wwPDB EM Validation Summary Report ⓘ

Nov 12, 2025 – 10:17 AM EST

PDB ID	:	9NDY / pdb_00009ndy
EMDB ID	:	EMD-49281
Title	:	Composite baseplate asymmetric unit of JohannRWettstein (Bas63)
Authors	:	Hodgkinson-Bean, J.
Deposited on	:	2025-02-18
Resolution	:	3.83 Å(reported)

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

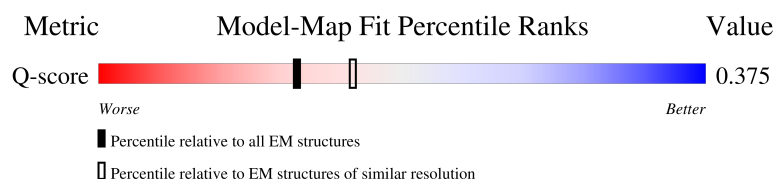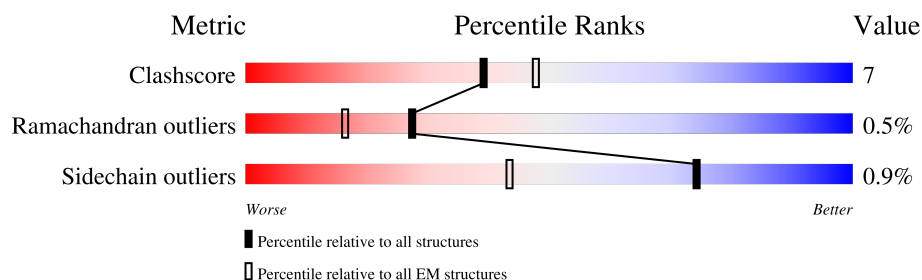|		
EMDB validation analysis	:	0.0.1.dev129
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
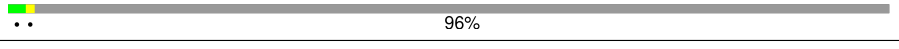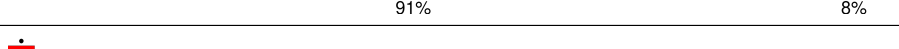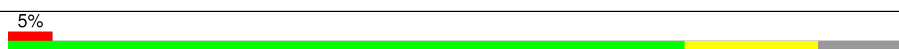
Metric	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		0.9%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Model-Map Fit Percentile Ranks	Value
Q-score		0.375

Worse   *Better*

▮ Percentile relative to all EM structures

▯ Percentile relative to EM structures of similar resolution

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	9087 (3.33 - 4.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	265	8% / 64% / 12% / 24%
1	B	265	13% / 67% / 9% / 24%
2	C	139	10% / 86% / · / 9%
2	D	139	9% / 78% / 12% / · / 9%

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Mol	Chain	Length	Quality of chain
3	E	325	85% 9% 6%
4	F	742	96%
5	G	207	91% 8%
6	H	489	79% 15% 6%
6	I	489	5% 76% 15% 10%
6	K	489	80% 11% 9%
6	L	489	82% 15%
7	J	285	5% 46% 9% 44%
7	M	285	46% 9% 43%
8	N	113	88% 12%
8	O	113	86% 12%
9	P	100	9% 97%
9	Q	100	11% 99%
9	R	100	8% 80% 15% 5%
9	S	100	14% 97%
9	T	100	6% 100%
9	U	100	11% 89% 8%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 30166 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 Tube initiator protein (gp018).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1519	933	262	317	7		
1	B	201	Total	C	N	O	S	0	0
			1513	930	261	315	7		

- Molecule 2 is a protein called Sheath initiator (gp022).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	126	Total	C	N	O	S	0	0
			995	628	170	194	3		
2	D	126	Total	C	N	O	S	0	0
			995	628	170	194	3		

- Molecule 3 is a protein called Hub protein (gp020).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	305	Total	C	N	O	S	0	0
			2463	1558	421	472	12		

- Molecule 4 is a protein called Tape measure protein (gp017).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	26	Total	C	N	O	S	0	0
			206	127	31	47	1		

- Molecule 5 is a protein called Puncture apparatus (gp021).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	206	Total	C	N	O	S	0	0
			1619	1021	269	319	10		

- Molecule 6 is a protein called Wedge protein 2 (gp023).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	459	Total 3541	C 2234	N 581	O 724	S 2	0	0
6	I	442	Total 3398	C 2140	N 564	O 692	S 2	0	0
6	K	446	Total 3436	C 2162	N 572	O 700	S 2	0	0
6	L	476	Total 3656	C 2304	N 604	O 746	S 2	0	0

- Molecule 7 is a protein called Wedge protein 1 (gp024).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	160	Total 1289	C 821	N 220	O 244	S 4	0	0
7	M	162	Total 1306	C 833	N 222	O 247	S 4	0	0

- Molecule 8 is a protein called Spacer protein (gp019).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	112	Total 919	C 584	N 150	O 180	S 5	0	0
8	O	111	Total 911	C 579	N 149	O 179	S 4	0	0

- Molecule 9 is a protein called LTF platform protein (gp025).

