



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:19 AM UTC

PDB ID : 6RWK / pdb_00006rwk
EMDB ID : EMD-10040
Title : MxiD N0 N1 and MxiG C-terminal domains of the Shigella type 3 secretion system
Authors : Kamprad, A.; Lunelli, M.
Deposited on : 2019-06-05
Resolution : 3.86 Å(reported)
Based on initial model : 3GR5

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

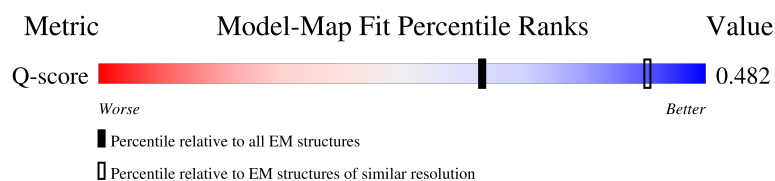
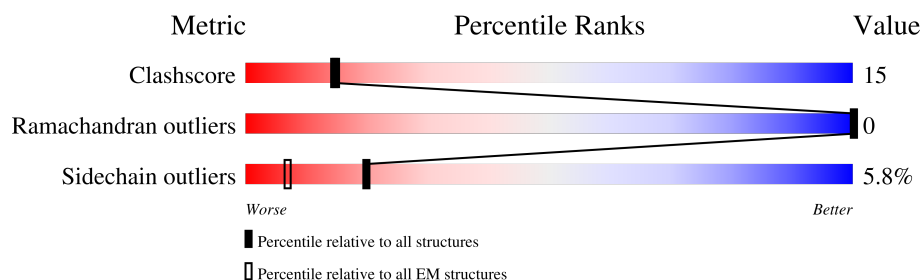
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.86 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.



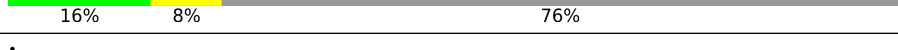
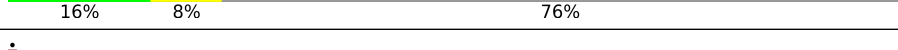
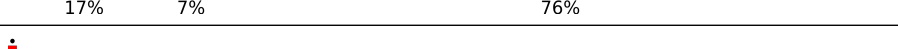
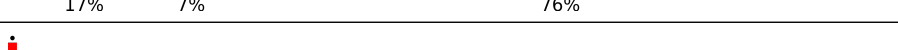
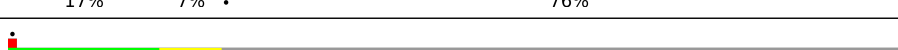
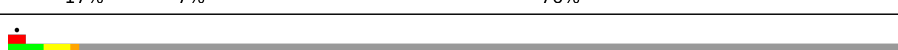
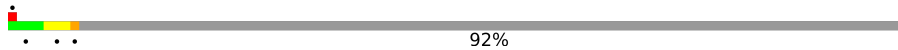
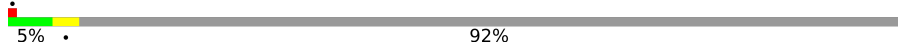
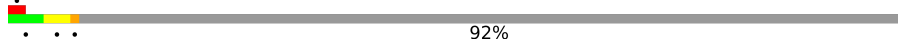
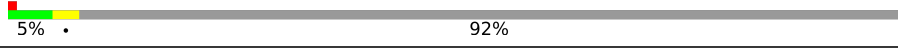
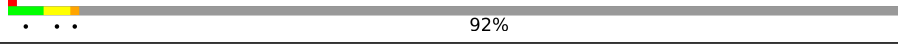
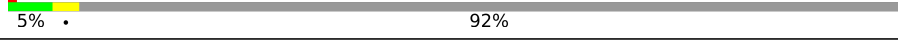
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8889 (3.36 - 4.35)

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	0	566	
1	1	566	
1	2	566	
1	3	566	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	4	566	 16% 8% 76%
1	5	566	 17% 7% 76%
1	6	566	 16% 8% 76%
1	7	566	 17% 7% 76%
1	8	566	 16% 8% 76%
1	9	566	 17% 7% 76%
1	X	566	 16% 8% 76%
1	Y	566	 16% 8% 76%
1	Z	566	 17% 7% 76%
1	x	566	 17% 7% 76%
1	y	566	 17% 7% 76%
1	z	566	 17% 7% 76%
2	A	371	 92%
2	B	371	 92%
2	D	371	 92%
2	E	371	 92%
2	G	371	 92%
2	H	371	 92%
2	J	371	 92%
2	K	371	 92%
2	M	371	 92%
2	N	371	 92%
2	P	371	 92%
2	Q	371	 92%
2	S	371	 92%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	T	371	 5% . 92%
2	U	371	 5% . . 92%
2	V	371	 5% . 92%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21760 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 Outer membrane protein MxiD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	Y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	Z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	0	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	2	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	4	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	6	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	8	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	x	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	y	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	z	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	1	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	3	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	5	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	7	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		
1	9	138	Total	C	N	O	S	0	0
			1102	718	174	209	1		

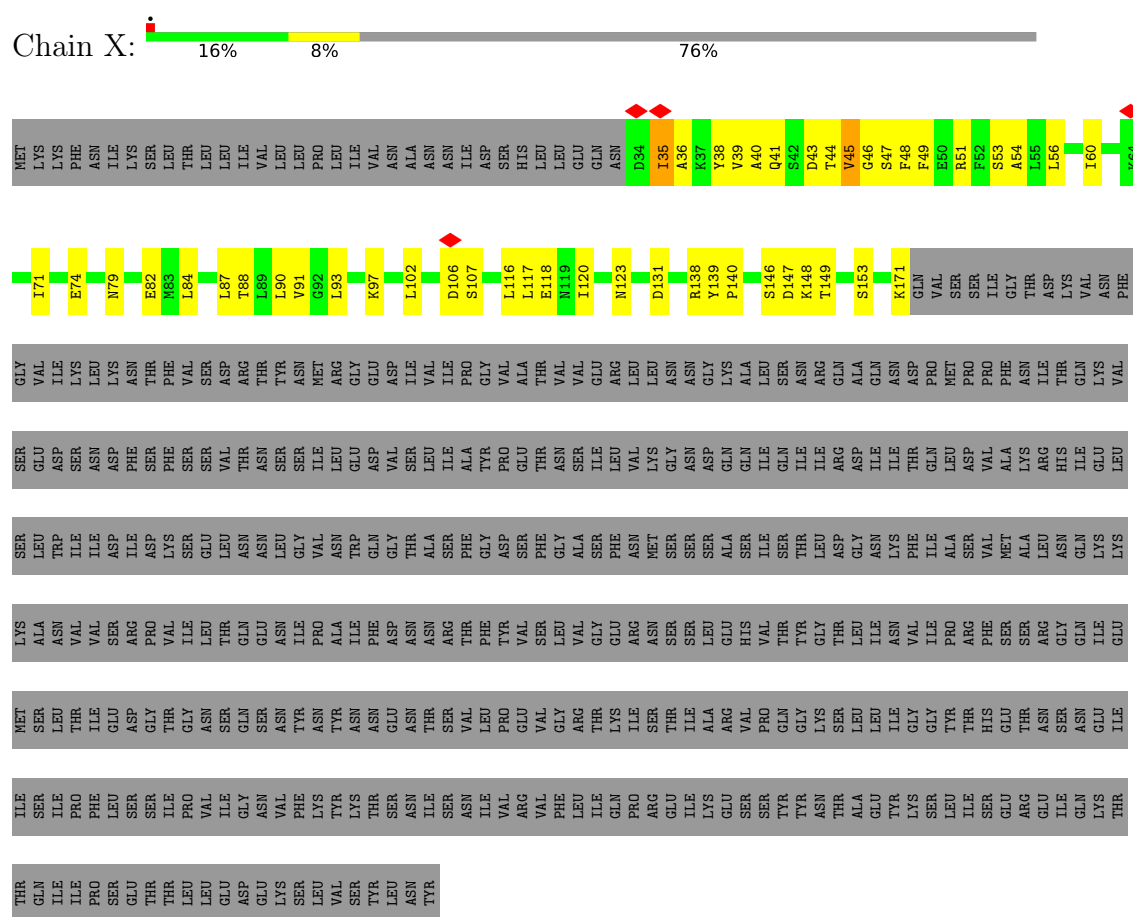
- Molecule 2 is a protein called Protein MxiG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	D	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	G	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	J	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	M	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	P	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	S	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	U	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	B	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	E	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	H	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	K	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	N	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	Q	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	T	30	Total	C	N	O	S	0	0
			258	171	39	47	1		
2	V	30	Total	C	N	O	S	0	0
			258	171	39	47	1		

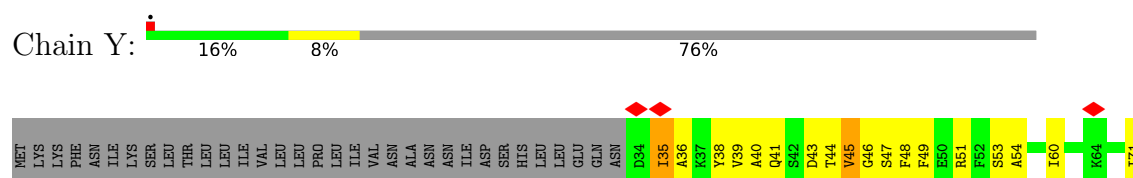
3 Residue-property plots

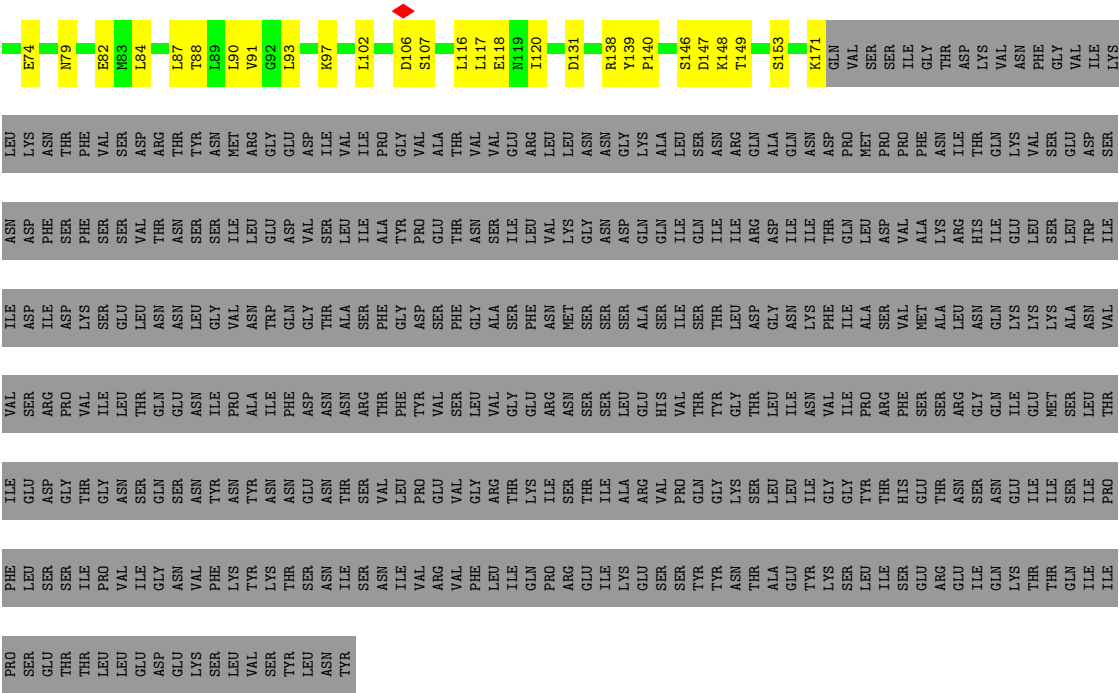
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Outer membrane protein MxiD



- Molecule 1: Outer membrane protein MxiD







THR	GLN	ILE	PRO	PRO	GLU	THR	LEU	LEU	GLU	ASP	GLU	ASN	VAL	LEU	LEU	ASN	THR	THR	THR	LYS	TYR	LYS	VAL	ASN	PHI	GLY	VAL	ILE	PRO	LEU	THR	ILE	SER	THR	GLN	ILE	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Outer membrane protein MxiD

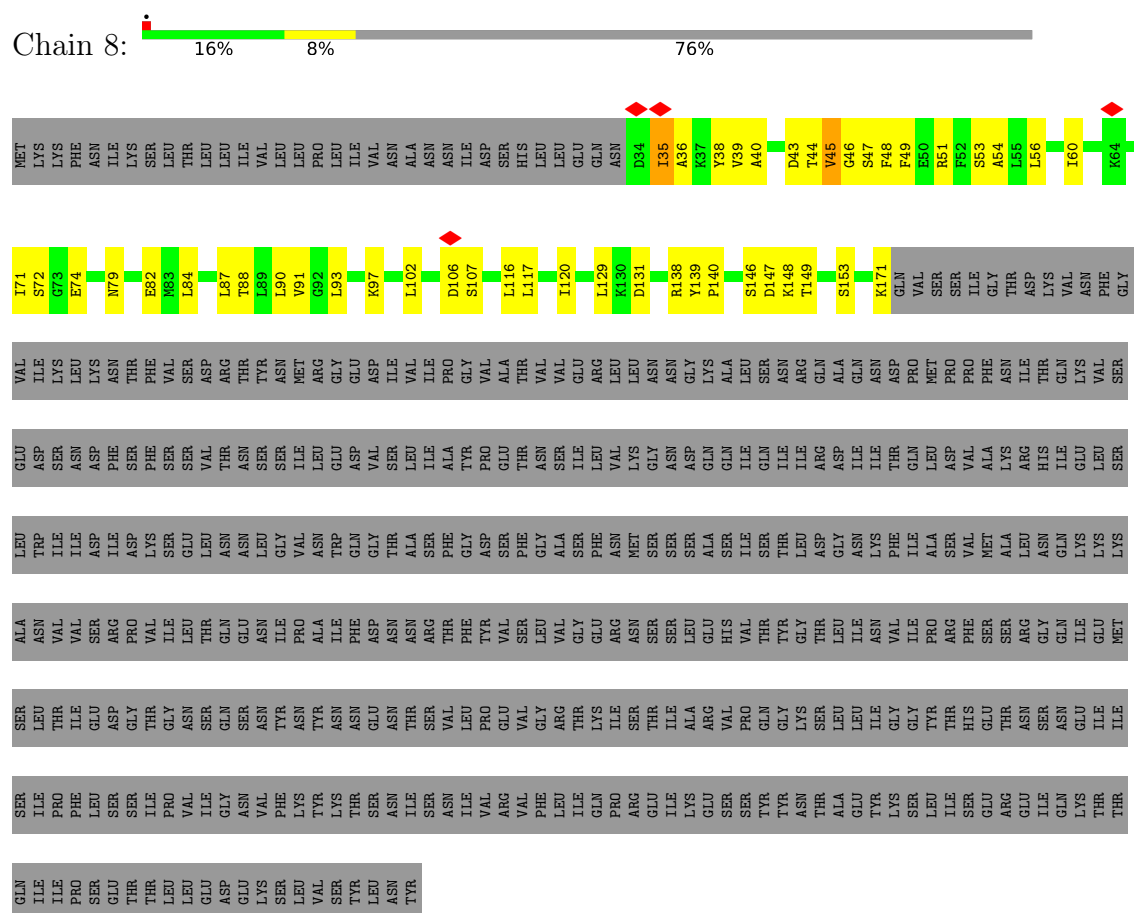
[illegible]

