Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 02:25 AM EST

PDB ID	:	6VE2
EMDB ID	:	EMD-21152
Title	:	Tetradecameric PilQ bound by TsaP heptamer from Pseudomonas aeruginosa
Authors	:	McCallum, M.; Tammam, S.; Rubinstein, J.L.; Burrows, L.L.; Howell, P.L.
Deposited on	:	2019-12-28
Resolution	:	4.30 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:

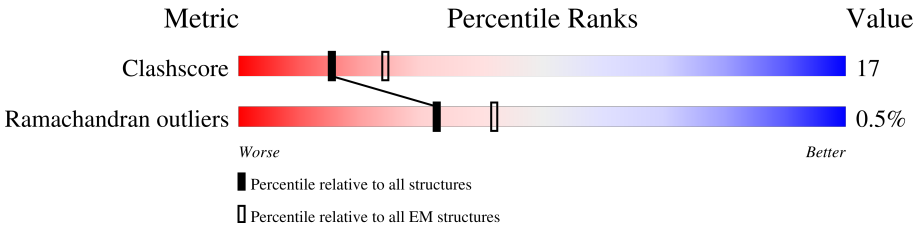
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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

Mol	Chain	Length	Quality of chain
1	A	731	5% 36% 8% 55%
1	B	731	5% 36% 9% 55%
1	C	731	5% 37% 8% 55%
1	D	731	37% 8% 55%
1	E	731	5% 36% 9% 55%
1	F	731	5% 36% 9% 55%
1	G	731	5% 36% 9% 55%
1	H	731	5% 36% 8% 55%
1	I	731	5% 37% 8% 55%

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Mol	Chain	Length	Quality of chain
1	J	731	5% 37% 8% 55%
1	K	731	5% 36% 9% 55%
1	L	731	5% 36% 9% 55%
1	M	731	5% 36% 9% 55%
1	N	731	37% 8% 55%
2	O	341	10% 50% 16% 34%
2	P	341	10% 51% 15% 34%
2	Q	341	10% 50% 16% 34%
2	R	341	9% 51% 15% 34%
2	S	341	10% 50% 16% 34%
2	T	341	10% 50% 16% 34%
2	U	341	10% 50% 16% 34%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30198 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 Fimbrial assembly protein PilQ.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	327	Total 1606	C 952	N 327	O 327	0	0
1	B	327	Total 1606	C 952	N 327	O 327	0	0
1	C	327	Total 1606	C 952	N 327	O 327	0	0
1	D	327	Total 1606	C 952	N 327	O 327	0	0
1	E	327	Total 1606	C 952	N 327	O 327	0	0
1	F	327	Total 1606	C 952	N 327	O 327	0	0
1	G	327	Total 1606	C 952	N 327	O 327	0	0
1	H	327	Total 1606	C 952	N 327	O 327	0	0
1	I	327	Total 1606	C 952	N 327	O 327	0	0
1	J	327	Total 1606	C 952	N 327	O 327	0	0
1	K	327	Total 1606	C 952	N 327	O 327	0	0
1	L	327	Total 1606	C 952	N 327	O 327	0	0
1	M	327	Total 1606	C 952	N 327	O 327	0	0
1	N	327	Total 1606	C 952	N 327	O 327	0	0