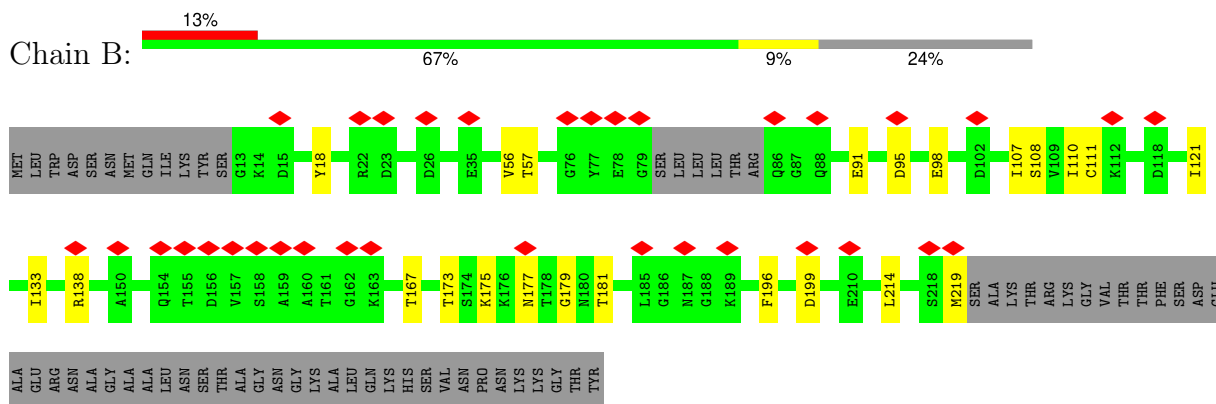| Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	100	Total 400	C 200	N 100	O 100	0	0
9	T	100	Total 400	C 200	N 100	O 100	0	0
9	U	100	Total 400	C 200	N 100	O 100	0	0
9	P	100	Total 400	C 200	N 100	O 100	0	0
9	Q	100	Total 400	C 200	N 100	O 100	0	0
9	R	100	Total 400	C 200	N 100	O 100	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
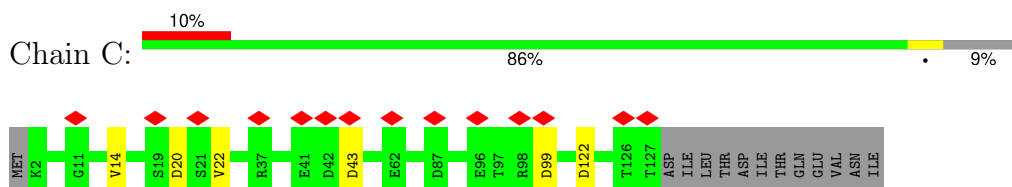
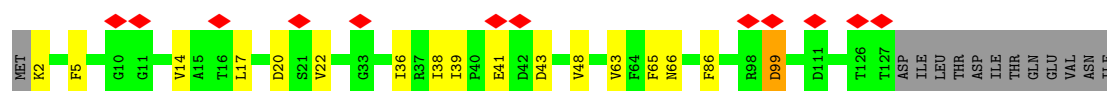- Molecule 1: Tube initiator protein (gp018)
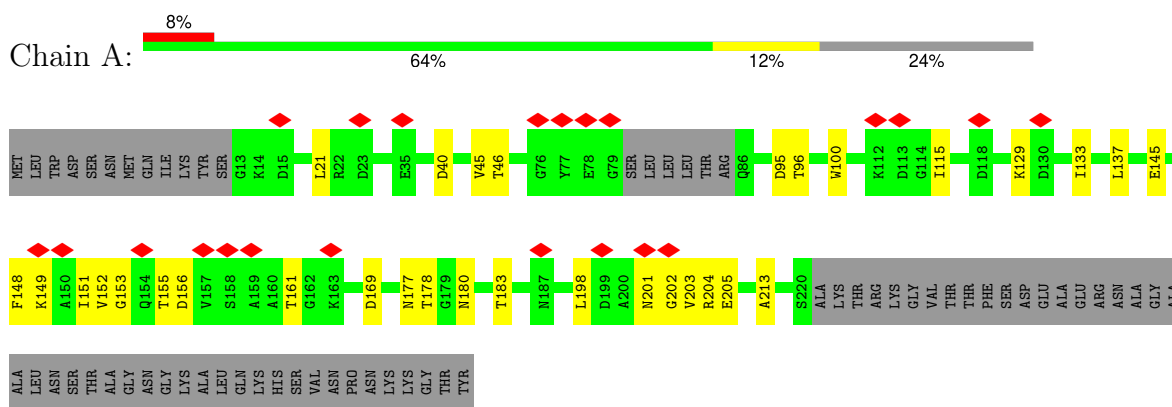
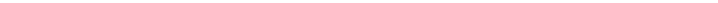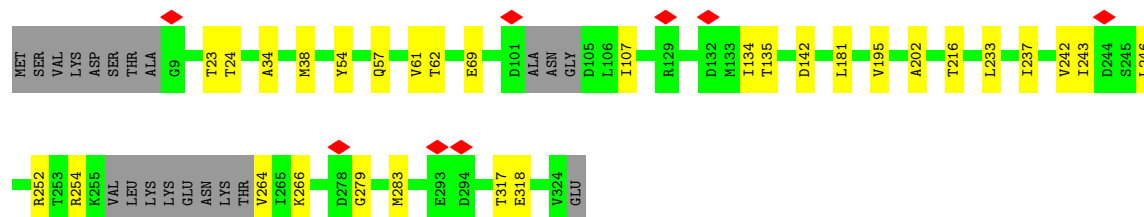- Molecule 1: Tube initiator protein (gp018)
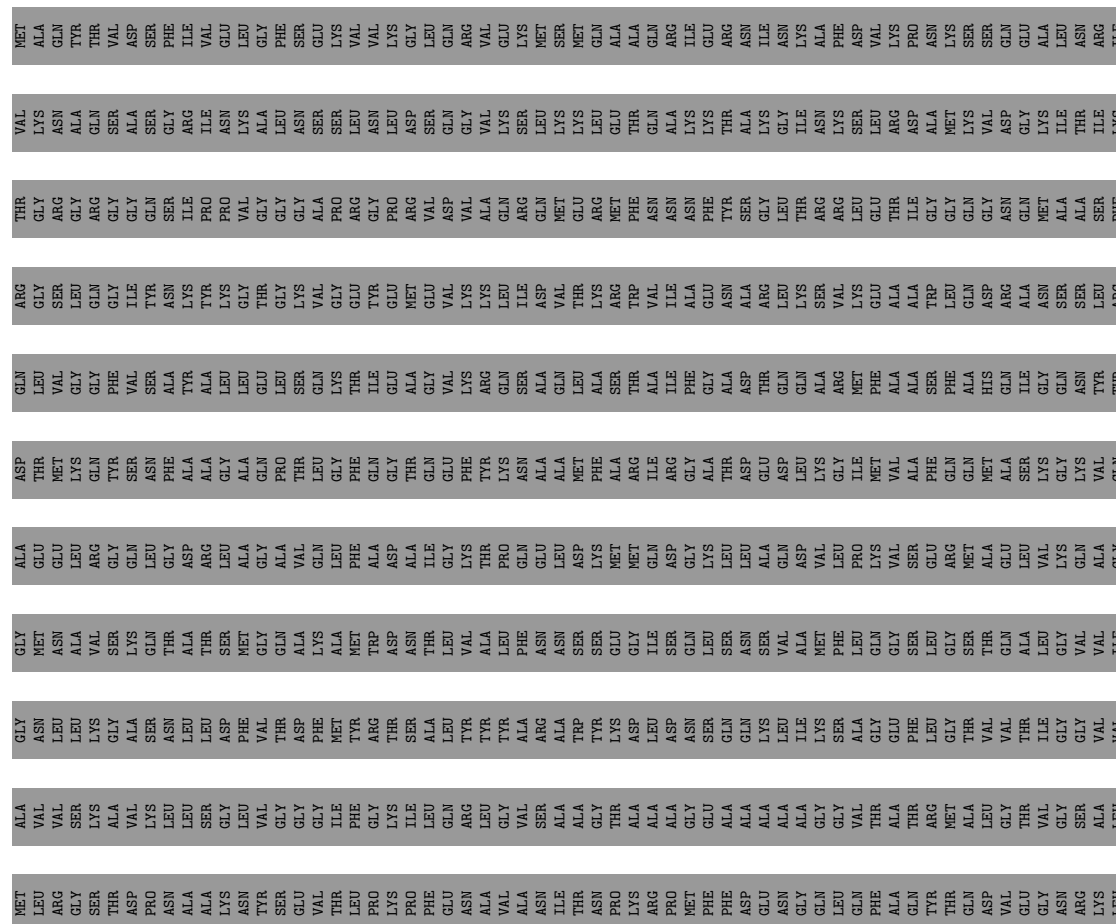

- Molecule 2: Sheath initiator (gp022)

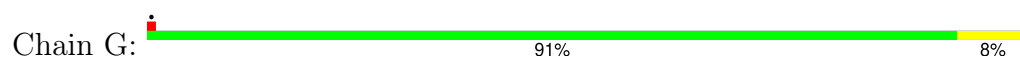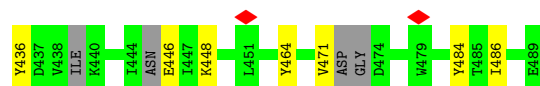- Molecule 2: Sheath initiator (gp022)
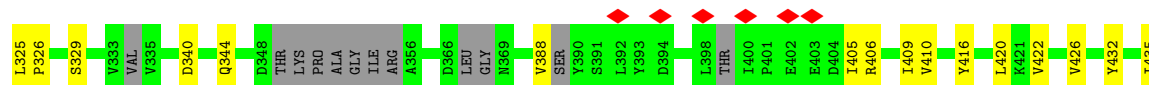
9%

Chain D:

78%   12% • 9%

MET K2 F5 G10 G11 V14 A15 T16 L17 D20 S21 V22 G33 I36 R37 I38 I39 P40 E41 D42 D43 V48 V63 F64 F65 N66 F86 R98 D99 D111 T126 T127 ASP ILE LEU THR ASP ILE THR GLN GLU VAL ASN ILE