- Molecule 1: Outer membrane protein MxiD

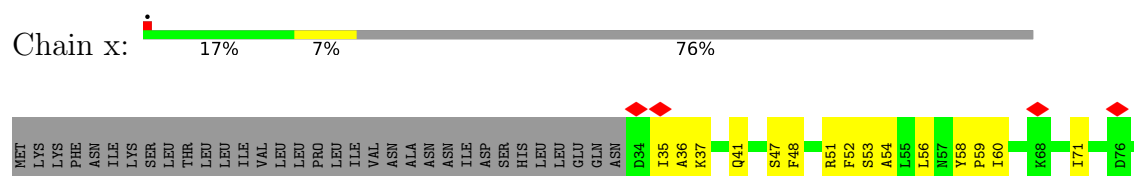


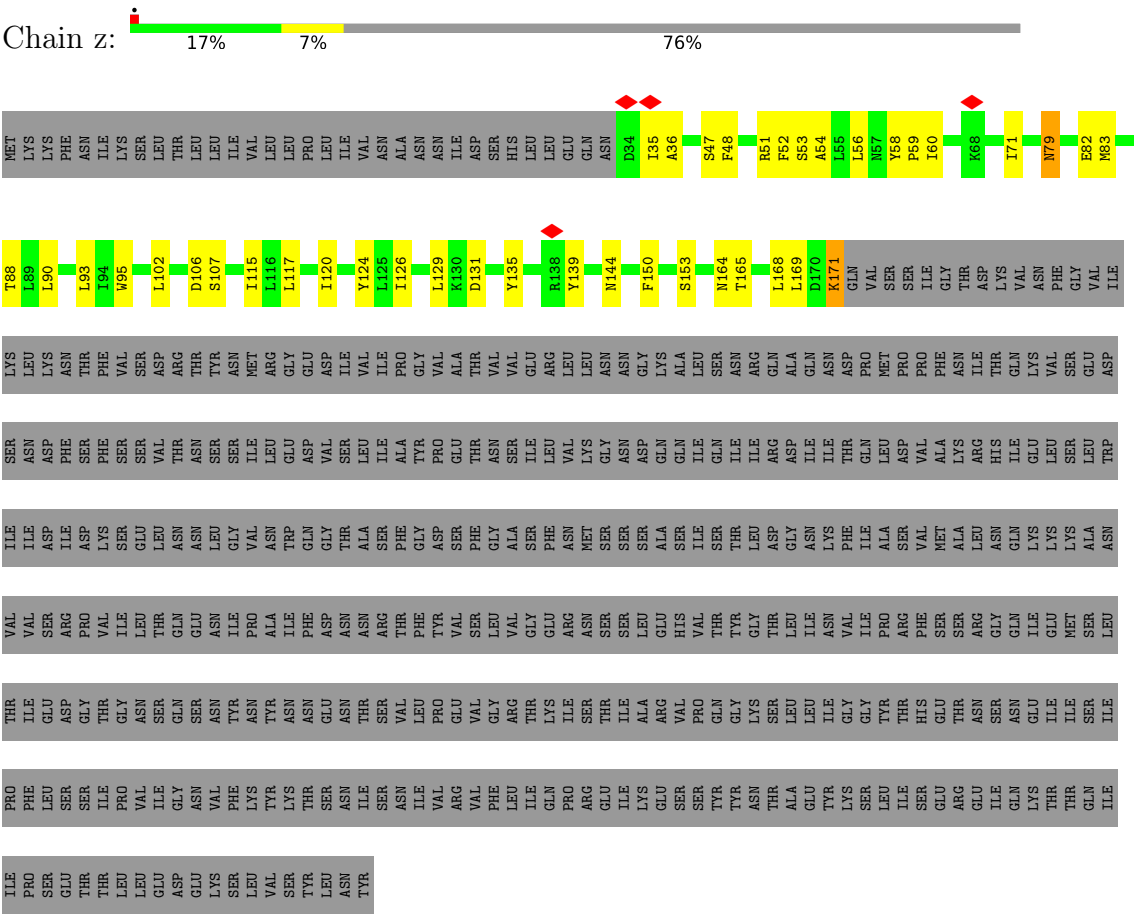
GLU	ASP	ILE	VAL	IT1	MET
SER	LYS	ILE	LYS	E74	LYS
ASN	LEU	LEU	LEU		PHE
ASP	ASN	ASN	LYS	N79	ASN
PHE	ILE	THR	THR	E82	ILE
SER	PHE	THR	VAL	M83	SER
SER	SER	VAL	VAL	L84	LEU
SER	SER	SER	SER		THR
VAL	VAL	ASP	ASP	L87	LEU
THR	THR	ARG	ARG	T88	LEU
ASN	ASN	THR	THR	L89	ILE
SER	SER	TYR	TYR	L90	VAL
SER	SER	ASN	ASN	V91	LEU
ILE	ILE	MET	MET	G92	LEU
LEU	LEU	ARG	ARG	L93	PRO
GLU	GLY	GLY	GLY		LEU
ASP	GLU	GLU	GLU	K97	ILE
VAL	VAL	ASP	ASP		VAL
SER	SER	ILE	ILE	L102	ASN
LEU	LEU	VAL	VAL		ALA
ALA	ALA	ILE	ILE	D106	ASN
TYR	TYR	GLY	GLY	S107	ASN
PRO	PRO	VAL	VAL	L116	ILE
GLU	GLU	ALA	ALA	L117	ASP
THR	THR	THR	THR	E118	SER
ASN	ASN	VAL	VAL	I119	HIS
SER	SER	VAL	VAL	R120	LEU
ILE	ILE	GLU	GLU		LEU
LEU	LEU	LEU	LEU	D131	GLN
VAL	VAL	LEU	LEU		ASN
LYS	LYS	LEU	LEU	R138	D34
GLY	GLY	ASN	ASN	Y139	I35
ASN	ASN	ASN	ASN	P140	A36
ASP	ASP	GLY	GLY		K37
GLN	GLN	LYS	LYS	S146	Y38
GLN	GLN	ALA	ALA	D147	V39
ILE	ILE	LEU	LEU	K148	A40
GLN	GLN	SER	SER	T149	
ILE	ILE	ASN	ASN		GLN
ILE	ILE	ARG	ARG	S153	D43
ARG	ARG	GLN	GLN		T44
ASP	ASP	ALA	ALA	L169	V45
ILE	ILE	GLN	GLN	D170	G46
ILE	ILE	ASN	ASN	K171	S47
THR	THR	ASP	ASP		F48
GLN	GLN	PRO	PRO	GLN	F49
LEU	LEU	PRO	PRO	VAL	E50
ASP	ASP	MET	MET	SER	R51
VAL	VAL	PRO	PRO	SER	F52
ALA	ALA	PHE	PHE	ILE	S53
LYS	LYS	ASN	ASN	THR	A54
ARG	ARG	ILE	ILE	ASP	L55
HIS	HIS	THR	THR	LYS	L56
ILE	ILE	GLN	GLN	VAL	
GLU	GLU	LYS	LYS	ASN	I60
LEU	LEU	VAL	VAL	PHE	
ASP	ASP	SER	SER		K64

- Molecule 1: Outer membrane protein MxiD

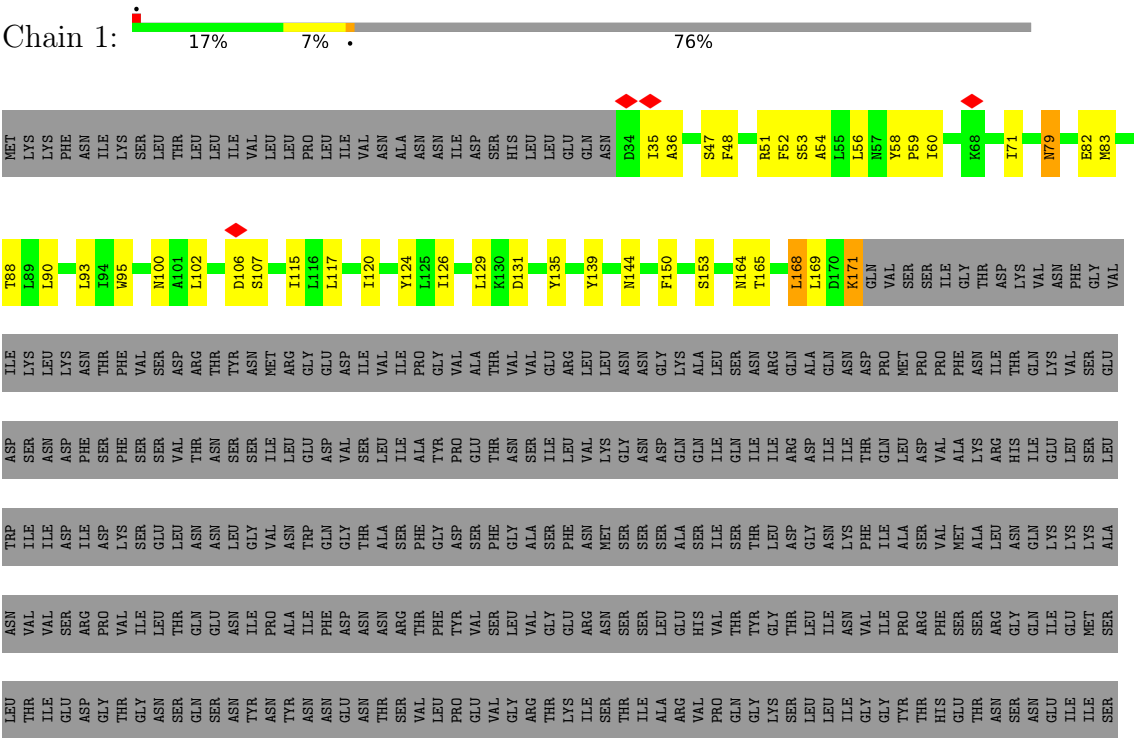


- Molecule 1: Outer membrane protein MxiD





● Molecule 1: Outer membrane protein MxiD



IIE	PRO	PHE	LEU	SER	SER	IIE	PRO	VAL	GLY	ASN	VAL	PHE	LYS	TYR	THR	SER	ASN	IIE	SER	SER	ASN	VAL	ARG	VAL	PHE	LEU	ILE	GLN	LYS	GLU	SER	SER	TYR	TYR	ASN	THR	ALA	GLU	TYR	TYR	LYS	SER	LEU	ILE	IIE	SER	GLU	ARG	GLU	ILE	GLN	THR	THR	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Outer membrane protein MxiD

[illegible]

- Molecule 1: Outer membrane protein MxiD

[illegible]

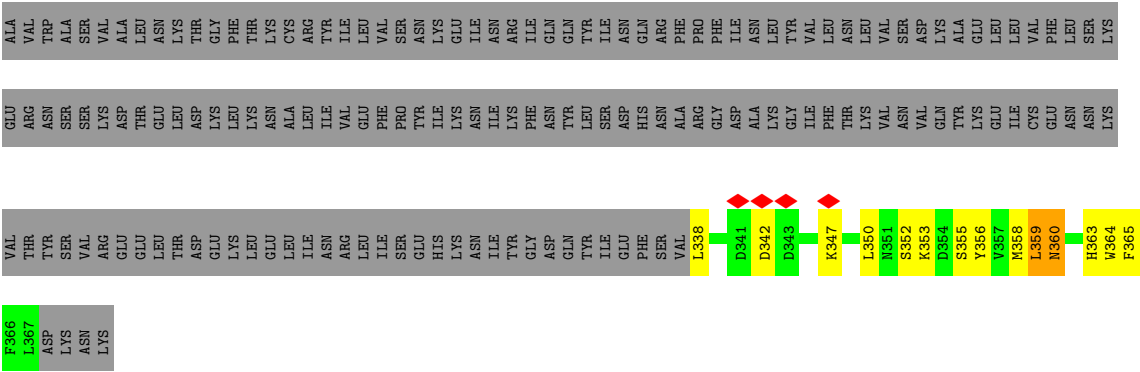


- Molecule 2: Protein MxiG

H363		L367	ASP
W364			LYS
			ASN
			LYS

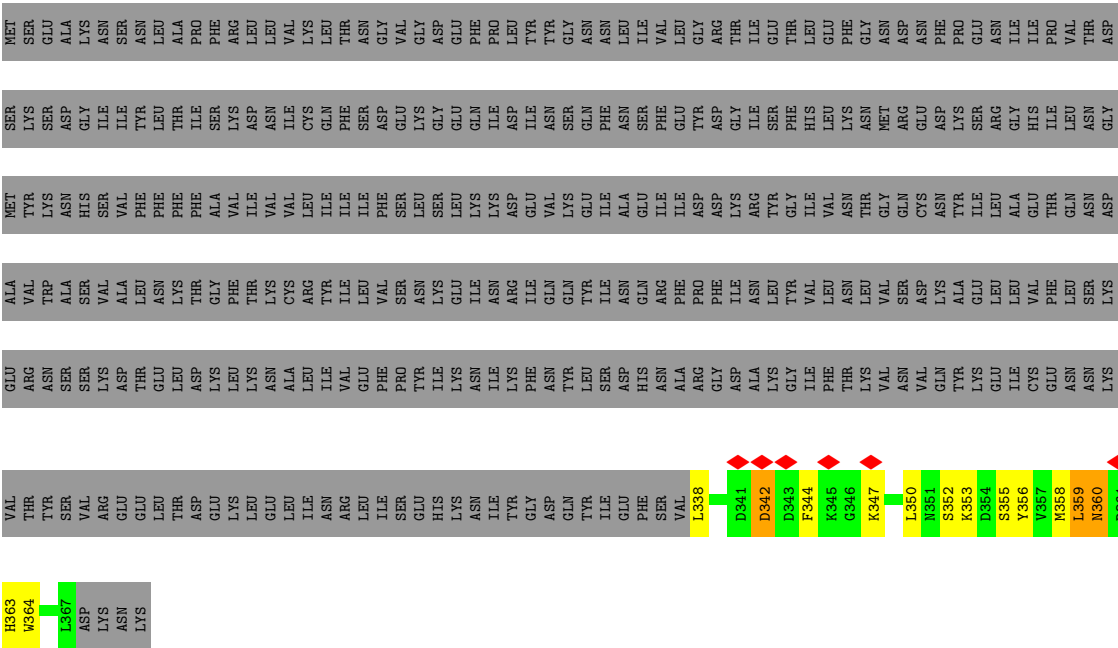
- Molecule 2: Protein MxiG

[illegible]



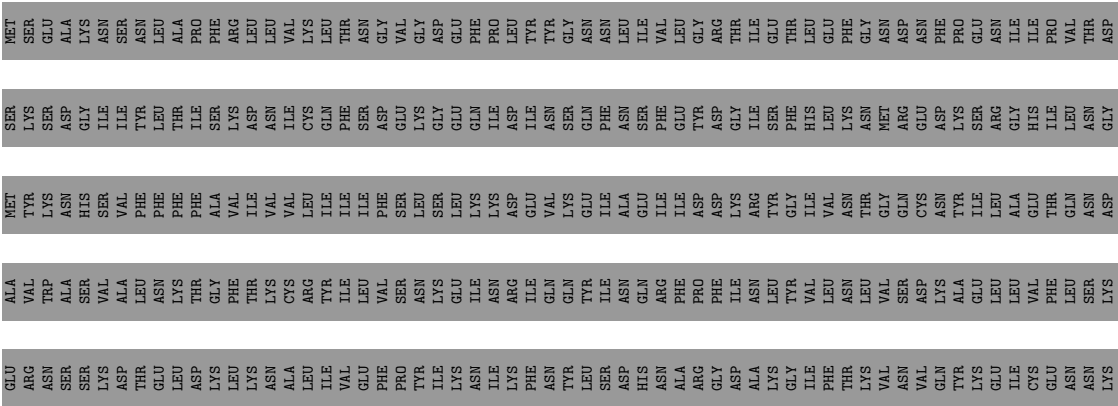
● Molecule 2: Protein MxiG

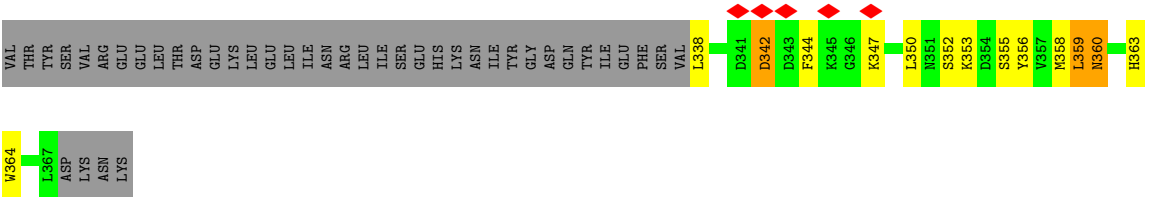
Chain M:  92%



● Molecule 2: Protein MxiG

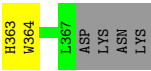
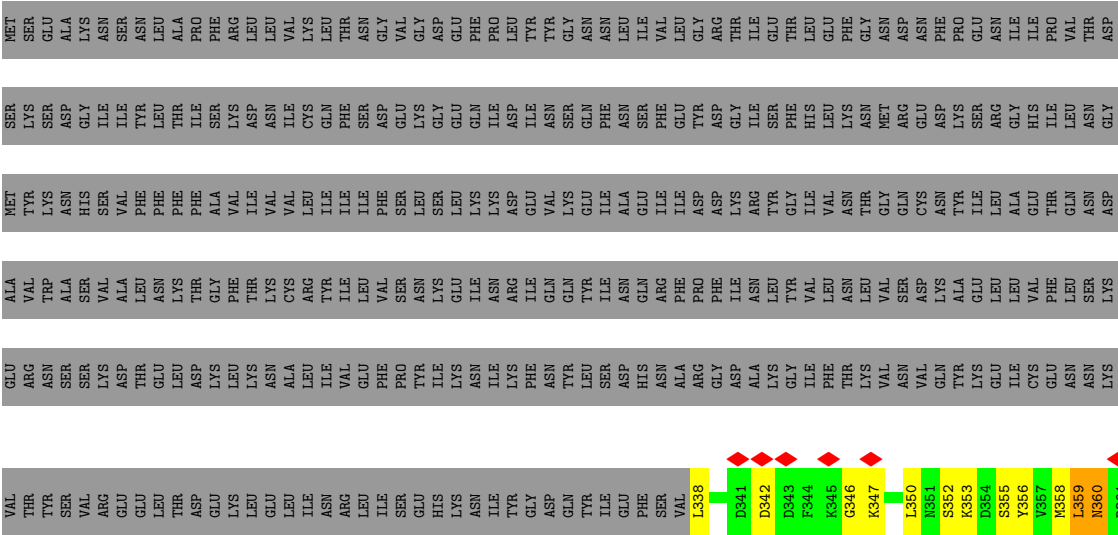
Chain P:  92%





