



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:21 AM UTC

PDB ID : 8V3X / pdb_00008v3x
EMDB ID : EMD-42959
Title : CryoEM Structure of Diffocin - precontracted - Trunk
Authors : Cai, X.Y.; He, Y.; Zhou, Z.H.
Deposited on : 2023-11-28
Resolution : 2.20 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:

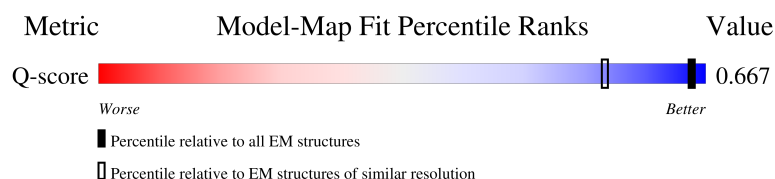
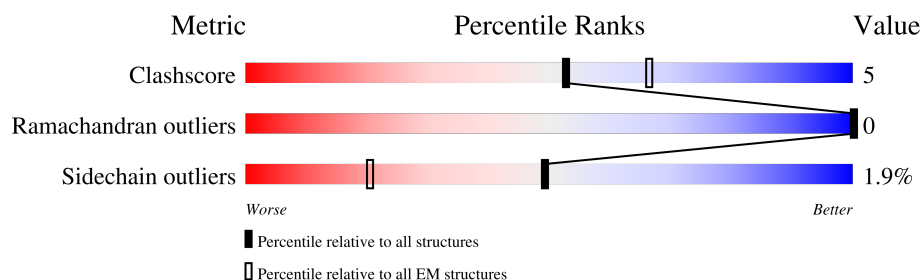
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	E	354	26% 81% 19% .
1	F	354	18% 85% 14% .
1	P	354	27% 80% 19% .
1	Q	354	19% 85% 14% ..

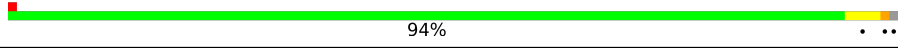
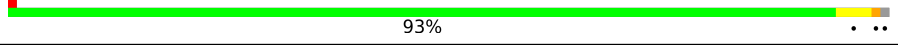
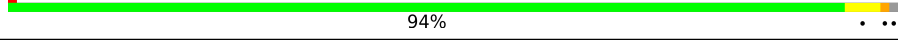
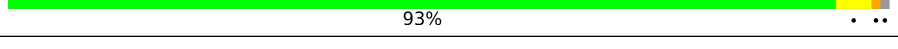
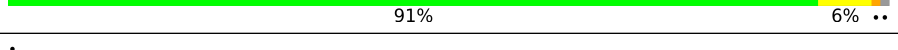
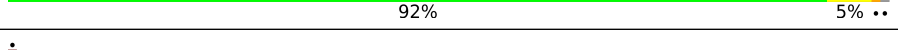
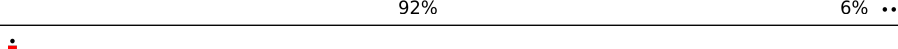
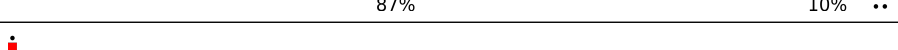
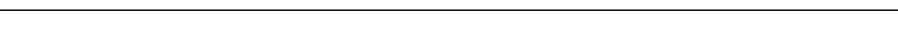
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	S	354	
1	T	354	
1	U	354	
1	V	354	
1	W	354	
1	X	354	
1	d	354	
1	e	354	
1	g	354	
1	n	354	
1	q	354	
1	r	354	
1	s	354	
1	z	354	
2	A	142	
2	B	142	
2	C	142	
2	D	142	
2	G	142	
2	H	142	
2	I	142	
2	J	142	
2	K	142	
2	L	142	
2	M	142	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	142	 83% 15% ..
2	O	142	 90% 8% .
2	R	142	 94% . ..
2	Y	142	 93% . ..
2	Z	142	 94% . ..
2	a	142	 93% . ..
2	b	142	 91% 6% ..
2	c	142	 92% 5% ..
2	i	142	 92% 6% ..
2	j	142	 87% 10% ..
2	k	142	 88% 9% ..
2	l	142	 87% 11% ..
2	m	142	 87% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 75948 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 Sheath (CD1363).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	d	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	V	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	S	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	W	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	T	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	F	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	E	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	X	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	U	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	Q	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	P	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	z	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	q	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	r	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	e	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
1	s	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	n	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		

- Molecule 2 is a protein called Tube (CD1364).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	A	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	B	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	Y	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	H	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	K	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	Z	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	I	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	L	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	G	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	C	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	D	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	a	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	J	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	M	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	R	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	N	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		
2	O	140	Total	C	N	O	S	0	0
			1111	711	183	211	6		

Continued on next page...

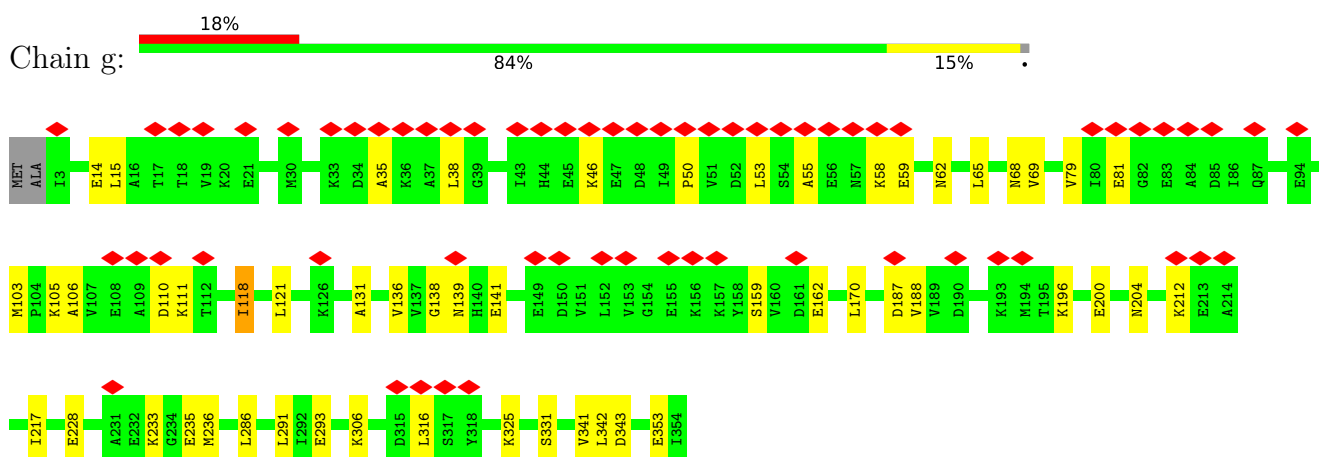
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	140	Total 1111	C 711	N 183	O 211	S 6	0	0
2	j	140	Total 1111	C 711	N 183	O 211	S 6	0	0
2	k	140	Total 1111	C 711	N 183	O 211	S 6	0	0
2	c	140	Total 1111	C 711	N 183	O 211	S 6	0	0
2	l	140	Total 1111	C 711	N 183	O 211	S 6	0	0
2	m	140	Total 1111	C 711	N 183	O 211	S 6	0	0

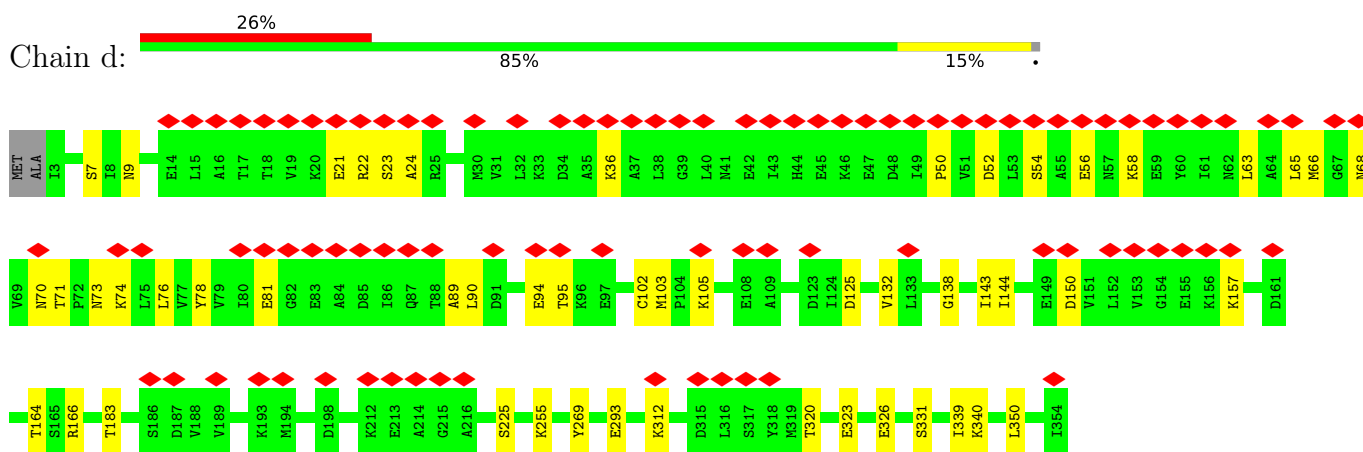
3 Residue-property plots

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.

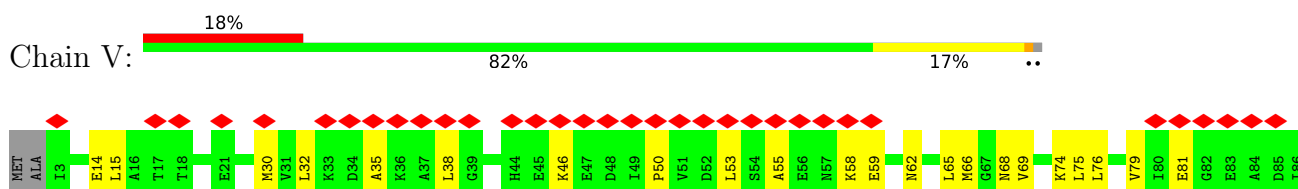
- Molecule 1: Sheath (CD1363)

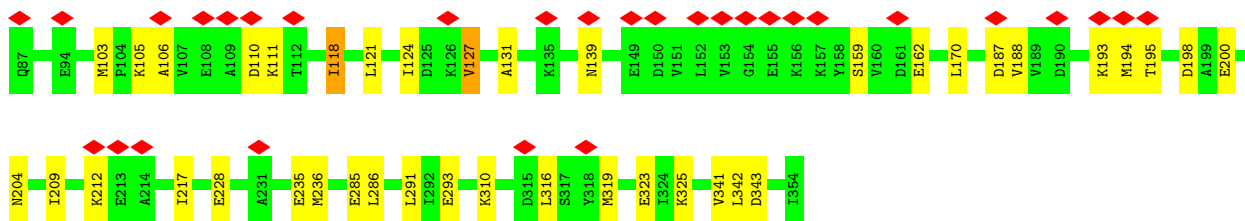


- Molecule 1: Sheath (CD1363)

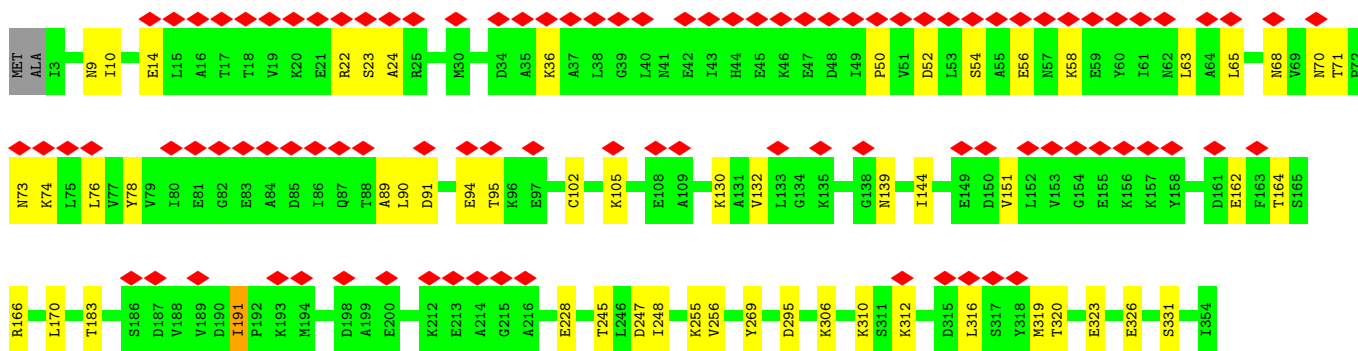
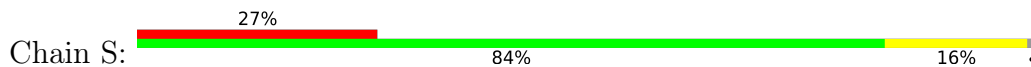


- Molecule 1: Sheath (CD1363)

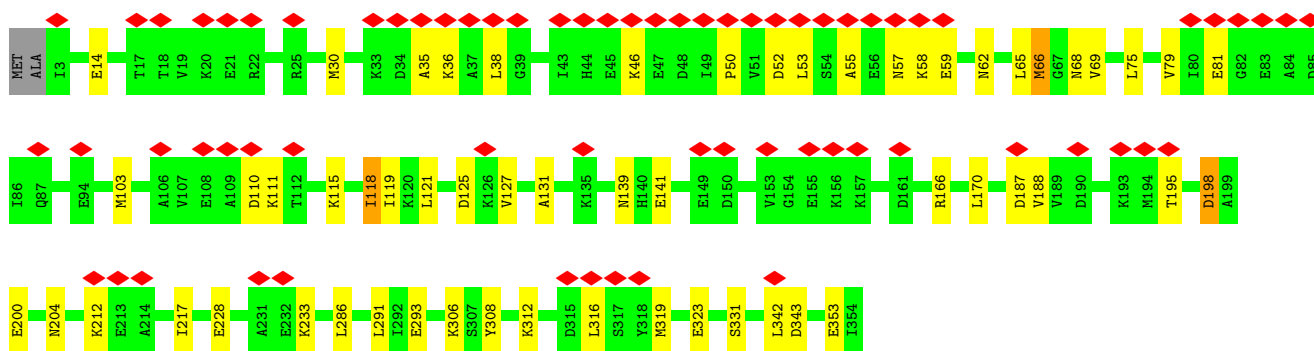
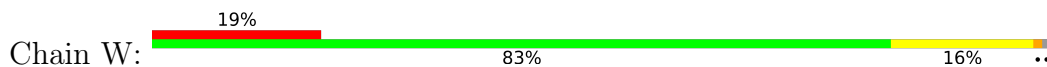




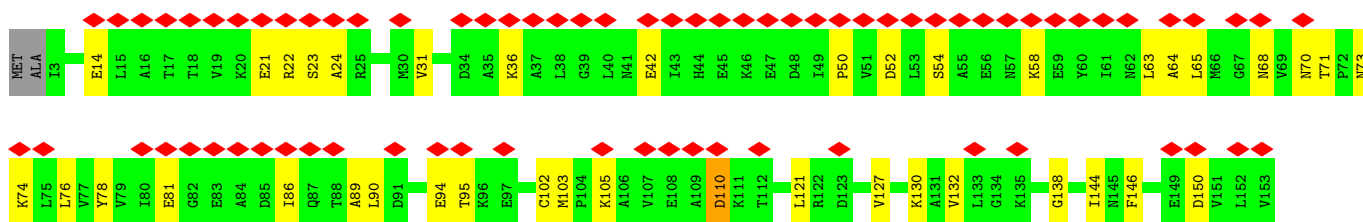
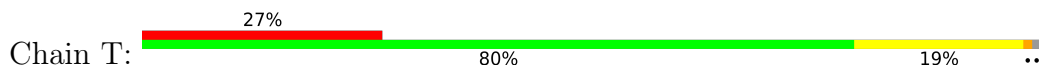
• Molecule 1: Sheath (CD1363)

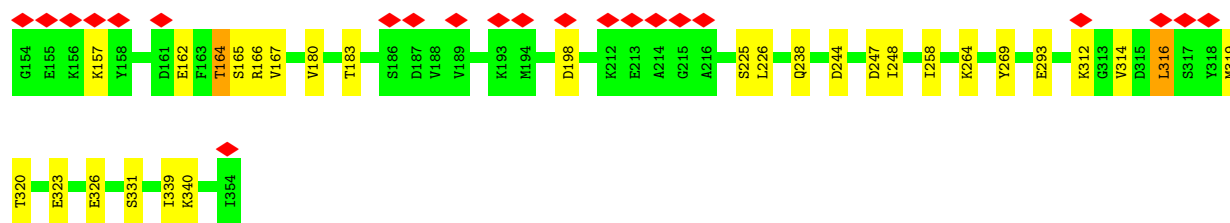


• Molecule 1: Sheath (CD1363)

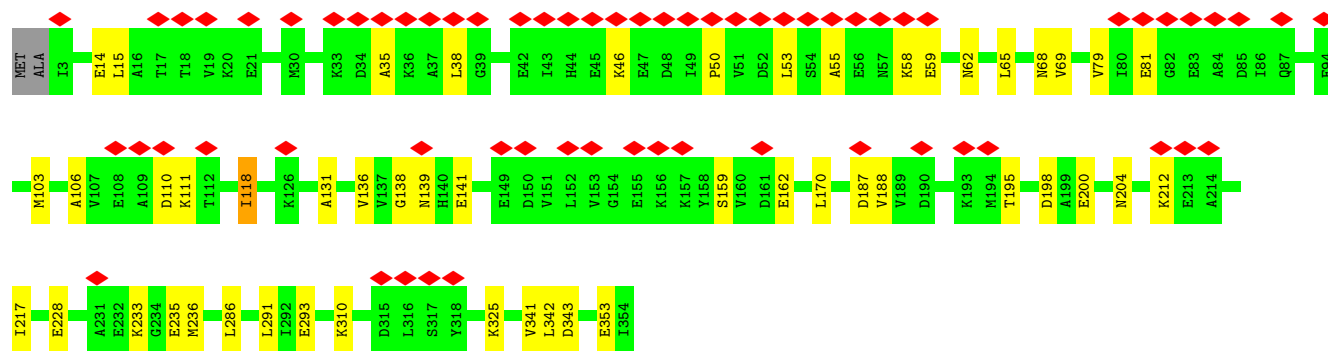
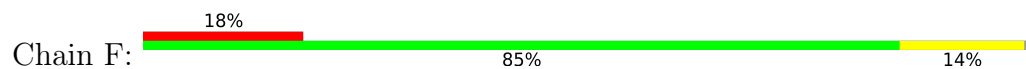


• Molecule 1: Sheath (CD1363)

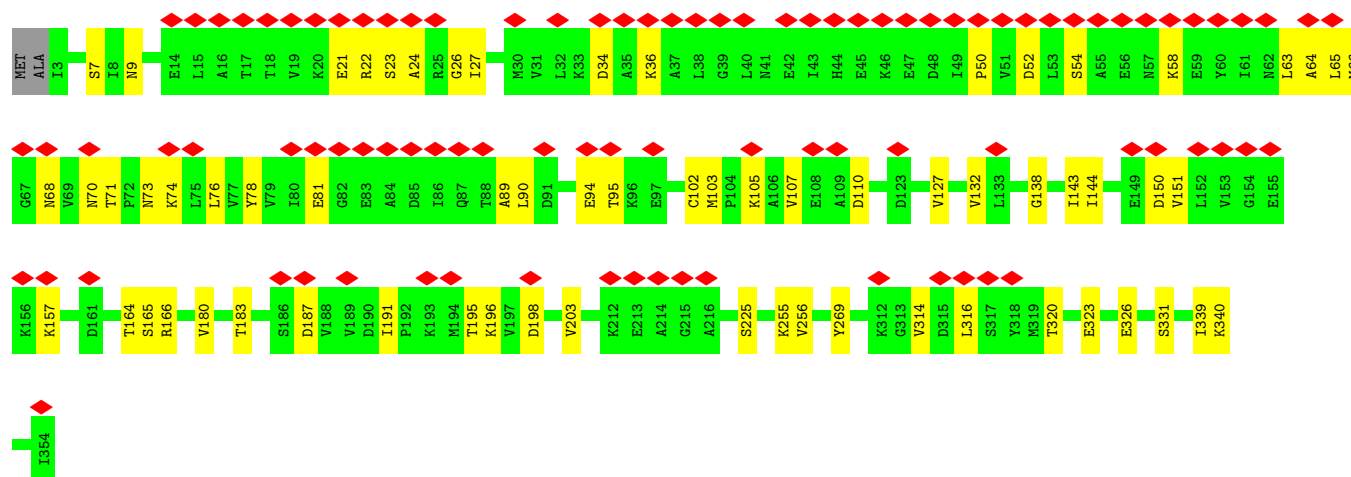
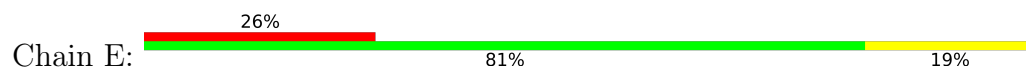




