



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:23 AM UTC

PDB ID : 6U5J / pdb_00006u5j
EMDB ID : EMD-20647
Title : CryoEM Structure of Pyocin R2 - postcontracted - collar
Authors : Ge, P.; Avaylon, J.; Scholl, D.; Shneider, M.M.; Browning, C.; Buth, S.A.; Plattner, M.; Ding, K.; Leiman, P.G.; Miller, J.F.; Zhou, Z.H.
Deposited on : 2019-08-27
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

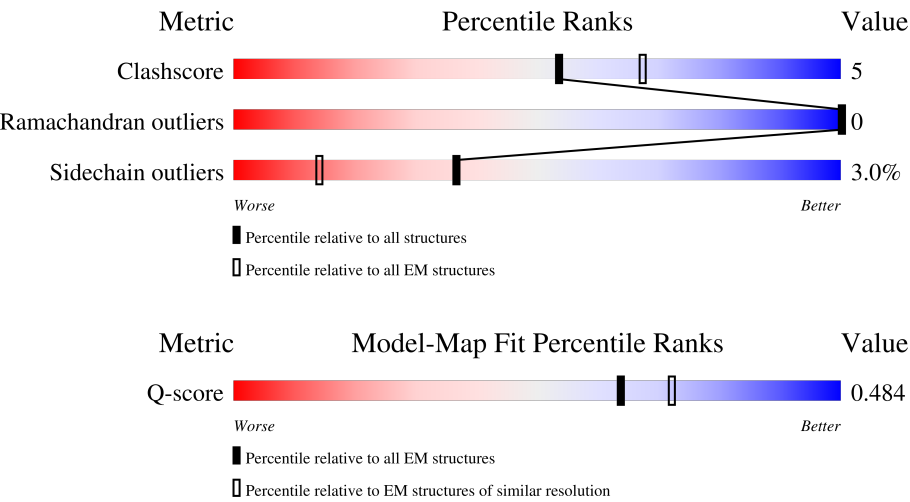
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	91% 85%11%.
1	B	171	92% 85%11%.
1	C	171	92% 85%11%.
1	D	171	92% 85%11%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	171	91% 85% 11% .
1	F	171	92% 85% 11% .
2	a	386	22% 80% 17% ..
2	b	386	24% 81% 17% ..
2	c	386	23% 81% 17% ..
2	d	386	23% 81% 16% ..
2	e	386	23% 80% 18% ..
2	f	386	22% 80% 17% ..
2	g	386	15% 85% 13% ..
2	h	386	15% 85% 13% ..
2	i	386	16% 86% 12% ..
2	j	386	16% 84% 14% ..
2	k	386	15% 85% 13% ..
2	l	386	16% 84% 14% ..
2	m	386	11% 87% 12% ..
2	n	386	12% 87% 11% ..
2	o	386	12% 87% 11% ..
2	p	386	12% 88% 11% ..
2	q	386	13% 87% 11% ..
2	r	386	12% 87% 12% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 59616 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 Collar PA0615.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		
1	B	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		
1	C	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		
1	D	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		
1	E	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		
1	F	164	Total	C	N	O	S	0	0
			1284	816	224	240	4		

- Molecule 2 is a protein called Sheath PA0622.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	b	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	c	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	d	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	e	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	f	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	g	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	h	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
2	l	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		

Continued on next page...

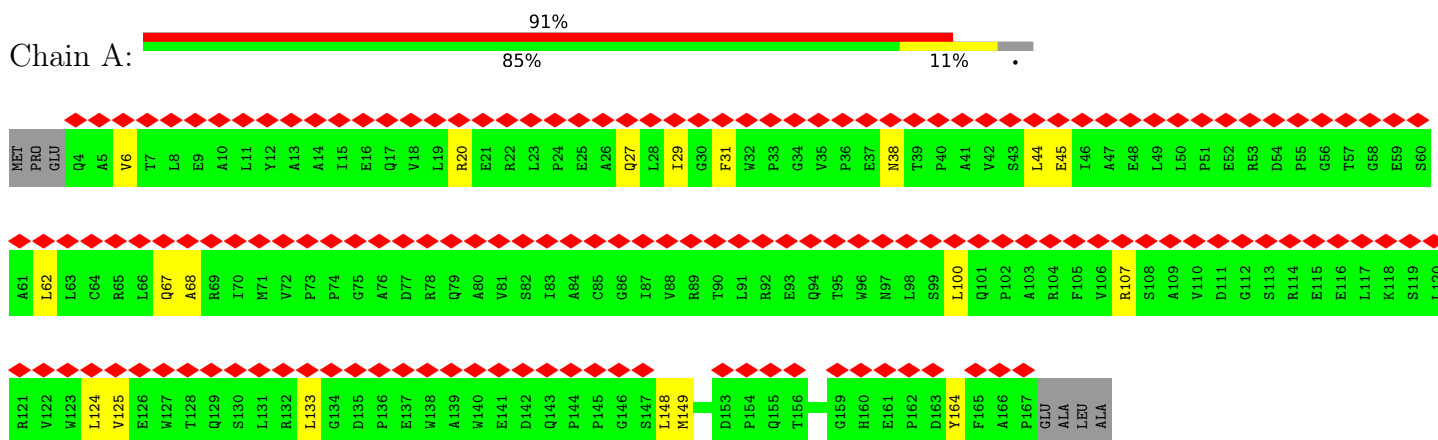
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	j	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	i	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	m	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	n	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	r	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	q	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	p	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
2	o	383	Total 2884	C 1817	N 504	O 555	S 8	0	0

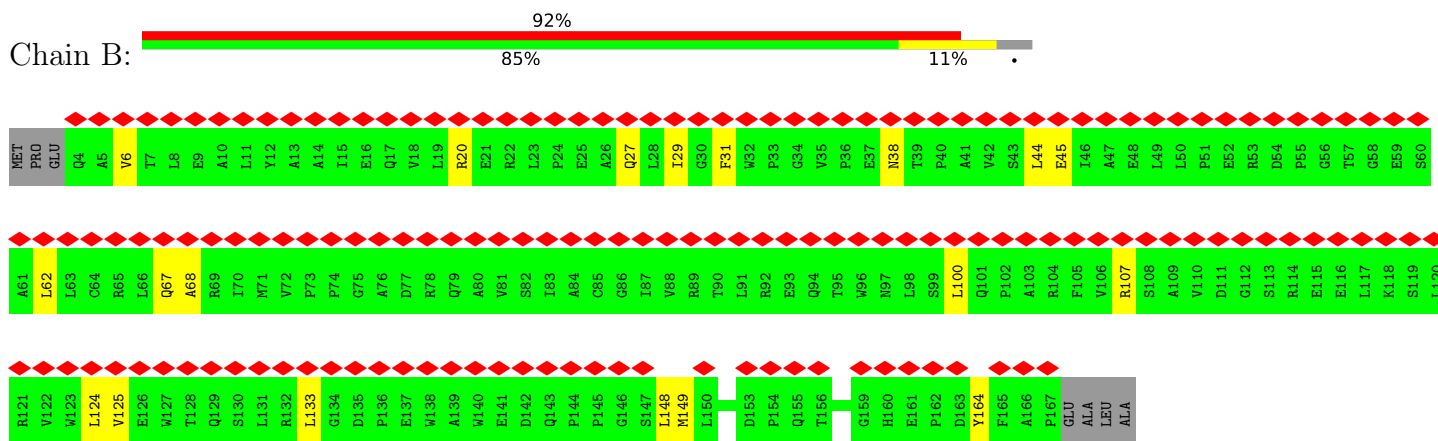
3 Residue-property plots

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.

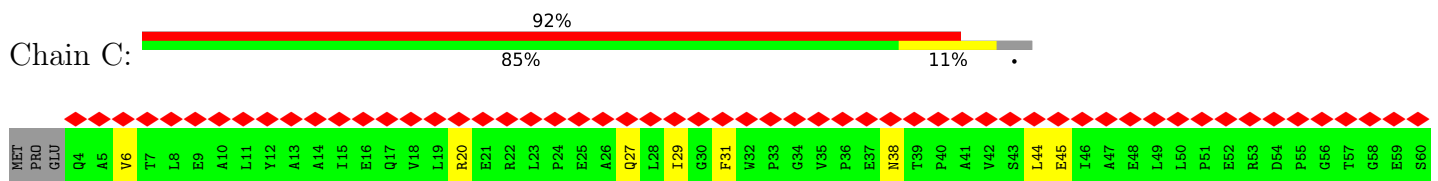
• Molecule 1: Collar PA0615

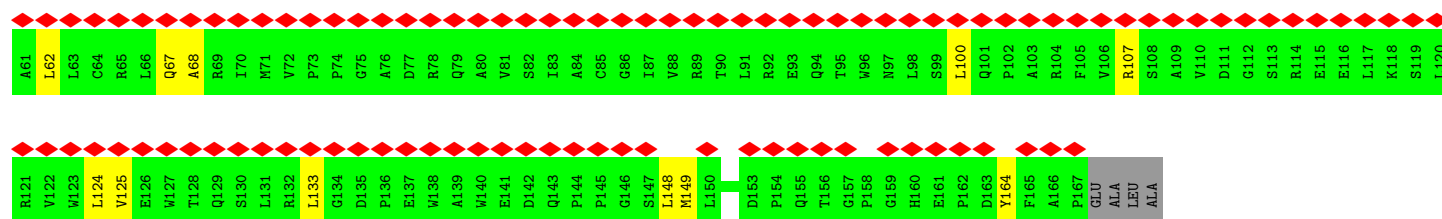


• Molecule 1: Collar PA0615

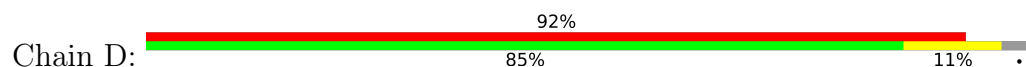


• Molecule 1: Collar PA0615

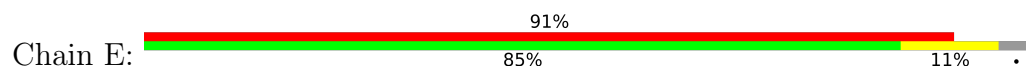




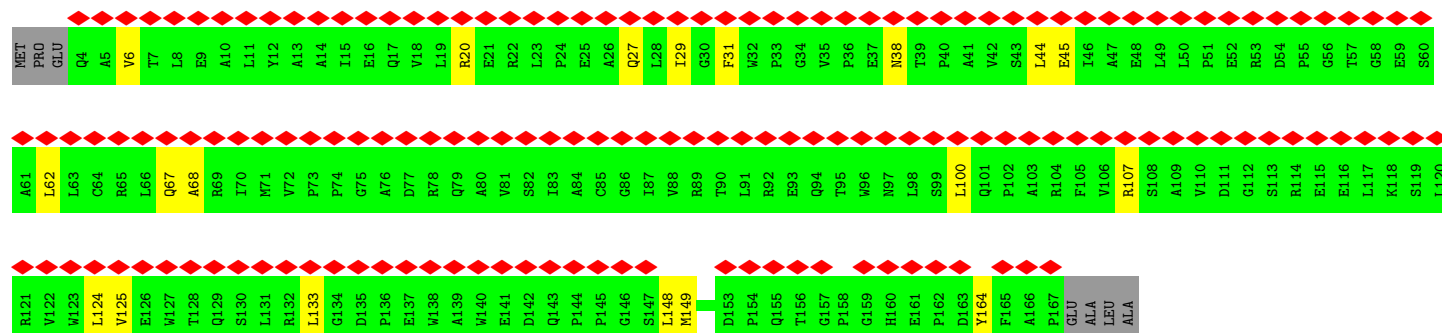
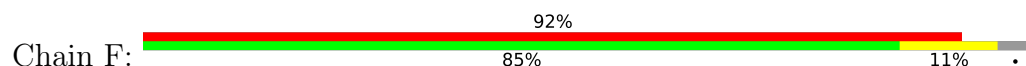
• Molecule 1: Collar PA0615



