Full wwPDB EM Validation Report (i)

May 11, 2024 – 03:10 pm BST

PDB ID	:	6RAO
EMDB ID	:	EMD-4782
Title	:	Cryo-EM structure of the anti-feeding prophage (AFP) baseplate, 6-fold symmetrised
Authors	:	Desfosses, A.
Deposited on	:	2019-04-06
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

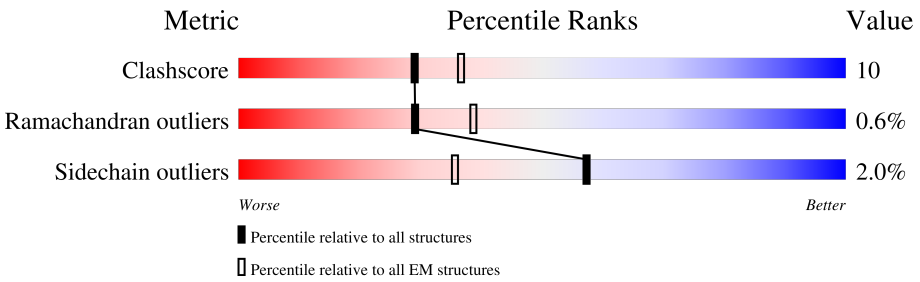
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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 <=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	149	9% 89% 10% •
1	B	149	• 85% 14% •
2	C	354	9% 85% 14% ••
3	D	451	10% 71% 8% 21%
4	F	149	• 84% 15% •
5	H	140	15% 64% 22% • 11%
6	E	417	15% 72% 20% • 7%
7	G	229	10% 79% 17% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	607	51% 59% 13% • 27%
9	J	963	31% 41% 15% • 43%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 22409 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 Afp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	148	1148	729	187	228	4	0	0
1	B	148	1148	729	187	228	4	0	0

- Molecule 2 is a protein called Afp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	351	2718	1740	450	522	6	0	0

- Molecule 3 is a protein called Afp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	358	2747	1753	462	525	7	0	0

- Molecule 4 is a protein called Afp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	149	1196	757	218	215	6	0	0

- Molecule 5 is a protein called Afp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	125	994	628	177	184	5	0	0

- Molecule 6 is a protein called Afp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	386	3005	1920	512	561	12	0	0

- Molecule 7 is a protein called Afp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	224	1737	1096	292	343	6	0	0

- Molecule 8 is a protein called Afp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	443	3441	2189	592	648	12	0	0

- Molecule 9 is a protein called Afp12.

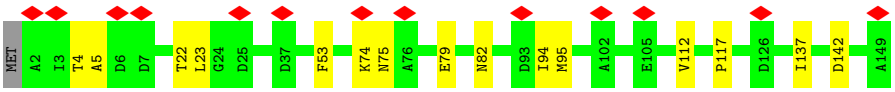
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	548	4275	2711	737	819	8	0	0

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.

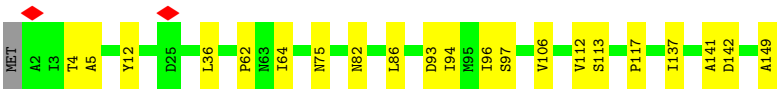
• Molecule 1: Afp1

Chain A:



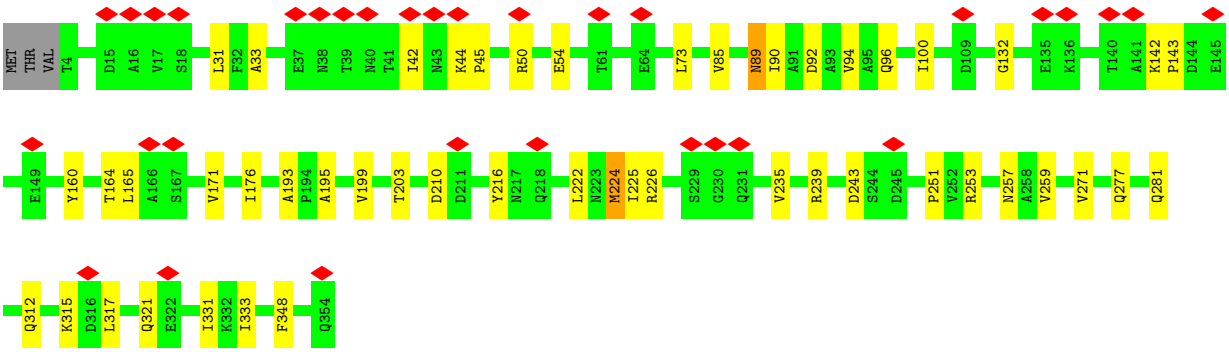
• Molecule 1: Afp1

Chain B:



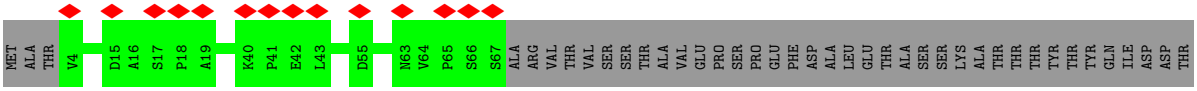
• Molecule 2: Afp2

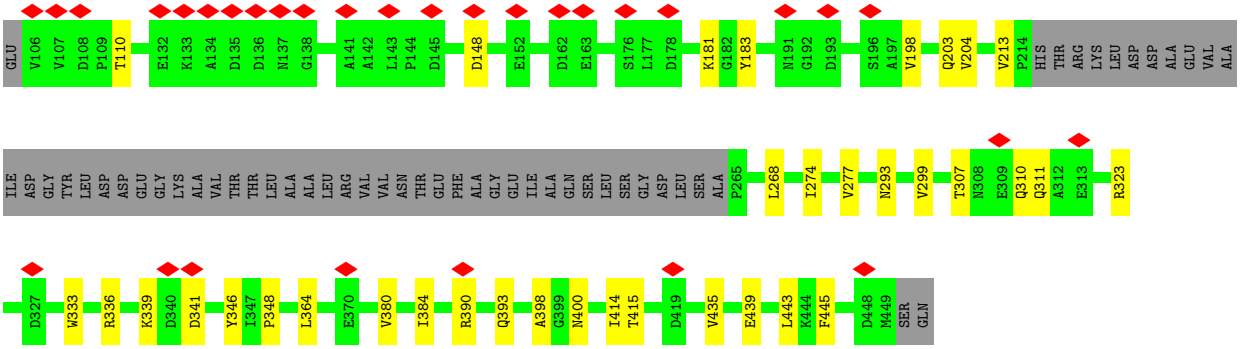
Chain C:



• Molecule 3: Afp3

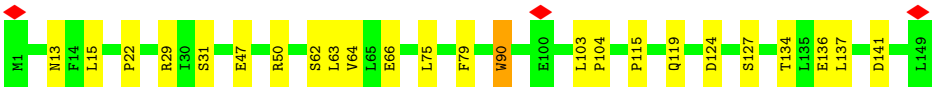
Chain D:





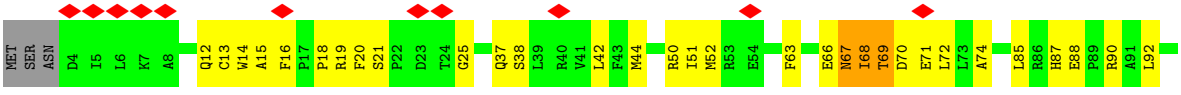
- Molecule 4: Afp5

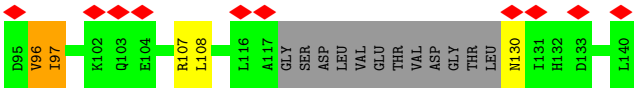
Chain F:



- Molecule 5: Afp9

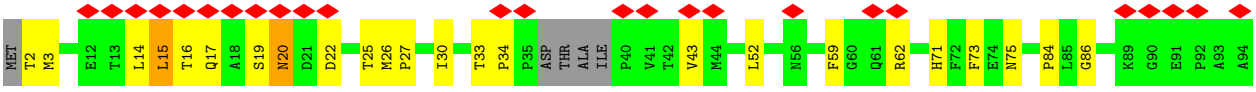
Chain H:

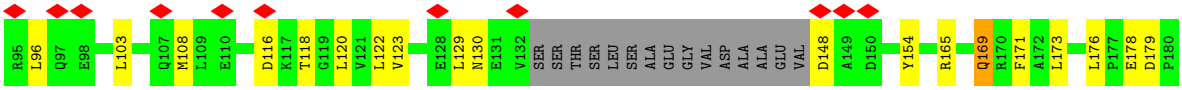


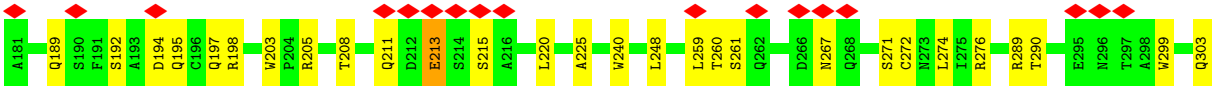


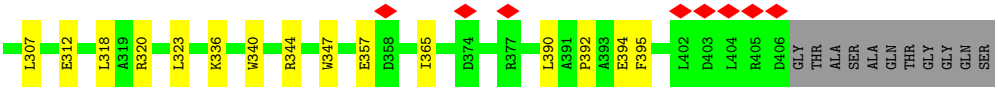
- Molecule 6: Afp4

Chain E:



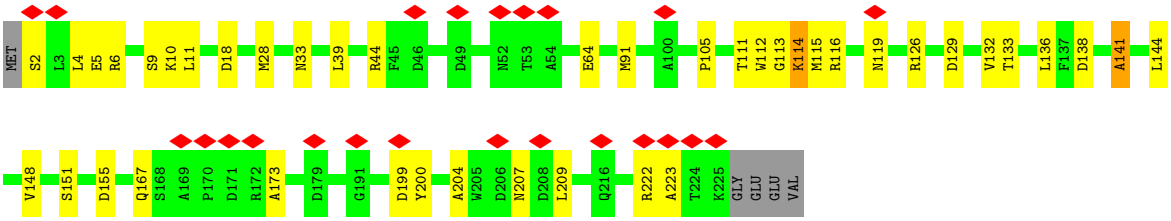






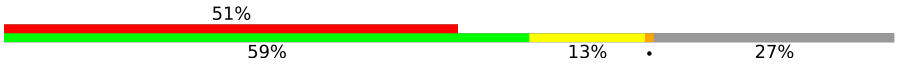
- Molecule 7: Afp7

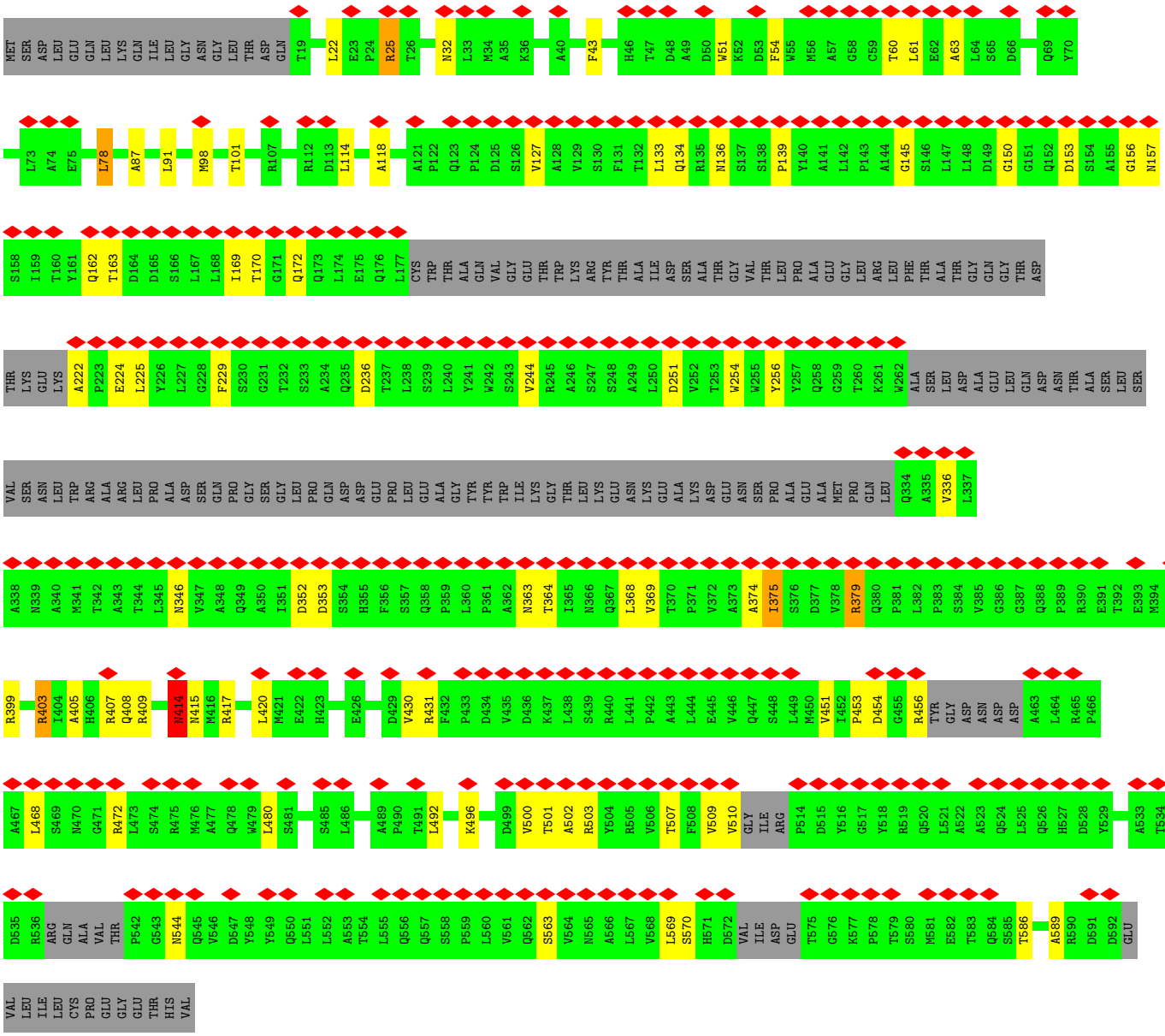
Chain G:



