:LYS:CE	2.68	0.41
4:2D:420:ASN:O	4:2D:421:PHE:C	2.57	0.41
4:2F:214:ILE:HB	4:2F:215:PRO:HD3	2.03	0.41
2:1B:222:ASN:HB3	2:1B:227:PHE:CE2	2.55	0.41
2:1E:202:ASN:OD1	2:1E:202:ASN:N	2.50	0.41
4:2D:214:ILE:HB	4:2D:215:PRO:HD3	2.03	0.41
4:2E:214:ILE:HB	4:2E:215:PRO:HD3	2.03	0.41
2:1A:92:GLU:O	4:2A:154:LYS:CE	2.68	0.41
2:1D:165:LEU:CD2	2:1D:170:LEU:HD12	2.50	0.41
2:1E:92:GLU:O	4:2E:154:LYS:CE	2.68	0.41
4:2C:437:LEU:O	4:2C:438:THR:C	2.55	0.41
4:2A:14:ILE:O	4:2B:686:SER:CB	2.68	0.41
4:2C:214:ILE:HB	4:2C:215:PRO:HD3	2.03	0.41
1:0A:118:THR:H	1:0A:121:ASN:HB2	1.85	0.41
2:1B:222:ASN:HD22	2:1B:227:PHE:HE2	1.20	0.41
2:1C:170:LEU:HD11	2:1C:179:ILE:HD11	2.03	0.41
2:1D:170:LEU:HD11	2:1D:179:ILE:HD11	2.03	0.41
2:1E:222:ASN:HB3	2:1E:227:PHE:CE2	2.55	0.41
4:2A:214:ILE:HB	4:2A:215:PRO:HD3	2.03	0.41
1:0F:128:LEU:HD23	1:0F:128:LEU:HA	1.95	0.41
4:2B:214:ILE:HB	4:2B:215:PRO:HD3	2.03	0.40
4:2E:169:LEU:HA	4:2E:170:PRO:HD3	1.94	0.40
1:0F:118:THR:H	1:0F:121:ASN:HB2	1.85	0.40
2:1F:165:LEU:CD2	2:1F:170:LEU:HD12	2.50	0.40
2:1E:170:LEU:HD11	2:1E:179:ILE:HD11	2.03	0.40
4:2F:45:ASP:OD1	4:2F:45:ASP:N	2.49	0.40
1:0C:118:THR:H	1:0C:121:ASN:HB2	1.85	0.40
4:2B:14:ILE:O	4:2C:686:SER:CB	2.68	0.40
4:2F:169:LEU:HA	4:2F:170:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0A	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0B	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0C	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0D	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0E	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
1	0F	195/197 (99%)	189 (97%)	6 (3%)	0	100	100
2	1A	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1B	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1C	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1D	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1E	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
2	1F	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
3	1a	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1b	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1c	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1d	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1e	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	1f	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	2a	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2b	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2c	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2d	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2e	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
3	2f	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
4	2A	651/692 (94%)	638 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2B	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2C	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2D	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
4	2E	651/692 (94%)	638 (98%)	13 (2%)	0	100	100
4	2F	651/692 (94%)	637 (98%)	14 (2%)	0	100	100
All	All	8436/8742 (96%)	8264 (98%)	172 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	0A	186/186 (100%)	185 (100%)	1 (0%)	88	96
1	0B	186/186 (100%)	185 (100%)	1 (0%)	88	96
1	0C	186/186 (100%)	185 (100%)	1 (0%)	88	96
1	0D	186/186 (100%)	185 (100%)	1 (0%)	88	96
1	0E	186/186 (100%)	185 (100%)	1 (0%)	88	96
1	0F	186/186 (100%)	185 (100%)	1 (0%)	88	96
2	1A	264/264 (100%)	264 (100%)	0	100	100
2	1B	264/264 (100%)	264 (100%)	0	100	100
2	1C	264/264 (100%)	264 (100%)	0	100	100
2	1D	264/264 (100%)	264 (100%)	0	100	100
2	1E	264/264 (100%)	264 (100%)	0	100	100
2	1F	264/264 (100%)	264 (100%)	0	100	100
3	1a	127/128 (99%)	127 (100%)	0	100	100
3	1b	127/128 (99%)	127 (100%)	0	100	100
3	1c	127/128 (99%)	127 (100%)	0	100	100
3	1d	127/128 (99%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1e	127/128 (99%)	127 (100%)	0	100	100
3	1f	127/128 (99%)	127 (100%)	0	100	100
3	2a	127/128 (99%)	127 (100%)	0	100	100
3	2b	127/128 (99%)	127 (100%)	0	100	100
3	2c	127/128 (99%)	127 (100%)	0	100	100
3	2d	127/128 (99%)	127 (100%)	0	100	100
3	2e	127/128 (99%)	127 (100%)	0	100	100
3	2f	127/128 (99%)	127 (100%)	0	100	100
4	2A	547/593 (92%)	547 (100%)	0	100	100
4	2B	547/593 (92%)	547 (100%)	0	100	100
4	2C	547/593 (92%)	547 (100%)	0	100	100
4	2D	547/593 (92%)	547 (100%)	0	100	100
4	2E	547/593 (92%)	547 (100%)	0	100	100
4	2F	547/593 (92%)	547 (100%)	0	100	100
All	All	7506/7794 (96%)	7500 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0A	82	LEU
1	0B	82	LEU
1	0C	82	LEU
1	0D	82	LEU
1	0E	82	LEU
1	0F	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	1a	123	ASN
3	1b	123	ASN
3	1c	123	ASN
3	1d	123	ASN
3	1e	123	ASN
3	1f	123	ASN
4	2A	36	GLN