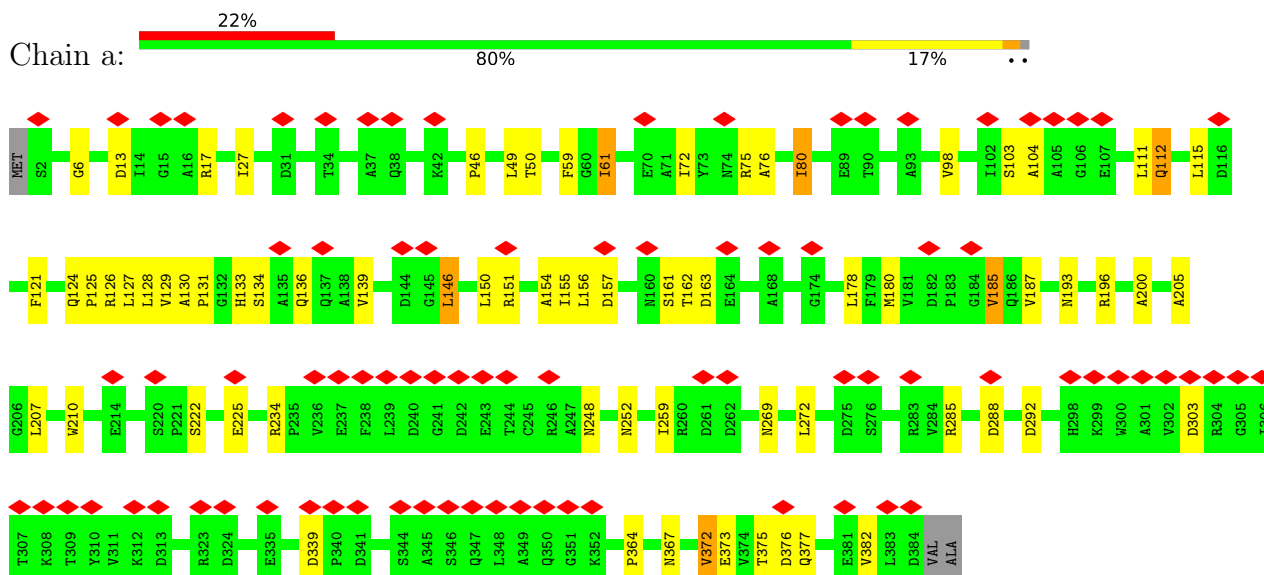
• Molecule 1: Collar PA0615



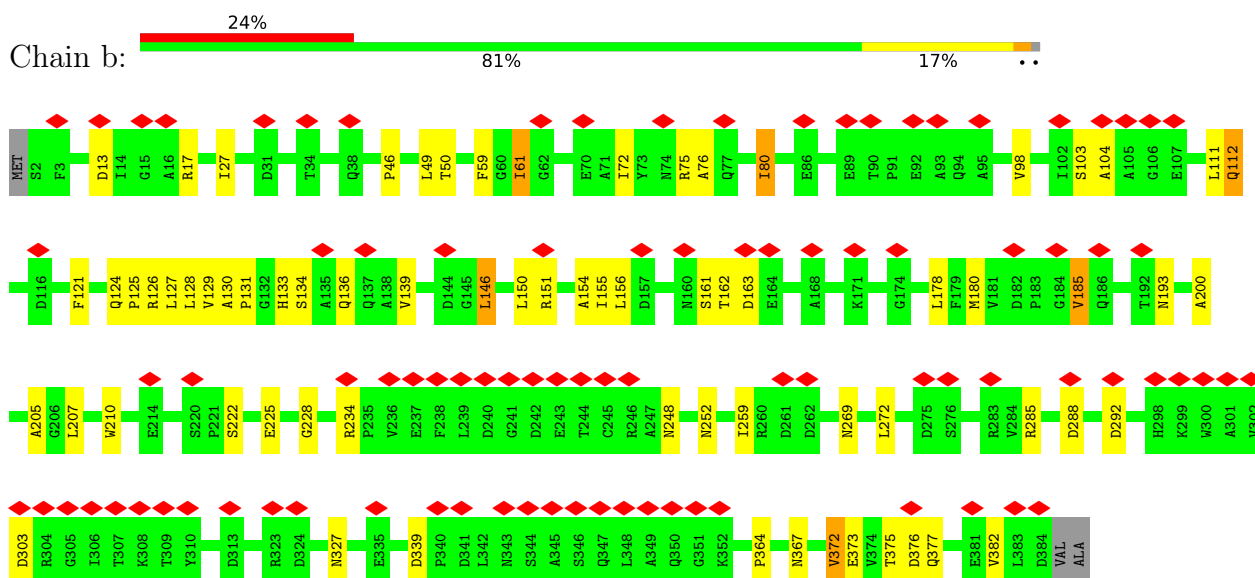
• Molecule 1: Collar PA0615



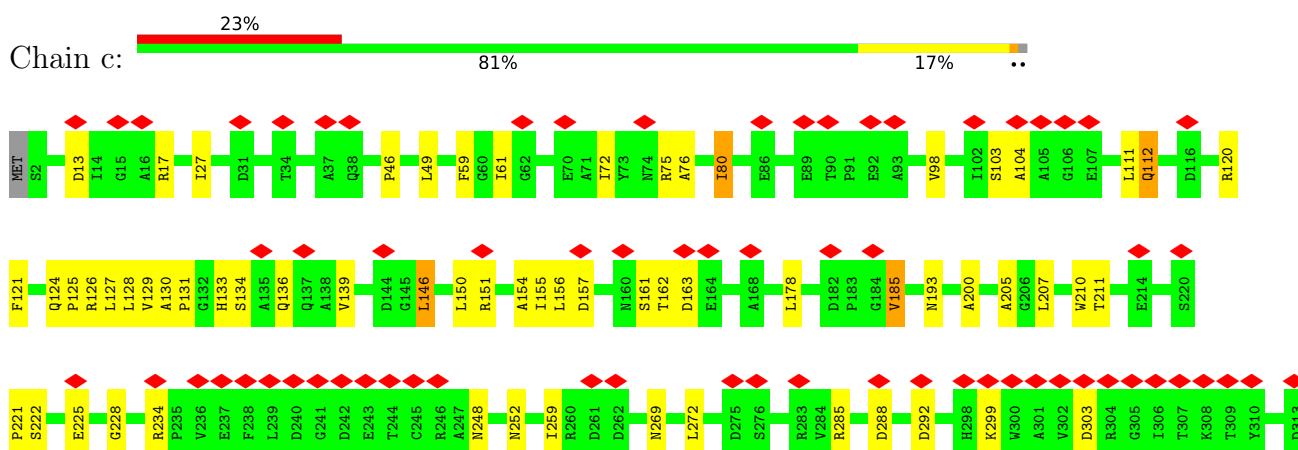
• Molecule 2: Sheath PA0622

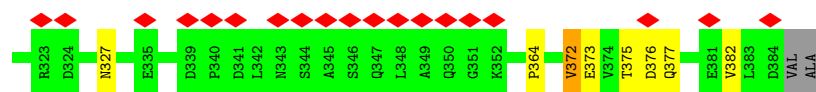


• Molecule 2: Sheath PA0622

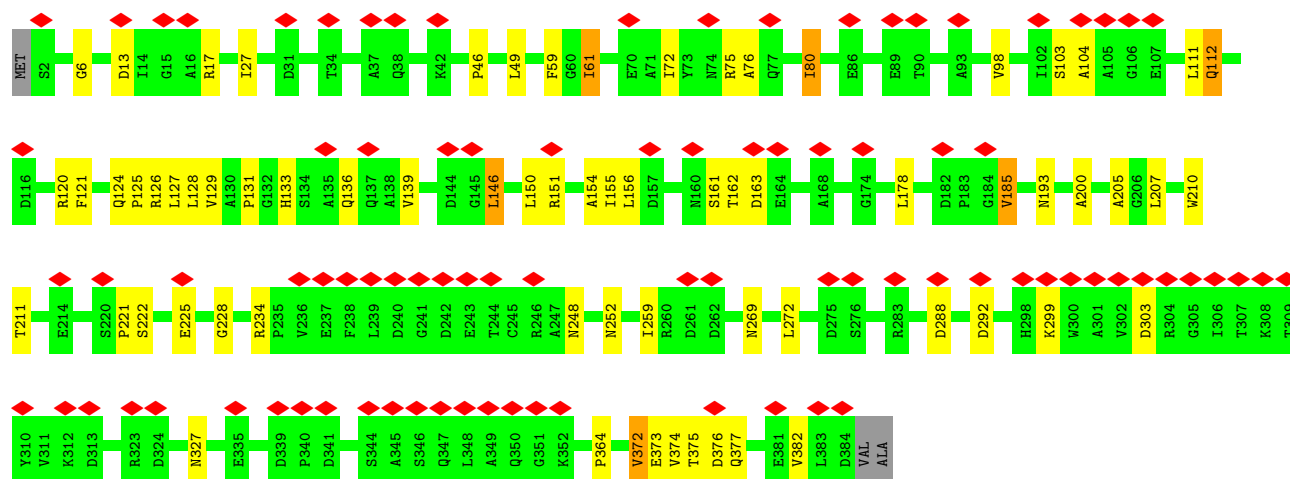
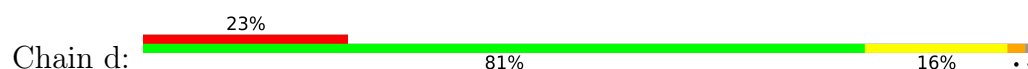


• Molecule 2: Sheath PA0622

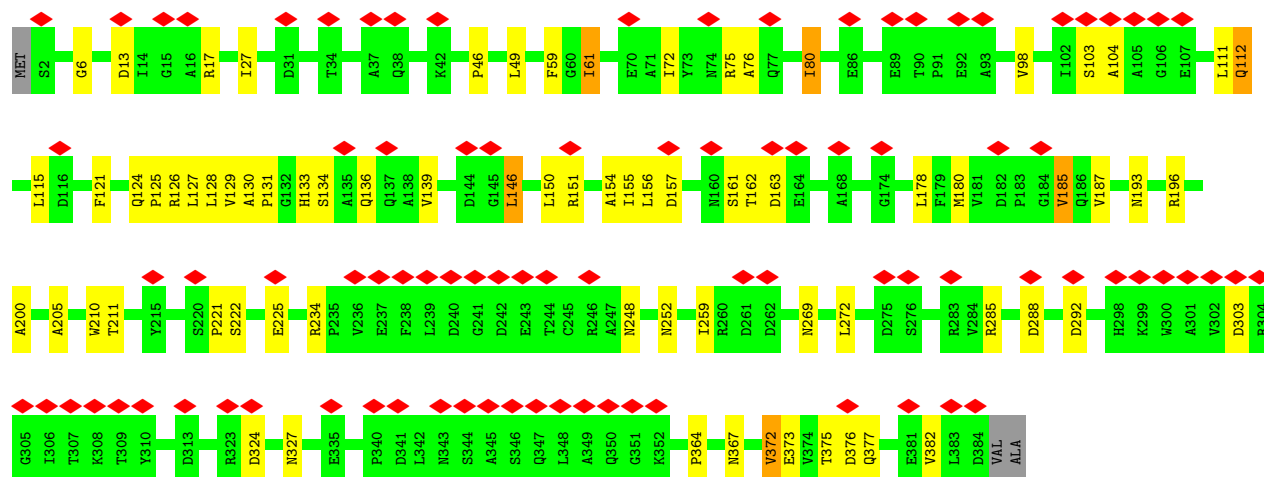
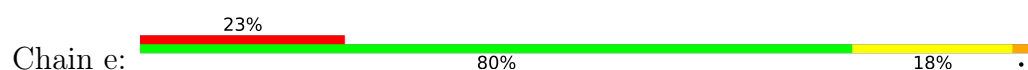




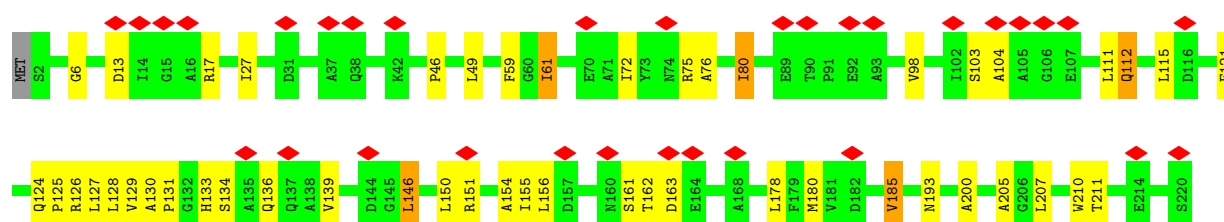
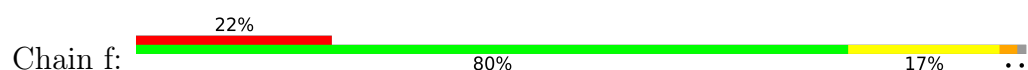
• Molecule 2: Sheath PA0622

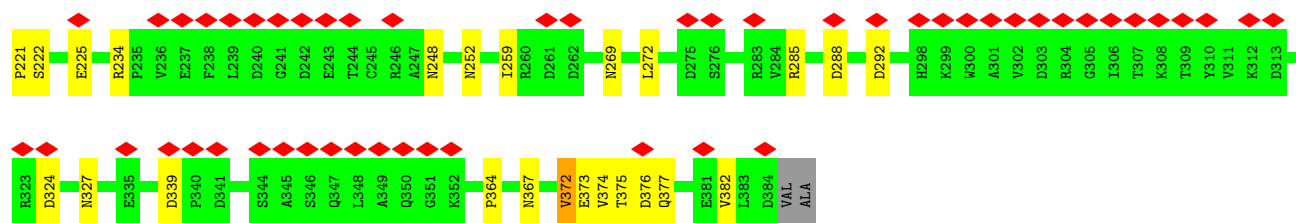


• Molecule 2: Sheath PA0622

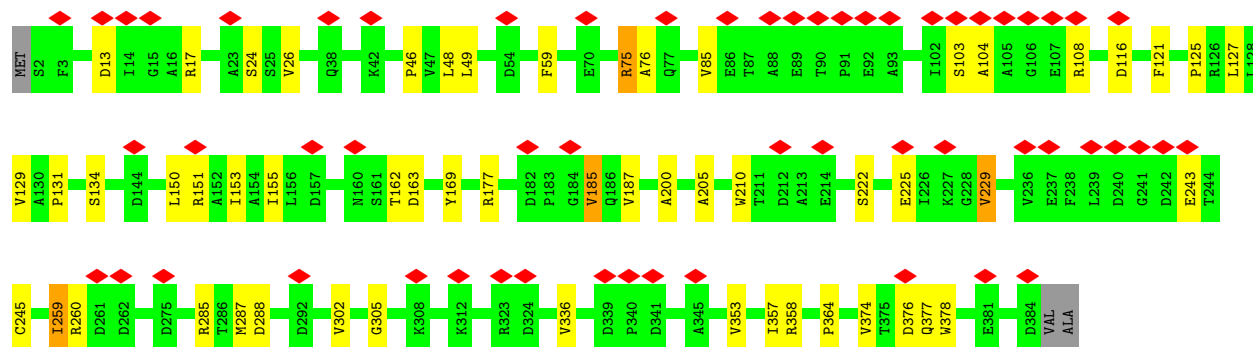
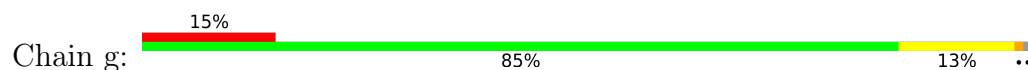


• Molecule 2: Sheath PA0622

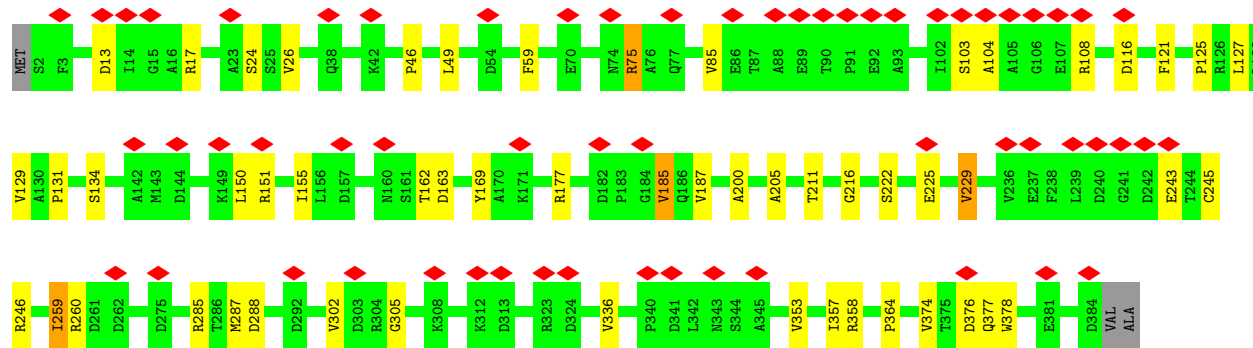
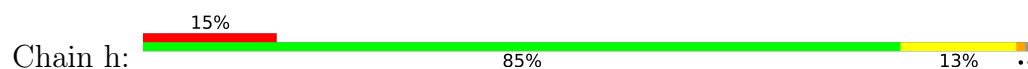




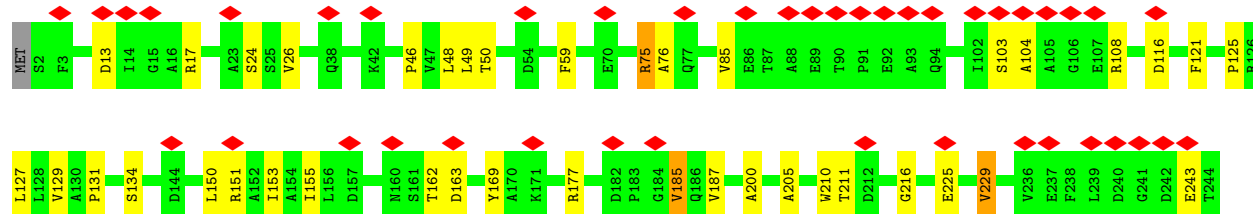
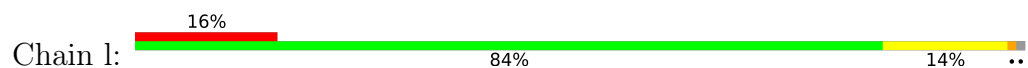
• Molecule 2: Sheath PA0622

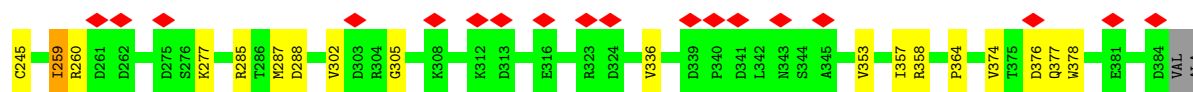


• Molecule 2: Sheath PA0622

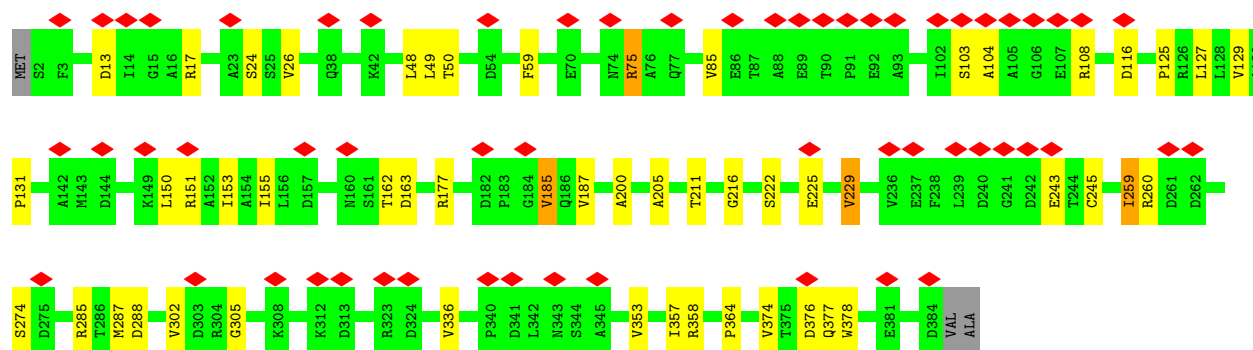
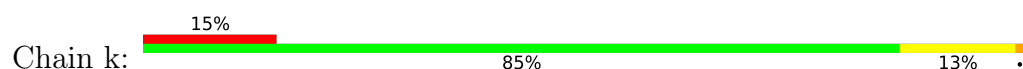


• Molecule 2: Sheath PA0622

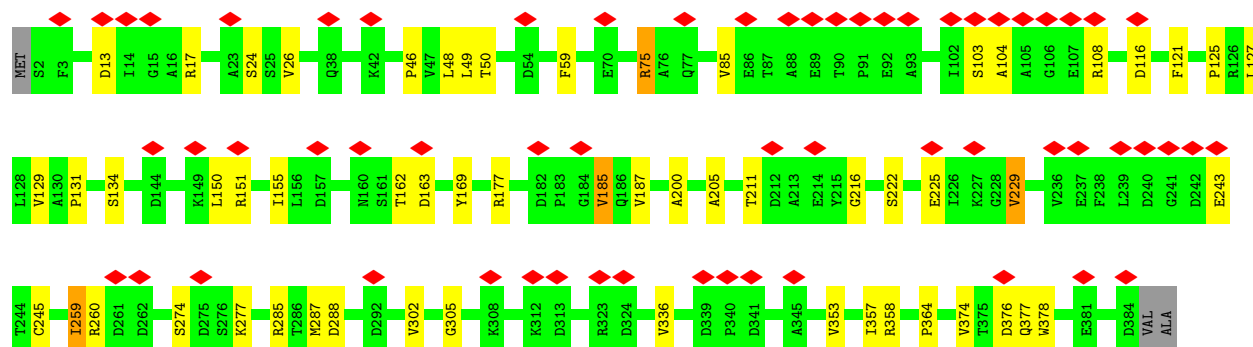
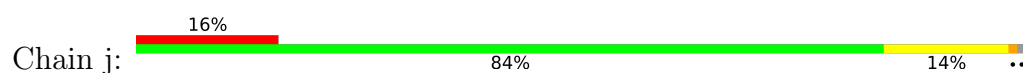




