



Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 10:03 am BST

PDB ID : 9SH2 / pdb_00009sh2
EMDB ID : EMD-54887
Title : Neisseria meningitidis Native PilQ tetradecamer
Authors : Fernandez-Martinez, D.; Dumenil, G.
Deposited on : 2025-08-24
Resolution : 2.14 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.dev133
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) : 2.50

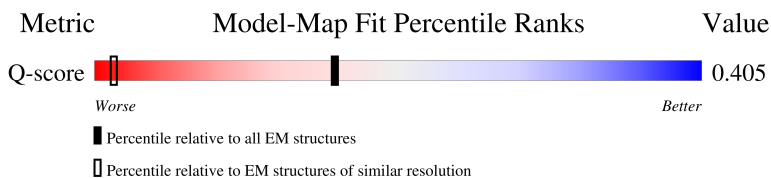
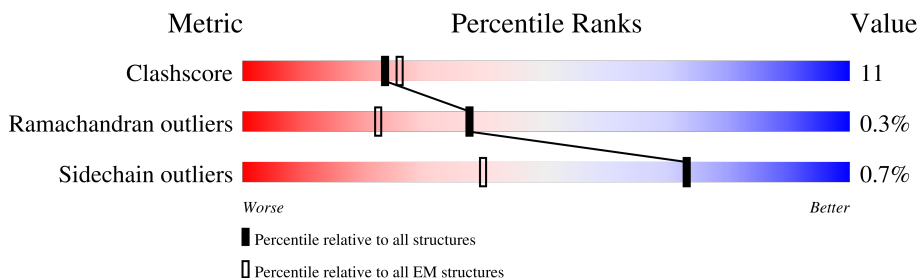
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 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	2493 (1.66 - 2.64)

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

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	
1	C	761	
1	D	761	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	761	
1	F	761	
1	G	761	
1	H	761	
1	I	761	
1	J	761	
1	K	761	
1	L	761	
1	M	761	
1	N	761	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43120 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 Type IV pilus biogenesis and competence protein PilQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	B	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	C	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	D	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	E	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	F	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	G	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	H	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	I	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	J	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	K	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	L	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	M	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		
1	N	404	Total	C	N	O	S	0	0
			3080	1930	537	604	9		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	HIS	-	expression tag	UNP A0A9K2PSI0
A	417	HIS	-	expression tag	UNP A0A9K2PSI0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	HIS	-	expression tag	UNP A0A9K2PSI0
A	419	HIS	-	expression tag	UNP A0A9K2PSI0
A	420	HIS	-	expression tag	UNP A0A9K2PSI0
A	421	HIS	-	expression tag	UNP A0A9K2PSI0
A	422	HIS	-	expression tag	UNP A0A9K2PSI0
A	423	HIS	-	expression tag	UNP A0A9K2PSI0
B	416	HIS	-	expression tag	UNP A0A9K2PSI0
B	417	HIS	-	expression tag	UNP A0A9K2PSI0
B	418	HIS	-	expression tag	UNP A0A9K2PSI0
B	419	HIS	-	expression tag	UNP A0A9K2PSI0
B	420	HIS	-	expression tag	UNP A0A9K2PSI0
B	421	HIS	-	expression tag	UNP A0A9K2PSI0
B	422	HIS	-	expression tag	UNP A0A9K2PSI0
B	423	HIS	-	expression tag	UNP A0A9K2PSI0
C	416	HIS	-	expression tag	UNP A0A9K2PSI0
C	417	HIS	-	expression tag	UNP A0A9K2PSI0
C	418	HIS	-	expression tag	UNP A0A9K2PSI0
C	419	HIS	-	expression tag	UNP A0A9K2PSI0
C	420	HIS	-	expression tag	UNP A0A9K2PSI0
C	421	HIS	-	expression tag	UNP A0A9K2PSI0
C	422	HIS	-	expression tag	UNP A0A9K2PSI0
C	423	HIS	-	expression tag	UNP A0A9K2PSI0
D	416	HIS	-	expression tag	UNP A0A9K2PSI0
D	417	HIS	-	expression tag	UNP A0A9K2PSI0
D	418	HIS	-	expression tag	UNP A0A9K2PSI0
D	419	HIS	-	expression tag	UNP A0A9K2PSI0
D	420	HIS	-	expression tag	UNP A0A9K2PSI0
D	421	HIS	-	expression tag	UNP A0A9K2PSI0
D	422	HIS	-	expression tag	UNP A0A9K2PSI0
D	423	HIS	-	expression tag	UNP A0A9K2PSI0
E	416	HIS	-	expression tag	UNP A0A9K2PSI0
E	417	HIS	-	expression tag	UNP A0A9K2PSI0
E	418	HIS	-	expression tag	UNP A0A9K2PSI0
E	419	HIS	-	expression tag	UNP A0A9K2PSI0
E	420	HIS	-	expression tag	UNP A0A9K2PSI0
E	421	HIS	-	expression tag	UNP A0A9K2PSI0
E	422	HIS	-	expression tag	UNP A0A9K2PSI0
E	423	HIS	-	expression tag	UNP A0A9K2PSI0
F	416	HIS	-	expression tag	UNP A0A9K2PSI0
F	417	HIS	-	expression tag	UNP A0A9K2PSI0
F	418	HIS	-	expression tag	UNP A0A9K2PSI0
F	419	HIS	-	expression tag	UNP A0A9K2PSI0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	420	HIS	-	expression tag	UNP A0A9K2PSI0
F	421	HIS	-	expression tag	UNP A0A9K2PSI0
F	422	HIS	-	expression tag	UNP A0A9K2PSI0
F	423	HIS	-	expression tag	UNP A0A9K2PSI0
G	416	HIS	-	expression tag	UNP A0A9K2PSI0
G	417	HIS	-	expression tag	UNP A0A9K2PSI0
G	418	HIS	-	expression tag	UNP A0A9K2PSI0
G	419	HIS	-	expression tag	UNP A0A9K2PSI0
G	420	HIS	-	expression tag	UNP A0A9K2PSI0
G	421	HIS	-	expression tag	UNP A0A9K2PSI0
G	422	HIS	-	expression tag	UNP A0A9K2PSI0
G	423	HIS	-	expression tag	UNP A0A9K2PSI0
H	416	HIS	-	expression tag	UNP A0A9K2PSI0
H	417	HIS	-	expression tag	UNP A0A9K2PSI0
H	418	HIS	-	expression tag	UNP A0A9K2PSI0
H	419	HIS	-	expression tag	UNP A0A9K2PSI0
H	420	HIS	-	expression tag	UNP A0A9K2PSI0
H	421	HIS	-	expression tag	UNP A0A9K2PSI0
H	422	HIS	-	expression tag	UNP A0A9K2PSI0
H	423	HIS	-	expression tag	UNP A0A9K2PSI0
I	416	HIS	-	expression tag	UNP A0A9K2PSI0
I	417	HIS	-	expression tag	UNP A0A9K2PSI0
I	418	HIS	-	expression tag	UNP A0A9K2PSI0
I	419	HIS	-	expression tag	UNP A0A9K2PSI0
I	420	HIS	-	expression tag	UNP A0A9K2PSI0
I	421	HIS	-	expression tag	UNP A0A9K2PSI0
I	422	HIS	-	expression tag	UNP A0A9K2PSI0
I	423	HIS	-	expression tag	UNP A0A9K2PSI0
J	416	HIS	-	expression tag	UNP A0A9K2PSI0
J	417	HIS	-	expression tag	UNP A0A9K2PSI0
J	418	HIS	-	expression tag	UNP A0A9K2PSI0
J	419	HIS	-	expression tag	UNP A0A9K2PSI0
J	420	HIS	-	expression tag	UNP A0A9K2PSI0
J	421	HIS	-	expression tag	UNP A0A9K2PSI0
J	422	HIS	-	expression tag	UNP A0A9K2PSI0
J	423	HIS	-	expression tag	UNP A0A9K2PSI0
K	416	HIS	-	expression tag	UNP A0A9K2PSI0
K	417	HIS	-	expression tag	UNP A0A9K2PSI0
K	418	HIS	-	expression tag	UNP A0A9K2PSI0
K	419	HIS	-	expression tag	UNP A0A9K2PSI0
K	420	HIS	-	expression tag	UNP A0A9K2PSI0
K	421	HIS	-	expression tag	UNP A0A9K2PSI0

Continued on next page...

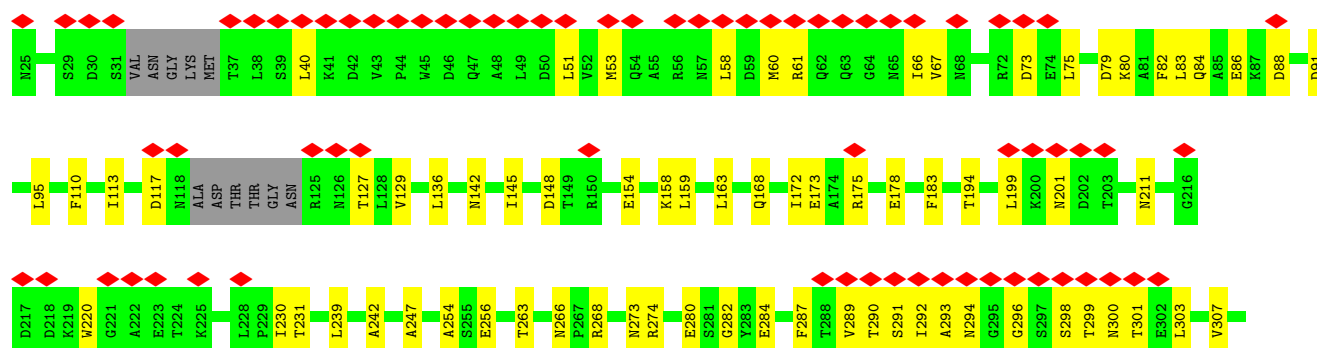
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	422	HIS	-	expression tag	UNP A0A9K2PSI0
K	423	HIS	-	expression tag	UNP A0A9K2PSI0
L	416	HIS	-	expression tag	UNP A0A9K2PSI0
L	417	HIS	-	expression tag	UNP A0A9K2PSI0
L	418	HIS	-	expression tag	UNP A0A9K2PSI0
L	419	HIS	-	expression tag	UNP A0A9K2PSI0
L	420	HIS	-	expression tag	UNP A0A9K2PSI0
L	421	HIS	-	expression tag	UNP A0A9K2PSI0
L	422	HIS	-	expression tag	UNP A0A9K2PSI0
L	423	HIS	-	expression tag	UNP A0A9K2PSI0
M	416	HIS	-	expression tag	UNP A0A9K2PSI0
M	417	HIS	-	expression tag	UNP A0A9K2PSI0
M	418	HIS	-	expression tag	UNP A0A9K2PSI0
M	419	HIS	-	expression tag	UNP A0A9K2PSI0
M	420	HIS	-	expression tag	UNP A0A9K2PSI0
M	421	HIS	-	expression tag	UNP A0A9K2PSI0
M	422	HIS	-	expression tag	UNP A0A9K2PSI0
M	423	HIS	-	expression tag	UNP A0A9K2PSI0
N	416	HIS	-	expression tag	UNP A0A9K2PSI0
N	417	HIS	-	expression tag	UNP A0A9K2PSI0
N	418	HIS	-	expression tag	UNP A0A9K2PSI0
N	419	HIS	-	expression tag	UNP A0A9K2PSI0
N	420	HIS	-	expression tag	UNP A0A9K2PSI0
N	421	HIS	-	expression tag	UNP A0A9K2PSI0
N	422	HIS	-	expression tag	UNP A0A9K2PSI0
N	423	HIS	-	expression tag	UNP A0A9K2PSI0

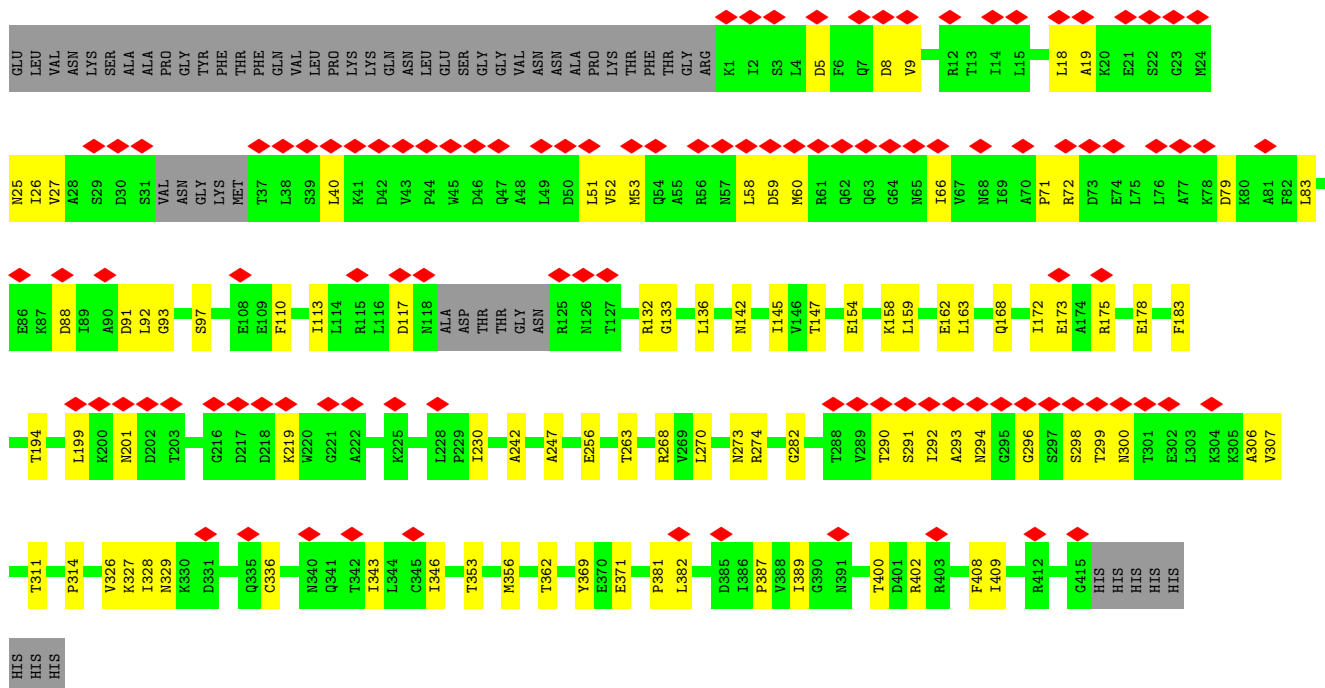
[illegible]

Chain C:

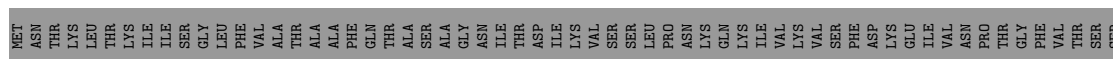
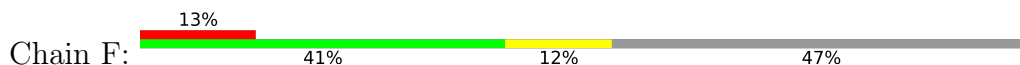
GLU	GLN	GLY	VAL	TRP	PRO	MET
LEU	GLN	GLY	VAL	ILE	ALA	ASN
VAL	PRO	ASP	VAL	PHE	ARG	THR
ASN	ASP	ILE	VAL	ILE	ILE	LYS
LYS	SER	SER	ALA	ASN	ALA	LEU
SER	GLN	SER	ALA	GLU	LEU	THR
ALA	GLN	SER	PRO	SER	ASP	LYS
ALA	HIS	GLN	PHE	ASP	PHE	ILE
PRO	HIS	ASP	SER	ASP	GLU	ILE
GLY	ASP	PRO	PRO	THR	THR	SER
THR	HIS	ILE	ALA	VAL	VAL	GLY
PHE	ILE	ILE	GLN	ALA	ILE	LEU
THR	VAL	VAL	GLN	PRO	ILE	PHE
GLN	THR	THR	ALA	ALA	VAL	VAL
VAL	LEU	LEU	ALA	ALA	MET	ALA
LEU	LYS	LYS	ALA	PRO	ASP	THR
PRO	ASN	ASN	SER	ALA	GLN	ALA
LYS	HIS	ASN	ALA	VAL	GLN	ALA
LYS	THR	THR	ALA	LYS	LEU	PHE
GLN	LEU	LEU	GLN	VAL	LEU	GLN
ASN	PRO	PRO	GLN	ALA	TYR	THR
LEU	THR	THR	THR	PRO	ALA	SER
GLU	THR	THR	ALA	ALA	ASP	ALA
SER	LEU	LEU	ALA	ALA	PRO	GLY
GLY	GLN	ARG	PRO	PRO	LEU	ASN
GLY	ARG	ILE	ALA	ALA	ILE	ASN
ASN	SER	LYS	LYS	LYS	THR	THR
VAL	LEU	ASP	GLN	GLN	ILE	ILE
ASN	ASP	VAL	ALA	ALA	SER	LYS
ALA	VAL	VAL	ALA	ALA	ALA	VAL
PRO	LYS	ASP	ALA	ALA	SER	VAL
PRO	LYS	PHE	PRO	PRO	GLN	SER
THR	THR	THR	PRO	PRO	ASN	LEU
PHE	LYS	THR	ALA	SER	ASN	LEU
THR	THR	THR	LYS	THR	SER	PRO
GLY	PRO	PRO	GLN	LYS	SER	ASN
ARG	VAL	VAL	THR	SER	ARG	LYS
K1	GLN	LYS	ASN	ALA	ALA	GLN
I2	LYS	ILE	ILE	VAL	ARG	LYS
I3	VAL	VAL	PHE	VAL	LEU	ILE
D5	LEU	THR	ARG	SER	VAL	VAL
F6	ARG	THR	THR	THR	SER	VAL
Q7	LEU	LEU	GLY	PHE	LEU	LYS
D8	ASN	ASN	LYS	THR	LYS	ASP
V9	ASP	ASP	ASN	PRO	PRO	LYS
	THR	THR	ALA	ALA	GLY	GLY
	GLN	THR	ILE	LYS	THR	THR
R12	GLN	GLN	ILE	GLN	GLY	VAL
T13	LEU	LEU	ILE	GLN	TYR	VAL
I14	ILE	ILE	GLU	ALA	THR	PRO
L15	THR	THR	LEU	ALA	GLU	THR
	ALA	ALA	ALA	PRO	VAL	GLY
L16	GLY	GLY	LEU	PHE	ARG	PHE
A19	ASN	THR	GLY	THR	ASN	THR
P20	THR	THR	PHE	GLU	LYS	SER
	ALA	ALA	THR	SER	VAL	SER