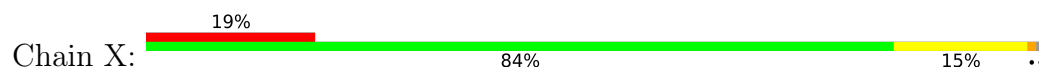
• Molecule 1: Sheath (CD1363)

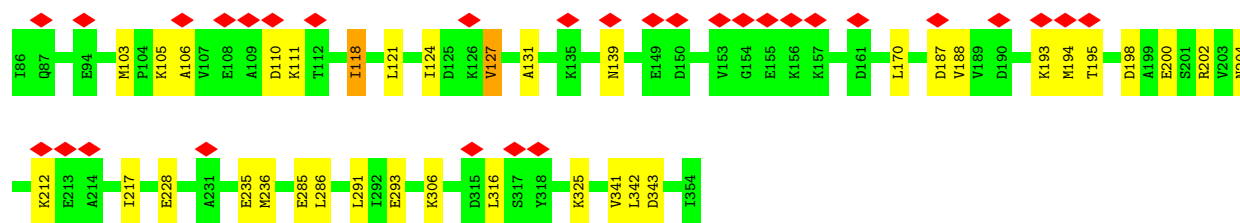


• Molecule 1: Sheath (CD1363)

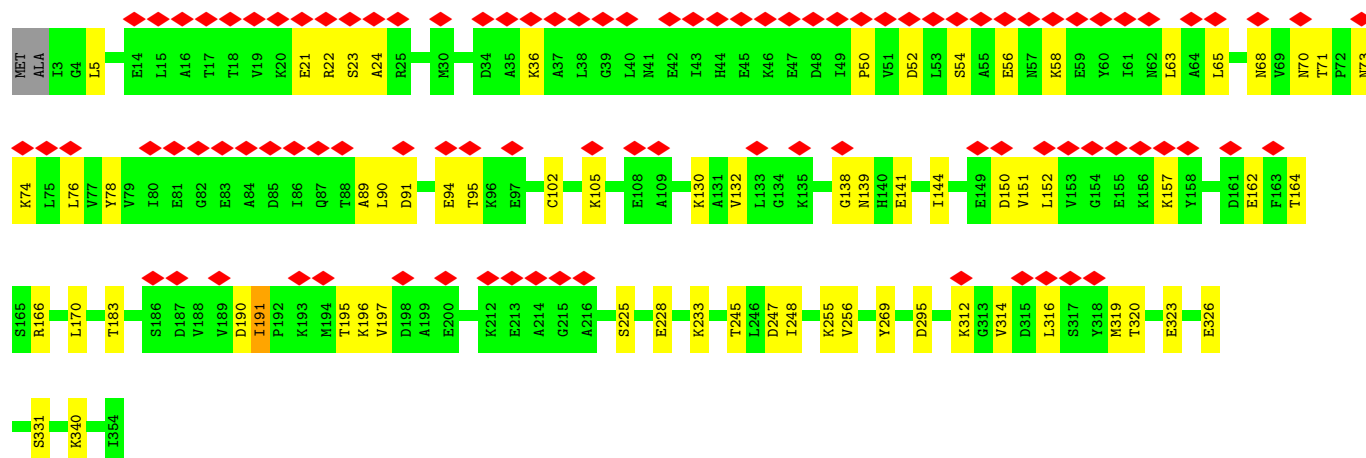
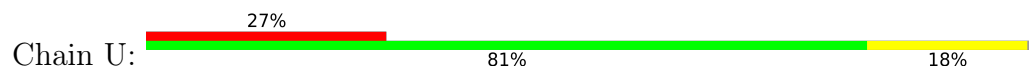


• Molecule 1: Sheath (CD1363)

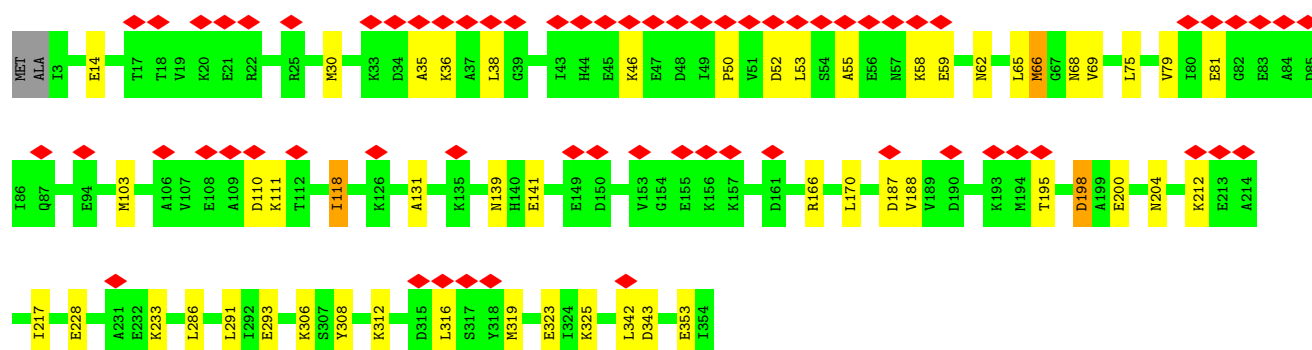
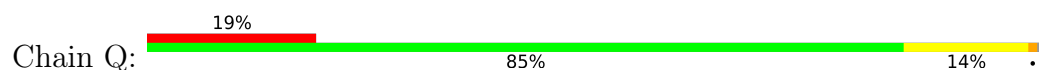




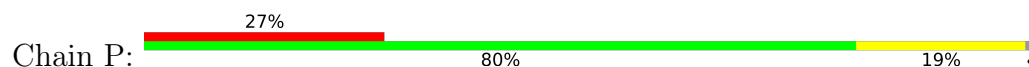
• Molecule 1: Sheath (CD1363)

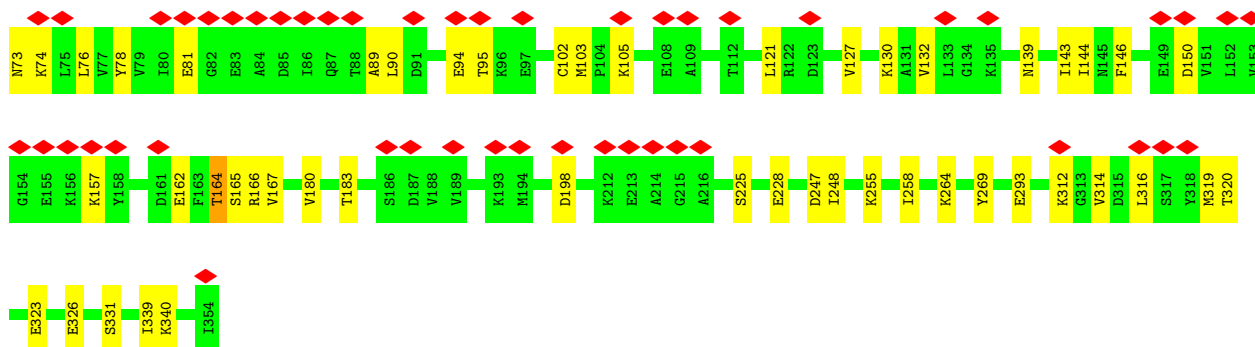


• Molecule 1: Sheath (CD1363)

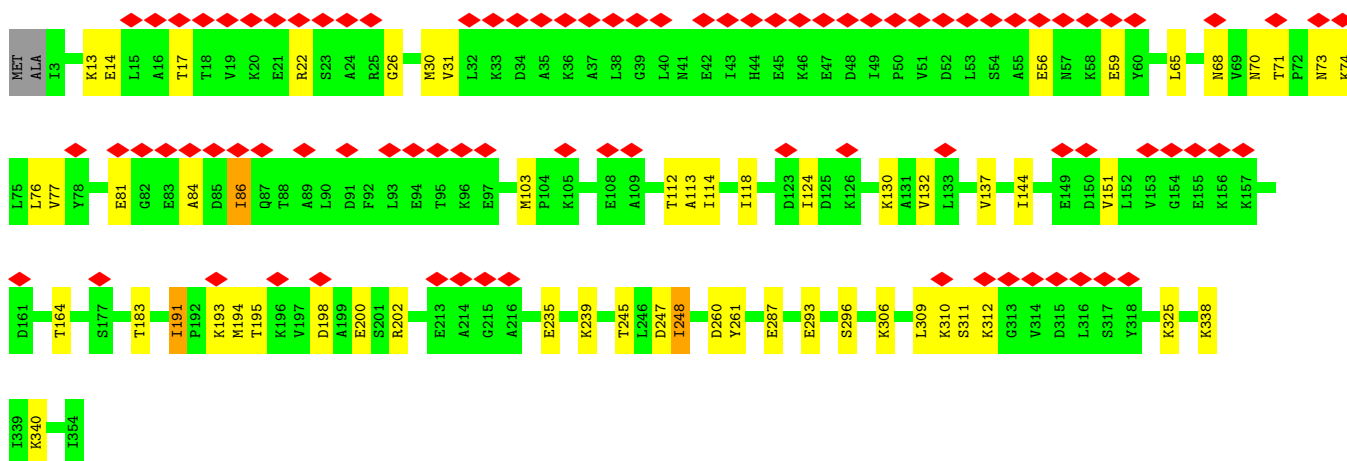
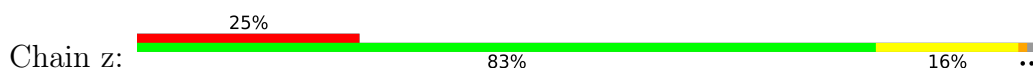


• Molecule 1: Sheath (CD1363)

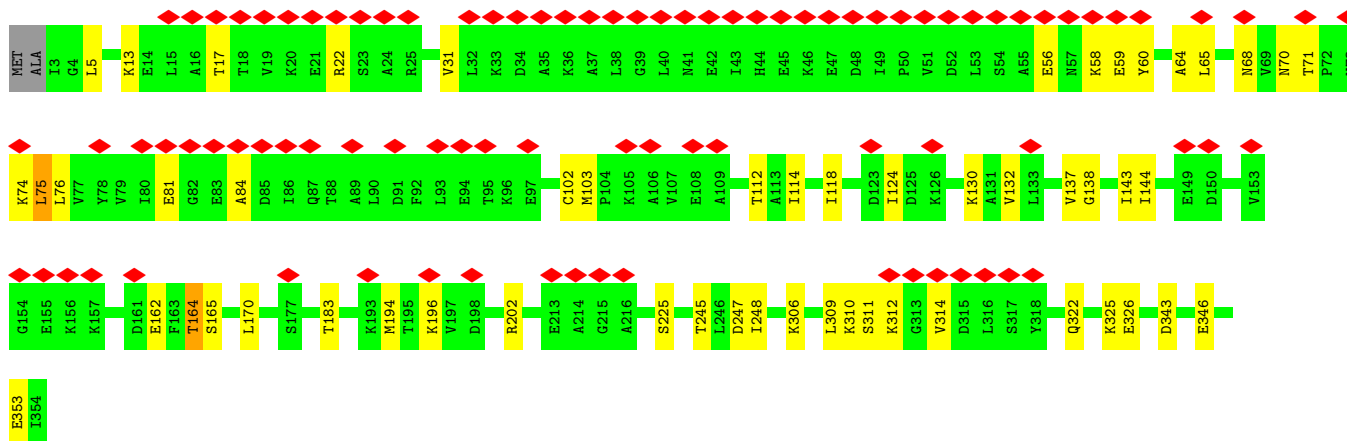
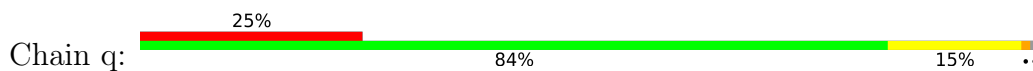




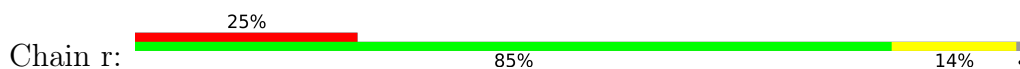
• Molecule 1: Sheath (CD1363)

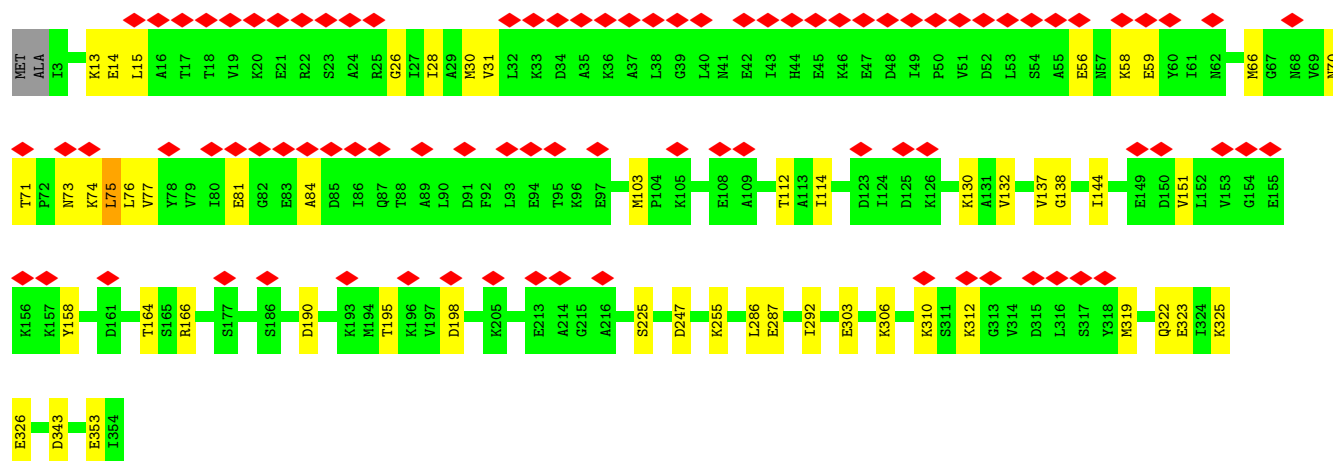


• Molecule 1: Sheath (CD1363)

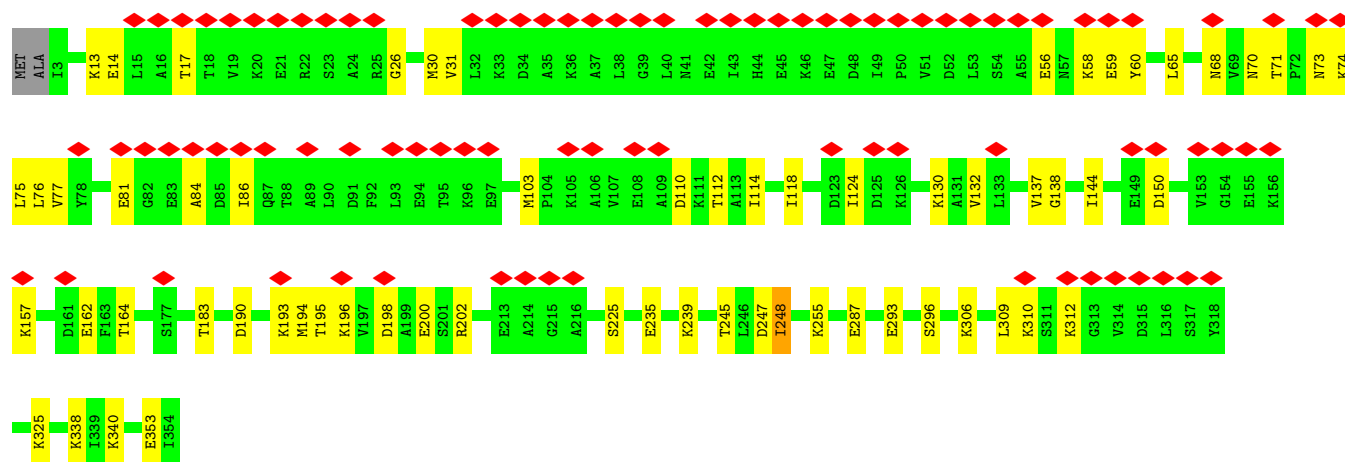
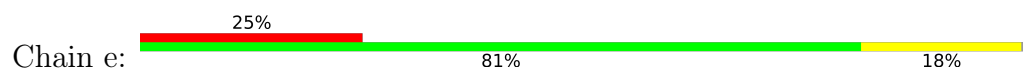


• Molecule 1: Sheath (CD1363)

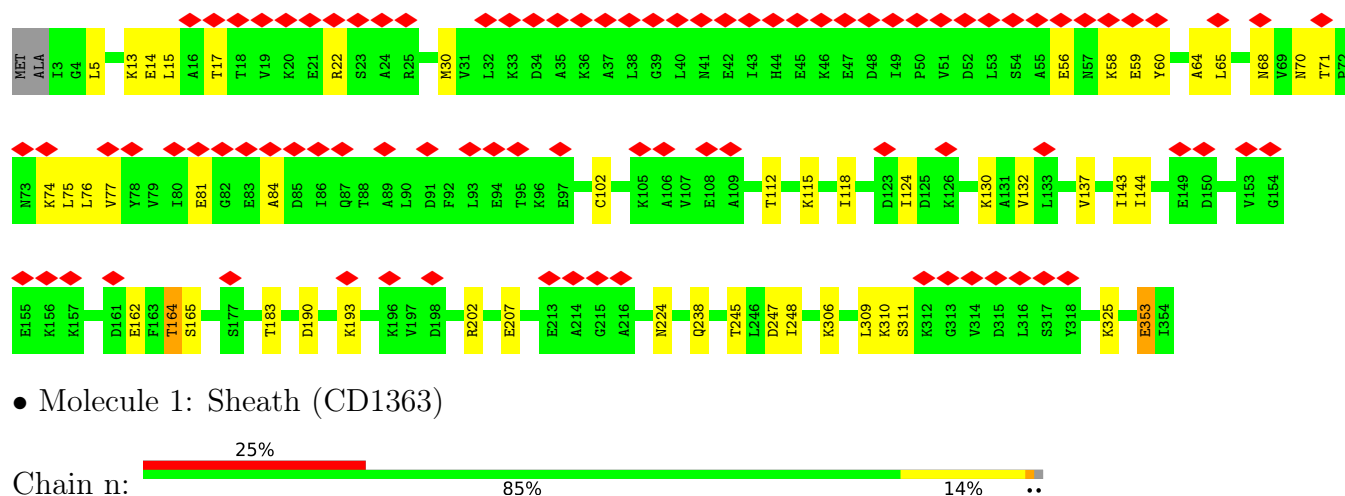
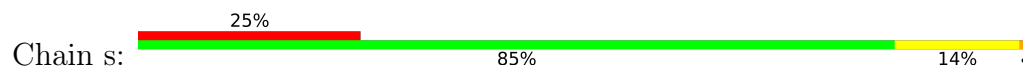




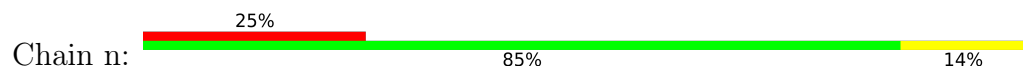
• Molecule 1: Sheath (CD1363)

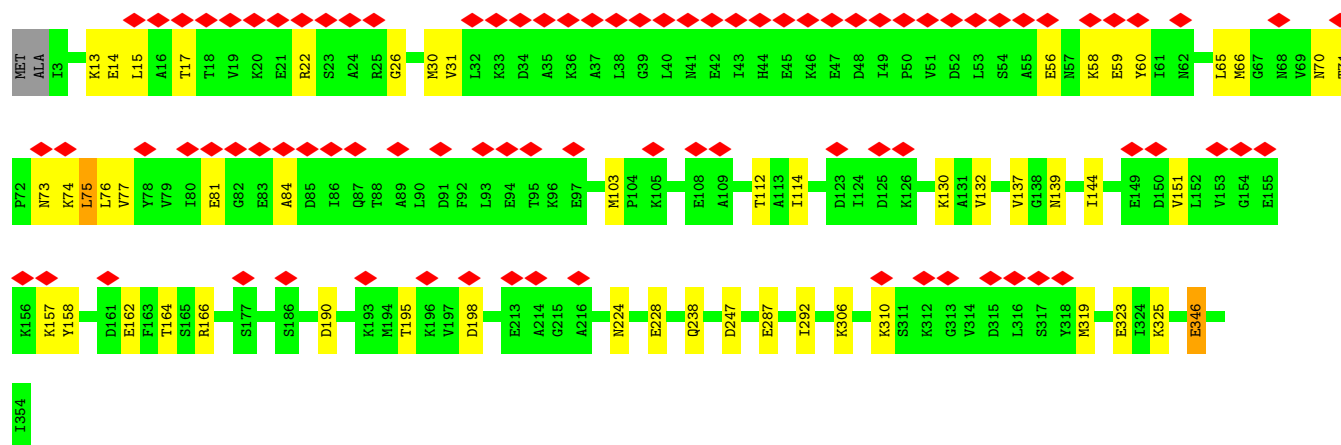


• Molecule 1: Sheath (CD1363)



• Molecule 1: Sheath (CD1363)

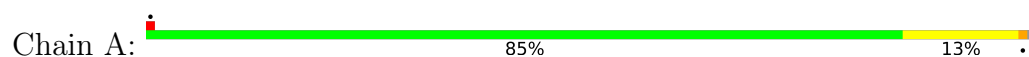




• Molecule 2: Tube (CD1364)



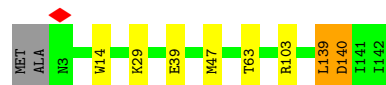
• Molecule 2: Tube (CD1364)



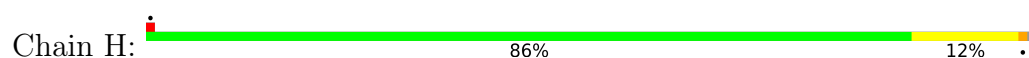
• Molecule 2: Tube (CD1364)



• Molecule 2: Tube (CD1364)

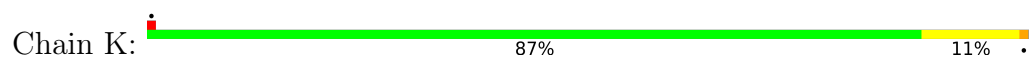


• Molecule 2: Tube (CD1364)





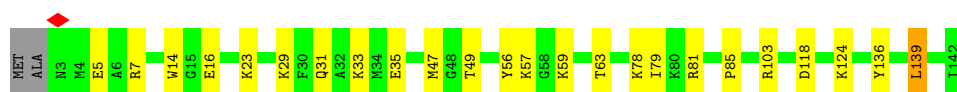
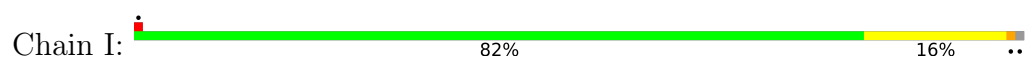
- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



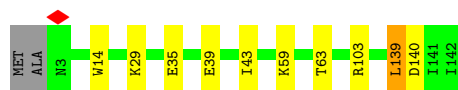
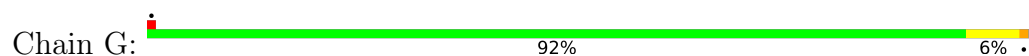
- Molecule 2: Tube (CD1364)



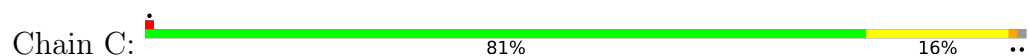
- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)

Chain D:  91% 7% ..