• Molecule 3: Hub protein (gp020)

Chain E:

85%   9%   6%

MET SER VAL LYS ASP SER THR ALA G9 T23 T24 A34 M38 Y54 Q57 V61 T62 E69 D101 ALA ASN GLY D105 L106 I107 R129 D132 M133 I134 T135 D142 L181 V195 A202 T216 L233 I237 V242 I243 D244 S245 L246

R252 T253 R254 K255 VAL LEU LYS LYS GLU ASN LYS THR V264 I265 K266 D278 G279 M283 E293 D294 T317 E318 V324 GLU

• Molecule 4: Tape measure protein (gp017)

Chain F: 96%

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

VAL LYS ASN ALA GLN SER ALA SER GLY ARG ILE ASN ALA LYS ALA LEU ASN SER LEU ASN LEU ASP SER GLN GLY VAL LYS SER MET LYS LEU LYS LEU GLU THR GLN ALA LYS LYS GLY ILE ILE ASN LYS SER LEU ARG ASP ALA MET LYS VAL ASP GLY LYS ILE THR ILE LYS

THR GLY ARG GLY ARG GLY GLY GLN SER ILE PRO PRO VAL GLY GLY ALA PRO ARG GLY PRO ARG ASP VAL ALA GLN ARG MET GLY ARG MET PHE ASN ASN PHE TYR SER GLY LEU THR ARG ARG LEU GLY THR ILE GLY LEU GLN GLY ASN MET ALA ALA SER PHE

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

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

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

ALA GLU GLU LEU ARG GLY GLN GLN LEU GLY ASP ARG LEU ALA GLY ALA VAL GLN LEU PHE ALA ASP ALA ILE GLY LYS THR PRO GLN GLU LEU ASP LYS MET LEU ASP GLY LYS LEU LEU ALA GLN ASP VAL GLY SER GLU MET ALA GLU LEU VAL LYS GLN ALA GLY

GLY MET ASN ALA VAL SER LYS GLN THR ALA THR SER MET GLY GLN ALA LYS ALA MET TRP ASP ASN THR LEU VAL ALA LEU PHE ASN ASN SER GLU GLY ILE SER GLU GLN ASN SER VAL ALA ALA MET PHE LEU GLN GLY SER LEU GLY SER THR ALA LEU GLY VAL VAL ILE

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

ALA VAL VAL SER LYS ALA VAL LYS LEU LEU LEU SER GLY LEU VAL GLY GLY ILE PHE GLY ILE ILE LEU GLN ARG LEU VAL SER ALA ALA GLY ALA ALA GLY GLU ALA ALA ALA ALA GLY VAL THR THR THR ARG MET ALA LEU GLY THR VAL GLY SER ALA LEU

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

ILE ASP ASN GLY LEU SER ASN TRP GLU ILE ILE MET ASP LYS LEU SER THR SER ILE ASP ASN PHE ALA ASN LYS PHE ASN GLN THR PRO MET MET THR PRO SER GLY LEU PRO MET GLN THR LYS GLN THR LEU ASN VAL THR PHE ASN LEU ASP GLY LYS Q716 M721 D726

K727 N728 Q729 E730 D731 I732 S737 Y738 P739 E740 E741 GLU

• Molecule 5: Puncture apparatus (gp021)

Chain G: 91%   8%

M1 K2 Y11 E18 E22 A29 I30 I49 N50 V60 K77 T78 D93 E104 C123 L138 T181 G182 V183 A206 GLN

• Molecule 6: Wedge protein 2 (gp023)

Chain H: 79%   15%   6%

MET ALA G3 I29 S30 D34 D38 L52 T55 H56 I62 Y63 D64 T67 F74 N75 L76 D77 D78 I79 T80 V89 A90 Q91 T102 T103 R112 L113 N119 V135 S143 LEU R145 I152 D155 P163 LYS SER SER ASP T168 L172

L176 I180 N181 G182 GLY ILE V185 A188 I191 ASN ASP GLY SER A196 L197 R198 K201 M213 L221 V233 A234 V237 GLY A239 I240 L243 D265 L266 L278 Y282 L283 L286 T293 L294 A299 K302 D309 N315 E323 G324

L325 P326 S329 V333 VAL V335 D340 Q344 D348 THR LYS PRO ALA GLY ILE ARG A356 D366 LEU GLY N369 V388 SER Y390 S391 L392 Y393 D394 L398 THR I400 P401 E402 E403 D404 I405 R406 I409 V410 Y416 L420 K421 V422 V426 Y432 I435

Y436 D437 V438 ILE K440 I444 ASN E446 I447 K448 L451 Y464 V471 ASP GLY D474 W479 Y484 T485 I486 E489

• Molecule 6: Wedge protein 2 (gp023)

Chain I: 5%   76%   15%   10%

MET ALA GLY L4 R13 Y14 Q15 E16 D19 I29 S30 L33 D34 V35 D38 L43 F44 L45 D54 T55 H56 E61 I62 Y63 T67 L76 T80 A81 L82 V89 A90 Q91 A92 E98 I120 F121 L129 S132 V135 GLU A137 V138 L139

E140 V141 N142 SER L144 D147 ALA N149 Y150 V151 I152 I153 I154 S166 ASP T168 I169 G183 I184 V185 E189 D193 G194 V199 M213 V214 V215 T216 A217 L221 T222 F223 T224 K225 I226 I229 E235 E236 V237 G238 A239 I240 T252 R270 N271 L286 A287

VAL T289 G290 L294 R303 V304 Q305 G306 A310 SER GLY V313 S322 E323 G324 L325 P326 F330 K331 ILE V333 V334 V335 N339 D340 N341 G353 ILE R355 D366 LEU GLY N369 L370 A371 H372 N373 V374 Y375 P379 L392 Y393 D394 GLU GLU SER LEU THR ILE P401

- Molecule 6: Wedge protein 2 (gp023)

Chain K:

- Molecule 6: Wedge protein 2 (gp023)

Chain L:

- Molecule 7: Wedge protein 1 (gp024)

Chain J:

N136 N137 V138 T141 D161 VAL THR LEU ASN GLY THR ALA TRP THR PRO VAL GLU VAL ALA ASP SER ALA LEU ALA ILE VAL ASP ASP LYS ASP ASN TRP PHE VAL THR ASP ALA ASN LYS GLY LEU VAL VAL THR ASN ASN THR GLY SER LEU GLU LYS ASN LEU LEU GLY SER LEU

ALA ASP ALA GLY VAL ARG ASP ALA TYR PHE LYS VAL ASP ARG THR ALA ASN SER GLY SER VAL ASP TYR LEU LYS VAL ASN LYS ASN LYS TYR ASN ALA THR ASP ASN ASN TYR ILE VAL GLY LYS GLU THR VAL ALA GLY ASP TYR GLY VAL MET ALA GLU VAL ALA GLN ILE ILE LYS GLY

ARG LYS ASP LYS GLN GLN GLU GLY SER SER

- Molecule 7: Wedge protein 1 (gp024)

Chain M:

46%   9%   43%

MET F2 Q3 D6 E15 V18 K22 D23 L41 H49 T50 E51 R55 I69 K70 V71 Y82 R83 A84 M85 L86 Y87 I88 Q89 I90 F91 L92 D96 T97 T98 P99 T100 Q103 M107 Y110 N111 ALA T113 Q116 I117 I121 V132 V138