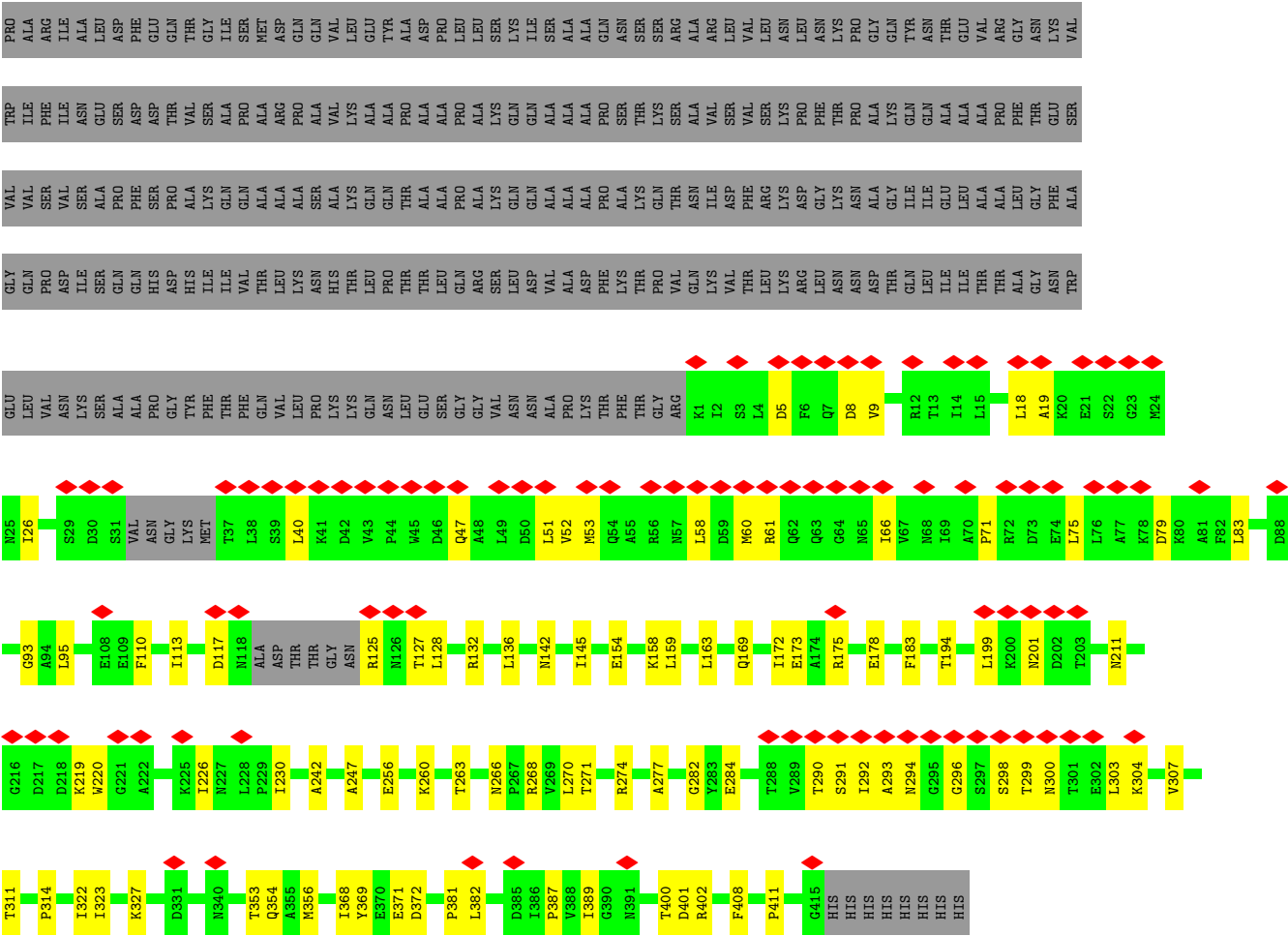


- Molecule 1: Type IV pilus biogenesis and competence protein PilQ

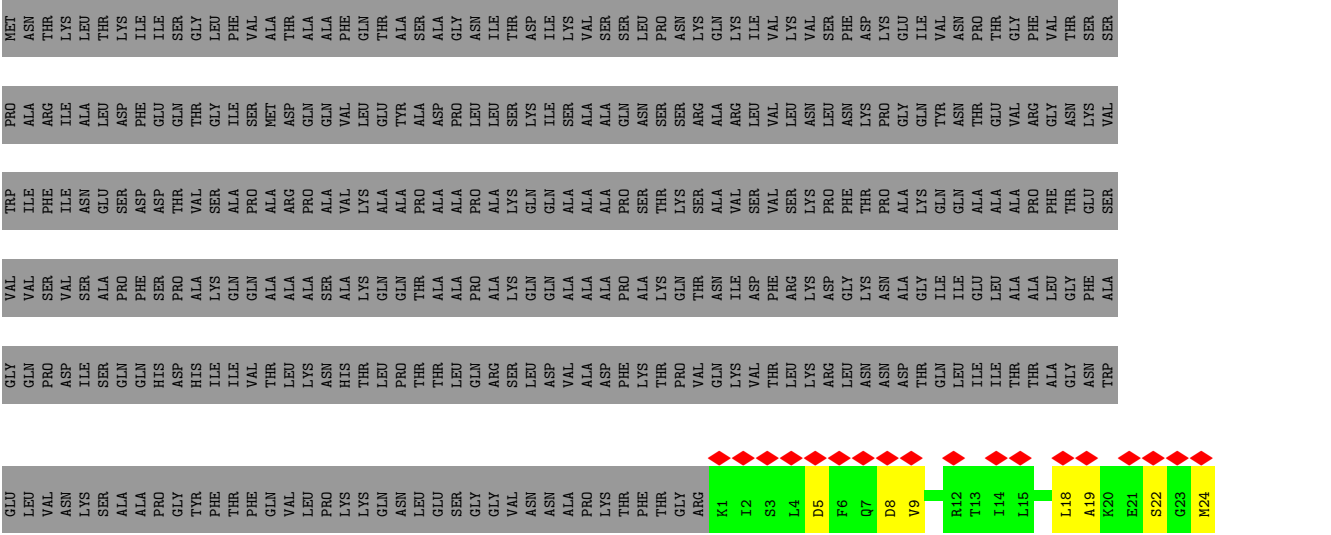
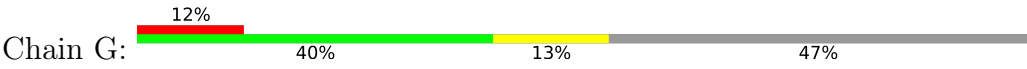


- Molecule 1: Type IV pilus biogenesis and competence protein PilQ

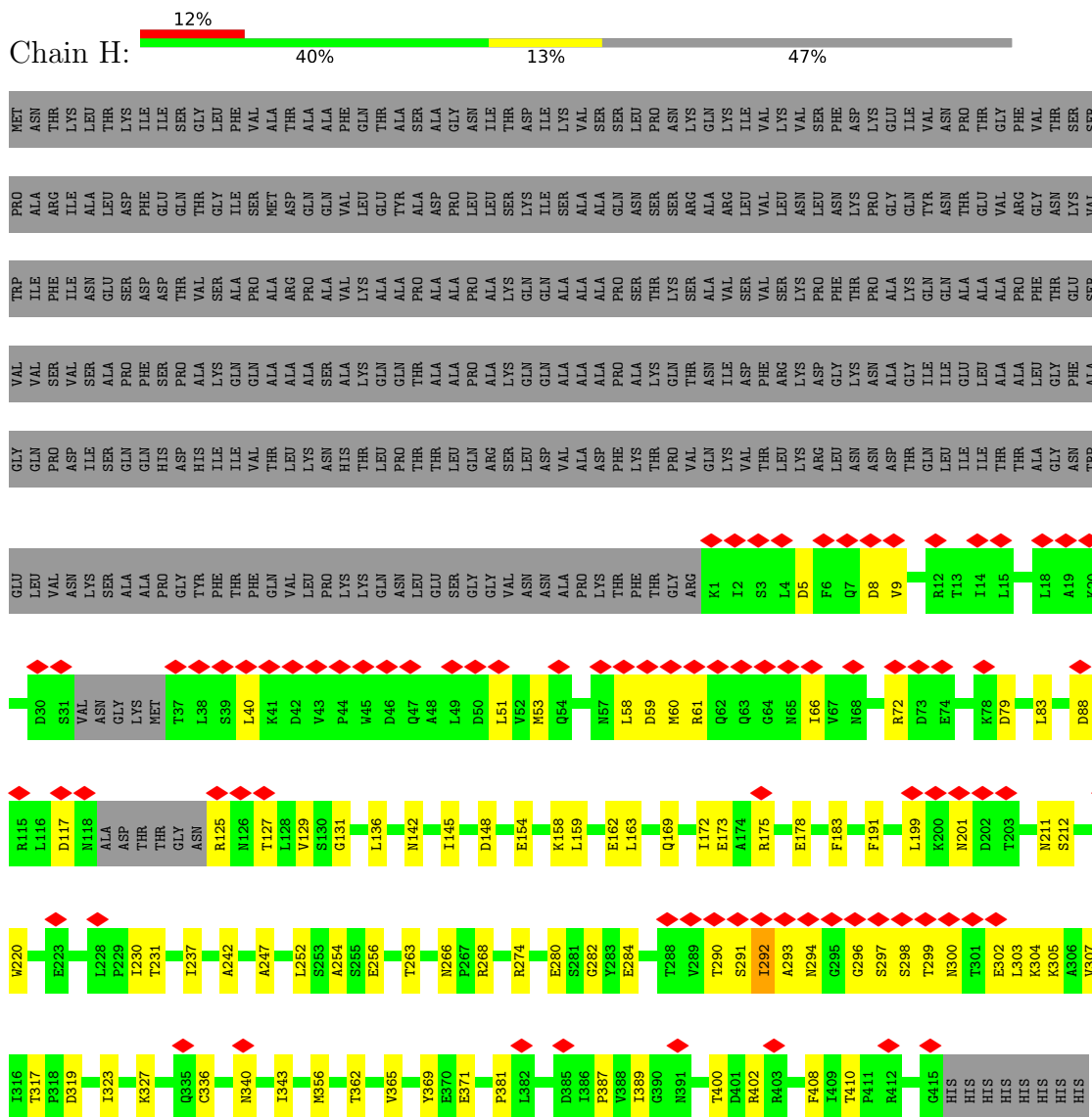




• Molecule 1: Type IV pilus biogenesis and competence protein PilQ

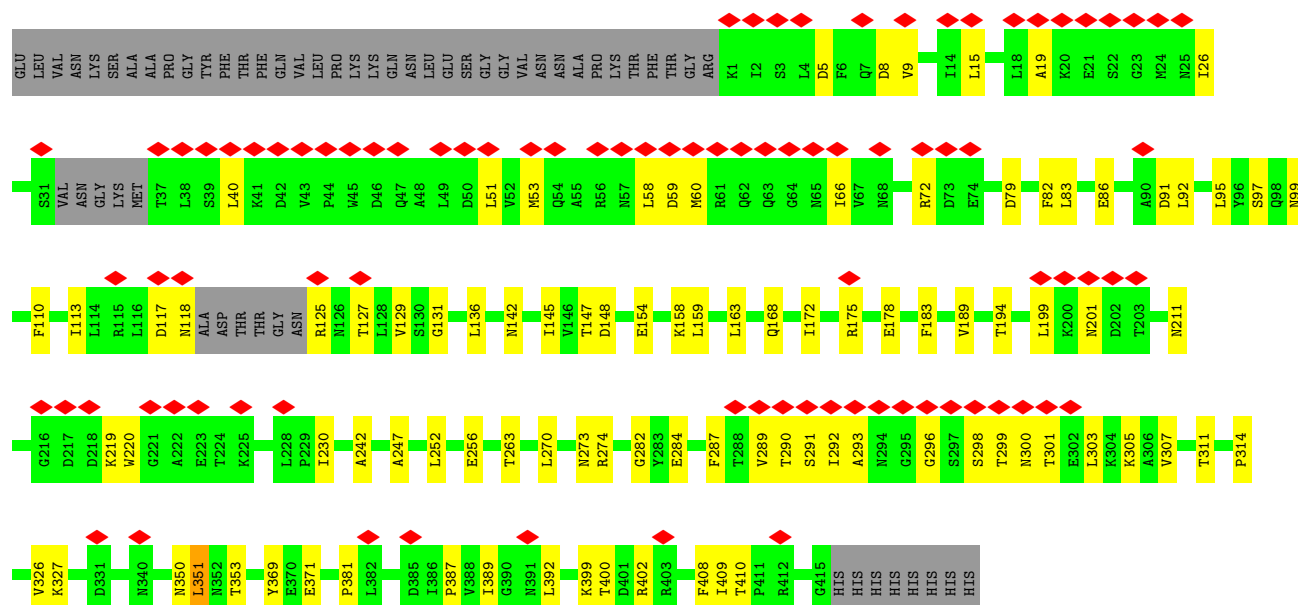


- Molecule 1: Type IV pilus biogenesis and competence protein PilQ

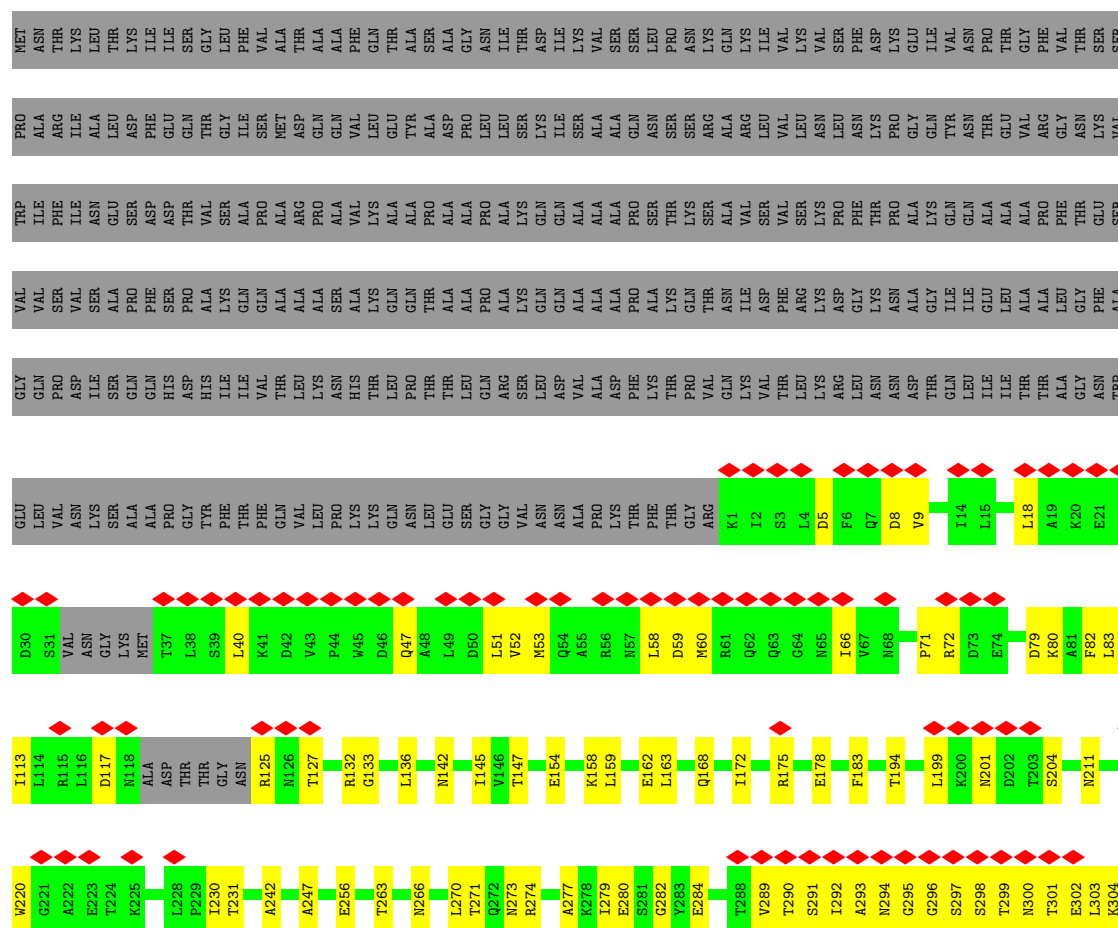


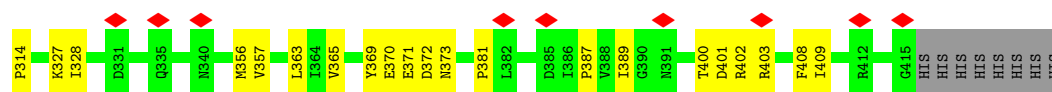
- Molecule 1: Type IV pilus biogenesis and competence protein PilQ



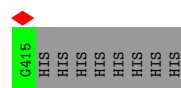
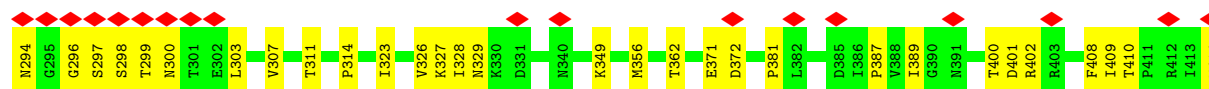
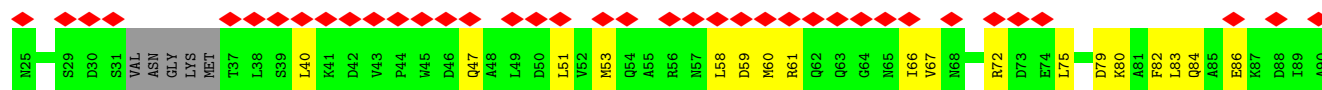
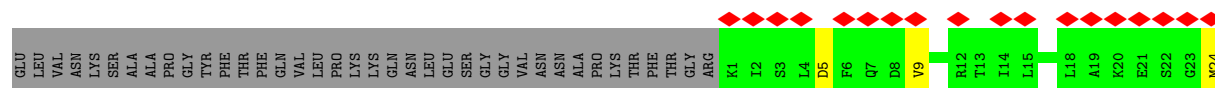
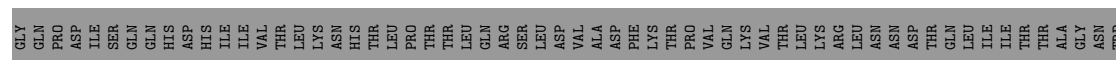
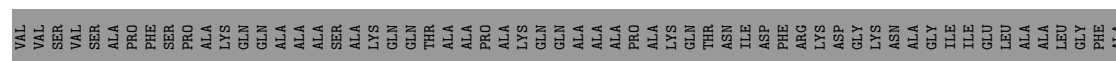
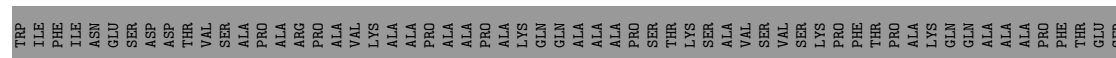
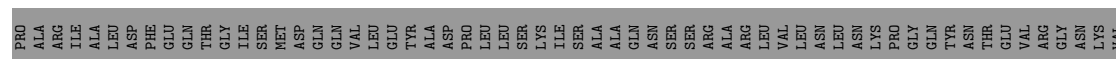
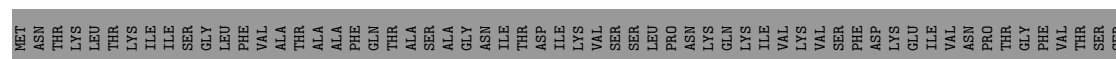


• Molecule 1: Type IV pilus biogenesis and competence protein PilQ

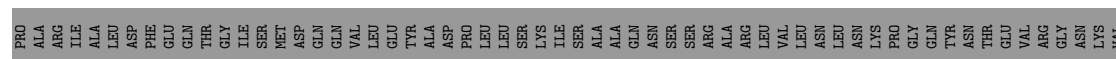
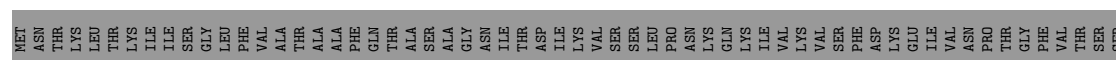


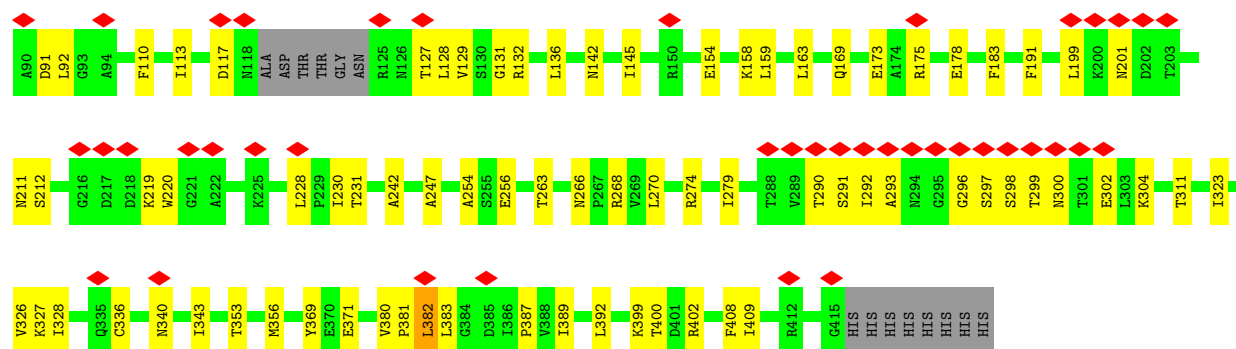


• Molecule 1: Type IV pilus biogenesis and competence protein PilQ



• Molecule 1: Type IV pilus biogenesis and competence protein PilQ





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C14	Depositor
Number of particles used	154572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.611	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.201	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/3112	0.34	0/4203
1	B	0.12	0/3112	0.32	0/4203
1	C	0.12	0/3112	0.34	0/4203
1	D	0.13	0/3112	0.35	0/4203
1	E	0.11	0/3112	0.32	0/4203
1	F	0.11	0/3112	0.32	0/4203
1	G	0.12	0/3112	0.34	0/4203
1	H	0.11	0/3112	0.33	0/4203
1	I	0.12	0/3112	0.34	0/4203
1	J	0.11	0/3112	0.33	0/4203
1	K	0.14	0/3112	0.35	0/4203
1	L	0.13	0/3112	0.32	0/4203
1	M	0.11	0/3112	0.33	0/4203
1	N	0.11	0/3112	0.32	0/4203
All	All	0.12	0/43568	0.33	0/58842

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3080	0	3181	96	0
1	B	3080	0	3181	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3080	0	3181	99	0
1	D	3080	0	3181	91	0
1	E	3080	0	3181	81	0
1	F	3080	0	3181	90	0
1	G	3080	0	3181	92	0
1	H	3080	0	3181	88	0
1	I	3080	0	3181	82	0
1	J	3080	0	3181	83	0
1	K	3080	0	3181	95	0
1	L	3080	0	3181	97	0
1	M	3080	0	3181	94	0
1	N	3080	0	3181	94	0
All	All	43120	0	44534	961	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 11.