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Mol	Chain	Res	Type
4	2A	219	ASN
4	2A	552	HIS
4	2B	36	GLN
4	2B	219	ASN
4	2B	552	HIS
4	2C	36	GLN
4	2C	219	ASN
4	2C	552	HIS
4	2D	36	GLN
4	2D	219	ASN
4	2D	552	HIS
4	2E	36	GLN
4	2E	219	ASN
4	2E	552	HIS
4	2F	36	GLN
4	2F	219	ASN
4	2F	552	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	0A	1
1	0B	1
1	0C	1
1	0D	1
1	0E	1
1	0F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0A	82:LEU	C	83:ASN	N	1.17
1	0B	82:LEU	C	83:ASN	N	1.17
1	0C	82:LEU	C	83:ASN	N	1.17
1	0D	82:LEU	C	83:ASN	N	1.17
1	0E	82:LEU	C	83:ASN	N	1.17
1	0F	82:LEU	C	83:ASN	N	1.17

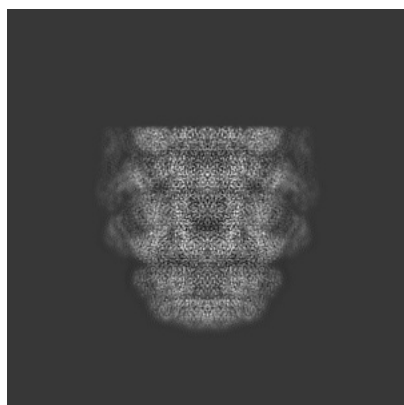
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11734. These allow visual inspection of the internal detail of the map and identification of artifacts.

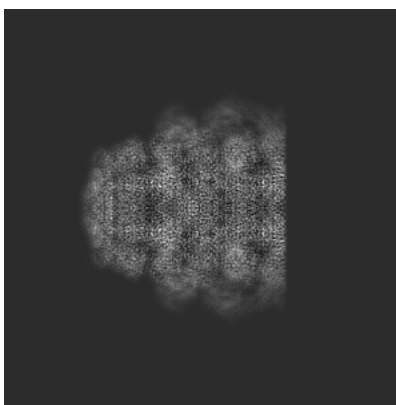
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

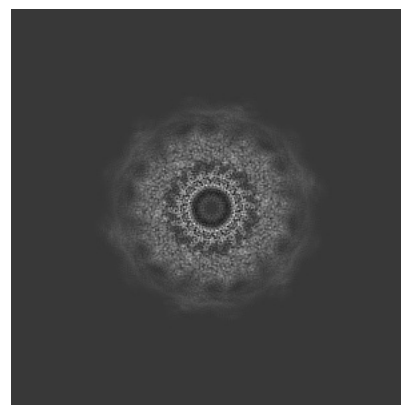
6.1.1 Primary map



X



Y



Z

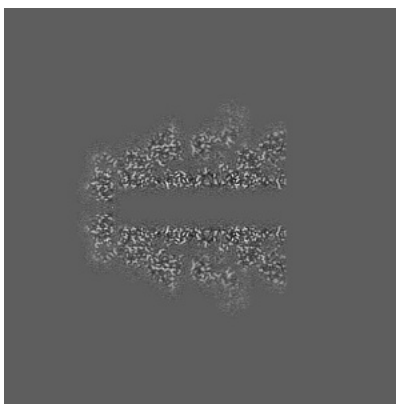
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