I139 D140 T144 T151 R160 D161 V162 T163 L164 ASN GLY THR ALA TRP THR PRO VAL GLU VAL ALA ASP SER ALA LEU ALA ILE VAL ASP ASP LYS ASP ASN TRP PHE VAL THR ASP ALA ASN LYS GLY LEU VAL VAL THR ASN ASN THR GLY SER LEU GLU LYS ASN LEU LEU GLY

SER LEU ALA ASP ALA GLY VAL ARG ASP ALA TYR PHE LYS VAL ASP ARG THR ALA ASN SER GLY SER VAL ASP TYR LEU LYS VAL ASN LYS ASN LYS TYR ASN ALA THR ASP ASN ASN TYR ILE VAL GLY LYS GLU THR VAL ALA GLY ASP TYR GLY VAL MET ALA GLU VAL ALA GLN ILE ILE

LYS GLY ARG ASP LYS ASP LYS SER GLN GLN GLU GLY SER SER

- Molecule 8: Spacer protein (gp019)

Chain N:

88%   12%

M1 Y4 D9 T14 Q15 L34 G46 N47 V48 L56 V76 M79 D83 E98 L99 T103 Q104 E105 D106 M110 E111 N112 LEU

- Molecule 8: Spacer protein (gp019)

Chain O:

86%   12%

MET S2 Q3 W12 V17 G21 E32 R33 L34 D35 D45 L50 L56 I61 V76 E77 R78 M79 D83 N100 N112 LEU

- Molecule 9: LTF platform protein (gp025)

Chain S:

14%   97%

M1 A2 I26 L32 R33 G55 T56 V57 T82 G83 T84 A85 S86 T87 S88 V98 G99 A100

- Molecule 9: LTF platform protein (gp025)

Chain T:

6%

100%

M1 D14 S86 T87 S88 A100

• Molecule 9: LTF platform protein (gp025)

Chain U:

11%

89%   8%

M1 A13 D14 L18 G34 G38 R39 Q40 W41 F42 N43 Y44 I45 L46 N47 T56 N76 L77 G83 S86 T87 G99 A100

• Molecule 9: LTF platform protein (gp025)

Chain P:

9%

97%

M1 A2 A13 I26 L32 R33 G83 T84 A85 S86 T87 G99 A100

• Molecule 9: LTF platform protein (gp025)

Chain Q:

11%

99%

M1 A2 F3 A13 D14 E35 T56 V57 G83 S86 T87 S88 A100

• Molecule 9: LTF platform protein (gp025)

Chain R:

8%

80%   15%   5%

M1 A13 N16 K19 V20 L21 P22 P23 P24 P36 M37 G38 R39 Q40 W41 F42 N43 Y44 I45 L46 N47 E66 N76 L77 G83 S86 T87 S88 A100

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	49.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.048	Depositor
Minimum map value	-8.973	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.044	Depositor
Recommended contour level	4.78	Depositor
Map size (Å)	554.8, 554.8, 554.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.387, 1.387, 1.387	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| >5$	RMSZ	$\#|Z| >5$
1	A	0.13	0/1532	0.36	0/2069
1	B	0.12	0/1526	0.30	0/2061
2	C	0.12	0/1012	0.32	0/1369
2	D	0.12	0/1012	0.31	0/1369
3	E	0.11	0/2507	0.29	0/3378
4	F	0.19	0/207	0.47	0/279
5	G	0.12	0/1661	0.29	0/2260
6	H	0.10	0/3586	0.27	0/4877
6	I	0.12	0/3441	0.30	1/4676 (0.0%)
6	K	0.11	0/3474	0.29	0/4708
6	L	0.11	0/3709	0.28	0/5051
7	J	0.13	0/1310	0.35	0/1779
7	M	0.15	0/1326	0.36	0/1800
8	N	0.14	0/937	0.31	0/1269
8	O	0.13	0/929	0.31	0/1259
9	P	0.21	0/399	0.57	0/497
9	Q	0.23	0/399	0.54	0/497
9	R	0.62	0/399	0.97	1/497 (0.2%)
9	S	0.20	0/399	0.56	0/497
9	T	0.23	0/399	0.54	0/497
9	U	0.49	0/399	0.93	3/497 (0.6%)
All	All	0.15	0/30563	0.35	5/41186 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	36	PRO	N-CA-C	6.92	126.72	112.47
6	I	185	VAL	N-CA-C	-6.29	106.80	111.90
9	U	44	TYR	N-CA-C	-6.00	104.75	111.28
9	U	43	ASN	N-CA-C	-5.25	105.46	111.07
9	U	39	ARG	N-CA-C	-5.12	106.72	112.87

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	A	1519	0	1500	25	0
1	B	1513	0	1495	16	0
2	C	995	0	980	4	0
2	D	995	0	980	13	0
3	E	2463	0	2441	26	0
4	F	206	0	200	23	0
5	G	1619	0	1540	23	0
6	H	3541	0	3479	50	0
6	I	3398	0	3340	61	0
6	K	3436	0	3373	39	0
6	L	3656	0	3616	69	0
7	J	1289	0	1310	27	0
7	M	1306	0	1331	33	0
8	N	919	0	900	10	0
8	O	911	0	888	16	0
9	P	400	0	115	1	0
9	Q	400	0	115	3	0
9	R	400	0	115	14	0
9	S	400	0	115	1	0
9	T	400	0	115	0	0
9	U	400	0	115	7	0
All	All	30166	0	28063	405	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 7.

The worst 5 of 405 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)
7:J:118:PHE:CE2	9:Q:35:GLU:CA	1.85	1.41
7:J:118:PHE:HE2	9:Q:35:GLU:CA	1.28	1.32

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PROTEIN DATA BANK

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:738:TYR:CD2	5:G:18:GLU:OE1	1.83	1.29
4:F:738:TYR:CG	5:G:18:GLU:OE1	1.84	1.28
9:R:19:LYS:CA	9:R:40:GLN:CA	2.25	1.14

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/265 (75%)	175 (88%)	21 (11%)	2 (1%)	13	46
1	B	197/265 (74%)	186 (94%)	11 (6%)	0	100	100
2	C	124/139 (89%)	119 (96%)	5 (4%)	0	100	100
2	D	124/139 (89%)	116 (94%)	8 (6%)	0	100	100
3	E	299/325 (92%)	287 (96%)	12 (4%)	0	100	100
4	F	24/742 (3%)	24 (100%)	0	0	100	100
5	G	204/207 (99%)	189 (93%)	15 (7%)	0	100	100
6	H	431/489 (88%)	407 (94%)	24 (6%)	0	100	100
6	I	414/489 (85%)	383 (92%)	30 (7%)	1 (0%)	44	75
6	K	409/489 (84%)	382 (93%)	26 (6%)	1 (0%)	44	75
6	L	462/489 (94%)	426 (92%)	34 (7%)	2 (0%)	30	65
7	J	158/285 (55%)	139 (88%)	16 (10%)	3 (2%)	6	35
7	M	158/285 (55%)	147 (93%)	9 (6%)	2 (1%)	10	41
8	N	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
8	O	109/113 (96%)	102 (94%)	7 (6%)	0	100	100
9	P	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	13	46
9	Q	98/100 (98%)	90 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	R	98/100 (98%)	80 (82%)	11 (11%)	7 (7%)	1	14
9	S	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	13	46
9	T	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
9	U	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	13	46
All	All	4009/5434 (74%)	3703 (92%)	285 (7%)	21 (0%)	27	60