All (961) 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:L:53:MET:HG3	1:L:60:MET:HG2	1.49	0.93
1:J:53:MET:HG3	1:J:60:MET:HG2	1.49	0.92
1:K:53:MET:HG3	1:K:60:MET:HG2	1.52	0.90
1:I:53:MET:HG3	1:I:60:MET:HG2	1.57	0.87
1:J:292:ILE:HB	1:K:298:SER:HB3	1.61	0.82
1:F:53:MET:HG3	1:F:60:MET:HG2	1.61	0.81
1:H:53:MET:HG3	1:H:60:MET:HG2	1.61	0.81
1:D:53:MET:HG3	1:D:60:MET:HG2	1.61	0.80
1:C:53:MET:HG3	1:C:60:MET:HG2	1.63	0.80
1:J:292:ILE:HG12	1:K:293:ALA:HB3	1.65	0.79
1:J:290:THR:HB	1:K:299:THR:N	1.96	0.79
1:B:53:MET:HG3	1:B:60:MET:HG2	1.64	0.79
1:C:292:ILE:HD13	1:D:293:ALA:H	1.49	0.77
1:C:290:THR:HB	1:D:299:THR:N	2.00	0.76
1:F:51:LEU:HD11	1:G:66:ILE:HG21	1.67	0.76
1:N:53:MET:HG3	1:N:60:MET:HG2	1.69	0.74
1:A:95:LEU:HD21	1:A:132:ARG:HG3	1.70	0.74
1:F:292:ILE:HB	1:G:298:SER:HB3	1.68	0.74
1:K:290:THR:H	1:L:300:ASN:HA	1.52	0.74
1:I:290:THR:HG23	1:I:298:SER:C	2.13	0.73
1:D:290:THR:HB	1:E:299:THR:N	2.02	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:ILE:HD13	1:G:293:ALA:H	1.53	0.73
1:C:292:ILE:HB	1:D:298:SER:HB3	1.70	0.72
1:J:289:VAL:HG22	1:K:301:THR:H	1.53	0.72
1:J:290:THR:HG23	1:J:298:SER:C	2.14	0.72
1:F:290:THR:HG23	1:F:298:SER:C	2.15	0.72
1:B:290:THR:HG23	1:B:298:SER:C	2.15	0.72
1:A:293:ALA:H	1:N:292:ILE:HD13	1.53	0.72
1:G:53:MET:HG3	1:G:60:MET:HG2	1.72	0.71
1:F:292:ILE:HG12	1:G:293:ALA:HB3	1.72	0.71
1:G:292:ILE:HG12	1:H:293:ALA:HB3	1.71	0.71
1:M:290:THR:HG23	1:M:298:SER:C	2.16	0.71
1:G:290:THR:H	1:H:300:ASN:HA	1.55	0.70
1:L:290:THR:HG23	1:L:298:SER:C	2.16	0.70
1:N:290:THR:HG23	1:N:298:SER:C	2.17	0.70
1:C:284:GLU:HB3	1:C:303:LEU:HB3	1.74	0.70
1:H:290:THR:HG23	1:H:298:SER:C	2.17	0.69
1:M:290:THR:HB	1:N:299:THR:N	2.07	0.69
1:C:290:THR:HG23	1:C:298:SER:C	2.18	0.69
1:K:292:ILE:HD13	1:L:292:ILE:HA	1.73	0.69
1:H:292:ILE:HG12	1:I:293:ALA:HB3	1.75	0.69
1:L:292:ILE:HG12	1:M:293:ALA:HB3	1.74	0.69
1:J:284:GLU:HB3	1:J:303:LEU:HB3	1.74	0.68
1:M:159:LEU:O	1:M:163:LEU:HB2	1.93	0.68
1:J:284:GLU:OE1	1:J:305:LYS:NZ	2.26	0.68
1:A:292:ILE:HG12	1:B:293:ALA:HB3	1.76	0.68
1:I:93:GLY:O	1:I:132:ARG:NH2	2.26	0.68
1:H:290:THR:HG22	1:I:298:SER:HA	1.75	0.68
1:A:298:SER:HB3	1:N:292:ILE:HB	1.76	0.67
1:D:292:ILE:HG12	1:E:293:ALA:HB3	1.75	0.67
1:E:292:ILE:HD13	1:F:292:ILE:HA	1.76	0.67
1:G:178:GLU:HB2	1:G:263:THR:HB	1.77	0.67
1:M:178:GLU:HB2	1:M:263:THR:HB	1.77	0.67
1:D:284:GLU:HB3	1:D:303:LEU:HB3	1.77	0.67
1:E:290:THR:HG23	1:E:298:SER:C	2.20	0.67
1:K:175:ARG:HB3	1:K:408:PHE:HB2	1.77	0.66
1:A:93:GLY:O	1:A:132:ARG:NH1	2.28	0.66
1:I:291:SER:O	1:I:298:SER:OG	2.12	0.66
1:L:291:SER:O	1:L:298:SER:OG	2.13	0.66
1:I:175:ARG:HB3	1:I:408:PHE:HB2	1.78	0.66
1:N:175:ARG:HB3	1:N:408:PHE:HB2	1.76	0.66
1:A:290:THR:HG23	1:A:298:SER:C	2.20	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:ARG:HB3	1:J:408:PHE:HB2	1.78	0.66
1:B:178:GLU:HB2	1:B:263:THR:HB	1.76	0.66
1:D:178:GLU:HB2	1:D:263:THR:HB	1.77	0.66
1:F:290:THR:HB	1:G:299:THR:N	2.11	0.66
1:G:290:THR:HB	1:H:299:THR:N	2.11	0.65
1:F:381:PRO:HG3	1:G:256:GLU:HB2	1.79	0.65
1:C:292:ILE:HG12	1:D:293:ALA:HB3	1.78	0.65
1:A:290:THR:H	1:B:300:ASN:HA	1.62	0.65
1:H:336:CYS:HB3	1:H:343:ILE:HG13	1.79	0.65
1:K:93:GLY:O	1:K:132:ARG:NH2	2.25	0.65
1:L:93:GLY:O	1:L:132:ARG:NH2	2.25	0.65
1:F:178:GLU:HB2	1:F:263:THR:HB	1.78	0.65
1:M:381:PRO:HG3	1:N:256:GLU:HB2	1.79	0.65
1:B:159:LEU:O	1:B:163:LEU:HB2	1.96	0.65
1:D:290:THR:H	1:E:300:ASN:HA	1.60	0.65
1:I:292:ILE:HD13	1:J:292:ILE:HA	1.77	0.65
1:I:328:ILE:HD11	1:I:409:ILE:HD11	1.77	0.65
1:J:136:LEU:HB2	1:J:145:ILE:HB	1.78	0.65
1:M:389:ILE:HD12	1:M:389:ILE:H	1.62	0.65
1:H:175:ARG:HB3	1:H:408:PHE:HB2	1.80	0.64
1:K:294:ASN:HA	1:L:294:ASN:HB2	1.77	0.64
1:A:293:ALA:HB3	1:N:292:ILE:HG12	1.79	0.64
1:E:381:PRO:HG3	1:F:256:GLU:HB2	1.78	0.64
1:J:290:THR:HG22	1:K:298:SER:HA	1.79	0.64
1:D:159:LEU:O	1:D:163:LEU:HB2	1.97	0.64
1:J:292:ILE:HD13	1:K:293:ALA:H	1.63	0.64
1:M:290:THR:HG22	1:N:298:SER:HA	1.78	0.64
1:A:175:ARG:HB3	1:A:408:PHE:HB2	1.78	0.63
1:B:292:ILE:HD13	1:C:292:ILE:HA	1.79	0.63
1:K:178:GLU:HB2	1:K:263:THR:HB	1.79	0.63
1:K:290:THR:HG23	1:K:298:SER:C	2.23	0.63
1:K:290:THR:HG23	1:K:299:THR:N	2.14	0.63
1:F:159:LEU:O	1:F:163:LEU:HB2	1.98	0.63
1:E:291:SER:O	1:E:298:SER:OG	2.16	0.63
1:G:290:THR:HG23	1:G:298:SER:C	2.23	0.63
1:A:381:PRO:HG3	1:B:256:GLU:HB2	1.81	0.63
1:N:159:LEU:O	1:N:163:LEU:HB2	1.98	0.63
1:F:51:LEU:HG	1:G:66:ILE:HG12	1.80	0.63
1:L:284:GLU:HB3	1:L:303:LEU:HD23	1.80	0.63
1:A:83:LEU:HD13	1:B:92:LEU:HD12	1.81	0.62
1:B:292:ILE:HG12	1:C:293:ALA:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:THR:HG23	1:D:298:SER:C	2.24	0.62
1:G:323:ILE:HG12	1:G:356:MET:HB2	1.81	0.62
1:M:93:GLY:O	1:M:132:ARG:NH1	2.31	0.62
1:B:175:ARG:HB3	1:B:408:PHE:HB2	1.80	0.62
1:C:289:VAL:HG22	1:D:301:THR:H	1.62	0.62
1:F:93:GLY:O	1:F:132:ARG:NH1	2.32	0.62
1:C:93:GLY:O	1:C:132:ARG:NH1	2.29	0.62
1:I:91:ASP:O	1:I:132:ARG:NH1	2.32	0.62
1:B:291:SER:O	1:B:298:SER:OG	2.16	0.62
1:I:292:ILE:HG12	1:J:293:ALA:HB3	1.81	0.62
1:D:290:THR:HG22	1:E:298:SER:HA	1.81	0.62
1:D:311:THR:HB	1:D:327:LYS:HB3	1.81	0.62
1:L:175:ARG:HB3	1:L:408:PHE:HB2	1.82	0.62
1:F:284:GLU:HB3	1:F:303:LEU:HD23	1.81	0.62
1:N:5:ASP:HB3	1:N:40:LEU:HB2	1.82	0.62
1:E:311:THR:HB	1:E:327:LYS:HB3	1.82	0.62
1:M:290:THR:H	1:N:300:ASN:HA	1.65	0.62
1:H:356:MET:O	1:I:169:GLN:NE2	2.28	0.62
1:D:175:ARG:HB3	1:D:408:PHE:HB2	1.81	0.61
1:C:183:PHE:HB3	1:C:400:THR:HB	1.82	0.61
1:C:381:PRO:HG3	1:D:256:GLU:HB2	1.82	0.61
1:N:291:SER:O	1:N:298:SER:OG	2.18	0.61
1:G:159:LEU:O	1:G:163:LEU:HB2	1.99	0.61
1:A:60:MET:HE2	1:A:60:MET:HA	1.82	0.61
1:M:91:ASP:O	1:M:132:ARG:NH1	2.33	0.61
1:C:291:SER:O	1:C:298:SER:OG	2.18	0.61
1:L:311:THR:HB	1:L:327:LYS:HB3	1.82	0.61
1:B:183:PHE:HB3	1:B:400:THR:HB	1.81	0.61
1:H:290:THR:H	1:I:300:ASN:HA	1.66	0.61
1:H:88:ASP:O	1:H:92:LEU:HB3	2.01	0.60
1:K:183:PHE:HB3	1:K:400:THR:HB	1.82	0.60
1:A:300:ASN:HA	1:N:290:THR:H	1.64	0.60
1:A:292:ILE:HD11	1:B:296:GLY:H	1.66	0.60
1:H:291:SER:O	1:H:298:SER:OG	2.18	0.60
1:N:91:ASP:O	1:N:132:ARG:NH1	2.34	0.60
1:C:91:ASP:O	1:C:132:ARG:NH1	2.34	0.60
1:B:311:THR:HB	1:B:327:LYS:HB3	1.83	0.60
1:J:381:PRO:HG3	1:K:256:GLU:HB2	1.82	0.60
1:M:311:THR:HB	1:M:327:LYS:HB3	1.83	0.60
1:I:183:PHE:HB3	1:I:400:THR:HB	1.83	0.60
1:C:311:THR:HB	1:C:327:LYS:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:ARG:HB3	1:F:408:PHE:HB2	1.84	0.60
1:F:291:SER:O	1:F:298:SER:OG	2.16	0.60
1:G:381:PRO:HG3	1:H:256:GLU:HB2	1.83	0.60
1:H:183:PHE:HB3	1:H:400:THR:HB	1.84	0.60
1:E:290:THR:H	1:F:300:ASN:HA	1.66	0.60
1:E:175:ARG:HB3	1:E:408:PHE:HB2	1.82	0.60
1:J:183:PHE:HB3	1:J:400:THR:HB	1.84	0.60
1:N:291:SER:OG	1:N:302:GLU:OE2	2.20	0.60
1:A:291:SER:O	1:A:298:SER:OG	2.19	0.59
1:A:136:LEU:HB2	1:A:145:ILE:HB	1.84	0.59
1:D:381:PRO:HG3	1:E:256:GLU:HB2	1.83	0.59
1:G:290:THR:HG22	1:H:298:SER:HA	1.84	0.59
1:H:290:THR:HB	1:I:299:THR:N	2.17	0.59
1:D:183:PHE:HB3	1:D:400:THR:HB	1.84	0.59
1:L:381:PRO:HG3	1:M:256:GLU:HB2	1.83	0.59
1:I:136:LEU:HB2	1:I:145:ILE:HB	1.83	0.59
1:L:183:PHE:HB3	1:L:400:THR:HB	1.85	0.59
1:C:290:THR:HG22	1:D:298:SER:HA	1.84	0.59
1:H:311:THR:HB	1:H:327:LYS:HB3	1.83	0.59
1:A:92:LEU:HD13	1:N:83:LEU:HD22	1.83	0.59
1:B:219:LYS:HB3	1:C:231:THR:HB	1.83	0.59
1:D:290:THR:HG23	1:D:299:THR:N	2.18	0.59
1:J:5:ASP:HB3	1:J:40:LEU:HB2	1.84	0.59
1:B:290:THR:HG22	1:C:298:SER:HA	1.83	0.59
1:M:292:ILE:HD11	1:N:296:GLY:H	1.68	0.59
1:B:290:THR:H	1:C:300:ASN:HA	1.68	0.59
1:C:336:CYS:HB3	1:C:343:ILE:HG13	1.85	0.59
1:G:291:SER:O	1:G:298:SER:OG	2.21	0.59
1:K:284:GLU:HB2	1:K:303:LEU:HD23	1.85	0.59
1:D:172:ILE:HD11	1:D:314:PRO:HG3	1.86	0.58
1:J:159:LEU:O	1:J:163:LEU:HB2	2.02	0.58
1:K:292:ILE:HD11	1:L:296:GLY:H	1.66	0.58
1:M:136:LEU:HB2	1:M:145:ILE:HB	1.84	0.58
1:B:381:PRO:HG3	1:C:256:GLU:HB2	1.84	0.58
1:K:136:LEU:HB2	1:K:145:ILE:HB	1.84	0.58
1:K:290:THR:HB	1:L:299:THR:N	2.19	0.58
1:K:328:ILE:HD11	1:K:409:ILE:HD11	1.85	0.58
1:D:136:LEU:HB2	1:D:145:ILE:HB	1.84	0.58
1:L:117:ASP:OD1	1:L:117:ASP:N	2.36	0.58
1:E:136:LEU:HB2	1:E:145:ILE:HB	1.83	0.58
1:G:175:ARG:HB3	1:G:408:PHE:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:292:ILE:HG12	1:L:293:ALA:HB3	1.83	0.58
1:J:296:GLY:HA2	1:K:296:GLY:HA3	1.84	0.58
1:M:292:ILE:HG12	1:N:293:ALA:HB3	1.85	0.58
1:E:5:ASP:HB3	1:E:40:LEU:HB2	1.85	0.58
1:E:274:ARG:HD3	1:F:142:ASN:HB2	1.84	0.58
1:K:274:ARG:HD3	1:L:142:ASN:HB2	1.85	0.58
1:D:292:ILE:HD11	1:E:296:GLY:H	1.68	0.58
1:A:299:THR:N	1:N:290:THR:HB	2.18	0.58
1:D:5:ASP:HB3	1:D:40:LEU:HB2	1.85	0.58
1:E:183:PHE:HB3	1:E:400:THR:HB	1.84	0.58
1:I:159:LEU:O	1:I:163:LEU:HB2	2.02	0.58
1:N:136:LEU:HB2	1:N:145:ILE:HB	1.85	0.58
1:C:175:ARG:HB3	1:C:408:PHE:HB2	1.85	0.58
1:M:291:SER:O	1:M:298:SER:OG	2.19	0.57
1:A:291:SER:OG	1:A:302:GLU:OE2	2.23	0.57
1:F:290:THR:H	1:G:300:ASN:HA	1.69	0.57
1:K:371:GLU:HG3	1:K:402:ARG:HG2	1.85	0.57
1:M:117:ASP:N	1:M:117:ASP:OD1	2.36	0.57
1:A:256:GLU:HB2	1:N:381:PRO:HG3	1.86	0.57
1:I:292:ILE:HD12	1:J:298:SER:HB3	1.86	0.57
1:J:117:ASP:N	1:J:117:ASP:OD2	2.37	0.57
1:N:178:GLU:HB2	1:N:263:THR:HB	1.86	0.57
1:B:5:ASP:HB3	1:B:40:LEU:HB2	1.86	0.57
1:D:291:SER:O	1:D:298:SER:OG	2.22	0.57
1:G:136:LEU:HB2	1:G:145:ILE:HB	1.86	0.57
1:G:183:PHE:HB3	1:G:400:THR:HB	1.85	0.57
1:M:219:LYS:HB3	1:N:231:THR:HB	1.85	0.57
1:A:298:SER:HA	1:N:290:THR:HG22	1.87	0.57
1:B:136:LEU:HB2	1:B:145:ILE:HB	1.86	0.57
1:H:178:GLU:HB2	1:H:263:THR:HB	1.84	0.57
1:I:339:GLY:O	1:I:340:ASN:ND2	2.34	0.57
1:K:311:THR:HB	1:K:327:LYS:HB3	1.85	0.57
1:L:292:ILE:HD13	1:M:292:ILE:HA	1.86	0.57
1:E:292:ILE:HG12	1:F:293:ALA:HB3	1.86	0.57
1:F:136:LEU:HB2	1:F:145:ILE:HB	1.85	0.57
1:K:381:PRO:HG3	1:L:256:GLU:HB2	1.86	0.57
1:N:183:PHE:HB3	1:N:400:THR:HB	1.85	0.57
1:A:290:THR:HG23	1:A:299:THR:N	2.20	0.57
1:A:284:GLU:HB3	1:A:303:LEU:HB3	1.86	0.57
1:B:292:ILE:HD11	1:C:296:GLY:H	1.70	0.57
1:F:183:PHE:HB3	1:F:400:THR:HB	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ILE:HD12	1:F:298:SER:HB3	1.87	0.56
1:A:311:THR:HB	1:A:327:LYS:HB3	1.88	0.56
1:J:371:GLU:HG3	1:J:402:ARG:HG2	1.87	0.56
1:M:175:ARG:HB3	1:M:408:PHE:HB2	1.87	0.56
1:F:219:LYS:HB3	1:G:231:THR:HB	1.86	0.56
1:M:183:PHE:HB3	1:M:400:THR:HB	1.86	0.56
1:G:290:THR:HG23	1:G:299:THR:N	2.21	0.56
1:I:340:ASN:ND2	1:I:340:ASN:C	2.63	0.56
1:B:371:GLU:HG3	1:B:402:ARG:HG2	1.87	0.56
1:D:387:PRO:O	1:D:389:ILE:N	2.38	0.56
1:E:290:THR:HG23	1:E:299:THR:N	2.19	0.56
1:F:117:ASP:OD2	1:F:117:ASP:N	2.39	0.56
1:C:292:ILE:HB	1:D:298:SER:CB	2.35	0.56
1:L:79:ASP:O	1:L:83:LEU:HG	2.06	0.56
1:M:5:ASP:HB3	1:M:40:LEU:HB2	1.88	0.56
1:F:290:THR:HG22	1:G:298:SER:HA	1.87	0.56
1:G:53:MET:HE3	1:G:60:MET:SD	2.45	0.56
1:I:5:ASP:HB3	1:I:40:LEU:HB2	1.87	0.56
1:M:371:GLU:HG3	1:M:402:ARG:HG2	1.87	0.56
1:K:290:THR:HG22	1:L:298:SER:HA	1.88	0.56
1:M:323:ILE:HG12	1:M:356:MET:HB2	1.87	0.56
1:A:162:GLU:HG2	1:A:163:LEU:HD12	1.87	0.55
1:A:317:THR:OG1	1:A:319:ASP:OD1	2.18	0.55
1:C:389:ILE:HD12	1:C:389:ILE:H	1.71	0.55
1:F:371:GLU:HG3	1:F:402:ARG:HG2	1.86	0.55
1:A:292:ILE:HD13	1:B:293:ALA:H	1.72	0.55
1:L:297:SER:O	1:L:297:SER:OG	2.21	0.55
1:F:292:ILE:HD11	1:G:296:GLY:H	1.71	0.55
1:F:389:ILE:HD12	1:F:389:ILE:H	1.71	0.55
1:I:311:THR:HB	1:I:327:LYS:HB3	1.87	0.55
1:K:280:GLU:OE1	1:K:305:LYS:NZ	2.28	0.55
1:M:59:ASP:HB2	1:M:72:ARG:HA	1.87	0.55
1:B:290:THR:HG23	1:B:299:THR:N	2.22	0.55
1:L:292:ILE:HB	1:M:298:SER:CB	2.36	0.55
1:A:290:THR:HB	1:B:299:THR:N	2.22	0.55
1:B:274:ARG:HD3	1:C:142:ASN:HB2	1.87	0.55
1:C:5:ASP:HB3	1:C:40:LEU:HB2	1.89	0.55
1:C:296:GLY:HA2	1:D:296:GLY:HA3	1.88	0.55
1:C:387:PRO:O	1:C:389:ILE:N	2.38	0.55
1:J:291:SER:O	1:J:298:SER:OG	2.24	0.55
1:M:289:VAL:HG11	1:M:302:GLU:HG2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:GLU:HG3	1:G:402:ARG:HG2	1.87	0.55
1:H:381:PRO:HG3	1:I:256:GLU:HB2	1.88	0.55
1:I:274:ARG:HD3	1:J:142:ASN:HB2	1.89	0.55
1:I:371:GLU:HG3	1:I:402:ARG:HG2	1.88	0.55
1:F:274:ARG:HD3	1:G:142:ASN:HB2	1.87	0.55
1:G:292:ILE:HD13	1:H:293:ALA:H	1.71	0.55
1:L:219:LYS:HB3	1:M:231:THR:HB	1.87	0.55
1:B:304:LYS:HG3	1:C:303:LEU:HD21	1.89	0.55
1:N:311:THR:HB	1:N:327:LYS:HB3	1.89	0.55
1:B:290:THR:HB	1:C:299:THR:N	2.22	0.54
1:L:136:LEU:HB2	1:L:145:ILE:HB	1.88	0.54
1:L:371:GLU:HG3	1:L:402:ARG:HG2	1.88	0.54
1:E:91:ASP:O	1:E:132:ARG:NH1	2.40	0.54
1:L:290:THR:H	1:M:300:ASN:HA	1.72	0.54
1:H:51:LEU:HD11	1:I:66:ILE:HG21	1.88	0.54
1:H:371:GLU:HG3	1:H:402:ARG:HG2	1.89	0.54
1:M:91:ASP:OD1	1:M:92:LEU:N	2.40	0.54
1:C:136:LEU:HB2	1:C:145:ILE:HB	1.88	0.54
1:C:219:LYS:HB3	1:D:231:THR:HB	1.89	0.54
1:C:290:THR:HG23	1:C:299:THR:N	2.23	0.54
1:L:178:GLU:HB3	1:L:263:THR:HB	1.89	0.54
1:N:336:CYS:HB3	1:N:343:ILE:HG13	1.89	0.54
1:A:298:SER:CB	1:N:292:ILE:HB	2.37	0.54
1:G:84:GLN:HE22	1:H:92:LEU:HD21	1.73	0.54
1:G:292:ILE:HB	1:H:298:SER:CB	2.38	0.54
1:L:274:ARG:HD3	1:M:142:ASN:HB2	1.88	0.54
1:L:389:ILE:HD12	1:L:389:ILE:H	1.72	0.54
1:F:5:ASP:HB3	1:F:40:LEU:HB2	1.89	0.54
1:F:311:THR:HB	1:F:327:LYS:HB3	1.89	0.54
1:H:297:SER:O	1:H:297:SER:OG	2.24	0.54
1:H:292:ILE:HD11	1:I:296:GLY:H	1.71	0.54
1:L:5:ASP:HB3	1:L:40:LEU:HB2	1.90	0.54
1:N:290:THR:HG23	1:N:299:THR:N	2.23	0.54
1:A:296:GLY:H	1:N:292:ILE:HD11	1.72	0.53
1:B:173:GLU:HG2	1:B:268:ARG:HB3	1.90	0.53
1:G:292:ILE:HD11	1:H:296:GLY:H	1.73	0.53
1:E:51:LEU:HD11	1:F:66:ILE:HG21	1.90	0.53
1:G:79:ASP:O	1:G:83:LEU:HD13	2.08	0.53
1:H:136:LEU:HB2	1:H:145:ILE:HB	1.88	0.53
1:K:5:ASP:HB3	1:K:40:LEU:HB2	1.91	0.53
1:M:356:MET:O	1:N:169:GLN:NE2	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:88:ASP:O	1:N:92:LEU:HB3	2.07	0.53
1:E:53:MET:HE3	1:E:60:MET:SD	2.49	0.53
1:J:274:ARG:HD3	1:K:142:ASN:HB2	1.88	0.53
1:K:92:LEU:O	1:K:92:LEU:HD13	2.08	0.53
1:M:280:GLU:OE1	1:M:305:LYS:HE3	2.08	0.53
1:M:292:ILE:HD13	1:N:293:ALA:H	1.73	0.53
1:A:231:THR:HB	1:N:219:LYS:HB3	1.89	0.53
1:A:326:VAL:HG11	1:A:409:ILE:HD13	1.89	0.53
1:C:371:GLU:HG3	1:C:402:ARG:HG2	1.89	0.53
1:L:290:THR:HG23	1:L:299:THR:N	2.22	0.53
1:H:162:GLU:HG2	1:H:163:LEU:HD12	1.90	0.53
1:L:172:ILE:HD11	1:L:314:PRO:HG3	1.90	0.53
1:L:323:ILE:HG12	1:L:356:MET:HB2	1.89	0.53
1:A:18:LEU:HD11	1:A:52:VAL:HG21	1.91	0.53
1:B:297:SER:O	1:B:297:SER:OG	2.24	0.53
1:C:274:ARG:HD3	1:D:142:ASN:HB2	1.91	0.53