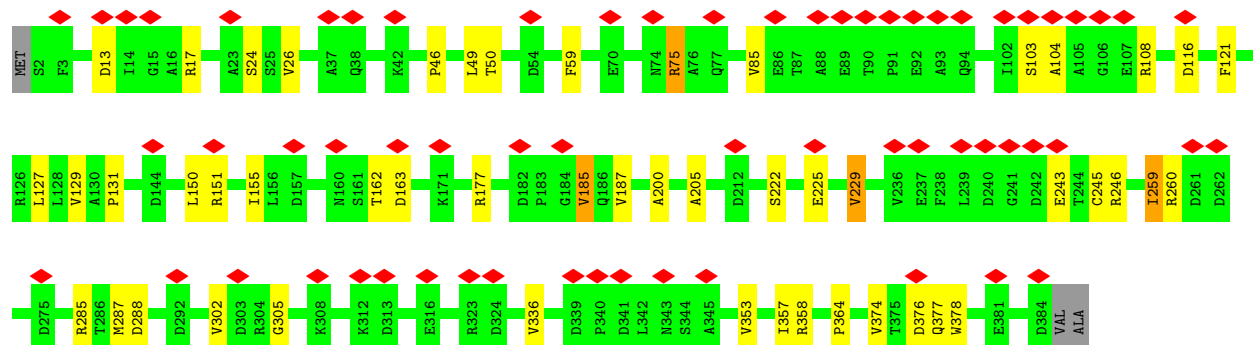
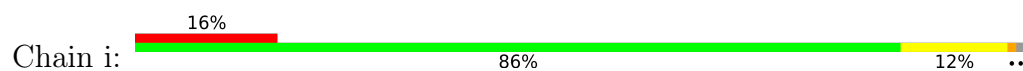
• Molecule 2: Sheath PA0622



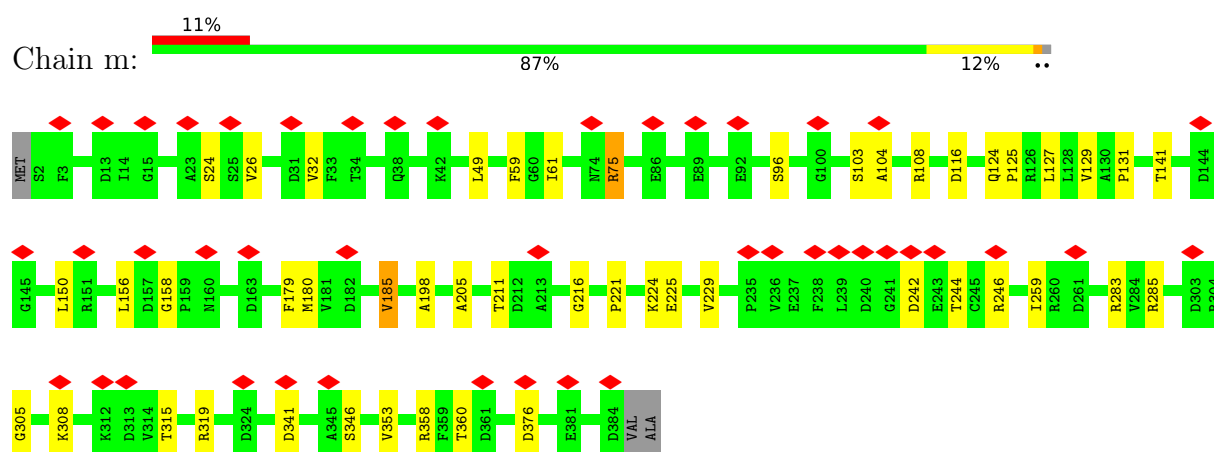
• Molecule 2: Sheath PA0622



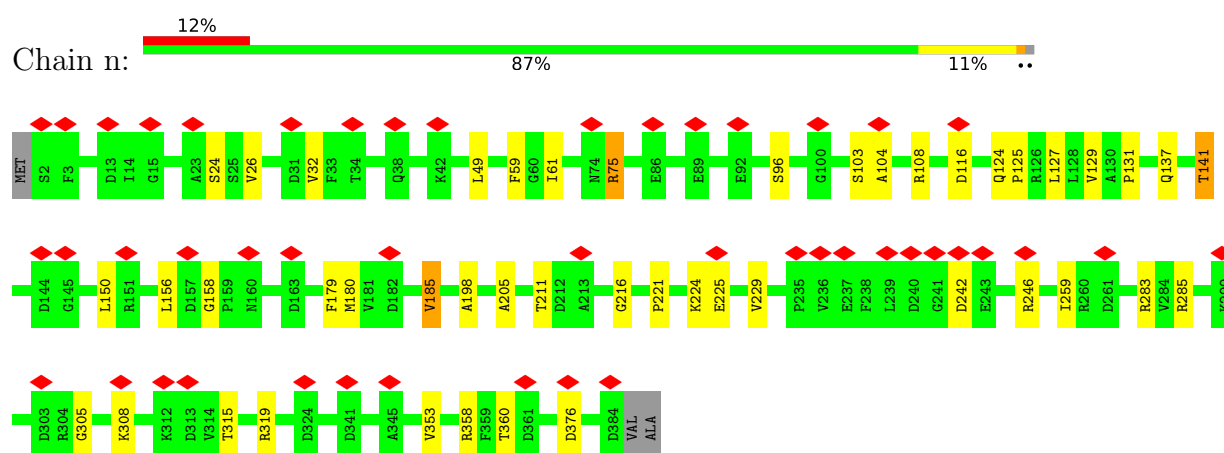
• Molecule 2: Sheath PA0622



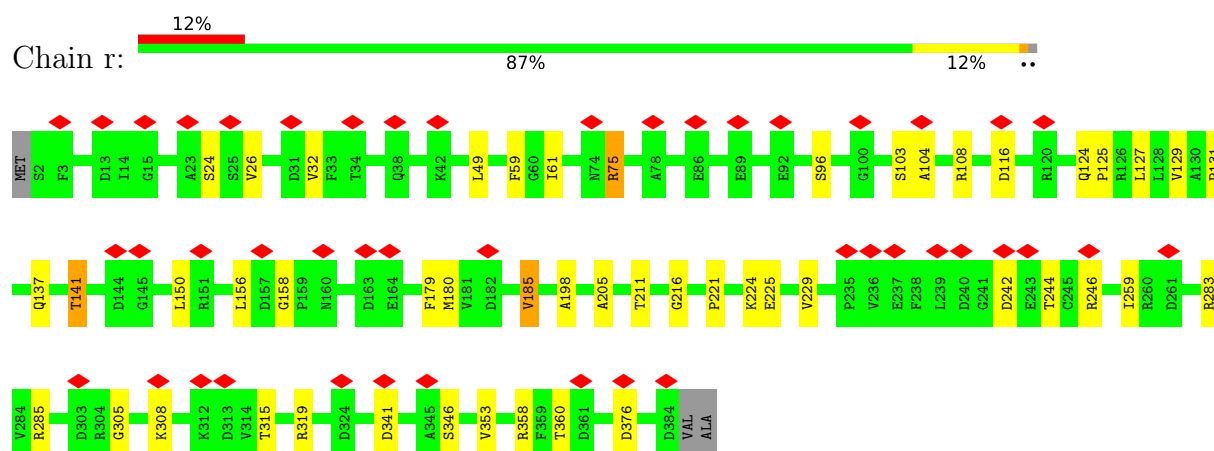
• Molecule 2: Sheath PA0622



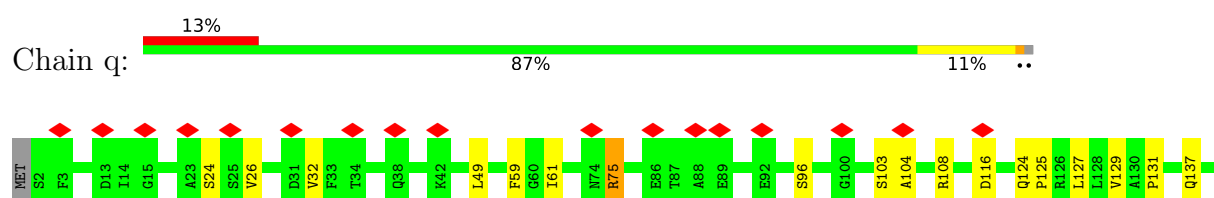
• Molecule 2: Sheath PA0622

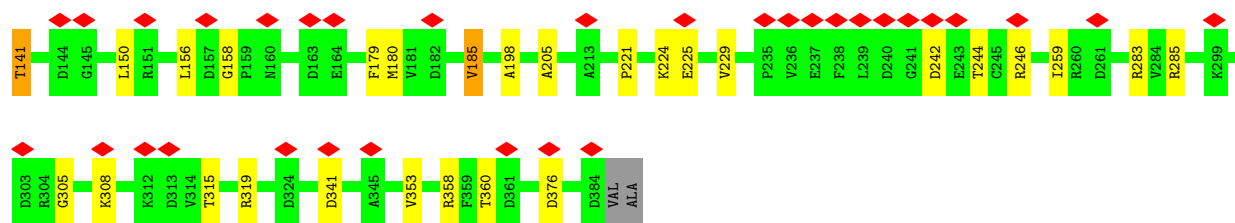


• Molecule 2: Sheath PA0622

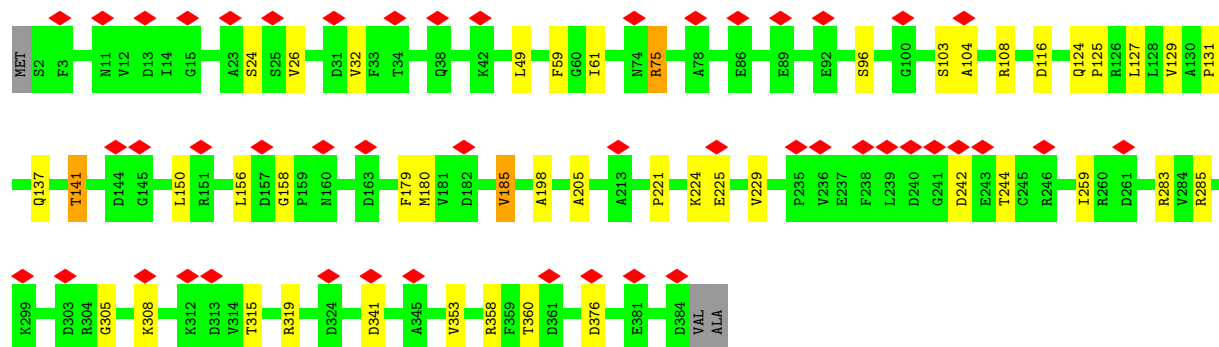
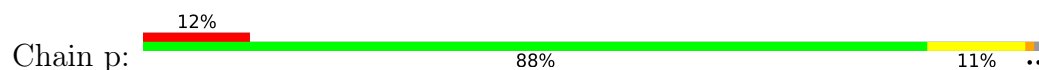


• Molecule 2: Sheath PA0622

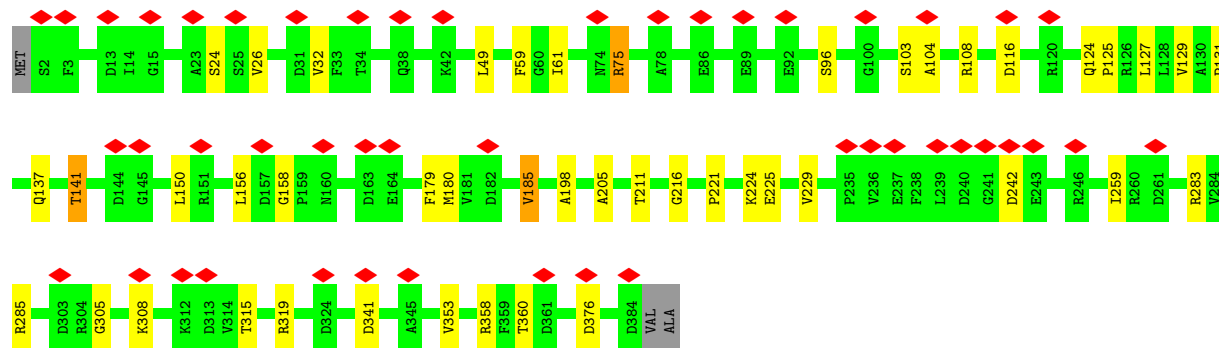
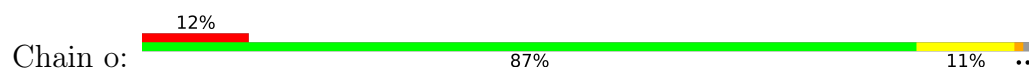




• Molecule 2: Sheath PA0622



• Molecule 2: Sheath PA0622



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	9933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	437.22, 437.22, 437.22	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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	0.18	0/1318	0.50	0/1803
1	B	0.18	0/1318	0.50	0/1803
1	C	0.18	0/1318	0.50	0/1803
1	D	0.19	0/1318	0.50	0/1803
1	E	0.18	0/1318	0.50	0/1803
1	F	0.18	0/1318	0.50	0/1803
2	a	0.21	0/2942	0.41	0/4010
2	b	0.21	0/2942	0.40	0/4010
2	c	0.21	0/2942	0.40	0/4010
2	d	0.21	0/2942	0.40	0/4010
2	e	0.21	0/2942	0.40	0/4010
2	f	0.21	0/2942	0.40	0/4010
2	g	0.23	0/2942	0.41	0/4010
2	h	0.23	0/2942	0.40	0/4010
2	i	0.23	0/2942	0.40	0/4010
2	j	0.23	0/2942	0.40	0/4010
2	k	0.23	0/2942	0.40	0/4010
2	l	0.23	0/2942	0.40	0/4010
2	m	0.23	0/2942	0.42	0/4010
2	n	0.23	0/2942	0.42	0/4010
2	o	0.23	0/2942	0.42	0/4010
2	p	0.23	0/2942	0.42	0/4010
2	q	0.23	0/2942	0.42	0/4010
2	r	0.23	0/2942	0.42	0/4010
All	All	0.22	0/60864	0.42	0/82998

There are no bond length outliers.

There are no bond angle outliers.

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	1284	0	1264	10	0
1	B	1284	0	1264	10	0
1	C	1284	0	1264	9	0
1	D	1284	0	1264	9	0
1	E	1284	0	1264	9	0
1	F	1284	0	1264	10	0
2	a	2884	0	2841	50	0
2	b	2884	0	2841	46	0
2	c	2884	0	2841	45	0
2	d	2884	0	2841	44	0
2	e	2884	0	2841	48	0
2	f	2884	0	2841	49	0
2	g	2884	0	2841	32	0
2	h	2884	0	2841	31	0
2	i	2884	0	2841	31	0
2	j	2884	0	2841	34	0
2	k	2884	0	2841	32	0
2	l	2884	0	2841	34	0
2	m	2884	0	2841	27	0
2	n	2884	0	2841	25	0
2	o	2884	0	2841	26	0
2	p	2884	0	2841	27	0
2	q	2884	0	2841	28	0
2	r	2884	0	2841	28	0
All	All	59616	0	58722	603	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 5.