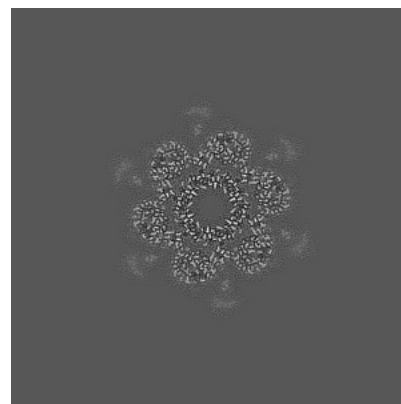
6.2.1 Primary map



X Index: 200



Y Index: 200

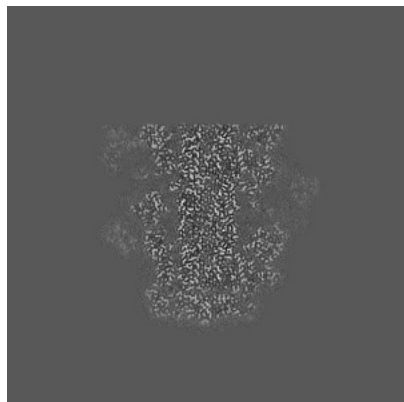


Z Index: 200

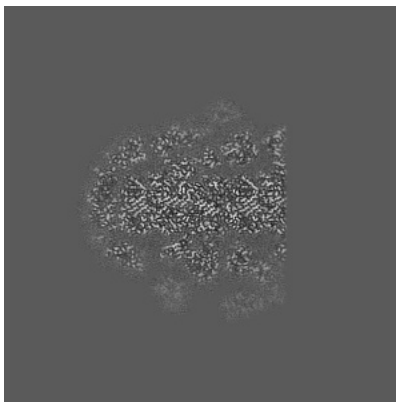
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

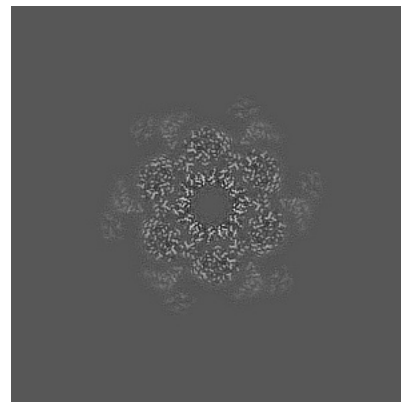
6.3.1 Primary map



X Index: 179



Y Index: 177

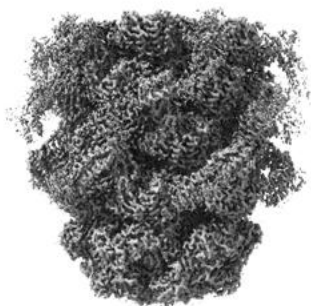


Z Index: 234

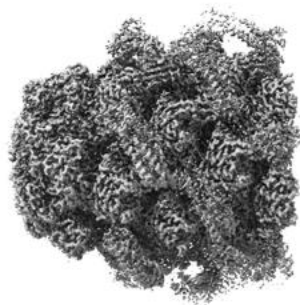
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

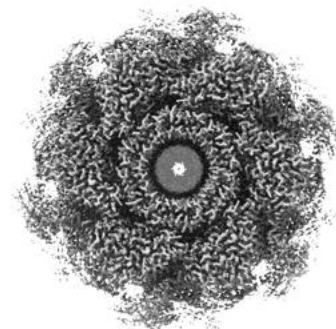
6.4.1 Primary map



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.