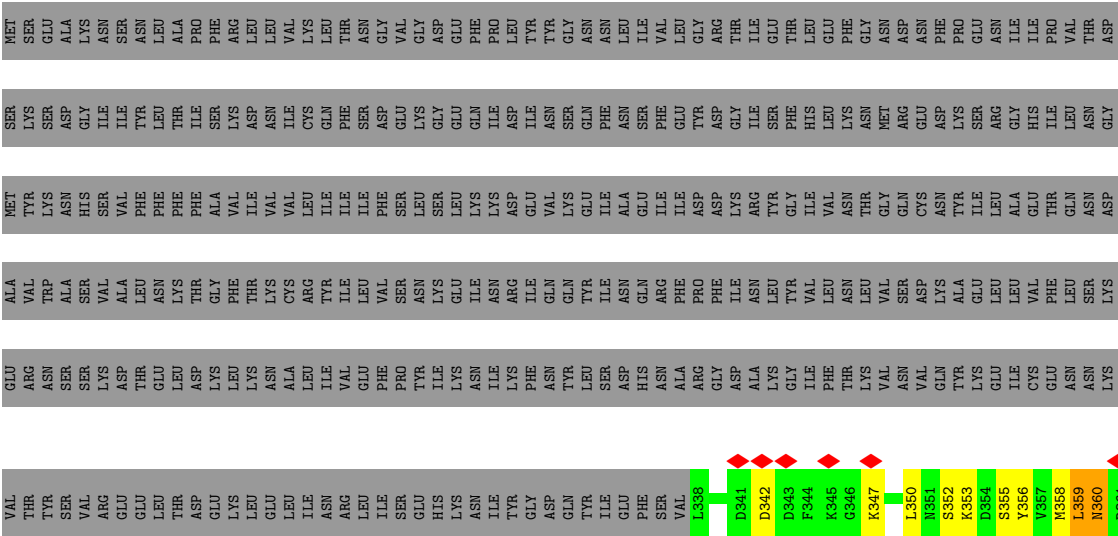
● Molecule 2: Protein MxiG

Chain S: 92%



● Molecule 2: Protein MxiG

Chain U: 5% 92%



L367
ASP
LYS
ASN
LYS

W364	L367	ASP
		LYS
		ASN
		LYS

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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of particles used	72298	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	4	Depositor
Magnification	101179	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.471	Depositor
Minimum map value	-0.240	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	664.1712, 664.1712, 664.1712	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38369, 1.38369, 1.38369	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	0	0.33	0/1124	0.44	0/1525
1	1	0.33	0/1124	0.41	0/1525
1	2	0.33	0/1124	0.44	0/1525
1	3	0.33	0/1124	0.42	0/1525
1	4	0.33	0/1124	0.44	0/1525
1	5	0.33	0/1124	0.41	0/1525
1	6	0.33	0/1124	0.44	0/1525
1	7	0.33	0/1124	0.41	0/1525
1	8	0.33	0/1124	0.44	0/1525
1	9	0.33	0/1124	0.42	0/1525
1	X	0.33	0/1124	0.44	0/1525
1	Y	0.33	0/1124	0.44	0/1525
1	Z	0.33	0/1124	0.44	0/1525
1	x	0.33	0/1124	0.41	0/1525
1	y	0.33	0/1124	0.41	0/1525
1	z	0.33	0/1124	0.41	0/1525
2	A	0.30	0/265	0.52	0/355
2	B	0.30	0/265	0.40	0/355
2	D	0.30	0/265	0.53	0/355
2	E	0.29	0/265	0.40	0/355
2	G	0.30	0/265	0.53	0/355
2	H	0.30	0/265	0.40	0/355
2	J	0.30	0/265	0.53	0/355
2	K	0.30	0/265	0.40	0/355
2	M	0.30	0/265	0.53	0/355
2	N	0.30	0/265	0.40	0/355
2	P	0.30	0/265	0.52	0/355
2	Q	0.30	0/265	0.40	0/355
2	S	0.30	0/265	0.53	0/355
2	T	0.29	0/265	0.40	0/355
2	U	0.30	0/265	0.53	0/355
2	V	0.30	0/265	0.40	0/355
All	All	0.33	0/22224	0.44	0/30080

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	0	1102	0	1118	35	0
1	1	1102	0	1118	26	0
1	2	1102	0	1118	37	0
1	3	1102	0	1118	31	0
1	4	1102	0	1118	40	0
1	5	1102	0	1118	29	0
1	6	1102	0	1118	37	0
1	7	1102	0	1118	32	0
1	8	1102	0	1118	37	0
1	9	1102	0	1118	31	0
1	X	1102	0	1118	37	0
1	Y	1102	0	1118	37	0
1	Z	1102	0	1118	33	0
1	x	1102	0	1118	32	0
1	y	1102	0	1118	32	0
1	z	1102	0	1118	27	0
2	A	258	0	247	18	0
2	B	258	0	247	12	0
2	D	258	0	247	19	0
2	E	258	0	247	13	0
2	G	258	0	247	17	0
2	H	258	0	247	11	0
2	J	258	0	247	17	0
2	K	258	0	247	11	0
2	M	258	0	247	16	0
2	N	258	0	247	9	0
2	P	258	0	247	17	0
2	Q	258	0	247	12	0
2	S	258	0	247	16	0
2	T	258	0	247	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	258	0	247	17	0
2	V	258	0	247	12	0
All	All	21760	0	21840	656	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 15.