All (603) 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)
2:e:129:VAL:HG21	2:e:205:ALA:HB2	1.83	0.60
2:f:129:VAL:HG21	2:f:205:ALA:HB2	1.83	0.60
2:r:24:SER:O	2:r:285:ARG:NH2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:129:VAL:HG21	2:d:205:ALA:HB2	1.84	0.60
2:a:129:VAL:HG21	2:a:205:ALA:HB2	1.84	0.60
2:n:24:SER:O	2:n:285:ARG:NH2	2.34	0.60
2:q:24:SER:O	2:q:285:ARG:NH2	2.34	0.60
2:o:24:SER:O	2:o:285:ARG:NH2	2.34	0.60
2:b:129:VAL:HG21	2:b:205:ALA:HB2	1.84	0.60
2:c:129:VAL:HG21	2:c:205:ALA:HB2	1.84	0.59
2:m:24:SER:O	2:m:285:ARG:NH2	2.34	0.59
2:p:24:SER:O	2:p:285:ARG:NH2	2.34	0.59
1:B:27:GLN:HE22	1:B:38:ASN:HB3	1.68	0.58
1:C:27:GLN:HE22	1:C:38:ASN:HB3	1.68	0.58
2:a:151:ARG:HB3	2:a:288:ASP:HB3	1.86	0.58
2:b:151:ARG:HB3	2:b:288:ASP:HB3	1.86	0.58
2:e:151:ARG:HB3	2:e:288:ASP:HB3	1.86	0.57
1:D:27:GLN:HE22	1:D:38:ASN:HB3	1.68	0.57
2:d:151:ARG:HB3	2:d:288:ASP:HB3	1.86	0.57
1:A:27:GLN:HE22	1:A:38:ASN:HB3	1.68	0.57
1:E:27:GLN:HE22	1:E:38:ASN:HB3	1.68	0.57
1:F:27:GLN:HE22	1:F:38:ASN:HB3	1.68	0.57
2:e:75:ARG:NH1	2:e:225:GLU:O	2.38	0.57
1:C:20:ARG:NH2	1:C:29:ILE:O	2.38	0.57
2:c:151:ARG:HB3	2:c:288:ASP:HB3	1.86	0.57
2:c:75:ARG:NH1	2:c:225:GLU:O	2.38	0.57
1:B:20:ARG:NH2	1:B:29:ILE:O	2.38	0.56
2:f:151:ARG:HB3	2:f:288:ASP:HB3	1.86	0.56
1:D:20:ARG:NH2	1:D:29:ILE:O	2.38	0.56
1:A:20:ARG:NH2	1:A:29:ILE:O	2.38	0.56
2:c:163:ASP:OD1	2:c:234:ARG:NH1	2.39	0.56
2:f:193:ASN:ND2	2:m:96:SER:OG	2.39	0.56
1:F:20:ARG:NH2	1:F:29:ILE:O	2.38	0.55
2:f:75:ARG:NH1	2:f:225:GLU:O	2.38	0.55
1:E:20:ARG:NH2	1:E:29:ILE:O	2.38	0.55
2:b:163:ASP:OD1	2:b:234:ARG:NH1	2.39	0.55
2:g:129:VAL:HG21	2:g:205:ALA:HB2	1.89	0.55
2:k:129:VAL:HG21	2:k:205:ALA:HB2	1.89	0.55
2:n:108:ARG:NH1	2:n:116:ASP:OD1	2.40	0.55
2:o:108:ARG:NH1	2:o:116:ASP:OD1	2.39	0.55
2:d:163:ASP:OD1	2:d:234:ARG:NH1	2.39	0.55
2:e:163:ASP:OD1	2:e:234:ARG:NH1	2.39	0.55
2:m:108:ARG:NH1	2:m:116:ASP:OD1	2.40	0.55
2:b:75:ARG:NH1	2:b:225:GLU:O	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:108:ARG:NH1	2:p:116:ASP:OD1	2.40	0.55
2:f:163:ASP:OD1	2:f:234:ARG:NH1	2.39	0.55
2:r:108:ARG:NH1	2:r:116:ASP:OD1	2.40	0.55
2:l:129:VAL:HG21	2:l:205:ALA:HB2	1.89	0.55
2:q:108:ARG:NH1	2:q:116:ASP:OD1	2.40	0.55
2:j:129:VAL:HG21	2:j:205:ALA:HB2	1.89	0.55
2:a:163:ASP:OD1	2:a:234:ARG:NH1	2.39	0.55
2:p:129:VAL:HG21	2:p:205:ALA:HB2	1.89	0.55
2:b:373:GLU:OE2	2:h:358:ARG:NH1	2.40	0.54
2:h:129:VAL:HG21	2:h:205:ALA:HB2	1.89	0.54
2:a:75:ARG:NH1	2:a:225:GLU:O	2.38	0.54
2:d:373:GLU:OE2	2:j:358:ARG:NH1	2.40	0.54
2:e:373:GLU:OE2	2:k:358:ARG:NH1	2.40	0.54
2:a:373:GLU:OE2	2:g:358:ARG:NH1	2.40	0.54
2:d:193:ASN:ND2	2:q:96:SER:OG	2.41	0.54
2:i:129:VAL:HG21	2:i:205:ALA:HB2	1.89	0.54
2:o:129:VAL:HG21	2:o:205:ALA:HB2	1.89	0.54
2:f:373:GLU:OE2	2:l:358:ARG:NH1	2.40	0.54
2:q:129:VAL:HG21	2:q:205:ALA:HB2	1.89	0.54
2:k:24:SER:O	2:k:285:ARG:NH2	2.41	0.54
2:h:24:SER:O	2:h:285:ARG:NH2	2.41	0.54
2:l:187:VAL:HG23	2:l:229:VAL:HA	1.90	0.54
2:k:187:VAL:HG23	2:k:229:VAL:HA	1.90	0.54
2:m:129:VAL:HG21	2:m:205:ALA:HB2	1.89	0.54
2:g:24:SER:O	2:g:285:ARG:NH2	2.41	0.53
2:l:24:SER:O	2:l:285:ARG:NH2	2.41	0.53
2:j:24:SER:O	2:j:285:ARG:NH2	2.41	0.53
2:d:303:ASP:OD1	2:d:303:ASP:N	2.41	0.53
2:i:24:SER:O	2:i:285:ARG:NH2	2.41	0.53
2:c:373:GLU:OE2	2:i:358:ARG:NH1	2.40	0.53
2:g:187:VAL:HG23	2:g:229:VAL:HA	1.90	0.53
2:j:13:ASP:OD1	2:j:17:ARG:NH2	2.42	0.53
2:e:193:ASN:ND2	2:r:96:SER:OG	2.41	0.53
2:h:187:VAL:HG23	2:h:229:VAL:HA	1.90	0.53
2:l:108:ARG:NH1	2:l:116:ASP:OD1	2.42	0.53
2:a:222:SER:OG	2:a:269:ASN:OD1	2.27	0.53
2:f:222:SER:OG	2:f:269:ASN:OD1	2.27	0.53
2:l:13:ASP:OD1	2:l:17:ARG:NH2	2.42	0.53
2:n:129:VAL:HG21	2:n:205:ALA:HB2	1.89	0.53
2:a:303:ASP:OD1	2:a:303:ASP:N	2.42	0.53
2:k:103:SER:OG	2:k:104:ALA:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:129:VAL:HG21	2:r:205:ALA:HB2	1.89	0.53
2:l:103:SER:OG	2:l:104:ALA:N	2.42	0.53
2:j:50:THR:OG1	2:q:244:THR:O	2.27	0.53
2:j:187:VAL:HG23	2:j:229:VAL:HA	1.91	0.53
2:k:108:ARG:NH1	2:k:116:ASP:OD1	2.42	0.52
2:g:108:ARG:NH1	2:g:116:ASP:OD1	2.42	0.52
2:j:364:PRO:HA	2:p:305:GLY:HA2	1.91	0.52
2:i:187:VAL:HG23	2:i:229:VAL:HA	1.90	0.52
2:d:372:VAL:HG22	2:j:287:MET:HE1	1.92	0.52
2:e:372:VAL:HG22	2:k:287:MET:HE1	1.92	0.52
2:j:103:SER:OG	2:j:104:ALA:N	2.42	0.52
2:j:108:ARG:NH1	2:j:116:ASP:OD1	2.42	0.52
2:f:185:VAL:H	2:f:200:ALA:HB2	1.75	0.52
2:g:103:SER:OG	2:g:104:ALA:N	2.42	0.52
2:i:364:PRO:HA	2:o:305:GLY:HA2	1.91	0.52
2:k:13:ASP:OD1	2:k:17:ARG:NH2	2.42	0.52
2:r:75:ARG:NH1	2:r:225:GLU:O	2.43	0.52
2:q:75:ARG:NH1	2:q:225:GLU:O	2.43	0.52
2:b:222:SER:OG	2:b:269:ASN:OD1	2.27	0.52
2:e:222:SER:OG	2:e:269:ASN:OD1	2.27	0.52
2:c:372:VAL:HG22	2:i:287:MET:HE1	1.92	0.52
2:i:13:ASP:OD1	2:i:17:ARG:NH2	2.42	0.52
2:i:103:SER:OG	2:i:104:ALA:N	2.42	0.52
2:i:108:ARG:NH1	2:i:116:ASP:OD1	2.42	0.52
2:c:185:VAL:H	2:c:200:ALA:HB2	1.75	0.52
2:f:372:VAL:HG22	2:l:287:MET:HE1	1.92	0.52
2:h:103:SER:OG	2:h:104:ALA:N	2.42	0.52
2:g:364:PRO:HA	2:m:305:GLY:HA2	1.91	0.51
2:a:185:VAL:H	2:a:200:ALA:HB2	1.75	0.51
2:a:193:ASN:ND2	2:n:96:SER:OG	2.44	0.51
2:h:108:ARG:NH1	2:h:116:ASP:OD1	2.42	0.51
2:k:364:PRO:HA	2:q:305:GLY:HA2	1.91	0.51
2:e:185:VAL:H	2:e:200:ALA:HB2	1.75	0.51
2:l:50:THR:OG1	2:m:244:THR:O	2.29	0.51
2:p:221:PRO:HA	2:p:224:LYS:HD3	1.92	0.51
2:e:303:ASP:OD1	2:e:303:ASP:N	2.41	0.51
2:h:364:PRO:HA	2:n:305:GLY:HA2	1.91	0.51
2:b:129:VAL:HG12	2:b:131:PRO:HD3	1.93	0.51
2:n:75:ARG:NH1	2:n:225:GLU:O	2.43	0.51
2:o:75:ARG:NH1	2:o:225:GLU:O	2.43	0.51
2:c:129:VAL:HG12	2:c:131:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:222:SER:OG	2:c:269:ASN:OD1	2.27	0.51
2:d:222:SER:OG	2:d:269:ASN:OD1	2.27	0.51
2:m:75:ARG:NH1	2:m:225:GLU:O	2.43	0.51
2:b:185:VAL:H	2:b:200:ALA:HB2	1.75	0.51
2:h:185:VAL:H	2:h:200:ALA:HB2	1.76	0.51
2:g:185:VAL:H	2:g:200:ALA:HB2	1.76	0.51
2:l:185:VAL:H	2:l:200:ALA:HB2	1.76	0.51
2:i:185:VAL:H	2:i:200:ALA:HB2	1.76	0.51
2:b:372:VAL:HG22	2:h:287:MET:HE1	1.92	0.51
2:d:75:ARG:NH1	2:d:225:GLU:O	2.38	0.51
2:d:129:VAL:HG12	2:d:131:PRO:HD3	1.93	0.51
2:g:13:ASP:OD1	2:g:17:ARG:NH2	2.42	0.51
2:l:364:PRO:HA	2:r:305:GLY:HA2	1.91	0.51
2:p:75:ARG:NH1	2:p:225:GLU:O	2.43	0.51
2:o:221:PRO:HA	2:o:224:LYS:HD3	1.92	0.51
2:f:377:GLN:OE1	2:l:358:ARG:NH2	2.44	0.50
2:h:13:ASP:OD1	2:h:17:ARG:NH2	2.42	0.50
2:k:129:VAL:HG12	2:k:131:PRO:HD3	1.93	0.50
2:k:185:VAL:H	2:k:200:ALA:HB2	1.76	0.50
2:j:129:VAL:HG12	2:j:131:PRO:HD3	1.93	0.50
2:q:221:PRO:HA	2:q:224:LYS:HD3	1.92	0.50
2:a:372:VAL:HG22	2:g:287:MET:HE1	1.92	0.50
2:h:129:VAL:HG12	2:h:131:PRO:HD3	1.93	0.50
2:j:185:VAL:H	2:j:200:ALA:HB2	1.76	0.50
2:d:185:VAL:H	2:d:200:ALA:HB2	1.75	0.50
2:i:129:VAL:HG12	2:i:131:PRO:HD3	1.93	0.50
2:a:377:GLN:OE1	2:g:358:ARG:NH2	2.44	0.50
2:n:221:PRO:HA	2:n:224:LYS:HD3	1.92	0.50
2:c:377:GLN:OE1	2:i:358:ARG:NH2	2.44	0.50
2:r:221:PRO:HA	2:r:224:LYS:HD3	1.92	0.50
2:e:129:VAL:HG12	2:e:131:PRO:HD3	1.93	0.50
2:m:221:PRO:HA	2:m:224:LYS:HD3	1.92	0.50
2:a:49:LEU:HD11	2:a:59:PHE:HE2	1.77	0.50
2:b:124:GLN:OE1	2:b:126:ARG:NH2	2.45	0.50
2:d:124:GLN:OE1	2:d:126:ARG:NH2	2.45	0.50
2:g:129:VAL:HG12	2:g:131:PRO:HD3	1.93	0.50
2:h:125:PRO:HG2	2:h:150:LEU:HD13	1.94	0.50
2:e:124:GLN:OE1	2:e:126:ARG:NH2	2.45	0.49
2:f:129:VAL:HG12	2:f:131:PRO:HD3	1.93	0.49
2:l:129:VAL:HG12	2:l:131:PRO:HD3	1.93	0.49
2:e:49:LEU:HD11	2:e:59:PHE:HE2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:124:GLN:OE1	2:f:126:ARG:NH2	2.45	0.49
2:g:125:PRO:HG2	2:g:150:LEU:HD13	1.94	0.49
2:a:129:VAL:HG12	2:a:131:PRO:HD3	1.93	0.49
2:i:125:PRO:HG2	2:i:150:LEU:HD13	1.94	0.49
2:a:124:GLN:OE1	2:a:126:ARG:NH2	2.45	0.49
2:b:377:GLN:OE1	2:h:358:ARG:NH2	2.44	0.49
2:c:49:LEU:HD11	2:c:59:PHE:HE2	1.77	0.49
2:j:125:PRO:HG2	2:j:150:LEU:HD13	1.94	0.49
2:l:125:PRO:HG2	2:l:150:LEU:HD13	1.94	0.49
2:c:124:GLN:OE1	2:c:126:ARG:NH2	2.45	0.49
2:f:49:LEU:HD11	2:f:59:PHE:HE2	1.77	0.49
2:d:374:VAL:O	2:j:277:LYS:NZ	2.44	0.49
2:k:125:PRO:HG2	2:k:150:LEU:HD13	1.94	0.49
2:a:13:ASP:OD1	2:a:17:ARG:NH2	2.44	0.48
1:C:68:ALA:HB3	1:C:125:VAL:HB	1.95	0.48
2:d:49:LEU:HD11	2:d:59:PHE:HE2	1.77	0.48
2:d:327:ASN:ND2	2:q:341:ASP:O	2.45	0.48
1:A:68:ALA:HB3	1:A:125:VAL:HB	1.95	0.48
2:d:377:GLN:OE1	2:j:358:ARG:NH2	2.44	0.48
1:F:68:ALA:HB3	1:F:125:VAL:HB	1.95	0.48
2:b:49:LEU:HD11	2:b:59:PHE:HE2	1.77	0.48
2:a:367:ASN:ND2	2:f:6:GLY:O	2.41	0.48
2:l:48:LEU:O	2:m:246:ARG:NH2	2.45	0.48
2:k:50:THR:OG1	2:r:244:THR:O	2.30	0.48
1:D:68:ALA:HB3	1:D:125:VAL:HB	1.95	0.48
2:e:377:GLN:OE1	2:k:358:ARG:NH2	2.44	0.48
1:B:68:ALA:HB3	1:B:125:VAL:HB	1.95	0.48
1:E:62:LEU:HD12	1:E:133:LEU:HD12	1.96	0.48
2:c:303:ASP:OD1	2:c:303:ASP:N	2.41	0.48
2:j:377:GLN:OE1	2:p:358:ARG:NH2	2.46	0.48
1:E:68:ALA:HB3	1:E:125:VAL:HB	1.95	0.48
1:F:62:LEU:HD12	1:F:133:LEU:HD12	1.96	0.48
1:A:62:LEU:HD12	1:A:133:LEU:HD12	1.96	0.48
1:D:62:LEU:HD12	1:D:133:LEU:HD12	1.96	0.47
2:b:303:ASP:OD1	2:b:303:ASP:N	2.41	0.47
2:q:185:VAL:HG12	2:q:198:ALA:HB3	1.96	0.47
2:c:327:ASN:ND2	2:p:341:ASP:O	2.47	0.47
1:B:62:LEU:HD12	1:B:133:LEU:HD12	1.96	0.47
2:b:248:ASN:O	2:b:252:ASN:ND2	2.46	0.47
2:f:13:ASP:OD1	2:f:17:ARG:NH2	2.44	0.47
2:h:222:SER:O	2:h:222:SER:OG	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:185:VAL:HG12	2:n:198:ALA:HB3	1.97	0.47
2:r:185:VAL:HG12	2:r:198:ALA:HB3	1.96	0.47
2:l:377:GLN:OE1	2:r:358:ARG:NH2	2.46	0.47
2:i:377:GLN:OE1	2:o:358:ARG:NH2	2.46	0.47
1:C:62:LEU:HD12	1:C:133:LEU:HD12	1.96	0.47
2:b:13:ASP:OD1	2:b:17:ARG:NH2	2.44	0.47
2:b:136:GLN:HB2	2:b:139:VAL:HG12	1.97	0.47
2:c:98:VAL:O	2:c:111:LEU:N	2.48	0.47
2:f:136:GLN:HB2	2:f:139:VAL:HG12	1.97	0.47
2:g:222:SER:O	2:g:222:SER:OG	2.33	0.47
2:m:185:VAL:HG12	2:m:198:ALA:HB3	1.97	0.47
2:p:185:VAL:HG12	2:p:198:ALA:HB3	1.96	0.47
2:f:248:ASN:O	2:f:252:ASN:ND2	2.46	0.47
2:g:377:GLN:OE1	2:m:358:ARG:NH2	2.46	0.47
2:o:185:VAL:HG12	2:o:198:ALA:HB3	1.97	0.47
2:e:98:VAL:O	2:e:111:LEU:N	2.48	0.47
2:d:98:VAL:O	2:d:111:LEU:N	2.48	0.46
2:l:151:ARG:HB3	2:l:288:ASP:HB3	1.97	0.46
2:i:222:SER:O	2:i:222:SER:OG	2.33	0.46
2:h:377:GLN:OE1	2:n:358:ARG:NH2	2.46	0.46
1:C:45:GLU:N	1:C:67:GLN:O	2.49	0.46
2:c:46:PRO:HB2	2:c:121:PHE:HE2	1.81	0.46
2:g:151:ARG:HB3	2:g:288:ASP:HB3	1.97	0.46
1:D:45:GLU:N	1:D:67:GLN:O	2.49	0.46
2:c:136:GLN:HB2	2:c:139:VAL:HG12	1.97	0.46
2:e:46:PRO:HB2	2:e:121:PHE:HE2	1.81	0.46
2:e:136:GLN:HB2	2:e:139:VAL:HG12	1.97	0.46
1:B:107:ARG:HH21	1:B:124:LEU:HD22	1.81	0.46
1:D:107:ARG:HH21	1:D:124:LEU:HD22	1.81	0.46
2:b:375:THR:OG1	2:b:376:ASP:N	2.49	0.46
2:c:193:ASN:ND2	2:p:96:SER:OG	2.49	0.46
2:d:375:THR:OG1	2:d:376:ASP:N	2.49	0.46
2:e:375:THR:OG1	2:e:376:ASP:N	2.49	0.46
1:C:107:ARG:HH21	1:C:124:LEU:HD22	1.81	0.46
1:F:31:PHE:HA	1:F:44:LEU:HB2	1.98	0.46
2:c:375:THR:OG1	2:c:376:ASP:N	2.49	0.46
2:f:375:THR:OG1	2:f:376:ASP:N	2.49	0.46
2:k:151:ARG:HB3	2:k:288:ASP:HB3	1.97	0.46
2:a:375:THR:OG1	2:a:376:ASP:N	2.49	0.46
1:B:45:GLU:N	1:B:67:GLN:O	2.49	0.46
2:e:13:ASP:OD1	2:e:17:ARG:NH2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:377:GLN:OE1	2:q:358:ARG:NH2	2.46	0.45
2:j:222:SER:O	2:j:222:SER:OG	2.33	0.45
2:a:46:PRO:HB2	2:a:121:PHE:HE2	1.81	0.45
2:e:125:PRO:HG2	2:e:150:LEU:HD13	1.99	0.45
2:g:26:VAL:HB	2:g:125:PRO:HA	1.98	0.45
2:k:222:SER:O	2:k:222:SER:OG	2.33	0.45
2:a:136:GLN:HB2	2:a:139:VAL:HG12	1.97	0.45
1:D:31:PHE:HA	1:D:44:LEU:HB2	1.98	0.45
2:b:46:PRO:HB2	2:b:121:PHE:HE2	1.81	0.45
2:f:98:VAL:O	2:f:111:LEU:N	2.48	0.45
1:A:31:PHE:HA	1:A:44:LEU:HB2	1.98	0.45
1:A:107:ARG:HH21	1:A:124:LEU:HD22	1.81	0.45
2:a:98:VAL:O	2:a:111:LEU:N	2.48	0.45
1:C:31:PHE:HA	1:C:44:LEU:HB2	1.98	0.45
2:d:125:PRO:HG2	2:d:150:LEU:HD13	1.99	0.45
2:f:178:LEU:HB3	2:f:272:LEU:HD12	1.99	0.45
2:f:327:ASN:ND2	2:m:341:ASP:O	2.49	0.45
2:h:26:VAL:HB	2:h:125:PRO:HA	1.98	0.45
2:i:151:ARG:HB3	2:i:288:ASP:HB3	1.97	0.45
2:b:98:VAL:O	2:b:111:LEU:N	2.48	0.45
2:c:178:LEU:HB3	2:c:272:LEU:HD12	1.99	0.45
2:d:248:ASN:O	2:d:252:ASN:ND2	2.46	0.45
1:F:107:ARG:HH21	1:F:124:LEU:HD22	1.81	0.45
2:c:13:ASP:OD1	2:c:17:ARG:NH2	2.44	0.45
2:f:154:ALA:HB3	2:f:178:LEU:HD23	1.99	0.45
2:h:151:ARG:HB3	2:h:288:ASP:HB3	1.97	0.45
2:a:178:LEU:HB3	2:a:272:LEU:HD12	1.99	0.45
1:E:107:ARG:HH21	1:E:124:LEU:HD22	1.81	0.45
2:b:178:LEU:HB3	2:b:272:LEU:HD12	1.99	0.45
2:i:129:VAL:HG22	2:i:155:ILE:HB	1.99	0.45
2:i:376:ASP:N	2:i:376:ASP:OD1	2.50	0.45
1:E:45:GLU:N	1:E:67:GLN:O	2.48	0.45
2:c:130:ALA:O	2:c:134:SER:OG	2.35	0.45
2:f:125:PRO:HG2	2:f:150:LEU:HD13	1.99	0.45
2:f:161:SER:OG	2:f:162:THR:N	2.50	0.45
2:h:129:VAL:HG22	2:h:155:ILE:HB	1.99	0.45
2:l:26:VAL:HB	2:l:125:PRO:HA	1.98	0.45
2:a:6:GLY:O	2:b:367:ASN:ND2	2.44	0.45
1:E:31:PHE:HA	1:E:44:LEU:HB2	1.98	0.45
1:F:149:MET:HB3	1:F:164:TYR:HB3	1.99	0.45
1:A:149:MET:HB3	1:A:164:TYR:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB3	1:B:164:TYR:HB3	1.99	0.45
2:c:125:PRO:HG2	2:c:150:LEU:HD13	1.99	0.45
2:d:46:PRO:HB2	2:d:121:PHE:HE2	1.81	0.45
2:d:136:GLN:HB2	2:d:139:VAL:HG12	1.97	0.45
2:d:178:LEU:HB3	2:d:272:LEU:HD12	1.99	0.45
2:h:376:ASP:OD1	2:h:376:ASP:N	2.50	0.45
2:k:26:VAL:HB	2:k:125:PRO:HA	1.98	0.45
2:o:376:ASP:OD1	2:o:376:ASP:N	2.50	0.45
2:e:178:LEU:HB3	2:e:272:LEU:HD12	1.99	0.44
2:j:129:VAL:HG22	2:j:155:ILE:HB	1.99	0.44
2:a:112:GLN:HE21	2:a:112:GLN:HB3	1.63	0.44
2:d:13:ASP:OD1	2:d:17:ARG:NH2	2.44	0.44
2:e:154:ALA:HB3	2:e:178:LEU:HD23	1.99	0.44
2:e:324:ASP:OD2	2:r:346:SER:OG	2.33	0.44
2:f:46:PRO:HB2	2:f:121:PHE:HE2	1.81	0.44
2:p:376:ASP:OD1	2:p:376:ASP:N	2.50	0.44
1:A:164:TYR:OH	2:a:339:ASP:OD2	2.33	0.44
2:c:154:ALA:HB3	2:c:178:LEU:HD23	1.99	0.44
2:j:26:VAL:HB	2:j:125:PRO:HA	1.98	0.44
2:j:151:ARG:HB3	2:j:288:ASP:HB3	1.97	0.44
2:a:382:VAL:HG13	2:m:308:LYS:HA	2.00	0.44
2:b:382:VAL:HG13	2:n:308:LYS:HA	2.00	0.44
2:e:327:ASN:ND2	2:r:341:ASP:O	2.50	0.44
1:A:45:GLU:N	1:A:67:GLN:O	2.48	0.44
2:a:125:PRO:HG2	2:a:150:LEU:HD13	1.99	0.44
2:a:207:LEU:HD23	2:a:207:LEU:HA	1.87	0.44
2:c:129:VAL:HG22	2:c:155:ILE:HB	2.00	0.44
2:g:129:VAL:HG22	2:g:155:ILE:HB	1.99	0.44
2:b:125:PRO:HG2	2:b:150:LEU:HD13	1.99	0.44
2:b:161:SER:OG	2:b:162:THR:N	2.50	0.44
2:d:129:VAL:HG22	2:d:155:ILE:HB	2.00	0.44
2:d:161:SER:OG	2:d:162:THR:N	2.50	0.44
2:e:129:VAL:HG22	2:e:155:ILE:HB	2.00	0.44
2:k:378:TRP:HE3	2:q:360:THR:HG23	1.82	0.44
2:a:129:VAL:HG22	2:a:155:ILE:HB	2.00	0.44
1:E:149:MET:HB3	1:E:164:TYR:HB3	1.99	0.44
2:b:72:ILE:HG21	2:b:80:ILE:HD11	2.00	0.44
2:b:130:ALA:O	2:b:134:SER:OG	2.35	0.44
2:c:72:ILE:HG21	2:c:80:ILE:HD11	2.00	0.44
2:f:129:VAL:HG22	2:f:155:ILE:HB	2.00	0.44