- Molecule 8: Afp11

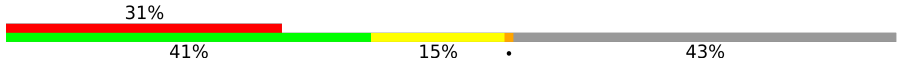
Chain I:

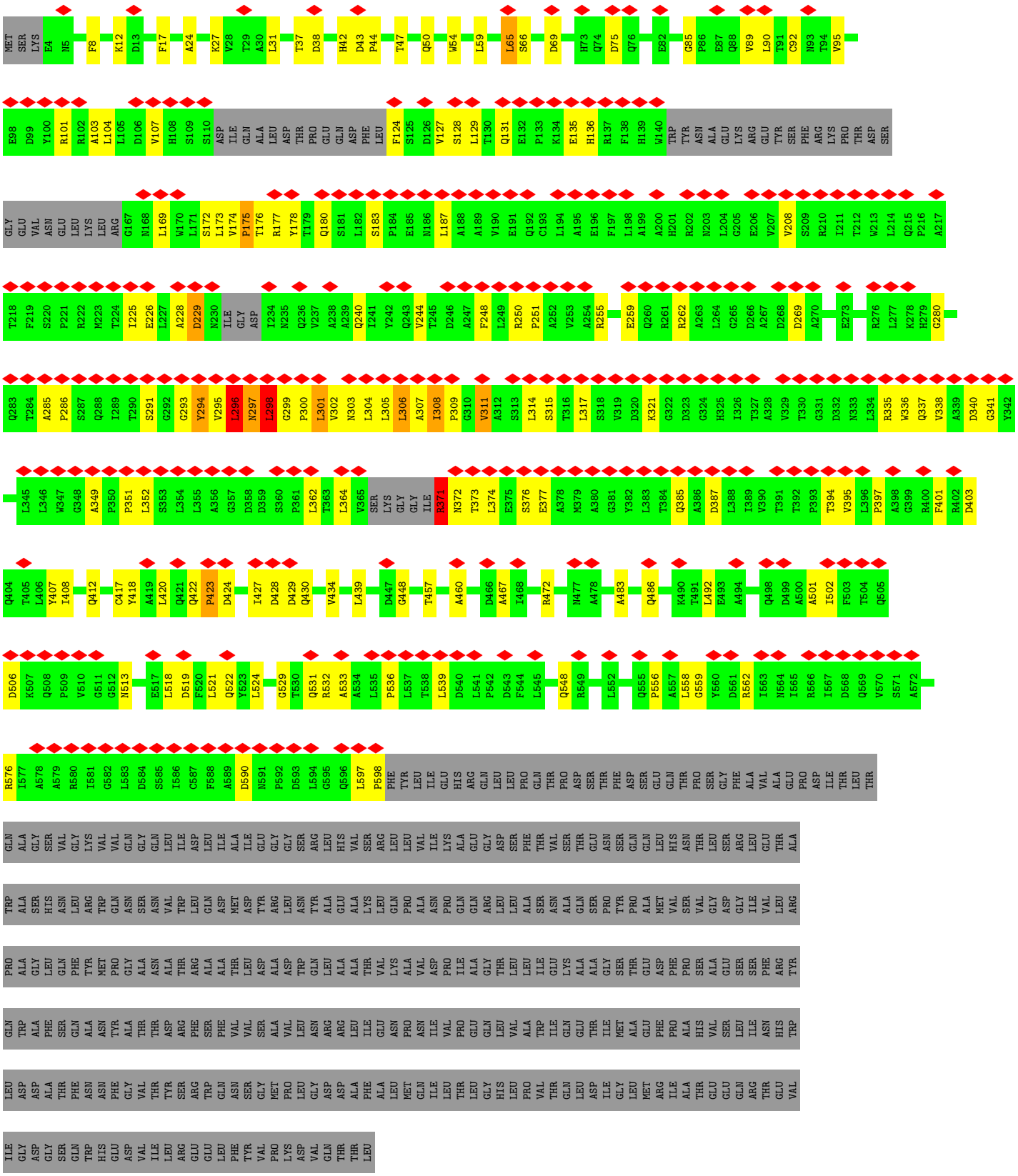




- Molecule 9: Afp12

Chain J:


31%
41%
15%
43%


MET SER LYS E4 N5 F8 K12 D13 F17 A24 K27 V28 T29 A30 L31 T37 D38 H42 D43 P44 T47 Q50 W54 L59 L65 S66 D69 H73 Q74 D75 Q76 E82 G85 P86 E87 Q88 V89 L90 T91 C92 N93 T94 V95
E98 D99 Y100 R101 R102 A103 L104 L105 D106 V107 H108 S109 S110 ASP ILE GLN ALA LEU ASP THR PRO GLU GLN ASP PHE LEU F124 S125 D126 V127 S128 L129 T130 Q131 E132 P133 K134 E135 H136 R137 F138 H139 W140 TRP TYR ASN ALA GLU LYS ARG GLU TYR SER PHE ARG LYS PRO THR ASP SER
GLY GLU VAL ASN GLU LEU LYS LEU ARG G167 N168 L169 W170 L171 S172 L173 V174 P175 T176 R177 Y178 T179 Q180 S181 L182 S183 P184 E185 N186 L187 A188 A189 V190 E191 Q192 C193 L194 A195 E196 F197 L198 A199 A200 H201 R202 N203 L204 G205 E206 V207 V208 S209 R210 I211 T212 W213 L214 Q215 P216 A217
T218 F219 S220 P221 R222 M223 T224 I225 E226 L227 A228 D229 N230 ILE GLY ASP I234 N235 Q236 V237 A238 A239 Q240 I241 Y242 Q243 V244 T245 D246 A247 F248 F249 R250 P251 A252 V253 A254 R255 E259 Q260 R261 R262 A263 L264 G265 D266 A267 D268 D269 A270 E273 R276 L277 K278 H279 G280
Q283 T284 A285 P286 S287 Q288 I289 T290 S291 G292 G293 Y294 V295 L296 N297 L298 G299 P300 L301 V302 N303 L304 L305 L306 A307 I308 P309 G310 V311 A312 S313 L314 S315 T316 L317 S318 V319 D320 K321 G322 D323 G324 H325 I326 T327 A328 V329 T330 G331 D332 N333 L334 R335 W336 Q337 V338 A339 D340 G341 Y342
L345 L346 W347 G348 A349 P350 P351 L352 S353 L354 L355 A356 G357 D358 D359 S360 P361 L362 T363 L364 V365 SER LYS GLY GLY ILE R371 N372 T373 L374 E375 S376 E377 A378 M379 A380 G381 Y382 L383 T384 Q385 A386 D387 L388 I389 V390 T391 T392 P393 T394 V395 L396 P397 A398 G399 R400 F401 R402 D403
Q404 T405 L406 Y407 I408 Q412 C417 Y418 A419 L420 Q421 Q422 P423 D424 I427 D428 D429 Q430 V434 L439 D447 G448 T457 A460 D466 A467 I468 R472 N477 A478 A483 Q486 K490 T491 L492 E493 A494 Q498 D499 A500 A501 I502 F503 T504 Q505
D506 K507 Q508 P509 V510 G511 G512 N513 E517 L518 D519 F520 L521 Q522 Y523 L524 G529 T530 Q531 R532 A533 A534 L535 P536 L537 T538 L539 D540 L541 P542 D543 F544 L545 Q548 R549 L552 Q555 P556 A557 L558 G559 Y560 D561 R562 I563 N564 I565 R566 I567 D568 Q569 V570 S571 A572
R576 I577 A578 A579 R580 I581 G582 L583 D584 S585 I586 C587 F588 A589 D590 N591 P592 D593 L594 G595 Q596 L597 P598 PHE TYR LEU VAL ILE GLU HIS ARG GLN LEU LEU PRO GLN THR PRO ASP SER THR PHE ASP SER GLU GLN THR PRO SER GLY PHE ALA VAL ALA GLU PRO ASP ILE THR LEU THR
GLN ALA GLY SER VAL GLY LYS VAL VAL GLN GLY GLN LEU ILE ASP LEU ILE ALA ILE GLU GLY GLY SER ARG LEU HIS VAL SER ARG LEU LEU VAL ILE LYS ALA GLU GLY ASP SER PHE THR VAL SER THR GLU ASN SER GLN GLN LEU HIS ASN THR LEU SER GLY PHE ALA VAL ALA GLU PRO ASP
TRP ALA SER HIS ASN LEU ARG TRP GLN ASN SER ASN VAL TRP LEU GLN ASP MET ASP TYR ARG LEU ASN TYR ALA GLU ALA ALA LYS GLN GLN PRO ALA ASN PRO GLN GLN ARG LEU LEU ALA SER ASN ALA GLN SER PRO TYR PRO ALA MET VAL SER VAL GLY ASP GLY ILE VAL LEU ARG
PRO ALA GLY LEU GLN PHE TYR MET PRO GLY ALA ASN ALA THR ARG ALA ALA THR LEU ASP ALA ALA ASP TRP GLN LEU ALA ALA THR LEU LYS ALA VAL ASP PRO ILE ALA GLY THR LEU LEU ILE GLU LYS ALA ALA GLY SER THR GLU ASP PHE PRO SER ALA GLU SER SER PHE ARG TYR
GLN TRP ALA PHE SER GLN ALA ASN TYR ALA THR ASP ARG PHE SER ARG PHE VAL VAL SER ALA VAL LEU ASN ARG ARG LEU ILE GLU ASN PRO ASN ILE VAL PRO GLU GLN LEU VAL ALA TRP ILE GLN GLU THR ILE MET ALA GLU PHE PRO ALA HIS VAL SER LEU ILE ASN HIS TRP
LEU ASP ASP ALA THR PHE ASN ASN PHE GLY VAL THR TYR SER ARG TRP GLN ASN SER GLY MET PRO LEU GLY ASP ASP ALA PHE ALA LEU MET GLN ILE LEU THR LEU GLY HIS LEU PRO VAL THR GLN LEU ASP ILE GLY LEU MET ARG ILE ALA THR GLU GLU GLN ARG THR GLU VAL
ILE GLY ASP GLY SER GLN TRP HIS GLU ASP VAL ILE LEU ARG GLU GLU LEU PHE TYR VAL PRO LYS ASP VAL GLN THR THR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	46991	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 ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.524	Depositor
Minimum map value	-0.368	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.34	0/1172	0.60	1/1601 (0.1%)
1	B	0.42	0/1172	0.65	2/1601 (0.1%)
2	C	0.40	0/2789	0.62	1/3812 (0.0%)
3	D	0.32	0/2809	0.56	0/3833
4	F	0.45	0/1220	0.66	1/1658 (0.1%)
5	H	0.36	0/1011	0.69	0/1366
6	E	0.38	0/3073	0.66	4/4195 (0.1%)
7	G	0.40	0/1770	0.75	4/2410 (0.2%)
8	I	0.41	0/3524	0.68	6/4815 (0.1%)
9	J	0.44	0/4370	0.71	5/5974 (0.1%)
All	All	0.40	0/22910	0.66	24/31265 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	I	0	5
9	J	0	6
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	423	PRO	CA-N-CD	-8.46	99.65	111.50
7	G	144	LEU	CA-CB-CG	8.25	134.27	115.30
1	B	86	LEU	CA-CB-CG	7.08	131.58	115.30
4	F	75	LEU	CA-CB-CG	6.62	130.51	115.30
8	I	133	LEU	CA-CB-CG	6.36	129.92	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	199	ASP	CB-CG-OD1	6.32	123.99	118.30
7	G	11	LEU	CA-CB-CG	6.03	129.17	115.30
1	B	86	LEU	CB-CG-CD1	-5.77	101.19	111.00
8	I	379	ARG	C-N-CA	-5.76	107.31	121.70
2	C	73	LEU	CA-CB-CG	5.70	128.40	115.30
6	E	116	ASP	CB-CG-OD1	5.69	123.42	118.30
7	G	39	LEU	CA-CB-CG	5.56	128.10	115.30
8	I	78	LEU	CA-CB-CG	5.55	128.06	115.30
8	I	22	LEU	CA-CB-CG	5.53	128.02	115.30
8	I	25	ARG	CA-CB-CG	5.35	125.18	113.40
6	E	194	ASP	CB-CG-OD2	5.21	122.99	118.30
9	J	429	ASP	CB-CG-OD2	5.21	122.99	118.30
6	E	179	ASP	CB-CG-OD2	5.21	122.99	118.30
9	J	229	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	23	LEU	CA-CB-CG	5.16	127.16	115.30
9	J	519	ASP	CB-CG-OD2	5.15	122.93	118.30
9	J	424	ASP	CB-CG-OD2	5.09	122.88	118.30
6	E	318	LEU	CA-CB-CG	5.08	126.97	115.30
8	I	61	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	141	ALA	Peptide
8	I	254	TRP	Peptide
8	I	353	ASP	Peptide
8	I	368	LEU	Peptide
8	I	375	ILE	Peptide
8	I	414	ASN	Peptide
9	J	175	PRO	Peptide
9	J	285	ALA	Peptide
9	J	298	LEU	Peptide
9	J	371	ARG	Sidechain
9	J	394	THR	Peptide
9	J	506	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1148	0	1123	7	0
1	B	1148	0	1123	12	0
2	C	2718	0	2630	35	0
3	D	2747	0	2721	21	0
4	F	1196	0	1206	12	0
5	H	994	0	998	76	0
6	E	3005	0	3004	83	0
7	G	1737	0	1720	26	0
8	I	3441	0	3352	59	0
9	J	4275	0	4189	231	0
All	All	22409	0	22066	459	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 10.