All (656) 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:X:47:SER:OG	1:X:51:ARG:NH1	2.18	0.76
1:Y:47:SER:OG	1:Y:51:ARG:NH1	2.18	0.76
1:Z:47:SER:OG	1:Z:51:ARG:NH1	2.18	0.76
1:8:47:SER:OG	1:8:51:ARG:NH1	2.18	0.76
1:6:47:SER:OG	1:6:51:ARG:NH1	2.18	0.76
1:4:47:SER:OG	1:4:51:ARG:NH1	2.18	0.76
1:2:47:SER:OG	1:2:51:ARG:NH1	2.18	0.76
1:0:47:SER:OG	1:0:51:ARG:NH1	2.18	0.75
1:5:47:SER:OG	1:5:51:ARG:NH1	2.23	0.72
1:3:47:SER:OG	1:3:51:ARG:NH1	2.23	0.72
1:1:47:SER:OG	1:1:51:ARG:NH1	2.23	0.71
1:x:47:SER:OG	1:x:51:ARG:NH1	2.23	0.70
1:y:47:SER:OG	1:y:51:ARG:NH1	2.23	0.70
1:z:47:SER:OG	1:z:51:ARG:NH1	2.23	0.70
1:9:47:SER:OG	1:9:51:ARG:NH1	2.23	0.70
1:7:47:SER:OG	1:7:51:ARG:NH1	2.23	0.68
1:4:60:ILE:HG12	1:4:102:LEU:HB3	1.76	0.68
1:6:60:ILE:HG12	1:6:102:LEU:HB3	1.76	0.68
1:8:60:ILE:HG12	1:8:102:LEU:HB3	1.76	0.68
1:y:88:THR:HG23	1:y:93:LEU:HB2	1.76	0.67
1:X:60:ILE:HG12	1:X:102:LEU:HB3	1.76	0.67
1:Z:147:ASP:OD2	1:z:171:LYS:NZ	2.24	0.67
1:Z:60:ILE:HG12	1:Z:102:LEU:HB3	1.76	0.67
1:x:88:THR:HG23	1:x:93:LEU:HB2	1.76	0.67
1:z:88:THR:HG23	1:z:93:LEU:HB2	1.76	0.67
1:5:47:SER:HG	1:5:51:ARG:HH12	1.43	0.66
1:9:88:THR:HG23	1:9:93:LEU:HB2	1.76	0.66
1:3:88:THR:HG23	1:3:93:LEU:HB2	1.76	0.66
1:0:60:ILE:HG12	1:0:102:LEU:HB3	1.76	0.66
1:5:88:THR:HG23	1:5:93:LEU:HB2	1.76	0.66
1:Y:60:ILE:HG12	1:Y:102:LEU:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:60:ILE:HG12	1:2:102:LEU:HB3	1.76	0.66
1:X:38:TYR:OH	1:X:51:ARG:NH2	2.25	0.65
1:7:88:THR:HG23	1:7:93:LEU:HB2	1.76	0.65
1:0:38:TYR:OH	1:0:51:ARG:NH2	2.25	0.65
1:1:88:THR:HG23	1:1:93:LEU:HB2	1.76	0.65
1:6:79:ASN:ND2	1:6:82:GLU:OE1	2.30	0.65
2:B:352:SER:H	2:B:355:SER:HB3	1.62	0.65
2:V:352:SER:H	2:V:355:SER:HB3	1.62	0.65
1:4:79:ASN:ND2	1:4:82:GLU:OE1	2.30	0.65
2:K:352:SER:H	2:K:355:SER:HB3	1.62	0.64
1:8:79:ASN:ND2	1:8:82:GLU:OE1	2.30	0.64
2:T:352:SER:H	2:T:355:SER:HB3	1.62	0.64
1:2:79:ASN:ND2	1:2:82:GLU:OE1	2.30	0.64
1:8:38:TYR:OH	1:8:51:ARG:NH2	2.25	0.64
2:E:352:SER:H	2:E:355:SER:HB3	1.62	0.64
1:1:47:SER:HG	1:1:51:ARG:HH12	1.46	0.64
2:Q:352:SER:H	2:Q:355:SER:HB3	1.62	0.64
1:0:79:ASN:ND2	1:0:82:GLU:OE1	2.30	0.63
2:B:359:LEU:O	2:B:363:HIS:HB3	1.99	0.63
2:H:352:SER:H	2:H:355:SER:HB3	1.62	0.63
1:Z:79:ASN:ND2	1:Z:82:GLU:OE1	2.30	0.63
2:V:359:LEU:O	2:V:363:HIS:HB3	1.98	0.63
1:Y:79:ASN:ND2	1:Y:82:GLU:OE1	2.30	0.63
1:0:147:ASP:OD2	1:1:171:LYS:NZ	2.27	0.63
2:N:352:SER:H	2:N:355:SER:HB3	1.62	0.63
2:E:359:LEU:O	2:E:363:HIS:HB3	1.99	0.62
1:X:79:ASN:ND2	1:X:82:GLU:OE1	2.30	0.62
2:Q:359:LEU:O	2:Q:363:HIS:HB3	1.98	0.62
2:T:359:LEU:O	2:T:363:HIS:HB3	1.98	0.62
2:N:359:LEU:O	2:N:363:HIS:HB3	1.99	0.62
1:6:38:TYR:OH	1:6:51:ARG:NH2	2.25	0.62
2:K:359:LEU:O	2:K:363:HIS:HB3	1.98	0.62
2:H:359:LEU:O	2:H:363:HIS:HB3	1.98	0.62
1:4:139:TYR:HE1	1:5:59:PRO:HG3	1.65	0.62
1:7:47:SER:HG	1:7:51:ARG:HH12	1.46	0.61
1:X:51:ARG:HD3	2:D:358:MET:HE3	1.82	0.61
1:X:139:TYR:HE1	1:x:59:PRO:HG3	1.66	0.61
1:Z:38:TYR:OH	1:Z:51:ARG:NH2	2.25	0.61
1:Z:139:TYR:HE1	1:z:59:PRO:HG3	1.66	0.61
1:0:139:TYR:HE1	1:1:59:PRO:HG3	1.66	0.60
1:8:54:ALA:HB1	1:7:90:LEU:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:139:TYR:HE1	1:y:59:PRO:HG3	1.66	0.60
2:M:358:MET:HE1	2:M:364:TRP:CE2	2.37	0.60
1:6:51:ARG:HD3	2:U:358:MET:HE3	1.83	0.60
1:6:147:ASP:OD2	1:7:171:LYS:NZ	2.31	0.60
2:J:358:MET:HE1	2:J:364:TRP:CE2	2.37	0.60
2:P:358:MET:HE1	2:P:364:TRP:CE2	2.37	0.60
1:4:38:TYR:OH	1:4:51:ARG:NH2	2.25	0.59
2:M:347:LYS:HG2	2:M:359:LEU:HB3	1.85	0.59
2:U:358:MET:HE1	2:U:364:TRP:CE2	2.37	0.59
2:J:347:LYS:HG2	2:J:359:LEU:HB3	1.85	0.59
1:x:79:ASN:N	1:x:79:ASN:OD1	2.36	0.59
1:5:79:ASN:OD1	1:5:79:ASN:N	2.36	0.59
2:G:358:MET:HE1	2:G:364:TRP:CE2	2.37	0.59
2:P:347:LYS:HG2	2:P:359:LEU:HB3	1.85	0.59
2:S:358:MET:HE1	2:S:364:TRP:CE2	2.37	0.59
1:y:71:ILE:HG22	2:J:364:TRP:HB2	1.85	0.59
2:S:347:LYS:HG2	2:S:359:LEU:HB3	1.85	0.59
1:y:79:ASN:OD1	1:y:79:ASN:N	2.36	0.58
1:2:139:TYR:HE1	1:3:59:PRO:HG3	1.68	0.58
2:D:358:MET:HE1	2:D:364:TRP:CE2	2.37	0.58
1:X:43:ASP:OD2	1:X:51:ARG:NH2	2.36	0.58
1:3:79:ASN:N	1:3:79:ASN:OD1	2.36	0.58
2:U:347:LYS:HG2	2:U:359:LEU:HB3	1.85	0.58
1:4:43:ASP:OD2	1:4:51:ARG:NH2	2.36	0.58
1:7:79:ASN:OD1	1:7:79:ASN:N	2.36	0.58
1:Y:38:TYR:OH	1:Y:51:ARG:NH2	2.25	0.58
1:9:79:ASN:OD1	1:9:79:ASN:N	2.36	0.58
2:A:358:MET:HE1	2:A:364:TRP:CE2	2.37	0.58
1:3:71:ILE:HG22	2:S:364:TRP:HB2	1.85	0.58
2:G:347:LYS:HG2	2:G:359:LEU:HB3	1.85	0.58
1:0:43:ASP:OD2	1:0:51:ARG:NH2	2.36	0.58
1:8:43:ASP:OD2	1:8:51:ARG:NH2	2.36	0.58
1:Y:43:ASP:OD2	1:Y:51:ARG:NH2	2.36	0.57
1:Z:43:ASP:OD2	1:Z:51:ARG:NH2	2.36	0.57
1:6:43:ASP:OD2	1:6:51:ARG:NH2	2.36	0.57
2:D:347:LYS:HG2	2:D:359:LEU:HB3	1.85	0.57
1:2:43:ASP:OD2	1:2:51:ARG:NH2	2.36	0.57
1:2:147:ASP:OD2	1:3:171:LYS:NZ	2.28	0.57
1:z:79:ASN:N	1:z:79:ASN:OD1	2.36	0.57
2:A:347:LYS:HG2	2:A:359:LEU:HB3	1.85	0.57
1:1:79:ASN:N	1:1:79:ASN:OD1	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:139:TYR:HE1	1:9:59:PRO:HG3	1.69	0.57
1:6:139:TYR:HE1	1:7:59:PRO:HG3	1.69	0.56
1:Y:38:TYR:HH	1:Y:51:ARG:HH21	1.50	0.56
1:3:106:ASP:OD1	1:3:107:SER:N	2.39	0.56
1:y:106:ASP:OD1	1:y:107:SER:N	2.39	0.56
1:5:106:ASP:OD1	1:5:107:SER:N	2.39	0.56
1:9:106:ASP:OD1	1:9:107:SER:N	2.39	0.56
1:1:106:ASP:OD1	1:1:107:SER:N	2.39	0.56
1:7:106:ASP:OD1	1:7:107:SER:N	2.39	0.56
1:x:106:ASP:OD1	1:x:107:SER:N	2.39	0.56
1:z:106:ASP:OD1	1:z:107:SER:N	2.39	0.56
1:1:95:TRP:HE3	1:1:102:LEU:HD11	1.71	0.55
1:X:54:ALA:HB1	1:9:90:LEU:HA	1.88	0.55
1:7:95:TRP:HE3	1:7:102:LEU:HD11	1.71	0.55
1:2:38:TYR:OH	1:2:51:ARG:NH2	2.25	0.55
1:x:95:TRP:HE3	1:x:102:LEU:HD11	1.71	0.55
1:9:95:TRP:HE3	1:9:102:LEU:HD11	1.71	0.55
1:Z:54:ALA:HB1	1:y:90:LEU:HA	1.88	0.55
1:z:95:TRP:HE3	1:z:102:LEU:HD11	1.71	0.54
1:3:95:TRP:HE3	1:3:102:LEU:HD11	1.71	0.54
1:5:95:TRP:HE3	1:5:102:LEU:HD11	1.71	0.54
1:6:54:ALA:HB1	1:5:90:LEU:HA	1.88	0.54
1:y:95:TRP:HE3	1:y:102:LEU:HD11	1.71	0.54
1:2:54:ALA:HB1	1:1:90:LEU:HA	1.89	0.54
1:Y:54:ALA:HB1	1:x:90:LEU:HA	1.88	0.54
1:0:147:ASP:OD1	1:0:148:LYS:N	2.36	0.54
1:6:51:ARG:HH11	2:U:358:MET:HE3	1.72	0.54
1:4:88:THR:HG23	1:4:93:LEU:HB2	1.90	0.54
1:Z:147:ASP:OD1	1:Z:148:LYS:N	2.36	0.54
2:B:350:LEU:HD23	2:B:356:TYR:CE2	2.43	0.54
1:9:47:SER:HG	1:9:51:ARG:HH12	1.55	0.53
1:2:147:ASP:OD1	1:2:148:LYS:N	2.36	0.53
2:T:350:LEU:HD23	2:T:356:TYR:CE2	2.43	0.53
1:0:72:SER:O	2:N:365:PHE:HA	2.07	0.53
1:6:147:ASP:OD1	1:6:148:LYS:N	2.36	0.53
1:8:88:THR:HG23	1:8:93:LEU:HB2	1.90	0.53
2:G:352:SER:OG	2:G:353:LYS:N	2.42	0.53
1:4:147:ASP:OD1	1:4:148:LYS:N	2.36	0.53
1:x:51:ARG:HD3	2:E:358:MET:HE3	1.89	0.53
2:D:352:SER:OG	2:D:353:LYS:N	2.42	0.53
2:H:350:LEU:HD23	2:H:356:TYR:CE2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:90:LEU:HA	1:5:54:ALA:HB1	1.90	0.53
1:8:51:ARG:HD3	2:A:358:MET:HE3	1.90	0.53
2:E:350:LEU:HD23	2:E:356:TYR:CE2	2.43	0.53
1:Y:147:ASP:OD1	1:Y:148:LYS:N	2.36	0.53
2:K:350:LEU:HD23	2:K:356:TYR:CE2	2.43	0.53
2:V:350:LEU:HD23	2:V:356:TYR:CE2	2.43	0.53
1:2:38:TYR:HB2	2:P:350:LEU:HD13	1.91	0.53
1:8:106:ASP:OD1	1:8:107:SER:N	2.43	0.53
1:0:88:THR:HG23	1:0:93:LEU:HB2	1.90	0.52
1:4:54:ALA:HB1	1:3:90:LEU:HA	1.90	0.52
1:7:71:ILE:HG22	2:A:364:TRP:HB2	1.90	0.52
2:S:352:SER:OG	2:S:353:LYS:N	2.42	0.52
1:X:118:GLU:O	1:X:148:LYS:NZ	2.38	0.52
1:Z:106:ASP:OD1	1:Z:107:SER:N	2.43	0.52
2:M:352:SER:OG	2:M:353:LYS:N	2.42	0.52
2:K:358:MET:HE1	2:K:364:TRP:CE2	2.45	0.52
2:N:358:MET:HE1	2:N:364:TRP:CE2	2.45	0.52
1:Z:88:THR:HG23	1:Z:93:LEU:HB2	1.90	0.52
2:A:352:SER:OG	2:A:353:LYS:N	2.42	0.52
2:U:352:SER:OG	2:U:353:LYS:N	2.42	0.52
2:N:350:LEU:HD23	2:N:356:TYR:CE2	2.43	0.52
2:Q:350:LEU:HD23	2:Q:356:TYR:CE2	2.43	0.52
1:Y:88:THR:HG23	1:Y:93:LEU:HB2	1.90	0.52
1:6:88:THR:HG23	1:6:93:LEU:HB2	1.90	0.52
1:6:106:ASP:OD1	1:6:107:SER:N	2.43	0.52
1:2:88:THR:HG23	1:2:93:LEU:HB2	1.90	0.52
1:X:106:ASP:OD1	1:X:107:SER:N	2.43	0.52
2:P:352:SER:OG	2:P:353:LYS:N	2.42	0.52
2:Q:358:MET:HE1	2:Q:364:TRP:CE2	2.44	0.52
1:Y:51:ARG:HD3	2:G:358:MET:HE3	1.91	0.52
1:Y:106:ASP:OD1	1:Y:107:SER:N	2.43	0.52
2:H:358:MET:HE1	2:H:364:TRP:CE2	2.45	0.52
1:4:106:ASP:OD1	1:4:107:SER:N	2.43	0.52
1:3:48:PHE:CG	1:3:71:ILE:HD11	2.46	0.52
2:M:352:SER:O	2:M:355:SER:OG	2.28	0.52
1:X:88:THR:HG23	1:X:93:LEU:HB2	1.90	0.51
1:0:106:ASP:OD1	1:0:107:SER:N	2.43	0.51
2:D:352:SER:O	2:D:355:SER:OG	2.28	0.51
1:2:106:ASP:OD1	1:2:107:SER:N	2.43	0.51
1:x:48:PHE:CG	1:x:71:ILE:HD11	2.46	0.51
1:7:48:PHE:CG	1:7:71:ILE:HD11	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:51:ARG:HH11	2:G:358:MET:HE3	1.76	0.51
1:4:171:LYS:NZ	1:3:147:ASP:OD1	2.42	0.51
1:z:48:PHE:CG	1:z:71:ILE:HD11	2.46	0.51
1:z:51:ARG:NH1	2:K:358:MET:HE3	2.25	0.51
2:G:352:SER:O	2:G:355:SER:OG	2.29	0.51
2:P:352:SER:O	2:P:355:SER:OG	2.28	0.51
2:T:358:MET:HE1	2:T:364:TRP:CE2	2.45	0.51
1:4:51:ARG:HH11	2:S:358:MET:HE3	1.76	0.51
1:X:147:ASP:OD1	1:X:148:LYS:N	2.36	0.51
2:P:359:LEU:O	2:P:363:HIS:HB3	2.11	0.51
2:E:358:MET:HE1	2:E:364:TRP:CE2	2.44	0.51
1:X:51:ARG:HH11	2:D:358:MET:HE3	1.76	0.51
1:Z:90:LEU:HA	1:z:54:ALA:HB1	1.92	0.51
1:y:48:PHE:CG	1:y:71:ILE:HD11	2.46	0.51
2:V:358:MET:HE1	2:V:364:TRP:CE2	2.45	0.51
1:8:51:ARG:HH11	2:A:358:MET:HE3	1.76	0.51
1:9:48:PHE:CG	1:9:71:ILE:HD11	2.46	0.51
1:9:71:ILE:HG22	2:D:364:TRP:HB2	1.93	0.51
2:J:352:SER:O	2:J:355:SER:OG	2.28	0.51
2:J:359:LEU:O	2:J:363:HIS:HB3	2.11	0.51
2:P:352:SER:N	2:P:355:SER:OG	2.41	0.51
2:U:352:SER:N	2:U:355:SER:OG	2.41	0.51
2:B:358:MET:HE1	2:B:364:TRP:CE2	2.45	0.51
2:D:352:SER:N	2:D:355:SER:OG	2.41	0.51
2:S:352:SER:O	2:S:355:SER:OG	2.28	0.51
1:z:60:ILE:HG13	1:z:102:LEU:HB3	1.94	0.50
1:X:147:ASP:OD2	1:x:171:LYS:NZ	2.34	0.50
1:1:48:PHE:CG	1:1:71:ILE:HD11	2.46	0.50
1:5:48:PHE:CG	1:5:71:ILE:HD11	2.46	0.50
1:9:60:ILE:HG13	1:9:102:LEU:HB3	1.94	0.50
2:A:352:SER:O	2:A:355:SER:OG	2.29	0.50
1:Y:147:ASP:OD2	1:y:171:LYS:NZ	2.34	0.50
1:8:171:LYS:NZ	1:7:147:ASP:OD1	2.43	0.50
1:7:51:ARG:HH11	2:V:358:MET:HE3	1.76	0.50
2:S:359:LEU:O	2:S:363:HIS:HB3	2.11	0.50
2:G:359:LEU:O	2:G:363:HIS:HB3	2.11	0.50
2:M:359:LEU:O	2:M:363:HIS:HB3	2.11	0.50
1:0:90:LEU:HA	1:1:54:ALA:HB1	1.92	0.50
1:x:60:ILE:HG13	1:x:102:LEU:HB3	1.94	0.50
1:Y:44:THR:HG22	1:Y:46:GLY:H	1.77	0.50
2:U:352:SER:O	2:U:355:SER:OG	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:48:PHE:CD1	1:Z:71:ILE:HD11	2.47	0.50
1:Z:44:THR:HG22	1:Z:46:GLY:H	1.77	0.50
1:6:48:PHE:CD1	1:6:71:ILE:HD11	2.47	0.50
1:8:48:PHE:CD1	1:8:71:ILE:HD11	2.47	0.50
1:5:60:ILE:HG13	1:5:102:LEU:HB3	1.93	0.50
1:2:44:THR:HG22	1:2:46:GLY:H	1.77	0.50
1:4:39:VAL:HG13	1:4:74:GLU:HG2	1.94	0.50
1:4:44:THR:HG22	1:4:46:GLY:H	1.77	0.50
1:6:39:VAL:HG13	1:6:74:GLU:HG2	1.94	0.50
1:X:44:THR:HG22	1:X:46:GLY:H	1.77	0.49
1:Z:39:VAL:HG13	1:Z:74:GLU:HG2	1.94	0.49
1:2:48:PHE:CD1	1:2:71:ILE:HD11	2.47	0.49
1:4:147:ASP:OD2	1:5:171:LYS:NZ	2.27	0.49
1:6:44:THR:HG22	1:6:46:GLY:H	1.77	0.49
1:z:51:ARG:HH11	2:K:358:MET:HE3	1.77	0.49
1:X:48:PHE:CD1	1:X:71:ILE:HD11	2.47	0.49
1:Y:39:VAL:HG13	1:Y:74:GLU:HG2	1.94	0.49
1:Y:153:SER:HB3	1:y:100:ASN:HD21	1.77	0.49
1:0:39:VAL:HG13	1:0:74:GLU:HG2	1.94	0.49
1:0:48:PHE:CD1	1:0:71:ILE:HD11	2.47	0.49
1:4:48:PHE:CD1	1:4:71:ILE:HD11	2.47	0.49
1:y:60:ILE:HG13	1:y:102:LEU:HB3	1.94	0.49
2:D:359:LEU:O	2:D:363:HIS:HB3	2.11	0.49
1:X:153:SER:HB3	1:x:100:ASN:HD21	1.76	0.49
2:A:359:LEU:O	2:A:363:HIS:HB3	2.11	0.49
1:X:39:VAL:HG13	1:X:74:GLU:HG2	1.94	0.49
1:0:44:THR:HG22	1:0:46:GLY:H	1.77	0.49
1:2:39:VAL:HG13	1:2:74:GLU:HG2	1.94	0.49
1:7:60:ILE:HG13	1:7:102:LEU:HB3	1.93	0.49
2:G:352:SER:N	2:G:355:SER:OG	2.41	0.49
2:J:352:SER:OG	2:J:353:LYS:N	2.42	0.49
1:3:60:ILE:HG13	1:3:102:LEU:HB3	1.94	0.49
2:U:359:LEU:O	2:U:363:HIS:HB3	2.11	0.49
1:Y:48:PHE:CD1	1:Y:71:ILE:HD11	2.47	0.49
1:8:39:VAL:HG13	1:8:74:GLU:HG2	1.94	0.49
1:x:71:ILE:HG22	2:G:364:TRP:HB2	1.93	0.49
1:4:72:SER:O	2:T:365:PHE:HA	2.13	0.49
1:1:71:ILE:HG22	2:P:364:TRP:HB2	1.95	0.49
1:1:60:ILE:HG13	1:1:102:LEU:HB3	1.94	0.49
1:3:120:ILE:HG23	1:3:124:TYR:HB3	1.95	0.49
1:9:51:ARG:HD3	2:B:358:MET:HE3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:44:THR:HG22	1:8:46:GLY:H	1.77	0.48
1:5:71:ILE:HG22	2:U:364:TRP:HB2	1.95	0.48
1:9:129:LEU:HB3	1:9:135:TYR:HB2	1.95	0.48
1:x:37:LYS:O	2:E:350:LEU:HD12	2.13	0.48
1:x:129:LEU:HB3	1:x:135:TYR:HB2	1.95	0.48
1:z:71:ILE:HG22	2:M:364:TRP:HB2	1.94	0.48
1:1:120:ILE:HG23	1:1:124:TYR:HB3	1.95	0.48
1:5:120:ILE:HG23	1:5:124:TYR:HB3	1.95	0.48
1:7:51:ARG:NH1	2:V:358:MET:HE3	2.28	0.48
2:E:352:SER:OG	2:E:353:LYS:N	2.46	0.48
1:4:51:ARG:HD3	2:S:358:MET:HE3	1.95	0.48
1:8:90:LEU:HA	1:9:54:ALA:HB1	1.95	0.48
1:Z:45:VAL:HG13	1:Z:49:PHE:CD2	2.49	0.48
1:4:118:GLU:O	1:4:148:LYS:NZ	2.38	0.48
1:y:115:ILE:HB	1:y:150:PHE:CZ	2.49	0.48
1:7:129:LEU:HB3	1:7:135:TYR:HB2	1.95	0.48
2:H:352:SER:OG	2:H:353:LYS:N	2.46	0.48
1:8:147:ASP:OD1	1:8:148:LYS:N	2.36	0.48
1:8:153:SER:HB3	1:9:100:ASN:HD21	1.78	0.48
1:7:120:ILE:HG23	1:7:124:TYR:HB3	1.95	0.48
2:B:352:SER:OG	2:B:353:LYS:N	2.46	0.48
2:K:352:SER:OG	2:K:353:LYS:N	2.46	0.48
1:X:45:VAL:HG13	1:X:49:PHE:CD2	2.49	0.48
1:4:45:VAL:HG13	1:4:49:PHE:CD2	2.49	0.48
1:6:45:VAL:HG13	1:6:49:PHE:CD2	2.49	0.48
1:y:129:LEU:HB3	1:y:135:TYR:HB2	1.95	0.48
1:z:115:ILE:HB	1:z:150:PHE:CZ	2.49	0.48
1:3:129:LEU:HB3	1:3:135:TYR:HB2	1.95	0.48
1:9:51:ARG:HH11	2:B:358:MET:HE3	1.79	0.48
2:G:350:LEU:HD23	2:G:356:TYR:CE2	2.49	0.48
2:N:352:SER:OG	2:N:353:LYS:N	2.46	0.48
1:Z:39:VAL:HG22	1:Z:74:GLU:HG2	1.96	0.48
1:0:51:ARG:HH11	2:M:358:MET:HE3	1.79	0.48
1:6:118:GLU:O	1:6:148:LYS:NZ	2.38	0.48
1:8:45:VAL:HG13	1:8:49:PHE:CD2	2.49	0.48
1:x:82:GLU:OE1	1:x:82:GLU:N	2.45	0.48
1:3:115:ILE:HB	1:3:150:PHE:CZ	2.49	0.48
2:V:352:SER:OG	2:V:353:LYS:N	2.46	0.48
1:Y:45:VAL:HG13	1:Y:49:PHE:CD2	2.49	0.48
1:2:45:VAL:HG13	1:2:49:PHE:CD2	2.49	0.48
1:6:51:ARG:NH1	2:U:358:MET:HE3	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:LEU:HD23	2:A:356:TYR:CE2	2.49	0.48
2:D:350:LEU:HD23	2:D:356:TYR:CE2	2.49	0.48
2:S:350:LEU:HD23	2:S:356:TYR:CE2	2.49	0.48
1:y:72:SER:O	2:J:365:PHE:HA	2.13	0.48
2:J:350:LEU:HD23	2:J:356:TYR:CE2	2.49	0.48
2:Q:352:SER:OG	2:Q:353:LYS:N	2.46	0.48
1:0:39:VAL:HG22	1:0:74:GLU:HG2	1.96	0.47
1:x:115:ILE:HB	1:x:150:PHE:CZ	2.49	0.47
1:5:115:ILE:HB	1:5:150:PHE:CZ	2.49	0.47
1:9:120:ILE:HG23	1:9:124:TYR:HB3	1.95	0.47
2:M:350:LEU:HD23	2:M:356:TYR:CE2	2.49	0.47
2:P:350:LEU:HD23	2:P:356:TYR:CE2	2.49	0.47
1:0:51:ARG:HD3	2:M:358:MET:HE3	1.96	0.47
1:9:115:ILE:HB	1:9:150:PHE:CZ	2.49	0.47
2:S:352:SER:N	2:S:355:SER:OG	2.41	0.47
2:T:352:SER:OG	2:T:353:LYS:N	2.46	0.47
1:Y:39:VAL:HG22	1:Y:74:GLU:HG2	1.96	0.47
1:0:45:VAL:HG13	1:0:49:PHE:CD2	2.49	0.47
1:2:118:GLU:O	1:2:148:LYS:NZ	2.38	0.47
1:8:147:ASP:OD2	1:9:171:LYS:NZ	2.29	0.47
1:x:41:GLN:HG3	2:E:346:GLY:O	2.14	0.47
1:y:164:ASN:O	1:y:168:LEU:HB2	2.15	0.47
1:1:129:LEU:HB3	1:1:135:TYR:HB2	1.95	0.47
2:G:350:LEU:HD23	2:G:356:TYR:HE2	1.80	0.47
2:U:350:LEU:HD23	2:U:356:TYR:CE2	2.49	0.47
1:X:41:GLN:HG3	2:D:346:GLY:HA2	1.96	0.47
1:X:90:LEU:HA	1:x:54:ALA:HB1	1.96	0.47
1:z:120:ILE:HG23	1:z:124:TYR:HB3	1.96	0.47
1:5:129:LEU:HB3	1:5:135:TYR:HB2	1.95	0.47
1:2:39:VAL:HG22	1:2:74:GLU:HG2	1.96	0.47
1:x:164:ASN:O	1:x:168:LEU:HB2	2.15	0.47
1:7:115:ILE:HB	1:7:150:PHE:CZ	2.49	0.47
1:x:120:ILE:HG23	1:x:124:TYR:HB3	1.95	0.47
1:y:120:ILE:HG23	1:y:124:TYR:HB3	1.95	0.47
1:1:115:ILE:HB	1:1:150:PHE:CZ	2.49	0.47
1:5:164:ASN:O	1:5:168:LEU:HB2	2.15	0.47
1:7:164:ASN:O	1:7:168:LEU:HB2	2.15	0.47
2:A:350:LEU:HD23	2:A:356:TYR:HE2	1.80	0.47
2:U:350:LEU:HD23	2:U:356:TYR:HE2	1.80	0.47
1:X:39:VAL:HG22	1:X:74:GLU:HG2	1.96	0.47
1:5:82:GLU:OE1	1:5:82:GLU:N	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:164:ASN:O	1:9:168:LEU:HB2	2.15	0.47
2:J:350:LEU:HD23	2:J:356:TYR:HE2	1.80	0.47
2:P:358:MET:HB2	2:P:358:MET:HE2	1.53	0.47
1:y:51:ARG:HH11	2:H:358:MET:HE3	1.79	0.47
1:z:164:ASN:O	1:z:168:LEU:HB2	2.15	0.47
1:5:139:TYR:HB3	1:5:153:SER:O	2.15	0.47
2:A:352:SER:N	2:A:355:SER:OG	2.41	0.47
2:D:350:LEU:HD23	2:D:356:TYR:HE2	1.80	0.47
1:z:129:LEU:HB3	1:z:135:TYR:HB2	1.95	0.47
2:J:352:SER:N	2:J:355:SER:OG	2.41	0.47