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	I	14	TYR
7	J	5	ILE
9	S	26	ILE
9	P	26	ILE
9	R	36	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/222 (77%)	171 (100%)	0	100	100
1	B	170/222 (77%)	169 (99%)	1 (1%)	84	88
2	C	109/122 (89%)	108 (99%)	1 (1%)	75	83
2	D	109/122 (89%)	106 (97%)	3 (3%)	38	60
3	E	271/288 (94%)	268 (99%)	3 (1%)	70	79
4	F	25/590 (4%)	25 (100%)	0	100	100
5	G	183/184 (100%)	181 (99%)	2 (1%)	70	79
6	H	389/411 (95%)	388 (100%)	1 (0%)	91	92
6	I	373/411 (91%)	368 (99%)	5 (1%)	65	76
6	K	376/411 (92%)	372 (99%)	4 (1%)	70	79
6	L	402/411 (98%)	399 (99%)	3 (1%)	81	86
7	J	143/242 (59%)	141 (99%)	2 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	M	146/242 (60%)	144 (99%)	2 (1%)	62	75
8	N	103/104 (99%)	103 (100%)	0	100	100
8	O	102/104 (98%)	102 (100%)	0	100	100
All	All	3072/4086 (75%)	3045 (99%)	27 (1%)	74	83

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	189	GLU
7	J	92	LEU
6	L	416	TYR
7	J	37	GLU
6	K	29	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	429	ASN
6	I	453	ASN
8	N	85	GLN
6	L	56	HIS
8	N	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-49281. 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 ⓘ

6.1.1   Primary map

| X | Y | Z |
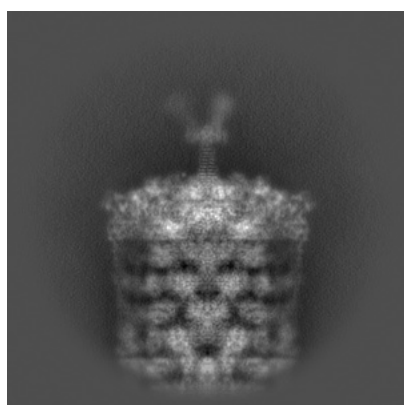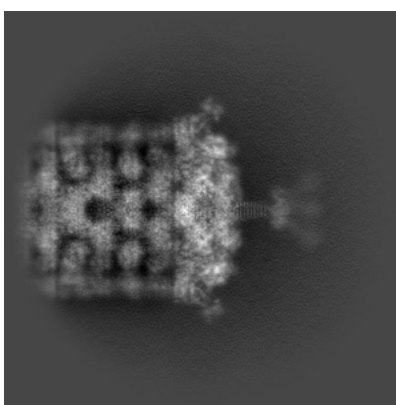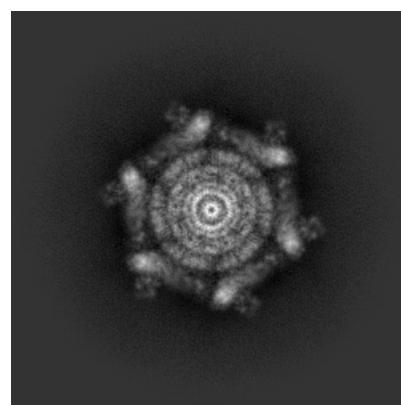
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
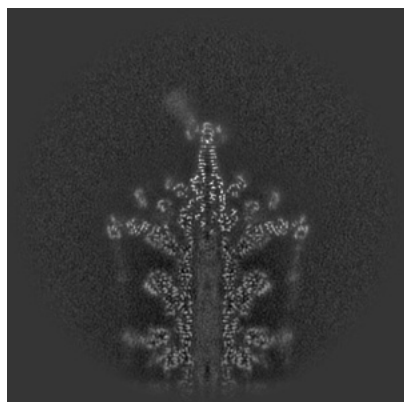
6.2.1   Primary map
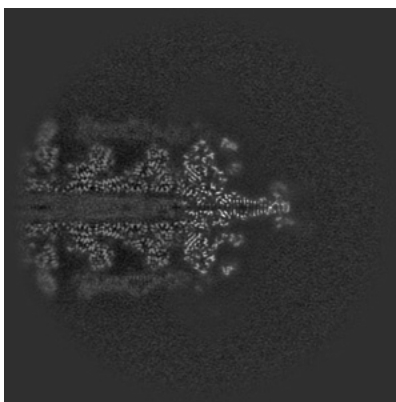
| X Index: 200 | Y Index: 200 | Z Index: 200 |
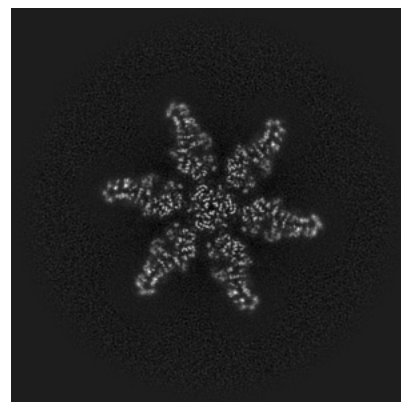
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
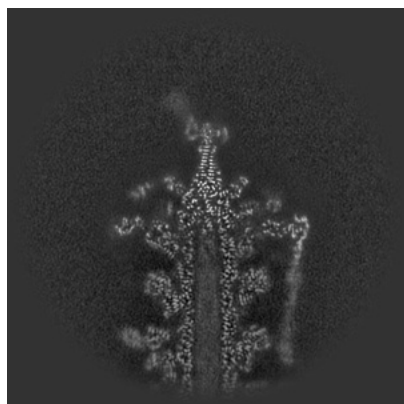
6.3.1   Primary map
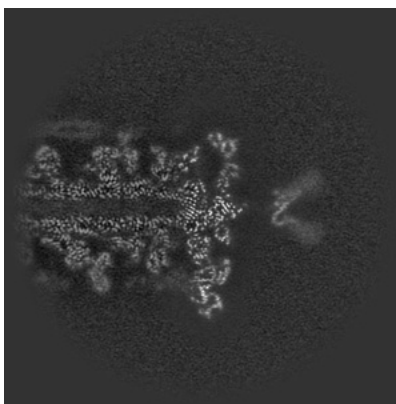
| X Index: 196 | Y Index: 212 | Z Index: 201 |
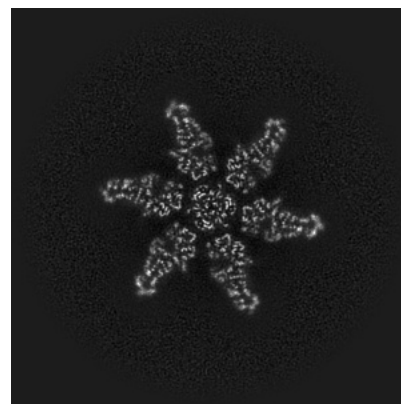
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1   Primary map

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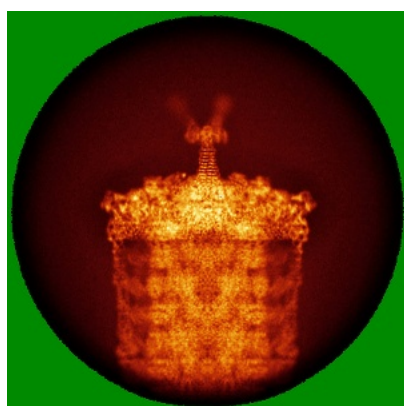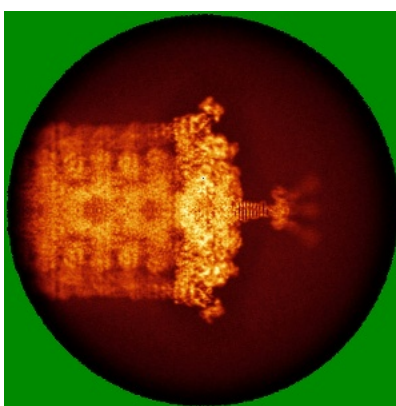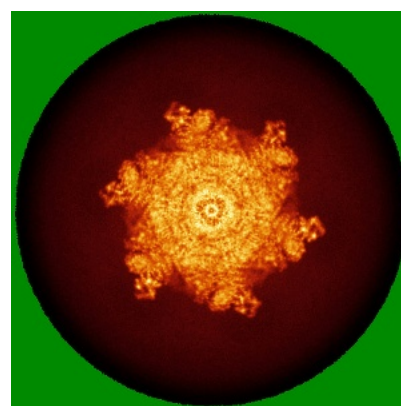
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views (i)