- Molecule 2: Tube (CD1364)

Chain a:  93% ..



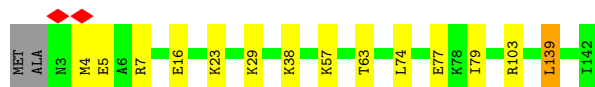
- Molecule 2: Tube (CD1364)

Chain J:  85% 13% ..

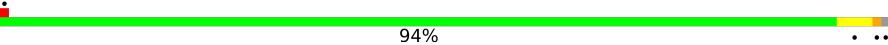


- Molecule 2: Tube (CD1364)

Chain M:  89% 9% ..



- Molecule 2: Tube (CD1364)

Chain R:  94% ..



- Molecule 2: Tube (CD1364)

Chain N:  83% 15% ..

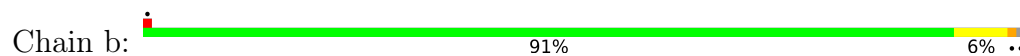


- Molecule 2: Tube (CD1364)

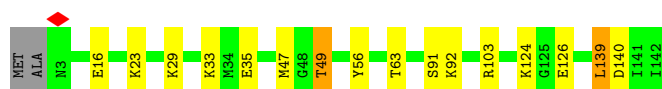
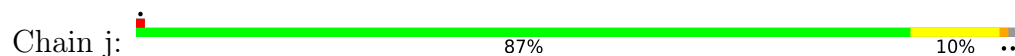
Chain O:  90% 8% ..



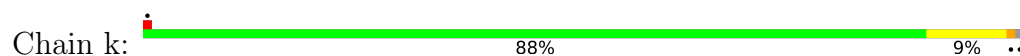
- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



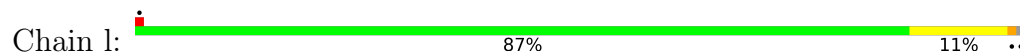
- Molecule 2: Tube (CD1364)



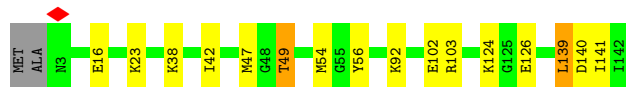
- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



- Molecule 2: Tube (CD1364)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	450732	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.55, 0.55, 0.55	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.19	0/2766	0.44	1/3729 (0.0%)
1	F	0.18	0/2766	0.38	1/3729 (0.0%)
1	P	0.18	0/2766	0.43	0/3729
1	Q	0.19	0/2766	0.38	1/3729 (0.0%)
1	S	0.19	0/2766	0.44	1/3729 (0.0%)
1	T	0.19	0/2766	0.44	1/3729 (0.0%)
1	U	0.19	0/2766	0.43	1/3729 (0.0%)
1	V	0.18	0/2766	0.39	1/3729 (0.0%)
1	W	0.19	0/2766	0.39	1/3729 (0.0%)
1	X	0.18	0/2766	0.39	1/3729 (0.0%)
1	d	0.18	0/2766	0.42	0/3729
1	e	0.18	0/2766	0.42	0/3729
1	g	0.18	0/2766	0.38	1/3729 (0.0%)
1	n	0.18	0/2766	0.43	0/3729
1	q	0.19	0/2766	0.43	0/3729
1	r	0.18	0/2766	0.43	0/3729
1	s	0.18	0/2766	0.43	0/3729
1	z	0.18	0/2766	0.43	0/3729
2	A	0.27	0/1133	0.49	0/1522
2	B	0.24	0/1133	0.48	0/1522
2	C	0.27	0/1133	0.49	0/1522
2	D	0.24	0/1133	0.47	0/1522
2	G	0.26	0/1133	0.49	0/1522
2	H	0.27	0/1133	0.47	0/1522
2	I	0.27	0/1133	0.48	0/1522
2	J	0.27	0/1133	0.47	0/1522
2	K	0.24	0/1133	0.47	0/1522
2	L	0.24	0/1133	0.47	0/1522
2	M	0.23	0/1133	0.47	0/1522
2	N	0.27	0/1133	0.48	0/1522
2	O	0.24	0/1133	0.48	0/1522
2	R	0.27	0/1133	0.49	0/1522
2	Y	0.27	0/1133	0.50	0/1522
2	Z	0.27	0/1133	0.49	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	a	0.27	0/1133	0.50	0/1522
2	b	0.24	0/1133	0.46	0/1522
2	c	0.24	0/1133	0.46	0/1522
2	i	0.26	0/1133	0.49	0/1522
2	j	0.24	0/1133	0.46	0/1522
2	k	0.24	0/1133	0.45	0/1522
2	l	0.25	0/1133	0.45	0/1522
2	m	0.24	0/1133	0.45	0/1522
All	All	0.21	0/76980	0.44	10/103650 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	68	ASN	N-CA-C	7.60	119.20	111.07
1	U	68	ASN	N-CA-C	7.55	119.15	111.07
1	E	68	ASN	N-CA-C	7.23	118.80	111.07
1	T	68	ASN	N-CA-C	7.19	118.77	111.07
1	X	69	VAL	N-CA-C	-6.37	106.59	112.96
1	V	69	VAL	N-CA-C	-6.26	106.70	112.96
1	W	69	VAL	N-CA-C	-5.75	107.21	112.96
1	Q	69	VAL	N-CA-C	-5.71	107.25	112.96
1	g	69	VAL	N-CA-C	-5.19	107.77	112.96
1	F	69	VAL	N-CA-C	-5.16	107.80	112.96