1:Y:90:LEU:HA	1:y:54:ALA:HB1	1.96	0.47
1:4:39:VAL:HG22	1:4:74:GLU:HG2	1.96	0.46
1:y:82:GLU:OE1	1:y:82:GLU:N	2.45	0.46
1:6:39:VAL:HG22	1:6:74:GLU:HG2	1.96	0.46
1:x:35:ILE:HG23	1:x:36:ALA:H	1.80	0.46
1:y:51:ARG:NH1	2:H:358:MET:HE3	2.31	0.46
1:1:164:ASN:O	1:1:168:LEU:HB2	2.15	0.46
1:9:139:TYR:HB3	1:9:153:SER:O	2.15	0.46
1:9:169:LEU:HA	1:9:169:LEU:HD23	1.62	0.46
2:M:350:LEU:HD23	2:M:356:TYR:HE2	1.80	0.46
2:K:358:MET:HE2	2:K:358:MET:HB2	1.60	0.46
1:x:139:TYR:HB3	1:x:153:SER:O	2.15	0.46
1:y:139:TYR:HB3	1:y:153:SER:O	2.15	0.46
1:7:35:ILE:HG23	1:7:36:ALA:H	1.81	0.46
1:9:35:ILE:HG23	1:9:36:ALA:H	1.80	0.46
1:8:39:VAL:HG22	1:8:74:GLU:HG2	1.96	0.46
1:1:139:TYR:HB3	1:1:153:SER:O	2.15	0.46
1:3:164:ASN:O	1:3:168:LEU:HB2	2.15	0.46
2:P:350:LEU:HD23	2:P:356:TYR:HE2	1.80	0.46
2:J:338:LEU:HD23	2:J:338:LEU:HA	1.77	0.46
1:0:54:ALA:HB1	1:z:90:LEU:HA	1.98	0.46
1:x:51:ARG:NH1	2:E:358:MET:HE3	2.31	0.46
1:z:35:ILE:HG23	1:z:36:ALA:H	1.81	0.46
1:z:169:LEU:HD23	1:z:169:LEU:HA	1.62	0.46
1:7:139:TYR:HB3	1:7:153:SER:O	2.15	0.46
1:Z:171:LYS:HB2	1:Z:171:LYS:HE3	1.58	0.46
1:0:171:LYS:HB2	1:0:171:LYS:HE3	1.58	0.46
1:7:169:LEU:HD23	1:7:169:LEU:HA	1.62	0.46
2:P:338:LEU:HD23	2:P:338:LEU:HA	1.77	0.46
1:z:139:TYR:HB3	1:z:153:SER:O	2.15	0.46
1:1:35:ILE:HG23	1:1:36:ALA:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:118:GLU:O	1:0:148:LYS:NZ	2.38	0.46
1:4:54:ALA:HB1	1:3:90:LEU:HD23	1.98	0.46
1:3:139:TYR:HB3	1:3:153:SER:O	2.15	0.46
1:7:82:GLU:OE1	1:7:82:GLU:N	2.45	0.46
1:Y:171:LYS:NZ	1:x:147:ASP:OD1	2.49	0.45
1:y:51:ARG:HD3	2:H:358:MET:HE3	1.98	0.45
1:5:35:ILE:HG23	1:5:36:ALA:H	1.81	0.45
1:Z:171:LYS:NZ	1:y:147:ASP:OD1	2.46	0.45
2:S:350:LEU:HD23	2:S:356:TYR:HE2	1.80	0.45
1:Z:146:SER:OG	1:Z:147:ASP:N	2.50	0.45
1:0:146:SER:OG	1:0:147:ASP:N	2.50	0.45
1:2:90:LEU:HA	1:3:54:ALA:HB1	1.98	0.45
1:2:146:SER:OG	1:2:147:ASP:N	2.50	0.45
1:6:90:LEU:HA	1:7:54:ALA:HB1	1.99	0.45
1:x:51:ARG:HH11	2:E:358:MET:HE3	1.81	0.45
1:3:51:ARG:HH11	2:Q:358:MET:HE3	1.81	0.45
2:M:338:LEU:HD23	2:M:338:LEU:HA	1.77	0.45
1:4:146:SER:OG	1:4:147:ASP:N	2.50	0.45
1:x:52:PHE:HZ	1:x:83:MET:HB3	1.82	0.45
1:y:52:PHE:HZ	1:y:83:MET:HB3	1.82	0.45
2:S:358:MET:HE2	2:S:358:MET:HB2	1.54	0.45
2:H:358:MET:HB2	2:H:358:MET:HE2	1.60	0.45
2:V:339:LEU:HD23	2:V:339:LEU:HA	1.80	0.45
1:Y:146:SER:OG	1:Y:147:ASP:N	2.50	0.45
1:z:82:GLU:OE1	1:z:82:GLU:N	2.45	0.45
1:9:51:ARG:NH1	2:B:358:MET:HE3	2.31	0.45
1:9:52:PHE:HZ	1:9:83:MET:HB3	1.82	0.45
1:2:51:ARG:HH11	2:P:358:MET:HE3	1.81	0.45
1:X:146:SER:OG	1:X:147:ASP:N	2.50	0.45
1:8:146:SER:OG	1:8:147:ASP:N	2.50	0.45
1:y:35:ILE:HG23	1:y:36:ALA:H	1.80	0.45
2:B:341:ASP:OD1	2:B:341:ASP:N	2.49	0.45
1:3:35:ILE:HG23	1:3:36:ALA:H	1.80	0.45
1:Y:171:LYS:HB2	1:Y:171:LYS:HE3	1.58	0.45
1:z:52:PHE:HZ	1:z:83:MET:HB3	1.82	0.45
1:5:51:ARG:HD3	2:T:358:MET:HE3	1.99	0.45
1:4:171:LYS:HB2	1:4:171:LYS:HE3	1.58	0.44
2:D:358:MET:HB2	2:D:358:MET:HE2	1.54	0.44
2:U:358:MET:HB2	2:U:358:MET:HE2	1.54	0.44
2:Q:358:MET:HB2	2:Q:358:MET:HE2	1.60	0.44
1:0:153:SER:HB3	1:1:100:ASN:HD21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:52:PHE:HZ	1:7:83:MET:HB3	1.82	0.44
2:S:362:LYS:HD3	2:S:362:LYS:HA	1.85	0.44
1:X:84:LEU:HD21	1:X:102:LEU:HD21	1.99	0.44
2:B:358:MET:HB2	2:B:358:MET:HE2	1.60	0.44
2:N:339:LEU:HD23	2:N:339:LEU:HA	1.80	0.44
1:Z:51:ARG:HD3	2:J:358:MET:HE3	1.99	0.44
1:6:171:LYS:HB2	1:6:171:LYS:HE3	1.58	0.44
1:5:169:LEU:HD23	1:5:169:LEU:HA	1.62	0.44
2:M:352:SER:N	2:M:355:SER:OG	2.41	0.44
1:Y:84:LEU:HD21	1:Y:102:LEU:HD21	2.00	0.44
1:2:84:LEU:HD21	1:2:102:LEU:HD21	2.00	0.44
2:K:339:LEU:HD23	2:K:339:LEU:HA	1.80	0.44
1:4:153:SER:HB3	1:5:100:ASN:HD21	1.83	0.44
1:8:53:SER:HB3	1:8:60:ILE:HB	2.00	0.44
1:1:52:PHE:HZ	1:1:83:MET:HB3	1.82	0.44
1:1:82:GLU:OE1	1:1:82:GLU:N	2.45	0.44
1:2:53:SER:HB3	1:2:60:ILE:HB	2.00	0.43
1:2:153:SER:HB3	1:3:100:ASN:HD21	1.83	0.43
1:5:52:PHE:HZ	1:5:83:MET:HB3	1.82	0.43
1:0:53:SER:HB3	1:0:60:ILE:HB	2.00	0.43
2:Q:339:LEU:HD23	2:Q:339:LEU:HA	1.80	0.43
2:V:358:MET:HE2	2:V:358:MET:HB2	1.60	0.43
1:X:53:SER:HB3	1:X:60:ILE:HB	2.00	0.43
1:Y:51:ARG:NH1	2:G:358:MET:HE3	2.33	0.43
1:4:84:LEU:HD21	1:4:102:LEU:HD21	1.99	0.43
1:3:51:ARG:NH1	2:Q:358:MET:HE3	2.33	0.43
1:6:53:SER:HB3	1:6:60:ILE:HB	2.01	0.43
1:8:54:ALA:HB1	1:7:90:LEU:HD23	2.01	0.43
1:3:52:PHE:HZ	1:3:83:MET:HB3	1.82	0.43
2:E:358:MET:HB2	2:E:358:MET:HE2	1.60	0.43
1:4:53:SER:HB3	1:4:60:ILE:HB	2.00	0.43
2:J:360:ASN:OD1	2:J:360:ASN:N	2.52	0.43
1:6:146:SER:OG	1:6:147:ASP:N	2.50	0.43
1:6:169:LEU:HD23	1:6:169:LEU:HA	1.84	0.43
2:K:360:ASN:C	2:K:362:LYS:H	2.27	0.43
1:Y:41:GLN:HG3	2:G:346:GLY:HA2	2.01	0.43
1:0:84:LEU:HD21	1:0:102:LEU:HD21	2.00	0.43
1:x:169:LEU:HD23	1:x:169:LEU:HA	1.62	0.43
1:y:169:LEU:HD23	1:y:169:LEU:HA	1.62	0.43
1:3:82:GLU:OE1	1:3:82:GLU:N	2.45	0.43
1:Y:45:VAL:HG13	1:Y:49:PHE:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:53:SER:HB3	1:Y:60:ILE:HB	2.00	0.43
1:6:84:LEU:HD21	1:6:102:LEU:HD21	1.99	0.43
1:z:48:PHE:CD1	1:z:71:ILE:HD11	2.54	0.43
1:9:82:GLU:OE1	1:9:82:GLU:N	2.45	0.43
2:M:360:ASN:OD1	2:M:360:ASN:N	2.52	0.43
2:U:360:ASN:OD1	2:U:360:ASN:N	2.52	0.43
2:H:360:ASN:C	2:H:362:LYS:H	2.26	0.43
1:Z:53:SER:HB3	1:Z:60:ILE:HB	2.00	0.43
1:4:97:LYS:HG3	1:4:102:LEU:HD13	2.01	0.43
1:8:72:SER:O	2:B:365:PHE:HA	2.19	0.43
1:3:171:LYS:HD3	1:3:171:LYS:N	2.34	0.43
2:G:358:MET:HB2	2:G:358:MET:HE2	1.54	0.43
2:B:360:ASN:C	2:B:362:LYS:H	2.27	0.43
1:Z:35:ILE:HG23	1:Z:36:ALA:H	1.84	0.43
1:Z:118:GLU:O	1:Z:148:LYS:NZ	2.38	0.43
1:2:35:ILE:HG23	1:2:36:ALA:H	1.84	0.43
1:7:171:LYS:HD3	1:7:171:LYS:N	2.34	0.43
2:H:339:LEU:HD23	2:H:339:LEU:HA	1.80	0.43
1:Y:35:ILE:HG23	1:Y:36:ALA:H	1.84	0.42
1:0:38:TYR:CE2	1:0:40:ALA:HB2	2.55	0.42
1:0:45:VAL:HG13	1:0:49:PHE:HD2	1.84	0.42
1:4:35:ILE:HG23	1:4:36:ALA:H	1.84	0.42
1:4:45:VAL:HG13	1:4:49:PHE:HD2	1.84	0.42
1:8:84:LEU:HD21	1:8:102:LEU:HD21	2.00	0.42
1:X:38:TYR:CE2	1:X:40:ALA:HB2	2.54	0.42
1:X:171:LYS:HE3	1:X:171:LYS:HB2	1.58	0.42
1:2:38:TYR:CE2	1:2:40:ALA:HB2	2.55	0.42
1:6:153:SER:HB3	1:7:100:ASN:HD21	1.83	0.42
1:x:48:PHE:CD1	1:x:71:ILE:HD11	2.54	0.42
1:y:70:ARG:O	2:J:363:HIS:HA	2.19	0.42
2:M:362:LYS:HD3	2:M:362:LYS:HA	1.85	0.42
2:T:360:ASN:C	2:T:362:LYS:H	2.27	0.42
1:2:171:LYS:HB2	1:2:171:LYS:HE3	1.58	0.42
1:8:38:TYR:CE2	1:8:40:ALA:HB2	2.55	0.42
1:5:48:PHE:CD1	1:5:71:ILE:HD11	2.54	0.42
2:D:360:ASN:OD1	2:D:360:ASN:N	2.52	0.42
2:J:358:MET:HB2	2:J:358:MET:HE2	1.54	0.42
1:Y:38:TYR:CE2	1:Y:40:ALA:HB2	2.55	0.42
1:Z:84:LEU:HD21	1:Z:102:LEU:HD21	2.00	0.42
1:4:38:TYR:CE2	1:4:40:ALA:HB2	2.54	0.42
1:4:41:GLN:HG3	2:S:346:GLY:HA2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:129:LEU:HD23	1:8:129:LEU:HA	1.84	0.42
1:8:171:LYS:HE3	1:8:171:LYS:HB2	1.58	0.42
1:1:48:PHE:CD1	1:1:71:ILE:HD11	2.54	0.42
2:N:360:ASN:C	2:N:362:LYS:H	2.26	0.42
1:Y:97:LYS:HG3	1:Y:102:LEU:HD13	2.01	0.42
1:6:38:TYR:CE2	1:6:40:ALA:HB2	2.55	0.42
1:8:138:ARG:C	1:8:140:PRO:HD3	2.45	0.42
1:z:171:LYS:HD3	1:z:171:LYS:N	2.34	0.42
1:3:48:PHE:CD1	1:3:71:ILE:HD11	2.54	0.42
1:9:48:PHE:CD1	1:9:71:ILE:HD11	2.54	0.42
1:9:53:SER:O	1:9:56:LEU:N	2.53	0.42
2:E:360:ASN:C	2:E:362:LYS:H	2.27	0.42
1:Z:97:LYS:HG3	1:Z:102:LEU:HD13	2.01	0.42
1:6:97:LYS:HG3	1:6:102:LEU:HD13	2.01	0.42
1:6:138:ARG:C	1:6:140:PRO:HD3	2.45	0.42
1:8:51:ARG:NH1	2:A:358:MET:HE3	2.34	0.42
1:x:53:SER:O	1:x:56:LEU:N	2.53	0.42
1:y:48:PHE:CD1	1:y:71:ILE:HD11	2.54	0.42
1:8:35:ILE:HG23	1:8:36:ALA:H	1.84	0.42
1:7:48:PHE:CD1	1:7:71:ILE:HD11	2.54	0.42
1:7:53:SER:O	1:7:56:LEU:N	2.53	0.42
1:Y:118:GLU:O	1:Y:148:LYS:NZ	2.38	0.42
1:Z:38:TYR:CE2	1:Z:40:ALA:HB2	2.55	0.42
1:0:35:ILE:HG23	1:0:36:ALA:H	1.84	0.42
1:2:45:VAL:HG13	1:2:49:PHE:HD2	1.84	0.42
1:x:171:LYS:N	1:x:171:LYS:HD3	2.34	0.42
1:z:53:SER:O	1:z:56:LEU:N	2.53	0.42
1:1:53:SER:O	1:1:56:LEU:N	2.53	0.42
1:7:51:ARG:HD3	2:V:358:MET:HE3	2.02	0.42
1:7:120:ILE:HD12	1:7:169:LEU:HB3	2.02	0.42
2:A:362:LYS:HA	2:A:362:LYS:HD3	1.85	0.42
1:2:51:ARG:NH1	2:P:358:MET:HE3	2.35	0.42
1:4:53:SER:O	1:4:56:LEU:N	2.53	0.42
1:6:35:ILE:HG23	1:6:36:ALA:H	1.84	0.42
1:9:120:ILE:HD12	1:9:169:LEU:HB3	2.02	0.42
1:9:171:LYS:HD3	1:9:171:LYS:N	2.34	0.42
1:X:97:LYS:HG3	1:X:102:LEU:HD13	2.01	0.42
1:Z:45:VAL:HG13	1:Z:49:PHE:HD2	1.84	0.42
1:4:38:TYR:HH	1:4:51:ARG:HH21	1.61	0.42
1:5:171:LYS:HD3	1:5:171:LYS:N	2.34	0.42
2:U:362:LYS:HD3	2:U:362:LYS:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:360:ASN:C	2:Q:362:LYS:H	2.27	0.42
1:X:87:LEU:O	1:X:91:VAL:HG23	2.20	0.41
1:X:138:ARG:C	1:X:140:PRO:HD3	2.45	0.41
1:O:53:SER:O	1:O:56:LEU:N	2.53	0.41
1:2:116:LEU:HD13	1:2:149:THR:OG1	2.20	0.41
1:y:171:LYS:HD3	1:y:171:LYS:N	2.34	0.41
1:5:120:ILE:HD12	1:5:169:LEU:HB3	2.02	0.41
2:G:360:ASN:OD1	2:G:360:ASN:N	2.52	0.41
2:P:360:ASN:OD1	2:P:360:ASN:N	2.52	0.41
1:X:45:VAL:HG13	1:X:49:PHE:HD2	1.84	0.41
1:8:87:LEU:O	1:8:91:VAL:HG23	2.20	0.41
1:y:120:ILE:HD12	1:y:169:LEU:HB3	2.02	0.41
1:3:120:ILE:HD12	1:3:169:LEU:HB3	2.02	0.41
2:D:359:LEU:HD12	2:D:363:HIS:HB3	2.03	0.41
2:J:353:LYS:H	2:J:353:LYS:HG2	1.68	0.41
2:V:360:ASN:C	2:V:362:LYS:H	2.27	0.41
1:2:53:SER:O	1:2:56:LEU:N	2.53	0.41
1:4:87:LEU:O	1:4:91:VAL:HG23	2.21	0.41
1:4:138:ARG:C	1:4:140:PRO:HD3	2.45	0.41
1:8:45:VAL:HG13	1:8:49:PHE:HD2	1.84	0.41
1:x:120:ILE:HD12	1:x:169:LEU:HB3	2.02	0.41
1:y:53:SER:O	1:y:56:LEU:N	2.53	0.41
1:5:53:SER:O	1:5:56:LEU:N	2.53	0.41
2:G:338:LEU:HD23	2:G:338:LEU:HA	1.77	0.41
1:X:35:ILE:HG23	1:X:36:ALA:H	1.84	0.41
1:Z:116:LEU:HD13	1:Z:149:THR:OG1	2.21	0.41
1:O:97:LYS:HG3	1:O:102:LEU:HD13	2.01	0.41
1:6:45:VAL:HG13	1:6:49:PHE:HD2	1.84	0.41
1:6:53:SER:O	1:6:56:LEU:N	2.53	0.41
1:8:116:LEU:HD13	1:8:149:THR:OG1	2.20	0.41
1:z:120:ILE:HD12	1:z:169:LEU:HB3	2.02	0.41
1:1:171:LYS:HD3	1:1:171:LYS:N	2.34	0.41
2:J:359:LEU:HD12	2:J:363:HIS:HB3	2.03	0.41
2:N:358:MET:HE2	2:N:358:MET:HB2	1.60	0.41
1:2:97:LYS:HG3	1:2:102:LEU:HD13	2.01	0.41
1:1:120:ILE:HD12	1:1:169:LEU:HB3	2.02	0.41
1:3:53:SER:O	1:3:56:LEU:N	2.53	0.41
1:X:82:GLU:CD	1:X:82:GLU:H	2.29	0.41
1:X:116:LEU:HD13	1:X:149:THR:OG1	2.20	0.41
1:6:116:LEU:HD13	1:6:149:THR:OG1	2.20	0.41
1:8:97:LYS:HG3	1:8:102:LEU:HD13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:LEU:HA	2:A:338:LEU:HD23	1.77	0.41
2:A:360:ASN:OD1	2:A:360:ASN:N	2.52	0.41
1:X:53:SER:O	1:X:56:LEU:N	2.53	0.41
1:Z:53:SER:O	1:Z:56:LEU:N	2.53	0.41
1:0:138:ARG:C	1:0:140:PRO:HD3	2.45	0.41
1:2:87:LEU:O	1:2:91:VAL:HG23	2.21	0.41
2:A:359:LEU:HD12	2:A:363:HIS:HB3	2.02	0.41
2:M:359:LEU:HD12	2:M:363:HIS:HB3	2.02	0.41
1:X:51:ARG:NH1	2:D:358:MET:HE3	2.34	0.41
1:Y:87:LEU:O	1:Y:91:VAL:HG23	2.20	0.41
1:Y:138:ARG:C	1:Y:140:PRO:HD3	2.45	0.41
1:Z:138:ARG:C	1:Z:140:PRO:HD3	2.45	0.41
1:0:82:GLU:H	1:0:82:GLU:CD	2.29	0.41
1:0:87:LEU:O	1:0:91:VAL:HG23	2.20	0.41
1:2:72:SER:O	2:Q:365:PHE:HA	2.21	0.41
1:2:82:GLU:H	1:2:82:GLU:CD	2.29	0.41
1:2:138:ARG:C	1:2:140:PRO:HD3	2.45	0.41
1:4:82:GLU:H	1:4:82:GLU:CD	2.29	0.41
1:6:38:TYR:HB2	2:U:350:LEU:HD13	2.03	0.41
1:6:87:LEU:O	1:6:91:VAL:HG23	2.21	0.41
2:D:362:LYS:HD3	2:D:362:LYS:HA	1.85	0.41
2:U:359:LEU:HD12	2:U:363:HIS:HB3	2.02	0.41
2:Q:356:TYR:HE1	2:Q:358:MET:HE2	1.86	0.41
2:V:356:TYR:HE1	2:V:358:MET:HE2	1.86	0.41
1:Y:116:LEU:HD13	1:Y:149:THR:OG1	2.20	0.41
1:4:116:LEU:HD13	1:4:149:THR:OG1	2.20	0.41
1:8:53:SER:O	1:8:56:LEU:N	2.53	0.41
2:K:356:TYR:HE1	2:K:358:MET:HE2	1.86	0.41
1:X:171:LYS:NZ	1:9:147:ASP:OD1	2.47	0.40
1:6:82:GLU:H	1:6:82:GLU:CD	2.29	0.40
2:G:359:LEU:HD12	2:G:363:HIS:HB3	2.02	0.40
2:S:338:LEU:HD23	2:S:338:LEU:HA	1.77	0.40
2:E:356:TYR:HE1	2:E:358:MET:HE2	1.86	0.40
2:T:339:LEU:HA	2:T:339:LEU:HD23	1.80	0.40
1:Z:82:GLU:CD	1:Z:82:GLU:H	2.29	0.40
1:Z:87:LEU:O	1:Z:91:VAL:HG23	2.21	0.40
1:2:129:LEU:HD23	1:2:129:LEU:HA	1.84	0.40
1:4:145:ILE:HD13	1:4:145:ILE:HA	1.93	0.40
1:3:169:LEU:HD23	1:3:169:LEU:HA	1.62	0.40
2:A:358:MET:HE2	2:A:358:MET:HB2	1.53	0.40
1:Y:82:GLU:CD	1:Y:82:GLU:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:78:SER:OG	1:5:79:ASN:OD1	2.39	0.40
2:A:342:ASP:OD1	2:A:342:ASP:N	2.55	0.40
2:D:342:ASP:OD1	2:D:342:ASP:N	2.55	0.40
2:P:342:ASP:O	2:P:344:PHE:N	2.55	0.40
2:P:359:LEU:HD12	2:P:363:HIS:HB3	2.03	0.40
2:S:360:ASN:OD1	2:S:360:ASN:N	2.52	0.40
1:0:116:LEU:HD13	1:0:149:THR:OG1	2.21	0.40
1:3:122:LEU:HD13	1:3:150:PHE:HB3	2.03	0.40
2:D:342:ASP:O	2:D:344:PHE:N	2.55	0.40
2:M:342:ASP:O	2:M:344:PHE:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	1	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	2	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	3	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	4	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	5	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	6	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	7	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	8	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	9	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	X	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	Y	136/566 (24%)	121 (89%)	15 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	x	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	y	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
1	z	136/566 (24%)	121 (89%)	15 (11%)	0	100	100
2	A	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	B	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	D	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	E	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	G	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	H	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	J	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	K	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	M	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	N	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	P	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	Q	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	S	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	T	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
2	U	28/371 (8%)	21 (75%)	7 (25%)	0	100	100
2	V	28/371 (8%)	25 (89%)	3 (11%)	0	100	100
All	All	2624/14992 (18%)	2304 (88%)	320 (12%)	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	0	121/513 (24%)	116 (96%)	5 (4%)	27	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	121/513 (24%)	112 (93%)	9 (7%)	13	39
1	2	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	3	121/513 (24%)	113 (93%)	8 (7%)	15	42
1	4	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	5	121/513 (24%)	113 (93%)	8 (7%)	15	42
1	6	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	7	121/513 (24%)	112 (93%)	9 (7%)	13	39
1	8	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	9	121/513 (24%)	113 (93%)	8 (7%)	15	42
1	X	121/513 (24%)	115 (95%)	6 (5%)	22	47
1	Y	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	Z	121/513 (24%)	116 (96%)	5 (4%)	27	51
1	x	121/513 (24%)	113 (93%)	8 (7%)	15	42
1	y	121/513 (24%)	112 (93%)	9 (7%)	13	39
1	z	121/513 (24%)	113 (93%)	8 (7%)	15	42
2	A	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	B	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	D	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	E	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	G	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	H	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	J	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	K	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	M	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	N	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	P	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	Q	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	S	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	T	29/342 (8%)	28 (97%)	1 (3%)	32	56
2	U	29/342 (8%)	26 (90%)	3 (10%)	7	26
2	V	29/342 (8%)	28 (97%)	1 (3%)	32	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2400/13680 (18%)	2260 (94%)	140 (6%)	20	45