There are 238 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-256	HIS	-	insertion	UNP P34750
A	-255	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-254	HIS	-	insertion	UNP P34750
A	-253	HIS	-	insertion	UNP P34750
A	-252	HIS	-	insertion	UNP P34750
A	-251	HIS	-	insertion	UNP P34750
A	-250	HIS	-	insertion	UNP P34750
A	-249	HIS	-	insertion	UNP P34750
A	330	GLY	-	expression tag	UNP P34750
A	331	HIS	-	expression tag	UNP P34750
A	332	HIS	-	expression tag	UNP P34750
A	333	HIS	-	expression tag	UNP P34750
A	334	HIS	-	expression tag	UNP P34750
A	335	HIS	-	expression tag	UNP P34750
A	336	HIS	-	expression tag	UNP P34750
A	337	HIS	-	expression tag	UNP P34750
A	338	HIS	-	expression tag	UNP P34750
B	-256	HIS	-	insertion	UNP P34750
B	-255	HIS	-	insertion	UNP P34750
B	-254	HIS	-	insertion	UNP P34750
B	-253	HIS	-	insertion	UNP P34750
B	-252	HIS	-	insertion	UNP P34750
B	-251	HIS	-	insertion	UNP P34750
B	-250	HIS	-	insertion	UNP P34750
B	-249	HIS	-	insertion	UNP P34750
B	330	GLY	-	expression tag	UNP P34750
B	331	HIS	-	expression tag	UNP P34750
B	332	HIS	-	expression tag	UNP P34750
B	333	HIS	-	expression tag	UNP P34750
B	334	HIS	-	expression tag	UNP P34750
B	335	HIS	-	expression tag	UNP P34750
B	336	HIS	-	expression tag	UNP P34750
B	337	HIS	-	expression tag	UNP P34750
B	338	HIS	-	expression tag	UNP P34750
C	-256	HIS	-	insertion	UNP P34750
C	-255	HIS	-	insertion	UNP P34750
C	-254	HIS	-	insertion	UNP P34750
C	-253	HIS	-	insertion	UNP P34750
C	-252	HIS	-	insertion	UNP P34750
C	-251	HIS	-	insertion	UNP P34750
C	-250	HIS	-	insertion	UNP P34750
C	-249	HIS	-	insertion	UNP P34750
C	330	GLY	-	expression tag	UNP P34750
C	331	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	HIS	-	expression tag	UNP P34750
C	333	HIS	-	expression tag	UNP P34750
C	334	HIS	-	expression tag	UNP P34750
C	335	HIS	-	expression tag	UNP P34750
C	336	HIS	-	expression tag	UNP P34750
C	337	HIS	-	expression tag	UNP P34750
C	338	HIS	-	expression tag	UNP P34750
D	-256	HIS	-	insertion	UNP P34750
D	-255	HIS	-	insertion	UNP P34750
D	-254	HIS	-	insertion	UNP P34750
D	-253	HIS	-	insertion	UNP P34750
D	-252	HIS	-	insertion	UNP P34750
D	-251	HIS	-	insertion	UNP P34750
D	-250	HIS	-	insertion	UNP P34750
D	-249	HIS	-	insertion	UNP P34750
D	330	GLY	-	expression tag	UNP P34750
D	331	HIS	-	expression tag	UNP P34750
D	332	HIS	-	expression tag	UNP P34750
D	333	HIS	-	expression tag	UNP P34750
D	334	HIS	-	expression tag	UNP P34750
D	335	HIS	-	expression tag	UNP P34750
D	336	HIS	-	expression tag	UNP P34750
D	337	HIS	-	expression tag	UNP P34750
D	338	HIS	-	expression tag	UNP P34750
E	-256	HIS	-	insertion	UNP P34750
E	-255	HIS	-	insertion	UNP P34750
E	-254	HIS	-	insertion	UNP P34750
E	-253	HIS	-	insertion	UNP P34750
E	-252	HIS	-	insertion	UNP P34750
E	-251	HIS	-	insertion	UNP P34750
E	-250	HIS	-	insertion	UNP P34750
E	-249	HIS	-	insertion	UNP P34750
E	330	GLY	-	expression tag	UNP P34750
E	331	HIS	-	expression tag	UNP P34750
E	332	HIS	-	expression tag	UNP P34750
E	333	HIS	-	expression tag	UNP P34750
E	334	HIS	-	expression tag	UNP P34750
E	335	HIS	-	expression tag	UNP P34750
E	336	HIS	-	expression tag	UNP P34750
E	337	HIS	-	expression tag	UNP P34750
E	338	HIS	-	expression tag	UNP P34750
F	-256	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-255	HIS	-	insertion	UNP P34750
F	-254	HIS	-	insertion	UNP P34750
F	-253	HIS	-	insertion	UNP P34750
F	-252	HIS	-	insertion	UNP P34750
F	-251	HIS	-	insertion	UNP P34750
F	-250	HIS	-	insertion	UNP P34750
F	-249	HIS	-	insertion	UNP P34750
F	330	GLY	-	expression tag	UNP P34750
F	331	HIS	-	expression tag	UNP P34750
F	332	HIS	-	expression tag	UNP P34750
F	333	HIS	-	expression tag	UNP P34750
F	334	HIS	-	expression tag	UNP P34750
F	335	HIS	-	expression tag	UNP P34750
F	336	HIS	-	expression tag	UNP P34750
F	337	HIS	-	expression tag	UNP P34750
F	338	HIS	-	expression tag	UNP P34750
G	-256	HIS	-	insertion	UNP P34750
G	-255	HIS	-	insertion	UNP P34750
G	-254	HIS	-	insertion	UNP P34750
G	-253	HIS	-	insertion	UNP P34750
G	-252	HIS	-	insertion	UNP P34750
G	-251	HIS	-	insertion	UNP P34750
G	-250	HIS	-	insertion	UNP P34750
G	-249	HIS	-	insertion	UNP P34750
G	330	GLY	-	expression tag	UNP P34750
G	331	HIS	-	expression tag	UNP P34750
G	332	HIS	-	expression tag	UNP P34750
G	333	HIS	-	expression tag	UNP P34750
G	334	HIS	-	expression tag	UNP P34750
G	335	HIS	-	expression tag	UNP P34750
G	336	HIS	-	expression tag	UNP P34750
G	337	HIS	-	expression tag	UNP P34750
G	338	HIS	-	expression tag	UNP P34750
H	-256	HIS	-	insertion	UNP P34750
H	-255	HIS	-	insertion	UNP P34750
H	-254	HIS	-	insertion	UNP P34750
H	-253	HIS	-	insertion	UNP P34750
H	-252	HIS	-	insertion	UNP P34750
H	-251	HIS	-	insertion	UNP P34750
H	-250	HIS	-	insertion	UNP P34750
H	-249	HIS	-	insertion	UNP P34750
H	330	GLY	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
H	331	HIS	-	expression tag	UNP P34750
H	332	HIS	-	expression tag	UNP P34750
H	333	HIS	-	expression tag	UNP P34750
H	334	HIS	-	expression tag	UNP P34750
H	335	HIS	-	expression tag	UNP P34750
H	336	HIS	-	expression tag	UNP P34750
H	337	HIS	-	expression tag	UNP P34750
H	338	HIS	-	expression tag	UNP P34750
I	-256	HIS	-	insertion	UNP P34750
I	-255	HIS	-	insertion	UNP P34750
I	-254	HIS	-	insertion	UNP P34750
I	-253	HIS	-	insertion	UNP P34750
I	-252	HIS	-	insertion	UNP P34750
I	-251	HIS	-	insertion	UNP P34750
I	-250	HIS	-	insertion	UNP P34750
I	-249	HIS	-	insertion	UNP P34750
I	330	GLY	-	expression tag	UNP P34750
I	331	HIS	-	expression tag	UNP P34750
I	332	HIS	-	expression tag	UNP P34750
I	333	HIS	-	expression tag	UNP P34750
I	334	HIS	-	expression tag	UNP P34750
I	335	HIS	-	expression tag	UNP P34750
I	336	HIS	-	expression tag	UNP P34750
I	337	HIS	-	expression tag	UNP P34750
I	338	HIS	-	expression tag	UNP P34750
J	-256	HIS	-	insertion	UNP P34750
J	-255	HIS	-	insertion	UNP P34750
J	-254	HIS	-	insertion	UNP P34750
J	-253	HIS	-	insertion	UNP P34750
J	-252	HIS	-	insertion	UNP P34750
J	-251	HIS	-	insertion	UNP P34750
J	-250	HIS	-	insertion	UNP P34750
J	-249	HIS	-	insertion	UNP P34750
J	330	GLY	-	expression tag	UNP P34750
J	331	HIS	-	expression tag	UNP P34750
J	332	HIS	-	expression tag	UNP P34750
J	333	HIS	-	expression tag	UNP P34750
J	334	HIS	-	expression tag	UNP P34750
J	335	HIS	-	expression tag	UNP P34750
J	336	HIS	-	expression tag	UNP P34750
J	337	HIS	-	expression tag	UNP P34750
J	338	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-256	HIS	-	insertion	UNP P34750
K	-255	HIS	-	insertion	UNP P34750
K	-254	HIS	-	insertion	UNP P34750
K	-253	HIS	-	insertion	UNP P34750
K	-252	HIS	-	insertion	UNP P34750
K	-251	HIS	-	insertion	UNP P34750
K	-250	HIS	-	insertion	UNP P34750
K	-249	HIS	-	insertion	UNP P34750
K	330	GLY	-	expression tag	UNP P34750
K	331	HIS	-	expression tag	UNP P34750
K	332	HIS	-	expression tag	UNP P34750
K	333	HIS	-	expression tag	UNP P34750
K	334	HIS	-	expression tag	UNP P34750
K	335	HIS	-	expression tag	UNP P34750
K	336	HIS	-	expression tag	UNP P34750
K	337	HIS	-	expression tag	UNP P34750
K	338	HIS	-	expression tag	UNP P34750
L	-256	HIS	-	insertion	UNP P34750
L	-255	HIS	-	insertion	UNP P34750
L	-254	HIS	-	insertion	UNP P34750
L	-253	HIS	-	insertion	UNP P34750
L	-252	HIS	-	insertion	UNP P34750
L	-251	HIS	-	insertion	UNP P34750
L	-250	HIS	-	insertion	UNP P34750
L	-249	HIS	-	insertion	UNP P34750
L	330	GLY	-	expression tag	UNP P34750
L	331	HIS	-	expression tag	UNP P34750
L	332	HIS	-	expression tag	UNP P34750
L	333	HIS	-	expression tag	UNP P34750
L	334	HIS	-	expression tag	UNP P34750
L	335	HIS	-	expression tag	UNP P34750
L	336	HIS	-	expression tag	UNP P34750
L	337	HIS	-	expression tag	UNP P34750
L	338	HIS	-	expression tag	UNP P34750
M	-256	HIS	-	insertion	UNP P34750
M	-255	HIS	-	insertion	UNP P34750
M	-254	HIS	-	insertion	UNP P34750
M	-253	HIS	-	insertion	UNP P34750
M	-252	HIS	-	insertion	UNP P34750
M	-251	HIS	-	insertion	UNP P34750
M	-250	HIS	-	insertion	UNP P34750
M	-249	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
M	330	GLY	-	expression tag	UNP P34750
M	331	HIS	-	expression tag	UNP P34750
M	332	HIS	-	expression tag	UNP P34750
M	333	HIS	-	expression tag	UNP P34750
M	334	HIS	-	expression tag	UNP P34750
M	335	HIS	-	expression tag	UNP P34750
M	336	HIS	-	expression tag	UNP P34750
M	337	HIS	-	expression tag	UNP P34750
M	338	HIS	-	expression tag	UNP P34750
N	-256	HIS	-	insertion	UNP P34750
N	-255	HIS	-	insertion	UNP P34750
N	-254	HIS	-	insertion	UNP P34750
N	-253	HIS	-	insertion	UNP P34750
N	-252	HIS	-	insertion	UNP P34750
N	-251	HIS	-	insertion	UNP P34750
N	-250	HIS	-	insertion	UNP P34750
N	-249	HIS	-	insertion	UNP P34750
N	330	GLY	-	expression tag	UNP P34750
N	331	HIS	-	expression tag	UNP P34750
N	332	HIS	-	expression tag	UNP P34750
N	333	HIS	-	expression tag	UNP P34750
N	334	HIS	-	expression tag	UNP P34750
N	335	HIS	-	expression tag	UNP P34750
N	336	HIS	-	expression tag	UNP P34750
N	337	HIS	-	expression tag	UNP P34750
N	338	HIS	-	expression tag	UNP P34750