1:H:173:GLU:HG2	1:H:268:ARG:HB3	1.91	0.53
1:K:289:VAL:HG11	1:K:302:GLU:HB2	1.91	0.53
1:A:117:ASP:OD2	1:A:117:ASP:N	2.40	0.53
1:A:218:ASP:OD1	1:A:218:ASP:N	2.36	0.53
1:D:274:ARG:HD3	1:E:142:ASN:HB2	1.89	0.53
1:E:371:GLU:HG3	1:E:402:ARG:HG2	1.89	0.53
1:A:5:ASP:HB3	1:A:40:LEU:HB2	1.91	0.53
1:B:356:MET:O	1:C:169:GLN:NE2	2.28	0.53
1:C:290:THR:H	1:D:300:ASN:HA	1.73	0.53
1:D:371:GLU:HG3	1:D:402:ARG:HG2	1.89	0.53
1:F:296:GLY:HA2	1:G:296:GLY:HA3	1.89	0.53
1:G:311:THR:HB	1:G:327:LYS:HB3	1.89	0.53
1:A:92:LEU:HD11	1:N:84:GLN:OE1	2.09	0.52
1:H:53:MET:SD	1:H:58:LEU:HB3	2.50	0.52
1:E:59:ASP:HB2	1:E:72:ARG:HA	1.91	0.52
1:I:290:THR:HG23	1:I:299:THR:N	2.24	0.52
1:A:183:PHE:HB3	1:A:400:THR:HB	1.90	0.52
1:D:284:GLU:HB2	1:D:303:LEU:HD23	1.91	0.52
1:E:326:VAL:HG11	1:E:409:ILE:HD13	1.90	0.52
1:M:292:ILE:HD13	1:N:292:ILE:HA	1.91	0.52
1:I:284:GLU:HB3	1:I:303:LEU:HB3	1.90	0.52
1:G:53:MET:SD	1:G:58:LEU:HB3	2.50	0.52
1:J:311:THR:HB	1:J:327:LYS:HB3	1.90	0.52
1:L:326:VAL:HG11	1:L:409:ILE:HD13	1.91	0.52
1:B:387:PRO:O	1:B:389:ILE:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:291:SER:O	1:K:298:SER:OG	2.23	0.52
1:F:53:MET:SD	1:F:58:LEU:HB3	2.50	0.52
1:I:117:ASP:OD2	1:I:117:ASP:N	2.43	0.52
1:I:336:CYS:HB3	1:I:343:ILE:HG13	1.92	0.52
1:N:323:ILE:HG12	1:N:356:MET:HB2	1.91	0.52
1:B:290:THR:CG2	1:C:298:SER:HA	2.40	0.52
1:E:387:PRO:O	1:E:389:ILE:N	2.43	0.52
1:L:24:MET:HE1	1:L:67:VAL:HG22	1.92	0.52
1:E:294:ASN:HA	1:F:294:ASN:HB2	1.92	0.51
1:G:274:ARG:HD3	1:H:142:ASN:HB2	1.92	0.51
1:H:290:THR:HG23	1:H:299:THR:N	2.23	0.51
1:J:289:VAL:HG22	1:K:301:THR:N	2.21	0.51
1:I:381:PRO:HG3	1:J:256:GLU:HB2	1.91	0.51
1:A:274:ARG:HD3	1:B:142:ASN:HB2	1.92	0.51
1:E:292:ILE:HD11	1:F:296:GLY:H	1.74	0.51
1:K:199:LEU:HG	1:K:201:ASN:H	1.75	0.51
1:A:51:LEU:HG	1:B:66:ILE:HG12	1.93	0.51
1:I:172:ILE:HD11	1:I:314:PRO:HG3	1.93	0.51
1:A:142:ASN:HB2	1:N:274:ARG:HD3	1.92	0.51
1:H:291:SER:OG	1:H:302:GLU:OE2	2.28	0.51
1:J:290:THR:H	1:K:300:ASN:HA	1.76	0.51
1:M:172:ILE:HD11	1:M:314:PRO:HG3	1.93	0.51
1:A:266:ASN:HB2	1:N:369:TYR:HB3	1.92	0.51
1:G:80:LYS:O	1:G:84:GLN:HG2	2.11	0.51
1:E:93:GLY:O	1:E:132:ARG:NH1	2.35	0.51
1:G:284:GLU:HB3	1:G:303:LEU:HB3	1.92	0.51
1:H:51:LEU:HG	1:I:66:ILE:HG12	1.93	0.51
1:A:303:LEU:HD11	1:N:304:LYS:HG3	1.93	0.51
1:B:53:MET:HE3	1:B:60:MET:SD	2.51	0.51
1:H:284:GLU:HB3	1:H:303:LEU:HB3	1.92	0.51
1:M:290:THR:HG23	1:M:299:THR:N	2.26	0.51
1:N:371:GLU:HG3	1:N:402:ARG:HG2	1.92	0.51
1:C:178:GLU:HB3	1:C:263:THR:HB	1.92	0.51
1:D:292:ILE:HB	1:E:298:SER:CB	2.41	0.51
1:M:242:ALA:HA	1:M:247:ALA:HA	1.93	0.51
1:A:53:MET:HG2	1:A:60:MET:HB2	1.93	0.50
1:A:68:ASN:OD1	1:A:68:ASN:N	2.45	0.50
1:E:336:CYS:HB3	1:E:343:ILE:HG13	1.93	0.50
1:G:356:MET:O	1:H:169:GLN:NE2	2.31	0.50
1:K:51:LEU:HG	1:L:66:ILE:HG12	1.94	0.50
1:A:371:GLU:HG3	1:A:402:ARG:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HD21	1:C:66:ILE:HB	1.93	0.50
1:K:154:GLU:OE1	1:K:158:LYS:NZ	2.44	0.50
1:K:242:ALA:HA	1:K:247:ALA:HA	1.93	0.50
1:I:199:LEU:HG	1:I:201:ASN:H	1.77	0.50
1:K:162:GLU:HG2	1:K:163:LEU:HD12	1.93	0.50
1:L:282:GLY:HA3	1:L:307:VAL:HA	1.92	0.50
1:M:292:ILE:HB	1:N:298:SER:CB	2.41	0.50
1:N:53:MET:HE3	1:N:60:MET:SD	2.51	0.50
1:F:290:THR:HG23	1:F:299:THR:N	2.27	0.50
1:H:274:ARG:HD3	1:I:142:ASN:HB2	1.91	0.50
1:L:292:ILE:HD13	1:M:293:ALA:H	1.75	0.50
1:E:328:ILE:HD11	1:E:409:ILE:HD11	1.94	0.50
1:C:326:VAL:HG11	1:C:409:ILE:HD13	1.93	0.50
1:E:172:ILE:HD11	1:E:314:PRO:HG3	1.94	0.50
1:A:58:LEU:HA	1:A:71:PRO:HA	1.94	0.50
1:B:61:ARG:HD3	1:B:75:LEU:HD21	1.94	0.50
1:F:47:GLN:O	1:F:51:LEU:HD13	2.12	0.50
1:F:53:MET:HE3	1:F:60:MET:SD	2.51	0.50
1:I:162:GLU:OE2	1:J:99:ASN:ND2	2.44	0.50
1:M:53:MET:SD	1:M:58:LEU:HB3	2.52	0.50
1:F:125:ARG:HH12	1:F:127:THR:HG22	1.76	0.50
1:K:172:ILE:HD11	1:K:314:PRO:HG3	1.94	0.49
1:L:271:THR:HB	1:L:277:ALA:HB2	1.94	0.49
1:A:59:ASP:HB2	1:A:72:ARG:HA	1.95	0.49
1:E:162:GLU:HG2	1:E:163:LEU:HD12	1.93	0.49
1:E:178:GLU:HB3	1:E:263:THR:HB	1.93	0.49
1:E:199:LEU:HG	1:E:201:ASN:H	1.77	0.49
1:J:219:LYS:HB3	1:K:231:THR:HB	1.93	0.49
1:A:290:THR:HG22	1:B:298:SER:HA	1.92	0.49
1:B:292:ILE:HB	1:C:298:SER:CB	2.42	0.49
1:M:292:ILE:HB	1:N:298:SER:HB3	1.94	0.49
1:E:290:THR:HB	1:F:299:THR:C	2.38	0.49
1:J:242:ALA:HA	1:J:247:ALA:HA	1.94	0.49
1:L:242:ALA:HA	1:L:247:ALA:HA	1.93	0.49
1:H:290:THR:HB	1:I:299:THR:C	2.36	0.49
1:M:79:ASP:O	1:M:83:LEU:HG	2.13	0.49
1:A:94:ALA:HB3	1:A:96:TYR:HE1	1.78	0.49
1:A:292:ILE:HB	1:B:298:SER:CB	2.42	0.49
1:A:293:ALA:H	1:N:292:ILE:CD1	2.25	0.49
1:F:194:THR:HG21	1:G:230:ILE:H	1.77	0.49
1:H:356:MET:H	1:I:169:GLN:NE2	2.09	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:GLU:HG2	1:I:268:ARG:HB3	1.95	0.49
1:J:178:GLU:HB3	1:J:263:THR:HB	1.93	0.49
1:H:59:ASP:HB2	1:H:72:ARG:HA	1.95	0.49
1:A:369:TYR:HB3	1:B:266:ASN:HB2	1.94	0.49
1:C:51:LEU:HD21	1:D:66:ILE:HB	1.93	0.49
1:C:53:MET:HE3	1:C:60:MET:SD	2.53	0.49
1:C:61:ARG:HD3	1:C:75:LEU:HD21	1.95	0.49
1:J:172:ILE:HD11	1:J:314:PRO:HG3	1.95	0.49
1:M:353:THR:OG1	1:N:270:LEU:O	2.24	0.49
1:C:302:GLU:OE2	1:C:304:LYS:NZ	2.41	0.49
1:G:154:GLU:OE1	1:G:158:LYS:NZ	2.45	0.49
1:H:117:ASP:N	1:H:117:ASP:OD1	2.46	0.49
1:N:380:VAL:HG11	1:N:383:LEU:HD12	1.94	0.49
1:A:296:GLY:HA3	1:N:296:GLY:HA2	1.95	0.49
1:B:356:MET:H	1:C:169:GLN:NE2	2.10	0.49
1:E:154:GLU:OE1	1:E:158:LYS:NZ	2.46	0.49
1:G:326:VAL:HG11	1:G:409:ILE:HD13	1.94	0.49
1:I:242:ALA:HA	1:I:247:ALA:HA	1.94	0.49
1:J:387:PRO:O	1:J:389:ILE:N	2.43	0.49
1:L:199:LEU:HG	1:L:201:ASN:H	1.76	0.49
1:N:173:GLU:HG2	1:N:268:ARG:HB3	1.95	0.49
1:D:242:ALA:HA	1:D:247:ALA:HA	1.95	0.48
1:F:387:PRO:O	1:F:389:ILE:N	2.45	0.48
1:G:315:ASN:N	1:G:323:ILE:O	2.44	0.48
1:K:53:MET:HE3	1:K:60:MET:SD	2.53	0.48
1:D:287:PHE:O	1:D:289:VAL:N	2.43	0.48
1:E:282:GLY:HA3	1:E:307:VAL:HA	1.94	0.48
1:F:154:GLU:OE1	1:F:158:LYS:NZ	2.45	0.48
1:F:356:MET:O	1:G:169:GLN:NE2	2.44	0.48
1:M:84:GLN:OE1	1:N:92:LEU:HD11	2.13	0.48
1:N:59:ASP:HB2	1:N:72:ARG:HA	1.95	0.48
1:B:199:LEU:HG	1:B:201:ASN:H	1.77	0.48
1:D:294:ASN:HA	1:E:294:ASN:HB2	1.94	0.48
1:I:387:PRO:O	1:I:389:ILE:N	2.43	0.48
1:H:292:ILE:HD13	1:I:293:ALA:H	1.78	0.48
1:N:199:LEU:HG	1:N:201:ASN:H	1.78	0.48
1:A:79:ASP:O	1:A:83:LEU:HG	2.13	0.48
1:C:211:ASN:HD21	1:C:220:TRP:HB3	1.79	0.48
1:F:369:TYR:HB3	1:G:266:ASN:HB2	1.94	0.48
1:G:51:LEU:HG	1:H:66:ILE:HG12	1.94	0.48
1:H:369:TYR:HB3	1:I:266:ASN:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:LEU:HG	1:J:201:ASN:H	1.77	0.48
1:K:387:PRO:O	1:K:389:ILE:N	2.43	0.48
1:E:53:MET:SD	1:E:58:LEU:HB3	2.54	0.48
1:G:290:THR:HA	1:G:299:THR:HA	1.95	0.48
1:H:199:LEU:HG	1:H:201:ASN:H	1.78	0.48
1:A:175:ARG:HH22	1:A:362:THR:HG21	1.78	0.48
1:B:284:GLU:HB3	1:B:303:LEU:HB3	1.96	0.48
1:E:117:ASP:OD1	1:E:117:ASP:N	2.45	0.48
1:E:242:ALA:HA	1:E:247:ALA:HA	1.95	0.48
1:G:5:ASP:HB3	1:G:40:LEU:HB2	1.94	0.48
1:H:315:ASN:N	1:H:323:ILE:O	2.43	0.48
1:L:154:GLU:OE1	1:L:158:LYS:NZ	2.45	0.48
1:M:154:GLU:OE1	1:M:158:LYS:NZ	2.45	0.48
1:B:51:LEU:HG	1:C:66:ILE:HG12	1.95	0.48
1:C:242:ALA:HA	1:C:247:ALA:HA	1.95	0.48
1:D:292:ILE:HD13	1:E:293:ALA:H	1.79	0.48
1:E:88:ASP:O	1:E:92:LEU:HB3	2.12	0.48
1:H:5:ASP:HB3	1:H:40:LEU:HB2	1.95	0.48
1:I:290:THR:H	1:J:300:ASN:HA	1.79	0.48
1:L:51:LEU:HG	1:M:66:ILE:HG12	1.95	0.48
1:B:242:ALA:HA	1:B:247:ALA:HA	1.96	0.48
1:B:91:ASP:O	1:B:132:ARG:NH1	2.47	0.48
1:D:154:GLU:OE1	1:D:158:LYS:NZ	2.47	0.48
1:F:172:ILE:HD11	1:F:314:PRO:HG3	1.95	0.48
1:F:242:ALA:HA	1:F:247:ALA:HA	1.95	0.48
1:H:356:MET:H	1:I:169:GLN:HE21	1.60	0.48
1:I:51:LEU:HD21	1:J:66:ILE:HB	1.96	0.48
1:N:129:VAL:HG12	1:N:131:GLY:H	1.79	0.48
1:C:53:MET:SD	1:C:58:LEU:HB3	2.54	0.47
1:C:199:LEU:HG	1:C:201:ASN:H	1.78	0.47
1:G:242:ALA:HA	1:G:247:ALA:HA	1.95	0.47
1:H:387:PRO:O	1:H:389:ILE:N	2.43	0.47
1:N:326:VAL:HG11	1:N:409:ILE:HD13	1.96	0.47
1:A:51:LEU:HD21	1:B:66:ILE:HB	1.97	0.47
1:J:282:GLY:HA3	1:J:307:VAL:HA	1.95	0.47
1:L:211:ASN:HD21	1:L:220:TRP:HB3	1.79	0.47
1:A:387:PRO:O	1:A:389:ILE:N	2.41	0.47
1:B:294:ASN:HA	1:C:294:ASN:HB2	1.95	0.47
1:C:60:MET:HE1	1:C:67:VAL:HB	1.96	0.47
1:C:239:LEU:HD12	1:C:250:LEU:HD22	1.95	0.47
1:E:290:THR:HG22	1:F:298:SER:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:MET:HE3	1:A:60:MET:HB2	1.96	0.47
1:H:242:ALA:HA	1:H:247:ALA:HA	1.95	0.47
1:N:242:ALA:HA	1:N:247:ALA:HA	1.96	0.47
1:D:287:PHE:O	1:D:301:THR:HG23	2.15	0.47
1:I:178:GLU:HB2	1:I:263:THR:HB	1.97	0.47
1:J:292:ILE:HD11	1:K:295:GLY:H	1.79	0.47
1:L:51:LEU:HD21	1:M:66:ILE:HB	1.97	0.47
1:A:299:THR:C	1:N:290:THR:HB	2.40	0.47
1:F:199:LEU:HG	1:F:201:ASN:H	1.78	0.47
1:F:323:ILE:HG12	1:F:356:MET:HB2	1.96	0.47
1:K:365:VAL:HA	1:L:270:LEU:HB3	1.95	0.47
1:M:292:ILE:CD1	1:N:293:ALA:H	2.28	0.47
1:C:24:MET:HE1	1:C:66:ILE:C	2.40	0.47
1:E:79:ASP:O	1:E:83:LEU:HD13	2.15	0.47
1:H:304:LYS:HG3	1:I:303:LEU:HD11	1.96	0.47
1:I:189:VAL:HG13	1:I:252:LEU:HD12	1.96	0.47
1:L:159:LEU:O	1:L:163:LEU:HB2	2.15	0.47
1:A:290:THR:HB	1:B:299:THR:C	2.40	0.47
1:D:328:ILE:HD11	1:D:409:ILE:HD11	1.97	0.47
1:N:53:MET:SD	1:N:58:LEU:HB3	2.54	0.47
1:B:315:ASN:N	1:B:323:ILE:O	2.46	0.47
1:D:88:ASP:HA	1:D:91:ASP:HB3	1.96	0.47
1:D:326:VAL:HG11	1:D:409:ILE:HD13	1.96	0.47
1:J:83:LEU:O	1:J:86:GLU:HG2	2.15	0.47
1:K:369:TYR:HB3	1:L:266:ASN:HB2	1.97	0.47
1:L:387:PRO:O	1:L:389:ILE:N	2.47	0.47
1:C:194:THR:HG21	1:D:230:ILE:H	1.80	0.47
1:D:315:ASN:N	1:D:323:ILE:O	2.43	0.47
1:E:290:THR:N	1:F:300:ASN:HA	2.30	0.47
1:J:82:PHE:CD1	1:J:82:PHE:C	2.93	0.47
1:K:290:THR:CG2	1:L:298:SER:HA	2.45	0.47
1:K:357:VAL:HB	1:K:363:LEU:HD13	1.97	0.47
1:N:128:LEU:HD12	1:N:128:LEU:HA	1.82	0.47
1:H:159:LEU:O	1:H:163:LEU:HB2	2.15	0.46
1:K:82:PHE:CD1	1:K:82:PHE:C	2.93	0.46
1:E:292:ILE:HD13	1:F:293:ALA:H	1.80	0.46
1:I:53:MET:SD	1:I:58:LEU:HB3	2.55	0.46
1:A:271:THR:HB	1:A:277:ALA:HB2	1.98	0.46
1:B:271:THR:HB	1:B:277:ALA:HB2	1.98	0.46
1:D:199:LEU:HG	1:D:201:ASN:H	1.79	0.46
1:G:356:MET:H	1:H:169:GLN:NE2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:125:ARG:HH12	1:K:127:THR:HG22	1.79	0.46
1:L:84:GLN:OE1	1:M:92:LEU:HD11	2.15	0.46
1:L:290:THR:HB	1:M:299:THR:C	2.39	0.46
1:M:24:MET:HE1	1:M:67:VAL:HG22	1.96	0.46
1:A:280:GLU:OE2	1:A:305:LYS:NZ	2.49	0.46
1:D:211:ASN:HD21	1:D:220:TRP:HB3	1.80	0.46
1:G:199:LEU:HG	1:G:201:ASN:H	1.81	0.46
1:G:387:PRO:O	1:G:389:ILE:N	2.42	0.46
1:J:154:GLU:OE1	1:J:158:LYS:NZ	2.47	0.46
1:E:356:MET:O	1:F:169:GLN:NE2	2.45	0.46
1:G:19:ALA:HB2	1:G:26:ILE:HB	1.97	0.46
1:G:211:ASN:HD21	1:G:220:TRP:HB3	1.81	0.46
1:G:290:THR:HB	1:H:299:THR:C	2.40	0.46
1:L:290:THR:HB	1:M:299:THR:N	2.31	0.46
1:L:372:ASP:HB2	1:L:401:ASP:HB2	1.97	0.46
1:M:51:LEU:HD21	1:N:66:ILE:HB	1.97	0.46
1:N:387:PRO:O	1:N:389:ILE:N	2.42	0.46
1:E:369:TYR:HB3	1:F:266:ASN:HB2	1.96	0.46
1:F:292:ILE:HB	1:G:298:SER:CB	2.40	0.46
1:B:172:ILE:HD11	1:B:314:PRO:HG3	1.98	0.46
1:D:79:ASP:O	1:D:83:LEU:HD13	2.15	0.46
1:B:92:LEU:HD13	1:B:92:LEU:O	2.16	0.46
1:C:117:ASP:OD2	1:C:117:ASP:N	2.47	0.46
1:D:53:MET:HE3	1:D:60:MET:SD	2.56	0.46
1:D:60:MET:HE1	1:D:67:VAL:HB	1.98	0.46
1:D:317:THR:OG1	1:D:319:ASP:OD2	2.32	0.46
1:H:79:ASP:O	1:H:83:LEU:HG	2.15	0.46
1:I:292:ILE:HD11	1:J:296:GLY:H	1.81	0.46
1:K:110:PHE:HA	1:K:113:ILE:HB	1.98	0.46
1:N:117:ASP:OD1	1:N:117:ASP:N	2.48	0.46
1:C:282:GLY:HA3	1:C:307:VAL:HA	1.98	0.46
1:M:83:LEU:HD12	1:N:92:LEU:HD12	1.97	0.46
1:N:154:GLU:OE1	1:N:158:LYS:NZ	2.48	0.46
1:A:61:ARG:HD3	1:A:75:LEU:HD21	1.97	0.46
1:C:292:ILE:HD11	1:D:296:GLY:H	1.80	0.46
1:K:292:ILE:HD12	1:L:298:SER:HB3	1.98	0.46
1:M:284:GLU:HB3	1:M:303:LEU:HB3	1.97	0.46
1:E:18:LEU:HD11	1:E:52:VAL:HG21	1.97	0.45
1:J:211:ASN:HD21	1:J:220:TRP:HB3	1.81	0.45
1:J:369:TYR:HB3	1:K:266:ASN:HB2	1.98	0.45
1:K:271:THR:HB	1:K:277:ALA:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:297:SER:O	1:K:297:SER:OG	2.28	0.45
1:L:328:ILE:HD11	1:L:409:ILE:HD11	1.97	0.45
1:N:80:LYS:O	1:N:84:GLN:HG2	2.16	0.45
1:D:53:MET:SD	1:D:58:LEU:HB3	2.56	0.45
1:H:172:ILE:HD11	1:H:314:PRO:HG3	1.98	0.45
1:I:340:ASN:C	1:I:340:ASN:HD22	2.22	0.45
1:K:18:LEU:HD11	1:K:52:VAL:HG21	1.98	0.45
1:B:194:THR:HG21	1:C:230:ILE:H	1.81	0.45
1:B:290:THR:HB	1:C:299:THR:C	2.41	0.45
1:E:175:ARG:HH22	1:E:362:THR:HG21	1.81	0.45
1:I:211:ASN:HD21	1:I:220:TRP:HB3	1.82	0.45
1:L:292:ILE:CD1	1:M:293:ALA:H	2.30	0.45
1:A:242:ALA:HA	1:A:247:ALA:HA	1.99	0.45
1:C:51:LEU:HD11	1:D:66:ILE:HG21	1.98	0.45
1:I:53:MET:HE3	1:I:60:MET:SD	2.57	0.45
1:K:51:LEU:HD21	1:L:66:ILE:HB	1.98	0.45
1:K:292:ILE:HB	1:L:298:SER:CB	2.47	0.45
1:M:110:PHE:HA	1:M:113:ILE:HB	1.99	0.45
1:M:290:THR:CG2	1:N:298:SER:HA	2.46	0.45
1:A:392:LEU:HD23	1:A:392:LEU:H	1.82	0.45
1:C:162:GLU:HG2	1:C:163:LEU:HD12	1.98	0.45
1:D:172:ILE:HG12	1:D:312:VAL:HG21	1.98	0.45
1:F:260:LYS:HB2	1:F:260:LYS:HE3	1.81	0.45
1:G:328:ILE:HD11	1:G:409:ILE:HD11	1.98	0.45
1:J:189:VAL:HG13	1:J:252:LEU:HD12	1.98	0.45
1:K:47:GLN:O	1:K:51:LEU:HD13	2.16	0.45
1:K:297:SER:HB2	1:L:297:SER:O	2.16	0.45
1:A:199:LEU:HG	1:A:201:ASN:H	1.80	0.45
1:G:128:LEU:HD12	1:G:128:LEU:HA	1.81	0.45
1:B:296:GLY:HA2	1:C:296:GLY:HA3	1.97	0.45
1:D:82:PHE:C	1:D:82:PHE:CD1	2.95	0.45
1:D:290:THR:CG2	1:E:298:SER:HA	2.45	0.45
1:D:292:ILE:HD13	1:E:292:ILE:HA	1.99	0.45
1:A:110:PHE:HA	1:A:113:ILE:HB	1.99	0.45
1:D:40:LEU:HD23	1:E:25:ASN:HD22	1.82	0.45
1:E:194:THR:HG21	1:F:230:ILE:H	1.82	0.45
1:F:61:ARG:HD3	1:F:75:LEU:HD21	1.99	0.45
1:H:280:GLU:OE2	1:H:305:LYS:NZ	2.34	0.45
1:I:60:MET:HE1	1:I:67:VAL:HB	1.99	0.45
1:L:53:MET:SD	1:L:58:LEU:HB3	2.56	0.45
1:A:211:ASN:HD21	1:A:220:TRP:HB3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:HG	1:D:66:ILE:HG12	1.97	0.45
1:K:168:GLN:O	1:K:273:ASN:N	2.50	0.45
1:N:92:LEU:HD13	1:N:92:LEU:O	2.17	0.45
1:N:211:ASN:HD21	1:N:220:TRP:HB3	1.82	0.45
1:G:194:THR:HG21	1:H:230:ILE:H	1.82	0.45
1:H:60:MET:HE3	1:H:61:ARG:N	2.32	0.45
1:K:53:MET:SD	1:K:58:LEU:HB3	2.57	0.45
1:M:387:PRO:O	1:M:389:ILE:N	2.49	0.45
1:A:178:GLU:HB2	1:A:263:THR:HB	1.99	0.44
1:B:47:GLN:O	1:B:51:LEU:HD13	2.16	0.44
1:F:226:ILE:HG23	1:F:230:ILE:HD11	1.98	0.44
1:F:271:THR:HB	1:F:277:ALA:HB2	1.98	0.44
1:F:290:THR:CG2	1:G:298:SER:HA	2.46	0.44
1:H:51:LEU:HD21	1:I:66:ILE:HB	1.99	0.44
1:J:168:GLN:O	1:J:273:ASN:N	2.50	0.44
1:J:351:LEU:HD12	1:K:279:ILE:HB	1.99	0.44