2:h:134:SER:O	2:h:169:TYR:OH	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:259:ILE:HD12	2:l:260:ARG:HG3	2.00	0.44
2:a:72:ILE:HG21	2:a:80:ILE:HD11	2.00	0.44
2:a:154:ALA:HB3	2:a:178:LEU:HD23	1.99	0.44
1:B:31:PHE:HA	1:B:44:LEU:HB2	1.98	0.44
1:B:164:TYR:OH	2:b:339:ASP:OD2	2.33	0.44
2:b:129:VAL:HG22	2:b:155:ILE:HB	2.00	0.44
2:b:154:ALA:HB3	2:b:178:LEU:HD23	1.99	0.44
2:c:207:LEU:HD23	2:c:207:LEU:HA	1.87	0.44
2:e:364:PRO:HA	2:k:305:GLY:HA2	2.00	0.44
2:k:129:VAL:HG22	2:k:155:ILE:HB	1.99	0.44
2:k:374:VAL:HG21	2:q:283:ARG:HD3	2.00	0.44
2:r:124:GLN:NE2	2:r:150:LEU:O	2.51	0.44
2:p:158:GLY:HA3	2:p:180:MET:HE3	2.00	0.44
2:b:364:PRO:HA	2:h:305:GLY:HA2	2.00	0.44
2:e:130:ALA:O	2:e:134:SER:OG	2.35	0.44
2:f:364:PRO:HA	2:l:305:GLY:HA2	2.00	0.44
2:g:48:LEU:O	2:n:246:ARG:NH2	2.49	0.44
2:h:378:TRP:HE3	2:n:360:THR:HG23	1.82	0.44
2:l:129:VAL:HG22	2:l:155:ILE:HB	1.99	0.44
2:a:364:PRO:HA	2:g:305:GLY:HA2	2.00	0.43
1:D:149:MET:HB3	1:D:164:TYR:HB3	1.99	0.43
2:c:27:ILE:HG12	2:c:127:LEU:HD23	2.00	0.43
2:d:27:ILE:HG12	2:d:127:LEU:HD23	2.00	0.43
2:e:6:GLY:O	2:f:367:ASN:ND2	2.45	0.43
2:f:382:VAL:HG13	2:r:308:LYS:HA	2.00	0.43
2:i:26:VAL:HB	2:i:125:PRO:HA	1.98	0.43
2:r:137:GLN:O	2:r:141:THR:OG1	2.32	0.43
2:a:161:SER:OG	2:a:162:THR:N	2.50	0.43
2:b:180:MET:HE2	2:b:180:MET:HB2	1.90	0.43
2:c:382:VAL:HG13	2:o:308:LYS:HA	2.00	0.43
2:e:27:ILE:HG12	2:e:127:LEU:HD23	2.00	0.43
2:f:27:ILE:HG12	2:f:127:LEU:HD23	2.01	0.43
2:f:72:ILE:HG21	2:f:80:ILE:HD11	2.00	0.43
2:f:180:MET:HE2	2:f:180:MET:HB2	1.90	0.43
2:g:259:ILE:HD12	2:g:260:ARG:HG3	2.00	0.43
2:k:259:ILE:HD12	2:k:260:ARG:HG3	2.00	0.43
2:n:124:GLN:NE2	2:n:150:LEU:O	2.51	0.43
2:p:124:GLN:NE2	2:p:150:LEU:O	2.51	0.43
2:o:158:GLY:HA3	2:o:180:MET:HE3	2.00	0.43
2:c:364:PRO:HA	2:i:305:GLY:HA2	2.00	0.43
2:d:72:ILE:HG21	2:d:80:ILE:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:154:ALA:HB3	2:d:178:LEU:HD23	1.99	0.43
2:j:376:ASP:OD1	2:j:376:ASP:N	2.50	0.43
2:j:378:TRP:HE3	2:p:360:THR:HG23	1.83	0.43
2:a:103:SER:OG	2:a:104:ALA:N	2.52	0.43
2:e:72:ILE:HG21	2:e:80:ILE:HD11	2.00	0.43
2:f:103:SER:OG	2:f:104:ALA:N	2.52	0.43
2:g:374:VAL:HG21	2:m:283:ARG:HD3	2.00	0.43
2:q:185:VAL:O	2:q:198:ALA:N	2.51	0.43
1:C:149:MET:HB3	1:C:164:TYR:HB3	1.99	0.43
2:d:61:ILE:H	2:d:61:ILE:HG13	1.51	0.43
2:d:103:SER:OG	2:d:104:ALA:N	2.52	0.43
2:e:103:SER:OG	2:e:104:ALA:N	2.52	0.43
2:f:112:GLN:HE21	2:f:112:GLN:HB3	1.63	0.43
2:j:48:LEU:O	2:q:246:ARG:NH2	2.51	0.43
2:a:27:ILE:HG12	2:a:127:LEU:HD23	2.00	0.43
2:a:130:ALA:O	2:a:134:SER:OG	2.35	0.43
2:a:248:ASN:O	2:a:252:ASN:ND2	2.46	0.43
2:b:103:SER:OG	2:b:104:ALA:N	2.52	0.43
2:k:75:ARG:NH1	2:k:225:GLU:O	2.52	0.43
2:i:378:TRP:HE3	2:o:360:THR:HG23	1.82	0.43
2:a:50:THR:HG22	2:h:246:ARG:HH21	1.83	0.43
2:b:27:ILE:HG12	2:b:127:LEU:HD23	2.00	0.43
2:c:103:SER:OG	2:c:104:ALA:N	2.52	0.43
2:f:324:ASP:OD2	2:m:346:SER:OG	2.33	0.43
2:g:378:TRP:HE3	2:m:360:THR:HG23	1.82	0.43
2:l:75:ARG:NH1	2:l:225:GLU:O	2.52	0.43
2:l:378:TRP:HE3	2:r:360:THR:HG23	1.82	0.43
1:F:164:TYR:OH	2:f:339:ASP:OD2	2.33	0.43
2:d:364:PRO:HA	2:j:305:GLY:HA2	2.00	0.43
2:f:130:ALA:O	2:f:134:SER:OG	2.35	0.43
2:h:259:ILE:HD12	2:h:260:ARG:HG3	2.00	0.43
2:h:374:VAL:HG21	2:n:283:ARG:HD3	2.00	0.43
2:l:376:ASP:OD1	2:l:376:ASP:N	2.50	0.43
2:k:376:ASP:N	2:k:376:ASP:OD1	2.50	0.43
2:n:376:ASP:OD1	2:n:376:ASP:N	2.50	0.43
2:d:382:VAL:HG13	2:p:308:LYS:HA	2.00	0.43
2:e:382:VAL:HG13	2:q:308:LYS:HA	2.00	0.43
2:g:376:ASP:OD1	2:g:376:ASP:N	2.50	0.43
2:l:374:VAL:HG21	2:r:283:ARG:HD3	2.00	0.43
2:j:259:ILE:HD12	2:j:260:ARG:HG3	2.00	0.43
2:n:137:GLN:O	2:n:141:THR:OG1	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:GLU:N	1:F:67:GLN:O	2.49	0.43
2:j:75:ARG:NH1	2:j:225:GLU:O	2.52	0.43
2:j:374:VAL:HG21	2:p:283:ARG:HD3	2.00	0.43
2:n:49:LEU:HD11	2:n:59:PHE:HE2	1.84	0.43
2:r:158:GLY:HA3	2:r:180:MET:HE3	2.00	0.43
2:a:156:LEU:HD11	2:a:178:LEU:HD22	2.01	0.42
2:a:376:ASP:N	2:a:376:ASP:OD1	2.52	0.42
2:f:376:ASP:N	2:f:376:ASP:OD1	2.52	0.42
2:m:49:LEU:HD11	2:m:59:PHE:HE2	1.84	0.42
2:m:185:VAL:O	2:m:198:ALA:N	2.51	0.42
2:q:158:GLY:HA3	2:q:180:MET:HE3	2.00	0.42
2:q:376:ASP:OD1	2:q:376:ASP:N	2.50	0.42
2:p:129:VAL:HG12	2:p:131:PRO:HD3	2.01	0.42
2:p:185:VAL:O	2:p:198:ALA:N	2.51	0.42
2:b:76:ALA:HB2	2:b:210:TRP:HB2	2.02	0.42
2:d:376:ASP:N	2:d:376:ASP:OD1	2.52	0.42
2:e:376:ASP:N	2:e:376:ASP:OD1	2.52	0.42
2:f:127:LEU:HD13	2:f:285:ARG:HH12	1.84	0.42
2:i:259:ILE:HD12	2:i:260:ARG:HG3	2.00	0.42
2:m:158:GLY:HA3	2:m:180:MET:HE3	2.00	0.42
2:d:156:LEU:HD11	2:d:178:LEU:HD22	2.01	0.42
2:f:61:ILE:H	2:f:61:ILE:HG13	1.51	0.42
2:h:75:ARG:NH1	2:h:225:GLU:O	2.52	0.42
2:h:211:THR:O	2:h:216:GLY:N	2.51	0.42
2:i:374:VAL:HG21	2:o:283:ARG:HD3	2.00	0.42
2:n:185:VAL:O	2:n:198:ALA:N	2.51	0.42
2:q:49:LEU:HD11	2:q:59:PHE:HE2	1.84	0.42
2:q:103:SER:OG	2:q:104:ALA:N	2.52	0.42
2:p:103:SER:OG	2:p:104:ALA:N	2.52	0.42
2:o:129:VAL:HG12	2:o:131:PRO:HD3	2.01	0.42
2:a:127:LEU:HD13	2:a:285:ARG:HH12	1.85	0.42
2:b:228:GLY:H	2:o:141:THR:HG22	1.85	0.42
2:c:76:ALA:HB2	2:c:210:TRP:HB2	2.01	0.42
2:f:207:LEU:HD23	2:f:207:LEU:HA	1.87	0.42
2:m:26:VAL:HB	2:m:125:PRO:HA	2.02	0.42
2:m:376:ASP:OD1	2:m:376:ASP:N	2.50	0.42
2:n:26:VAL:HB	2:n:125:PRO:HA	2.02	0.42
2:b:112:GLN:HG2	2:b:146:LEU:HD11	2.02	0.42
2:b:156:LEU:HD11	2:b:178:LEU:HD22	2.01	0.42
2:f:156:LEU:HD11	2:f:178:LEU:HD22	2.01	0.42
2:h:336:VAL:HG22	2:h:357:ILE:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:336:VAL:HG22	2:l:357:ILE:HG23	2.02	0.42
2:a:76:ALA:HB2	2:a:210:TRP:HB2	2.02	0.42
2:g:75:ARG:NH1	2:g:225:GLU:O	2.52	0.42
2:g:336:VAL:HG22	2:g:357:ILE:HG23	2.02	0.42
2:q:129:VAL:HG12	2:q:131:PRO:HD3	2.01	0.42
2:o:156:LEU:N	2:o:179:PHE:O	2.53	0.42
2:b:327:ASN:ND2	2:o:341:ASP:O	2.53	0.42
2:d:76:ALA:HB2	2:d:210:TRP:HB2	2.02	0.42
2:e:161:SER:OG	2:e:162:THR:N	2.50	0.42
2:l:134:SER:O	2:l:169:TYR:OH	2.33	0.42
2:k:336:VAL:HG22	2:k:357:ILE:HG23	2.02	0.42
1:F:6:VAL:HG11	1:F:100:LEU:HD21	2.02	0.42
2:b:112:GLN:HE21	2:b:112:GLN:HB3	1.63	0.42
2:g:49:LEU:HD11	2:g:59:PHE:HE2	1.85	0.42
2:j:211:THR:O	2:j:216:GLY:N	2.51	0.42
2:i:75:ARG:NH1	2:i:225:GLU:O	2.52	0.42
2:r:26:VAL:HB	2:r:125:PRO:HA	2.02	0.42
2:o:26:VAL:HB	2:o:125:PRO:HA	2.02	0.42
2:o:49:LEU:HD11	2:o:59:PHE:HE2	1.84	0.42
2:c:156:LEU:HD11	2:c:178:LEU:HD22	2.01	0.42
2:c:161:SER:OG	2:c:162:THR:N	2.50	0.42
2:c:376:ASP:N	2:c:376:ASP:OD1	2.52	0.42
2:m:103:SER:OG	2:m:104:ALA:N	2.53	0.42
2:r:49:LEU:HD11	2:r:59:PHE:HE2	1.84	0.42
1:A:6:VAL:HG11	1:A:100:LEU:HD21	2.02	0.42
2:k:49:LEU:HD11	2:k:59:PHE:HE2	1.85	0.42
2:k:211:THR:O	2:k:216:GLY:N	2.51	0.42
2:j:336:VAL:HG22	2:j:357:ILE:HG23	2.02	0.42
2:i:336:VAL:HG22	2:i:357:ILE:HG23	2.02	0.42
2:m:124:GLN:NE2	2:m:150:LEU:O	2.51	0.42
2:n:315:THR:HG22	2:n:319:ARG:HD2	2.02	0.42
2:r:211:THR:O	2:r:216:GLY:N	2.52	0.42
2:r:376:ASP:OD1	2:r:376:ASP:N	2.50	0.42
2:b:127:LEU:HD13	2:b:285:ARG:HH12	1.84	0.41
2:b:207:LEU:HD23	2:b:207:LEU:HA	1.87	0.41
2:e:156:LEU:HD11	2:e:178:LEU:HD22	2.01	0.41
2:i:50:THR:OG1	2:p:244:THR:O	2.38	0.41
2:n:103:SER:OG	2:n:104:ALA:N	2.52	0.41
2:n:158:GLY:HA3	2:n:180:MET:HE3	2.00	0.41
2:r:129:VAL:HG12	2:r:131:PRO:HD3	2.01	0.41
2:p:156:LEU:N	2:p:179:PHE:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:124:GLN:NE2	2:o:150:LEU:O	2.51	0.41
1:E:6:VAL:HG11	1:E:100:LEU:HD21	2.02	0.41
2:e:127:LEU:HD13	2:e:285:ARG:HH12	1.85	0.41
2:k:48:LEU:O	2:r:246:ARG:NH2	2.53	0.41
2:j:49:LEU:HD11	2:j:59:PHE:HE2	1.85	0.41
2:r:185:VAL:O	2:r:198:ALA:N	2.51	0.41
2:q:137:GLN:O	2:q:141:THR:OG1	2.32	0.41
2:p:49:LEU:HD11	2:p:59:PHE:HE2	1.84	0.41
2:c:112:GLN:HG2	2:c:146:LEU:HD11	2.02	0.41
2:d:126:ARG:NH2	2:d:292:ASP:OD2	2.54	0.41
2:k:162:THR:OG1	2:k:163:ASP:N	2.53	0.41
2:a:187:VAL:O	2:a:196:ARG:N	2.43	0.41
1:C:6:VAL:HG11	1:C:100:LEU:HD21	2.02	0.41
2:b:126:ARG:NH2	2:b:292:ASP:OD2	2.54	0.41
2:b:193:ASN:ND2	2:o:96:SER:OG	2.53	0.41
2:e:76:ALA:HB2	2:e:210:TRP:HB2	2.01	0.41
2:l:162:THR:OG1	2:l:163:ASP:N	2.53	0.41
2:n:156:LEU:N	2:n:179:PHE:O	2.53	0.41
2:r:156:LEU:N	2:r:179:PHE:O	2.53	0.41
2:q:156:LEU:N	2:q:179:PHE:O	2.53	0.41
2:p:26:VAL:HB	2:p:125:PRO:HA	2.01	0.41
2:o:211:THR:O	2:o:216:GLY:N	2.52	0.41
2:o:315:THR:HG22	2:o:319:ARG:HD2	2.02	0.41
2:a:112:GLN:HG2	2:a:146:LEU:HD11	2.02	0.41
2:d:112:GLN:HG2	2:d:146:LEU:HD11	2.02	0.41
2:d:211:THR:HG21	2:d:221:PRO:HA	2.03	0.41
2:e:211:THR:HG21	2:e:221:PRO:HA	2.03	0.41
2:j:162:THR:OG1	2:j:163:ASP:N	2.53	0.41
2:i:49:LEU:HD11	2:i:59:PHE:HE2	1.85	0.41
2:m:129:VAL:HG12	2:m:131:PRO:HD3	2.01	0.41
2:m:156:LEU:N	2:m:179:PHE:O	2.53	0.41
2:m:211:THR:O	2:m:216:GLY:N	2.52	0.41
2:n:129:VAL:HG12	2:n:131:PRO:HD3	2.01	0.41
2:o:103:SER:OG	2:o:104:ALA:N	2.52	0.41
2:a:126:ARG:NH2	2:a:292:ASP:OD2	2.54	0.41
2:a:180:MET:HE2	2:a:180:MET:HB2	1.90	0.41
2:c:248:ASN:O	2:c:252:ASN:ND2	2.45	0.41
2:e:112:GLN:HG2	2:e:146:LEU:HD11	2.02	0.41
2:l:49:LEU:HD11	2:l:59:PHE:HE2	1.85	0.41
2:r:103:SER:OG	2:r:104:ALA:N	2.53	0.41
2:r:315:THR:HG22	2:r:319:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:163:ASP:OD1	2:a:163:ASP:N	2.54	0.41
2:b:50:THR:HG22	2:i:246:ARG:HH21	1.86	0.41
2:e:157:ASP:OD1	2:e:157:ASP:N	2.54	0.41
2:f:76:ALA:HB2	2:f:210:TRP:HB2	2.02	0.41
2:n:211:THR:O	2:n:216:GLY:N	2.52	0.41
2:q:26:VAL:HB	2:q:125:PRO:HA	2.02	0.41
2:q:315:THR:HG22	2:q:319:ARG:HD2	2.02	0.41
2:p:137:GLN:O	2:p:141:THR:OG1	2.32	0.41
2:c:299:LYS:HD3	2:j:274:SER:HB2	2.03	0.41
2:e:163:ASP:OD1	2:e:163:ASP:N	2.54	0.41
2:f:126:ARG:NH2	2:f:292:ASP:OD2	2.54	0.41
2:g:46:PRO:HB2	2:g:121:PHE:HE2	1.86	0.41
2:i:162:THR:OG1	2:i:163:ASP:N	2.53	0.41
2:q:124:GLN:NE2	2:q:150:LEU:O	2.51	0.41
2:p:24:SER:O	2:p:24:SER:OG	2.37	0.41
2:o:137:GLN:O	2:o:141:THR:OG1	2.32	0.41
2:b:367:ASN:HD22	2:b:367:ASN:HA	1.74	0.41
2:c:112:GLN:HE21	2:c:112:GLN:HB3	1.63	0.41
2:c:120:ARG:HE	2:c:120:ARG:HB3	1.72	0.41
2:c:126:ARG:NH2	2:c:292:ASP:OD2	2.54	0.41
2:d:120:ARG:HE	2:d:120:ARG:HB3	1.72	0.41
2:e:115:LEU:HA	2:e:150:LEU:HD21	2.03	0.41
2:f:163:ASP:OD1	2:f:163:ASP:N	2.54	0.41
2:f:211:THR:HG21	2:f:221:PRO:HA	2.03	0.41
2:g:134:SER:O	2:g:169:TYR:OH	2.33	0.41
2:h:46:PRO:HB2	2:h:121:PHE:HE2	1.86	0.41
2:j:46:PRO:HB2	2:j:121:PHE:HE2	1.86	0.41
2:i:116:ASP:OD1	2:i:116:ASP:N	2.54	0.41
2:q:24:SER:O	2:q:24:SER:OG	2.37	0.41
2:p:315:THR:HG22	2:p:319:ARG:HD2	2.02	0.41
1:D:6:VAL:HG11	1:D:100:LEU:HD21	2.02	0.41
2:c:211:THR:HG21	2:c:221:PRO:HA	2.03	0.41
2:e:61:ILE:H	2:e:61:ILE:HG13	1.51	0.41
2:i:46:PRO:HB2	2:i:121:PHE:HE2	1.86	0.41
2:o:24:SER:O	2:o:24:SER:OG	2.37	0.41
2:a:157:ASP:OD1	2:a:157:ASP:N	2.54	0.40
2:g:162:THR:OG1	2:g:163:ASP:N	2.53	0.40
2:h:162:THR:OG1	2:h:163:ASP:N	2.53	0.40
2:l:76:ALA:HB2	2:l:210:TRP:HB2	2.03	0.40
2:k:153:ILE:HD12	2:k:285:ARG:HH11	1.87	0.40
1:B:6:VAL:HG11	1:B:100:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:127:LEU:HD13	2:c:285:ARG:HH12	1.85	0.40
2:c:228:GLY:H	2:p:141:THR:HG22	1.86	0.40
2:d:6:GLY:O	2:e:367:ASN:ND2	2.52	0.40
2:d:228:GLY:H	2:q:141:THR:HG22	1.86	0.40
2:e:126:ARG:NH2	2:e:292:ASP:OD2	2.54	0.40
2:e:187:VAL:O	2:e:196:ARG:N	2.43	0.40
2:f:115:LEU:HA	2:f:150:LEU:HD21	2.03	0.40
2:l:153:ILE:HD12	2:l:285:ARG:HH11	1.87	0.40
2:b:61:ILE:H	2:b:61:ILE:HG13	1.51	0.40
2:f:374:VAL:O	2:l:277:LYS:NZ	2.44	0.40
2:g:153:ILE:HD12	2:g:285:ARG:HH11	1.87	0.40
2:l:211:THR:O	2:l:216:GLY:N	2.51	0.40
2:m:315:THR:HG22	2:m:319:ARG:HD2	2.02	0.40
2:a:115:LEU:HA	2:a:150:LEU:HD21	2.03	0.40
2:d:207:LEU:HD23	2:d:207:LEU:HA	1.87	0.40
2:l:46:PRO:HB2	2:l:121:PHE:HE2	1.86	0.40
2:a:61:ILE:H	2:a:61:ILE:HG13	1.51	0.40
2:a:367:ASN:HD22	2:a:367:ASN:HA	1.74	0.40
2:c:157:ASP:OD1	2:c:157:ASP:N	2.54	0.40
2:d:299:LYS:HD3	2:k:274:SER:HB2	2.04	0.40
2:e:180:MET:HE2	2:e:180:MET:HB2	1.90	0.40
2:e:248:ASN:O	2:e:252:ASN:ND2	2.46	0.40
2:f:112:GLN:HG2	2:f:146:LEU:HD11	2.02	0.40
2:g:76:ALA:HB2	2:g:210:TRP:HB2	2.03	0.40
2:h:49:LEU:HD11	2:h:59:PHE:HE2	1.85	0.40
2:j:134:SER:O	2:j:169:TYR:OH	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
1	B	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
1	C	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
1	D	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
1	E	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
1	F	162/171 (95%)	148 (91%)	14 (9%)	0	100	100
2	a	381/386 (99%)	351 (92%)	30 (8%)	0	100	100
2	b	381/386 (99%)	351 (92%)	30 (8%)	0	100	100
2	c	381/386 (99%)	350 (92%)	31 (8%)	0	100	100
2	d	381/386 (99%)	351 (92%)	30 (8%)	0	100	100
2	e	381/386 (99%)	351 (92%)	30 (8%)	0	100	100
2	f	381/386 (99%)	351 (92%)	30 (8%)	0	100	100
2	g	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	h	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	i	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	j	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	k	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	l	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	m	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	n	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	o	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	p	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	q	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
2	r	381/386 (99%)	353 (93%)	28 (7%)	0	100	100
All	All	7830/7974 (98%)	7229 (92%)	601 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	136/141 (96%)	135 (99%)	1 (1%)	76	78
1	B	136/141 (96%)	135 (99%)	1 (1%)	76	78
1	C	136/141 (96%)	135 (99%)	1 (1%)	76	78
1	D	136/141 (96%)	135 (99%)	1 (1%)	76	78
1	E	136/141 (96%)	135 (99%)	1 (1%)	76	78
1	F	136/141 (96%)	135 (99%)	1 (1%)	76	78
2	a	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	b	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	c	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	d	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	e	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	f	296/298 (99%)	287 (97%)	9 (3%)	36	60
2	g	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	h	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	i	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	j	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	k	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	l	296/298 (99%)	285 (96%)	11 (4%)	30	56
2	m	296/298 (99%)	286 (97%)	10 (3%)	32	57
2	n	296/298 (99%)	286 (97%)	10 (3%)	32	57
2	o	296/298 (99%)	286 (97%)	10 (3%)	32	57
2	p	296/298 (99%)	286 (97%)	10 (3%)	32	57
2	q	296/298 (99%)	286 (97%)	10 (3%)	32	57
2	r	296/298 (99%)	286 (97%)	10 (3%)	32	57
All	All	6144/6210 (99%)	5958 (97%)	186 (3%)	37	60