- Molecule 2 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	225	Total	C	N	O	0	0
			1102	652	225	225		
2	P	225	Total	C	N	O	0	0
			1102	652	225	225		
2	Q	225	Total	C	N	O	0	0
			1102	652	225	225		
2	R	225	Total	C	N	O	0	0
			1102	652	225	225		
2	S	225	Total	C	N	O	0	0
			1102	652	225	225		
2	T	225	Total	C	N	O	0	0
			1102	652	225	225		

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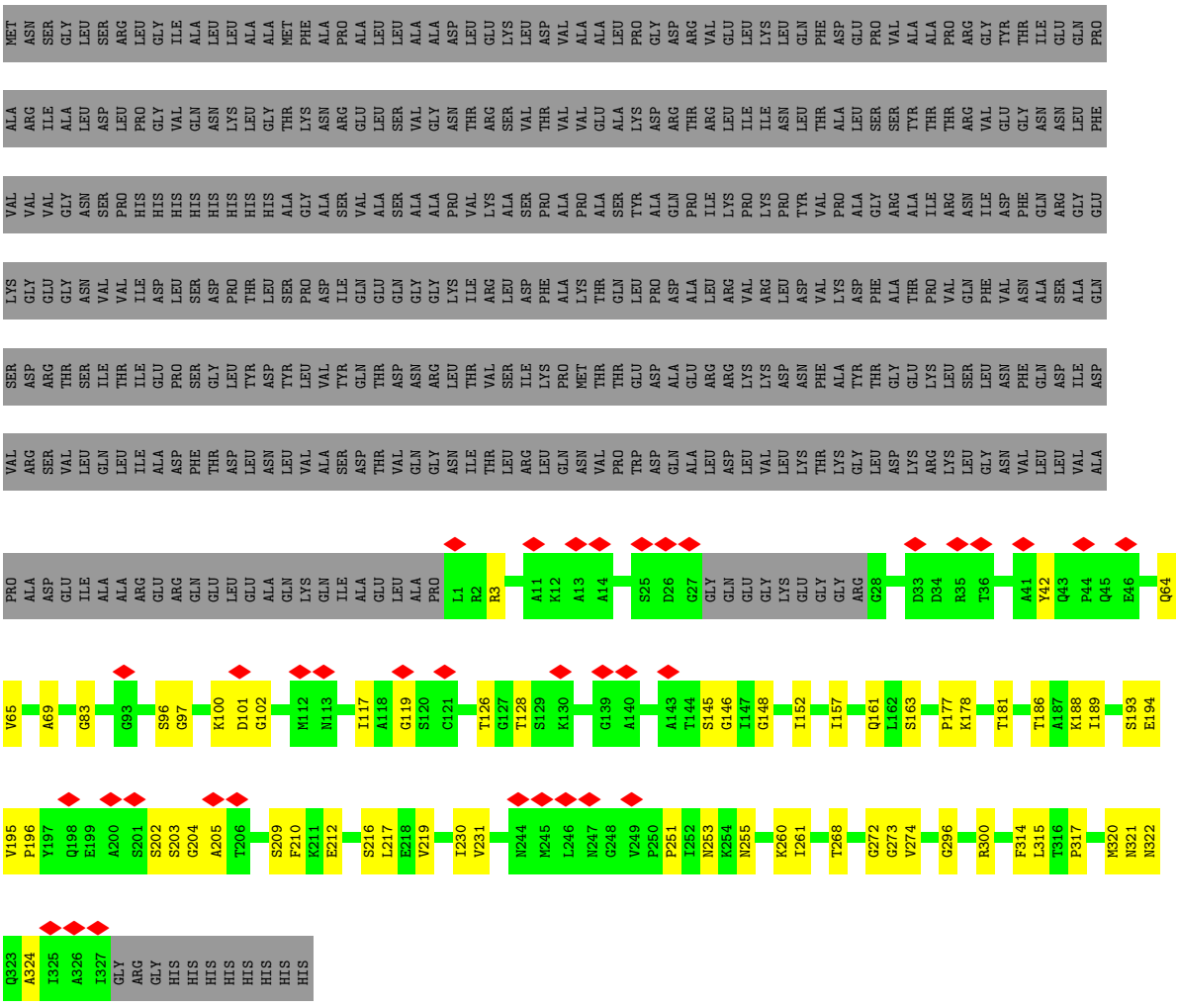
Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	225	Total 1102	C 652	N 225	O 225	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