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	35	ILE
1	X	45	VAL
1	X	117	LEU
1	X	120	ILE
1	X	123	ASN
1	X	131	ASP
1	Y	35	ILE
1	Y	45	VAL
1	Y	117	LEU
1	Y	120	ILE
1	Y	131	ASP
1	Z	35	ILE
1	Z	45	VAL
1	Z	117	LEU
1	Z	120	ILE
1	Z	131	ASP
1	0	35	ILE
1	0	45	VAL
1	0	117	LEU
1	0	120	ILE
1	0	131	ASP
1	2	35	ILE
1	2	45	VAL
1	2	117	LEU
1	2	120	ILE
1	2	131	ASP
1	4	35	ILE
1	4	45	VAL
1	4	117	LEU
1	4	120	ILE
1	4	131	ASP
1	6	35	ILE
1	6	45	VAL
1	6	117	LEU
1	6	120	ILE
1	6	131	ASP
1	8	35	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8	45	VAL
1	8	117	LEU
1	8	120	ILE
1	8	131	ASP
1	x	58	TYR
1	x	79	ASN
1	x	117	LEU
1	x	126	ILE
1	x	131	ASP
1	x	144	ASN
1	x	165	THR
1	x	171	LYS
1	y	58	TYR
1	y	79	ASN
1	y	117	LEU
1	y	126	ILE
1	y	131	ASP
1	y	144	ASN
1	y	165	THR
1	y	168	LEU
1	y	171	LYS
1	z	58	TYR
1	z	79	ASN
1	z	117	LEU
1	z	126	ILE
1	z	131	ASP
1	z	144	ASN
1	z	165	THR
1	z	171	LYS
1	1	58	TYR
1	1	79	ASN
1	1	117	LEU
1	1	126	ILE
1	1	131	ASP
1	1	144	ASN
1	1	165	THR
1	1	168	LEU
1	1	171	LYS
1	3	58	TYR
1	3	79	ASN
1	3	117	LEU
1	3	126	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	131	ASP
1	3	144	ASN
1	3	165	THR
1	3	171	LYS
1	5	58	TYR
1	5	79	ASN
1	5	117	LEU
1	5	126	ILE
1	5	131	ASP
1	5	144	ASN
1	5	165	THR
1	5	171	LYS
1	7	58	TYR
1	7	79	ASN
1	7	117	LEU
1	7	126	ILE
1	7	131	ASP
1	7	144	ASN
1	7	165	THR
1	7	168	LEU
1	7	171	LYS
1	9	58	TYR
1	9	79	ASN
1	9	117	LEU
1	9	126	ILE
1	9	131	ASP
1	9	144	ASN
1	9	165	THR
1	9	171	LYS
2	A	342	ASP
2	A	359	LEU
2	A	360	ASN
2	D	342	ASP
2	D	359	LEU
2	D	360	ASN
2	G	342	ASP
2	G	359	LEU
2	G	360	ASN
2	J	342	ASP
2	J	359	LEU
2	J	360	ASN
2	M	342	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	359	LEU
2	M	360	ASN
2	P	342	ASP
2	P	359	LEU
2	P	360	ASN
2	S	342	ASP
2	S	359	LEU
2	S	360	ASN
2	U	342	ASP
2	U	359	LEU
2	U	360	ASN
2	B	359	LEU
2	E	359	LEU
2	H	359	LEU
2	K	359	LEU
2	N	359	LEU
2	Q	359	LEU
2	T	359	LEU
2	V	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	65	GLN
1	X	137	HIS
1	Y	65	GLN
1	Y	137	HIS
1	Z	65	GLN
1	Z	137	HIS
1	0	65	GLN
1	0	137	HIS
1	2	65	GLN
1	2	137	HIS
1	4	65	GLN
1	4	137	HIS
1	6	65	GLN
1	6	137	HIS
1	8	65	GLN
1	8	137	HIS
1	x	65	GLN
1	x	100	ASN
1	x	144	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	y	65	GLN
1	y	100	ASN
1	y	144	ASN
1	z	65	GLN
1	z	144	ASN
1	1	65	GLN
1	1	100	ASN
1	1	144	ASN
1	3	65	GLN
1	3	100	ASN
1	3	144	ASN
1	5	65	GLN
1	5	100	ASN
1	5	144	ASN
1	7	65	GLN
1	7	100	ASN
1	7	144	ASN
1	9	65	GLN
1	9	100	ASN
1	9	144	ASN
2	A	351	ASN
2	D	351	ASN
2	G	351	ASN
2	J	351	ASN
2	M	351	ASN
2	B	351	ASN
2	E	351	ASN
2	H	351	ASN
2	K	351	ASN
2	N	351	ASN
2	Q	351	ASN
2	T	351	ASN
2	V	351	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 [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.