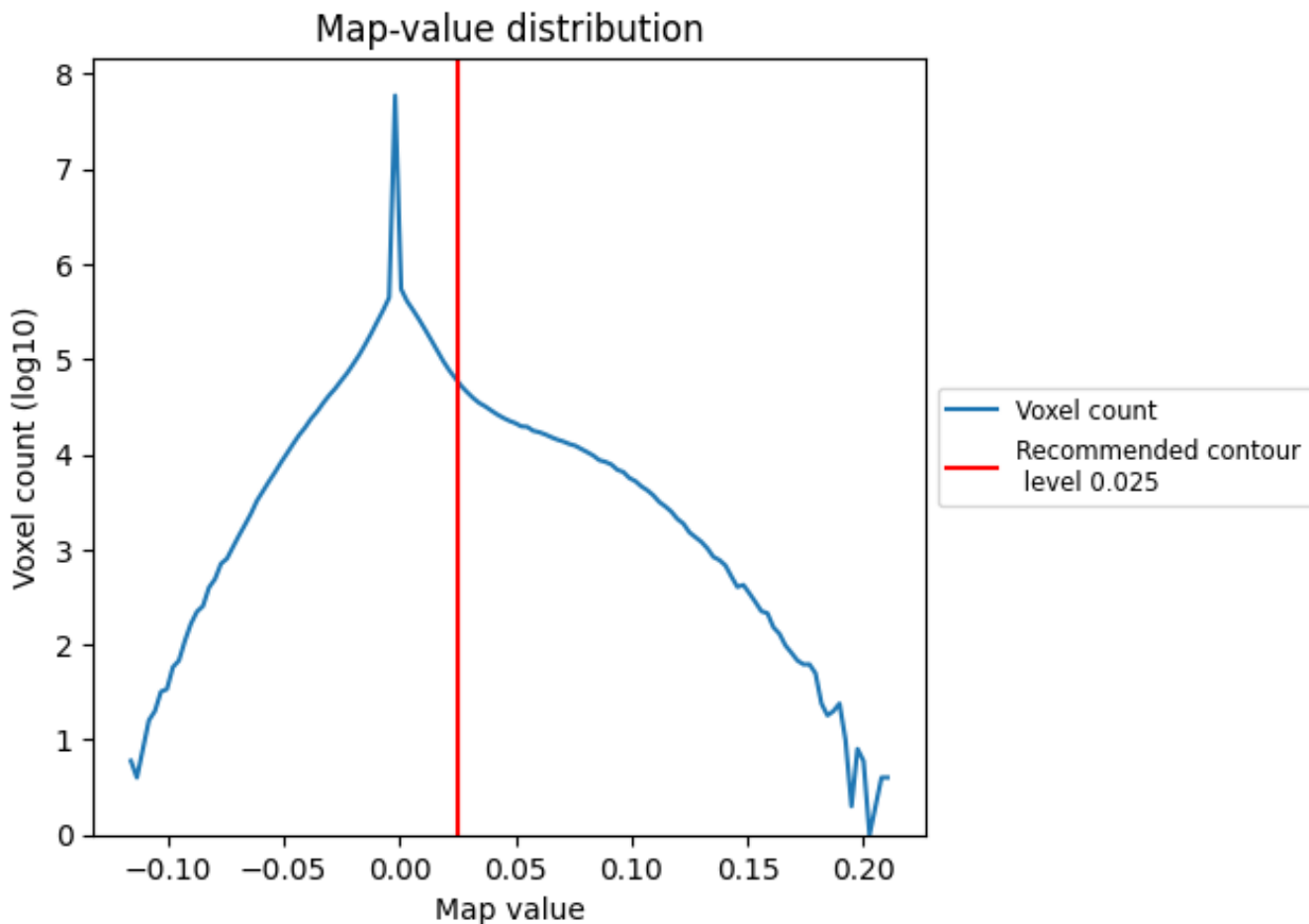
6.5 Mask visualisation

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

7 Map analysis [i](#)