6.5.1   Primary map

X   Y   Z
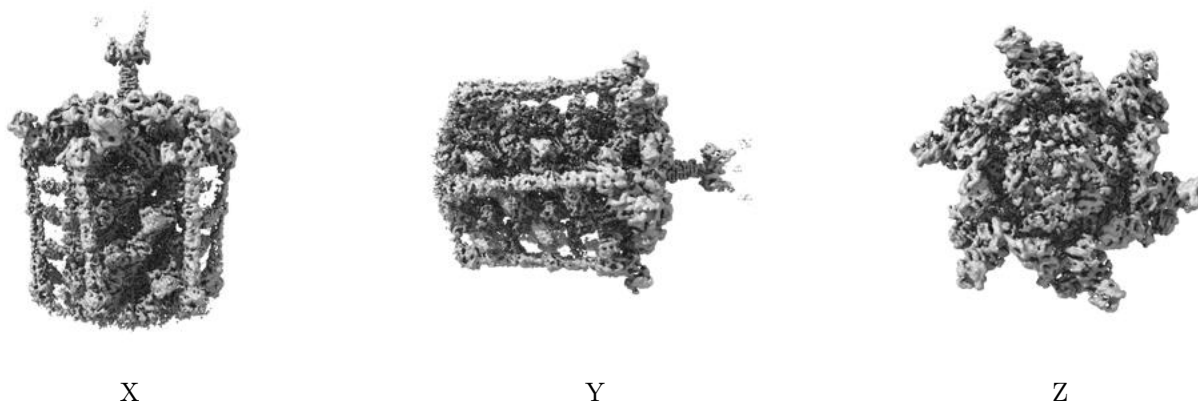
The images above show the 3D surface view of the map at the recommended contour level 4.78. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6   Mask visualisation (i)

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

7 Map analysis ⓘ

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

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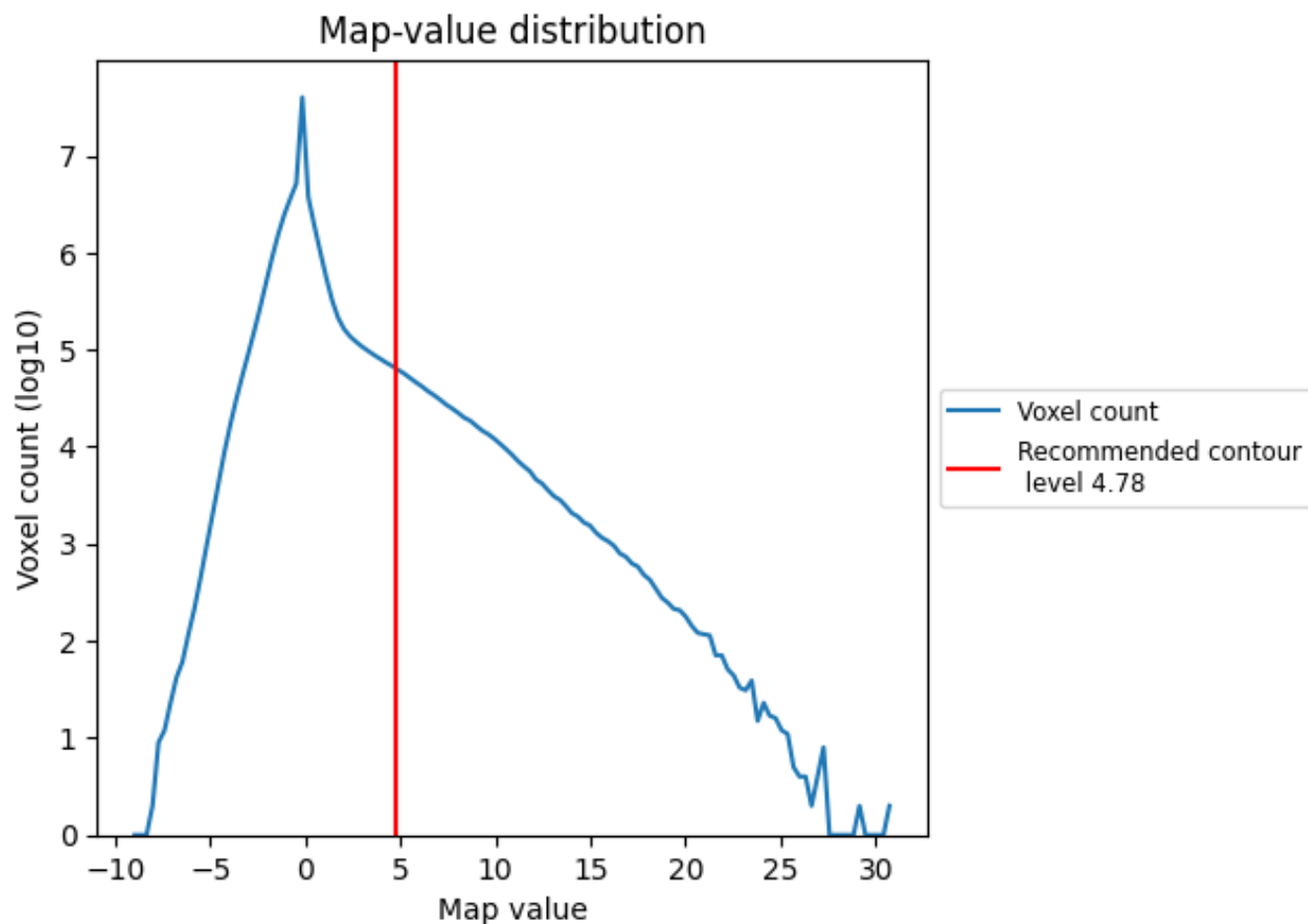
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
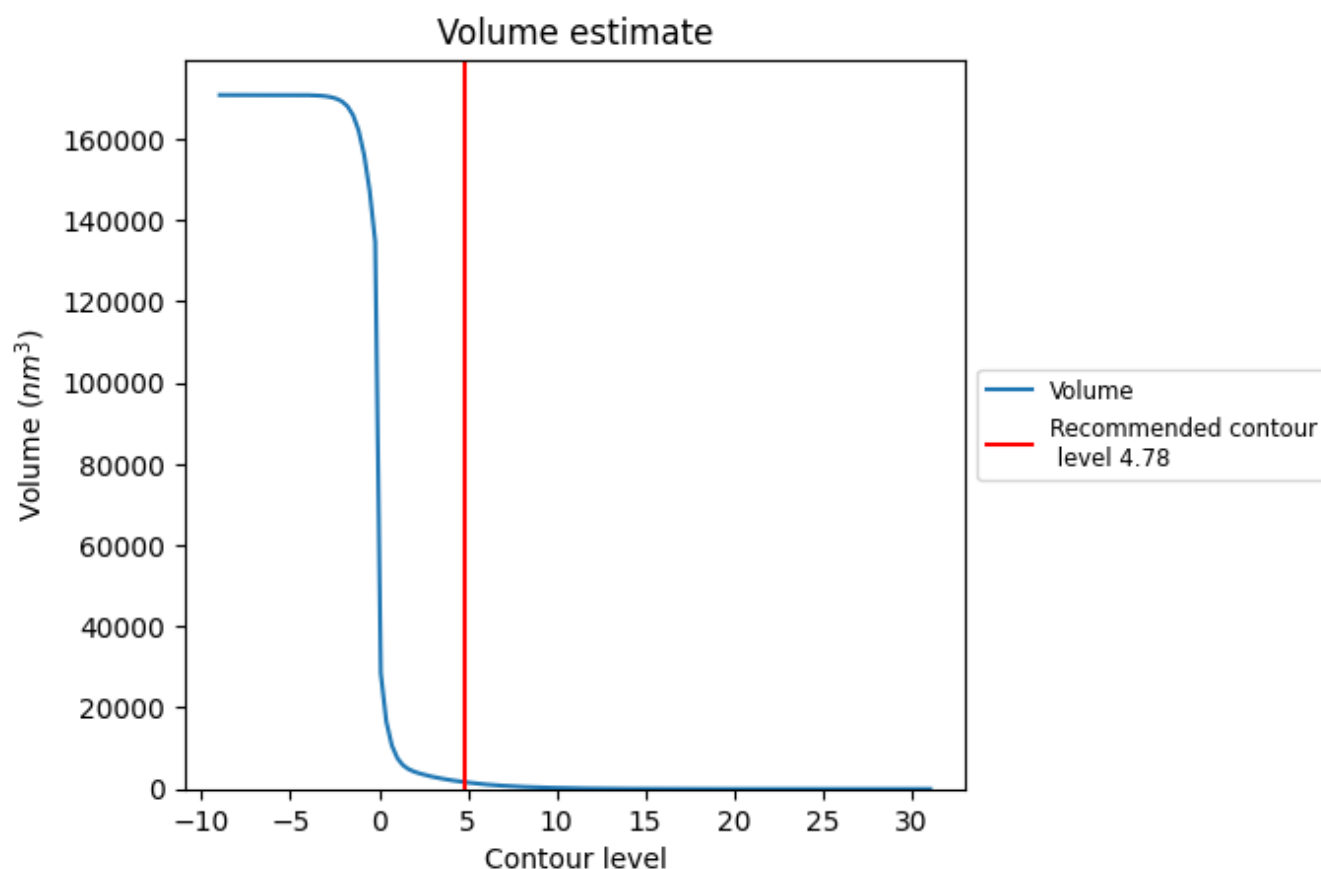
The volume at the recommended contour level is 1704 nm^3; this corresponds to an approximate mass of 1539 kDa.