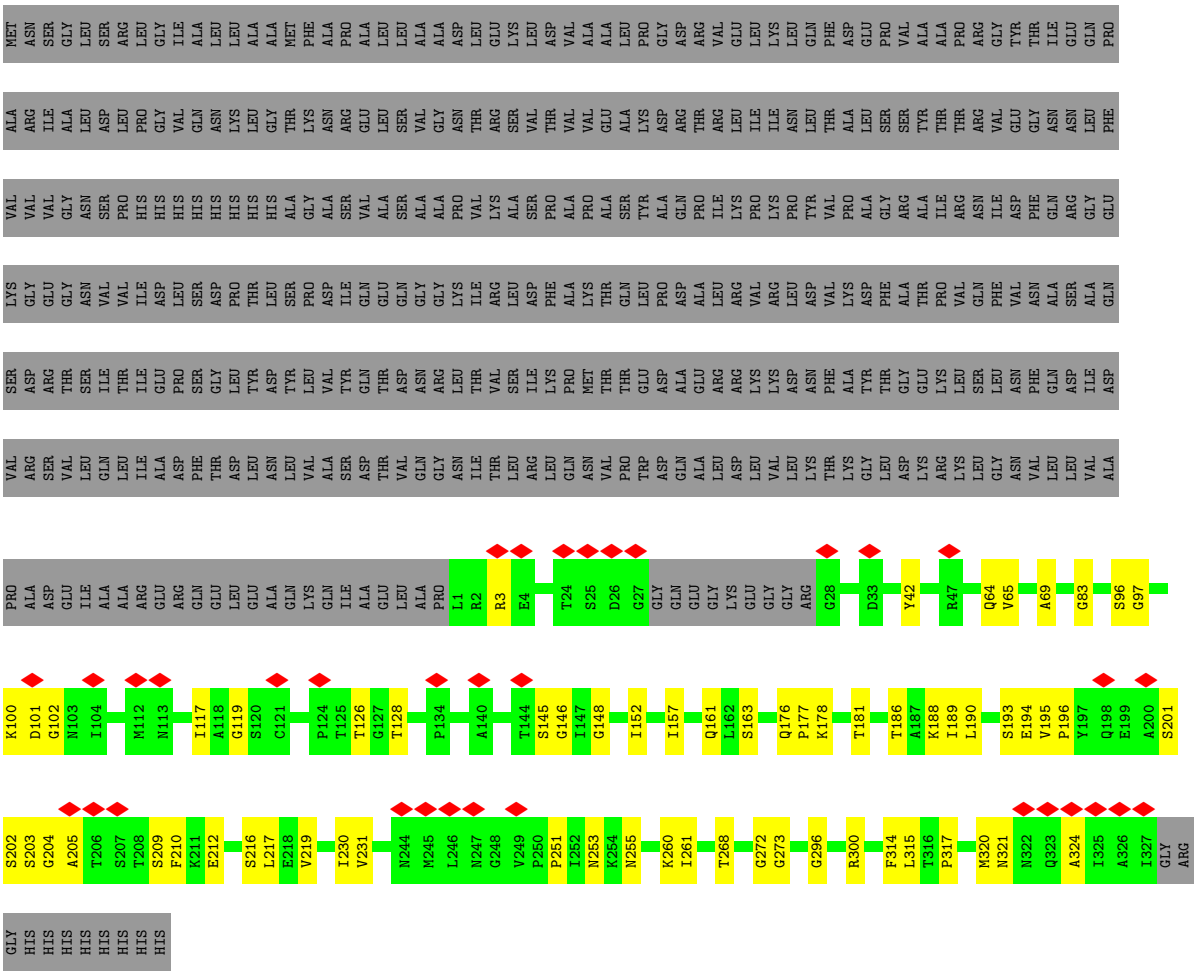
• Molecule 1: Fimbrial assembly protein PilQ

Chain A:



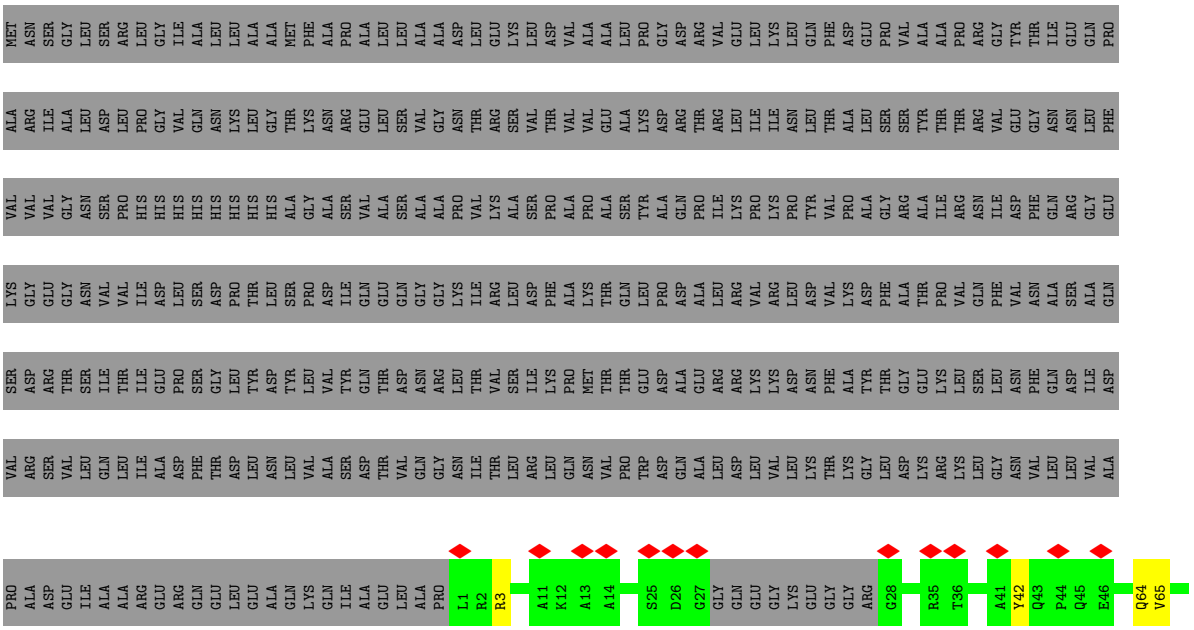
• Molecule 1: Fimbrial assembly protein PilQ

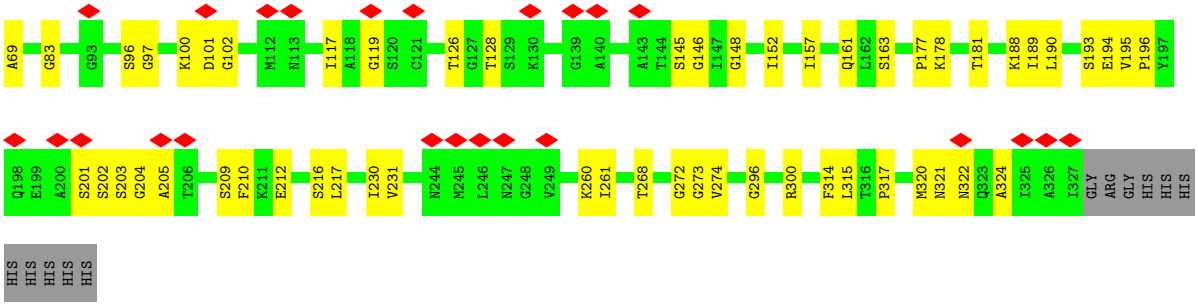
Chain B:



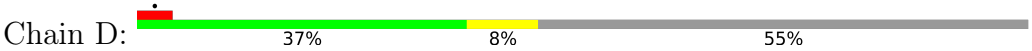
• Molecule 1: Fimbrial assembly protein PilQ