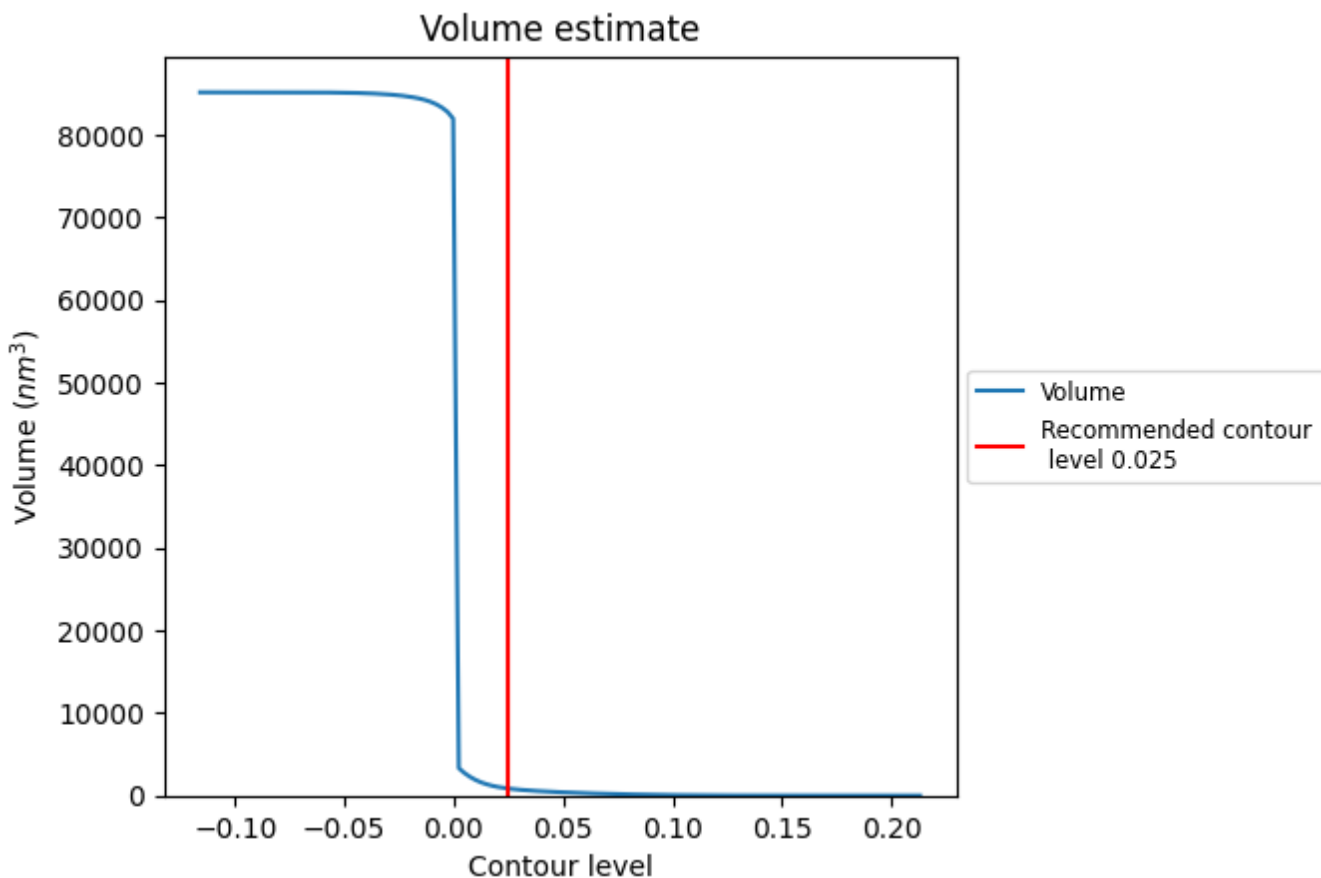
This section contains the results of statistical analysis of the map.

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.