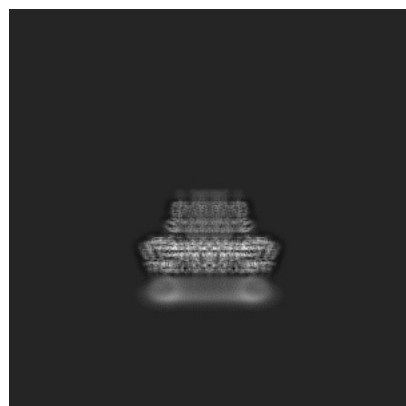
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10040. 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](#)

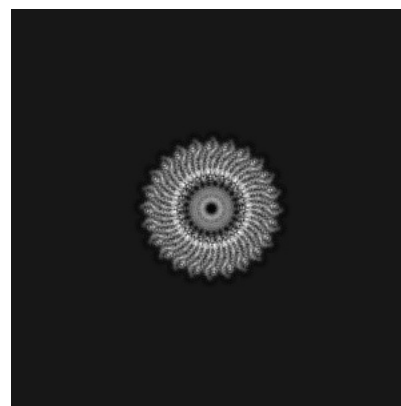
6.1.1 Primary map



X

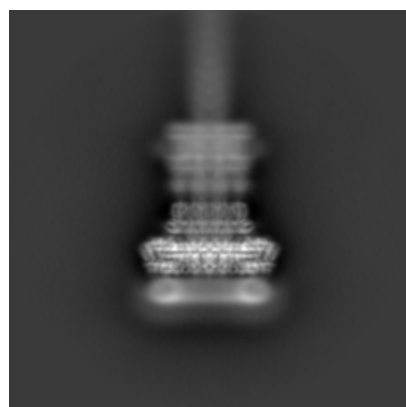


Y



Z

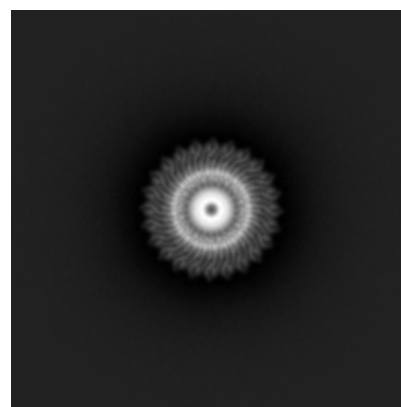
6.1.2 Raw map



X



Y



Z

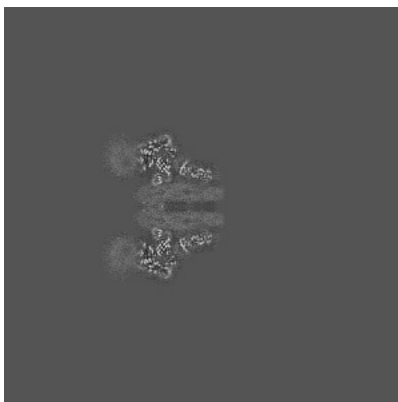
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

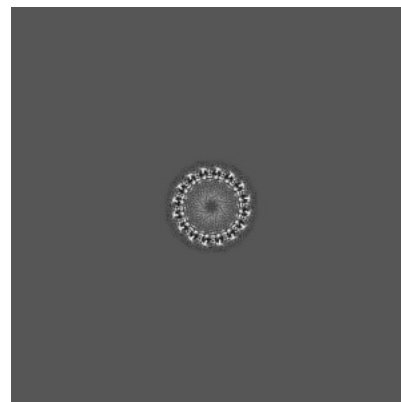
6.2.1 Primary map



X Index: 240

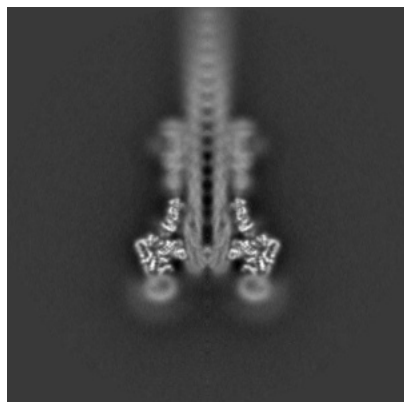


Y Index: 240

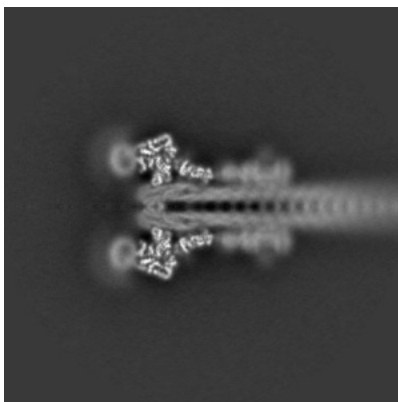


Z Index: 240

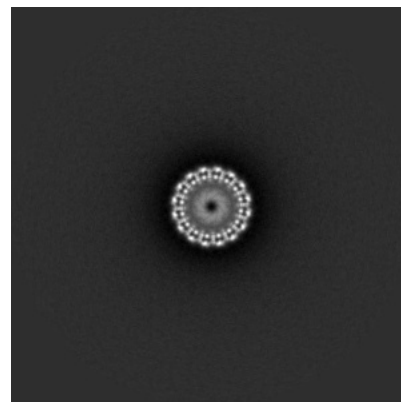
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

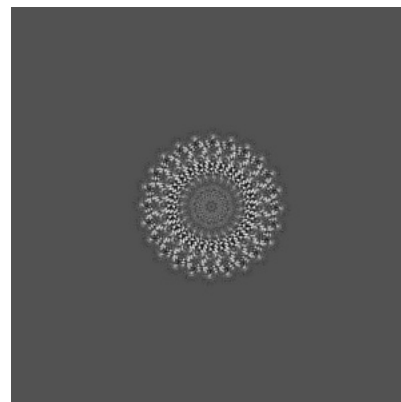
6.3.1 Primary map



X Index: 279

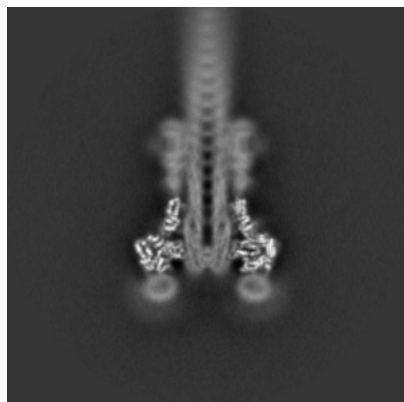


Y Index: 201

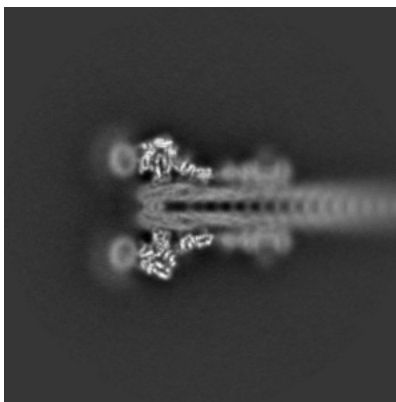


Z Index: 192

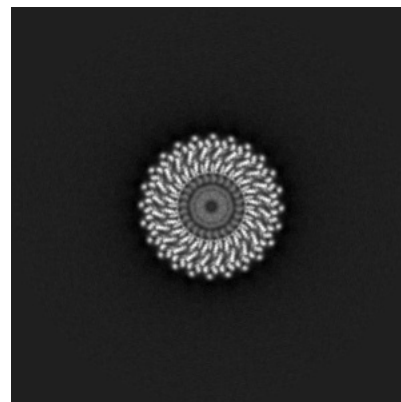
6.3.2 Raw map



X Index: 237



Y Index: 243

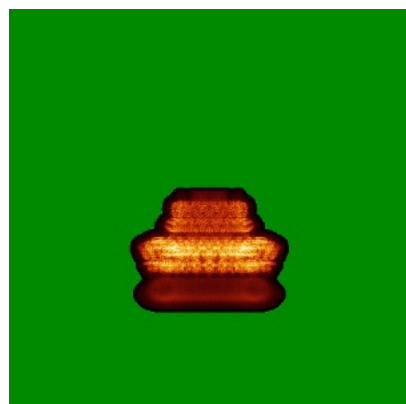


Z Index: 193

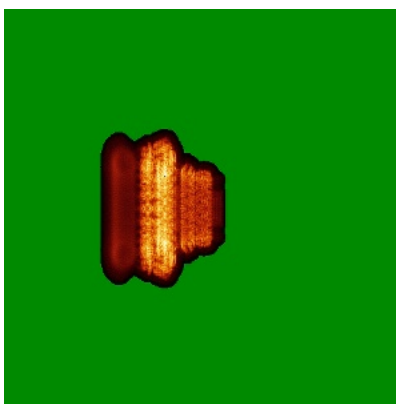
The images above show the largest variance slices of the map in three orthogonal directions.

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

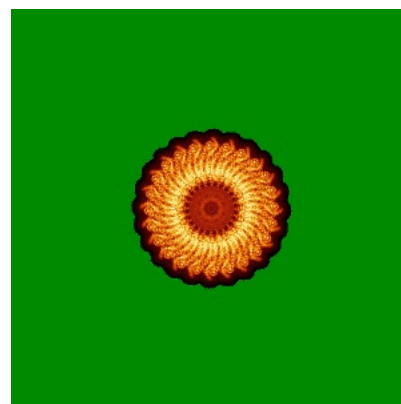
6.4.1 Primary map



X

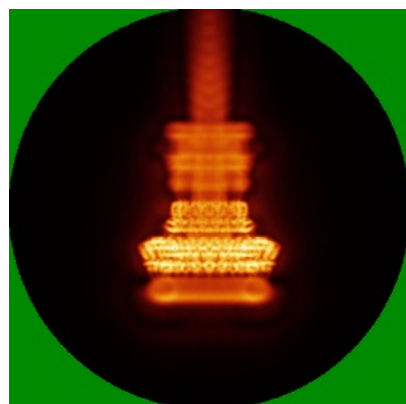


Y

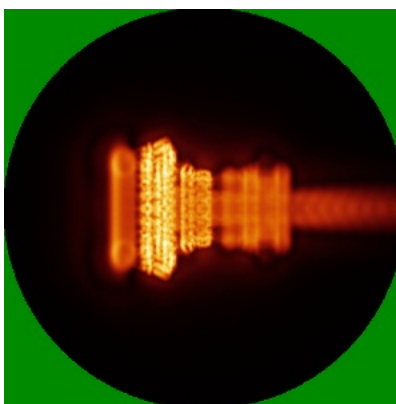


Z

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.

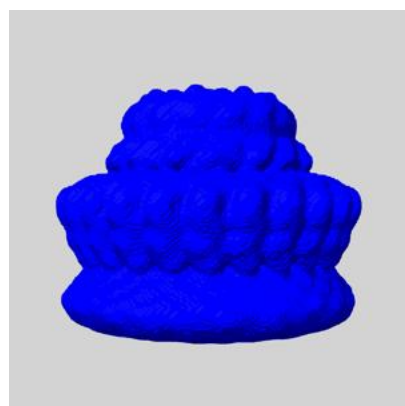
6.6 Mask visualisation [i](#)

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

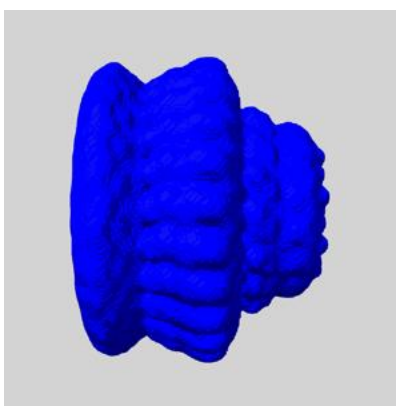
A mask typically either:

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

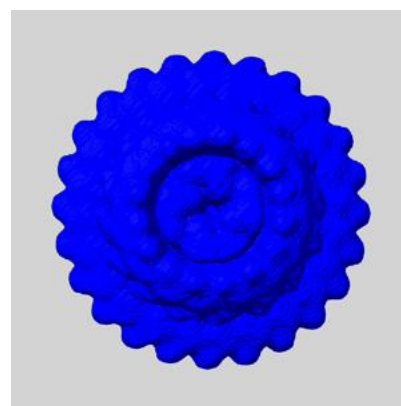
6.6.1 emd_10040_msk_1.map [i](#)



X



Y

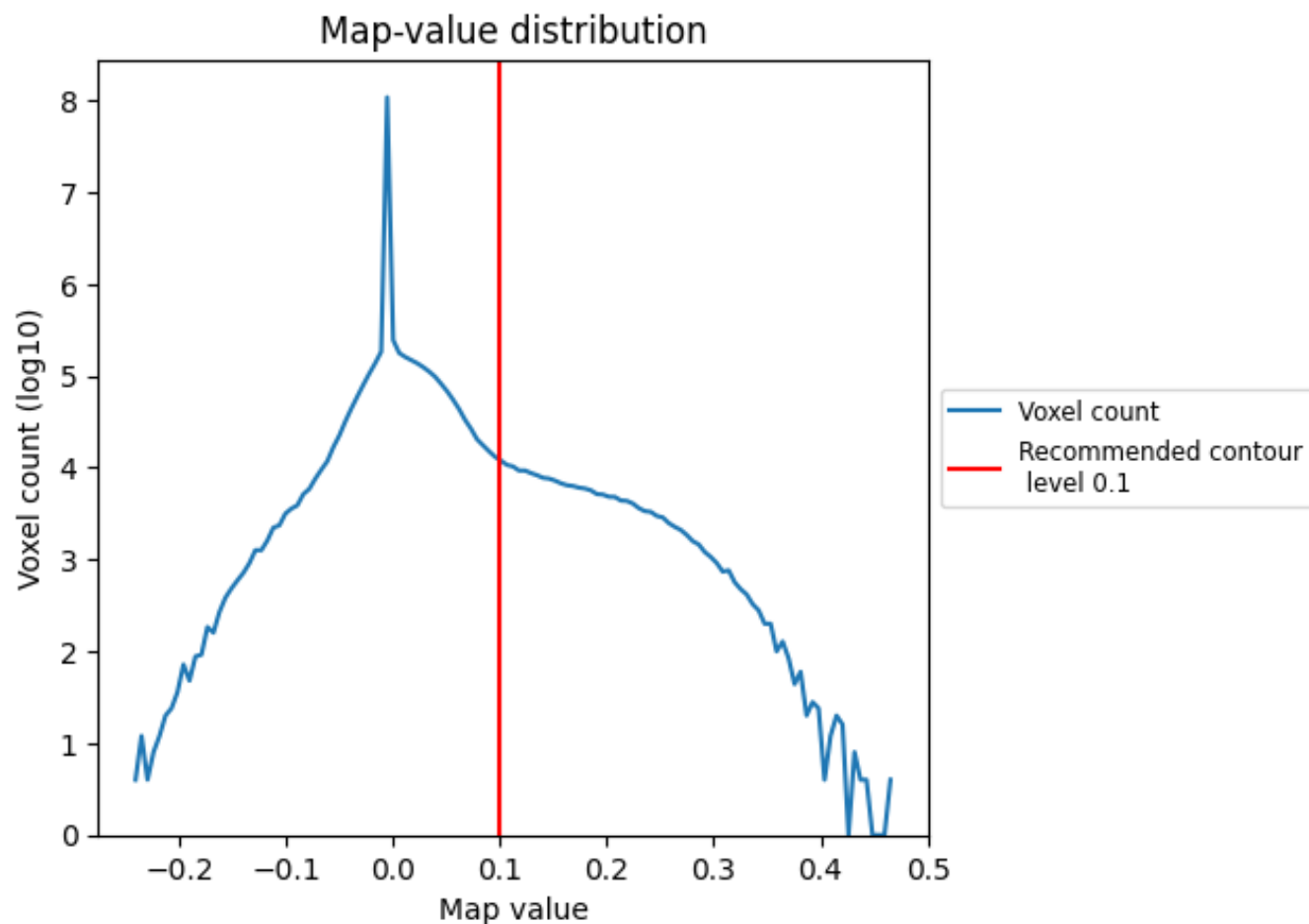


Z

7 Map analysis [i](#)

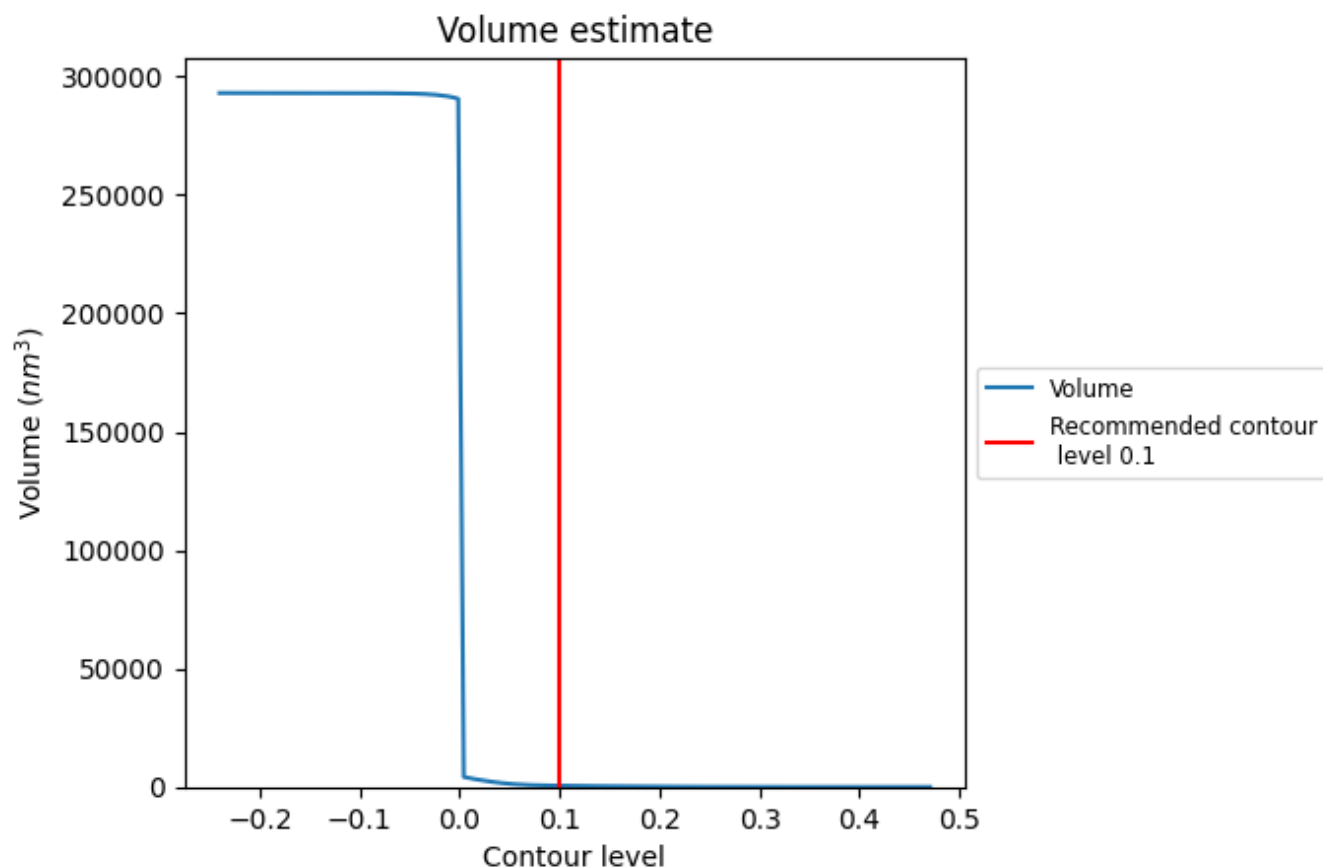
This section contains the results of statistical analysis of the map.