1:L:294:ASN:HA	1:M:294:ASN:HB2	1.99	0.44
1:M:129:VAL:HG12	1:M:131:GLY:H	1.82	0.44
1:E:292:ILE:HB	1:F:298:SER:CB	2.47	0.44
1:F:19:ALA:HB2	1:F:26:ILE:HB	1.99	0.44
1:H:8:ASP:OD1	1:H:8:ASP:N	2.50	0.44
1:J:129:VAL:HG12	1:J:131:GLY:H	1.82	0.44
1:N:61:ARG:HD3	1:N:75:LEU:HD21	1.99	0.44
1:A:159:LEU:O	1:A:163:LEU:HB2	2.17	0.44
1:A:211:ASN:ND2	1:A:220:TRP:HB3	2.32	0.44
1:B:129:VAL:HG12	1:B:131:GLY:H	1.82	0.44
1:H:129:VAL:HG12	1:H:131:GLY:H	1.82	0.44
1:M:274:ARG:HD3	1:N:142:ASN:HB2	1.99	0.44
1:A:254:ALA:HB1	1:N:381:PRO:HD2	1.99	0.44
1:D:168:GLN:O	1:D:273:ASN:N	2.51	0.44
1:F:8:ASP:OD1	1:F:8:ASP:N	2.50	0.44
1:I:110:PHE:HA	1:I:113:ILE:HB	2.00	0.44
1:I:290:THR:O	1:J:300:ASN:HB3	2.18	0.44
1:L:237:ILE:HD11	1:L:252:LEU:HD12	1.99	0.44
1:A:381:PRO:HD2	1:B:254:ALA:HB1	1.98	0.44
1:B:53:MET:SD	1:B:58:LEU:HB3	2.57	0.44
1:D:194:THR:HG21	1:E:230:ILE:H	1.82	0.44
1:G:172:ILE:HD11	1:G:314:PRO:HG3	1.99	0.44
1:I:59:ASP:HB2	1:I:72:ARG:HA	2.00	0.44
1:I:129:VAL:HG12	1:I:131:GLY:H	1.82	0.44
1:K:289:VAL:HG21	1:K:304:LYS:NZ	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:ARG:HH22	1:L:362:THR:HG21	1.82	0.44
1:D:336:CYS:HB3	1:D:343:ILE:HG13	2.00	0.44
1:G:51:LEU:HD21	1:H:66:ILE:HB	1.99	0.44
1:G:58:LEU:HA	1:G:71:PRO:HA	2.00	0.44
1:J:8:ASP:OD1	1:J:8:ASP:N	2.51	0.44
1:M:284:GLU:HB2	1:M:303:LEU:HD23	2.00	0.44
1:D:8:ASP:OD1	1:D:8:ASP:N	2.51	0.44
1:D:51:LEU:HD21	1:E:66:ILE:HB	2.00	0.44
1:E:353:THR:OG1	1:F:270:LEU:O	2.28	0.44
1:F:58:LEU:HD13	1:F:71:PRO:HA	1.99	0.44
1:F:110:PHE:HA	1:F:113:ILE:HB	2.00	0.44
1:L:296:GLY:HA2	1:M:296:GLY:HA3	1.99	0.44
1:D:80:LYS:O	1:D:84:GLN:HG2	2.17	0.44
1:G:61:ARG:HD3	1:G:75:LEU:HD21	1.98	0.44
1:H:53:MET:HE3	1:H:60:MET:SD	2.58	0.44
1:H:110:PHE:HA	1:H:113:ILE:HB	2.00	0.44
1:I:322:ILE:HG22	1:I:324:MET:HG2	1.98	0.44
1:K:58:LEU:HD13	1:K:71:PRO:HA	2.00	0.44
1:K:125:ARG:HG2	1:K:125:ARG:HH11	1.82	0.44
1:K:194:THR:HG21	1:L:230:ILE:H	1.83	0.44
1:M:8:ASP:OD1	1:M:8:ASP:N	2.50	0.44
1:B:211:ASN:HD21	1:B:220:TRP:HB3	1.83	0.44
1:C:159:LEU:O	1:C:163:LEU:HB2	2.17	0.44
1:C:172:ILE:HD11	1:C:314:PRO:HG3	1.99	0.44
1:H:175:ARG:HH22	1:H:362:THR:HG21	1.82	0.44
1:I:8:ASP:OD1	1:I:8:ASP:N	2.51	0.44
1:M:381:PRO:HD2	1:N:254:ALA:HB1	1.99	0.44
1:A:270:LEU:O	1:N:353:THR:OG1	2.27	0.43
1:B:365:VAL:HA	1:C:270:LEU:HB3	2.00	0.43
1:D:110:PHE:HA	1:D:113:ILE:HB	2.00	0.43
1:E:219:LYS:HD2	1:E:219:LYS:HA	1.82	0.43
1:F:51:LEU:HD21	1:G:66:ILE:HB	1.99	0.43
1:G:129:VAL:HG12	1:G:131:GLY:H	1.83	0.43
1:G:294:ASN:HA	1:H:294:ASN:HB2	1.99	0.43
1:K:290:THR:HB	1:L:299:THR:C	2.42	0.43
1:M:271:THR:HB	1:M:277:ALA:HB2	2.00	0.43
1:N:24:MET:HE1	1:N:67:VAL:HG22	1.99	0.43
1:N:382:LEU:HD13	1:N:382:LEU:O	2.18	0.43
1:A:282:GLY:HA3	1:A:307:VAL:HA	2.00	0.43
1:B:79:ASP:O	1:B:83:LEU:HD13	2.18	0.43
1:B:381:PRO:HD2	1:C:254:ALA:HB1	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ASP:OD1	1:C:8:ASP:N	2.51	0.43
1:G:292:ILE:HB	1:H:298:SER:HB3	1.99	0.43
1:G:292:ILE:CD1	1:H:293:ALA:H	2.31	0.43
1:H:292:ILE:HB	1:I:298:SER:CB	2.49	0.43
1:J:292:ILE:HD11	1:K:296:GLY:H	1.82	0.43
1:L:292:ILE:HB	1:M:298:SER:HB3	1.99	0.43
1:M:211:ASN:HD21	1:M:220:TRP:HB3	1.83	0.43
1:D:61:ARG:HD3	1:D:75:LEU:HD21	2.00	0.43
1:D:290:THR:HA	1:D:299:THR:HA	2.00	0.43
1:E:110:PHE:HA	1:E:113:ILE:HB	2.00	0.43
1:J:59:ASP:HB2	1:J:72:ARG:HA	2.01	0.43
1:J:110:PHE:HA	1:J:113:ILE:HB	2.01	0.43
1:J:290:THR:HG23	1:J:299:THR:N	2.33	0.43
1:B:356:MET:H	1:C:169:GLN:HE21	1.65	0.43
1:E:290:THR:HB	1:F:299:THR:N	2.33	0.43
1:E:292:ILE:CD1	1:F:293:ALA:H	2.30	0.43
1:F:211:ASN:HD21	1:F:220:TRP:HB3	1.82	0.43
1:F:304:LYS:HG3	1:G:303:LEU:HD11	2.00	0.43
1:F:368:ILE:HD11	1:G:279:ILE:HG12	2.01	0.43
1:J:326:VAL:HG11	1:J:409:ILE:HD13	2.00	0.43
1:L:211:ASN:ND2	1:L:220:TRP:HB3	2.33	0.43
1:A:290:THR:CG2	1:B:298:SER:HA	2.49	0.43
1:C:110:PHE:HA	1:C:113:ILE:HB	2.01	0.43
1:C:292:ILE:CD1	1:D:293:ALA:H	2.23	0.43
1:L:292:ILE:HD11	1:M:296:GLY:H	1.84	0.43
1:M:237:ILE:HD11	1:M:252:LEU:HD12	2.01	0.43
1:N:110:PHE:HA	1:N:113:ILE:HB	2.01	0.43
1:A:386:ILE:H	1:A:386:ILE:HG13	1.61	0.43
1:C:289:VAL:HG22	1:D:301:THR:N	2.32	0.43
1:F:18:LEU:HD11	1:F:52:VAL:HG21	2.00	0.43
1:H:211:ASN:HD21	1:H:220:TRP:HB3	1.83	0.43
1:I:88:ASP:HA	1:I:91:ASP:OD2	2.19	0.43
1:I:194:THR:HG21	1:J:230:ILE:H	1.83	0.43
1:J:392:LEU:HD23	1:J:392:LEU:H	1.83	0.43
1:A:66:ILE:HG21	1:N:51:LEU:HD11	2.01	0.43
1:A:199:LEU:HB3	1:A:204:SER:HB3	2.01	0.43
1:F:173:GLU:HG2	1:F:268:ARG:HB3	2.00	0.43
1:H:282:GLY:HA3	1:H:307:VAL:HA	1.99	0.43
1:K:80:LYS:HE3	1:K:80:LYS:HB3	1.77	0.43
1:K:356:MET:O	1:L:169:GLN:NE2	2.47	0.43
1:L:83:LEU:HA	1:L:86:GLU:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:LEU:HG	1:M:201:ASN:H	1.83	0.43
1:N:328:ILE:HD11	1:N:409:ILE:HD11	1.99	0.43
1:B:154:GLU:OE1	1:B:158:LYS:NZ	2.52	0.43
1:E:8:ASP:OD1	1:E:8:ASP:N	2.51	0.43
1:H:125:ARG:HH12	1:H:127:THR:HG22	1.83	0.43
1:J:51:LEU:HD11	1:K:66:ILE:HG21	2.01	0.43
1:L:82:PHE:C	1:L:82:PHE:CD2	2.97	0.43
1:M:290:THR:HB	1:N:299:THR:C	2.43	0.43
1:C:388:VAL:HB	1:C:389:ILE:HD12	2.00	0.43
1:G:22:SER:C	1:G:24:MET:N	2.77	0.43
1:N:392:LEU:H	1:N:392:LEU:HD23	1.84	0.43
1:H:292:ILE:CD1	1:I:293:ALA:H	2.31	0.43
1:A:27:VAL:HG23	1:A:66:ILE:HD11	2.00	0.42
1:A:353:THR:OG1	1:B:270:LEU:O	2.27	0.42
1:C:306:ALA:HB2	1:C:346:ILE:HD13	2.01	0.42
1:F:282:GLY:HA3	1:F:307:VAL:HA	2.00	0.42
1:G:8:ASP:OD1	1:G:8:ASP:N	2.50	0.42
1:H:154:GLU:OE1	1:H:158:LYS:NZ	2.50	0.42
1:I:47:GLN:O	1:I:51:LEU:HD13	2.19	0.42
1:J:53:MET:HE3	1:J:60:MET:SD	2.59	0.42
1:L:349:LYS:HB2	1:L:349:LYS:HE2	1.81	0.42
1:M:369:TYR:HB3	1:N:266:ASN:HB2	2.01	0.42
1:N:211:ASN:ND2	1:N:220:TRP:HB3	2.34	0.42
1:C:97:SER:HA	1:C:147:THR:HA	2.01	0.42
1:D:353:THR:OG1	1:E:270:LEU:O	2.26	0.42
1:I:95:LEU:HD11	1:I:132:ARG:HG2	2.00	0.42
1:I:292:ILE:HB	1:J:298:SER:CB	2.49	0.42
1:J:194:THR:HG21	1:K:230:ILE:H	1.83	0.42
1:L:92:LEU:HD13	1:L:92:LEU:O	2.19	0.42
1:L:110:PHE:HA	1:L:113:ILE:HB	2.02	0.42
1:M:53:MET:HE3	1:M:60:MET:SD	2.58	0.42
1:M:315:ASN:N	1:M:323:ILE:O	2.48	0.42
1:N:191:PHE:HB3	1:N:212:SER:HB3	2.02	0.42
1:A:191:PHE:HB3	1:A:212:SER:HB3	2.00	0.42
1:D:280:GLU:HB3	1:D:307:VAL:HG21	2.01	0.42
1:J:15:LEU:HD22	1:J:26:ILE:HD11	2.01	0.42
1:K:282:GLY:HA3	1:K:307:VAL:HA	2.00	0.42
1:L:125:ARG:HH12	1:L:127:THR:HG22	1.84	0.42
1:M:68:ASN:OD1	1:M:68:ASN:N	2.52	0.42
1:B:189:VAL:HG13	1:B:252:LEU:HD12	2.00	0.42
1:B:199:LEU:HB3	1:B:204:SER:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD23	1:C:128:LEU:HA	1.80	0.42
1:D:127:THR:HG21	1:E:133:GLY:HA2	2.01	0.42
1:F:353:THR:OG1	1:G:270:LEU:O	2.25	0.42
1:G:110:PHE:HA	1:G:113:ILE:HB	2.02	0.42
1:G:173:GLU:HG2	1:G:268:ARG:HB3	2.01	0.42
1:I:154:GLU:OE1	1:I:158:LYS:NZ	2.50	0.42
1:I:382:LEU:HD13	1:I:382:LEU:O	2.20	0.42
1:L:290:THR:HG22	1:M:298:SER:HA	2.02	0.42
1:A:172:ILE:HD11	1:A:314:PRO:HG3	2.02	0.42
1:A:297:SER:OG	1:N:297:SER:HB3	2.19	0.42
1:E:159:LEU:O	1:E:163:LEU:HB2	2.19	0.42
1:F:292:ILE:CD1	1:G:293:ALA:H	2.26	0.42
1:G:219:LYS:HB3	1:H:231:THR:HB	1.99	0.42
1:I:58:LEU:HD13	1:I:71:PRO:HA	2.02	0.42
1:K:8:ASP:OD1	1:K:8:ASP:N	2.51	0.42
1:K:211:ASN:HD21	1:K:220:TRP:HB3	1.84	0.42
1:A:298:SER:HA	1:N:290:THR:CG2	2.49	0.42
1:B:280:GLU:HB3	1:B:307:VAL:HG21	2.02	0.42
1:E:19:ALA:HB2	1:E:26:ILE:HB	2.01	0.42
1:G:381:PRO:HD2	1:H:254:ALA:HB1	2.00	0.42
1:I:353:THR:OG1	1:J:270:LEU:O	2.25	0.42
1:K:79:ASP:O	1:K:83:LEU:HD13	2.19	0.42
1:L:47:GLN:O	1:L:51:LEU:HD13	2.18	0.42
1:L:80:LYS:O	1:L:84:GLN:HG2	2.19	0.42
1:L:129:VAL:HG12	1:L:131:GLY:H	1.84	0.42
1:M:194:THR:HG21	1:N:230:ILE:H	1.85	0.42
1:A:292:ILE:CD1	1:B:293:ALA:H	2.30	0.42
1:C:19:ALA:HB2	1:C:26:ILE:HB	2.02	0.42
1:C:389:ILE:HD12	1:C:389:ILE:N	2.35	0.42
1:E:173:GLU:HG2	1:E:268:ARG:HB3	2.02	0.42
1:E:290:THR:CG2	1:F:298:SER:HA	2.49	0.42
1:F:79:ASP:O	1:F:83:LEU:HD13	2.19	0.42
1:H:365:VAL:HA	1:I:270:LEU:HB3	2.01	0.42
1:I:175:ARG:HH22	1:I:362:THR:HG21	1.85	0.42
1:A:328:ILE:HD11	1:A:409:ILE:HD11	2.01	0.42
1:B:110:PHE:HA	1:B:113:ILE:HB	2.02	0.42
1:C:175:ARG:HH22	1:C:362:THR:HG21	1.85	0.42
1:C:328:ILE:HD11	1:C:409:ILE:HD11	2.01	0.42
1:D:175:ARG:HH22	1:D:362:THR:HG21	1.84	0.42
1:E:27:VAL:HG23	1:E:66:ILE:HD11	2.01	0.42
1:F:290:THR:HB	1:G:299:THR:C	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:TYR:HB3	1:D:266:ASN:HB2	2.01	0.42
1:H:237:ILE:HD11	1:H:252:LEU:HD23	2.01	0.42
1:H:317:THR:OG1	1:H:319:ASP:OD2	2.30	0.42
1:N:68:ASN:OD1	1:N:68:ASN:N	2.52	0.42
1:C:154:GLU:OE1	1:C:158:LYS:NZ	2.52	0.42
1:G:175:ARG:HH22	1:G:362:THR:HG21	1.84	0.42
1:G:189:VAL:HG13	1:G:252:LEU:HD13	2.02	0.42
1:C:208:TRP:HB3	1:D:239:LEU:HD23	2.01	0.41
1:C:290:THR:CG2	1:D:298:SER:HA	2.50	0.41
1:D:173:GLU:HG2	1:D:268:ARG:HB3	2.02	0.41
1:I:282:GLY:HA3	1:I:307:VAL:HA	2.00	0.41
1:L:61:ARG:HD3	1:L:75:LEU:HD21	2.02	0.41
1:A:47:GLN:O	1:A:51:LEU:HD13	2.19	0.41
1:A:76:LEU:HD11	1:B:85:ALA:HB1	2.01	0.41
1:A:368:ILE:HD11	1:B:279:ILE:HG12	2.01	0.41
1:B:369:TYR:HB3	1:C:266:ASN:HB2	2.03	0.41
1:J:97:SER:HA	1:J:147:THR:HA	2.03	0.41
1:J:125:ARG:HH12	1:J:127:THR:HG22	1.85	0.41
1:L:59:ASP:HB2	1:L:72:ARG:HA	2.02	0.41
1:L:162:GLU:HG2	1:L:163:LEU:HD12	2.02	0.41
1:A:323:ILE:HG12	1:A:356:MET:HB2	2.01	0.41
1:B:93:GLY:O	1:B:132:ARG:NH1	2.39	0.41
1:J:127:THR:HG21	1:K:133:GLY:HA2	2.03	0.41
1:K:370:GLU:HB2	1:K:403:ARG:HB2	2.02	0.41
1:C:237:ILE:HD11	1:C:252:LEU:HD12	2.02	0.41
1:C:372:ASP:HB2	1:C:401:ASP:HB2	2.03	0.41
1:D:292:ILE:HB	1:E:298:SER:HB3	2.03	0.41
1:J:79:ASP:O	1:J:83:LEU:HD13	2.20	0.41
1:K:373:ASN:HB2	1:L:262:LYS:HB3	2.02	0.41
1:M:128:LEU:HD23	1:M:128:LEU:HA	1.81	0.41
1:D:282:GLY:HA3	1:D:307:VAL:HA	2.02	0.41
1:E:97:SER:HA	1:E:147:THR:HA	2.02	0.41
1:H:72:ARG:HE	1:H:72:ARG:HB3	1.77	0.41
1:H:323:ILE:HG12	1:H:356:MET:HB2	2.02	0.41
1:J:350:ASN:HD21	1:K:305:LYS:NZ	2.19	0.41
1:K:284:GLU:HB3	1:K:303:LEU:HB3	2.02	0.41
1:L:290:THR:CG2	1:M:298:SER:HA	2.51	0.41
1:M:47:GLN:O	1:M:51:LEU:HD13	2.20	0.41
1:M:224:THR:HG21	1:N:228:LEU:HB3	2.02	0.41
1:D:95:LEU:HD22	1:D:148:ASP:HA	2.03	0.41
1:E:168:GLN:O	1:E:273:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:ILE:HD11	1:G:295:GLY:H	1.84	0.41
1:G:18:LEU:HD11	1:G:52:VAL:HG21	2.01	0.41
1:I:292:ILE:CD1	1:J:293:ALA:H	2.34	0.41
1:L:97:SER:HA	1:L:147:THR:HA	2.02	0.41
1:M:84:GLN:HE22	1:N:92:LEU:HD21	1.85	0.41
1:B:386:ILE:H	1:B:386:ILE:HG13	1.72	0.41
1:C:47:GLN:O	1:C:51:LEU:HD13	2.20	0.41
1:D:292:ILE:CD1	1:E:293:ALA:H	2.33	0.41
1:H:95:LEU:HD22	1:H:148:ASP:HA	2.03	0.41
1:J:292:ILE:CD1	1:K:296:GLY:H	2.34	0.41
1:K:59:ASP:HB2	1:K:72:ARG:HA	2.03	0.41
1:K:127:THR:HG23	1:L:134:SER:HB3	2.02	0.41
1:K:159:LEU:O	1:K:163:LEU:HB2	2.20	0.41
1:L:53:MET:HE3	1:L:60:MET:SD	2.60	0.41
1:M:80:LYS:O	1:M:84:GLN:HG2	2.21	0.41
1:B:211:ASN:ND2	1:B:220:TRP:HB3	2.35	0.41
1:B:305:LYS:HE3	1:B:305:LYS:HB2	1.88	0.41
1:B:306:ALA:HB2	1:B:346:ILE:HD13	2.02	0.41
1:C:189:VAL:HG11	1:C:392:LEU:HB2	2.01	0.41
1:F:95:LEU:HD21	1:F:132:ARG:HG3	2.03	0.41
1:G:95:LEU:HD21	1:G:132:ARG:HG3	2.02	0.41
1:I:83:LEU:O	1:I:86:GLU:HG2	2.21	0.41
1:K:199:LEU:HB3	1:K:204:SER:HB3	2.03	0.41
1:L:387:PRO:O	1:L:389:ILE:HD12	2.19	0.41
1:B:95:LEU:HD22	1:B:148:ASP:HA	2.03	0.41
1:B:175:ARG:HH22	1:B:362:THR:HG21	1.86	0.41
1:C:83:LEU:O	1:C:86:GLU:HG2	2.20	0.41
1:D:83:LEU:HA	1:D:86:GLU:HG2	2.03	0.41
1:F:128:LEU:HD23	1:F:128:LEU:HA	1.80	0.41
1:G:58:LEU:HD13	1:G:71:PRO:HA	2.01	0.41
1:H:191:PHE:HB3	1:H:212:SER:HB3	2.02	0.41
1:J:92:LEU:HD13	1:J:92:LEU:O	2.21	0.41
1:M:368:ILE:HD11	1:N:279:ILE:HG12	2.03	0.41
1:C:381:PRO:HD2	1:D:254:ALA:HB1	2.02	0.41
1:D:73:ASP:OD1	1:D:73:ASP:N	2.54	0.41
1:D:91:ASP:C	1:D:91:ASP:OD1	2.64	0.41
1:F:211:ASN:ND2	1:F:220:TRP:HB3	2.35	0.41
1:G:369:TYR:HB3	1:H:266:ASN:HB2	2.03	0.41
1:K:211:ASN:ND2	1:K:220:TRP:HB3	2.36	0.41
1:A:294:ASN:HA	1:B:294:ASN:HB2	2.02	0.40
1:F:372:ASP:HB2	1:F:401:ASP:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:LEU:HD22	1:J:148:ASP:HA	2.03	0.40
1:K:372:ASP:HB2	1:K:401:ASP:HB2	2.03	0.40
1:L:290:THR:N	1:M:300:ASN:HA	2.35	0.40
1:M:356:MET:H	1:N:169:GLN:NE2	2.19	0.40
1:A:292:ILE:HB	1:B:298:SER:HB3	2.03	0.40
1:C:293:ALA:C	1:C:295:GLY:H	2.29	0.40
1:D:211:ASN:ND2	1:D:220:TRP:HB3	2.35	0.40
1:E:58:LEU:HD13	1:E:71:PRO:HA	2.02	0.40
1:G:191:PHE:HB3	1:G:212:SER:HB3	2.03	0.40
1:H:88:ASP:HA	1:H:91:ASP:OD2	2.22	0.40
1:I:290:THR:N	1:J:300:ASN:HA	2.35	0.40
1:J:53:MET:SD	1:J:58:LEU:HB3	2.61	0.40
1:J:287:PHE:O	1:J:301:THR:HG23	2.21	0.40
1:K:97:SER:HA	1:K:147:THR:HA	2.03	0.40
1:A:335:GLN:HB3	1:A:342:THR:HG21	2.03	0.40
1:I:51:LEU:HG	1:J:66:ILE:HG12	2.03	0.40
1:J:19:ALA:HB2	1:J:26:ILE:HB	2.02	0.40
1:M:175:ARG:HH22	1:M:362:THR:HG21	1.85	0.40
1:M:282:GLY:HA3	1:M:307:VAL:HA	2.02	0.40
1:A:133:GLY:HA2	1:N:127:THR:HG21	2.03	0.40
1:F:322:ILE:HD13	1:F:411:PRO:HB2	2.03	0.40
1:G:59:ASP:HB2	1:G:72:ARG:HA	2.04	0.40
1:J:91:ASP:OD1	1:J:92:LEU:N	2.53	0.40
1:J:292:ILE:HD13	1:K:293:ALA:N	2.32	0.40
1:J:353:THR:OG1	1:K:270:LEU:O	2.30	0.40
1:J:399:LYS:HE2	1:J:399:LYS:HB2	1.93	0.40
1:L:239:LEU:HB2	1:L:250:LEU:HB3	2.03	0.40
1:L:414:MET:N	1:L:414:MET:SD	2.94	0.40
1:B:105:LYS:NZ	1:B:109:GLU:OE1	2.50	0.40
1:C:58:LEU:HD13	1:C:71:PRO:HA	2.03	0.40
1:C:289:VAL:HG21	1:C:304:LYS:NZ	2.36	0.40
1:E:306:ALA:HB2	1:E:346:ILE:HD13	2.03	0.40
1:G:47:GLN:O	1:G:51:LEU:HD13	2.21	0.40
1:I:306:ALA:HB2	1:I:346:ILE:HD13	2.02	0.40
1:L:60:MET:HE1	1:L:67:VAL:HB	2.03	0.40
1:L:173:GLU:HG2	1:L:268:ARG:HB3	2.03	0.40
1:M:211:ASN:ND2	1:M:220:TRP:HB3	2.36	0.40
1:M:297:SER:HB3	1:N:297:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/761 (52%)	381 (96%)	16 (4%)	1 (0%)	36	33
1	B	398/761 (52%)	380 (96%)	17 (4%)	1 (0%)	36	33
1	C	398/761 (52%)	381 (96%)	16 (4%)	1 (0%)	36	33
1	D	398/761 (52%)	381 (96%)	16 (4%)	1 (0%)	36	33
1	E	398/761 (52%)	381 (96%)	16 (4%)	1 (0%)	36	33
1	F	398/761 (52%)	383 (96%)	14 (4%)	1 (0%)	36	33
1	G	398/761 (52%)	383 (96%)	14 (4%)	1 (0%)	36	33
1	H	398/761 (52%)	380 (96%)	17 (4%)	1 (0%)	36	33
1	I	398/761 (52%)	379 (95%)	18 (4%)	1 (0%)	36	33
1	J	398/761 (52%)	384 (96%)	13 (3%)	1 (0%)	36	33
1	K	398/761 (52%)	382 (96%)	15 (4%)	1 (0%)	36	33
1	L	398/761 (52%)	383 (96%)	14 (4%)	1 (0%)	36	33
1	M	398/761 (52%)	382 (96%)	15 (4%)	1 (0%)	36	33
1	N	398/761 (52%)	379 (95%)	18 (4%)	1 (0%)	36	33
All	All	5572/10654 (52%)	5339 (96%)	219 (4%)	14 (0%)	37	33