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
2	a	61	ILE
2	a	80	ILE
2	a	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	a	128	LEU
2	a	133	HIS
2	a	146	LEU
2	a	185	VAL
2	a	259	ILE
2	a	372	VAL
1	B	148	LEU
1	C	148	LEU
1	D	148	LEU
1	E	148	LEU
1	F	148	LEU
2	b	61	ILE
2	b	80	ILE
2	b	112	GLN
2	b	128	LEU
2	b	133	HIS
2	b	146	LEU
2	b	185	VAL
2	b	259	ILE
2	b	372	VAL
2	c	61	ILE
2	c	80	ILE
2	c	112	GLN
2	c	128	LEU
2	c	133	HIS
2	c	146	LEU
2	c	185	VAL
2	c	259	ILE
2	c	372	VAL
2	d	61	ILE
2	d	80	ILE
2	d	112	GLN
2	d	128	LEU
2	d	133	HIS
2	d	146	LEU
2	d	185	VAL
2	d	259	ILE
2	d	372	VAL
2	e	61	ILE
2	e	80	ILE
2	e	112	GLN
2	e	128	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	e	133	HIS
2	e	146	LEU
2	e	185	VAL
2	e	259	ILE
2	e	372	VAL
2	f	61	ILE
2	f	80	ILE
2	f	112	GLN
2	f	128	LEU
2	f	133	HIS
2	f	146	LEU
2	f	185	VAL
2	f	259	ILE
2	f	372	VAL
2	g	75	ARG
2	g	85	VAL
2	g	127	LEU
2	g	177	ARG
2	g	185	VAL
2	g	229	VAL
2	g	243	GLU
2	g	245	CYS
2	g	259	ILE
2	g	302	VAL
2	g	353	VAL
2	h	75	ARG
2	h	85	VAL
2	h	127	LEU
2	h	177	ARG
2	h	185	VAL
2	h	229	VAL
2	h	243	GLU
2	h	245	CYS
2	h	259	ILE
2	h	302	VAL
2	h	353	VAL
2	l	75	ARG
2	l	85	VAL
2	l	127	LEU
2	l	177	ARG
2	l	185	VAL
2	l	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	l	243	GLU
2	l	245	CYS
2	l	259	ILE
2	l	302	VAL
2	l	353	VAL
2	k	75	ARG
2	k	85	VAL
2	k	127	LEU
2	k	177	ARG
2	k	185	VAL
2	k	229	VAL
2	k	243	GLU
2	k	245	CYS
2	k	259	ILE
2	k	302	VAL
2	k	353	VAL
2	j	75	ARG
2	j	85	VAL
2	j	127	LEU
2	j	177	ARG
2	j	185	VAL
2	j	229	VAL
2	j	243	GLU
2	j	245	CYS
2	j	259	ILE
2	j	302	VAL
2	j	353	VAL
2	i	75	ARG
2	i	85	VAL
2	i	127	LEU
2	i	177	ARG
2	i	185	VAL
2	i	229	VAL
2	i	243	GLU
2	i	245	CYS
2	i	259	ILE
2	i	302	VAL
2	i	353	VAL
2	m	32	VAL
2	m	61	ILE
2	m	75	ARG
2	m	127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	m	141	THR
2	m	185	VAL
2	m	229	VAL
2	m	242	ASP
2	m	259	ILE
2	m	353	VAL
2	n	32	VAL
2	n	61	ILE
2	n	75	ARG
2	n	127	LEU
2	n	141	THR
2	n	185	VAL
2	n	229	VAL
2	n	242	ASP
2	n	259	ILE
2	n	353	VAL
2	r	32	VAL
2	r	61	ILE
2	r	75	ARG
2	r	127	LEU
2	r	141	THR
2	r	185	VAL
2	r	229	VAL
2	r	242	ASP
2	r	259	ILE
2	r	353	VAL
2	q	32	VAL
2	q	61	ILE
2	q	75	ARG
2	q	127	LEU
2	q	141	THR
2	q	185	VAL
2	q	229	VAL
2	q	242	ASP
2	q	259	ILE
2	q	353	VAL
2	p	32	VAL
2	p	61	ILE
2	p	75	ARG
2	p	127	LEU
2	p	141	THR
2	p	185	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	p	229	VAL
2	p	242	ASP
2	p	259	ILE
2	p	353	VAL
2	o	32	VAL
2	o	61	ILE
2	o	75	ARG
2	o	127	LEU
2	o	141	THR
2	o	185	VAL
2	o	229	VAL
2	o	242	ASP
2	o	259	ILE
2	o	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
2	a	11	ASN
2	a	112	GLN
2	a	172	ASN
2	a	193	ASN
2	a	223	ASN
2	a	248	ASN
1	B	27	GLN
1	C	27	GLN
1	D	27	GLN
1	E	27	GLN
1	F	27	GLN
2	b	5	HIS
2	b	11	ASN
2	b	112	GLN
2	b	172	ASN
2	b	193	ASN
2	b	223	ASN
2	c	5	HIS
2	c	11	ASN
2	c	112	GLN
2	c	172	ASN
2	c	193	ASN
2	c	223	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	c	367	ASN
2	d	11	ASN
2	d	112	GLN
2	d	172	ASN
2	d	193	ASN
2	d	223	ASN
2	d	367	ASN
2	e	11	ASN
2	e	112	GLN
2	e	122	ASN
2	e	172	ASN
2	e	193	ASN
2	e	223	ASN
2	e	367	ASN
2	f	11	ASN
2	f	112	GLN
2	f	172	ASN
2	f	193	ASN
2	f	223	ASN
2	f	248	ASN
2	f	367	ASN
2	g	44	ASN
2	g	254	ASN
2	h	44	ASN
2	h	254	ASN
2	l	44	ASN
2	l	254	ASN
2	k	44	ASN
2	k	254	ASN
2	j	44	ASN
2	j	254	ASN
2	j	369	ASN
2	i	44	ASN
2	i	254	ASN
2	i	369	ASN
2	m	137	GLN
2	m	172	ASN
2	m	367	ASN
2	n	137	GLN
2	n	172	ASN
2	r	11	ASN
2	r	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	r	367	ASN
2	q	172	ASN
2	q	367	ASN
2	p	11	ASN
2	p	172	ASN
2	p	367	ASN
2	o	11	ASN
2	o	172	ASN
2	o	367	ASN