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.

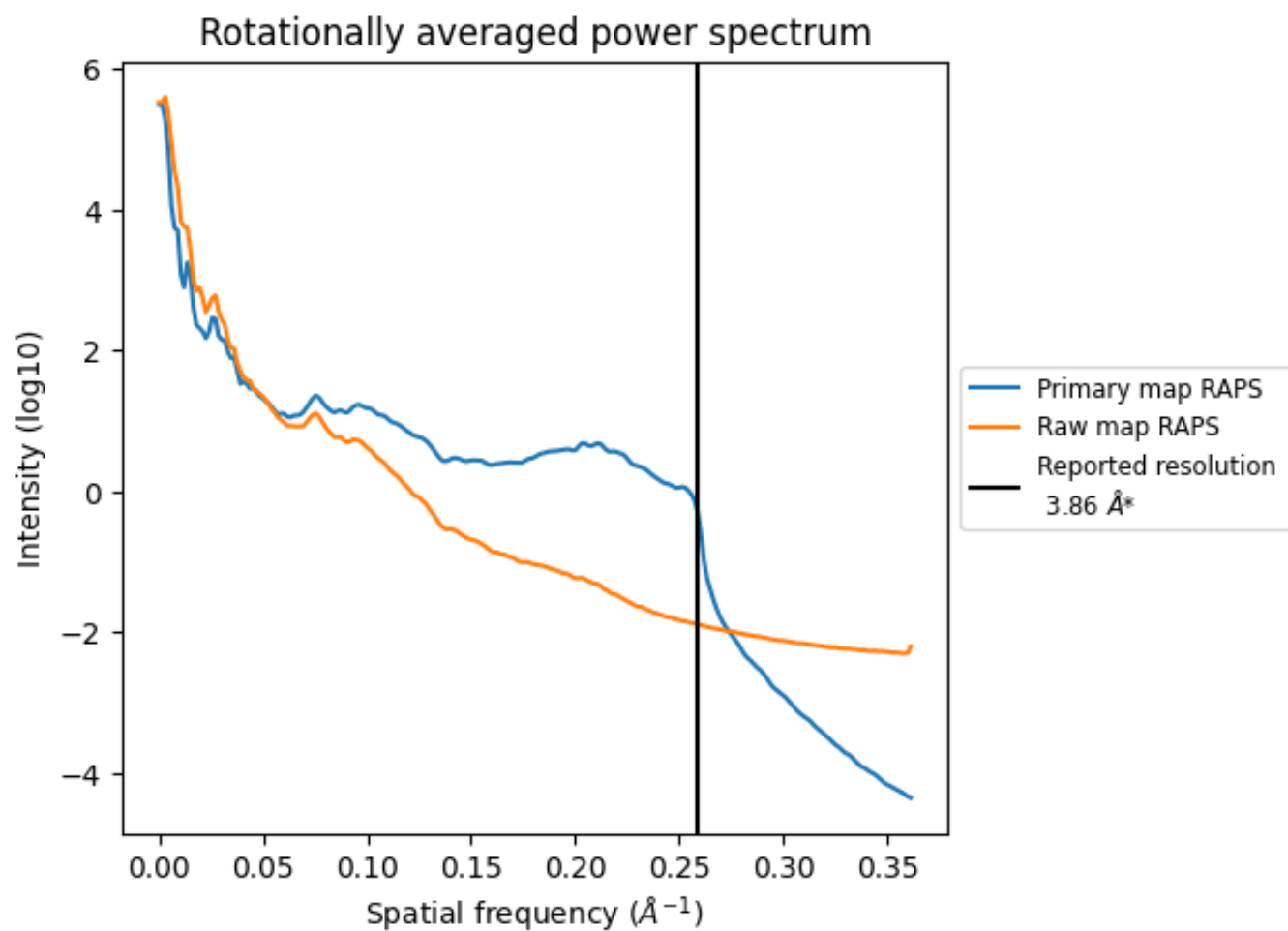
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 529 nm³; this corresponds to an approximate mass of 478 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

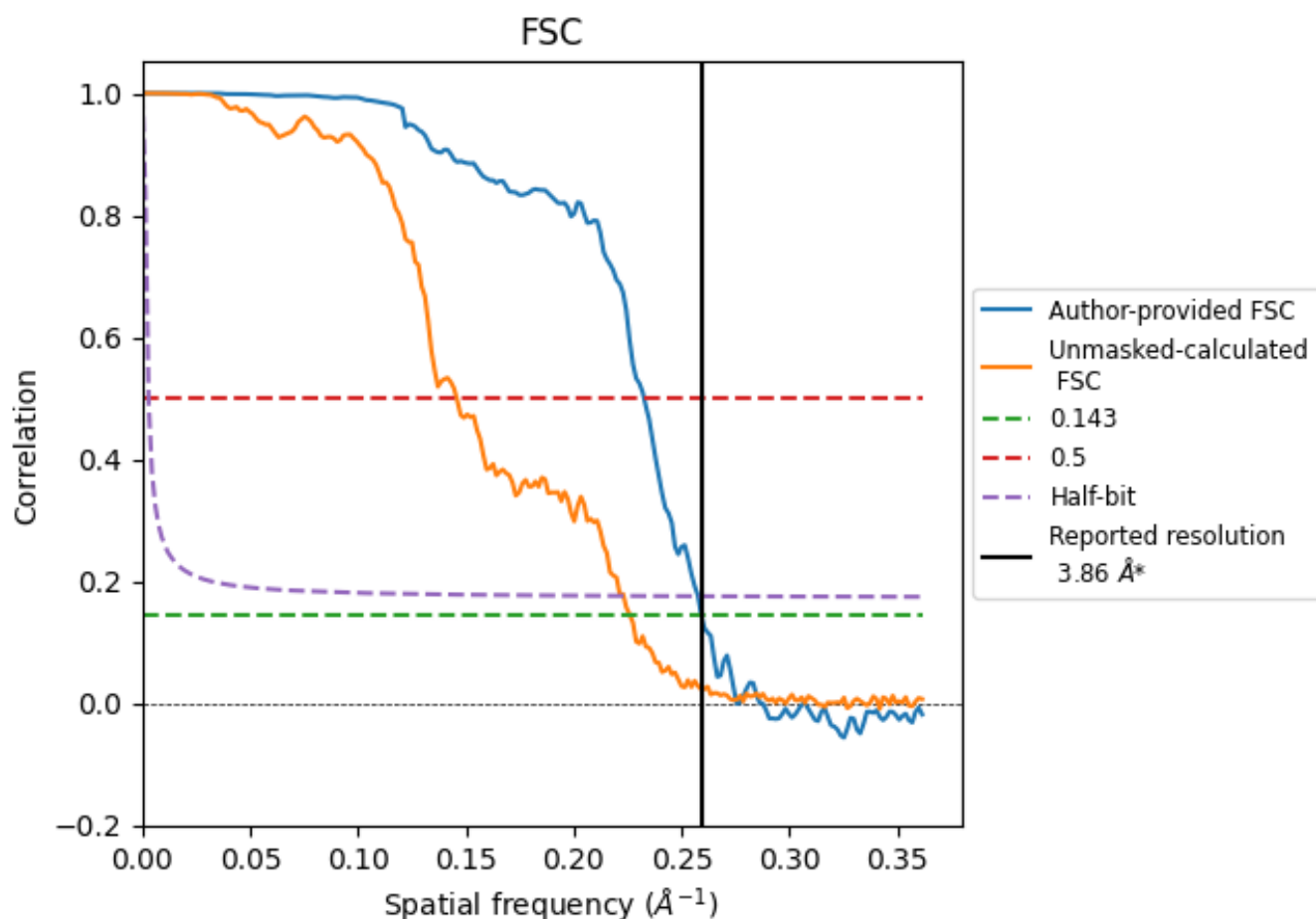


*Reported resolution corresponds to spatial frequency of $0.259 \text{ \AA}^{-1}$

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 $0.259 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.86	4.30	3.88
Unmasked-calculated*	4.42	6.86	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.86 by more than 10 %

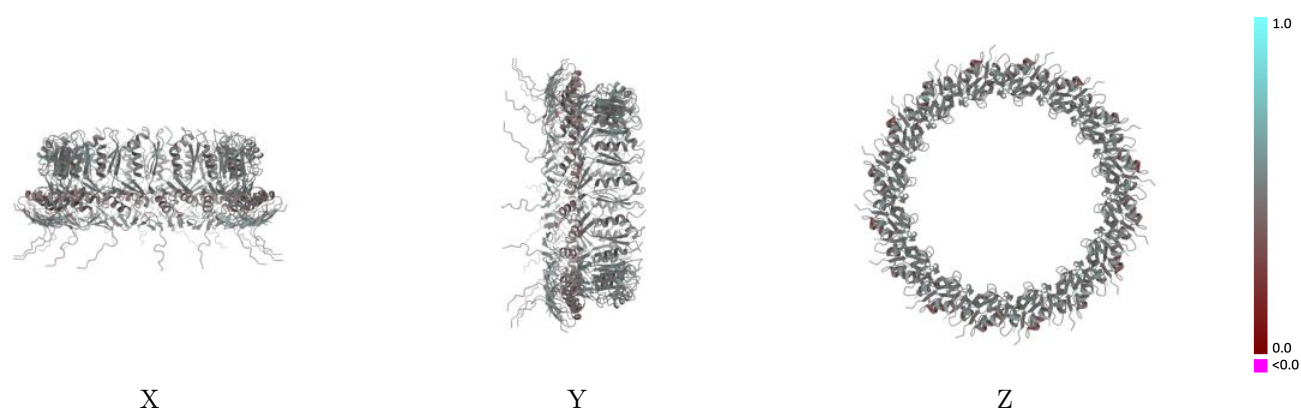
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10040 and PDB model 6RWK. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

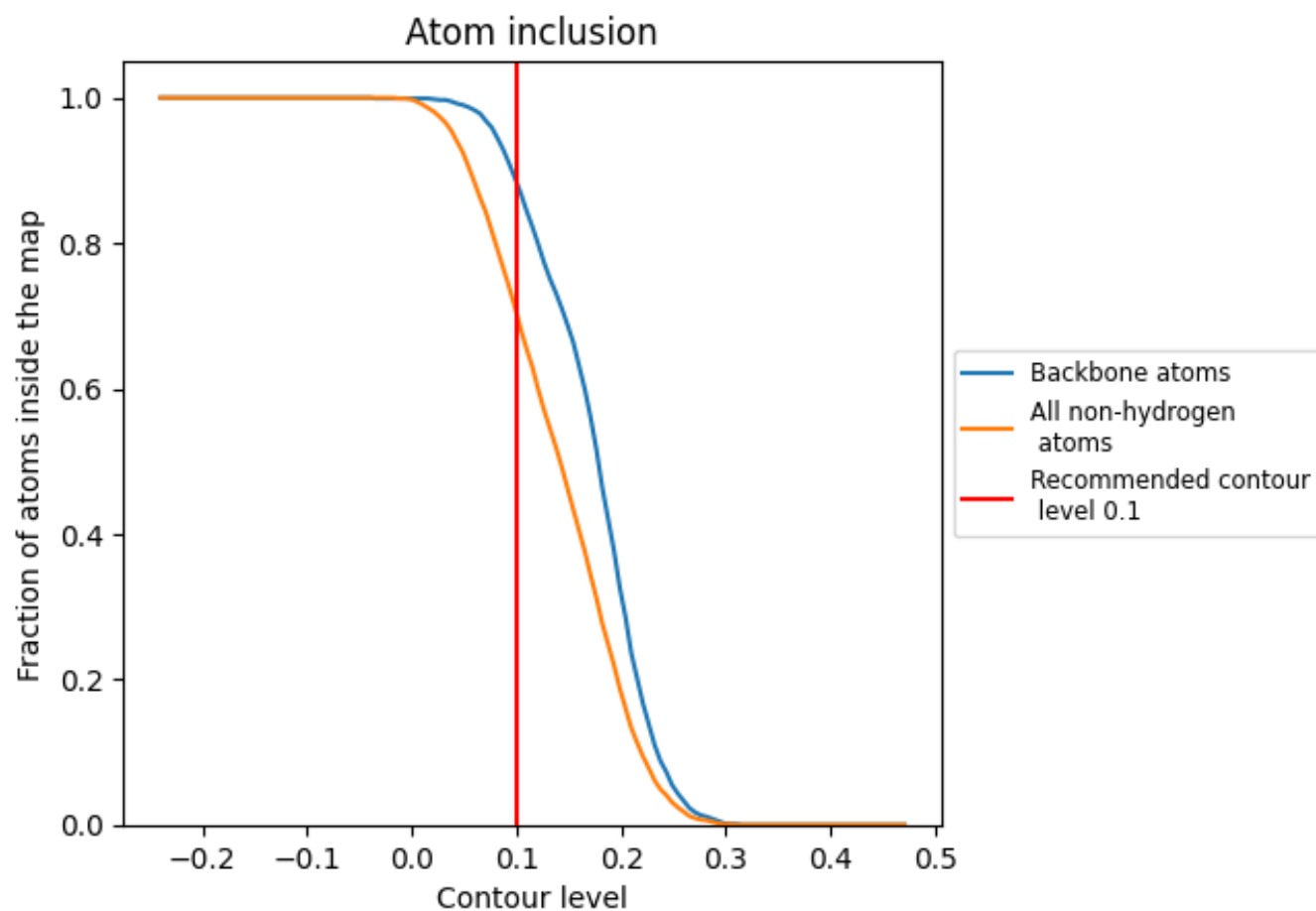


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7040	 0.4820
0	 0.7060	 0.4780
1	 0.7300	 0.4860
2	 0.7110	 0.4790
3	 0.7160	 0.4840
4	 0.7050	 0.4790
5	 0.7290	 0.4880
6	 0.7100	 0.4810
7	 0.7140	 0.4850
8	 0.7050	 0.4820
9	 0.7300	 0.4870
A	 0.6550	 0.4750
B	 0.6630	 0.4890
D	 0.6550	 0.4780
E	 0.6510	 0.4830
G	 0.6470	 0.4750
H	 0.6670	 0.4890
J	 0.6350	 0.4750
K	 0.6550	 0.4860
M	 0.6590	 0.4750
N	 0.6590	 0.4900
P	 0.6550	 0.4720
Q	 0.6430	 0.4870
S	 0.6510	 0.4760
T	 0.6590	 0.4840
U	 0.6550	 0.4720
V	 0.6470	 0.4810
X	 0.7120	 0.4800
Y	 0.7080	 0.4800
Z	 0.7110	 0.4790
x	 0.7170	 0.4830
y	 0.7290	 0.4880
z	 0.7190	 0.4840