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	E	2738	0	2864	45	0
1	F	2738	0	2864	33	0
1	P	2738	0	2864	49	0
1	Q	2738	0	2864	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2738	0	2864	41	0
1	T	2738	0	2864	47	0
1	U	2738	0	2864	48	0
1	V	2738	0	2864	38	0
1	W	2738	0	2864	36	0
1	X	2738	0	2864	36	0
1	d	2738	0	2864	37	0
1	e	2738	0	2864	39	0
1	g	2738	0	2864	35	0
1	n	2738	0	2864	30	0
1	q	2738	0	2864	36	0
1	r	2738	0	2864	30	0
1	s	2738	0	2864	30	0
1	z	2738	0	2864	35	0
2	A	1111	0	1103	14	0
2	B	1111	0	1103	5	0
2	C	1111	0	1103	18	0
2	D	1111	0	1103	8	0
2	G	1111	0	1103	8	0
2	H	1111	0	1103	14	0
2	I	1111	0	1103	20	0
2	J	1111	0	1103	14	0
2	K	1111	0	1103	7	0
2	L	1111	0	1103	8	0
2	M	1111	0	1103	8	0
2	N	1111	0	1103	18	0
2	O	1111	0	1103	5	0
2	R	1111	0	1103	4	0
2	Y	1111	0	1103	6	0
2	Z	1111	0	1103	3	0
2	a	1111	0	1103	6	0
2	b	1111	0	1103	9	0
2	c	1111	0	1103	7	0
2	i	1111	0	1103	7	0
2	j	1111	0	1103	11	0
2	k	1111	0	1103	10	0
2	l	1111	0	1103	11	0
2	m	1111	0	1103	12	0
All	All	75948	0	78024	819	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 (819) 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)
1:U:139:ASN:HD21	1:U:228:GLU:HG3	1.48	0.78
1:S:139:ASN:HD21	1:S:228:GLU:HG3	1.47	0.78
1:P:68:ASN:ND2	1:P:183:THR:OG1	2.20	0.74
1:e:130:LYS:NZ	1:e:247:ASP:OD2	2.22	0.73
1:T:78:TYR:HE2	1:T:89:ALA:HA	1.54	0.72
1:z:130:LYS:NZ	1:z:247:ASP:OD2	2.21	0.72
1:d:68:ASN:ND2	1:d:183:THR:OG1	2.22	0.72
1:s:353:GLU:HG3	1:n:13:LYS:HE3	1.73	0.71
2:j:16:GLU:OE2	2:j:23:LYS:NZ	2.24	0.70
1:s:68:ASN:ND2	1:s:183:THR:OG1	2.25	0.70
1:S:78:TYR:HE2	1:S:89:ALA:HA	1.56	0.69
1:q:68:ASN:ND2	1:q:183:THR:OG1	2.25	0.69
1:g:325:LYS:NZ	2:i:140:ASP:OD1	2.22	0.69
2:Y:39:GLU:HG2	2:I:124:LYS:HD3	1.74	0.69
2:M:16:GLU:OE1	2:M:23:LYS:NZ	2.20	0.69
2:l:16:GLU:OE2	2:l:23:LYS:NZ	2.25	0.69
1:P:22:ARG:NH2	1:P:23:SER:O	2.26	0.69
1:T:22:ARG:NH2	1:T:23:SER:O	2.25	0.68
1:U:78:TYR:HE2	1:U:89:ALA:HA	1.57	0.68
2:K:16:GLU:OE1	2:K:23:LYS:NZ	2.25	0.68
1:F:325:LYS:NZ	2:G:140:ASP:OD1	2.22	0.68
1:Q:35:ALA:HA	1:Q:81:GLU:HG2	1.76	0.68
1:U:151:VAL:HG22	1:U:191:ILE:HD11	1.74	0.67
1:V:53:LEU:O	1:V:58:LYS:NZ	2.23	0.67
2:a:39:GLU:HG2	2:N:124:LYS:HD3	1.77	0.67
1:W:35:ALA:HA	1:W:81:GLU:HG2	1.76	0.67
1:X:35:ALA:HA	1:X:81:GLU:HG2	1.76	0.67
1:g:35:ALA:HA	1:g:81:GLU:HG2	1.77	0.66
1:V:35:ALA:HA	1:V:81:GLU:HG2	1.75	0.66
1:F:53:LEU:O	1:F:58:LYS:NZ	2.25	0.66
1:g:212:LYS:HG2	1:d:95:THR:HG23	1.77	0.66
1:r:353:GLU:HG3	1:e:13:LYS:HE3	1.77	0.66
1:Q:38:LEU:HD21	1:Q:81:GLU:HG3	1.78	0.66
2:A:57:LYS:HE2	2:A:59:LYS:HZ3	1.59	0.66
2:C:57:LYS:HE2	2:C:59:LYS:HZ3	1.61	0.66
1:F:35:ALA:HA	1:F:81:GLU:HG2	1.77	0.65
1:g:53:LEU:O	1:g:58:LYS:NZ	2.25	0.65
1:z:68:ASN:ND2	1:z:183:THR:OG1	2.30	0.65
1:s:325:LYS:NZ	2:l:140:ASP:OD1	2.29	0.65
1:W:38:LEU:HD21	1:W:81:GLU:HG3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:LYS:HG2	2:D:63:THR:HB	1.79	0.64
1:W:212:LYS:HG2	1:T:95:THR:HG23	1.79	0.64
1:Q:212:LYS:HG2	1:P:95:THR:HG23	1.80	0.64
1:X:53:LEU:O	1:X:58:LYS:NZ	2.24	0.64
1:F:212:LYS:HG2	1:E:95:THR:HG23	1.80	0.64
1:Q:53:LEU:O	1:Q:58:LYS:NZ	2.24	0.64
1:e:68:ASN:ND2	1:e:183:THR:OG1	2.30	0.64
1:F:200:GLU:O	1:F:204:ASN:ND2	2.29	0.64
1:V:38:LEU:HD21	1:V:81:GLU:HG3	1.80	0.63
1:n:130:LYS:NZ	1:n:247:ASP:OD2	2.29	0.63
1:X:325:LYS:NZ	2:a:140:ASP:OD1	2.27	0.63
1:T:320:THR:OG1	1:T:323:GLU:HG3	1.98	0.63
1:q:325:LYS:NZ	2:j:140:ASP:OD1	2.29	0.63
2:Z:39:GLU:HG2	2:C:124:LYS:HD3	1.79	0.63
1:W:331:SER:HB2	1:q:346:GLU:OE1	1.99	0.62
1:X:38:LEU:HD21	1:X:81:GLU:HG3	1.81	0.62
1:g:38:LEU:HD21	1:g:81:GLU:HG3	1.82	0.62
1:S:22:ARG:NH2	1:S:23:SER:O	2.32	0.62
1:Q:200:GLU:O	1:Q:204:ASN:ND2	2.31	0.62
1:P:162:GLU:OE1	1:P:162:GLU:N	2.33	0.62
1:W:53:LEU:O	1:W:58:LYS:NZ	2.24	0.62
1:U:22:ARG:NH2	1:U:23:SER:O	2.33	0.62
2:A:124:LYS:HD3	2:R:39:GLU:HG2	1.82	0.62
1:X:139:ASN:HD21	1:X:228:GLU:HG3	1.64	0.62
1:z:81:GLU:HG2	1:z:84:ALA:HB2	1.82	0.62
2:L:29:LYS:HG2	2:L:63:THR:HB	1.81	0.61
1:d:22:ARG:NH2	1:d:23:SER:O	2.34	0.61
1:X:212:LYS:HG2	1:U:95:THR:HG23	1.81	0.61
1:e:325:LYS:NZ	2:c:140:ASP:OD1	2.29	0.61
1:V:212:LYS:HG2	1:S:95:THR:HG23	1.81	0.61
1:F:38:LEU:HD21	1:F:81:GLU:HG3	1.82	0.61
1:F:55:ALA:HA	1:F:58:LYS:HE2	1.83	0.61
1:W:68:ASN:HB2	1:W:170:LEU:HD22	1.83	0.61
1:V:139:ASN:HD21	1:V:228:GLU:HG3	1.66	0.61
1:S:162:GLU:N	1:S:162:GLU:OE1	2.34	0.60
1:W:200:GLU:O	1:W:204:ASN:ND2	2.33	0.60
1:U:162:GLU:OE1	1:U:162:GLU:N	2.34	0.60
2:m:124:LYS:NZ	2:m:126:GLU:OE1	2.34	0.60
1:S:151:VAL:HG22	1:S:191:ILE:HD11	1.82	0.60
2:m:16:GLU:OE2	2:m:23:LYS:NZ	2.34	0.60
1:g:55:ALA:HA	1:g:58:LYS:HE2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:162:GLU:OE2	1:T:162:GLU:N	2.33	0.60
2:k:124:LYS:NZ	2:k:126:GLU:OE1	2.34	0.60
1:S:70:ASN:OD1	1:S:71:THR:N	2.34	0.60
1:e:81:GLU:HG2	1:e:84:ALA:HB2	1.84	0.60
1:d:78:TYR:HE2	1:d:89:ALA:HA	1.66	0.60
1:Q:68:ASN:HB2	1:Q:170:LEU:HD22	1.84	0.60
1:P:70:ASN:OD1	1:P:71:THR:N	2.34	0.60
1:P:320:THR:OG1	1:P:323:GLU:HG3	2.01	0.60
1:z:325:LYS:NZ	2:b:140:ASP:OD1	2.30	0.60
1:r:325:LYS:NZ	2:k:140:ASP:OD1	2.29	0.60
2:k:16:GLU:OE2	2:k:23:LYS:NZ	2.34	0.60
1:d:70:ASN:OD1	1:d:71:THR:N	2.34	0.59
2:A:118:ASP:OD1	2:N:31:GLN:HG2	2.03	0.59
1:E:70:ASN:OD1	1:E:71:THR:N	2.33	0.59
2:C:29:LYS:HG2	2:C:63:THR:HB	1.85	0.59
1:q:81:GLU:HG2	1:q:84:ALA:HB2	1.84	0.59
1:q:130:LYS:NZ	1:q:247:ASP:OD2	2.29	0.59
2:I:31:GLN:HG2	2:C:118:ASP:OD1	2.02	0.59
1:n:325:LYS:NZ	2:m:140:ASP:OD1	2.29	0.59
1:s:81:GLU:HG2	1:s:84:ALA:HB2	1.84	0.58
2:H:31:GLN:HG2	2:I:118:ASP:OD1	2.03	0.58
1:q:64:ALA:HB2	1:q:165:SER:HB2	1.85	0.58
1:s:64:ALA:HB2	1:s:165:SER:HB2	1.85	0.58
1:g:200:GLU:O	1:g:204:ASN:ND2	2.31	0.58
2:A:29:LYS:HG2	2:A:63:THR:HB	1.85	0.58
1:T:132:VAL:HG22	1:T:144:ILE:HD11	1.85	0.58
1:T:70:ASN:OD1	1:T:71:THR:N	2.34	0.58
2:C:31:GLN:HG2	2:J:118:ASP:OD1	2.04	0.58
1:W:46:LYS:HA	1:W:65:LEU:HD13	1.86	0.58
1:g:62:ASN:HA	1:g:65:LEU:HD12	1.84	0.58
1:V:159:SER:N	1:V:162:GLU:OE2	2.25	0.58
1:g:68:ASN:HB2	1:g:170:LEU:HD22	1.86	0.58
2:i:14:TRP:CZ2	2:l:47:MET:HE3	2.39	0.58
2:A:31:GLN:HG2	2:H:118:ASP:OD1	2.04	0.58
2:B:29:LYS:HG2	2:B:63:THR:HB	1.86	0.58
1:E:78:TYR:HE2	1:E:89:ALA:HA	1.68	0.58
1:r:130:LYS:NZ	1:r:247:ASP:OD2	2.28	0.58
1:e:86:ILE:HD11	1:e:114:ILE:HG13	1.86	0.58
1:X:200:GLU:O	1:X:204:ASN:ND2	2.37	0.57
1:Q:139:ASN:HD21	1:Q:228:GLU:HG3	1.68	0.57
1:r:81:GLU:HG2	1:r:84:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ARG:NH2	1:E:23:SER:O	2.37	0.57
1:P:78:TYR:HE2	1:P:89:ALA:HA	1.68	0.57
1:z:287:GLU:OE1	1:z:296:SER:OG	2.21	0.57
1:V:200:GLU:O	1:V:204:ASN:ND2	2.38	0.57
2:J:31:GLN:HG2	2:N:118:ASP:OD1	2.04	0.57
1:Q:46:LYS:HA	1:Q:65:LEU:HD13	1.85	0.57
1:d:22:ARG:HH22	1:d:73:ASN:HA	1.70	0.57
1:W:118:ILE:HD12	1:W:131:ALA:HB2	1.87	0.57
1:F:62:ASN:HA	1:F:65:LEU:HD12	1.86	0.57
1:E:22:ARG:HH22	1:E:73:ASN:HA	1.69	0.57
1:Q:55:ALA:HA	1:Q:58:LYS:HE2	1.87	0.57
2:G:14:TRP:CZ2	2:j:47:MET:HE3	2.39	0.57
1:X:55:ALA:HA	1:X:58:LYS:HE2	1.87	0.56
2:M:29:LYS:HG2	2:M:63:THR:HB	1.87	0.56
2:O:29:LYS:HG2	2:O:63:THR:HB	1.87	0.56
2:I:29:LYS:HG2	2:I:63:THR:HB	1.87	0.56
2:N:29:LYS:HG2	2:N:63:THR:HB	1.87	0.56
1:e:287:GLU:OE2	1:e:296:SER:OG	2.21	0.56
1:E:320:THR:OG1	1:E:323:GLU:HG3	2.05	0.56
1:z:86:ILE:HD11	1:z:114:ILE:HG13	1.87	0.56
2:l:124:LYS:NZ	2:l:126:GLU:OE2	2.39	0.56
1:d:320:THR:OG1	1:d:323:GLU:HG3	2.05	0.56
2:L:4:MET:SD	2:D:26:GLU:HG3	2.46	0.56
1:F:159:SER:N	1:F:162:GLU:OE2	2.26	0.56
1:U:70:ASN:OD1	1:U:71:THR:N	2.34	0.56
2:j:124:LYS:NZ	2:j:126:GLU:OE1	2.38	0.56
2:C:57:LYS:HE2	2:C:59:LYS:NZ	2.21	0.56
2:J:29:LYS:HG2	2:J:63:THR:HB	1.88	0.56
1:d:132:VAL:HG22	1:d:144:ILE:HD11	1.86	0.56
1:Q:118:ILE:HD12	1:Q:131:ALA:HB2	1.87	0.56
1:s:130:LYS:NZ	1:s:247:ASP:OD2	2.29	0.56
1:P:132:VAL:HG22	1:P:144:ILE:HD11	1.88	0.56
1:q:194:MET:HE1	1:q:202:ARG:HD2	1.86	0.56
1:E:151:VAL:HG22	1:E:191:ILE:HD11	1.87	0.56
2:A:57:LYS:HE2	2:A:59:LYS:NZ	2.20	0.55
1:V:46:LYS:HA	1:V:65:LEU:HD13	1.88	0.55
2:K:29:LYS:HG2	2:K:63:THR:HB	1.87	0.55
1:r:132:VAL:HG22	1:r:144:ILE:HD11	1.88	0.55
1:V:55:ALA:HA	1:V:58:LYS:HE2	1.87	0.55
2:H:29:LYS:HG2	2:H:63:THR:HB	1.88	0.55
1:g:139:ASN:HD21	1:g:228:GLU:HG3	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:55:ALA:HA	1:W:58:LYS:HE2	1.87	0.55
1:F:118:ILE:HD12	1:F:131:ALA:HB2	1.89	0.55
1:n:81:GLU:HG2	1:n:84:ALA:HB2	1.87	0.55
1:g:106:ALA:HB1	1:g:111:LYS:HD2	1.88	0.55
1:E:50:PRO:O	1:E:58:LYS:NZ	2.40	0.55
1:q:138:GLY:O	1:q:225:SER:OG	2.23	0.55
2:H:31:GLN:HE22	2:H:33:LYS:HG3	1.71	0.55
1:X:46:LYS:HA	1:X:65:LEU:HD13	1.88	0.55
1:Q:343:ASP:OD2	1:P:331:SER:OG	2.25	0.55
1:d:50:PRO:O	1:d:58:LYS:NZ	2.39	0.55
2:B:14:TRP:CZ2	2:N:47:MET:HE3	2.41	0.55
1:T:22:ARG:NE	1:T:71:THR:HB	2.22	0.55
1:W:343:ASP:OD2	1:T:331:SER:OG	2.25	0.54
1:U:22:ARG:NE	1:U:71:THR:HB	2.22	0.54
2:J:31:GLN:HE22	2:J:33:LYS:HG3	1.72	0.54
1:S:22:ARG:NE	1:S:71:THR:HB	2.22	0.54
2:K:4:MET:SD	2:L:26:GLU:HG3	2.46	0.54
1:e:338:LYS:NZ	1:e:340:LYS:HG2	2.23	0.54
1:g:159:SER:N	1:g:162:GLU:OE2	2.25	0.54
1:P:22:ARG:NE	1:P:71:THR:HB	2.22	0.54
1:r:103:MET:HE2	1:r:114:ILE:HD11	1.89	0.54
2:I:47:MET:HE3	2:D:14:TRP:CZ2	2.43	0.54
1:g:103:MET:HE1	1:g:110:ASP:CG	2.33	0.54
1:g:188:VAL:HG12	1:g:217:ILE:HD13	1.90	0.53
1:g:343:ASP:OD2	1:d:331:SER:OG	2.27	0.53
1:E:78:TYR:CE2	1:E:89:ALA:HA	2.43	0.53
2:C:5:GLU:HG3	2:C:7:ARG:H	1.71	0.53
1:z:338:LYS:NZ	1:z:340:LYS:HG2	2.23	0.53
1:g:118:ILE:HD12	1:g:131:ALA:HB2	1.89	0.53
1:F:139:ASN:HD21	1:F:228:GLU:HG3	1.73	0.53
1:X:50:PRO:HG2	1:X:53:LEU:HD23	1.91	0.53
1:d:22:ARG:NE	1:d:71:THR:HB	2.23	0.53
1:d:138:GLY:O	1:d:225:SER:OG	2.24	0.53
1:n:132:VAL:HG22	1:n:144:ILE:HD11	1.89	0.53
1:S:22:ARG:HE	1:S:71:THR:HB	1.73	0.53
1:F:68:ASN:HB2	1:F:170:LEU:HD22	1.90	0.53
1:E:138:GLY:O	1:E:225:SER:OG	2.23	0.53
1:Q:319:MET:HE2	1:Q:323:GLU:HB3	1.91	0.53
1:E:22:ARG:NE	1:E:71:THR:HB	2.24	0.53
1:U:22:ARG:HE	1:U:71:THR:HB	1.73	0.53
1:V:62:ASN:HA	1:V:65:LEU:HD12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:106:ALA:HB1	1:V:111:LYS:HD2	1.91	0.53
1:z:338:LYS:HZ1	1:z:340:LYS:HG2	1.74	0.53
1:X:106:ALA:HB1	1:X:111:LYS:HD2	1.91	0.53
2:J:16:GLU:OE2	2:J:23:LYS:NZ	2.32	0.53
1:S:320:THR:HG1	1:S:323:GLU:HG3	1.72	0.53
1:W:319:MET:HE2	1:W:323:GLU:HB3	1.91	0.53
1:S:22:ARG:HH22	1:S:73:ASN:HA	1.74	0.53
1:X:103:MET:HE1	1:X:110:ASP:CG	2.33	0.53
2:N:16:GLU:OE1	2:N:23:LYS:NZ	2.31	0.53
2:B:16:GLU:OE1	2:B:23:LYS:NZ	2.38	0.52
1:V:103:MET:HE1	1:V:110:ASP:CG	2.34	0.52
1:V:343:ASP:OD2	1:S:331:SER:OG	2.27	0.52
1:F:188:VAL:HG12	1:F:217:ILE:HD13	1.91	0.52
1:e:138:GLY:O	1:e:225:SER:OG	2.23	0.52
1:U:22:ARG:HH22	1:U:73:ASN:HA	1.74	0.52
1:P:22:ARG:HH22	1:P:73:ASN:HA	1.74	0.52
1:P:78:TYR:CE2	1:P:89:ALA:HA	2.43	0.52
2:L:33:LYS:HD3	2:L:35:GLU:OE1	2.09	0.52
1:E:74:LYS:HE3	1:E:76:LEU:HD21	1.92	0.52
1:F:55:ALA:O	1:F:59:GLU:HG3	2.09	0.52
1:U:170:LEU:HD21	1:U:183:THR:HG21	1.91	0.52
1:d:74:LYS:HE3	1:d:76:LEU:HD21	1.92	0.52
1:F:343:ASP:OD2	1:E:331:SER:OG	2.27	0.52
1:n:74:LYS:HE3	1:n:76:LEU:HD21	1.91	0.52
1:d:22:ARG:HE	1:d:71:THR:HB	1.74	0.52
1:g:55:ALA:O	1:g:59:GLU:HG3	2.10	0.51
1:T:22:ARG:HE	1:T:71:THR:HB	1.75	0.51
2:N:33:LYS:HG2	2:N:35:GLU:OE1	2.11	0.51
1:S:170:LEU:HD21	1:S:183:THR:HG21	1.91	0.51
1:W:139:ASN:HD21	1:W:228:GLU:HG3	1.74	0.51
1:P:22:ARG:HE	1:P:71:THR:HB	1.75	0.51
1:P:50:PRO:O	1:P:58:LYS:NZ	2.44	0.51
2:i:39:GLU:HG2	2:H:124:LYS:HD3	1.92	0.51
2:G:39:GLU:HG2	2:J:124:LYS:HD3	1.92	0.51
1:X:343:ASP:OD2	1:U:331:SER:OG	2.27	0.51
1:q:306:LYS:O	1:q:310:LYS:HE3	2.11	0.51
1:d:78:TYR:CE2	1:d:89:ALA:HA	2.44	0.51
1:W:188:VAL:HG12	1:W:217:ILE:HD13	1.92	0.51
1:T:54:SER:O	1:T:58:LYS:N	2.44	0.51
1:U:54:SER:O	1:U:58:LYS:N	2.44	0.51
2:a:103:ARG:HB3	2:a:139:LEU:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:132:VAL:HG22	1:e:144:ILE:HD11	1.91	0.51
1:T:22:ARG:HH22	1:T:73:ASN:HA	1.75	0.51
1:T:50:PRO:O	1:T:58:LYS:NZ	2.44	0.51
1:X:188:VAL:HG12	1:X:217:ILE:HD13	1.93	0.51
1:U:102:CYS:HB2	1:U:164:THR:HG22	1.92	0.51
1:V:50:PRO:HG2	1:V:53:LEU:HD23	1.92	0.51
1:E:22:ARG:HE	1:E:71:THR:HB	1.74	0.51
1:P:54:SER:O	1:P:58:LYS:N	2.44	0.51
1:V:188:VAL:HG12	1:V:217:ILE:HD13	1.93	0.51
1:S:54:SER:O	1:S:58:LYS:N	2.44	0.51
1:E:54:SER:O	1:E:58:LYS:N	2.44	0.51
1:e:194:MET:HE1	1:e:202:ARG:HD2	1.94	0.50
2:j:33:LYS:HG2	2:j:35:GLU:OE1	2.12	0.50
1:U:138:GLY:O	1:U:225:SER:OG	2.20	0.50
2:a:29:LYS:HG2	2:a:63:THR:HB	1.94	0.50
1:Q:188:VAL:HG12	1:Q:217:ILE:HD13	1.93	0.50
1:T:130:LYS:HE2	1:T:247:ASP:OD2	2.11	0.50
2:I:16:GLU:OE2	2:I:23:LYS:NZ	2.31	0.50
2:G:43:ILE:HD12	2:C:4:MET:HE2	1.93	0.50
1:U:50:PRO:O	1:U:58:LYS:NZ	2.45	0.50
1:X:193:LYS:HD2	1:U:91:ASP:HB3	1.94	0.50
1:P:130:LYS:HE2	1:P:247:ASP:OD2	2.12	0.50
1:V:325:LYS:NZ	2:Y:140:ASP:OD1	2.27	0.50
2:a:14:TRP:CZ2	2:k:47:MET:HE3	2.47	0.50
1:Q:50:PRO:HG2	1:Q:53:LEU:HD23	1.94	0.50
1:d:21:GLU:O	1:d:70:ASN:ND2	2.41	0.50
1:S:130:LYS:HE2	1:S:247:ASP:OD2	2.12	0.50
1:S:139:ASN:ND2	1:S:228:GLU:HG3	2.23	0.50
2:Y:103:ARG:HB3	2:Y:139:LEU:O	2.11	0.49
1:V:55:ALA:O	1:V:59:GLU:HG3	2.13	0.49
1:q:65:LEU:HG	1:q:65:LEU:O	2.12	0.49
1:n:103:MET:HE2	1:n:114:ILE:HD11	1.92	0.49
1:S:74:LYS:HE3	1:S:76:LEU:HD21	1.94	0.49
1:z:132:VAL:HG22	1:z:144:ILE:HD11	1.95	0.49
1:n:26:GLY:O	1:n:73:ASN:N	2.45	0.49
2:Y:29:LYS:HG2	2:Y:63:THR:HB	1.93	0.49
2:Z:103:ARG:HB3	2:Z:139:LEU:O	2.12	0.49
1:F:106:ALA:HB1	1:F:111:LYS:HD2	1.94	0.49
2:R:103:ARG:HB3	2:R:139:LEU:O	2.13	0.49
1:z:31:VAL:O	1:z:103:MET:HG3	2.11	0.49
1:d:293:GLU:HB2	1:d:340:LYS:HE2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:102:CYS:HB2	1:S:164:THR:HG22	1.93	0.49
2:K:103:ARG:HB3	2:K:139:LEU:O	2.13	0.49
1:T:74:LYS:HE3	1:T:76:LEU:HD21	1.94	0.49
2:I:57:LYS:HE2	2:I:59:LYS:HZ3	1.77	0.49
2:L:103:ARG:HB3	2:L:139:LEU:O	2.12	0.49
1:X:118:ILE:HD12	1:X:131:ALA:HB2	1.94	0.49
2:N:103:ARG:HB3	2:N:139:LEU:O	2.13	0.49
2:O:103:ARG:HB3	2:O:139:LEU:O	2.12	0.49
1:V:103:MET:HE3	1:V:105:LYS:O	2.13	0.49
2:I:103:ARG:HB3	2:I:139:LEU:O	2.12	0.49
2:C:78:LYS:HD3	2:C:85:PRO:HG3	1.95	0.49
1:r:138:GLY:O	1:r:225:SER:OG	2.24	0.49
1:F:141:GLU:OE2	1:F:233:LYS:HE3	2.13	0.49
2:M:103:ARG:HB3	2:M:139:LEU:O	2.12	0.49
1:P:74:LYS:HE3	1:P:76:LEU:HD21	1.93	0.49
1:E:102:CYS:HB2	1:E:164:THR:HG22	1.94	0.49
2:D:40:ASP:OD1	2:M:57:LYS:HE3	2.13	0.49
1:s:306:LYS:O	1:s:310:LYS:HE3	2.12	0.49
1:g:141:GLU:OE2	1:g:233:LYS:HE3	2.13	0.49
1:U:130:LYS:HE2	1:U:247:ASP:OD2	2.13	0.49
1:s:202:ARG:HD2	1:s:207:GLU:OE1	2.13	0.49
1:e:103:MET:HE2	1:e:114:ILE:HD11	1.94	0.49
1:g:15:LEU:HD23	1:Q:353:GLU:HB3	1.95	0.48
1:X:103:MET:HE3	1:X:105:LYS:O	2.12	0.48
1:Q:103:MET:HE1	1:Q:110:ASP:CG	2.38	0.48
1:P:102:CYS:HB2	1:P:164:THR:HG22	1.95	0.48
1:W:50:PRO:HG2	1:W:53:LEU:HD23	1.95	0.48
1:T:21:GLU:O	1:T:70:ASN:ND2	2.40	0.48
2:M:4:MET:HE3	2:O:67:VAL:HG21	1.95	0.48
1:s:70:ASN:OD1	1:s:71:THR:N	2.46	0.48
1:d:102:CYS:HB2	1:d:164:THR:HG22	1.94	0.48
2:i:29:LYS:HG2	2:i:63:THR:HB	1.95	0.48
2:A:78:LYS:HD3	2:A:85:PRO:HG3	1.95	0.48
1:W:103:MET:HE1	1:W:110:ASP:CG	2.38	0.48
1:U:245:THR:O	1:U:248:ILE:HG22	2.13	0.48
1:d:54:SER:O	1:d:58:LYS:N	2.45	0.48
1:S:65:LEU:O	1:S:71:THR:HG23	2.14	0.48
1:T:102:CYS:HB2	1:T:164:THR:HG22	1.95	0.48
1:e:31:VAL:O	1:e:103:MET:HG3	2.13	0.48
1:g:286:LEU:HD22	1:g:291:LEU:HD12	1.95	0.48
1:V:118:ILE:HD12	1:V:131:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:62:ASN:HA	1:W:65:LEU:HD12	1.96	0.48
2:G:29:LYS:HG2	2:G:63:THR:HB	1.95	0.48
1:Q:308:TYR:CZ	1:Q:312:LYS:HD2	2.48	0.48
1:W:141:GLU:OE1	1:W:233:LYS:HE3	2.14	0.48
1:U:320:THR:OG1	1:U:323:GLU:HG3	2.14	0.48
1:Q:141:GLU:OE1	1:Q:233:LYS:HE3	2.14	0.48
1:z:103:MET:HE2	1:z:114:ILE:HD11	1.95	0.48
1:S:50:PRO:O	1:S:58:LYS:NZ	2.46	0.48
1:F:38:LEU:HA	1:F:79:VAL:HB	1.95	0.48
1:s:30:MET:O	1:s:77:VAL:HA	2.14	0.48
1:S:320:THR:OG1	1:S:323:GLU:HG3	2.14	0.48
1:W:308:TYR:CZ	1:W:312:LYS:HD2	2.48	0.48
1:T:180:VAL:O	1:T:183:THR:HG22	2.14	0.48
2:L:5:GLU:HG3	2:L:7:ARG:H	1.79	0.48
1:U:74:LYS:HE3	1:U:76:LEU:HD21	1.95	0.48
1:P:150:ASP:HB3	1:P:157:LYS:NZ	2.28	0.48
1:g:38:LEU:HA	1:g:79:VAL:HB	1.95	0.48
2:H:124:LYS:NZ	2:H:126:GLU:OE1	2.47	0.48
1:r:66:MET:HE2	1:r:166:ARG:NE	2.28	0.48
1:S:245:THR:O	1:S:248:ILE:HG22	2.14	0.47
1:U:65:LEU:O	1:U:71:THR:HG23	2.14	0.47
1:z:194:MET:HE1	1:z:202:ARG:HD2	1.95	0.47
2:Y:14:TRP:CZ2	2:m:47:MET:HE3	2.49	0.47
1:E:269:TYR:CD2	1:E:326:GLU:HG2	2.49	0.47
1:U:255:LYS:HD2	1:U:256:VAL:N	2.29	0.47
1:P:21:GLU:O	1:P:70:ASN:ND2	2.41	0.47
1:z:74:LYS:HE3	1:z:76:LEU:HD21	1.96	0.47
1:s:132:VAL:HG22	1:s:144:ILE:HD11	1.94	0.47
1:F:50:PRO:HG2	1:F:53:LEU:HD23	1.95	0.47
2:G:103:ARG:HB3	2:G:139:LEU:O	2.15	0.47
1:X:38:LEU:HA	1:X:79:VAL:HB	1.97	0.47
1:P:103:MET:HG2	1:P:105:LYS:O	2.15	0.47
1:d:269:TYR:CD2	1:d:326:GLU:HG2	2.50	0.47
2:I:33:LYS:HZ2	2:I:35:GLU:HG3	1.79	0.47
1:E:9:ASN:N	1:E:9:ASN:OD1	2.46	0.47
1:U:36:LYS:HE3	1:U:52:ASP:CG	2.39	0.47
1:e:338:LYS:HZ1	1:e:340:LYS:HG2	1.79	0.47
2:B:103:ARG:HB3	2:B:139:LEU:O	2.15	0.47
1:q:31:VAL:O	1:q:103:MET:HG3	2.15	0.47
1:n:319:MET:HE3	1:n:323:GLU:HG2	1.97	0.47
1:g:50:PRO:HG2	1:g:53:LEU:HD23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:9:ASN:N	1:S:9:ASN:OD1	2.47	0.47
1:W:125:ASP:OD1	1:q:196:LYS:NZ	2.38	0.47
1:F:286:LEU:HD22	1:F:291:LEU:HD12	1.95	0.47
1:q:70:ASN:OD1	1:q:71:THR:N	2.47	0.47
1:r:70:ASN:OD1	1:r:71:THR:N	2.48	0.47
1:g:353:GLU:HB3	1:V:15:LEU:HD23	1.97	0.47
2:i:103:ARG:HB3	2:i:139:LEU:O	2.15	0.47
1:S:78:TYR:CE2	1:S:89:ALA:HA	2.44	0.47
1:E:21:GLU:O	1:E:70:ASN:ND2	2.39	0.47
1:U:132:VAL:HG13	1:U:144:ILE:HD11	1.95	0.47
1:z:26:GLY:O	1:z:73:ASN:N	2.48	0.47
1:r:26:GLY:O	1:r:73:ASN:N	2.45	0.47
1:X:30:MET:HE2	1:X:32:LEU:HD11	1.96	0.47
1:U:139:ASN:ND2	1:U:228:GLU:HG3	2.23	0.47
2:J:124:LYS:NZ	2:J:126:GLU:OE1	2.47	0.47
1:P:36:LYS:HE3	1:P:52:ASP:CG	2.40	0.47
1:z:306:LYS:O	1:z:310:LYS:HE3	2.15	0.47
1:z:312:LYS:HA	1:z:312:LYS:HD3	1.67	0.47
2:b:124:LYS:NZ	2:b:126:GLU:OE2	2.48	0.47
1:r:137:VAL:HG12	1:r:137:VAL:O	2.15	0.47
1:e:70:ASN:OD1	1:e:71:THR:N	2.48	0.47
1:s:65:LEU:HG	1:s:65:LEU:O	2.14	0.47
1:W:115:LYS:HD3	1:W:119:ILE:HD12	1.97	0.47
1:Q:62:ASN:HA	1:Q:65:LEU:HD12	1.96	0.47
1:P:180:VAL:O	1:P:183:THR:HG22	2.14	0.47
2:N:33:LYS:HZ2	2:N:35:GLU:HG3	1.79	0.47
1:X:306:LYS:HG2	1:X:316:LEU:HD21	1.97	0.47
1:r:74:LYS:HE3	1:r:76:LEU:HD21	1.96	0.47
1:S:255:LYS:HD2	1:S:256:VAL:N	2.29	0.46
1:T:65:LEU:O	1:T:71:THR:HG23	2.15	0.46
1:T:138:GLY:O	1:T:225:SER:OG	2.30	0.46
2:I:33:LYS:HG2	2:I:35:GLU:OE1	2.15	0.46
1:E:191:ILE:HA	1:E:191:ILE:HD12	1.79	0.46
1:e:306:LYS:O	1:e:310:LYS:HE3	2.15	0.46
1:d:9:ASN:N	1:d:9:ASN:OD1	2.47	0.46
2:H:78:LYS:HD3	2:H:85:PRO:HG3	1.98	0.46
1:T:293:GLU:HB2	1:T:340:LYS:HE2	1.98	0.46
1:F:353:GLU:HB3	1:X:15:LEU:HD23	1.97	0.46
1:d:36:LYS:HE3	1:d:52:ASP:CG	2.40	0.46
1:W:353:GLU:HB3	1:F:15:LEU:HD23	1.96	0.46
1:E:63:LEU:HA	1:E:66:MET:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:286:LEU:HD22	1:Q:291:LEU:HD12	1.97	0.46
1:P:65:LEU:O	1:P:71:THR:HG23	2.16	0.46
1:d:90:LEU:O	1:d:94:GLU:HG3	2.16	0.46
1:S:36:LYS:HE3	1:S:52:ASP:CG	2.39	0.46
1:W:286:LEU:HD22	1:W:291:LEU:HD12	1.96	0.46
1:P:293:GLU:HB2	1:P:340:LYS:HE2	1.97	0.46
1:s:13:LYS:HG2	1:s:14:GLU:N	2.29	0.46
1:T:258:ILE:O	1:T:264:LYS:NZ	2.48	0.46
2:C:49:THR:HG22	2:J:56:TYR:O	2.16	0.46
1:P:258:ILE:O	1:P:264:LYS:NZ	2.48	0.46
2:R:47:MET:HE2	2:R:47:MET:HA	1.98	0.46
1:g:236:MET:HE1	1:g:341:VAL:O	2.15	0.46
1:E:27:ILE:HD12	1:E:74:LYS:HB3	1.98	0.46
1:q:132:VAL:HG22	1:q:144:ILE:HD11	1.98	0.46
1:d:65:LEU:O	1:d:71:THR:HG23	2.16	0.46
1:E:65:LEU:O	1:E:71:THR:HG23	2.16	0.46
1:e:312:LYS:HA	1:e:312:LYS:HD3	1.66	0.46
1:V:38:LEU:HA	1:V:79:VAL:HB	1.98	0.46
1:T:150:ASP:HB3	1:T:157:LYS:NZ	2.31	0.46
2:Z:47:MET:HE2	2:Z:47:MET:HA	1.98	0.46
1:E:36:LYS:HE3	1:E:52:ASP:CG	2.40	0.46
1:E:58:LYS:HB2	1:E:58:LYS:HE2	1.69	0.46
2:D:103:ARG:HB3	2:D:139:LEU:O	2.15	0.46
1:U:150:ASP:HB3	1:U:157:LYS:NZ	2.30	0.46
2:k:42:ILE:HD13	2:k:49:THR:HB	1.98	0.46
1:T:14:GLU:OE1	1:T:14:GLU:HA	2.15	0.46
1:T:42:GLU:CD	1:T:42:GLU:H	2.24	0.46
1:F:46:LYS:HA	1:F:65:LEU:HD13	1.98	0.46
1:X:139:ASN:HD21	1:X:228:GLU:CG	2.28	0.46
1:P:293:GLU:HB2	1:P:340:LYS:HB2	1.98	0.46
1:e:65:LEU:O	1:e:71:THR:HG23	2.16	0.46
2:m:42:ILE:HD13	2:m:49:THR:HB	1.98	0.46
1:S:269:TYR:CD2	1:S:326:GLU:HG2	2.51	0.45
1:W:38:LEU:HA	1:W:79:VAL:HB	1.97	0.45
1:T:36:LYS:HE3	1:T:52:ASP:CG	2.40	0.45
1:U:312:LYS:HA	1:U:312:LYS:HD3	1.83	0.45
1:r:303:GLU:OE1	1:r:303:GLU:N	2.49	0.45
1:e:58:LYS:HE2	1:e:58:LYS:HB2	1.64	0.45
2:K:5:GLU:HG3	2:K:7:ARG:H	1.81	0.45
1:U:314:VAL:HG12	1:U:316:LEU:HD23	1.97	0.45