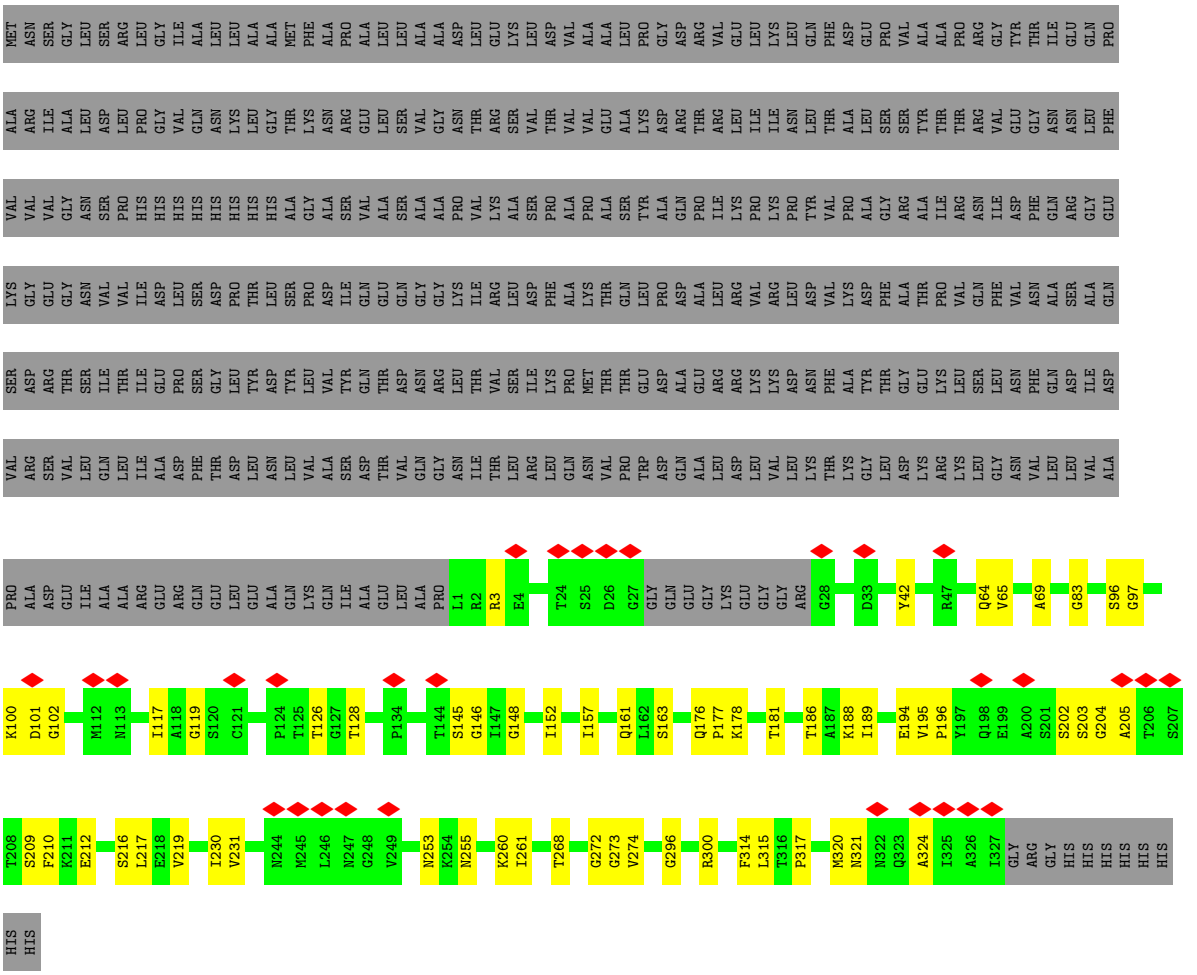
Chain C:



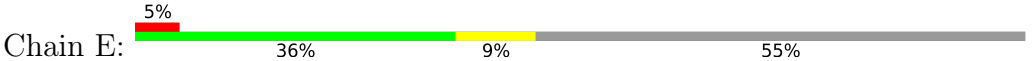


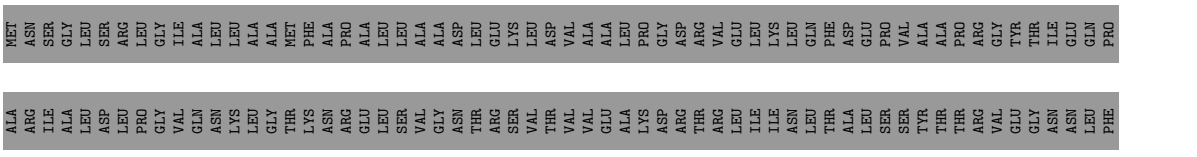
• Molecule 1: Fimbrial assembly protein PilQ