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 ⓘ

Rotationally averaged power spectrum
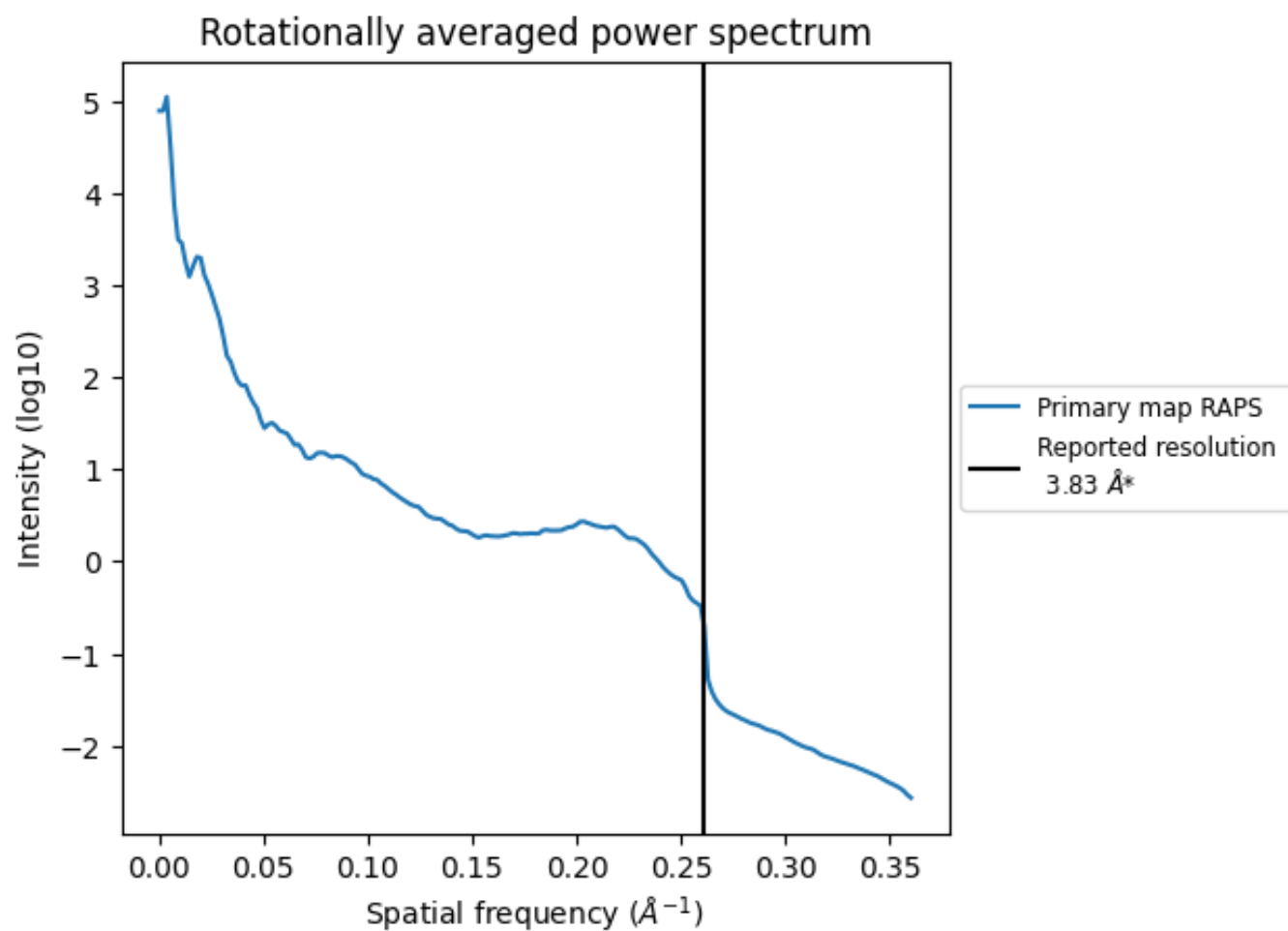
*Reported resolution corresponds to spatial frequency of 0.261 Å^{-1}

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-49281 and PDB model 9NDY. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlays

9.1.1   Map-model overlay (i)

| X | Y | Z |
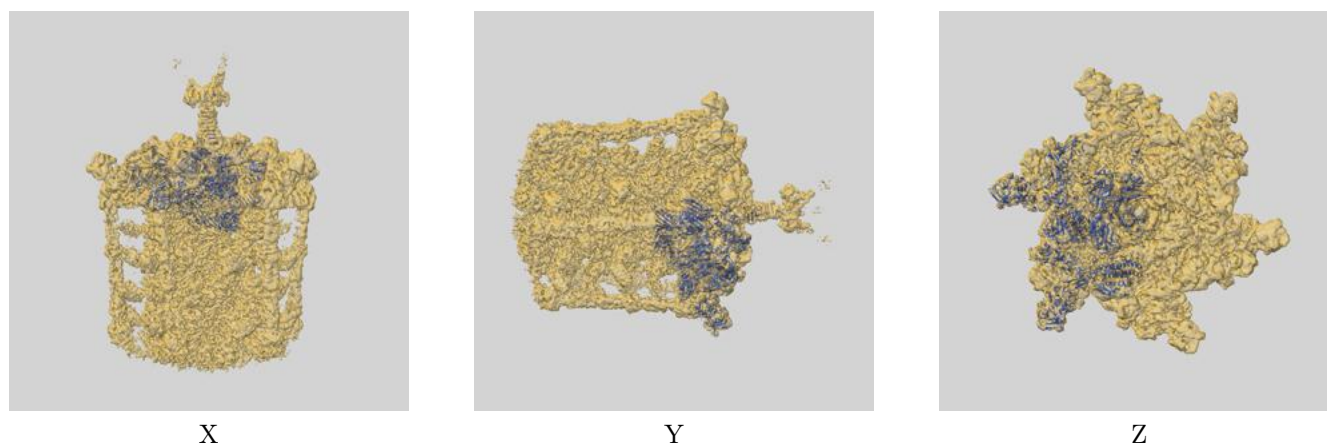
9.1.2   Map-model assembly overlay (i)

| X | Y | Z |
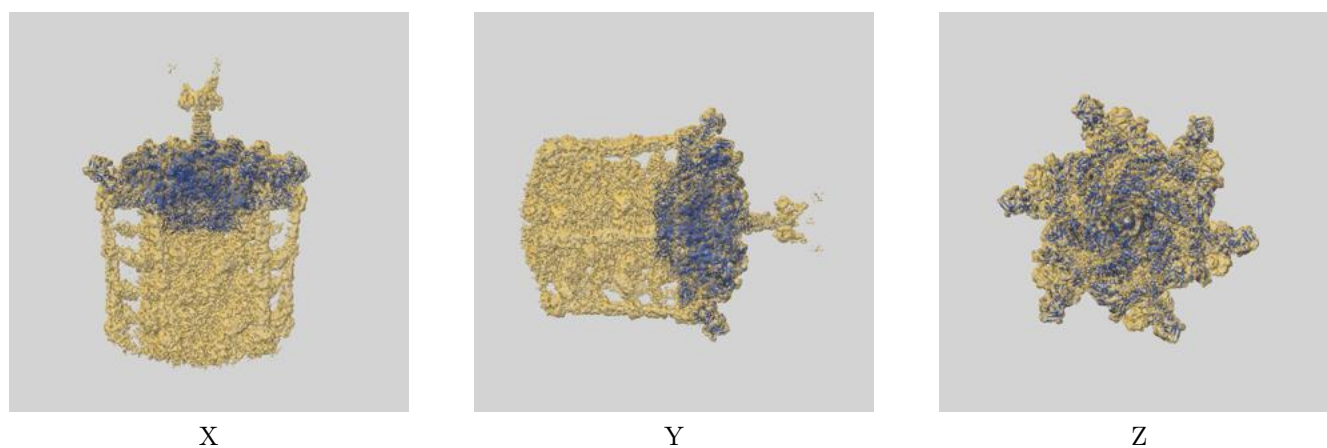
The images above show the 3D surface view of the map at the recommended contour level 4.78 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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 (4.78).

9.4   Atom inclusion ⓘ
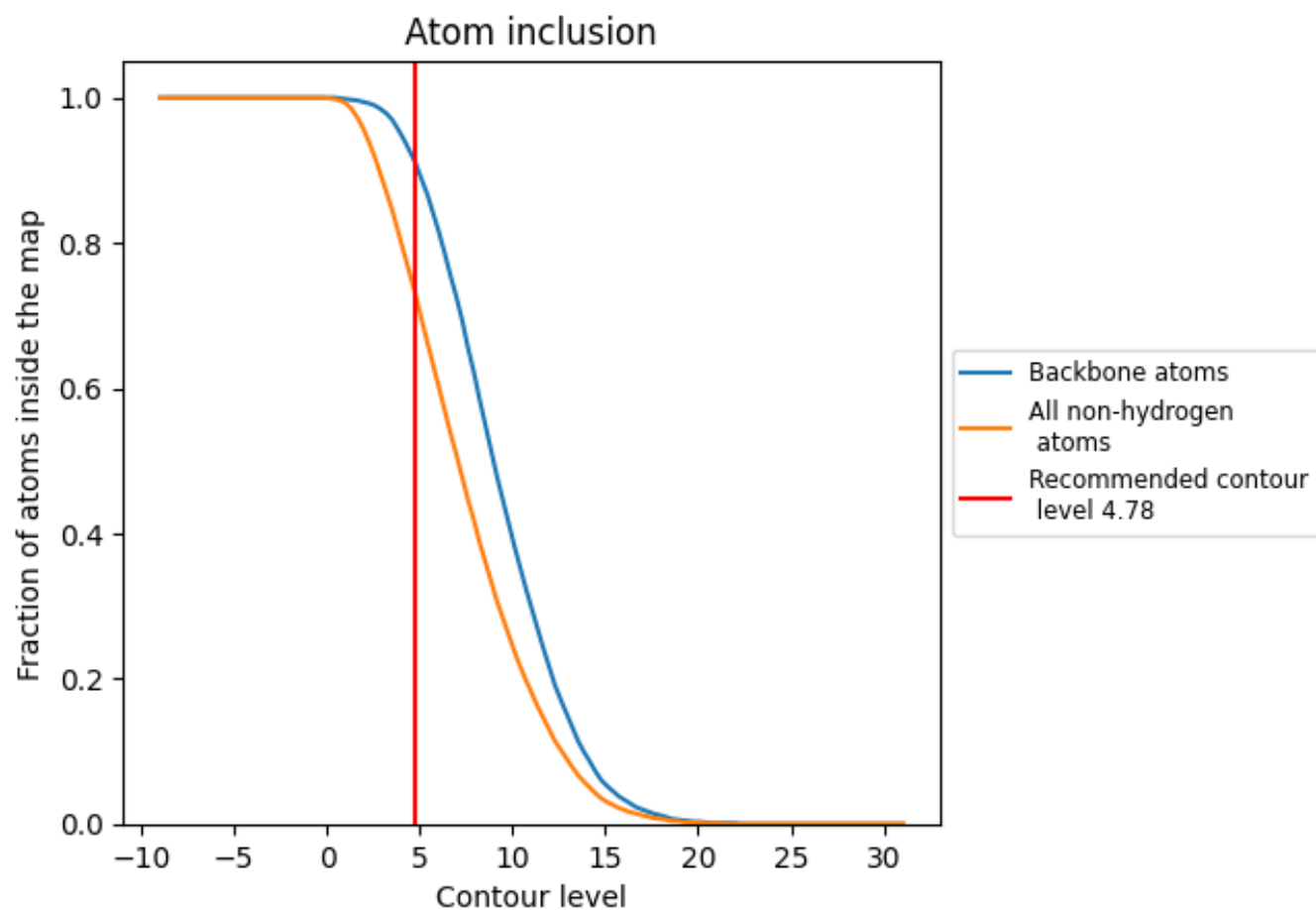
At the recommended contour level, 91% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.78) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.3750
A	0.5960	0.4410
B	0.5700	0.4400
C	0.6380	0.4510
D	0.6490	0.4550
E	0.7400	0.4690
F	0.6200	0.3940
G	0.8310	0.4350
H	0.7520	0.3280
I	0.7340	0.3380
J	0.6810	0.3400
K	0.7420	0.3290
L	0.7370	0.3430
M	0.6980	0.3770
N	0.7460	0.4440
O	0.7560	0.4450
P	0.8680	0.2610
Q	0.8400	0.2560
R	0.9000	0.2760
S	0.8000	0.3190
T	0.9000	0.3380
U	0.8480	0.3000

1.0

0.0
<0.0