2:M:38:LYS:NZ	2:O:112:ASP:OD1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:70:ASN:OD1	1:n:71:THR:N	2.50	0.45
1:d:63:LEU:HA	1:d:66:MET:HE2	1.98	0.45
1:d:103:MET:HG2	1:d:105:LYS:O	2.16	0.45
2:I:33:LYS:NZ	2:I:35:GLU:HG3	2.32	0.45
1:E:103:MET:HG2	1:E:105:LYS:O	2.17	0.45
1:X:194:MET:CE	1:X:202:ARG:HD2	2.47	0.45
1:U:58:LYS:HB2	1:U:58:LYS:HE2	1.71	0.45
1:U:269:TYR:CD2	1:U:326:GLU:HG2	2.51	0.45
1:z:70:ASN:OD1	1:z:71:THR:N	2.48	0.45
1:q:346:GLU:OE1	1:q:346:GLU:N	2.50	0.45
1:n:13:LYS:HG2	1:n:14:GLU:O	2.15	0.45
2:M:5:GLU:HG3	2:M:7:ARG:H	1.81	0.45
1:Q:55:ALA:O	1:Q:59:GLU:HG3	2.17	0.45
1:P:9:ASN:OD1	1:P:9:ASN:N	2.49	0.45
1:P:14:GLU:OE1	1:P:14:GLU:HA	2.15	0.45
1:z:65:LEU:O	1:z:71:THR:HG23	2.17	0.45
1:z:200:GLU:OE2	1:q:5:LEU:HG	2.16	0.45
1:s:245:THR:O	1:s:248:ILE:HG22	2.17	0.45
1:n:58:LYS:HE2	1:n:58:LYS:HB2	1.65	0.45
1:n:139:ASN:HD21	1:n:228:GLU:HB2	1.80	0.45
1:n:306:LYS:O	1:n:310:LYS:HE3	2.17	0.45
1:r:195:THR:HG22	1:r:198:ASP:HB2	1.99	0.45
1:e:200:GLU:OE2	1:s:5:LEU:HG	2.16	0.45
1:s:137:VAL:HG12	1:s:137:VAL:O	2.16	0.45
2:B:33:LYS:HG2	2:K:115:THR:HA	1.98	0.45
1:V:193:LYS:HD2	1:S:91:ASP:HB3	1.99	0.45
1:V:286:LEU:HD22	1:V:291:LEU:HD12	1.99	0.45
1:T:63:LEU:HG	1:T:166:ARG:HB2	1.99	0.45
1:T:269:TYR:CD2	1:T:326:GLU:HG2	2.51	0.45
2:J:78:LYS:HD3	2:J:85:PRO:HG3	1.99	0.45
1:P:42:GLU:H	1:P:42:GLU:CD	2.25	0.45
2:b:47:MET:HE2	2:b:47:MET:HA	1.99	0.45
1:r:151:VAL:O	1:r:158:TYR:HB2	2.17	0.45
1:e:137:VAL:O	1:e:137:VAL:HG12	2.17	0.45
1:n:31:VAL:O	1:n:103:MET:HG3	2.16	0.45
1:d:24:ALA:O	1:d:73:ASN:ND2	2.49	0.45
1:W:139:ASN:HD21	1:W:228:GLU:CG	2.29	0.45
1:T:293:GLU:HB2	1:T:340:LYS:HB2	1.98	0.45
1:E:90:LEU:O	1:E:94:GLU:HG3	2.16	0.45
1:U:78:TYR:CE2	1:U:89:ALA:HA	2.44	0.45
1:Q:38:LEU:HA	1:Q:79:VAL:HB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:139:ASN:HD21	1:Q:228:GLU:CG	2.30	0.45
1:g:46:LYS:HA	1:g:65:LEU:HD13	1.99	0.45
1:S:90:LEU:O	1:S:94:GLU:HG3	2.17	0.45
2:I:57:LYS:HE2	2:I:59:LYS:NZ	2.32	0.45
1:P:269:TYR:CD2	1:P:326:GLU:HG2	2.51	0.45
1:P:314:VAL:HG12	1:P:316:LEU:HD23	1.98	0.45
1:e:65:LEU:CD2	1:e:75:LEU:HD22	2.47	0.45
2:c:47:MET:HE2	2:c:47:MET:HA	1.99	0.45
1:n:60:TYR:OH	1:n:162:GLU:HG2	2.17	0.45
1:n:65:LEU:HG	1:n:75:LEU:HD22	1.98	0.45
1:W:55:ALA:O	1:W:59:GLU:HG3	2.17	0.44
1:P:255:LYS:HE3	1:P:255:LYS:HB3	1.84	0.44
1:g:139:ASN:HD21	1:g:228:GLU:CG	2.30	0.44
1:X:68:ASN:HB2	1:X:170:LEU:HD22	1.98	0.44
1:P:146:PHE:CD2	1:P:167:VAL:HG21	2.52	0.44
1:z:13:LYS:HG2	1:z:14:GLU:N	2.31	0.44
1:q:137:VAL:O	1:q:137:VAL:HG12	2.18	0.44
2:c:42:ILE:HD13	2:c:49:THR:HB	1.99	0.44
2:c:124:LYS:NZ	2:c:126:GLU:OE2	2.49	0.44
1:n:151:VAL:O	1:n:158:TYR:HB2	2.17	0.44
1:X:55:ALA:O	1:X:59:GLU:HG3	2.17	0.44
1:X:62:ASN:HA	1:X:65:LEU:HD12	1.99	0.44
2:b:42:ILE:HD13	2:b:49:THR:HB	1.99	0.44
1:s:65:LEU:O	1:s:71:THR:HG23	2.17	0.44
1:n:137:VAL:HG12	1:n:137:VAL:O	2.17	0.44
1:T:58:LYS:HE2	1:T:58:LYS:HB2	1.71	0.44
1:X:286:LEU:HD22	1:X:291:LEU:HD12	1.99	0.44
1:e:195:THR:HG22	1:e:198:ASP:HB2	2.00	0.44
1:d:312:LYS:HA	1:d:312:LYS:HD3	1.81	0.44
1:F:200:GLU:CD	1:F:204:ASN:HD21	2.25	0.44
1:F:236:MET:HE1	1:F:341:VAL:O	2.16	0.44
1:q:58:LYS:HB2	1:q:58:LYS:HE2	1.65	0.44
1:T:264:LYS:HE2	1:T:264:LYS:HB2	1.81	0.44
1:U:90:LEU:O	1:U:94:GLU:HG3	2.17	0.44
2:J:47:MET:HA	2:J:47:MET:HE2	1.98	0.44
2:N:57:LYS:HE2	2:N:59:LYS:NZ	2.33	0.44
1:e:60:TYR:OH	1:e:162:GLU:HG2	2.17	0.44
2:A:35:GLU:OE2	2:A:59:LYS:HD2	2.18	0.44
1:P:63:LEU:HG	1:P:166:ARG:HB2	2.00	0.44
1:P:121:LEU:HD22	1:P:127:VAL:HG11	1.99	0.44
1:q:65:LEU:O	1:q:71:THR:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:75:LEU:HD12	1:q:75:LEU:HA	1.79	0.44
1:q:309:LEU:HB3	1:q:314:VAL:CG2	2.48	0.44
1:q:312:LYS:HA	1:q:312:LYS:HD3	1.68	0.44
1:s:60:TYR:OH	1:s:162:GLU:HG2	2.18	0.44
2:m:92:LYS:HD2	2:m:103:ARG:NH2	2.32	0.44
2:i:35:GLU:OE1	2:i:59:LYS:HD2	2.18	0.44
1:V:74:LYS:HD2	1:V:76:LEU:HD21	2.00	0.44
2:J:49:THR:HG22	2:N:56:TYR:O	2.17	0.44
1:P:150:ASP:HB3	1:P:157:LYS:HZ2	1.82	0.44
2:N:5:GLU:HG3	2:N:7:ARG:H	1.82	0.44
1:q:74:LYS:HE3	1:q:76:LEU:HD21	1.99	0.44
1:r:306:LYS:O	1:r:310:LYS:HE3	2.17	0.44
2:l:103:ARG:HB3	2:l:139:LEU:O	2.17	0.44
1:d:150:ASP:HB3	1:d:157:LYS:NZ	2.33	0.44
2:A:49:THR:HG22	2:H:56:TYR:O	2.17	0.44
1:V:68:ASN:HB2	1:V:170:LEU:HD22	1.99	0.44
1:V:319:MET:HE2	1:V:323:GLU:HB3	1.99	0.44
2:H:47:MET:HA	2:H:47:MET:HE2	1.98	0.44
1:T:78:TYR:CE2	1:T:89:ALA:HA	2.44	0.44
1:T:314:VAL:HG12	1:T:316:LEU:HD23	1.99	0.44
2:I:78:LYS:HD3	2:I:85:PRO:HG3	1.99	0.44
1:E:180:VAL:O	1:E:183:THR:HG22	2.18	0.44
1:X:187:ASP:OD1	1:X:187:ASP:N	2.51	0.44
1:P:90:LEU:O	1:P:94:GLU:HG3	2.18	0.44
1:r:287:GLU:HG3	1:r:292:ILE:HG13	1.99	0.44
1:e:75:LEU:HD12	1:e:75:LEU:HA	1.80	0.44
1:n:66:MET:HE2	1:n:166:ARG:NE	2.33	0.44
1:V:139:ASN:HD21	1:V:228:GLU:CG	2.29	0.43
1:V:194:MET:HE1	1:V:209:ILE:HD13	2.00	0.43
1:P:58:LYS:HE2	1:P:58:LYS:HB2	1.72	0.43
1:z:137:VAL:HG12	1:z:137:VAL:O	2.17	0.43
1:e:13:LYS:HG2	1:e:14:GLU:O	2.18	0.43
1:T:121:LEU:HD22	1:T:127:VAL:HG11	1.99	0.43
2:I:5:GLU:HG3	2:I:7:ARG:H	1.83	0.43
1:X:195:THR:HG23	1:X:198:ASP:HB2	2.00	0.43
1:q:143:ILE:O	1:q:143:ILE:HG13	2.18	0.43
2:j:103:ARG:HB3	2:j:139:LEU:O	2.18	0.43
1:r:30:MET:O	1:r:77:VAL:HA	2.18	0.43
1:s:102:CYS:HB2	1:s:164:THR:HG23	2.00	0.43
1:T:312:LYS:HD3	1:T:312:LYS:HA	1.82	0.43
1:E:340:LYS:HB2	1:E:340:LYS:HE2	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:35:GLU:OE1	2:G:59:LYS:HD2	2.17	0.43
2:C:35:GLU:OE2	2:C:59:LYS:HD2	2.18	0.43
1:U:316:LEU:O	1:U:319:MET:HB2	2.18	0.43
1:z:81:GLU:CD	1:z:81:GLU:H	2.27	0.43
2:b:49:THR:HG22	2:j:56:TYR:O	2.19	0.43
1:r:319:MET:HE3	1:r:323:GLU:HG2	1.99	0.43
1:d:63:LEU:HG	1:d:166:ARG:HB2	1.99	0.43
1:T:146:PHE:CD2	1:T:167:VAL:HG21	2.53	0.43
1:E:63:LEU:HG	1:E:166:ARG:HB2	2.00	0.43
1:E:339:ILE:C	1:E:340:LYS:HD3	2.43	0.43
1:U:56:GLU:OE2	1:U:105:LYS:NZ	2.48	0.43
2:a:47:MET:HE3	2:N:14:TRP:CZ2	2.54	0.43
1:P:339:ILE:C	1:P:340:LYS:HD3	2.43	0.43
1:z:56:GLU:O	1:z:59:GLU:HG2	2.18	0.43
2:j:92:LYS:HD2	2:j:103:ARG:NH2	2.32	0.43
1:W:66:MET:HB3	1:W:166:ARG:NH1	2.33	0.43
1:T:90:LEU:O	1:T:94:GLU:HG3	2.18	0.43
1:T:339:ILE:C	1:T:340:LYS:HD3	2.43	0.43
1:F:187:ASP:OD1	1:F:187:ASP:N	2.51	0.43
1:E:24:ALA:O	1:E:73:ASN:ND2	2.51	0.43
1:Q:66:MET:HB3	1:Q:166:ARG:NH1	2.33	0.43
1:z:13:LYS:HB3	1:z:13:LYS:HE3	1.75	0.43
1:r:58:LYS:HB2	1:r:58:LYS:HE2	1.64	0.43
2:k:92:LYS:HD2	2:k:103:ARG:NH2	2.33	0.43
1:d:339:ILE:C	1:d:340:LYS:HD3	2.43	0.43
2:H:49:THR:HG22	2:I:56:TYR:O	2.18	0.43
1:F:293:GLU:OE2	1:F:342:LEU:HG	2.19	0.43
1:e:150:ASP:OD1	1:e:157:LYS:HD2	2.19	0.43
1:d:56:GLU:OE2	1:d:105:LYS:NZ	2.40	0.43
2:A:33:LYS:NZ	2:A:35:GLU:HG3	2.34	0.43
1:X:121:LEU:HB3	1:X:127:VAL:HG13	2.01	0.43
1:P:30:MET:HG3	1:P:102:CYS:SG	2.59	0.43
1:z:195:THR:HG22	1:z:198:ASP:HB2	1.99	0.43
1:q:245:THR:O	1:q:248:ILE:HG22	2.19	0.43
2:k:46:GLN:NE2	2:k:48:GLY:O	2.50	0.43
1:n:287:GLU:HG3	1:n:292:ILE:HG13	1.99	0.43
1:S:316:LEU:O	1:S:319:MET:HB2	2.18	0.43
1:P:316:LEU:O	1:P:319:MET:HB2	2.17	0.43
1:z:235:GLU:OE1	1:z:239:LYS:NZ	2.51	0.43
1:g:293:GLU:OE2	1:g:342:LEU:HG	2.19	0.43
1:V:293:GLU:OE2	1:V:342:LEU:HG	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:47:MET:HE3	2:I:14:TRP:CZ2	2.54	0.43
1:z:151:VAL:HG22	1:z:191:ILE:HD11	2.01	0.43
1:e:81:GLU:CD	1:e:81:GLU:H	2.27	0.43
1:e:235:GLU:OE1	1:e:239:LYS:NZ	2.51	0.43
1:s:22:ARG:NE	1:s:71:THR:HB	2.34	0.43
1:g:136:VAL:HG12	1:g:138:GLY:H	1.84	0.43
1:V:30:MET:SD	1:V:75:LEU:HD21	2.59	0.43
1:V:195:THR:HG23	1:V:198:ASP:HB2	2.01	0.43
1:W:121:LEU:HB3	1:W:127:VAL:HG13	1.99	0.43
1:q:81:GLU:CD	1:q:81:GLU:H	2.27	0.43
1:r:81:GLU:CD	1:r:81:GLU:H	2.27	0.43
2:l:29:LYS:HG2	2:l:63:THR:HB	2.01	0.43
1:W:36:LYS:HG2	1:W:52:ASP:HB3	2.01	0.42
1:W:306:LYS:HG2	1:W:316:LEU:HD21	2.00	0.42
1:F:139:ASN:HD21	1:F:228:GLU:CG	2.31	0.42
1:F:195:THR:HG23	1:F:198:ASP:HB2	2.01	0.42
1:E:107:VAL:H	1:E:110:ASP:HB2	1.84	0.42
2:b:69:SER:OG	2:m:102:GLU:OE2	2.35	0.42
1:r:13:LYS:HG2	1:r:14:GLU:N	2.34	0.42
1:r:312:LYS:HD3	1:r:312:LYS:HA	1.68	0.42
1:e:30:MET:O	1:e:77:VAL:HA	2.19	0.42
1:s:74:LYS:HE3	1:s:76:LEU:HD21	2.00	0.42
1:g:187:ASP:OD1	1:g:187:ASP:N	2.51	0.42
1:F:103:MET:HE1	1:F:110:ASP:CG	2.44	0.42
1:F:136:VAL:HG12	1:F:138:GLY:H	1.84	0.42
1:U:150:ASP:HB3	1:U:157:LYS:HZ2	1.84	0.42
2:l:92:LYS:HD2	2:l:103:ARG:NH2	2.34	0.42
1:T:226:LEU:O	1:T:238:GLN:NE2	2.45	0.42
1:T:340:LYS:HE2	1:T:340:LYS:HB2	1.80	0.42
1:E:150:ASP:HB3	1:E:157:LYS:NZ	2.33	0.42
1:X:236:MET:HE1	1:X:341:VAL:O	2.19	0.42
1:U:340:LYS:HB2	1:U:340:LYS:HE2	1.74	0.42
1:P:143:ILE:O	1:P:225:SER:OG	2.28	0.42
1:e:74:LYS:HE3	1:e:76:LEU:HD21	2.01	0.42
2:c:49:THR:HG22	2:l:56:TYR:O	2.19	0.42
1:n:81:GLU:H	1:n:81:GLU:CD	2.27	0.42
1:S:312:LYS:HA	1:S:312:LYS:HD3	1.83	0.42
1:T:64:ALA:HB2	1:T:165:SER:OG	2.20	0.42
2:O:5:GLU:HG3	2:O:7:ARG:H	1.85	0.42
1:r:28:ILE:HB	1:r:75:LEU:HD22	2.01	0.42
1:n:195:THR:HG22	1:n:198:ASP:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:121:LEU:HB3	1:V:127:VAL:HG13	2.01	0.42
1:W:195:THR:HG23	1:W:198:ASP:HB2	2.01	0.42
1:T:103:MET:HG2	1:T:105:LYS:O	2.20	0.42
1:z:293:GLU:HB2	1:z:340:LYS:HB2	2.02	0.42
2:b:103:ARG:HB3	2:b:139:LEU:O	2.20	0.42
1:e:255:LYS:HB2	1:e:255:LYS:HE3	1.85	0.42
1:e:293:GLU:HB2	1:e:340:LYS:HB2	2.02	0.42
1:s:81:GLU:H	1:s:81:GLU:CD	2.28	0.42
1:g:331:SER:HB2	1:n:346:GLU:HG2	2.01	0.42
1:V:236:MET:HE1	1:V:341:VAL:O	2.19	0.42
1:E:81:GLU:H	1:E:81:GLU:CD	2.28	0.42
1:z:260:ASP:HB2	1:z:261:TYR:CD1	2.54	0.42
1:g:196:LYS:HG3	1:d:125:ASP:OD2	2.19	0.42
2:i:14:TRP:CE2	2:l:47:MET:HE3	2.55	0.42
1:V:187:ASP:OD1	1:V:187:ASP:N	2.51	0.42
1:V:310:LYS:HZ3	1:V:316:LEU:HD22	1.85	0.42
2:C:33:LYS:NZ	2:C:35:GLU:HG3	2.34	0.42
2:C:124:LYS:NZ	2:C:126:GLU:OE2	2.52	0.42
1:U:24:ALA:O	1:U:73:ASN:ND2	2.52	0.42
1:Q:187:ASP:OD1	1:Q:187:ASP:N	2.52	0.42
1:Q:195:THR:HG23	1:Q:198:ASP:HB2	2.01	0.42
1:q:22:ARG:NE	1:q:71:THR:HB	2.34	0.42
1:s:58:LYS:HB2	1:s:58:LYS:HE2	1.65	0.42
1:V:235:GLU:N	1:V:235:GLU:CD	2.78	0.42
1:S:63:LEU:HG	1:S:166:ARG:HB2	2.02	0.42
2:H:5:GLU:HG3	2:H:7:ARG:H	1.85	0.42
1:Q:36:LYS:HG2	1:Q:52:ASP:HB3	2.01	0.42
1:s:115:LYS:HG3	1:s:143:ILE:HD13	2.02	0.42
1:s:118:ILE:HD13	1:s:118:ILE:HA	1.90	0.42
1:n:22:ARG:NH2	1:n:71:THR:O	2.53	0.42
2:A:56:TYR:O	2:N:49:THR:HG22	2.19	0.42
1:X:293:GLU:OE2	1:X:342:LEU:HG	2.19	0.42
1:P:64:ALA:HB2	1:P:165:SER:OG	2.19	0.42
1:P:81:GLU:CD	1:P:81:GLU:H	2.28	0.42
2:H:16:GLU:OE2	2:H:23:LYS:NZ	2.41	0.42
2:I:49:THR:HG22	2:C:56:TYR:O	2.19	0.42
1:E:196:LYS:HD3	1:E:196:LYS:HA	1.89	0.42
1:X:66:MET:HE3	1:X:66:MET:HB3	1.96	0.42
1:X:235:GLU:CD	1:X:235:GLU:N	2.78	0.42
1:P:132:VAL:HG13	1:P:144:ILE:HD11	2.02	0.42
1:z:30:MET:O	1:z:77:VAL:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:56:GLU:O	1:r:59:GLU:HG2	2.20	0.42
2:k:49:THR:HG22	2:c:56:TYR:O	2.19	0.42
1:n:30:MET:O	1:n:77:VAL:HA	2.20	0.42
1:g:103:MET:HE3	1:g:105:LYS:O	2.20	0.41
1:d:255:LYS:HE3	1:d:255:LYS:HB3	1.90	0.41
1:S:56:GLU:OE2	1:S:105:LYS:NZ	2.48	0.41
1:W:187:ASP:OD1	1:W:187:ASP:N	2.52	0.41
2:J:5:GLU:HG3	2:J:7:ARG:H	1.84	0.41
1:q:102:CYS:HB2	1:q:164:THR:HG23	2.01	0.41
2:m:103:ARG:HB3	2:m:139:LEU:O	2.20	0.41
1:d:81:GLU:H	1:d:81:GLU:CD	2.28	0.41
1:V:30:MET:HE2	1:V:32:LEU:HD11	2.02	0.41
1:V:66:MET:HE3	1:V:66:MET:HB3	1.96	0.41
1:W:286:LEU:HD23	1:W:286:LEU:HA	1.90	0.41
1:T:24:ALA:O	1:T:73:ASN:ND2	2.54	0.41
1:U:23:SER:OG	1:U:71:THR:O	2.37	0.41
1:z:118:ILE:HD13	1:z:118:ILE:HA	1.91	0.41
1:q:56:GLU:O	1:q:59:GLU:HG2	2.20	0.41
1:q:118:ILE:HD13	1:q:118:ILE:HA	1.90	0.41
1:S:306:LYS:HE3	1:S:306:LYS:HB3	1.77	0.41
1:W:293:GLU:OE2	1:W:342:LEU:HG	2.20	0.41
2:L:4:MET:HB2	2:D:26:GLU:OE2	2.20	0.41
1:P:139:ASN:HD21	1:P:228:GLU:CG	2.32	0.41
1:q:103:MET:HE2	1:q:114:ILE:HD11	2.02	0.41
2:k:103:ARG:HB3	2:k:139:LEU:O	2.20	0.41
1:s:22:ARG:NH2	1:s:71:THR:O	2.52	0.41
1:n:157:LYS:HE2	1:n:157:LYS:HB2	1.95	0.41
1:S:295:ASP:CG	2:I:81:ARG:HH21	2.29	0.41
1:F:235:GLU:N	1:F:235:GLU:CD	2.79	0.41
1:F:310:LYS:HB2	1:F:310:LYS:HE2	1.83	0.41
1:z:245:THR:O	1:z:248:ILE:HG22	2.20	0.41
1:r:286:LEU:HD23	1:r:286:LEU:HA	1.92	0.41
1:e:245:THR:O	1:e:248:ILE:HG22	2.20	0.41
1:s:56:GLU:O	1:s:59:GLU:HG2	2.20	0.41
1:E:255:LYS:HE3	1:E:255:LYS:HB3	1.90	0.41
2:J:31:GLN:HE22	2:J:33:LYS:CG	2.33	0.41
2:J:103:ARG:HB3	2:J:139:LEU:O	2.20	0.41
2:N:33:LYS:NZ	2:N:35:GLU:HG3	2.35	0.41
1:q:60:TYR:OH	1:q:162:GLU:HG2	2.19	0.41
1:q:353:GLU:OE1	1:r:15:LEU:HD12	2.20	0.41
1:e:353:GLU:OE2	1:s:15:LEU:HD12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:56:GLU:O	1:n:59:GLU:HG2	2.20	0.41
1:S:65:LEU:HD23	1:S:65:LEU:HA	1.91	0.41
1:U:141:GLU:OE2	1:U:233:LYS:HE3	2.19	0.41
1:P:312:LYS:HD3	1:P:312:LYS:HA	1.82	0.41
1:q:322:GLN:O	1:q:326:GLU:HG3	2.21	0.41
2:j:29:LYS:HG2	2:j:63:THR:HB	2.03	0.41
1:r:255:LYS:HB2	1:r:255:LYS:HE3	1.83	0.41
2:l:33:LYS:HG2	2:l:35:GLU:OE2	2.20	0.41
1:g:306:LYS:HG2	1:g:316:LEU:HD21	2.03	0.41
2:H:31:GLN:HE22	2:H:33:LYS:CG	2.33	0.41
1:E:65:LEU:HA	1:E:65:LEU:HD23	1.88	0.41
2:G:14:TRP:CE2	2:j:47:MET:HE3	2.55	0.41
2:N:124:LYS:NZ	2:N:126:GLU:OE2	2.54	0.41
1:e:56:GLU:O	1:e:59:GLU:HG2	2.20	0.41
1:g:121:LEU:HD23	1:g:121:LEU:HA	1.94	0.41
1:U:295:ASP:CG	2:N:81:ARG:HH21	2.29	0.41
1:Q:306:LYS:HG2	1:Q:316:LEU:HD21	2.02	0.41
2:l:49:THR:HG22	2:m:56:TYR:O	2.21	0.41
1:d:58:LYS:HE2	1:d:58:LYS:HB2	1.70	0.41
2:A:103:ARG:HB3	2:A:139:LEU:O	2.21	0.41
2:H:103:ARG:HB3	2:H:139:LEU:O	2.20	0.41
1:W:30:MET:HG2	1:W:75:LEU:HD11	2.03	0.41
1:T:81:GLU:CD	1:T:81:GLU:H	2.28	0.41
2:I:79:ILE:HD13	2:I:79:ILE:HA	1.98	0.41
2:I:136:TYR:CE2	2:C:80:LYS:HD2	2.56	0.41
1:X:200:GLU:HG3	1:X:204:ASN:ND2	2.36	0.41
1:U:21:GLU:O	1:U:70:ASN:ND2	2.42	0.41
1:U:63:LEU:HG	1:U:166:ARG:HB2	2.02	0.41
1:U:144:ILE:O	1:U:144:ILE:HG13	2.21	0.41
2:M:74:LEU:HD23	2:M:74:LEU:HA	1.96	0.41
1:Q:30:MET:HG2	1:Q:75:LEU:HD11	2.03	0.41
1:Q:293:GLU:OE2	1:Q:342:LEU:HG	2.20	0.41
1:P:24:ALA:O	1:P:73:ASN:ND2	2.54	0.41
2:b:56:TYR:O	2:m:49:THR:HG22	2.20	0.41
2:j:49:THR:HG22	2:k:56:TYR:O	2.21	0.41
1:e:118:ILE:HD13	1:e:118:ILE:HA	1.91	0.41
2:c:103:ARG:HB3	2:c:139:LEU:O	2.20	0.41
2:m:54:MET:HE3	2:m:54:MET:HB3	1.94	0.41
1:g:235:GLU:N	1:g:235:GLU:CD	2.78	0.41
1:X:30:MET:SD	1:X:75:LEU:HD21	2.61	0.41
1:U:152:LEU:HD12	1:U:190:ASP:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:22:ARG:NH2	1:z:71:THR:O	2.54	0.41
1:q:170:LEU:HD21	1:q:183:THR:HG21	2.02	0.41
1:S:24:ALA:O	1:S:73:ASN:ND2	2.53	0.40
1:S:132:VAL:HG13	1:S:144:ILE:HD11	2.02	0.40
1:S:306:LYS:O	1:S:310:LYS:HE3	2.21	0.40
1:W:53:LEU:HD12	1:W:57:ASN:HD22	1.86	0.40
1:T:31:VAL:O	1:T:103:MET:HG3	2.21	0.40
2:C:16:GLU:OE2	2:C:23:LYS:NZ	2.40	0.40
2:b:112:ASP:OD1	2:m:38:LYS:NZ	2.50	0.40
1:e:26:GLY:O	1:e:73:ASN:N	2.53	0.40
1:d:350:LEU:HD23	1:S:10:ILE:HG23	2.03	0.40
1:E:203:VAL:HG21	1:U:5:LEU:HD23	2.04	0.40
2:C:103:ARG:HB3	2:C:139:LEU:O	2.21	0.40
1:z:151:VAL:HG22	1:z:191:ILE:CD1	2.50	0.40
1:e:198:ASP:O	1:e:202:ARG:HG3	2.21	0.40
1:s:353:GLU:OE1	1:n:15:LEU:HD12	2.20	0.40
1:n:224:ASN:HB2	1:n:238:GLN:O	2.21	0.40
2:A:80:LYS:HD2	2:N:136:TYR:CE2	2.56	0.40
1:S:23:SER:OG	1:S:71:THR:O	2.39	0.40
2:K:84:GLU:HA	2:K:85:PRO:HD3	1.96	0.40
1:T:316:LEU:O	1:T:319:MET:HB2	2.21	0.40
2:L:38:LYS:NZ	2:D:112:ASP:OD1	2.49	0.40
1:E:314:VAL:HG12	1:E:316:LEU:HD23	2.03	0.40
2:C:47:MET:HA	2:C:47:MET:HE2	2.02	0.40
1:Q:200:GLU:HG3	1:Q:204:ASN:ND2	2.37	0.40
1:r:31:VAL:O	1:r:103:MET:HG3	2.22	0.40
2:A:124:LYS:NZ	2:A:126:GLU:OE1	2.54	0.40
1:T:86:ILE:HD13	1:T:110:ASP:OD1	2.22	0.40
1:E:34:ASP:O	1:E:81:GLU:HA	2.22	0.40
1:E:64:ALA:HB2	1:E:165:SER:OG	2.22	0.40
1:z:86:ILE:HD13	1:z:113:ALA:HB3	2.03	0.40
1:r:322:GLN:O	1:r:326:GLU:HG3	2.21	0.40
1:E:26:GLY:C	1:E:27:ILE:HD13	2.47	0.40
1:E:132:VAL:HG13	1:E:144:ILE:HD11	2.03	0.40
1:E:255:LYS:HD2	1:E:256:VAL:N	2.37	0.40
2:D:47:MET:HE2	2:D:47:MET:HA	2.04	0.40
1:U:195:THR:HG22	1:U:197:VAL:HG12	2.03	0.40
1:U:196:LYS:HA	1:U:196:LYS:HD3	1.89	0.40
1:Q:325:LYS:NZ	2:R:140:ASP:OD1	2.32	0.40
1:q:309:LEU:HB3	1:q:314:VAL:HG21	2.03	0.40
1:s:224:ASN:HB2	1:s:238:GLN:O	2.21	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	E	350/354 (99%)	341 (97%)	9 (3%)	0	100	100
1	F	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
1	P	350/354 (99%)	341 (97%)	9 (3%)	0	100	100
1	Q	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
1	S	350/354 (99%)	341 (97%)	9 (3%)	0	100	100
1	T	350/354 (99%)	343 (98%)	7 (2%)	0	100	100
1	U	350/354 (99%)	342 (98%)	8 (2%)	0	100	100
1	V	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
1	W	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
1	X	350/354 (99%)	338 (97%)	12 (3%)	0	100	100
1	d	350/354 (99%)	340 (97%)	10 (3%)	0	100	100
1	e	350/354 (99%)	338 (97%)	12 (3%)	0	100	100
1	g	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
1	n	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
1	q	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
1	r	350/354 (99%)	340 (97%)	10 (3%)	0	100	100
1	s	350/354 (99%)	338 (97%)	12 (3%)	0	100	100
1	z	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
2	A	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
2	B	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
2	C	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
2	D	138/142 (97%)	134 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
2	H	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
2	I	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	J	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	K	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	L	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
2	M	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	N	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	O	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
2	R	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	Y	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	Z	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	a	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	b	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	c	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
2	i	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	j	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
2	k	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	l	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
2	m	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
All	All	9612/9780 (98%)	9311 (97%)	301 (3%)	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	E	308/309 (100%)	302 (98%)	6 (2%)	50	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	308/309 (100%)	306 (99%)	2 (1%)	78	89
1	P	308/309 (100%)	305 (99%)	3 (1%)	68	81
1	Q	308/309 (100%)	303 (98%)	5 (2%)	55	71
1	S	308/309 (100%)	306 (99%)	2 (1%)	78	89
1	T	308/309 (100%)	302 (98%)	6 (2%)	50	66
1	U	308/309 (100%)	307 (100%)	1 (0%)	86	93
1	V	308/309 (100%)	303 (98%)	5 (2%)	55	71
1	W	308/309 (100%)	303 (98%)	5 (2%)	55	71
1	X	308/309 (100%)	303 (98%)	5 (2%)	55	71
1	d	308/309 (100%)	306 (99%)	2 (1%)	78	89
1	e	308/309 (100%)	298 (97%)	10 (3%)	34	47
1	g	308/309 (100%)	306 (99%)	2 (1%)	78	89
1	n	308/309 (100%)	302 (98%)	6 (2%)	50	66
1	q	308/309 (100%)	300 (97%)	8 (3%)	40	55
1	r	308/309 (100%)	303 (98%)	5 (2%)	55	71
1	s	308/309 (100%)	298 (97%)	10 (3%)	34	47
1	z	308/309 (100%)	298 (97%)	10 (3%)	34	47
2	A	117/118 (99%)	113 (97%)	4 (3%)	32	44
2	B	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	C	117/118 (99%)	113 (97%)	4 (3%)	32	44
2	D	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	G	117/118 (99%)	116 (99%)	1 (1%)	70	84
2	H	117/118 (99%)	116 (99%)	1 (1%)	70	84
2	I	117/118 (99%)	116 (99%)	1 (1%)	70	84
2	J	117/118 (99%)	115 (98%)	2 (2%)	53	69
2	K	117/118 (99%)	112 (96%)	5 (4%)	26	35
2	L	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	M	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	N	117/118 (99%)	116 (99%)	1 (1%)	70	84
2	O	117/118 (99%)	113 (97%)	4 (3%)	32	44
2	R	117/118 (99%)	115 (98%)	2 (2%)	53	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	117/118 (99%)	115 (98%)	2 (2%)	53	69
2	Z	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	a	117/118 (99%)	115 (98%)	2 (2%)	53	69
2	b	117/118 (99%)	115 (98%)	2 (2%)	53	69
2	c	117/118 (99%)	115 (98%)	2 (2%)	53	69
2	i	117/118 (99%)	116 (99%)	1 (1%)	70	84
2	j	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	k	117/118 (99%)	114 (97%)	3 (3%)	40	55
2	l	117/118 (99%)	113 (97%)	4 (3%)	32	44
2	m	117/118 (99%)	114 (97%)	3 (3%)	40	55
All	All	8352/8394 (100%)	8197 (98%)	155 (2%)	49	66