All (459) 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)
5:H:21:SER:CA	8:I:43:PHE:HZ	1.00	1.58
5:H:50:ARG:HH22	9:J:47:THR:CG2	1.14	1.55
5:H:21:SER:CA	8:I:43:PHE:CZ	1.88	1.54
9:J:298:LEU:CB	9:J:304:LEU:HD12	1.04	1.50
5:H:21:SER:HA	8:I:43:PHE:CZ	1.44	1.48
9:J:298:LEU:HB2	9:J:304:LEU:CD1	1.03	1.48
5:H:21:SER:C	8:I:43:PHE:CZ	1.83	1.25
5:H:50:ARG:NH2	9:J:47:THR:CG2	1.99	1.24
9:J:362:LEU:O	9:J:373:THR:HG21	1.38	1.23
5:H:50:ARG:NH2	9:J:47:THR:HG22	1.53	1.22
6:E:260:THR:CA	9:J:422:GLN:HE21	1.56	1.17
9:J:371:ARG:NH2	9:J:372:ASN:HD21	1.42	1.14
5:H:50:ARG:HH22	9:J:47:THR:HG21	1.09	1.13
6:E:259:LEU:O	9:J:422:GLN:CG	1.96	1.13
9:J:299:GLY:N	9:J:304:LEU:HB3	1.60	1.12
9:J:298:LEU:CB	9:J:304:LEU:CD1	1.80	1.11
5:H:13:CYS:CB	9:J:43:ASP:OD2	2.00	1.09
5:H:16:PHE:CE1	9:J:418:TYR:HE1	1.74	1.06
5:H:21:SER:C	8:I:43:PHE:HZ	1.32	1.03
9:J:293:GLY:HA2	9:J:341:GLY:N	1.73	1.03
6:E:260:THR:CA	9:J:422:GLN:NE2	2.21	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:50:ARG:HH22	9:J:47:THR:HG22	0.88	1.01
6:E:259:LEU:O	9:J:422:GLN:HG2	1.61	1.01
6:E:274:LEU:HD21	6:E:276:ARG:HD2	1.42	1.00
9:J:371:ARG:NH2	9:J:372:ASN:ND2	2.08	1.00
5:H:20:PHE:HE2	9:J:434:VAL:HG12	1.24	1.00
6:E:62:ARG:HH12	6:E:213:GLU:HB3	1.27	1.00
9:J:298:LEU:HB3	9:J:304:LEU:CD1	1.92	0.99
5:H:69:THR:O	7:G:5:GLU:OE2	1.81	0.99
5:H:21:SER:HA	8:I:43:PHE:CE2	1.90	0.99
6:E:260:THR:C	9:J:422:GLN:NE2	2.16	0.99
5:H:50:ARG:NH1	9:J:50:GLN:HE22	1.59	0.98
9:J:225:ILE:HG21	9:J:314:LEU:HB2	1.45	0.98
9:J:362:LEU:O	9:J:373:THR:CG2	2.12	0.98
5:H:50:ARG:NH1	9:J:50:GLN:NE2	2.13	0.96
9:J:299:GLY:O	9:J:305:LEU:HB2	1.65	0.96
9:J:298:LEU:H	9:J:298:LEU:HD22	1.30	0.95
9:J:299:GLY:O	9:J:305:LEU:CB	2.14	0.95
9:J:225:ILE:CG2	9:J:314:LEU:HB2	1.96	0.94
6:E:261:SER:N	9:J:422:GLN:HE22	1.65	0.94
9:J:298:LEU:CA	9:J:304:LEU:HD12	1.98	0.94
9:J:298:LEU:CB	9:J:304:LEU:HD11	1.96	0.93
9:J:294:TYR:HD2	9:J:296:LEU:H	1.07	0.93
9:J:299:GLY:H	9:J:304:LEU:HB3	1.21	0.93
6:E:260:THR:N	9:J:422:GLN:HE21	1.65	0.92
9:J:124:PHE:N	9:J:176:THR:HG1	1.67	0.92
6:E:15:LEU:HD12	6:E:15:LEU:H	1.33	0.92
6:E:62:ARG:HH12	6:E:213:GLU:CB	1.82	0.91
6:E:62:ARG:NH1	6:E:213:GLU:HB3	1.84	0.91
6:E:260:THR:HA	9:J:422:GLN:HE21	1.35	0.91
6:E:62:ARG:NH1	6:E:213:GLU:CB	2.35	0.89
9:J:293:GLY:HA2	9:J:341:GLY:H	1.28	0.89
9:J:294:TYR:HE2	9:J:296:LEU:CA	1.86	0.89
5:H:13:CYS:HB3	9:J:43:ASP:OD2	1.69	0.89
5:H:50:ARG:NH2	9:J:47:THR:HG21	1.76	0.88
5:H:16:PHE:CE1	9:J:418:TYR:CE1	2.61	0.88
2:C:331:ILE:O	3:D:443:LEU:O	1.90	0.87
5:H:20:PHE:CE2	9:J:434:VAL:HG12	2.10	0.87
5:H:52:MET:HG3	9:J:17:PHE:CD2	2.11	0.86
5:H:50:ARG:CZ	9:J:47:THR:HG22	2.06	0.86
6:E:20:ASN:O	6:E:20:ASN:ND2	2.08	0.85
2:C:85:VAL:CG1	2:C:89:ASN:O	2.24	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:309:PRO:HA	9:J:314:LEU:HD11	1.59	0.84
6:E:259:LEU:C	9:J:422:GLN:HE21	1.79	0.83
9:J:299:GLY:N	9:J:300:PRO:HD3	1.92	0.83
9:J:244:VAL:HG11	9:J:307:ALA:O	1.79	0.83
5:H:13:CYS:HB2	9:J:43:ASP:OD2	1.63	0.82
6:E:260:THR:C	9:J:422:GLN:HE22	1.78	0.82
9:J:294:TYR:CE2	9:J:296:LEU:HB2	2.14	0.82
5:H:50:ARG:HH11	9:J:50:GLN:HE22	1.22	0.82
9:J:294:TYR:CD2	9:J:296:LEU:N	2.47	0.81
6:E:259:LEU:O	9:J:422:GLN:HG3	1.79	0.81
9:J:301:LEU:HD22	9:J:301:LEU:O	1.81	0.80
9:J:371:ARG:HH21	9:J:372:ASN:ND2	1.74	0.80
5:H:12:GLN:H	9:J:37:THR:HG1	1.28	0.80
5:H:68:ILE:O	7:G:4:LEU:HD22	1.82	0.79
6:E:274:LEU:HD21	6:E:276:ARG:CD	2.14	0.76
6:E:22:ASP:OD2	6:E:25:THR:OG1	2.04	0.76
9:J:305:LEU:HD22	9:J:308:ILE:HG13	1.68	0.75
5:H:68:ILE:HG22	7:G:4:LEU:HD21	1.68	0.75
9:J:225:ILE:HG21	9:J:314:LEU:CB	2.15	0.75
2:C:85:VAL:HG11	2:C:89:ASN:O	1.86	0.75
5:H:21:SER:C	8:I:43:PHE:CE1	2.56	0.75
9:J:225:ILE:HG12	9:J:317:LEU:HG	1.69	0.74
9:J:294:TYR:CE2	9:J:296:LEU:CA	2.70	0.73
9:J:299:GLY:O	9:J:305:LEU:HB3	1.86	0.73
9:J:299:GLY:N	9:J:300:PRO:CD	2.50	0.73
9:J:308:ILE:H	9:J:309:PRO:HD2	1.52	0.73
9:J:293:GLY:HA3	9:J:340:ASP:HA	1.69	0.73
9:J:422:GLN:HB3	9:J:423:PRO:HD3	1.69	0.73
6:E:261:SER:N	9:J:422:GLN:NE2	2.35	0.72
9:J:371:ARG:HH21	9:J:372:ASN:HD21	1.33	0.72
9:J:298:LEU:HA	9:J:304:LEU:HG	1.69	0.72
9:J:225:ILE:HG22	9:J:226:GLU:N	2.06	0.71
6:E:259:LEU:C	9:J:422:GLN:NE2	2.43	0.71
2:C:271:VAL:O	3:D:293:ASN:ND2	2.23	0.70
9:J:294:TYR:CE2	9:J:296:LEU:N	2.60	0.70
5:H:52:MET:HG3	9:J:17:PHE:CE2	2.27	0.70
6:E:62:ARG:NH1	6:E:213:GLU:HB2	2.05	0.70
5:H:13:CYS:HB3	9:J:38:ASP:HB3	1.74	0.69
9:J:298:LEU:HD22	9:J:298:LEU:N	2.07	0.69
9:J:305:LEU:HD13	9:J:305:LEU:O	1.93	0.69
2:C:143:PRO:HA	2:C:216:TYR:HE1	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:17:GLN:H	6:E:17:GLN:NE2	1.90	0.69
9:J:304:LEU:HD13	9:J:304:LEU:O	1.92	0.69
9:J:301:LEU:HD22	9:J:301:LEU:C	2.14	0.69
6:E:260:THR:HA	9:J:422:GLN:NE2	2.00	0.69
9:J:298:LEU:HB3	9:J:304:LEU:HD11	1.63	0.69
9:J:304:LEU:O	9:J:304:LEU:HD22	1.93	0.68
9:J:305:LEU:HD22	9:J:305:LEU:O	1.93	0.68
9:J:306:LEU:HD13	9:J:306:LEU:O	1.92	0.68
9:J:294:TYR:HE2	9:J:296:LEU:CB	2.07	0.68
9:J:296:LEU:C	9:J:296:LEU:HD13	2.13	0.68
6:E:154:TYR:CD1	6:E:189:GLN:HG2	2.29	0.68
6:E:271:SER:HB2	6:E:290:THR:O	1.93	0.68
1:A:74:LYS:HE2	1:A:79:GLU:HG3	1.77	0.67
5:H:50:ARG:NH1	9:J:47:THR:HG22	2.09	0.67
8:I:139:PRO:HA	8:I:169:ILE:O	1.94	0.67
9:J:298:LEU:HA	9:J:304:LEU:CG	2.25	0.67
9:J:362:LEU:O	9:J:373:THR:CB	2.41	0.67
5:H:15:ALA:O	9:J:44:PRO:HG2	1.96	0.66
9:J:294:TYR:CE2	9:J:296:LEU:CB	2.78	0.66
7:G:129:ASP:HB3	7:G:151:SER:HB3	1.76	0.66
6:E:260:THR:N	9:J:422:GLN:NE2	2.37	0.66
9:J:293:GLY:CA	9:J:341:GLY:N	2.55	0.65
9:J:299:GLY:H	9:J:300:PRO:CD	2.08	0.65
5:H:74:ALA:HB1	7:G:113:GLY:O	1.95	0.65
9:J:308:ILE:N	9:J:309:PRO:HD2	2.11	0.65
5:H:12:GLN:N	9:J:37:THR:OG1	2.14	0.65
9:J:522:GLN:HE22	9:J:531:GLN:HG3	1.62	0.65
6:E:33:THR:HG23	6:E:86:GLY:H	1.62	0.65
9:J:308:ILE:H	9:J:309:PRO:CD	2.10	0.65
9:J:298:LEU:CB	9:J:304:LEU:CG	2.71	0.64
9:J:248:PHE:CE2	9:J:304:LEU:HD11	2.32	0.64
9:J:294:TYR:HE2	9:J:296:LEU:HA	1.59	0.64
2:C:45:PRO:HB2	2:C:89:ASN:ND2	2.13	0.63
5:H:21:SER:N	8:I:43:PHE:HZ	1.90	0.63
5:H:52:MET:CB	9:J:17:PHE:CE2	2.81	0.63
9:J:95:VAL:HG11	9:J:103:ALA:HB2	1.81	0.63
9:J:225:ILE:HD13	9:J:314:LEU:HD22	1.81	0.63
8:I:153:ASP:HB3	8:I:156:GLY:H	1.64	0.62
9:J:298:LEU:CA	9:J:304:LEU:CD1	2.70	0.62
9:J:128:SER:HB3	9:J:172:SER:HB2	1.82	0.62
9:J:225:ILE:CG2	9:J:226:GLU:N	2.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HG	1:B:64:ILE:HD12	1.82	0.61
4:F:63:LEU:HD23	4:F:137:LEU:HD12	1.81	0.61
9:J:101:ARG:NH2	9:J:286:PRO:O	2.33	0.61
5:H:68:ILE:HG22	7:G:4:LEU:CD2	2.30	0.61
6:E:274:LEU:HG	6:E:276:ARG:HG3	1.82	0.61
3:D:414:ILE:HG22	3:D:415:THR:HG23	1.81	0.60
6:E:43:VAL:HG12	6:E:43:VAL:O	2.00	0.60
5:H:38:SER:HB3	9:J:42:HIS:CD2	2.36	0.60
9:J:298:LEU:HD23	9:J:298:LEU:C	2.22	0.60
8:I:157:ASN:ND2	8:I:352:ASP:OD2	2.33	0.60
5:H:18:PRO:HB2	9:J:434:VAL:CG1	2.32	0.60
5:H:16:PHE:HB2	5:H:37:GLN:HE21	1.66	0.60
2:C:225:ILE:HG12	2:C:235:VAL:HG12	1.83	0.60
2:C:132:GLY:HA3	2:C:160:TYR:HA	1.84	0.60
6:E:347:TRP:CZ2	7:G:6:ARG:HG3	2.36	0.60
1:A:94:ILE:HB	1:A:112:VAL:HB	1.83	0.59
6:E:274:LEU:CD2	6:E:276:ARG:HD2	2.26	0.59
9:J:294:TYR:HE2	9:J:296:LEU:HB2	1.60	0.59
6:E:259:LEU:O	9:J:422:GLN:NE2	2.35	0.59
9:J:225:ILE:CG2	9:J:226:GLU:H	2.15	0.59
9:J:308:ILE:N	9:J:309:PRO:CD	2.65	0.59
9:J:408:ILE:HG23	9:J:412:GLN:HE21	1.68	0.59
8:I:145:GLY:HA2	8:I:162:GLN:HB2	1.84	0.59
9:J:302:VAL:HG22	9:J:302:VAL:O	2.02	0.59
9:J:309:PRO:HA	9:J:314:LEU:CD1	2.31	0.59
5:H:97:ILE:HG12	5:H:97:ILE:O	2.02	0.59
5:H:25:GLY:O	8:I:54:PHE:HE1	1.86	0.59
9:J:66:SER:H	9:J:69:ASP:HB2	1.68	0.58
8:I:430:VAL:HG22	8:I:451:VAL:HG22	1.86	0.58
8:I:454:ASP:O	8:I:456:ARG:NH2	2.36	0.58
9:J:293:GLY:CA	9:J:341:GLY:H	2.09	0.57
6:E:71:HIS:O	6:E:75:ASN:ND2	2.37	0.57
2:C:92:ASP:OD2	2:C:96:GLN:NE2	2.37	0.57
9:J:300:PRO:HD2	9:J:304:LEU:H	1.69	0.57
7:G:132:VAL:HG12	7:G:148:VAL:HG22	1.85	0.57
5:H:50:ARG:HH12	9:J:47:THR:HG22	1.68	0.57
9:J:364:LEU:HD23	9:J:373:THR:HG22	1.87	0.57
9:J:124:PHE:N	9:J:176:THR:OG1	2.36	0.57
2:C:31:LEU:HD21	2:C:90:ILE:HG12	1.85	0.57
9:J:300:PRO:HB2	9:J:303:ASN:HB2	1.85	0.57
9:J:373:THR:O	9:J:373:THR:OG1	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:TYR:HB2	2:C:222:LEU:HD21	1.86	0.56
4:F:119:GLN:HB3	4:F:134:THR:HB	1.88	0.56
5:H:69:THR:HB	7:G:5:GLU:OE2	2.04	0.56
6:E:192:SER:H	6:E:195:GLN:HE21	1.52	0.56
8:I:139:PRO:HB3	8:I:170:THR:HG22	1.88	0.56
9:J:301:LEU:HD13	9:J:302:VAL:HG12	1.87	0.56
4:F:29:ARG:HB3	4:F:66:GLU:HB2	1.87	0.56
1:A:22:THR:HB	1:A:95:MET:HB3	1.86	0.56
8:I:222:ALA:N	8:I:229:PHE:O	2.38	0.56
8:I:150:GLY:HA2	8:I:364:THR:HG22	1.88	0.56
9:J:299:GLY:H	9:J:300:PRO:HD3	1.69	0.56
1:B:113:SER:OG	1:B:142:ASP:OD1	2.23	0.55
5:H:18:PRO:HB2	9:J:434:VAL:HG11	1.88	0.55
9:J:295:VAL:HA	9:J:338:VAL:HA	1.87	0.55
9:J:259:GLU:HA	9:J:262:ARG:HG2	1.88	0.55
9:J:297:ASN:HB2	9:J:336:TRP:CB	2.37	0.55
9:J:298:LEU:CA	9:J:304:LEU:CG	2.84	0.55
9:J:371:ARG:HD2	9:J:371:ARG:C	2.27	0.55
6:E:130:ASN:HD21	6:E:178:GLU:H	1.53	0.55
9:J:298:LEU:H	9:J:298:LEU:CD2	2.12	0.55
5:H:85:LEU:HD23	7:G:167:GLN:NE2	2.22	0.55
6:E:15:LEU:H	6:E:15:LEU:CD1	2.12	0.55
8:I:407:ARG:NH2	9:J:92:CYS:O	2.35	0.54
9:J:129:LEU:HD11	9:J:169:LEU:HD13	1.89	0.54
9:J:427:ILE:HG22	9:J:428:ASP:N	2.22	0.54
5:H:19:ARG:NE	9:J:430:GLN:HB3	2.22	0.54
9:J:364:LEU:HG	9:J:371:ARG:HA	1.89	0.54
6:E:22:ASP:O	6:E:26:MET:HG2	2.08	0.54
6:E:122:LEU:HD13	6:E:173:LEU:HB2	1.90	0.54
5:H:88:GLU:HA	5:H:88:GLU:OE2	2.07	0.54
9:J:299:GLY:C	9:J:305:LEU:HB2	2.27	0.54
3:D:213:VAL:HG22	3:D:299:VAL:HG12	1.90	0.54
8:I:502:ALA:HB2	8:I:569:LEU:HD23	1.89	0.54
9:J:412:GLN:CB	9:J:420:LEU:HD21	2.38	0.54
9:J:502:ILE:HG22	9:J:513:ASN:HB3	1.90	0.54
1:B:117:PRO:HB3	1:B:137:ILE:HD11	1.89	0.53
2:C:333:ILE:HD12	3:D:445:PHE:CE1	2.43	0.53
9:J:423:PRO:O	9:J:423:PRO:HD2	2.08	0.53
9:J:349:ALA:H	9:J:352:LEU:HD12	1.74	0.53
5:H:69:THR:CG2	6:E:390:LEU:HD13	2.39	0.53
9:J:467:ALA:HA	9:J:501:ALA:HA	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:177:ARG:HA	9:J:180:GLN:HE21	1.74	0.53
6:E:289:ARG:NH1	6:E:394:GLU:OE1	2.42	0.52
8:I:134:GLN:NE2	8:I:375:ILE:O	2.42	0.52
8:I:414:ASN:HA	8:I:417:ARG:HB3	1.92	0.52
9:J:296:LEU:HD13	9:J:296:LEU:O	2.08	0.52
8:I:501:THR:HG1	8:I:570:SER:HG	1.49	0.52
2:C:160:TYR:HB2	2:C:222:LEU:HD11	1.91	0.52
9:J:412:GLN:HB3	9:J:420:LEU:HD21	1.91	0.52
9:J:183:SER:HB3	9:J:187:LEU:HB2	1.91	0.52
9:J:362:LEU:O	9:J:373:THR:OG1	2.28	0.52