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	B	9	VAL
1	C	9	VAL
1	D	9	VAL
1	E	9	VAL
1	F	9	VAL
1	G	9	VAL
1	H	9	VAL
1	I	9	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	9	VAL
1	K	9	VAL
1	L	9	VAL
1	M	9	VAL
1	N	9	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/632 (54%)	339 (99%)	3 (1%)	70	77
1	B	342/632 (54%)	340 (99%)	2 (1%)	78	84
1	C	342/632 (54%)	341 (100%)	1 (0%)	86	90
1	D	342/632 (54%)	339 (99%)	3 (1%)	70	77
1	E	342/632 (54%)	340 (99%)	2 (1%)	78	84
1	F	342/632 (54%)	340 (99%)	2 (1%)	78	84
1	G	342/632 (54%)	342 (100%)	0	100	100
1	H	342/632 (54%)	339 (99%)	3 (1%)	70	77
1	I	342/632 (54%)	339 (99%)	3 (1%)	70	77
1	J	342/632 (54%)	339 (99%)	3 (1%)	70	77
1	K	342/632 (54%)	341 (100%)	1 (0%)	86	90
1	L	342/632 (54%)	338 (99%)	4 (1%)	63	69
1	M	342/632 (54%)	341 (100%)	1 (0%)	86	90
1	N	342/632 (54%)	338 (99%)	4 (1%)	63	69
All	All	4788/8848 (54%)	4756 (99%)	32 (1%)	73	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	329	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	THR
1	B	117	ASP
1	B	410	THR
1	C	297	SER
1	D	117	ASP
1	D	129	VAL
1	D	324	MET
1	E	329	ASN
1	E	382	LEU
1	F	354	GLN
1	F	382	LEU
1	H	292	ILE
1	H	340	ASN
1	H	410	THR
1	I	329	ASN
1	I	340	ASN
1	I	382	LEU
1	J	118	ASN
1	J	351	LEU
1	J	410	THR
1	K	117	ASP
1	L	91	ASP
1	L	128	LEU
1	L	329	ASN
1	L	410	THR
1	M	382	LEU
1	N	83	LEU
1	N	340	ASN
1	N	382	LEU
1	N	399	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	A	352	ASN
1	B	101	GLN
1	B	329	ASN
1	C	329	ASN
1	C	341	GLN
1	D	235	ASN
1	D	329	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	350	ASN
1	E	352	ASN
1	F	235	ASN
1	F	354	GLN
1	H	235	ASN
1	J	84	GLN
1	J	315	ASN
1	K	235	ASN
1	K	329	ASN
1	L	329	ASN
1	L	341	GLN
1	M	329	ASN
1	N	235	ASN
1	N	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