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	g	14	GLU
1	g	118	ILE
1	d	7	SER
1	d	143	ILE
2	i	139	LEU
2	A	4	MET
2	A	24	VAL
2	A	139	LEU
2	A	141	ILE
2	B	24	VAL
2	B	139	LEU
2	B	141	ILE
1	V	14	GLU
1	V	118	ILE
1	V	124	ILE
1	V	127	VAL
1	V	285	GLU
1	S	14	GLU
1	S	191	ILE
2	Y	139	LEU
2	Y	140	ASP
2	H	139	LEU
2	K	24	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	77	GLU
2	K	79	ILE
2	K	139	LEU
2	K	141	ILE
1	W	14	GLU
1	W	66	MET
1	W	111	LYS
1	W	118	ILE
1	W	198	ASP
1	T	110	ASP
1	T	164	THR
1	T	198	ASP
1	T	244	ASP
1	T	248	ILE
1	T	316	LEU
2	Z	49	THR
2	Z	139	LEU
2	Z	141	ILE
2	I	139	LEU
2	L	77	GLU
2	L	79	ILE
2	L	141	ILE
1	F	14	GLU
1	F	118	ILE
1	E	7	SER
1	E	127	VAL
1	E	143	ILE
1	E	187	ASP
1	E	195	THR
1	E	198	ASP
2	G	139	LEU
2	C	4	MET
2	C	24	VAL
2	C	139	LEU
2	C	141	ILE
2	D	79	ILE
2	D	139	LEU
2	D	141	ILE
1	X	14	GLU
1	X	118	ILE
1	X	124	ILE
1	X	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	285	GLU
1	U	191	ILE
2	a	139	LEU
2	a	140	ASP
2	J	139	LEU
2	J	141	ILE
2	M	77	GLU
2	M	79	ILE
2	M	139	LEU
1	Q	14	GLU
1	Q	66	MET
1	Q	111	LYS
1	Q	118	ILE
1	Q	198	ASP
1	P	164	THR
1	P	198	ASP
1	P	248	ILE
2	R	49	THR
2	R	139	LEU
2	N	139	LEU
2	O	57	LYS
2	O	77	GLU
2	O	79	ILE
2	O	141	ILE
1	z	17	THR
1	z	86	ILE
1	z	112	THR
1	z	124	ILE
1	z	164	THR
1	z	191	ILE
1	z	193	LYS
1	z	248	ILE
1	z	309	LEU
1	z	311	SER
2	b	49	THR
2	b	139	LEU
1	q	13	LYS
1	q	17	THR
1	q	75	LEU
1	q	112	THR
1	q	124	ILE
1	q	164	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	q	311	SER
1	q	343	ASP
2	j	49	THR
2	j	91	SER
2	j	139	LEU
1	r	75	LEU
1	r	112	THR
1	r	164	THR
1	r	190	ASP
1	r	343	ASP
2	k	49	THR
2	k	139	LEU
2	k	141	ILE
1	e	17	THR
1	e	110	ASP
1	e	112	THR
1	e	124	ILE
1	e	164	THR
1	e	190	ASP
1	e	193	LYS
1	e	196	LYS
1	e	248	ILE
1	e	309	LEU
2	c	49	THR
2	c	139	LEU
1	s	17	THR
1	s	75	LEU
1	s	112	THR
1	s	124	ILE
1	s	164	THR
1	s	190	ASP
1	s	193	LYS
1	s	309	LEU
1	s	311	SER
1	s	353	GLU
2	l	31	GLN
2	l	49	THR
2	l	91	SER
2	l	139	LEU
1	n	17	THR
1	n	75	LEU
1	n	112	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	n	164	THR
1	n	190	ASP
1	n	346	GLU
2	m	49	THR
2	m	139	LEU
2	m	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	g	62	ASN
1	g	139	ASN
1	g	224	ASN
1	g	322	GLN
1	d	57	ASN
1	d	68	ASN
1	d	145	ASN
1	d	271	ASN
2	B	22	ASN
1	V	62	ASN
1	V	139	ASN
1	V	224	ASN
1	S	57	ASN
1	S	145	ASN
2	H	31	GLN
1	W	62	ASN
1	W	139	ASN
1	W	224	ASN
1	W	322	GLN
1	T	57	ASN
1	T	145	ASN
2	Z	108	ASN
1	F	62	ASN
1	F	139	ASN
1	F	322	GLN
1	E	57	ASN
1	E	145	ASN
1	E	271	ASN
2	D	22	ASN
1	X	62	ASN
1	X	139	ASN
1	X	224	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	57	ASN
1	U	145	ASN
2	J	31	GLN
1	Q	62	ASN
1	Q	224	ASN
1	Q	322	GLN
1	P	57	ASN
1	P	68	ASN
1	P	145	ASN
2	R	108	ASN
1	z	57	ASN
1	z	68	ASN
2	b	8	ASN
2	b	31	GLN
1	q	57	ASN
1	q	68	ASN
1	q	140	HIS
1	r	57	ASN
2	k	31	GLN
1	e	57	ASN
1	e	68	ASN
2	c	31	GLN
1	s	57	ASN
1	s	68	ASN
1	s	140	HIS
2	l	31	GLN
1	n	57	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