5:H:52:MET:HB2	9:J:17:PHE:CE2	2.43	0.52
6:E:30:ILE:HB	6:E:123:VAL:HG22	1.90	0.52
9:J:169:LEU:HB2	9:J:208:VAL:HG12	1.89	0.52
9:J:296:LEU:HD12	9:J:337:GLN:HB2	1.92	0.52
9:J:422:GLN:HB3	9:J:423:PRO:CD	2.38	0.52
5:H:74:ALA:CB	7:G:113:GLY:O	2.58	0.52
9:J:225:ILE:HG22	9:J:226:GLU:H	1.72	0.51
6:E:211:GLN:OE1	6:E:211:GLN:HA	2.08	0.51
2:C:45:PRO:HB2	2:C:89:ASN:HD21	1.74	0.51
9:J:127:VAL:HG22	9:J:173:LEU:HD11	1.93	0.51
8:I:405:ALA:HB2	9:J:529:GLY:HA3	1.92	0.51
6:E:96:LEU:CD2	6:E:129:LEU:HD23	2.41	0.50
5:H:19:ARG:HE	9:J:430:GLN:HB3	1.76	0.50
5:H:52:MET:CB	9:J:17:PHE:HE2	2.22	0.50
6:E:34:PRO:HG2	6:E:59:PHE:HB3	1.94	0.50
9:J:59:LEU:HD21	9:J:448:GLY:HA3	1.93	0.50
1:B:36:LEU:HD21	1:B:96:ILE:HD12	1.93	0.50
2:C:222:LEU:HD23	2:C:224:MET:HE1	1.94	0.50
1:A:117:PRO:HB3	1:A:137:ILE:HD11	1.94	0.50
2:C:348:PHE:HE2	6:E:312:GLU:HG2	1.77	0.50
1:A:53:PHE:HD1	1:B:12:TYR:CE1	2.30	0.50
5:H:71:GLU:OE1	7:G:9:SER:HB2	2.12	0.50
5:H:96:VAL:O	5:H:96:VAL:HG22	2.11	0.50
6:E:52:LEU:HD12	6:E:73:PHE:HB2	1.94	0.50
2:C:195:ALA:HA	2:C:235:VAL:HG23	1.94	0.49
5:H:12:GLN:N	9:J:37:THR:HG1	2.04	0.49
9:J:225:ILE:CG1	9:J:317:LEU:HG	2.39	0.49
9:J:294:TYR:HD2	9:J:296:LEU:N	1.91	0.49
9:J:427:ILE:CG2	9:J:428:ASP:N	2.75	0.49
6:E:96:LEU:HG	6:E:129:LEU:HD21	1.94	0.49
6:E:240:TRP:HB3	6:E:307:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:141:ASP:OD2	6:E:344:ARG:NH1	2.46	0.49
2:C:176:ILE:HG23	2:C:199:VAL:HG11	1.94	0.49
4:F:124:ASP:HB3	4:F:127:SER:HB3	1.93	0.49
8:I:172:GLN:NE2	8:I:236:ASP:O	2.45	0.49
3:D:390:ARG:HA	3:D:393:GLN:HG2	1.93	0.49
6:E:27:PRO:HA	6:E:120:LEU:HB2	1.94	0.49
7:G:10:LYS:HA	7:G:33:ASN:HD21	1.78	0.49
8:I:407:ARG:HH11	9:J:559:GLY:HA3	1.78	0.49
9:J:240:GLN:OE1	9:J:311:VAL:HG13	2.13	0.49
3:D:311:GLN:HE22	3:D:333:TRP:HD1	1.59	0.49
6:E:176:LEU:HD12	6:E:203:TRP:HB2	1.93	0.49
6:E:259:LEU:O	9:J:422:GLN:CD	2.51	0.49
8:I:43:PHE:HA	8:I:51:TRP:HE3	1.78	0.49
8:I:496:LYS:HB2	8:I:586:THR:HG22	1.95	0.49
5:H:38:SER:CB	9:J:42:HIS:CD2	2.95	0.48
5:H:52:MET:CG	9:J:17:PHE:CE2	2.94	0.48
9:J:294:TYR:CD2	9:J:294:TYR:C	2.85	0.48
3:D:198:VAL:HB	3:D:204:VAL:HG21	1.94	0.48
3:D:307:THR:H	3:D:310:GLN:HE21	1.60	0.48
9:J:8:PHE:O	9:J:12:LYS:HB2	2.13	0.48
6:E:96:LEU:HD23	6:E:129:LEU:HD23	1.94	0.48
6:E:165:ARG:HA	6:E:198:ARG:HD2	1.94	0.48
7:G:207:ASN:HD21	7:G:222:ARG:H	1.61	0.48
5:H:107:ARG:HG2	6:E:395:PHE:HB2	1.95	0.48
6:E:2:THR:OG1	6:E:3:MET:N	2.46	0.48
9:J:376:SER:OG	9:J:377:GLU:N	2.47	0.48
2:C:315:LYS:HE3	2:C:321:GLN:HB2	1.94	0.48
3:D:183:TYR:O	3:D:203:GLN:NE2	2.42	0.48
6:E:274:LEU:HD21	6:E:276:ARG:CG	2.43	0.48
2:C:312:GLN:HE21	2:C:317:LEU:HD22	1.77	0.48
6:E:22:ASP:CG	6:E:25:THR:OG1	2.52	0.48
8:I:78:LEU:HD21	9:J:31:LEU:HD12	1.96	0.48
9:J:427:ILE:CG2	9:J:428:ASP:H	2.27	0.48
4:F:47:GLU:OE2	4:F:50:ARG:NE	2.47	0.47
2:C:253:ARG:NH1	2:C:257:ASN:OD1	2.47	0.47
6:E:33:THR:HG22	6:E:84:PRO:CB	2.44	0.47
9:J:533:ALA:H	9:J:548:GLN:HE22	1.61	0.47
2:C:33:ALA:CB	2:C:90:ILE:HD11	2.45	0.47
5:H:63:PHE:HB3	5:H:72:LEU:HD11	1.96	0.47
6:E:274:LEU:CD2	6:E:276:ARG:CD	2.88	0.47
6:E:336:LYS:HD2	6:E:365:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:299:GLY:HA2	9:J:305:LEU:N	2.30	0.47
9:J:371:ARG:CZ	9:J:372:ASN:ND2	2.75	0.47
1:B:62:PRO:HG2	1:B:141:ALA:HB3	1.97	0.47
6:E:340:TRP:NE1	6:E:357:GLU:OE2	2.47	0.47
9:J:321:LYS:HE2	9:J:335:ARG:HD3	1.97	0.47
5:H:51:ILE:HD13	9:J:54:TRP:CD1	2.50	0.47
5:H:68:ILE:HG23	5:H:108:LEU:HD21	1.96	0.47
6:E:17:GLN:NE2	6:E:17:GLN:N	2.61	0.47
8:I:453:PRO:HG3	8:I:468:LEU:HB2	1.96	0.47
5:H:42:LEU:HD11	5:H:87:HIS:HB2	1.98	0.46
9:J:299:GLY:C	9:J:305:LEU:CB	2.81	0.46
1:B:142:ASP:OD1	1:B:142:ASP:N	2.42	0.46
3:D:339:LYS:HG3	3:D:341:ASP:H	1.80	0.46
9:J:558:LEU:O	9:J:576:ARG:NH2	2.39	0.46
9:J:293:GLY:HA3	9:J:340:ASP:CA	2.39	0.46
9:J:518:LEU:HD23	9:J:521:LEU:HD12	1.97	0.46
5:H:44:MET:CE	9:J:417:CYS:SG	3.03	0.46
4:F:15:LEU:HD13	4:F:22:PRO:HG3	1.98	0.46
7:G:114:LYS:HD2	7:G:114:LYS:HA	1.68	0.46
9:J:107:VAL:O	9:J:178:TYR:OH	2.34	0.46
9:J:304:LEU:HD13	9:J:304:LEU:C	2.36	0.46
8:I:145:GLY:N	8:I:163:THR:O	2.49	0.46
9:J:300:PRO:HD2	9:J:303:ASN:HB2	1.97	0.46
2:C:222:LEU:HD23	2:C:224:MET:CE	2.46	0.46
3:D:110:THR:HB	3:D:268:LEU:HD21	1.98	0.46
9:J:349:ALA:HB1	9:J:351:PRO:HD2	1.98	0.46
6:E:62:ARG:CZ	6:E:213:GLU:HB2	2.45	0.45
8:I:415:ASN:HD21	9:J:562:ARG:HH12	1.64	0.45
9:J:385:GLN:NE2	9:J:387:ASP:OD2	2.48	0.45
5:H:21:SER:N	8:I:43:PHE:CZ	2.73	0.45
6:E:197:GLN:HG3	6:E:299:TRP:HB3	1.97	0.45
9:J:298:LEU:C	9:J:298:LEU:CD2	2.85	0.45
1:B:149:ALA:HB3	2:C:281:GLN:HE22	1.82	0.45
2:C:239:ARG:NH1	2:C:243:ASP:OD1	2.48	0.45
7:G:204:ALA:HA	7:G:209:LEU:HD13	1.98	0.45
8:I:251:ASP:OD1	8:I:251:ASP:N	2.50	0.45
8:I:468:LEU:HD21	8:I:472:ARG:HD2	1.97	0.45
8:I:403:ARG:HE	9:J:269:ASP:HB2	1.80	0.45
9:J:225:ILE:HG12	9:J:317:LEU:CG	2.42	0.45
7:G:116:ARG:NH1	7:G:119:ASN:O	2.49	0.45
6:E:169:GLN:HE21	6:E:169:GLN:HB3	1.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:255:ARG:HB3	9:J:280:GLY:HA3	1.99	0.45
7:G:28:MET:HB3	7:G:91:MET:HG2	1.98	0.45
8:I:408:GLN:O	8:I:409:ARG:NH1	2.43	0.45
3:D:364:LEU:HD22	3:D:380:VAL:HG13	1.99	0.45
7:G:105:PRO:HB2	7:G:126:ARG:HD2	1.98	0.45
8:I:43:PHE:HA	8:I:51:TRP:CE3	2.52	0.45
5:H:70:ASP:OD2	7:G:2:SER:O	2.35	0.44
5:H:85:LEU:HD23	7:G:167:GLN:HE22	1.81	0.44
8:I:509:VAL:HG23	8:I:510:VAL:HG23	1.99	0.44
6:E:274:LEU:CG	6:E:276:ARG:HG3	2.47	0.44
8:I:500:VAL:N	8:I:589:ALA:O	2.45	0.44
9:J:226:GLU:HG3	9:J:315:SER:HB2	1.98	0.44
2:C:210:ASP:HB3	2:C:226:ARG:HH12	1.83	0.44
7:G:18:ASP:N	7:G:18:ASP:OD1	2.48	0.44
6:E:225:ALA:HB1	6:E:248:LEU:HD22	1.99	0.44
6:E:274:LEU:CD2	6:E:276:ARG:HG3	2.47	0.44
8:I:91:LEU:HD11	9:J:24:ALA:HB2	1.98	0.44
8:I:145:GLY:H	8:I:163:THR:HB	1.82	0.44
9:J:483:ALA:HA	9:J:486:GLN:HB2	2.00	0.44
1:B:97:SER:HB3	1:B:106:VAL:HG13	2.00	0.44
2:C:193:ALA:HA	2:C:251:PRO:HG3	2.00	0.43
5:H:16:PHE:HE1	9:J:418:TYR:CE1	2.26	0.43
6:E:103:LEU:HA	6:E:108:MET:HG3	2.00	0.43
6:E:176:LEU:HD11	6:E:272:CYS:SG	2.58	0.43
8:I:98:MET:O	8:I:101:THR:OG1	2.35	0.43
8:I:244:VAL:HG23	8:I:336:VAL:HG12	2.00	0.43
6:E:71:HIS:CE1	6:E:75:ASN:HD21	2.35	0.43
3:D:346:TYR:HB3	3:D:348:PRO:HD2	2.00	0.43
1:A:142:ASP:OD1	1:A:142:ASP:N	2.46	0.43
1:B:94:ILE:HB	1:B:112:VAL:HB	2.00	0.43
3:D:274:ILE:HA	3:D:277:VAL:HG22	2.01	0.43
9:J:174:VAL:HA	9:J:175:PRO:HD3	1.76	0.43
6:E:120:LEU:HD23	6:E:171:PHE:HB3	2.01	0.43
2:C:50:ARG:NH2	2:C:54:GLU:OE2	2.52	0.43
7:G:138:ASP:H	7:G:141:ALA:HA	1.84	0.43
8:I:87:ALA:HA	9:J:27:LYS:HG2	1.99	0.43
8:I:114:LEU:HD23	9:J:85:GLY:HA2	1.99	0.43
9:J:225:ILE:HG23	9:J:314:LEU:HB2	1.94	0.43
9:J:532:ARG:HG3	9:J:548:GLN:HE21	1.82	0.43
8:I:420:LEU:HD21	8:I:492:LEU:HD21	2.00	0.43
8:I:431:ARG:HG2	8:I:544:ASN:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:ASP:OD2	3:D:181:LYS:NZ	2.50	0.43
9:J:65:LEU:H	9:J:65:LEU:HG	1.54	0.43
9:J:131:GLN:HA	9:J:169:LEU:HA	2.01	0.43
9:J:439:LEU:HD21	9:J:492:LEU:HD11	1.99	0.43
4:F:62:SER:OG	4:F:136:GLU:OE2	2.26	0.43
9:J:401:PHE:CE1	9:J:403:ASP:HB2	2.53	0.43
6:E:303:GLN:HE22	6:E:392:PRO:HG3	1.83	0.43
5:H:63:PHE:HA	5:H:66:GLU:HG3	2.00	0.42
8:I:507:THR:HG1	8:I:563:SER:HG	1.62	0.42
4:F:79:PHE:CE1	4:F:115:PRO:HB3	2.55	0.42
8:I:417:ARG:NH2	8:I:430:VAL:H	2.17	0.42
9:J:244:VAL:CG1	9:J:307:ALA:O	2.61	0.42
3:D:398:ALA:HB2	3:D:435:VAL:HB	2.00	0.42
3:D:364:LEU:HD11	3:D:384:ILE:HD11	2.02	0.42
2:C:143:PRO:HB3	2:C:216:TYR:CD1	2.54	0.42
9:J:295:VAL:HG12	9:J:338:VAL:HG22	2.01	0.42
9:J:457:THR:HA	9:J:460:ALA:HB2	2.02	0.42
4:F:90:TRP:HD1	4:F:90:TRP:O	2.03	0.42
8:I:134:GLN:HG2	8:I:374:ALA:HA	2.01	0.42
5:H:44:MET:HE3	9:J:417:CYS:SG	2.60	0.42
6:E:33:THR:HG22	6:E:84:PRO:HB2	2.02	0.42
1:B:93:ASP:OD1	1:B:93:ASP:N	2.47	0.42
8:I:127:VAL:O	8:I:346:ASN:N	2.53	0.42
8:I:224:GLU:HG3	8:I:225:LEU:H	1.84	0.42
9:J:75:ASP:OD1	9:J:75:ASP:N	2.51	0.42
9:J:104:LEU:HB2	9:J:127:VAL:HG21	2.01	0.42
9:J:597:LEU:HD22	9:J:598:PRO:HD2	2.01	0.42
5:H:44:MET:HE2	9:J:417:CYS:SG	2.60	0.41
8:I:118:ALA:O	8:I:399:ARG:NH1	2.52	0.41
9:J:300:PRO:CB	9:J:303:ASN:HB2	2.49	0.41
2:C:164:THR:HG23	2:C:203:THR:HB	2.02	0.41
7:G:173:ALA:HB3	7:G:223:ALA:HB3	2.02	0.41
9:J:371:ARG:C	9:J:371:ARG:CD	2.87	0.41
9:J:407:TYR:HB2	9:J:472:ARG:HH22	1.85	0.41
6:E:17:GLN:N	6:E:17:GLN:CD	2.73	0.41
2:C:42:ILE:HG22	2:C:44:LYS:H	1.85	0.41
2:C:259:VAL:HG12	3:D:445:PHE:HE2	1.86	0.41
5:H:67:ASN:O	5:H:69:THR:N	2.43	0.41
8:I:136:ASN:OD1	8:I:136:ASN:N	2.53	0.41
3:D:311:GLN:OE1	3:D:323:ARG:NH1	2.47	0.41
7:G:112:TRP:HB3	7:G:115:MET:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:420:LEU:HD13	8:I:480:LEU:HD12	2.02	0.41
1:A:53:PHE:HD1	1:B:12:TYR:CD1	2.39	0.41
6:E:26:MET:HB2	6:E:118:THR:HA	2.02	0.41
8:I:407:ARG:NH2	9:J:90:LEU:HA	2.35	0.41
2:C:94:VAL:HA	2:C:100:ILE:HD12	2.02	0.41
3:D:336:ARG:NH2	3:D:439:GLU:OE2	2.54	0.41
5:H:14:TRP:HB2	9:J:44:PRO:HD2	2.03	0.41
9:J:228:ALA:O	9:J:229:ASP:OD1	2.38	0.41
2:C:165:LEU:HB2	2:C:171:VAL:HG23	2.02	0.41
5:H:68:ILE:O	5:H:70:ASP:N	2.54	0.41
5:H:68:ILE:H	5:H:68:ILE:HG13	1.49	0.41
6:E:178:GLU:OE2	6:E:205:ARG:NE	2.53	0.41
6:E:208:THR:HG21	6:E:220:LEU:HD12	2.02	0.41
6:E:320:ARG:HA	6:E:323:LEU:HB2	2.03	0.41
7:G:44:ARG:NE	7:G:64:GLU:OE2	2.51	0.41
9:J:524:LEU:HD23	9:J:524:LEU:HA	1.92	0.41
8:I:114:LEU:HD11	9:J:397:PRO:HG3	2.01	0.41
4:F:31:SER:HB3	4:F:64:VAL:HB	2.02	0.40
4:F:103:LEU:HA	4:F:104:PRO:HD3	1.96	0.40
8:I:60:THR:HG23	8:I:63:ALA:H	1.87	0.40
2:C:33:ALA:HB2	2:C:90:ILE:HD11	2.03	0.40
6:E:14:LEU:O	6:E:14:LEU:HD12	2.22	0.40
9:J:89:VAL:HA	9:J:556:PRO:HB3	2.03	0.40
9:J:135:GLU:HG3	9:J:136:HIS:CD2	2.57	0.40
9:J:300:PRO:CG	9:J:303:ASN:HB2	2.51	0.40
9:J:305:LEU:HD13	9:J:305:LEU:C	2.41	0.40
9:J:536:PRO:HB2	9:J:539:LEU:HB2	2.03	0.40
9:J:590:ASP:OD1	9:J:590:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/149 (98%)	136 (93%)	8 (6%)	2 (1%)	11	40
1	B	146/149 (98%)	133 (91%)	11 (8%)	2 (1%)	11	40
2	C	349/354 (99%)	314 (90%)	34 (10%)	1 (0%)	41	73
3	D	352/451 (78%)	328 (93%)	24 (7%)	0	100	100
4	F	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
5	H	121/140 (86%)	109 (90%)	8 (7%)	4 (3%)	4	21
6	E	380/417 (91%)	338 (89%)	41 (11%)	1 (0%)	41	73
7	G	222/229 (97%)	187 (84%)	33 (15%)	2 (1%)	17	52
8	I	429/607 (71%)	365 (85%)	63 (15%)	1 (0%)	47	79
9	J	538/963 (56%)	438 (81%)	97 (18%)	3 (1%)	25	59
All	All	2830/3608 (78%)	2480 (88%)	334 (12%)	16 (1%)	29	59