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 oligosaccharides 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.

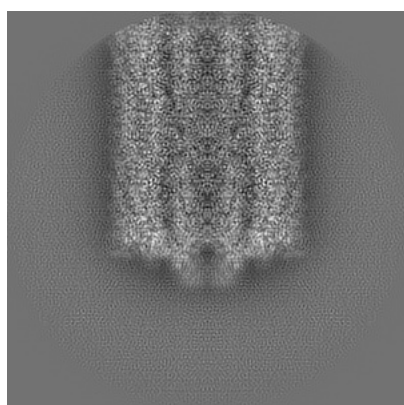
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20647. These allow visual inspection of the internal detail of the map and identification of artifacts.

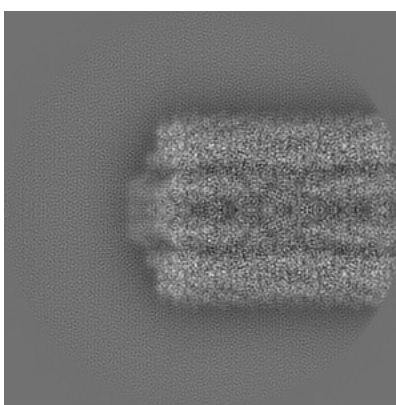
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

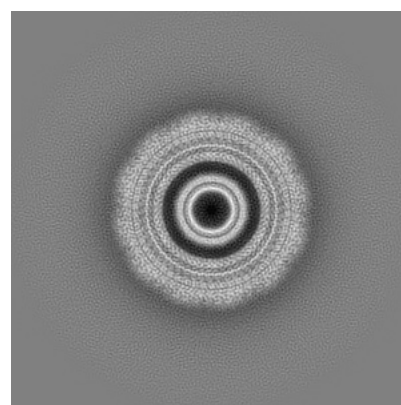
6.1.1 Primary map



X



Y

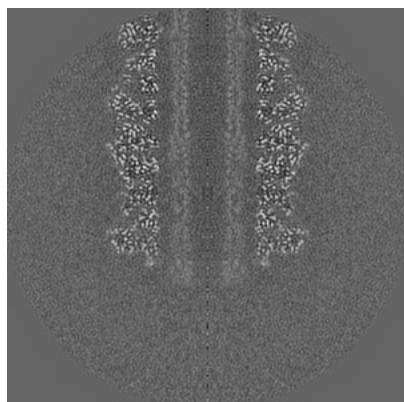


Z

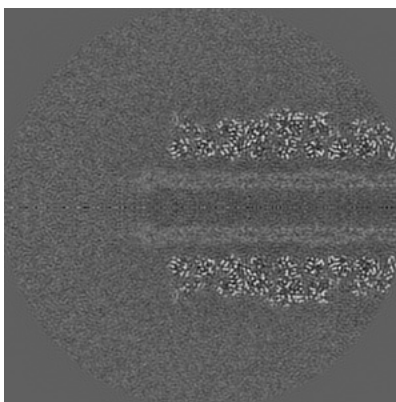
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

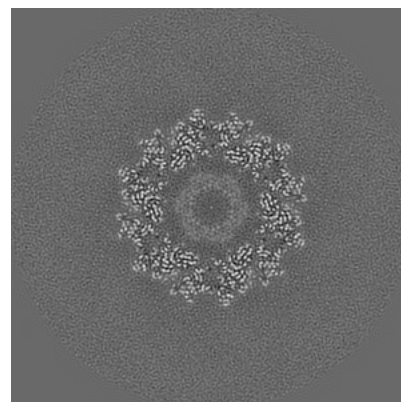
6.2.1 Primary map



X Index: 210



Y Index: 210

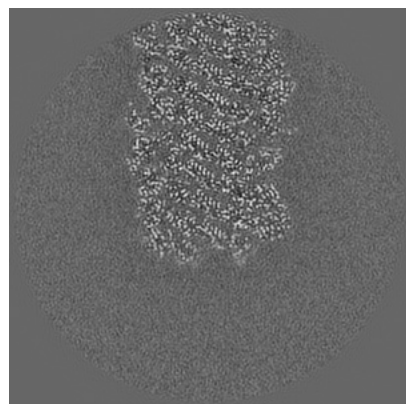


Z Index: 210

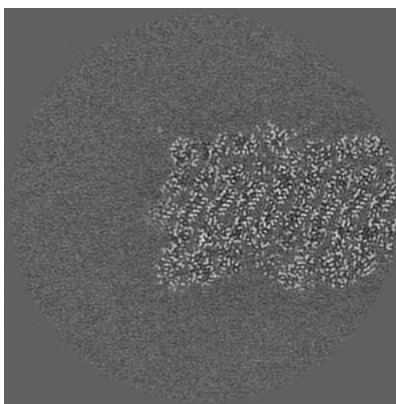
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

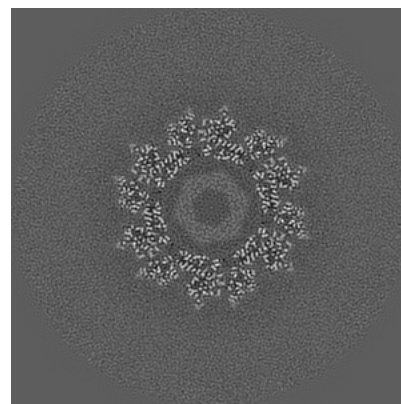
6.3.1 Primary map



X Index: 155



Y Index: 154

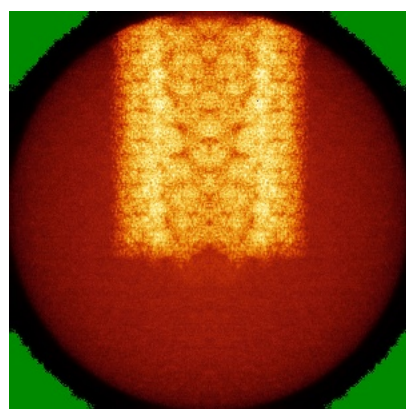


Z Index: 246

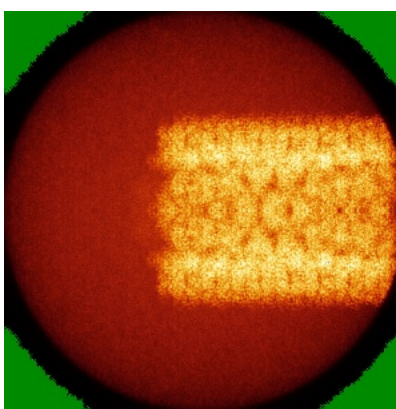
The images above show the largest variance slices of the map in three orthogonal directions.

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

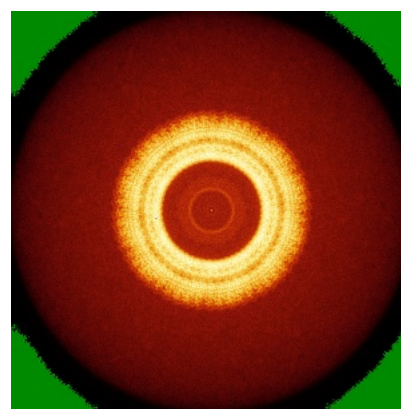
6.4.1 Primary map



X



Y

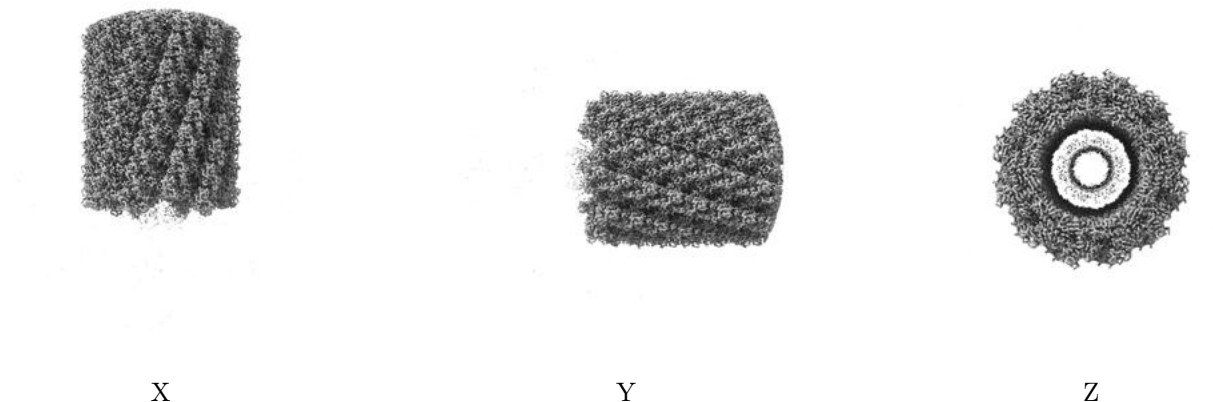


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

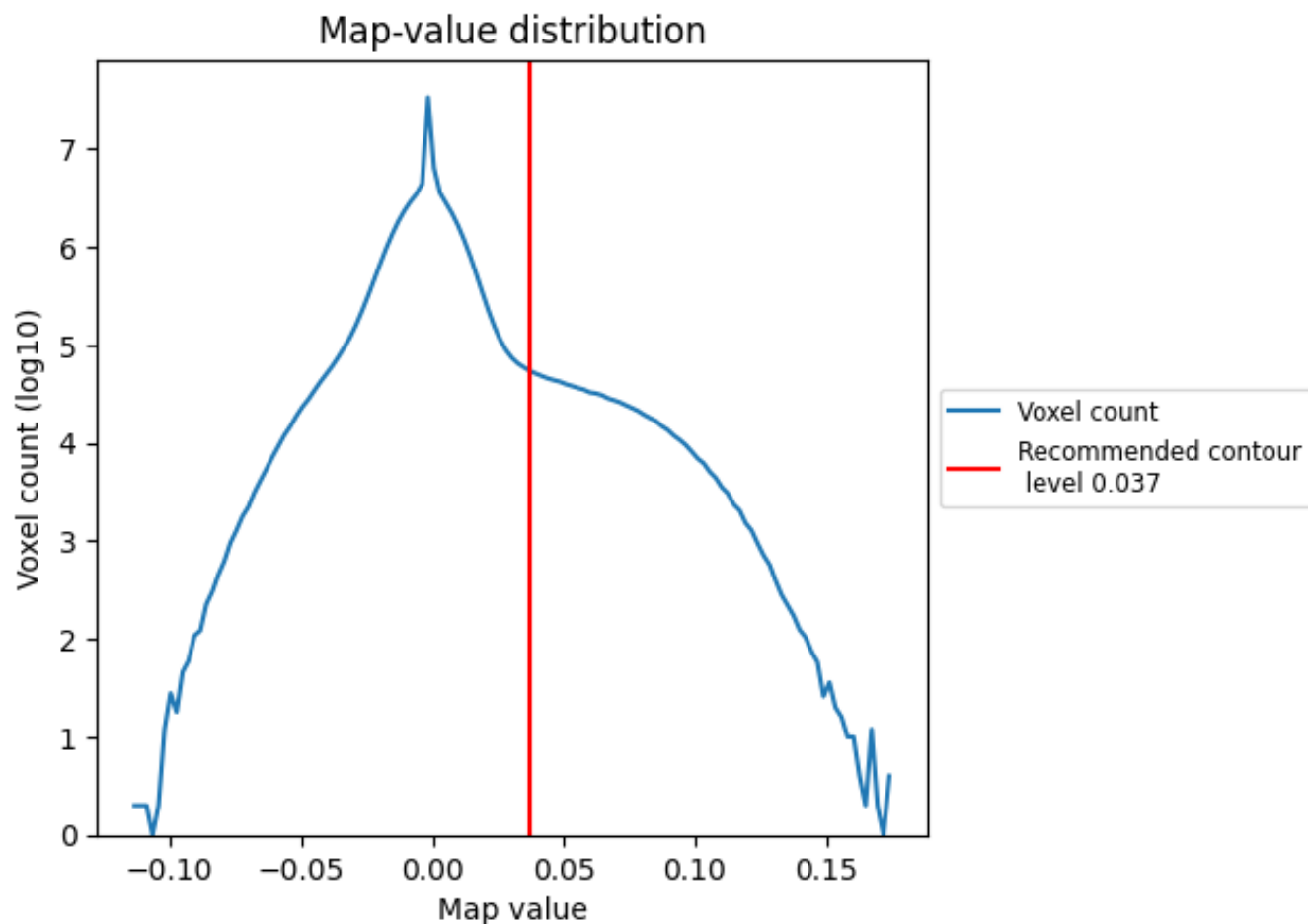
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