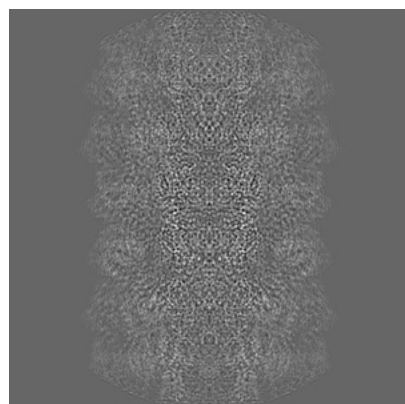
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42959. These allow visual inspection of the internal detail of the map and identification of artifacts.

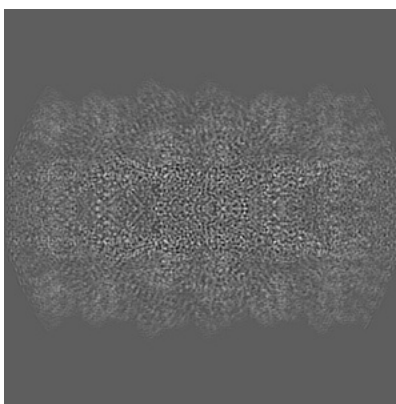
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

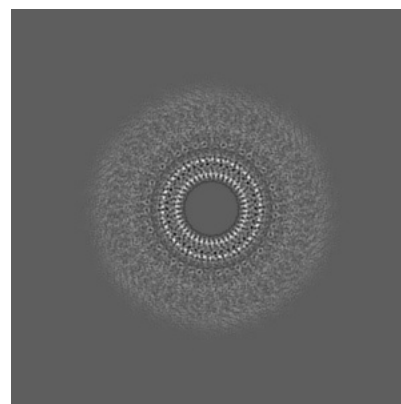
6.1.1 Primary map



X

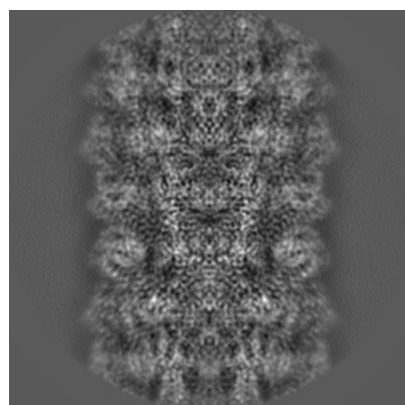


Y

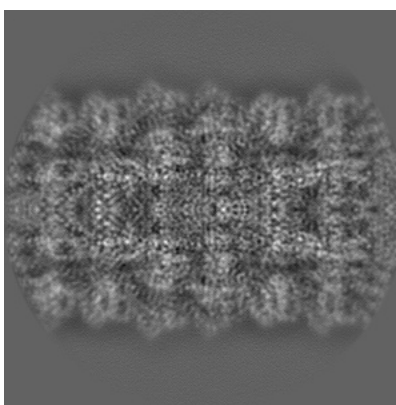


Z

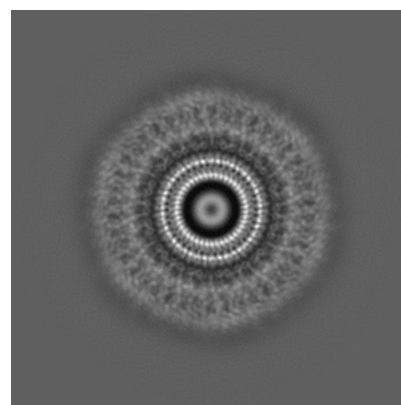
6.1.2 Raw map



X



Y

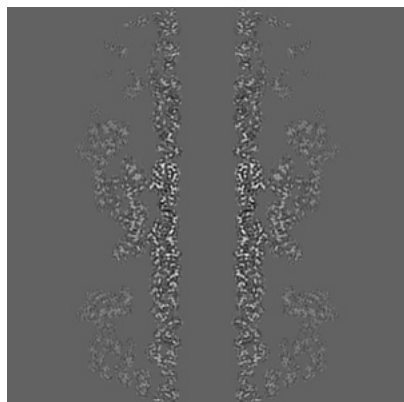


Z

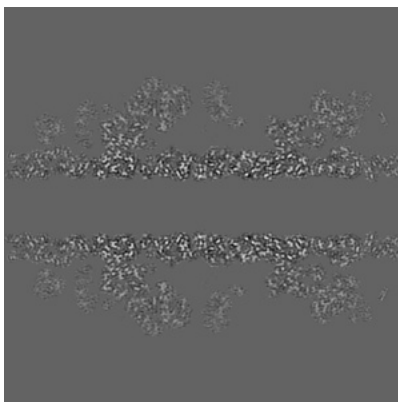
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

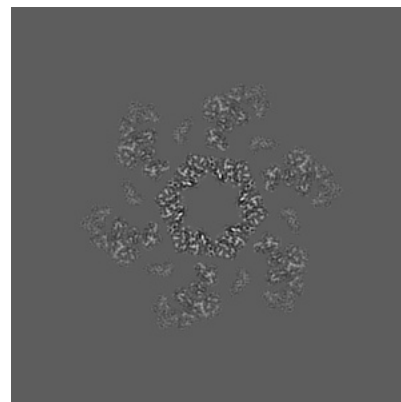
6.2.1 Primary map



X Index: 256

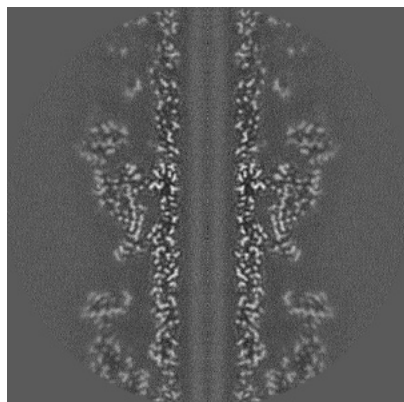


Y Index: 256

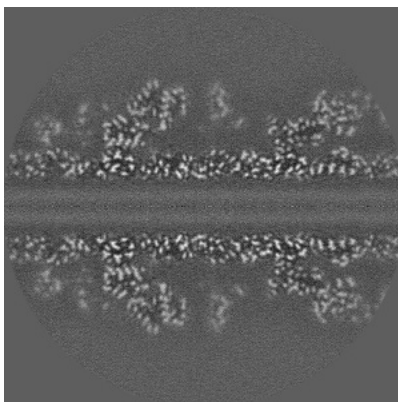


Z Index: 256

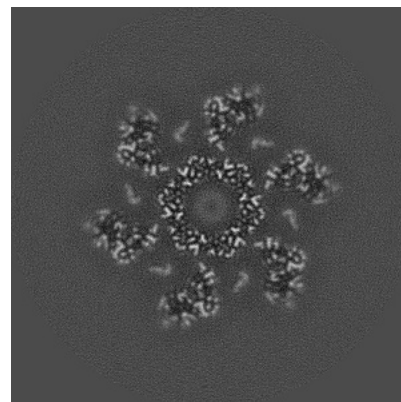
6.2.2 Raw map



X Index: 256



Y Index: 256

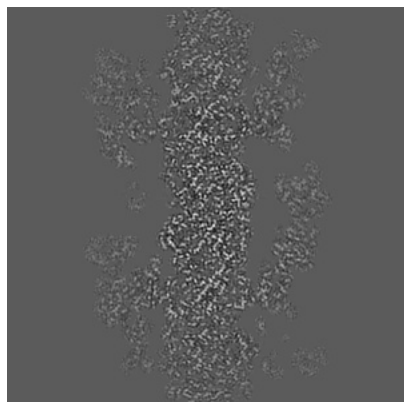


Z Index: 256

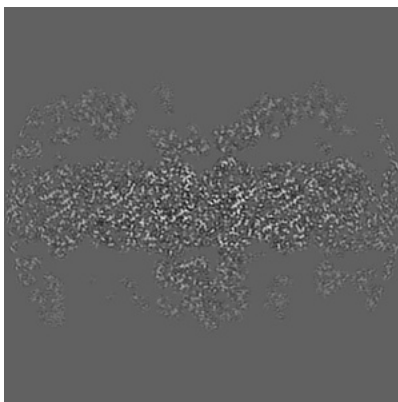
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

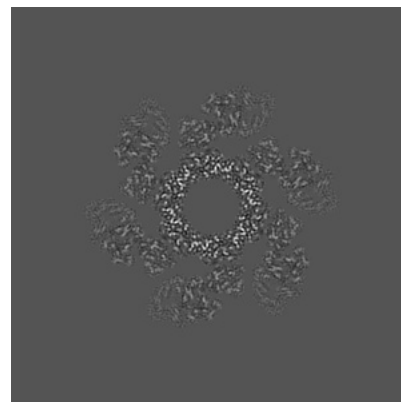
6.3.1 Primary map



X Index: 299

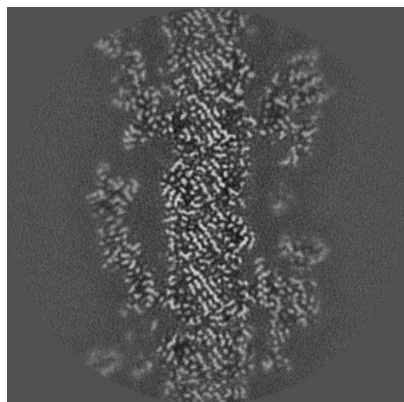


Y Index: 214

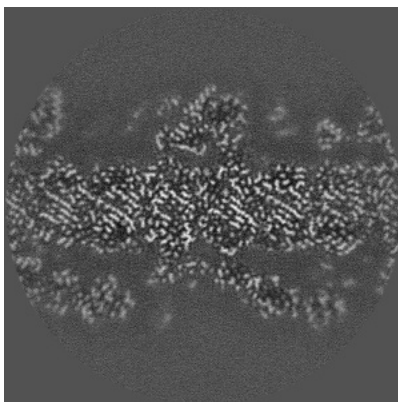


Z Index: 274

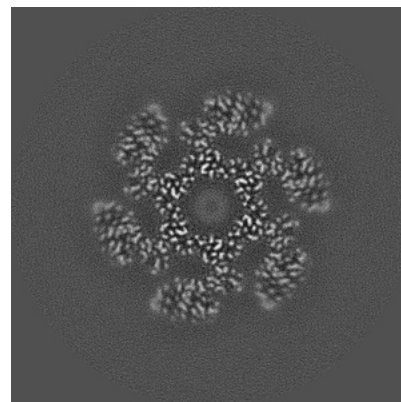
6.3.2 Raw map



X Index: 213



Y Index: 298

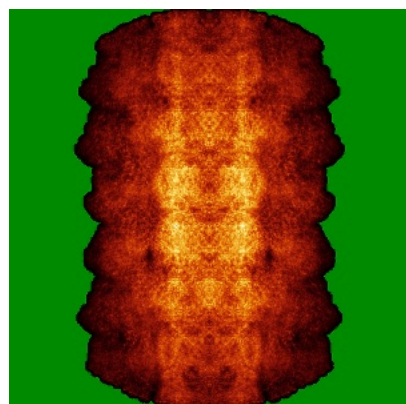


Z Index: 278

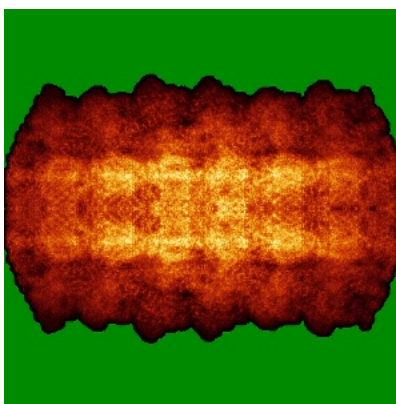
The images above show the largest variance slices of the map in three orthogonal directions.

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

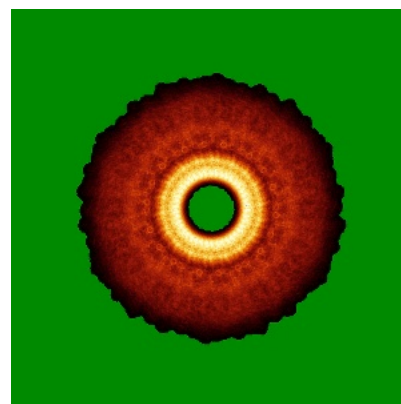
6.4.1 Primary map



X

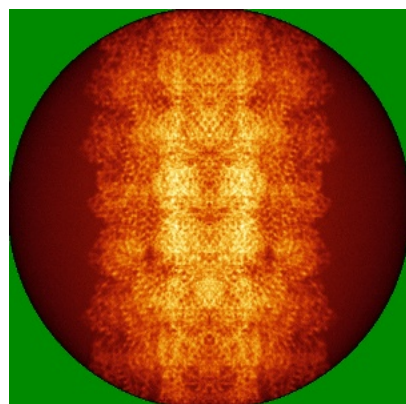


Y

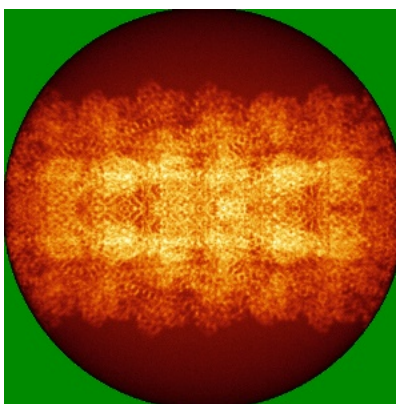


Z

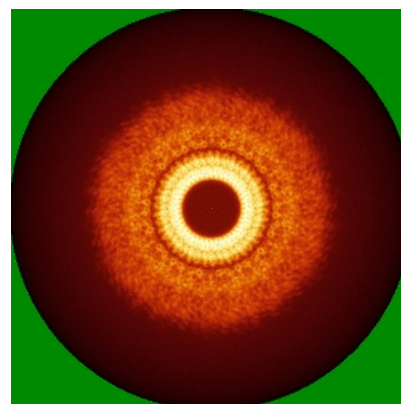
6.4.2 Raw map



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](#)

This section was not generated.

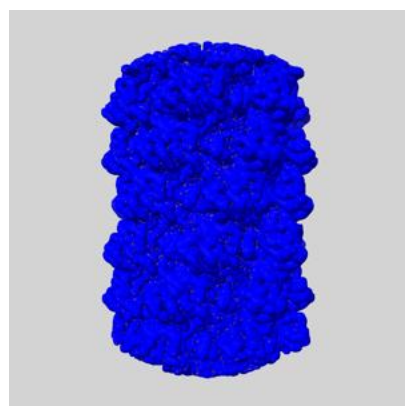
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

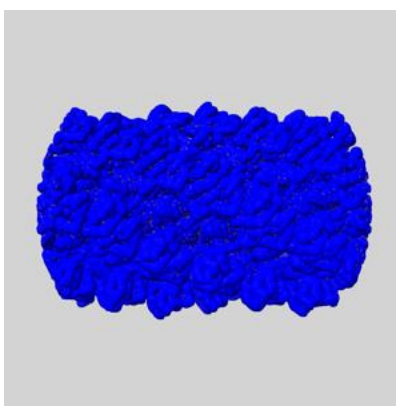
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

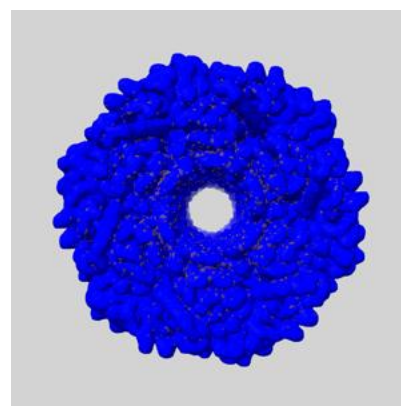
6.6.1 emd_42959_msk_1.map [i](#)