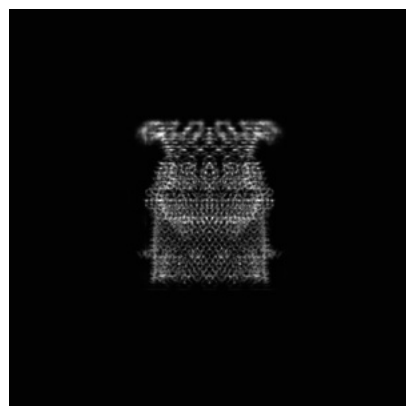
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54887. These allow visual inspection of the internal detail of the map and identification of artifacts.

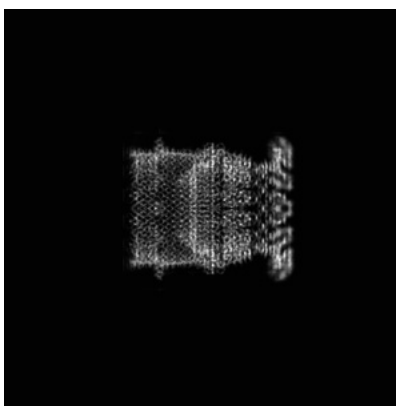
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

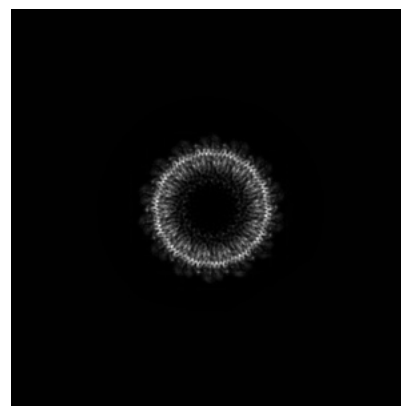
6.1.1 Primary map



X

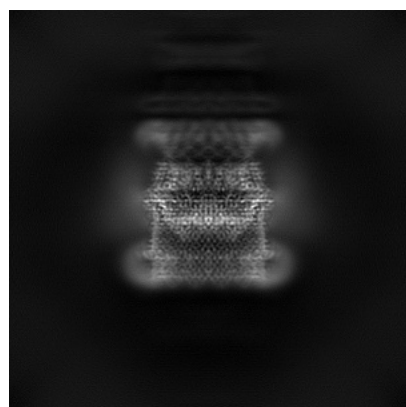


Y

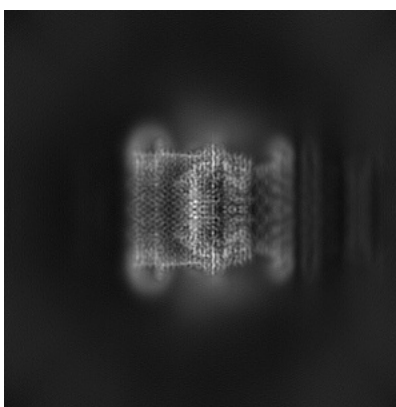


Z

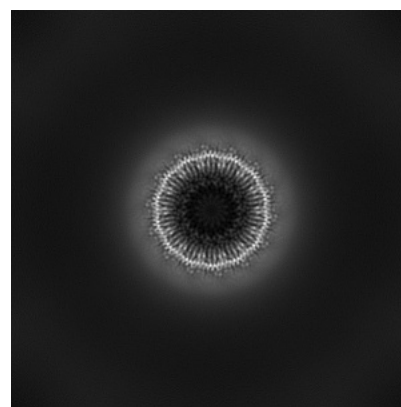
6.1.2 Raw map



X



Y

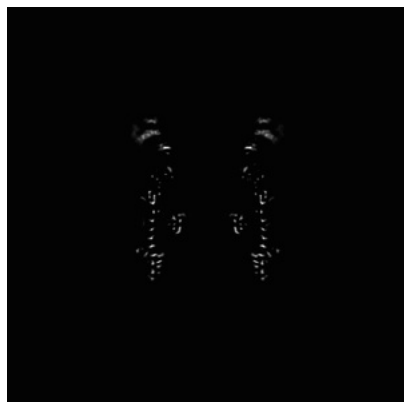


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

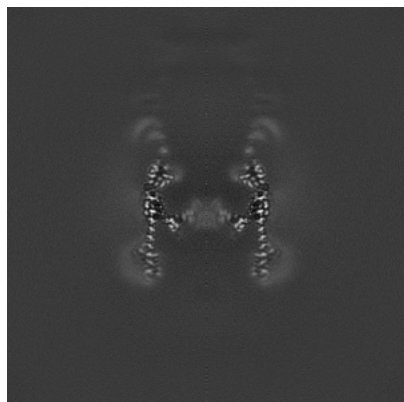


Y Index: 200

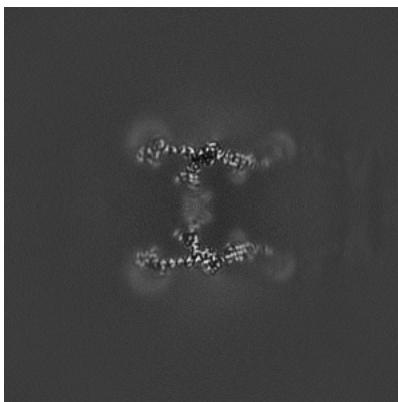


Z Index: 200

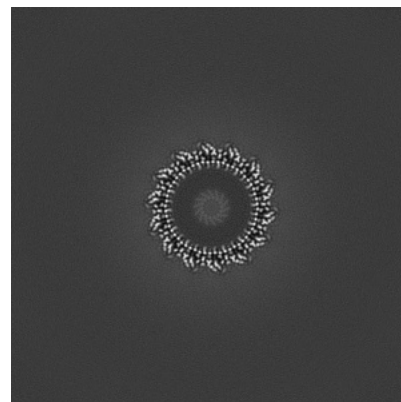
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 157

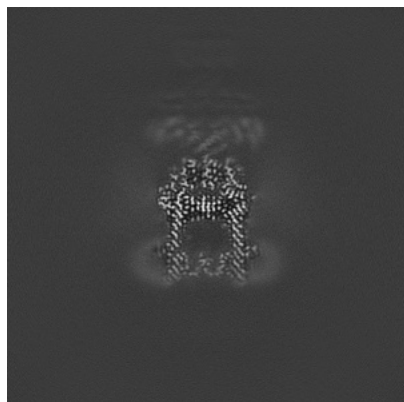


Y Index: 153

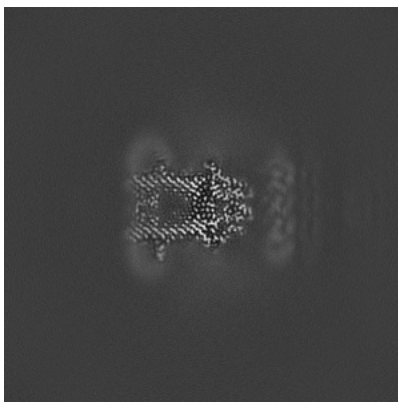


Z Index: 208

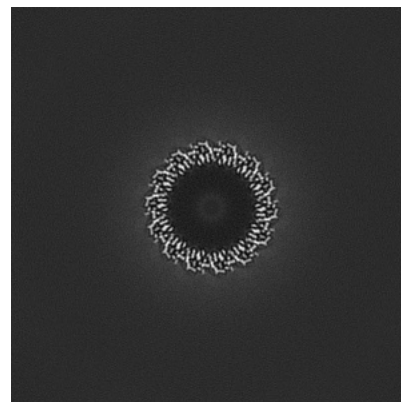
6.3.2 Raw map



X Index: 154



Y Index: 249

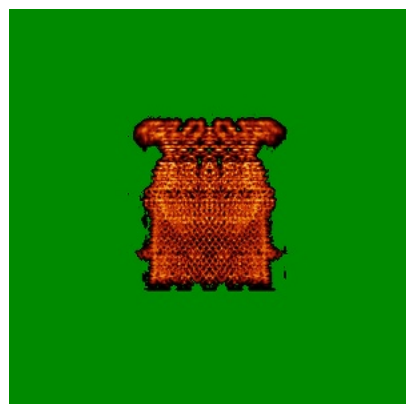


Z Index: 209

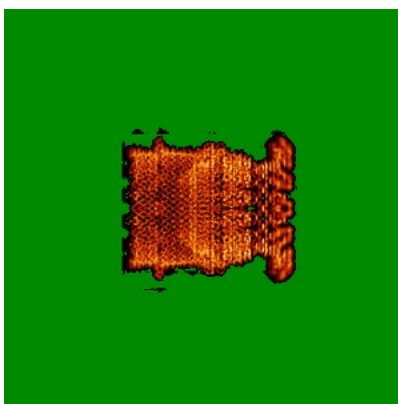
The images above show the largest variance slices of the map in three orthogonal directions.

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

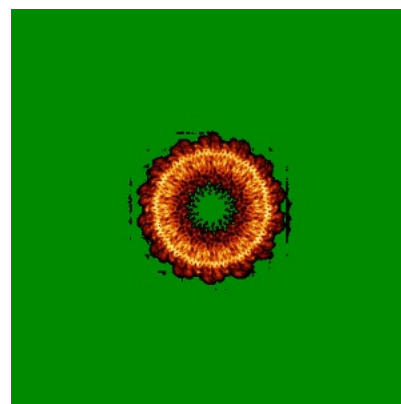
6.4.1 Primary map



X

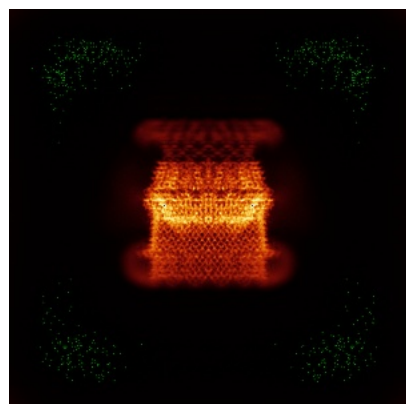


Y

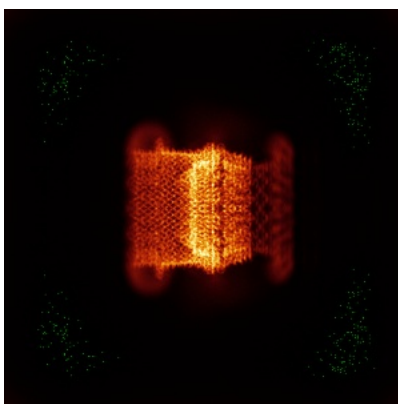


Z

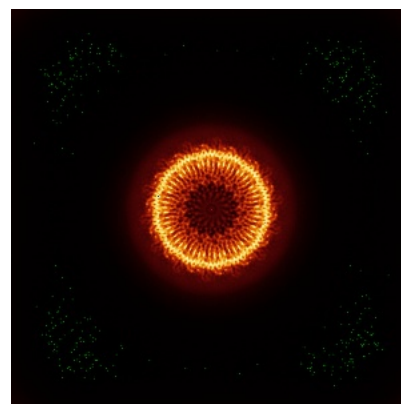
6.4.2 Raw map



X



Y

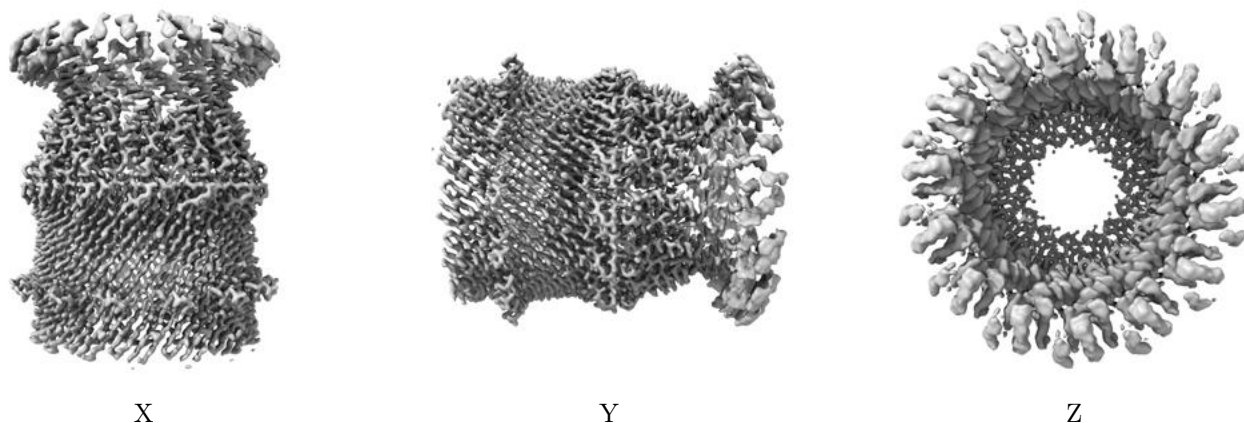


Z

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

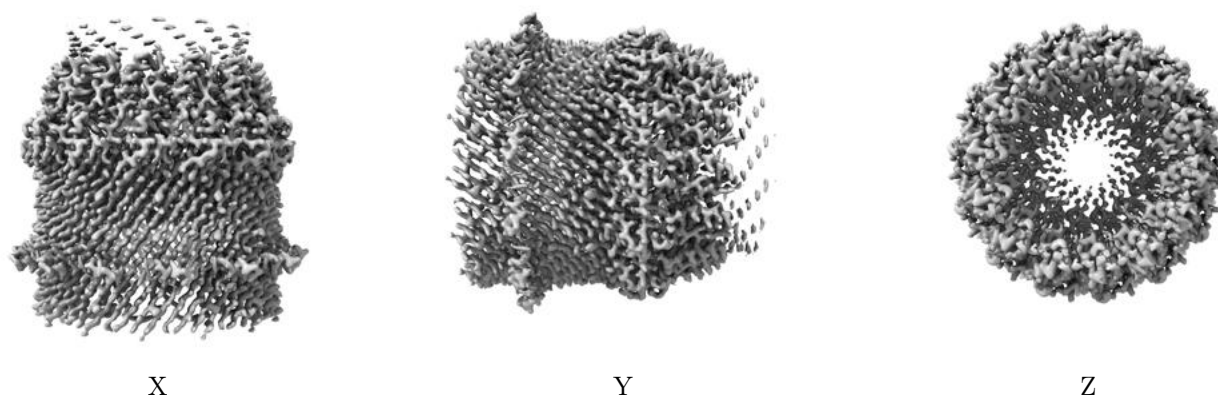
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.201. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

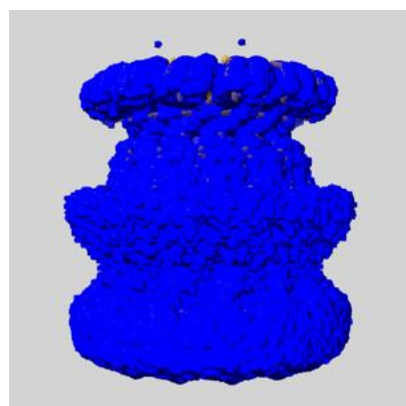
6.6 Mask visualisation [i](#)

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

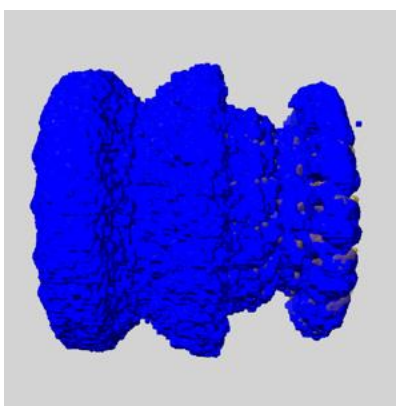
A mask typically either:

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

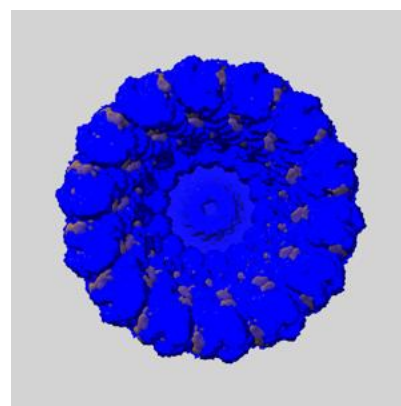
6.6.1 emd_54887_msk_1.map [i](#)