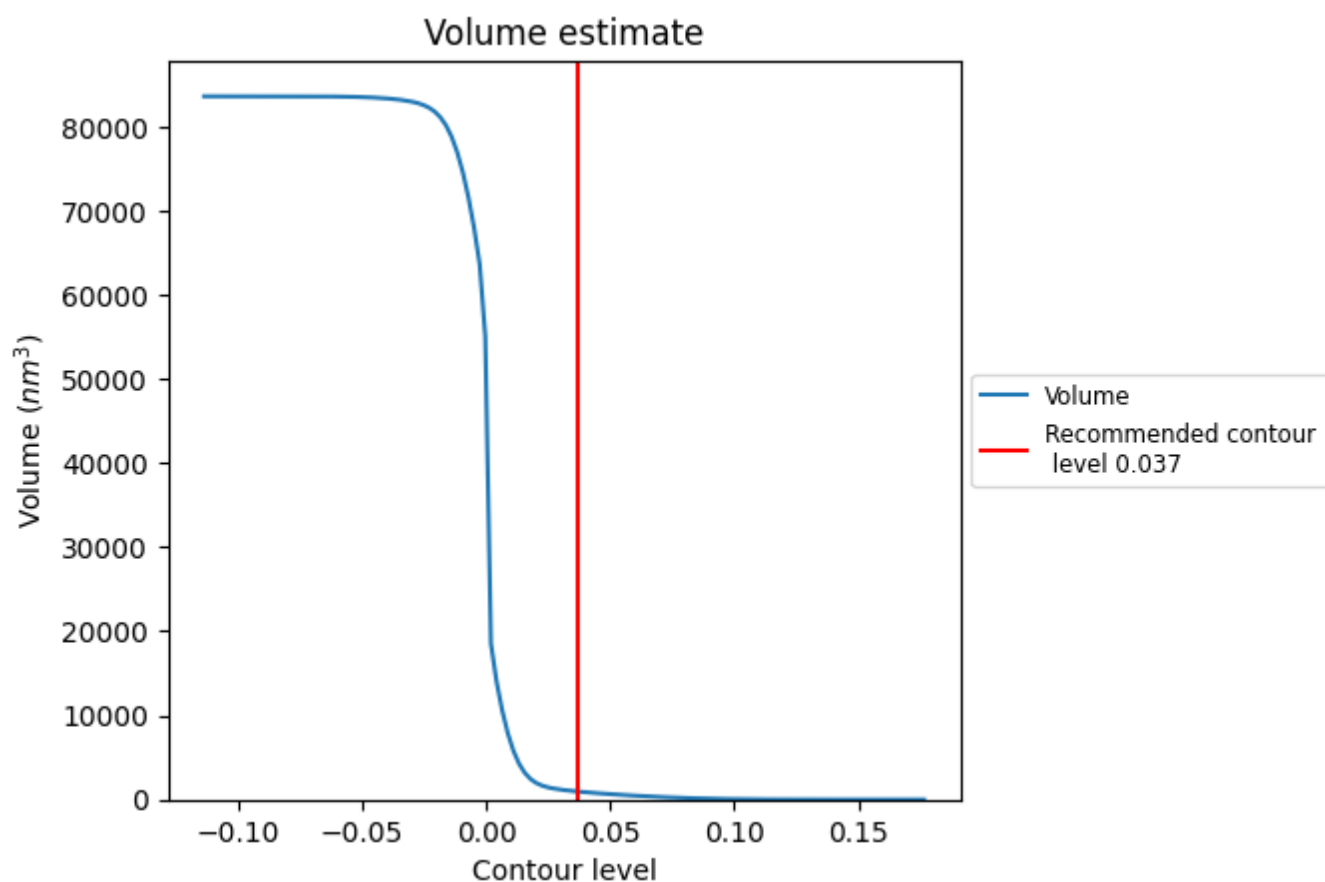
This section contains the results of statistical analysis of the map.

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.

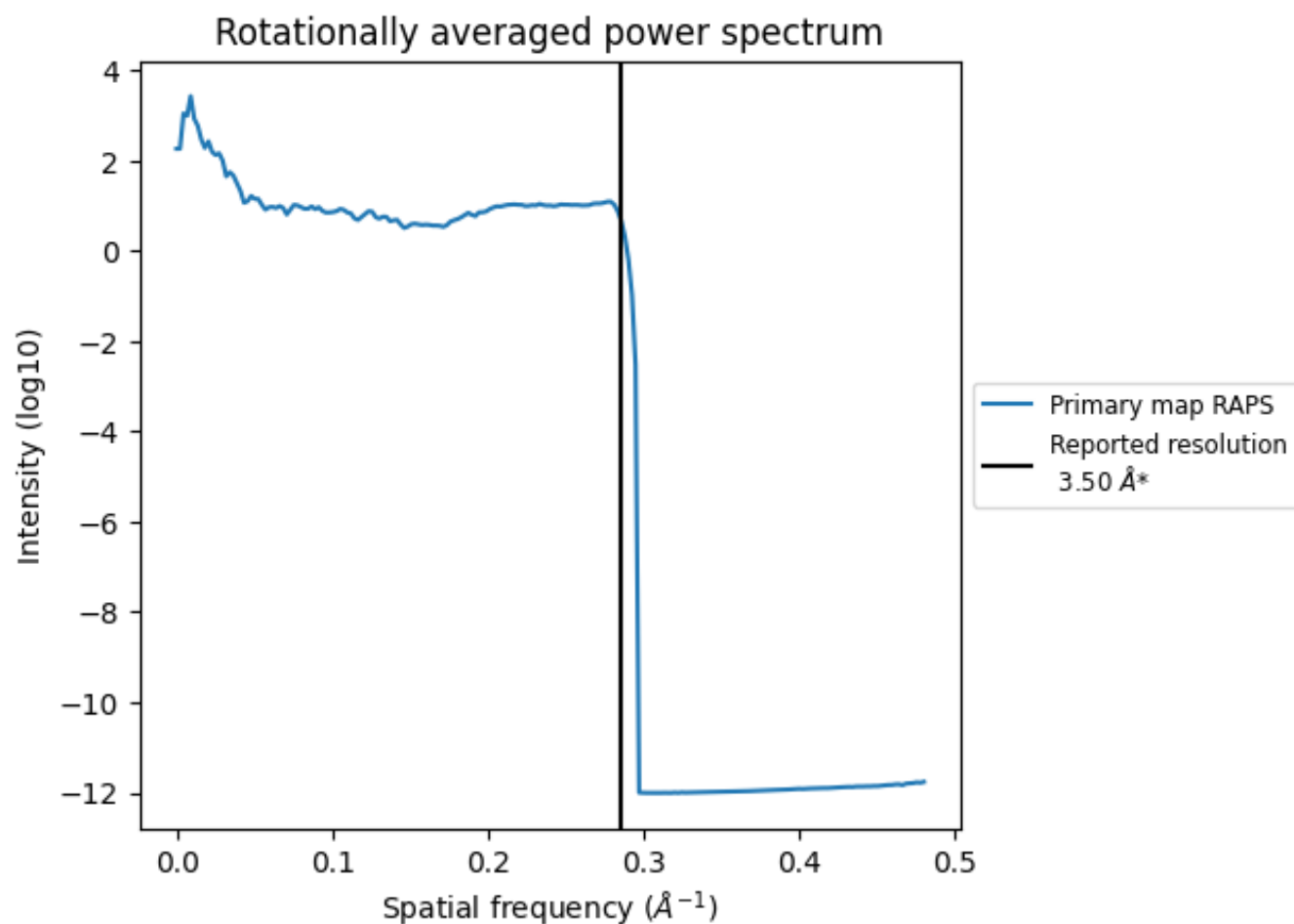
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 953 nm³; this corresponds to an approximate mass of 861 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 ⓘ

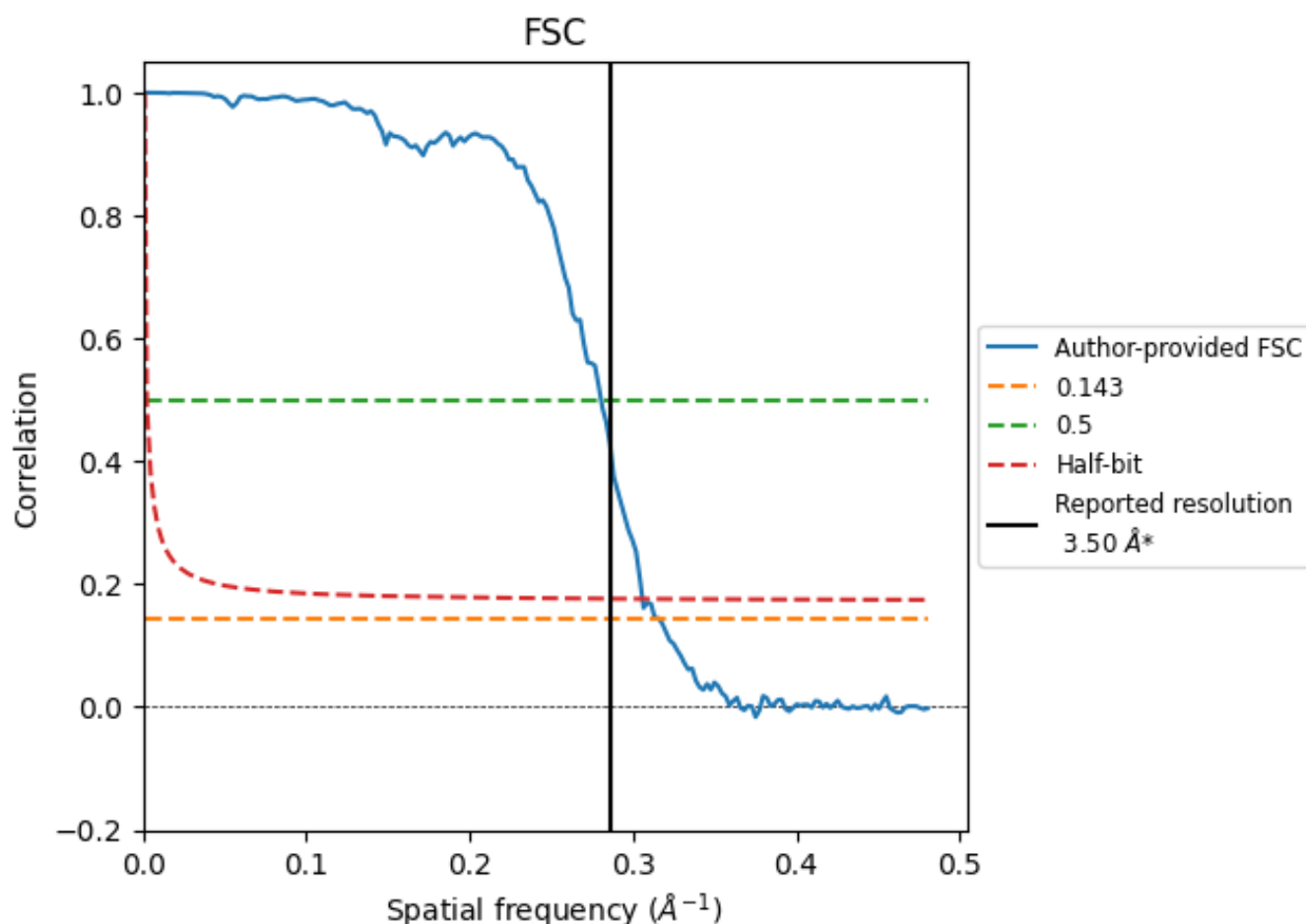


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.16	3.57	3.27
Unmasked-calculated*	-	-	-

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

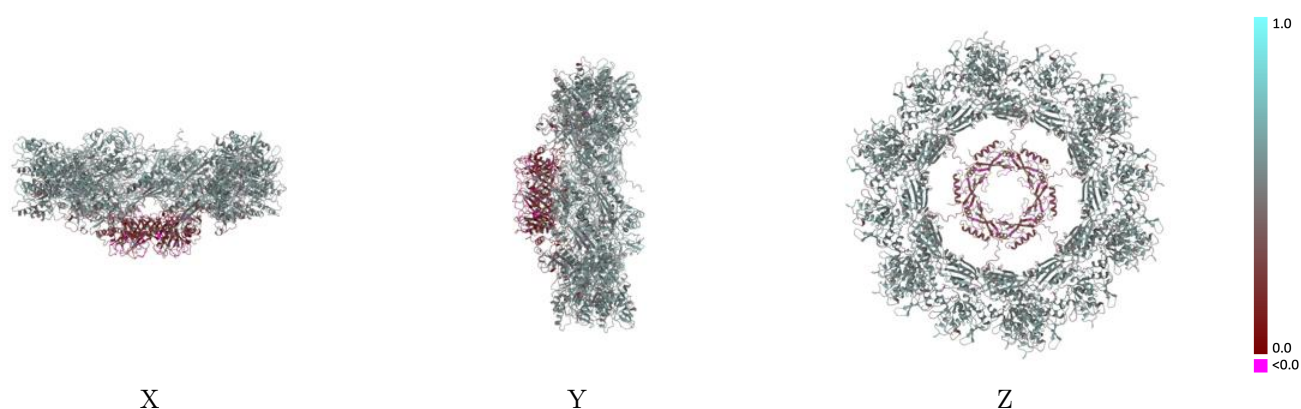
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20647 and PDB model 6U5J. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

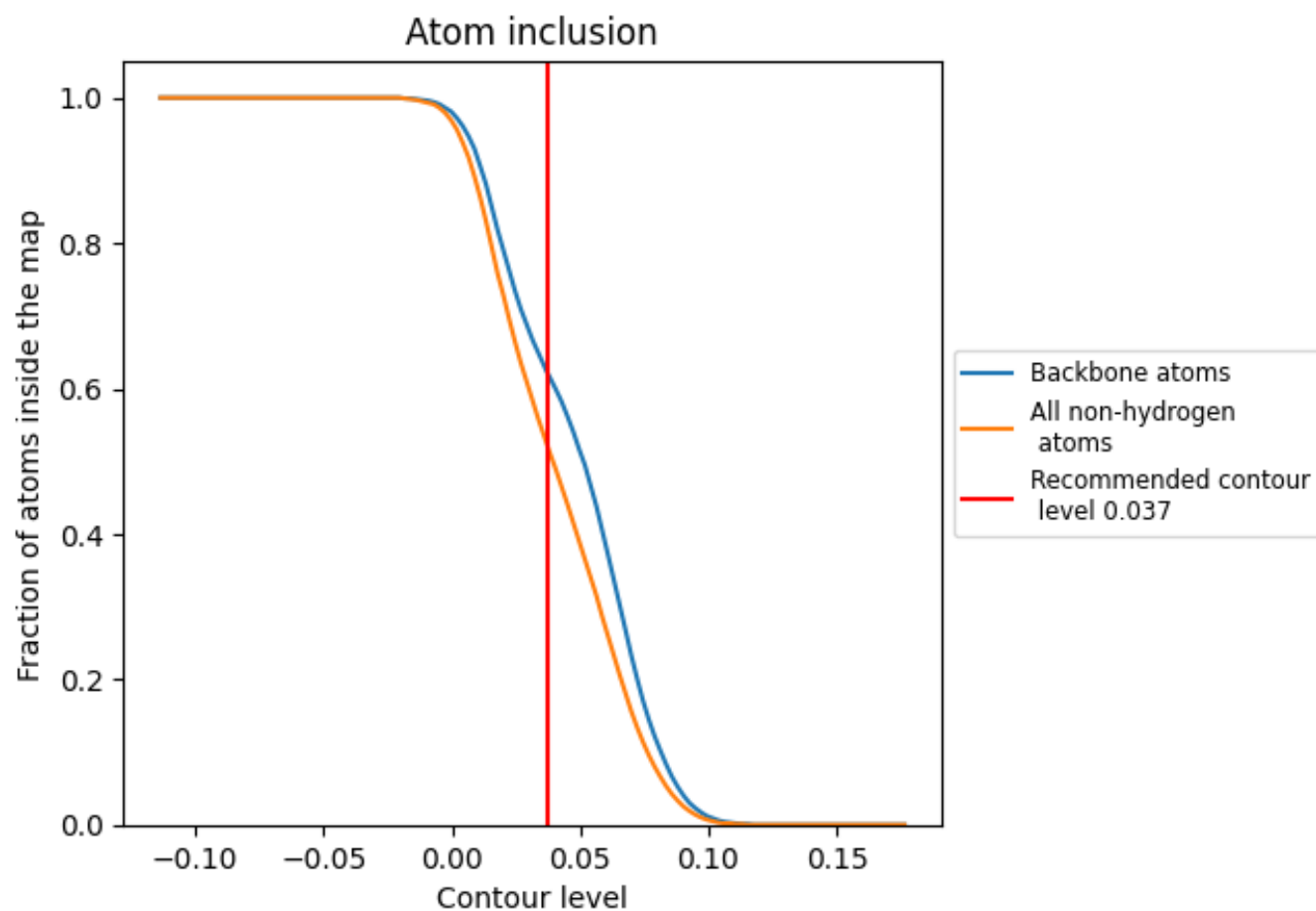


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5230	 0.4840
A	 0.0570	 0.2370
B	 0.0580	 0.2380
C	 0.0540	 0.2380
D	 0.0580	 0.2380
E	 0.0560	 0.2370
F	 0.0570	 0.2370
a	 0.5450	 0.5010
b	 0.5430	 0.5010
c	 0.5470	 0.5010
d	 0.5440	 0.5000
e	 0.5400	 0.5000
f	 0.5440	 0.5010
g	 0.6070	 0.5280
h	 0.6060	 0.5290
i	 0.6040	 0.5280
j	 0.6080	 0.5270
k	 0.6100	 0.5280
l	 0.6050	 0.5270
m	 0.6250	 0.5350
n	 0.6260	 0.5350
o	 0.6250	 0.5340
p	 0.6230	 0.5340
q	 0.6270	 0.5330
r	 0.6240	 0.5320