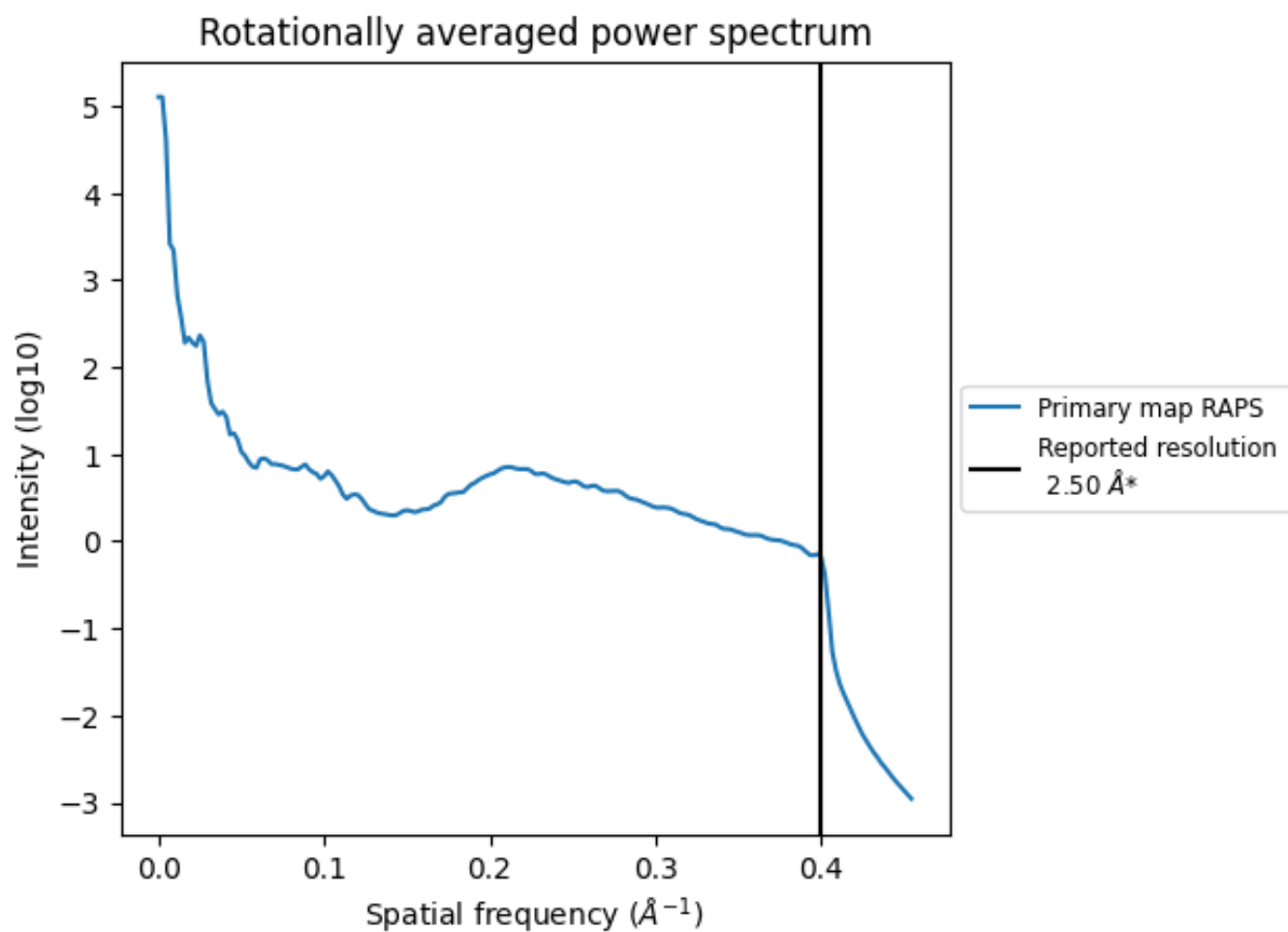
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 851 nm^3 ; this corresponds to an approximate mass of 769 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 0.400 Å⁻¹

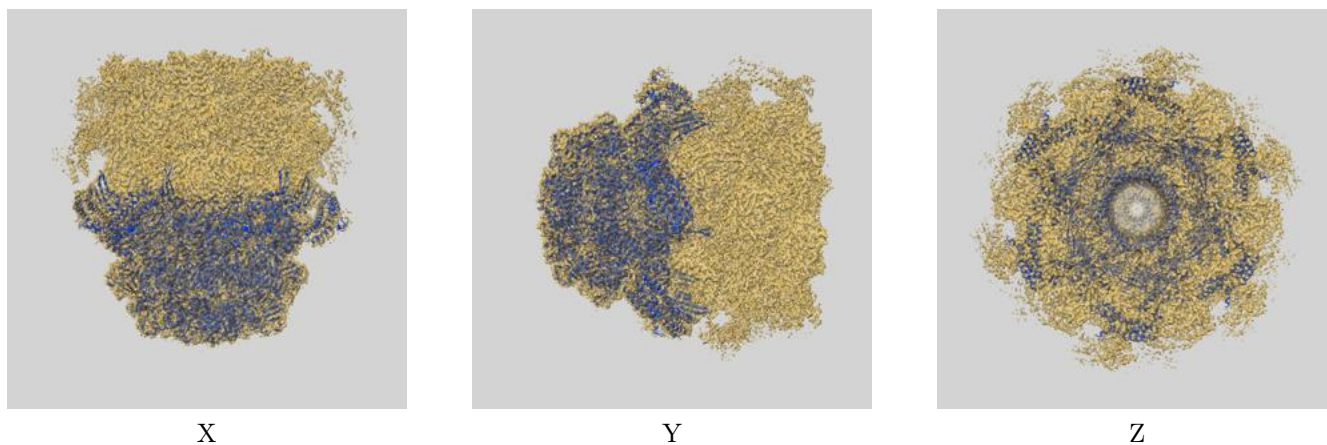
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