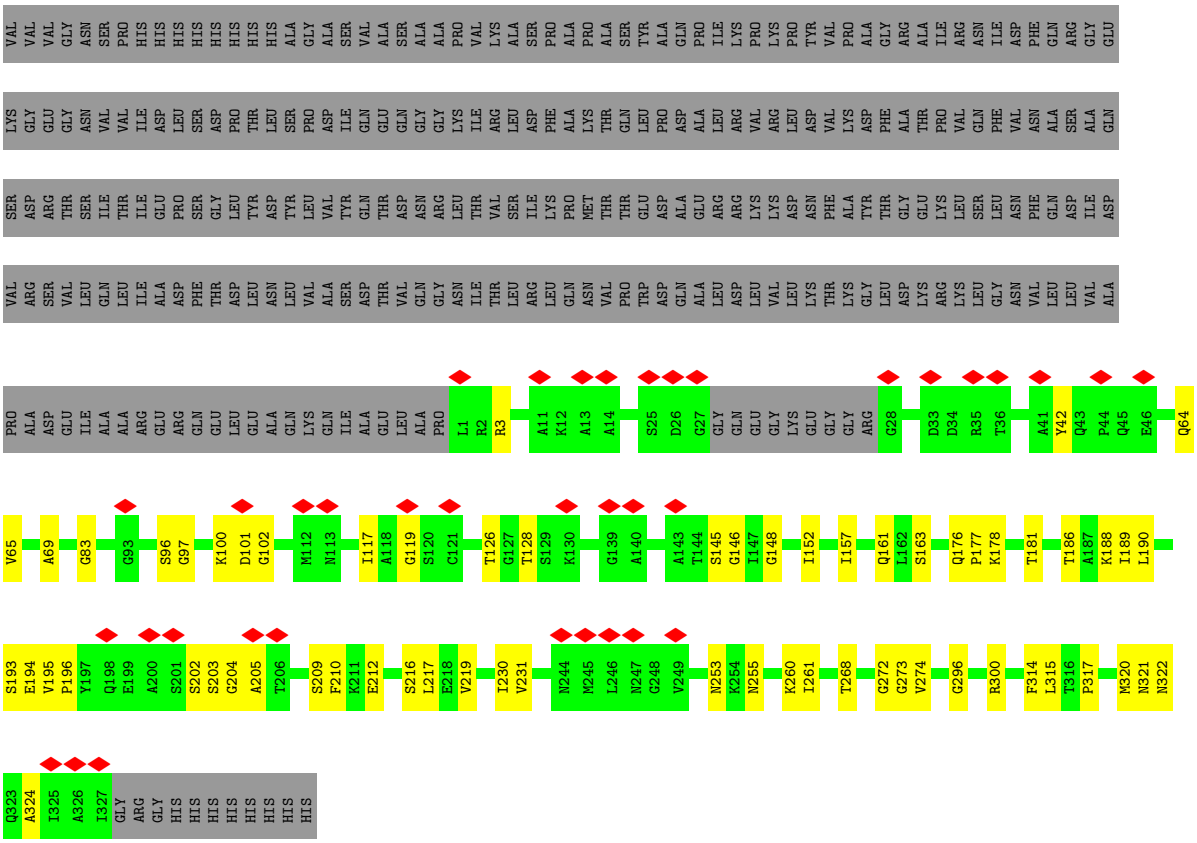




• Molecule 1: Fimbrial assembly protein PilQ

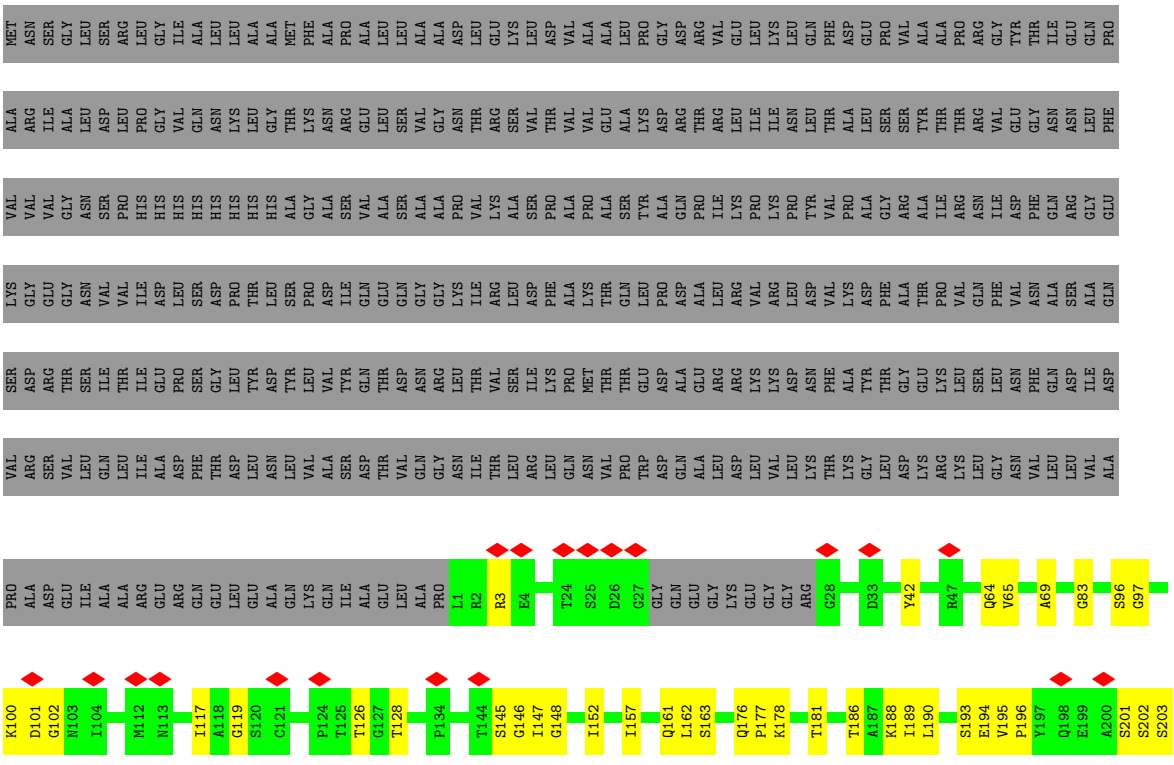


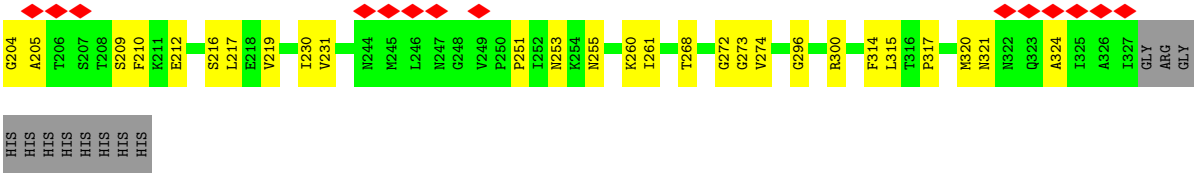




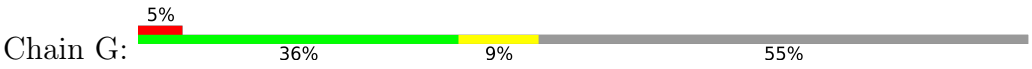
• Molecule 1: Fimbrial assembly protein PilQ

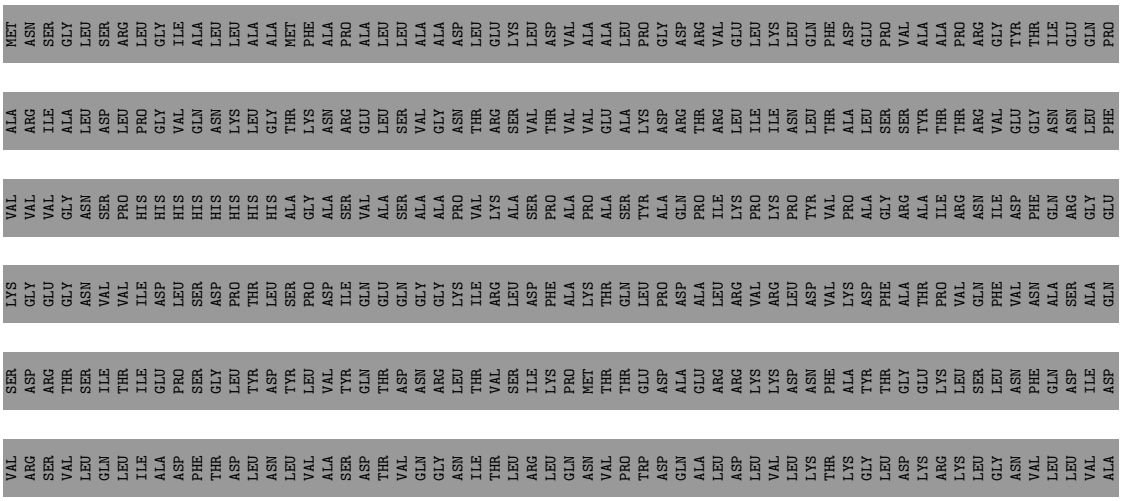
Chain F:



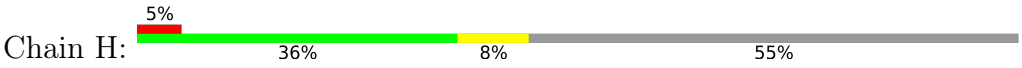


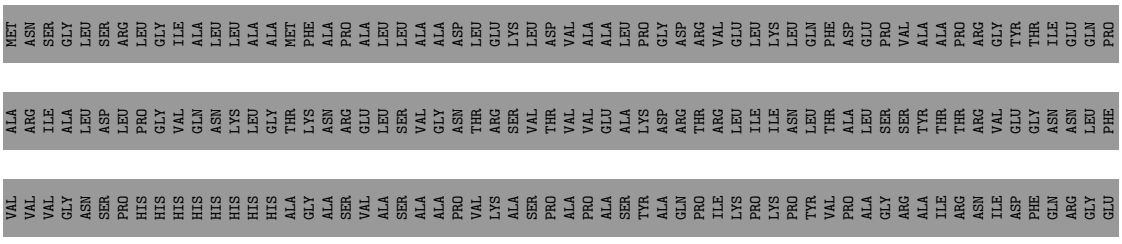
• Molecule 1: Fimbrial assembly protein PilQ