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	68	ILE
5	H	69	THR
9	J	296	LEU
9	J	395	VAL
1	A	5	ALA
1	B	5	ALA
5	H	92	LEU
7	G	155	ASP
7	G	200	TYR
6	E	19	SER
1	B	4	THR
2	C	142	LYS
5	H	67	ASN
9	J	251	PRO
1	A	4	THR
8	I	369	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/128 (99%)	125 (98%)	2 (2%)	62	84
1	B	127/128 (99%)	125 (98%)	2 (2%)	62	84
2	C	284/287 (99%)	281 (99%)	3 (1%)	73	89
3	D	293/368 (80%)	292 (100%)	1 (0%)	92	96
4	F	134/134 (100%)	132 (98%)	2 (2%)	65	85
5	H	108/121 (89%)	104 (96%)	4 (4%)	34	66
6	E	324/345 (94%)	316 (98%)	8 (2%)	47	75
7	G	191/195 (98%)	187 (98%)	4 (2%)	53	79
8	I	364/509 (72%)	356 (98%)	8 (2%)	52	78
9	J	455/807 (56%)	442 (97%)	13 (3%)	42	72
All	All	2407/3022 (80%)	2360 (98%)	47 (2%)	57	80

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	82	ASN
1	B	75	ASN
1	B	82	ASN
2	C	89	ASN
2	C	224	MET
2	C	277	GLN
3	D	400	ASN
4	F	13	ASN
4	F	90	TRP
5	H	90	ARG
5	H	96	VAL
5	H	97	ILE
5	H	130	ASN
6	E	15	LEU
6	E	16	THR
6	E	20	ASN
6	E	148	ASP
6	E	169	GLN
6	E	213	GLU
6	E	215	SER
6	E	267	ASN
7	G	111	THR
7	G	114	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	133	THR
7	G	136	LEU
8	I	25	ARG
8	I	32	ASN
8	I	256	TYR
8	I	363	ASN
8	I	379	ARG
8	I	403	ARG
8	I	414	ASN
8	I	503	ARG
9	J	65	LEU
9	J	250	ARG
9	J	291	SER
9	J	294	TYR
9	J	296	LEU
9	J	297	ASN
9	J	298	LEU
9	J	301	LEU
9	J	306	LEU
9	J	308	ILE
9	J	311	VAL
9	J	371	ARG
9	J	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
2	C	89	ASN
2	C	277	GLN
2	C	281	GLN
2	C	312	GLN
2	C	321	GLN
3	D	310	GLN
3	D	400	ASN
3	D	447	GLN
4	F	89	GLN
5	H	37	GLN
5	H	130	ASN
6	E	17	GLN
6	E	71	HIS
6	E	130	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	169	GLN
6	E	195	GLN
6	E	231	GLN
6	E	267	ASN
7	G	33	ASN
7	G	149	GLN
7	G	167	GLN
7	G	207	ASN
8	I	32	ASN
8	I	134	GLN
8	I	258	GLN
8	I	358	GLN
8	I	363	ASN
8	I	414	ASN
9	J	25	HIS
9	J	50	GLN
9	J	136	HIS
9	J	180	GLN
9	J	337	GLN
9	J	372	ASN
9	J	385	GLN
9	J	412	GLN
9	J	414	GLN
9	J	422	GLN
9	J	522	GLN
9	J	548	GLN
9	J	564	ASN
9	J	574	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

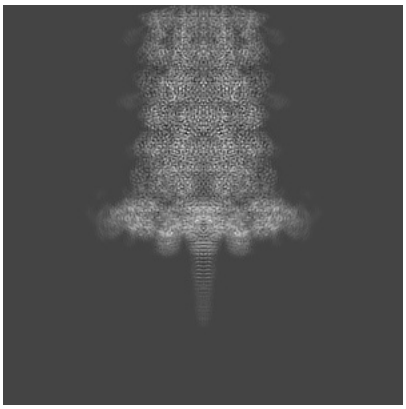
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4782. These allow visual inspection of the internal detail of the map and identification of artifacts.