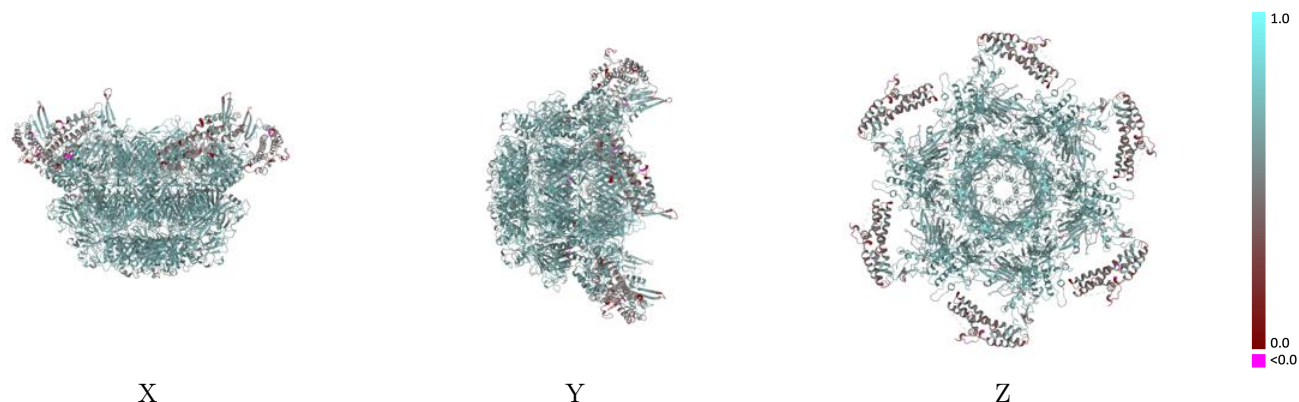
This section contains information regarding the fit between EMDB map EMD-11734 and PDB model 7ADZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



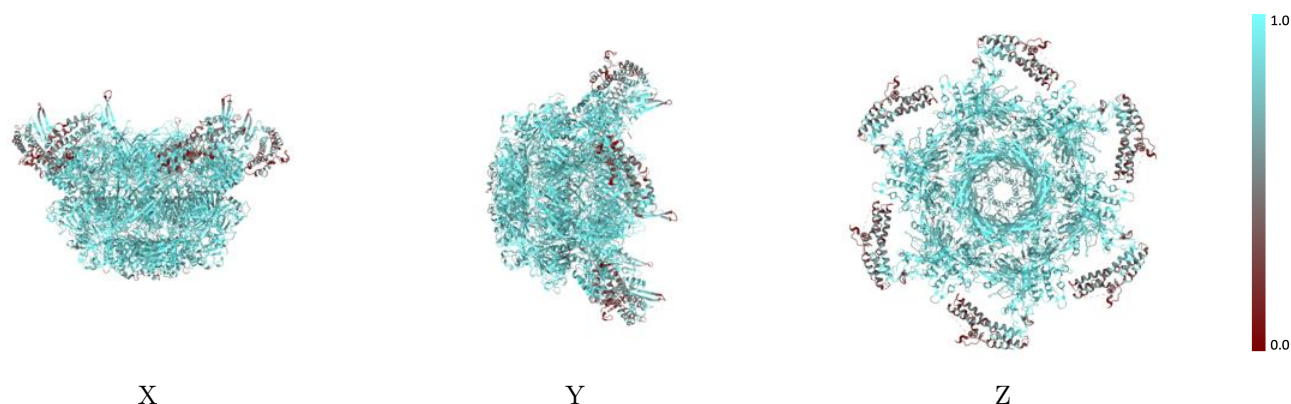
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