X



Y

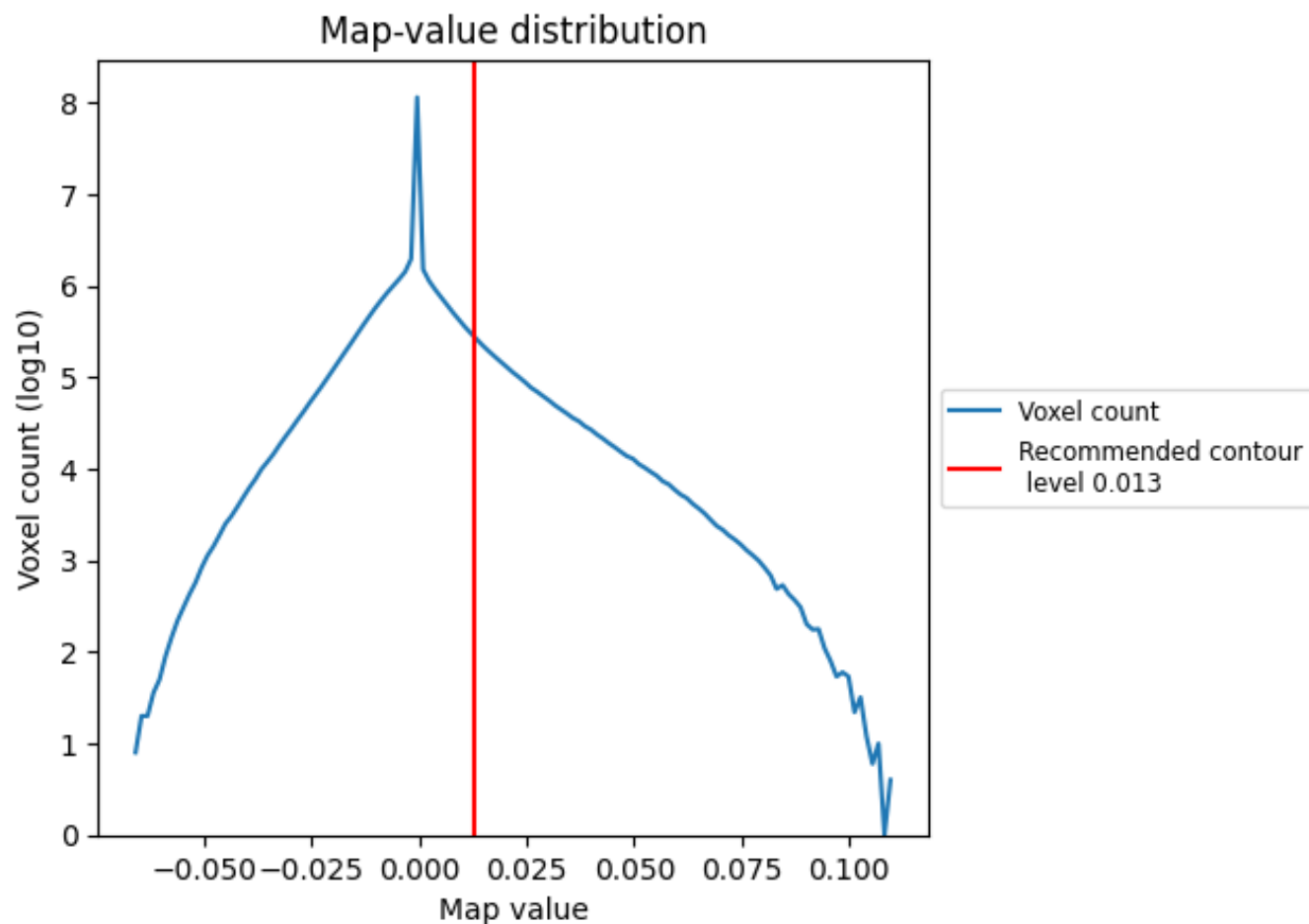


Z

7 Map analysis [i](#)

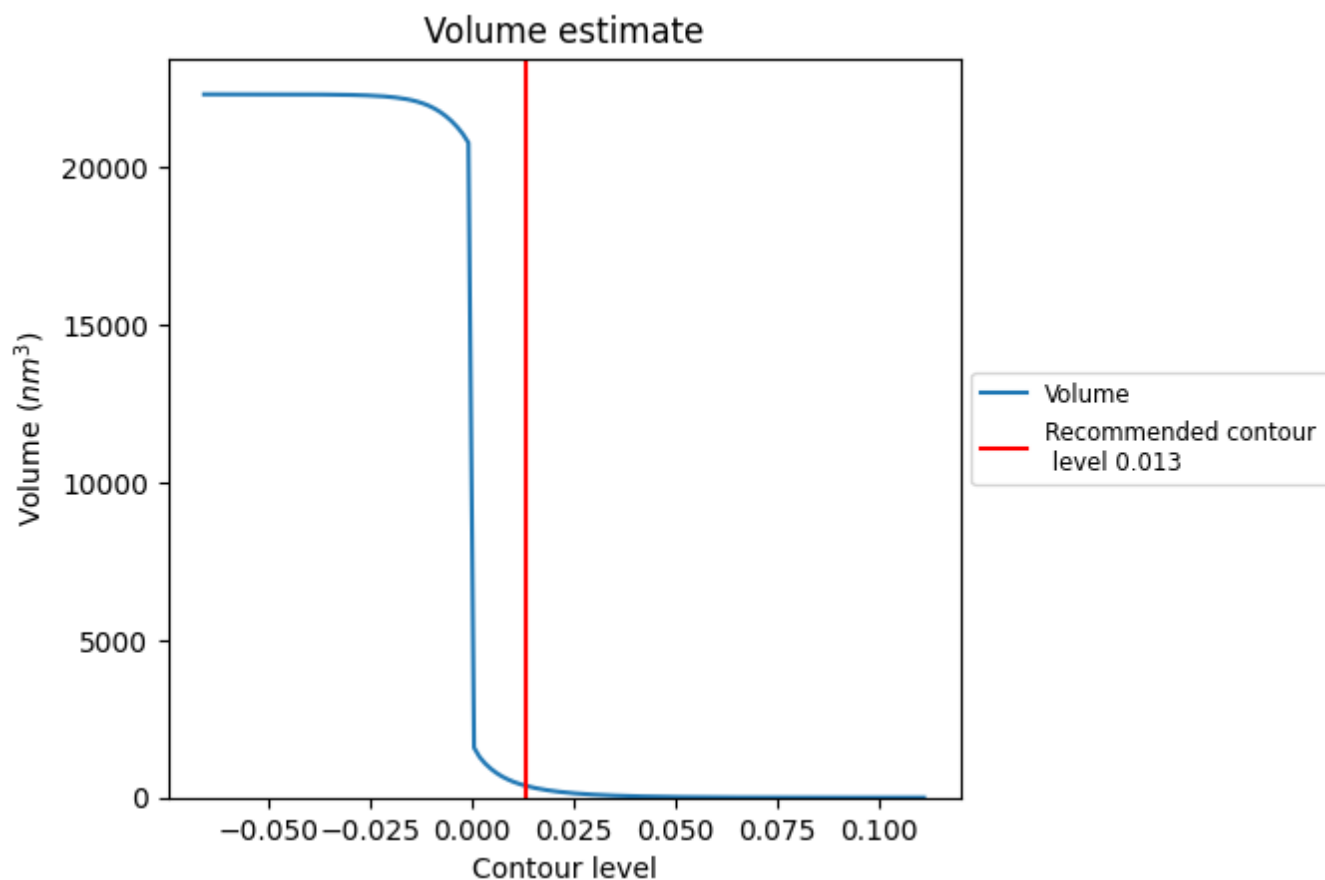
This section contains the results of statistical analysis of the map.

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.

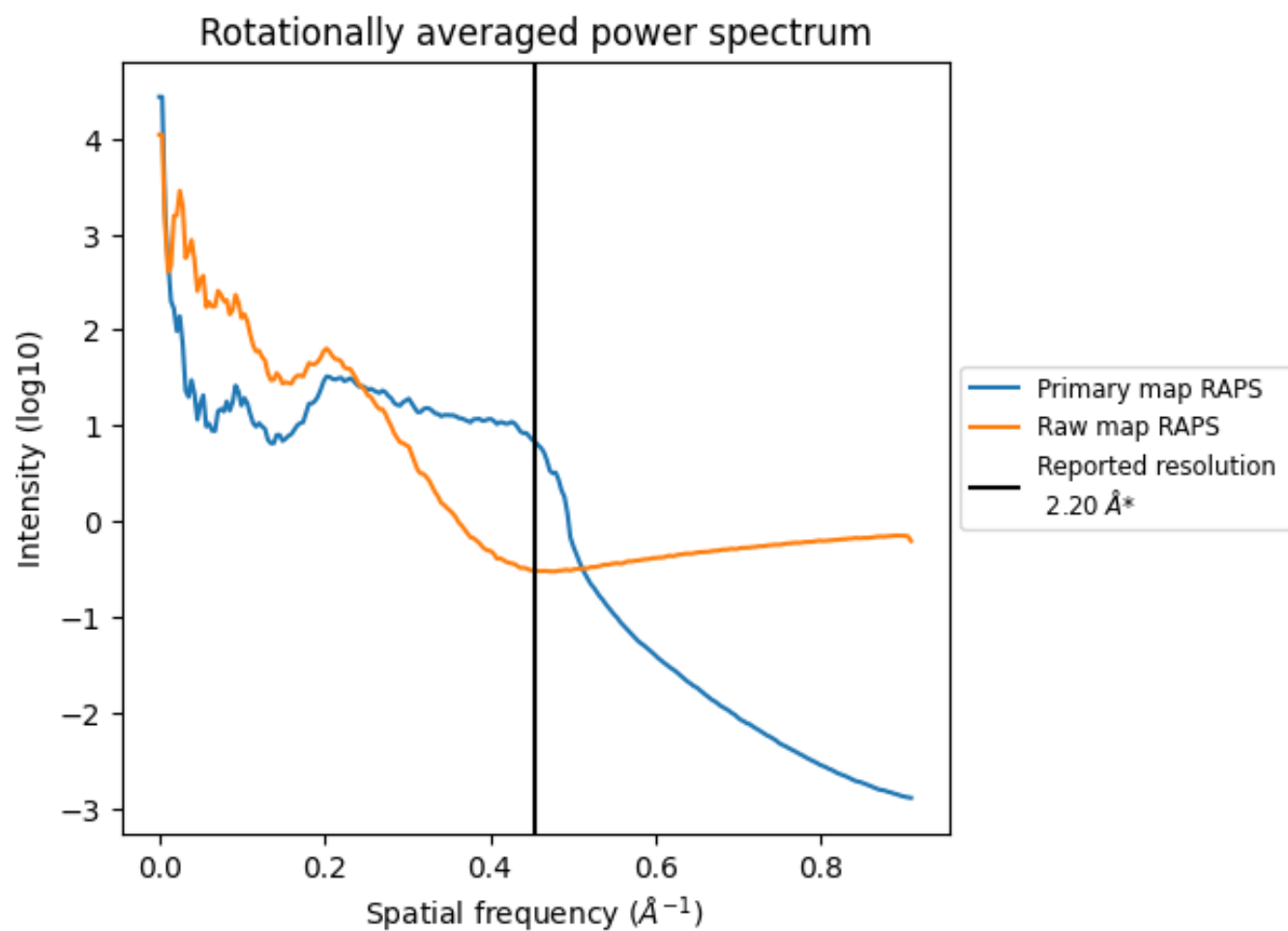
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 342 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 ⓘ

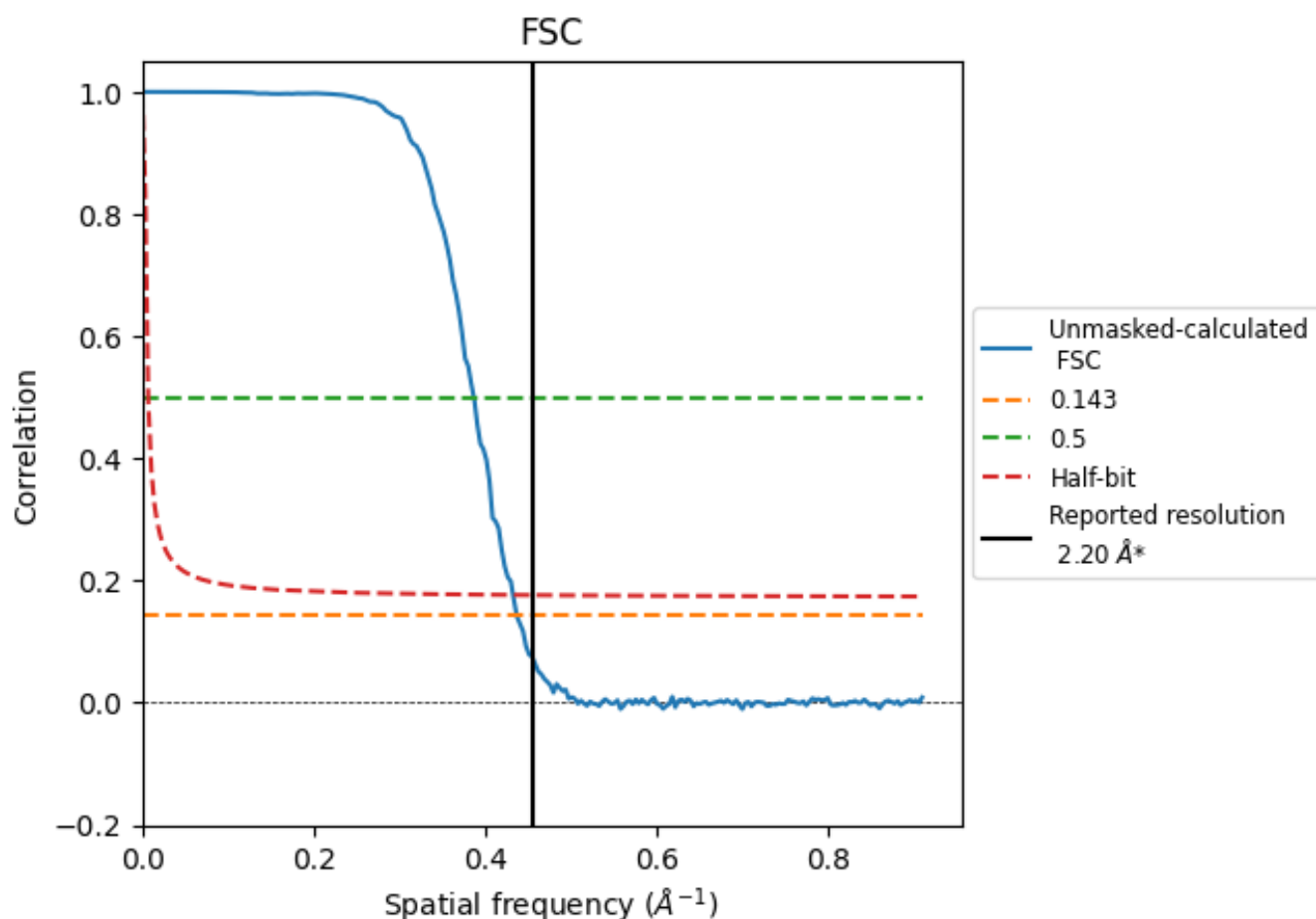


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

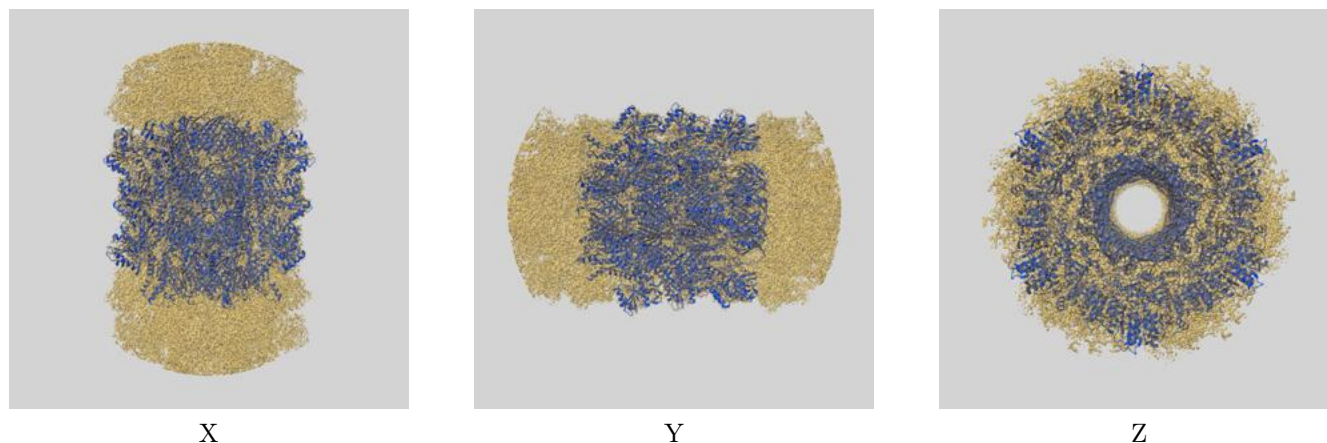
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.29	2.59	2.31

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

9 Map-model fit [i](#)

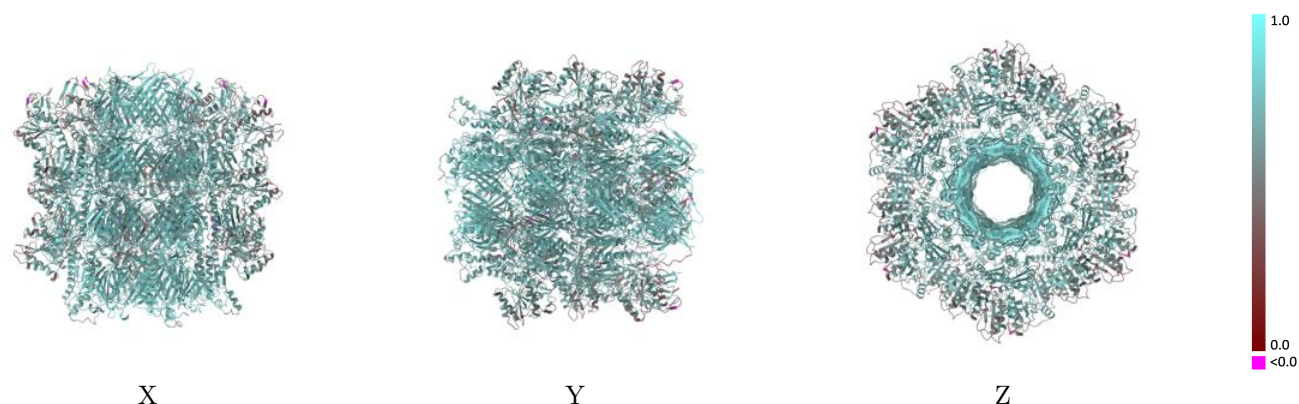
This section contains information regarding the fit between EMDB map EMD-42959 and PDB model 8V3X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

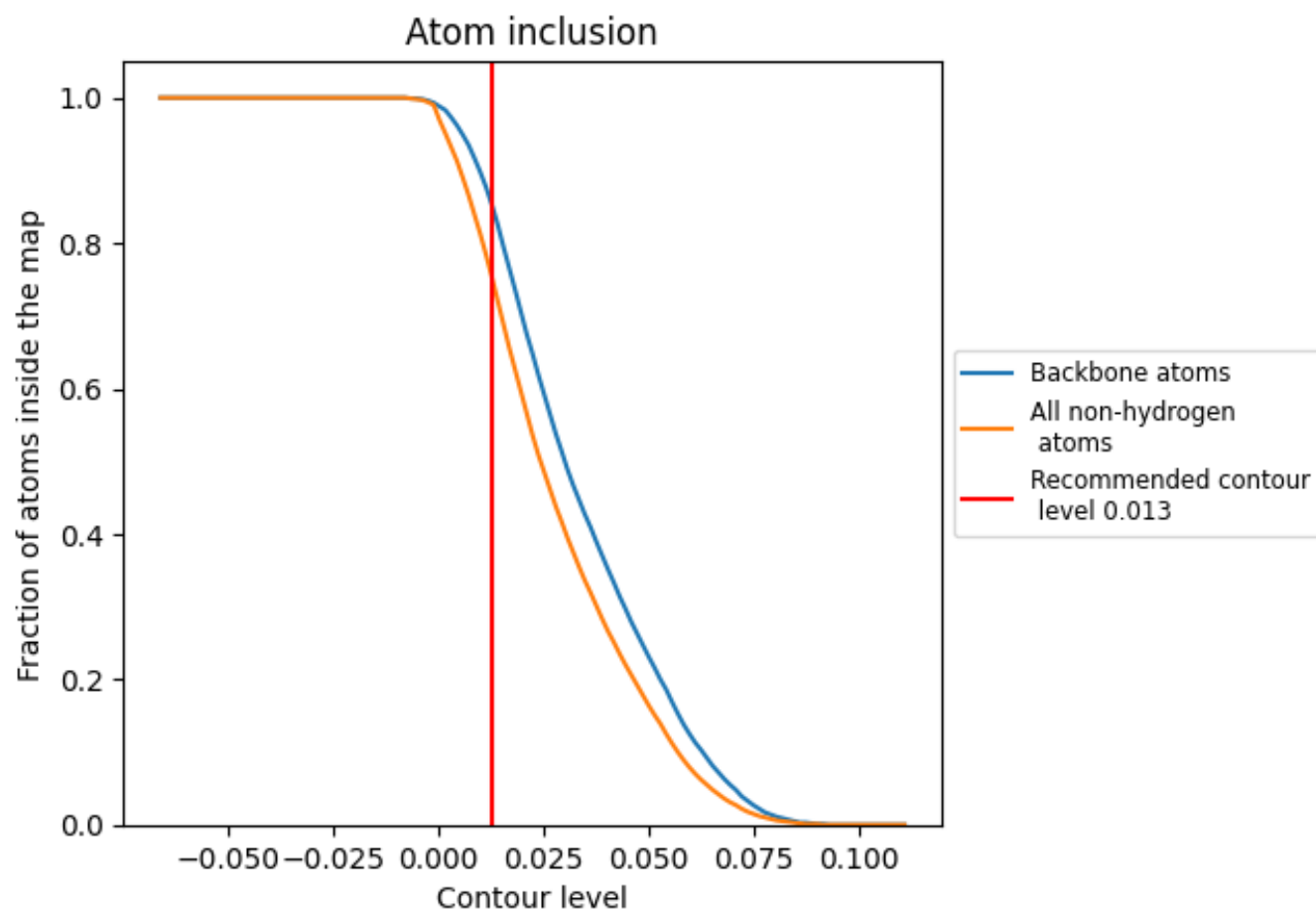


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.6670
A	 0.9280	 0.7590
B	 0.9130	 0.7570
C	 0.9270	 0.7590
D	 0.9080	 0.7540
E	 0.6330	 0.6000
F	 0.6980	 0.6420
G	 0.9320	 0.7630
H	 0.9250	 0.7610
I	 0.9260	 0.7620
J	 0.9260	 0.7610
K	 0.9110	 0.7560
L	 0.9130	 0.7540
M	 0.9080	 0.7550
N	 0.9270	 0.7620
O	 0.9120	 0.7540
P	 0.6330	 0.6010
Q	 0.6980	 0.6430
R	 0.9310	 0.7610
S	 0.6310	 0.5990
T	 0.6310	 0.6000
U	 0.6340	 0.6020
V	 0.6940	 0.6420
W	 0.6970	 0.6420
X	 0.6950	 0.6430
Y	 0.9370	 0.7610
Z	 0.9330	 0.7610
a	 0.9350	 0.7610
b	 0.9140	 0.7560
c	 0.9140	 0.7570
d	 0.6330	 0.5990
e	 0.6460	 0.6120
g	 0.6990	 0.6410
i	 0.9320	 0.7620
j	 0.9160	 0.7580



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.9160	 0.7570
l	 0.9150	 0.7590
m	 0.9150	 0.7570
n	 0.6420	 0.6070
q	 0.6390	 0.6050
r	 0.6410	 0.6080
s	 0.6390	 0.6070
z	 0.6440	 0.6110