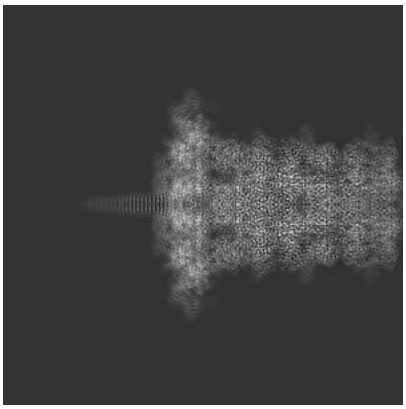
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

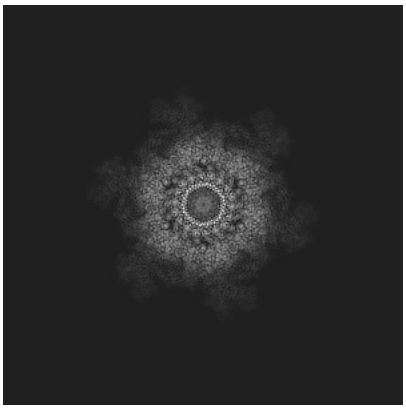
6.1.1 Primary map



X

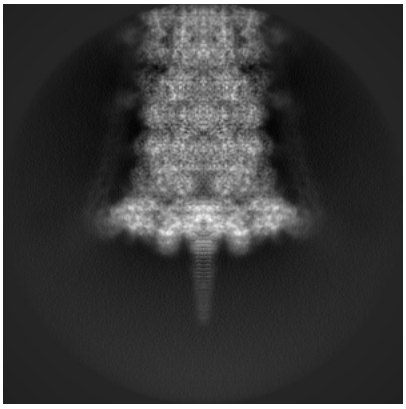


Y

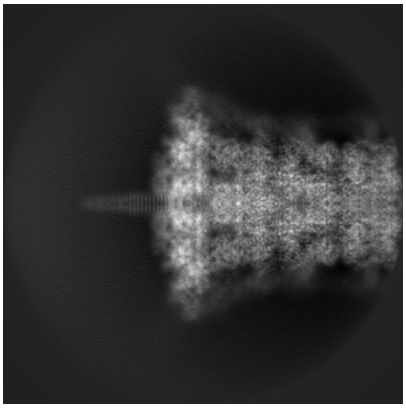


Z

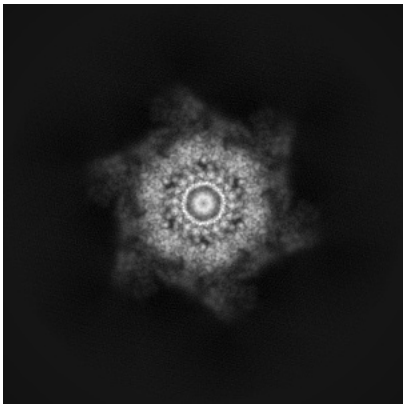
6.1.2 Raw map



X



Y

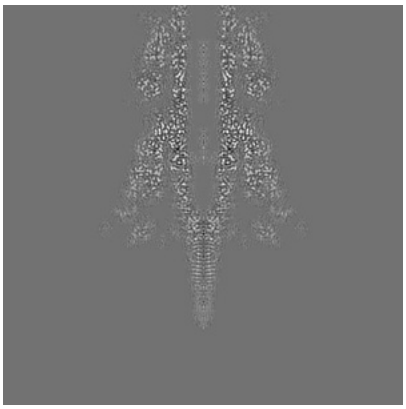


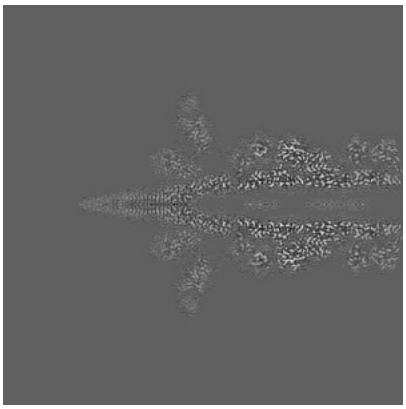
Z

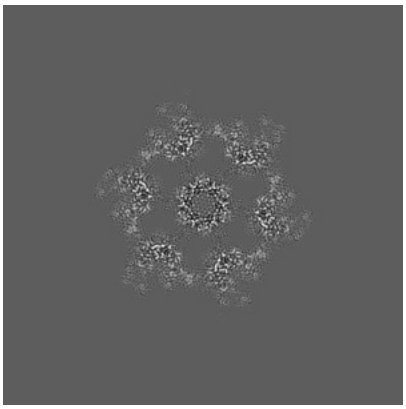
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

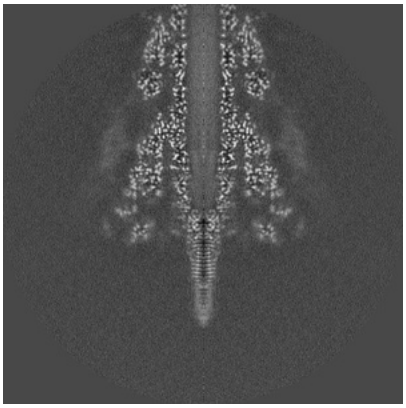
6.2.1 Primary map

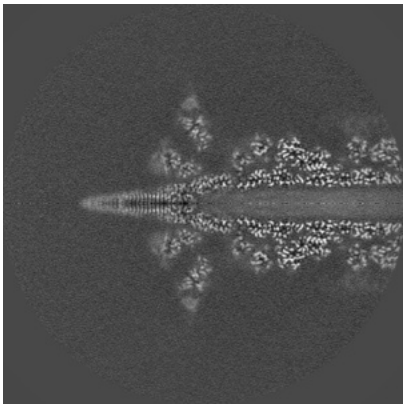

X Index: 180

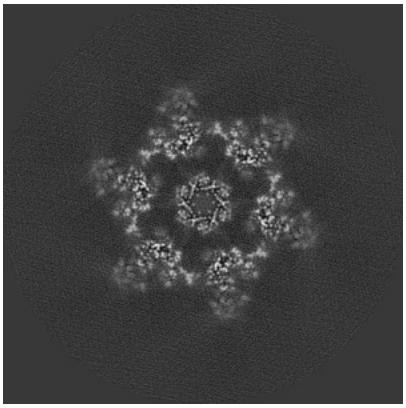

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

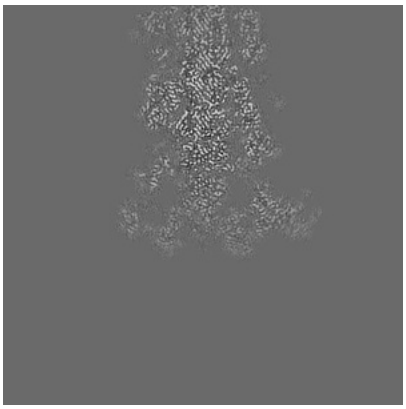

Y Index: 180


Z Index: 180

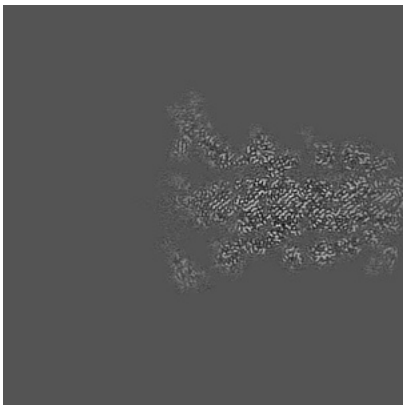
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

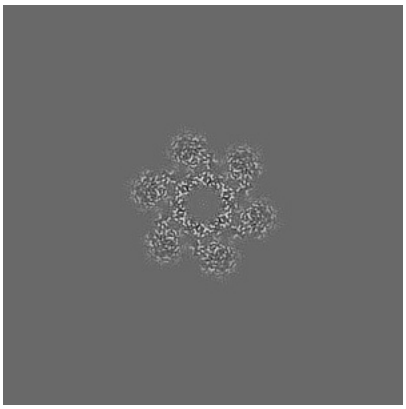
6.3.1 Primary map



X Index: 162

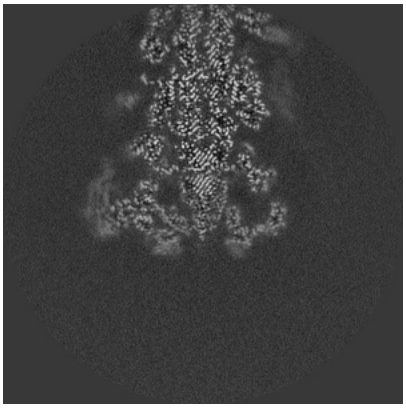


Y Index: 163

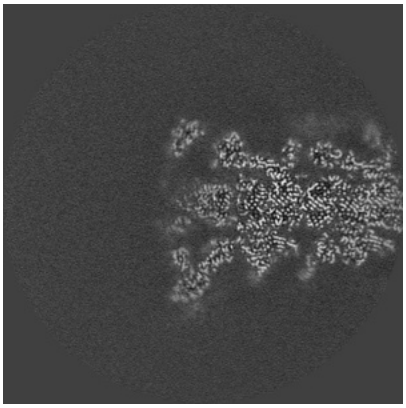


Z Index: 232

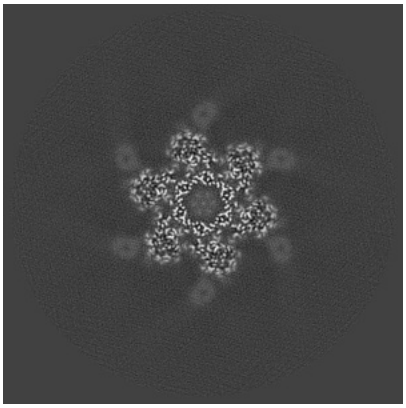
6.3.2 Raw map



X Index: 196



Y Index: 199

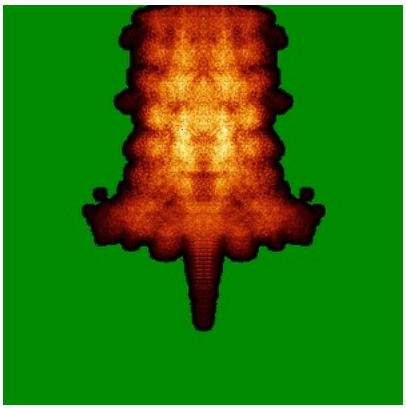


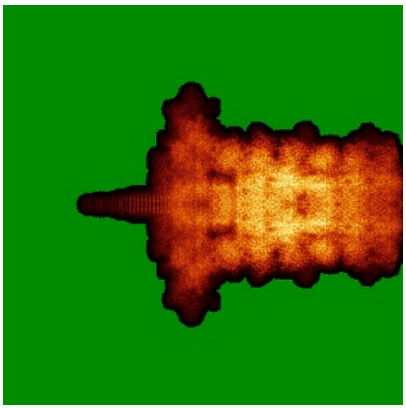
Z Index: 232

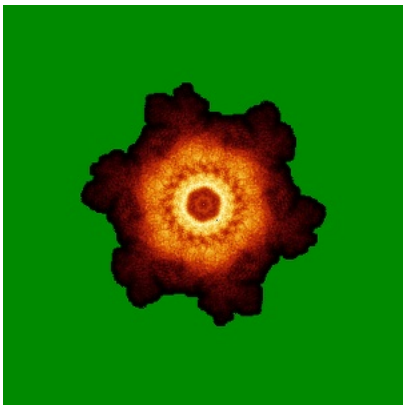
The images above show the largest variance slices of the map in three orthogonal directions.

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

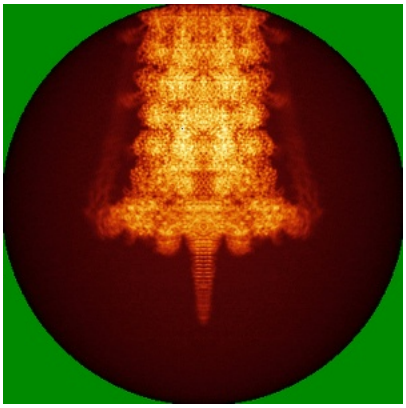
6.4.1 Primary map

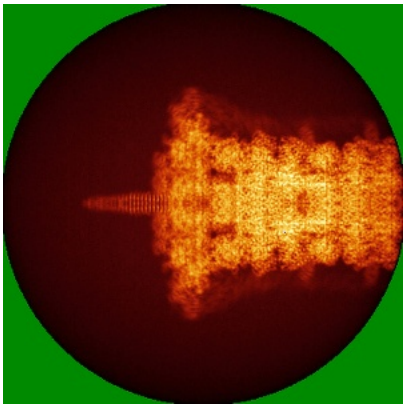

X

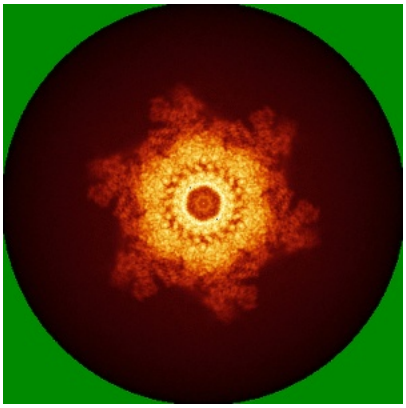

Y


Z

6.4.2 Raw map


X

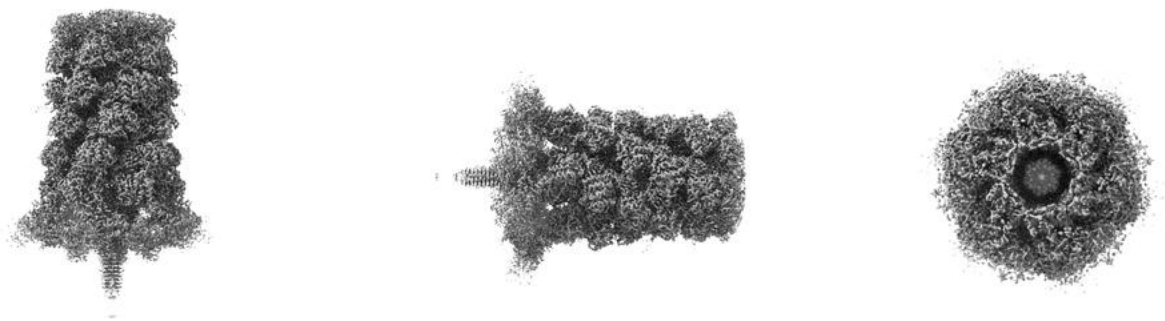

Y


Z

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

6.5 Orthogonal surface views (i)

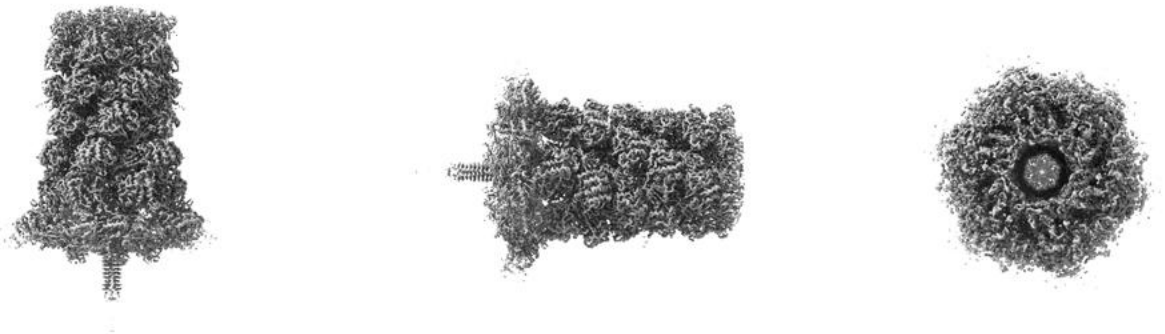
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