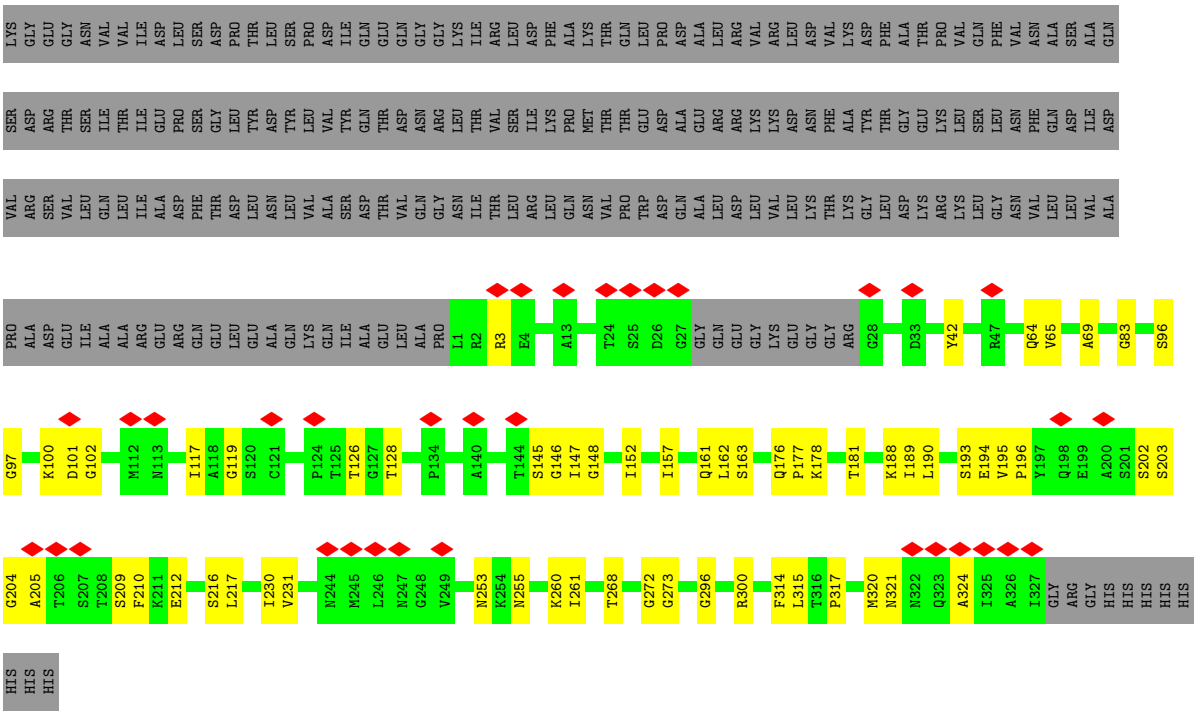




• Molecule 1: Fimbrial assembly protein PilQ

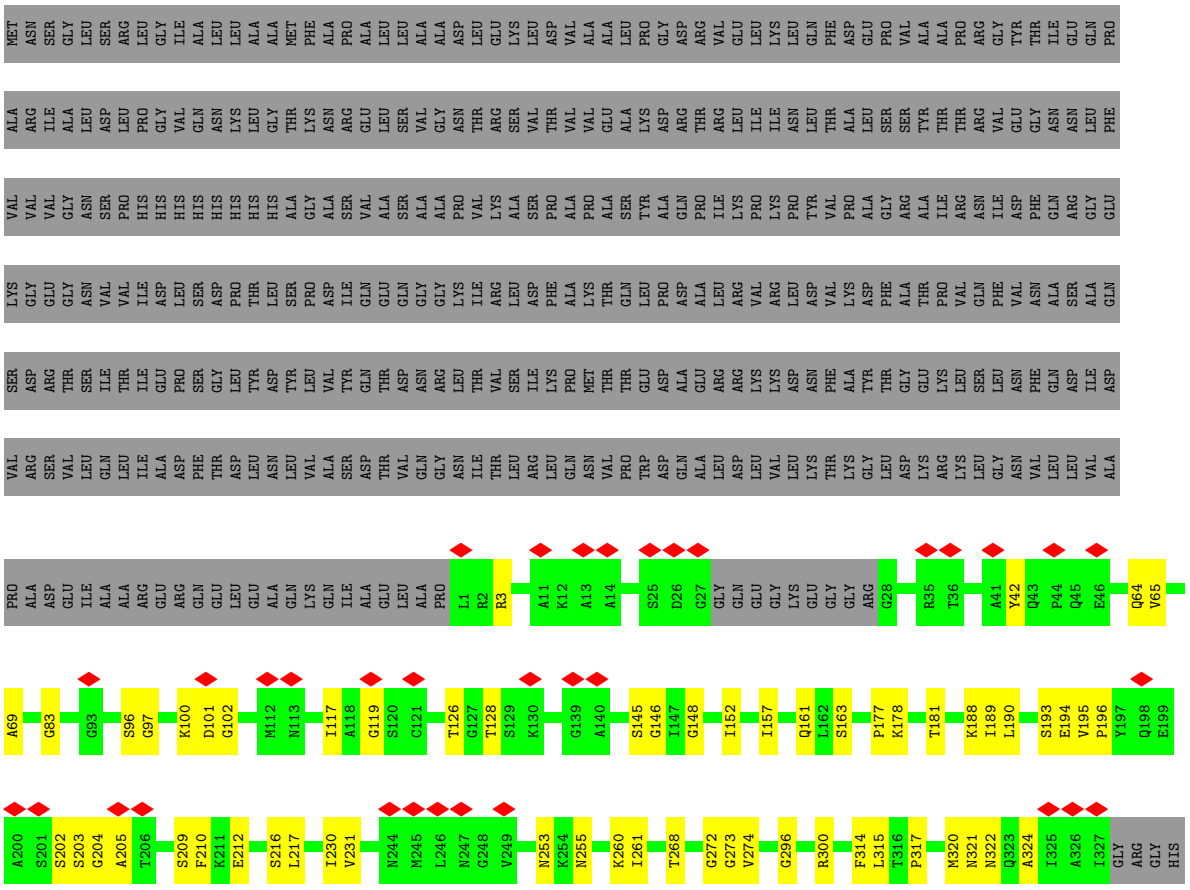






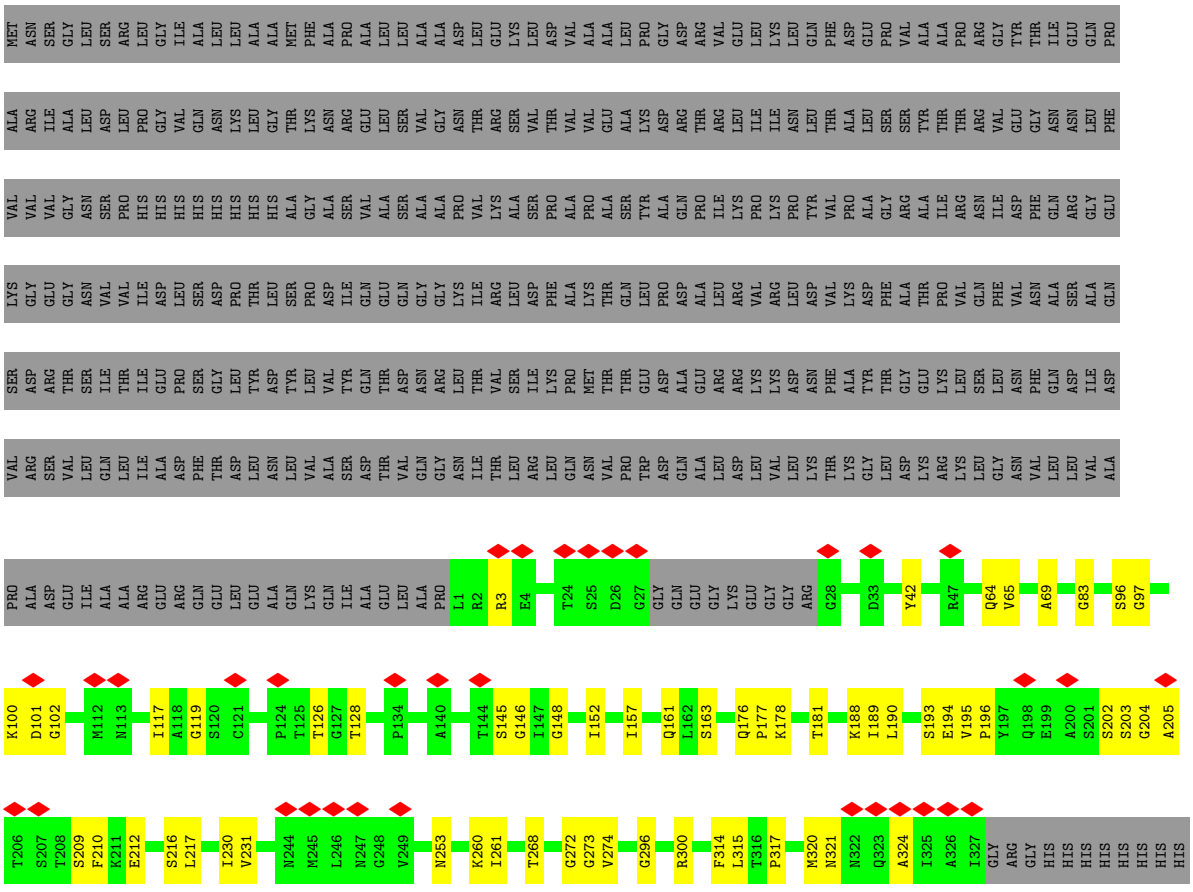
• Molecule 1: Fimbrial assembly protein PilQ