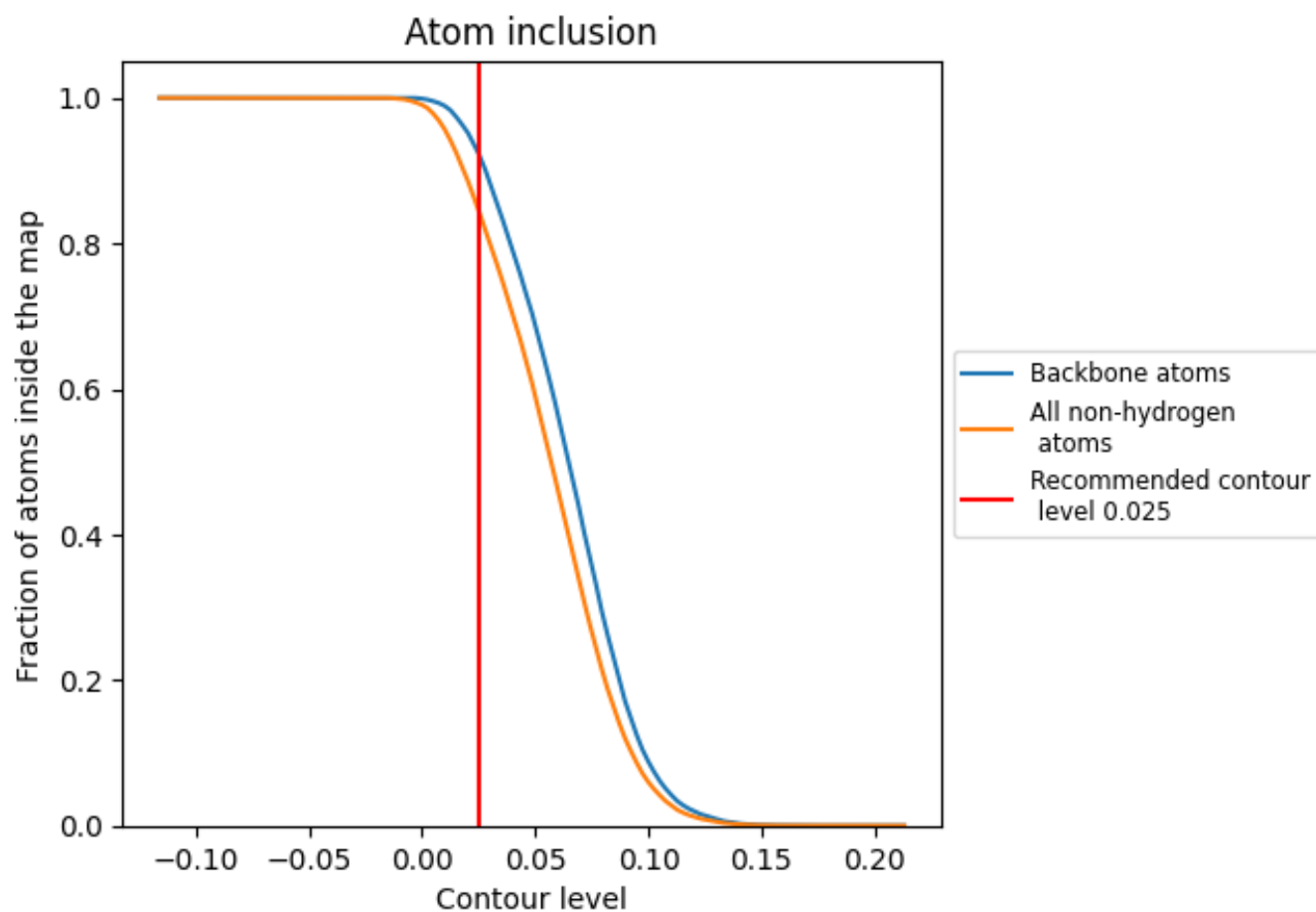
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 85% 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	 0.8457	 0.6110
0A	 0.9077	 0.6570
0B	 0.9064	 0.6540
0C	 0.9083	 0.6530
0D	 0.9077	 0.6580
0E	 0.9070	 0.6530
0F	 0.9083	 0.6520
1A	 0.8623	 0.6070
1B	 0.8722	 0.6080
1C	 0.8666	 0.6090
1D	 0.8636	 0.6070
1E	 0.8727	 0.6070
1F	 0.8666	 0.6080
1a	 0.9362	 0.6880
1b	 0.9344	 0.6820
1c	 0.9335	 0.6830
1d	 0.9371	 0.6890
1e	 0.9344	 0.6830
1f	 0.9335	 0.6840
2A	 0.7733	 0.5710
2B	 0.7735	 0.5710
2C	 0.7789	 0.5690
2D	 0.7741	 0.5710
2E	 0.7747	 0.5700
2F	 0.7769	 0.5690
2a	 0.9353	 0.6660
2b	 0.9353	 0.6630
2c	 0.9371	 0.6650
2d	 0.9335	 0.6660
2e	 0.9362	 0.6640
2f	 0.9379	 0.6660