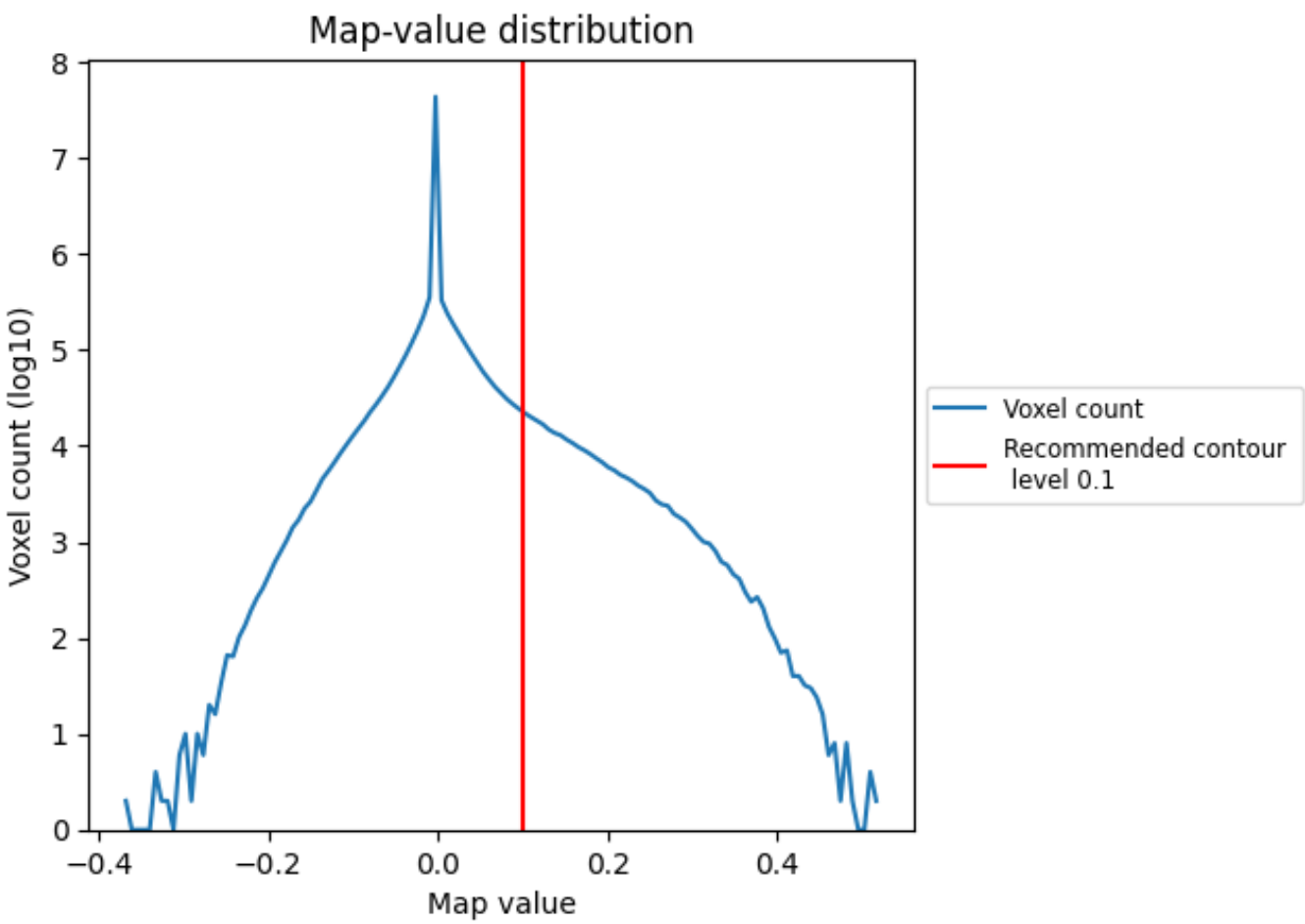
6.6 Mask visualisation (i)

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

7 Map analysis (i)

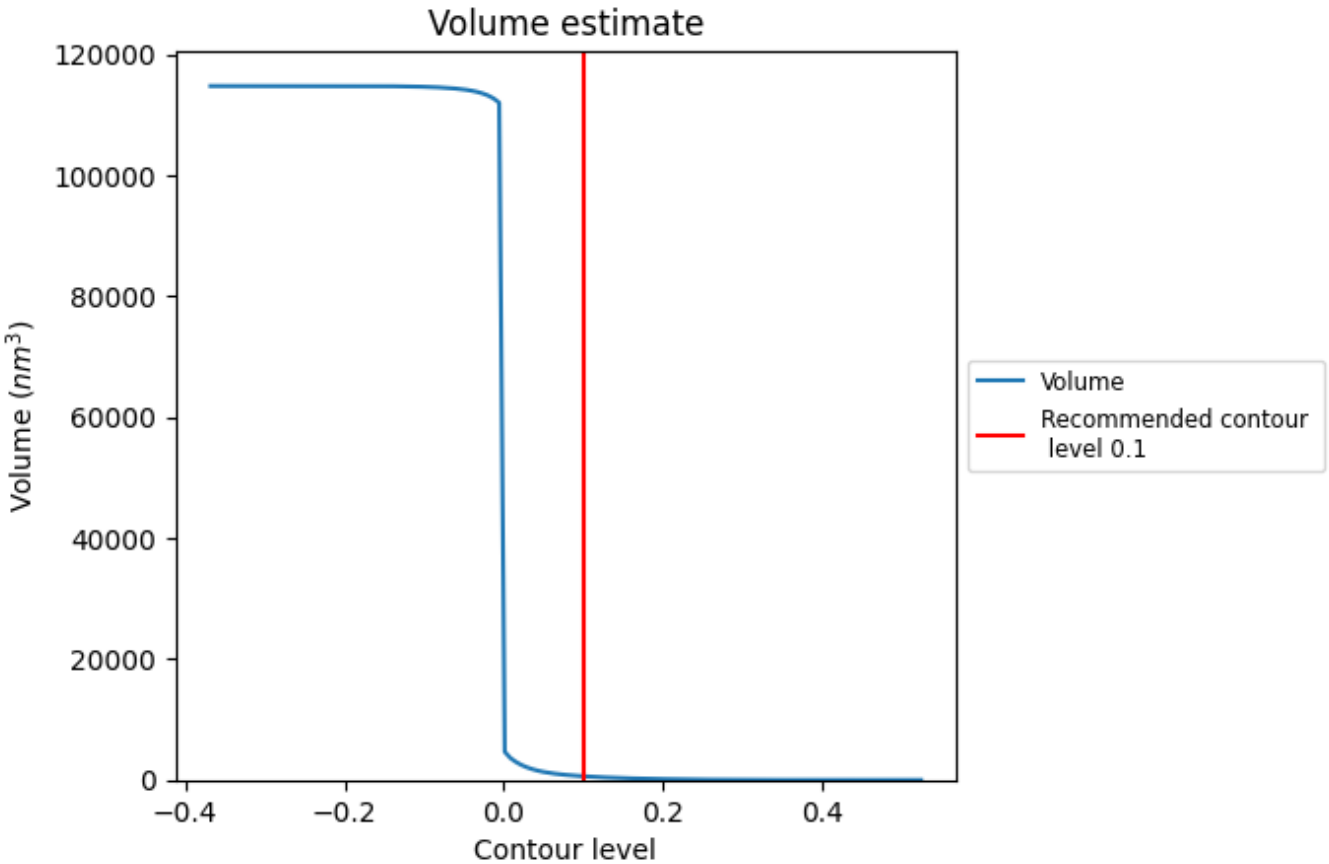
This section contains the results of statistical analysis of the map.

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.

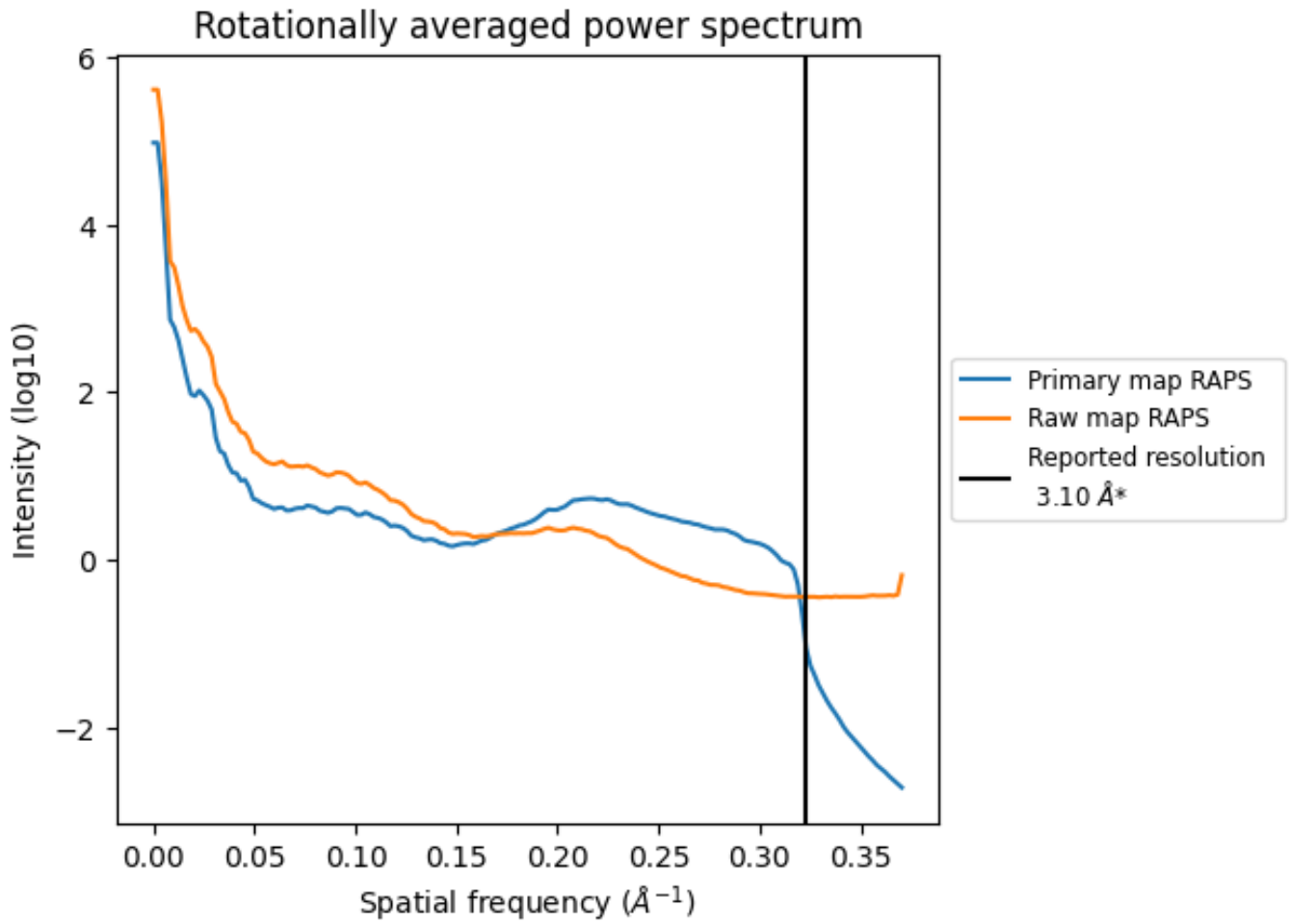
7.2 Volume estimate (i)



The volume at the recommended contour level is 613 nm^3; this corresponds to an approximate mass of 554 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)