X



Y

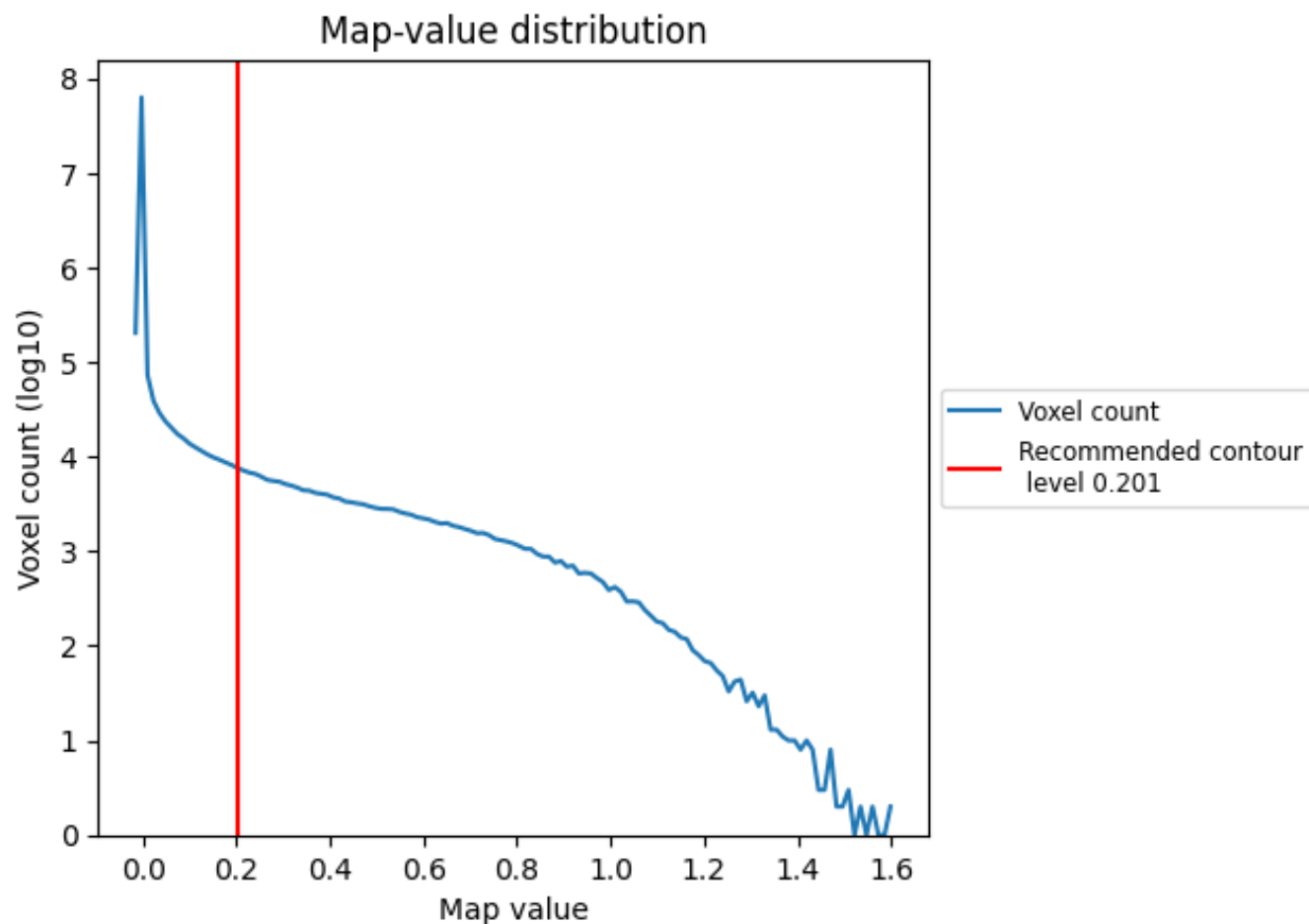


Z

7 Map analysis [i](#)

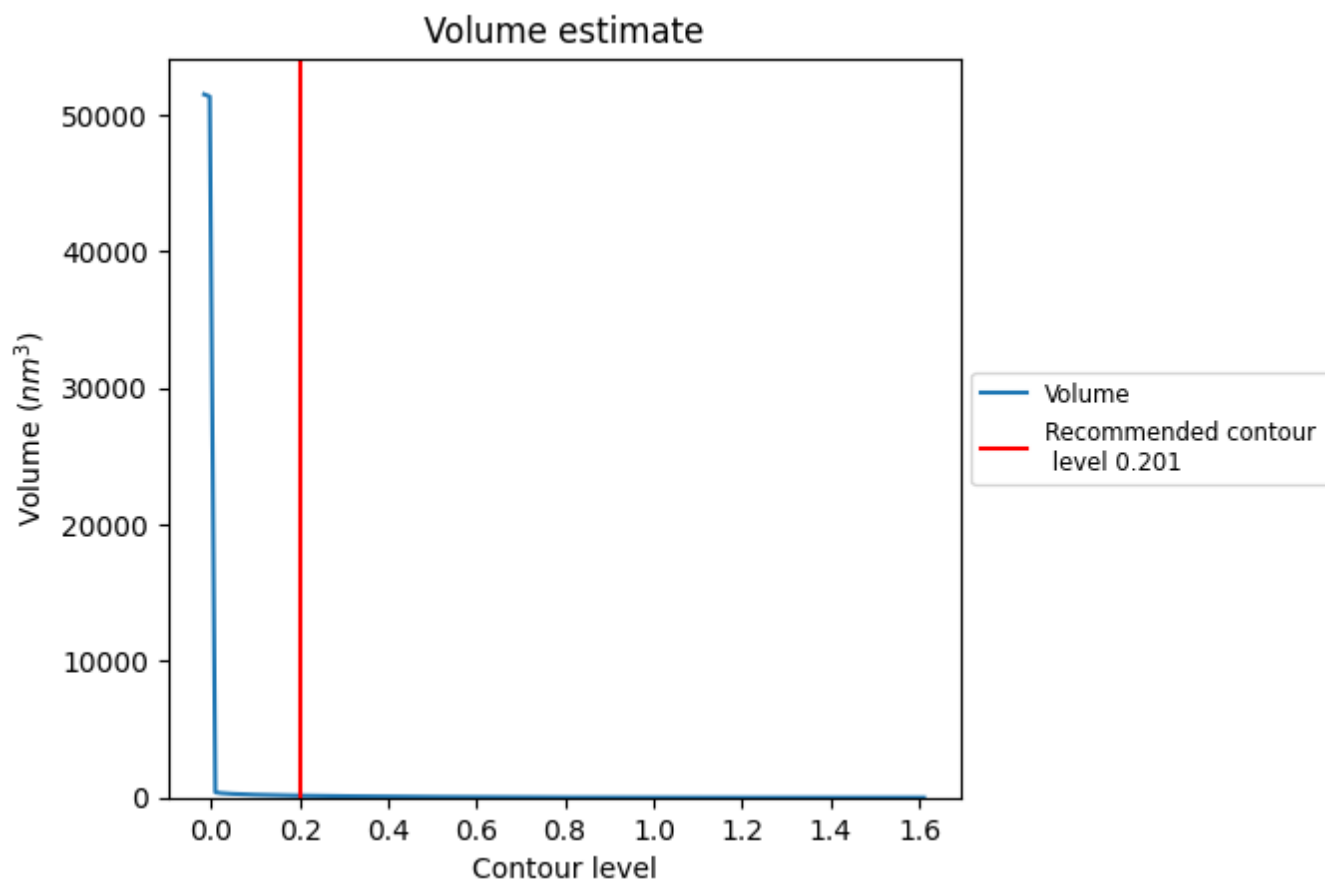
This section contains the results of statistical analysis of the map.

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.

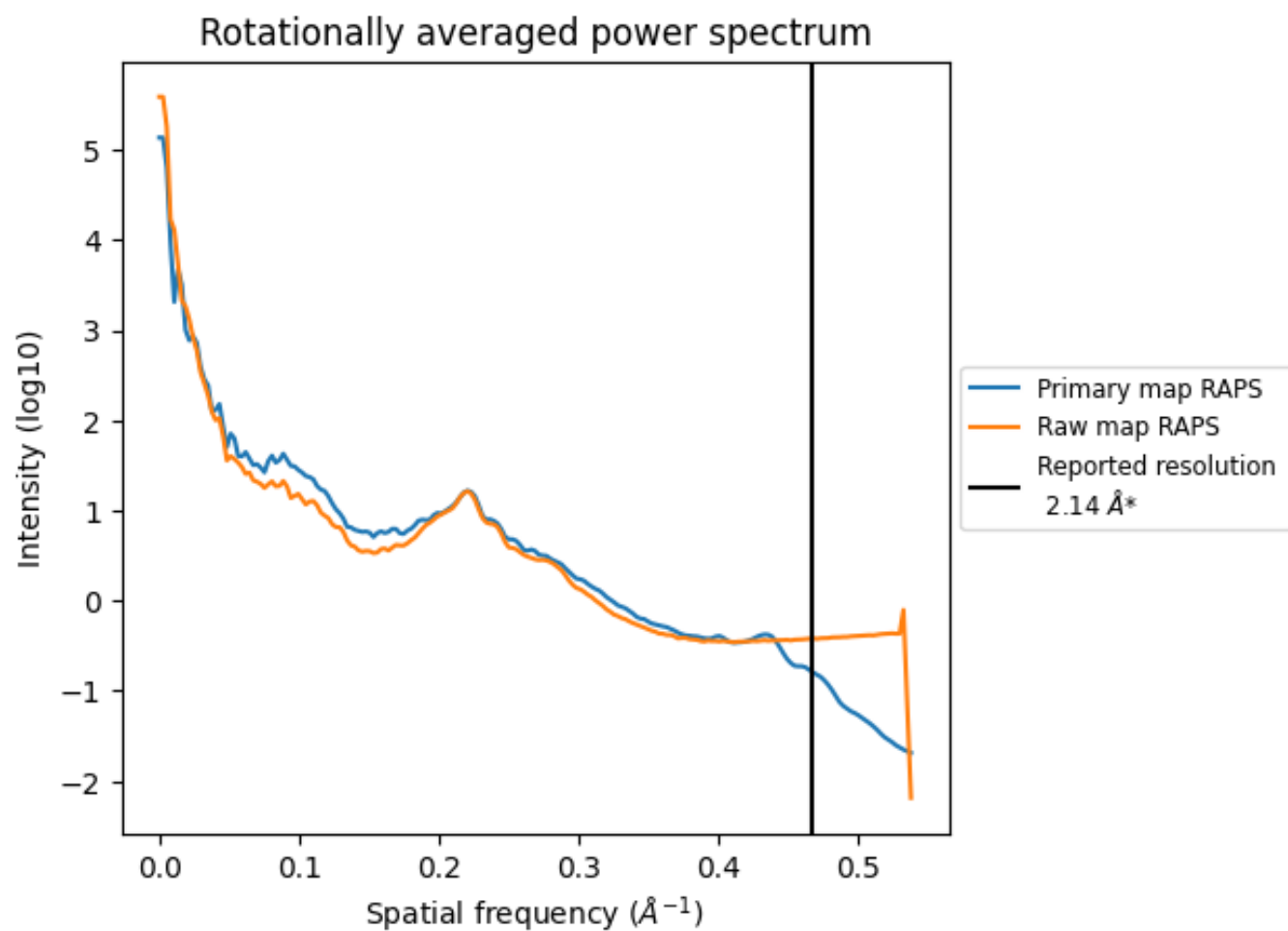
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

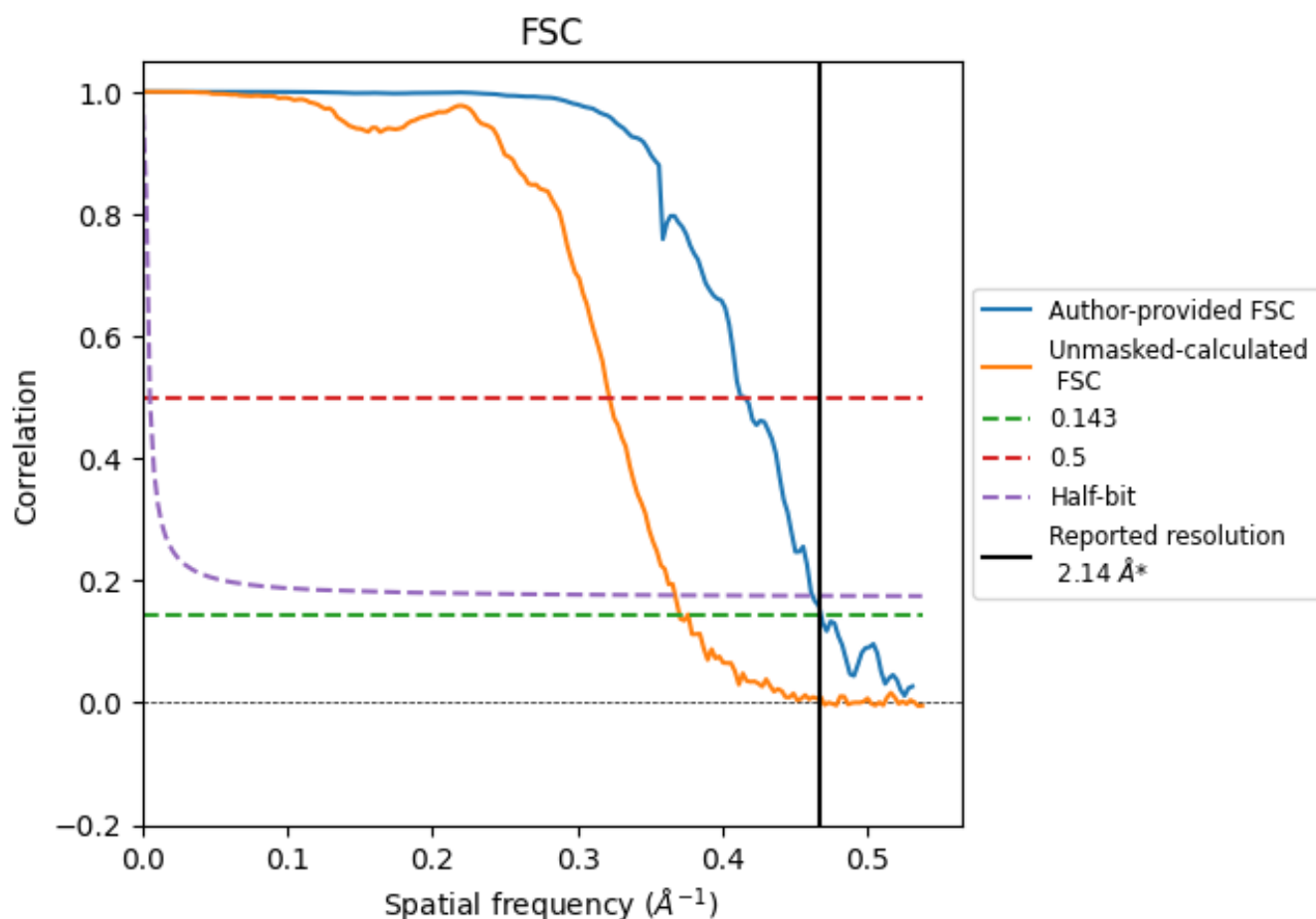


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

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 0.467 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

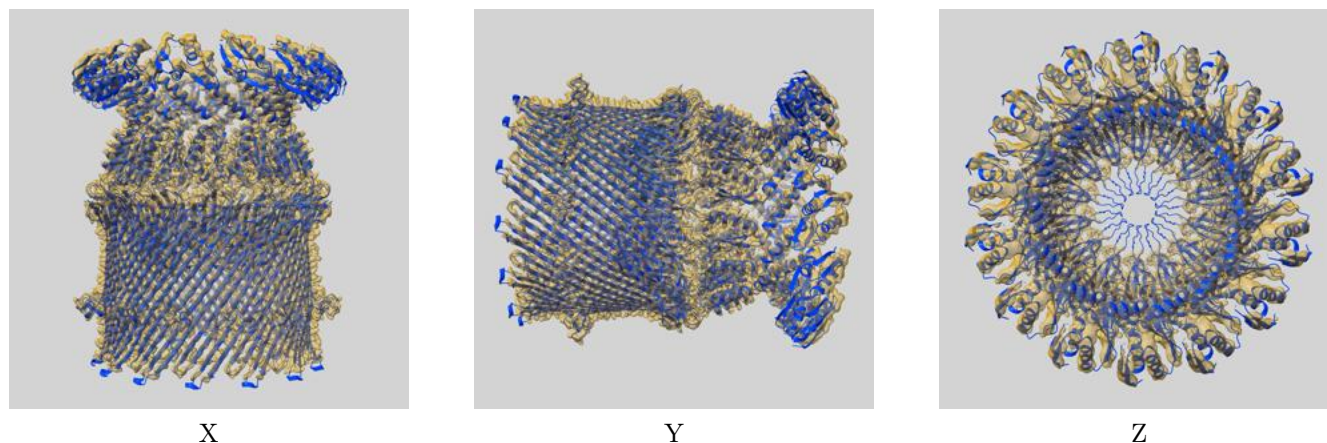
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.42	2.16
Unmasked-calculated*	2.70	3.11	2.72

*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 2.70 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

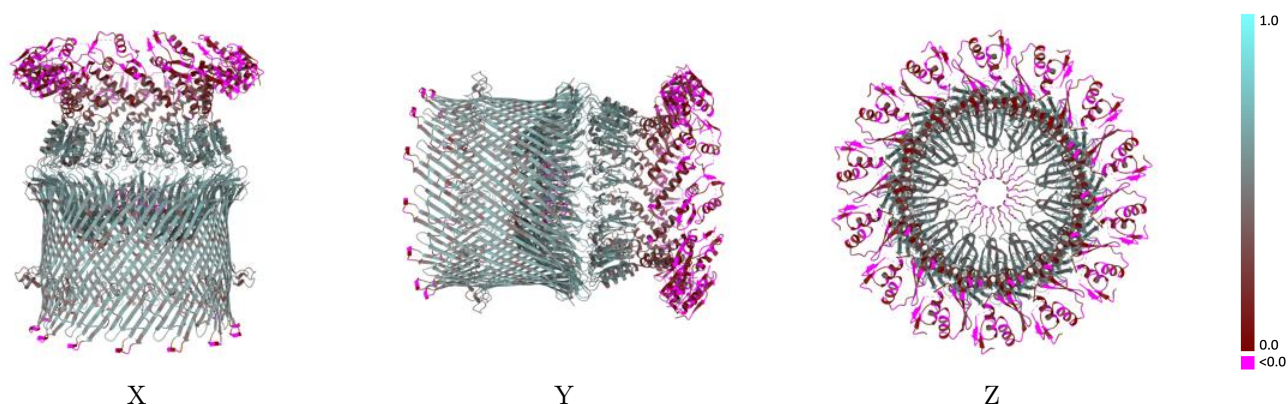
This section contains information regarding the fit between EMDB map EMD-54887 and PDB model 9SH2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



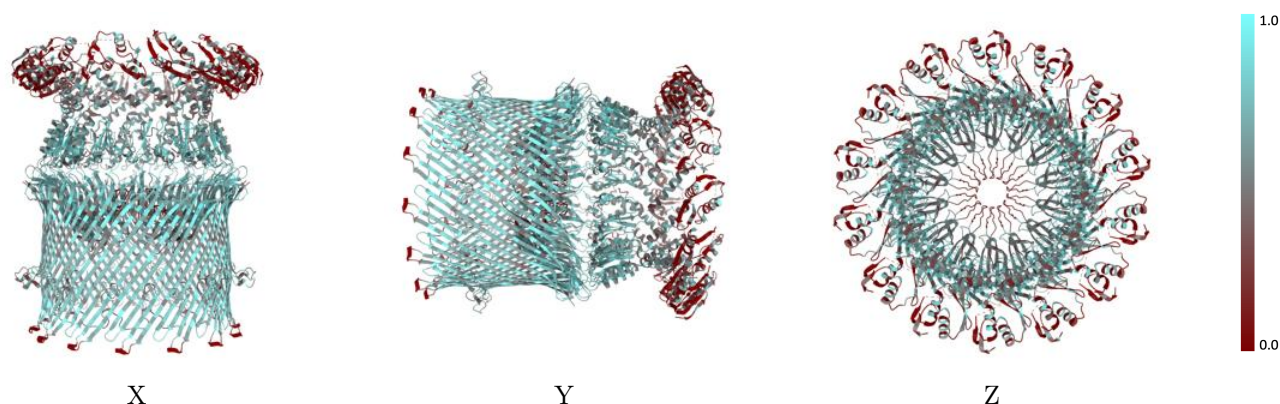
The images above show the 3D surface view of the map at the recommended contour level 0.201 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



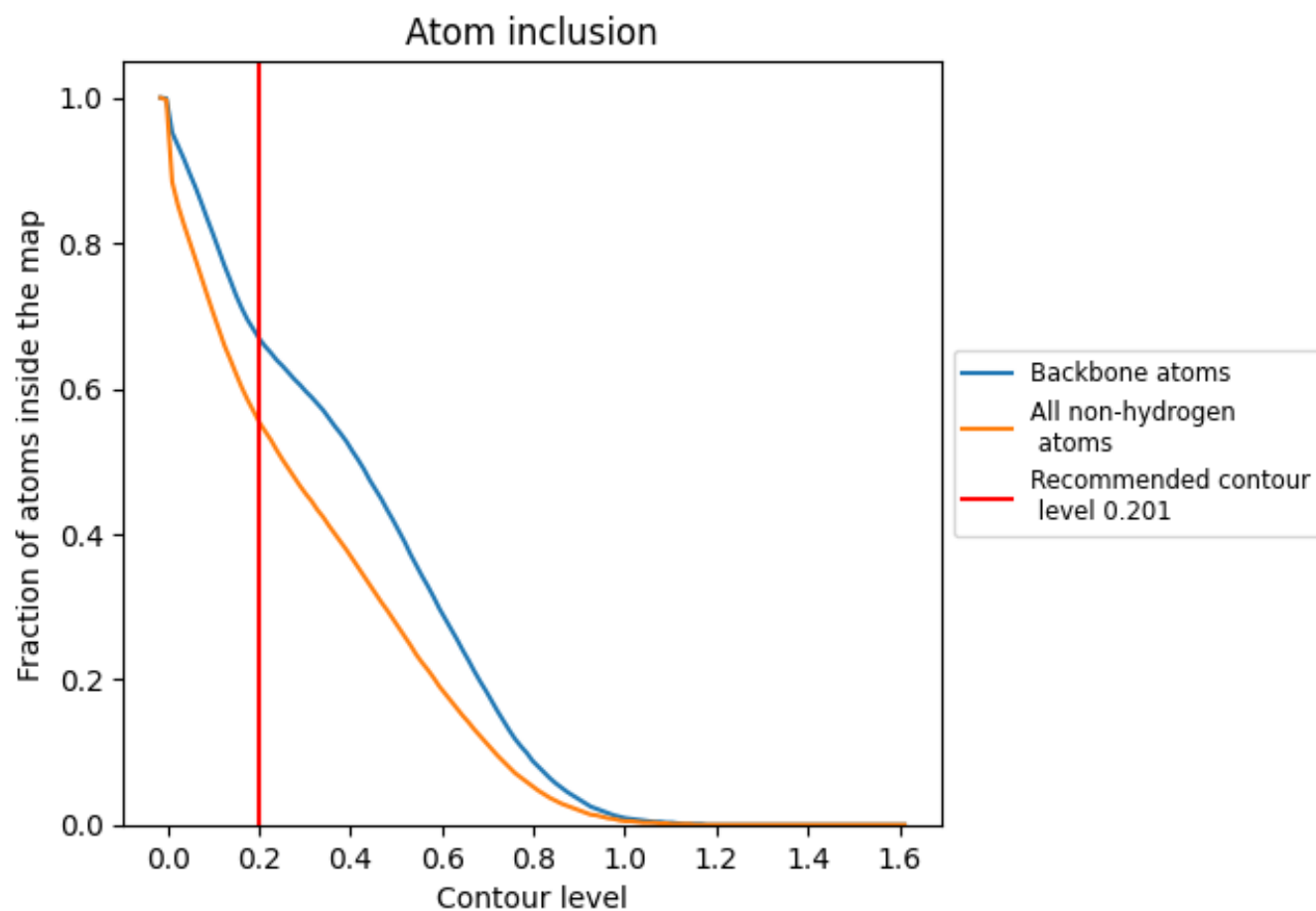
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.201).

9.4 Atom inclusion ⓘ



At the recommended contour level, 67% of all backbone atoms, 55% 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 (0.201) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5530	0.4050
A	0.5650	0.4200
B	0.5630	0.4080
C	0.5450	0.4040
D	0.5420	0.3970
E	0.5390	0.3930
F	0.5460	0.4020
G	0.5540	0.4030
H	0.5620	0.4100
I	0.5620	0.4070
J	0.5580	0.4110
K	0.5530	0.4040
L	0.5540	0.3980
M	0.5520	0.4060
N	0.5520	0.4090

1.0

0.0

<0.0