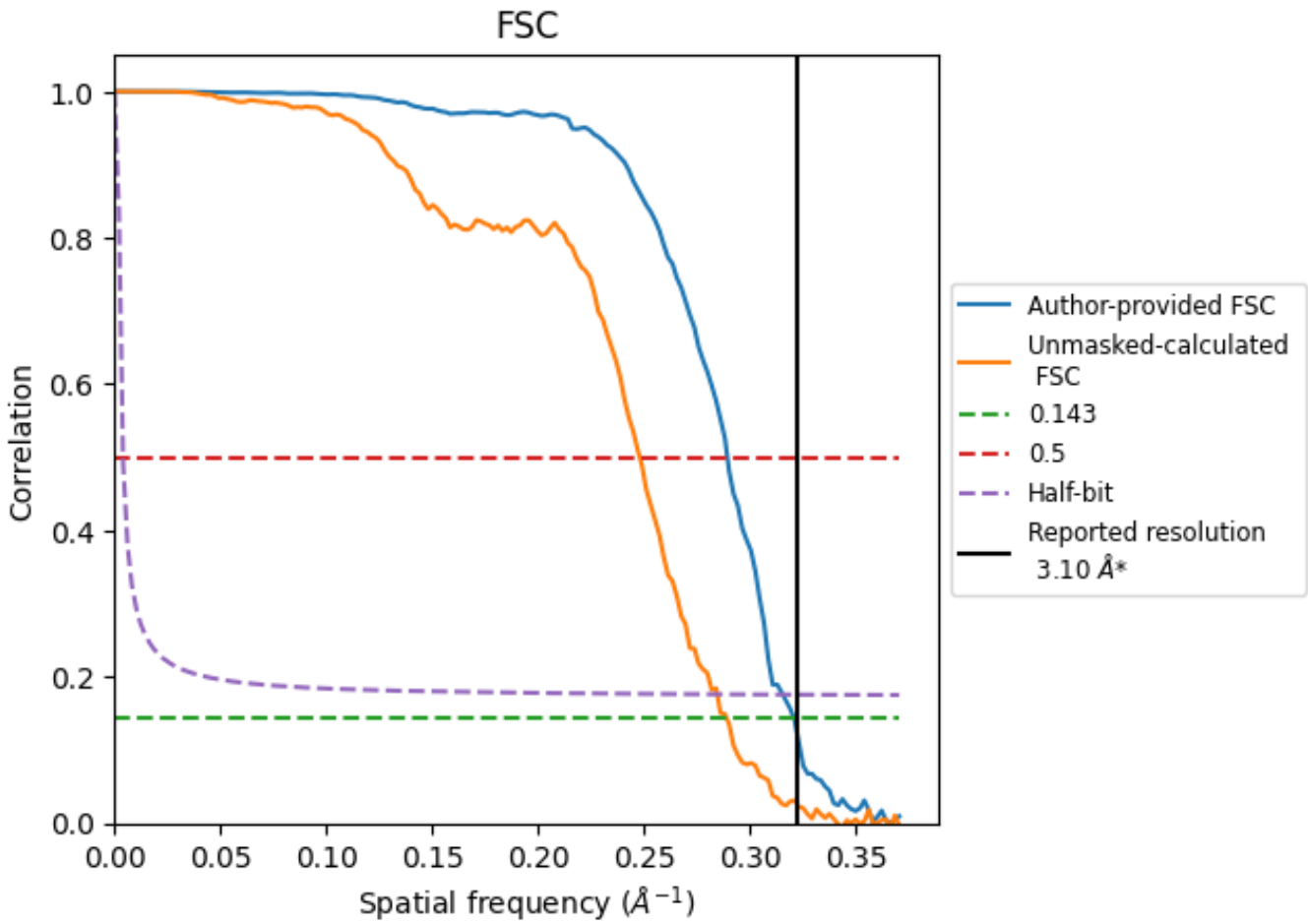


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.46	3.17
Unmasked-calculated*	3.46	4.03	3.51

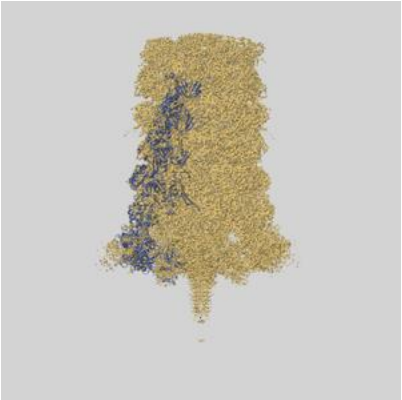
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 3.1 by more than 10 %

9 Map-model fit (i)

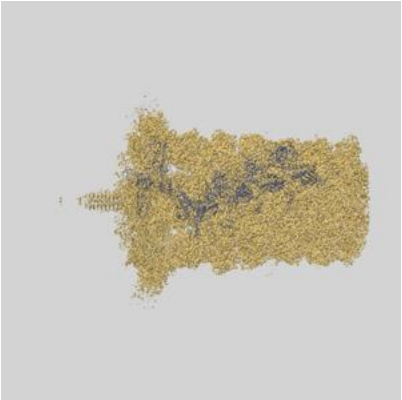
This section contains information regarding the fit between EMDB map EMD-4782 and PDB model 6RAO. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

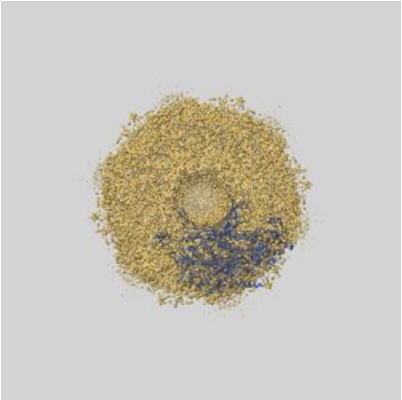
9.1.1 Map-model overlay (i)



X

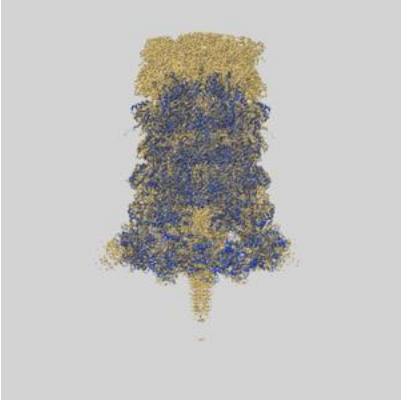


Y

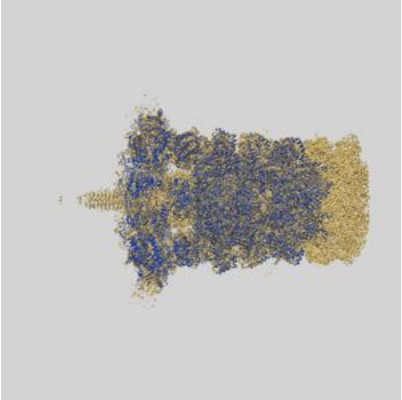


Z

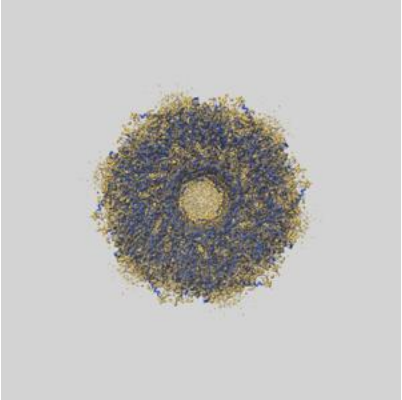
9.1.2 Map-model assembly overlay (i)



X



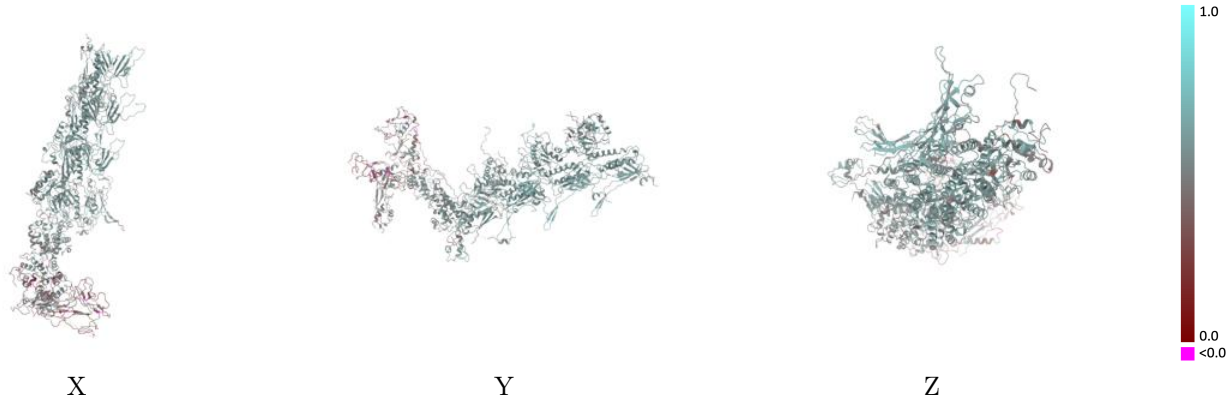
Y



Z

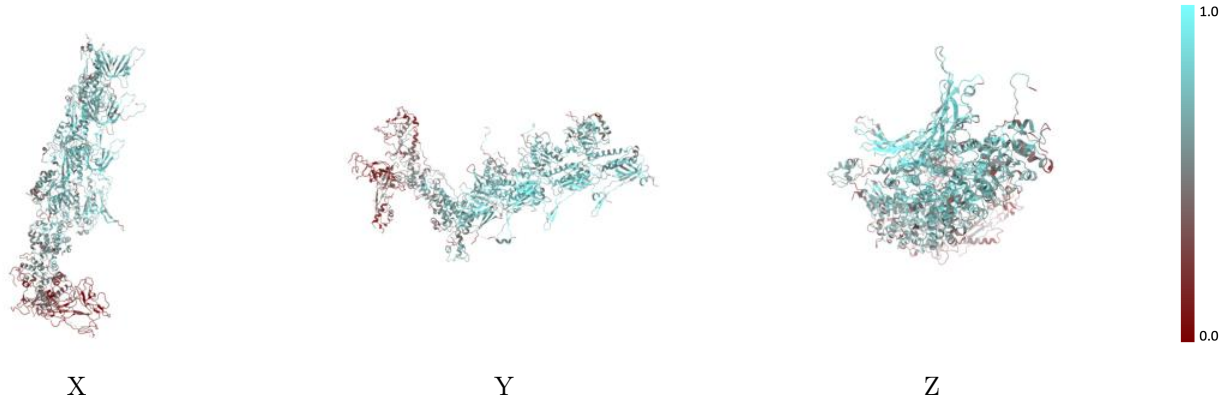
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



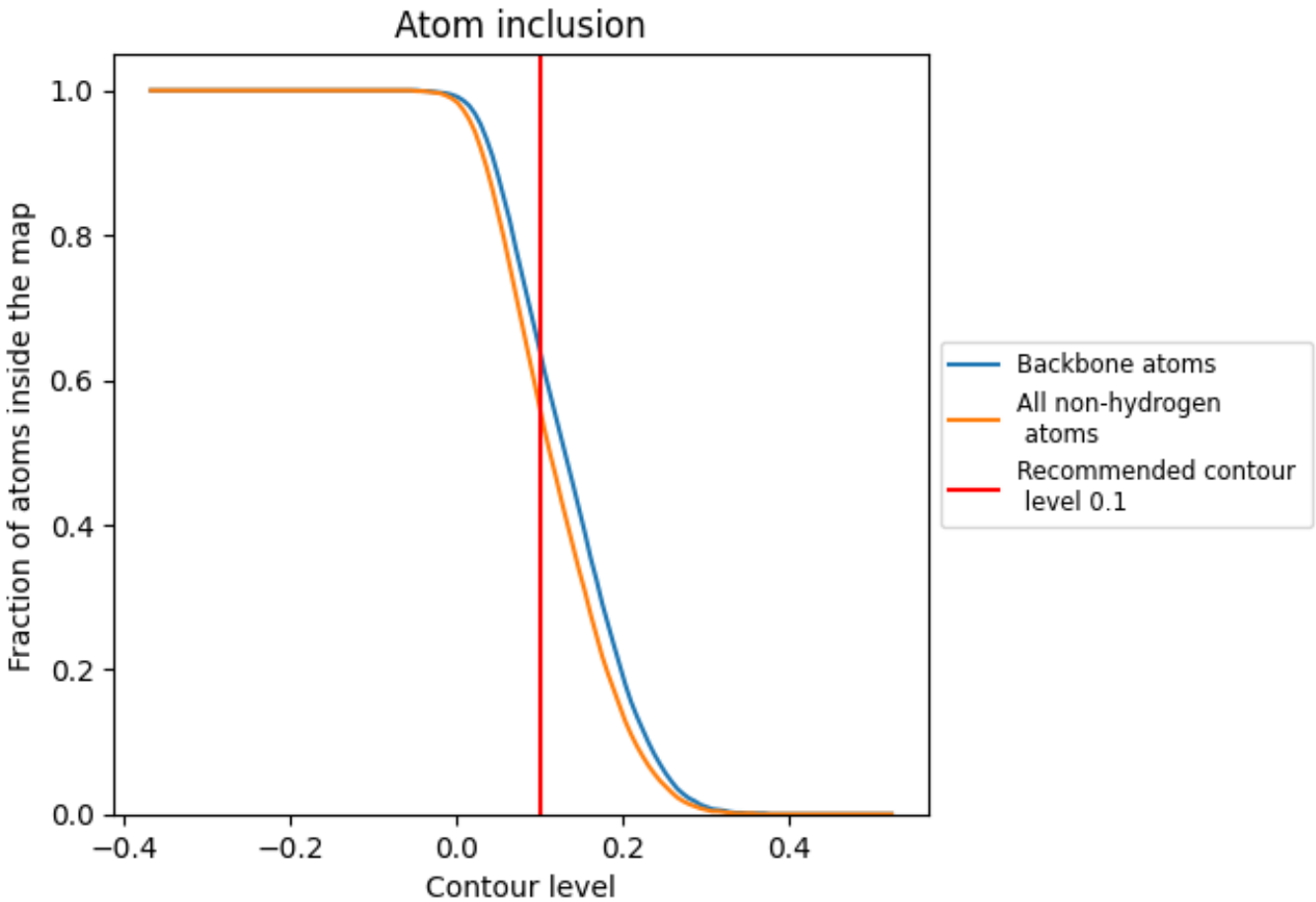
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 56% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.5100
A	0.6860	0.5610
B	0.7450	0.5830
C	0.6920	0.5710
D	0.6390	0.5360
E	0.6470	0.5550
F	0.7860	0.5880
G	0.6690	0.5290
H	0.6260	0.5420
I	0.2970	0.4120
J	0.3900	0.4300