Chain I:



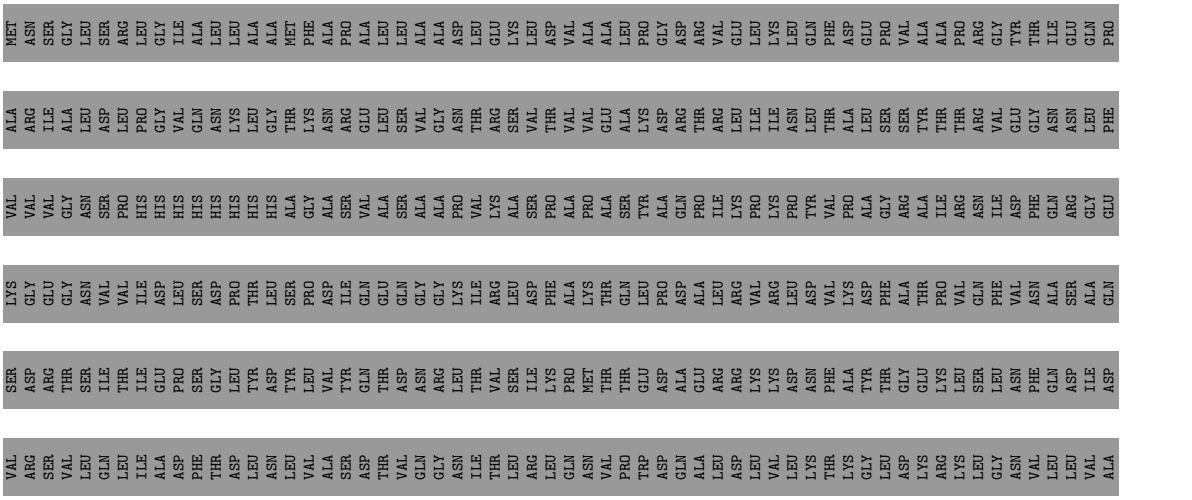
- Molecule 1: Fimbrial assembly protein PilQ

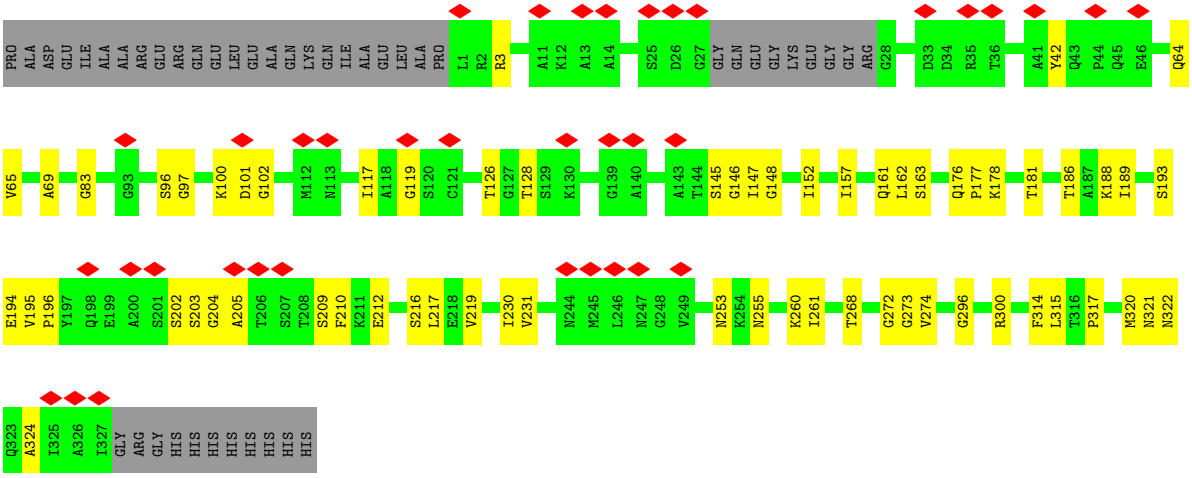
Chain J:



- Molecule 1: Fimbrial assembly protein PilQ

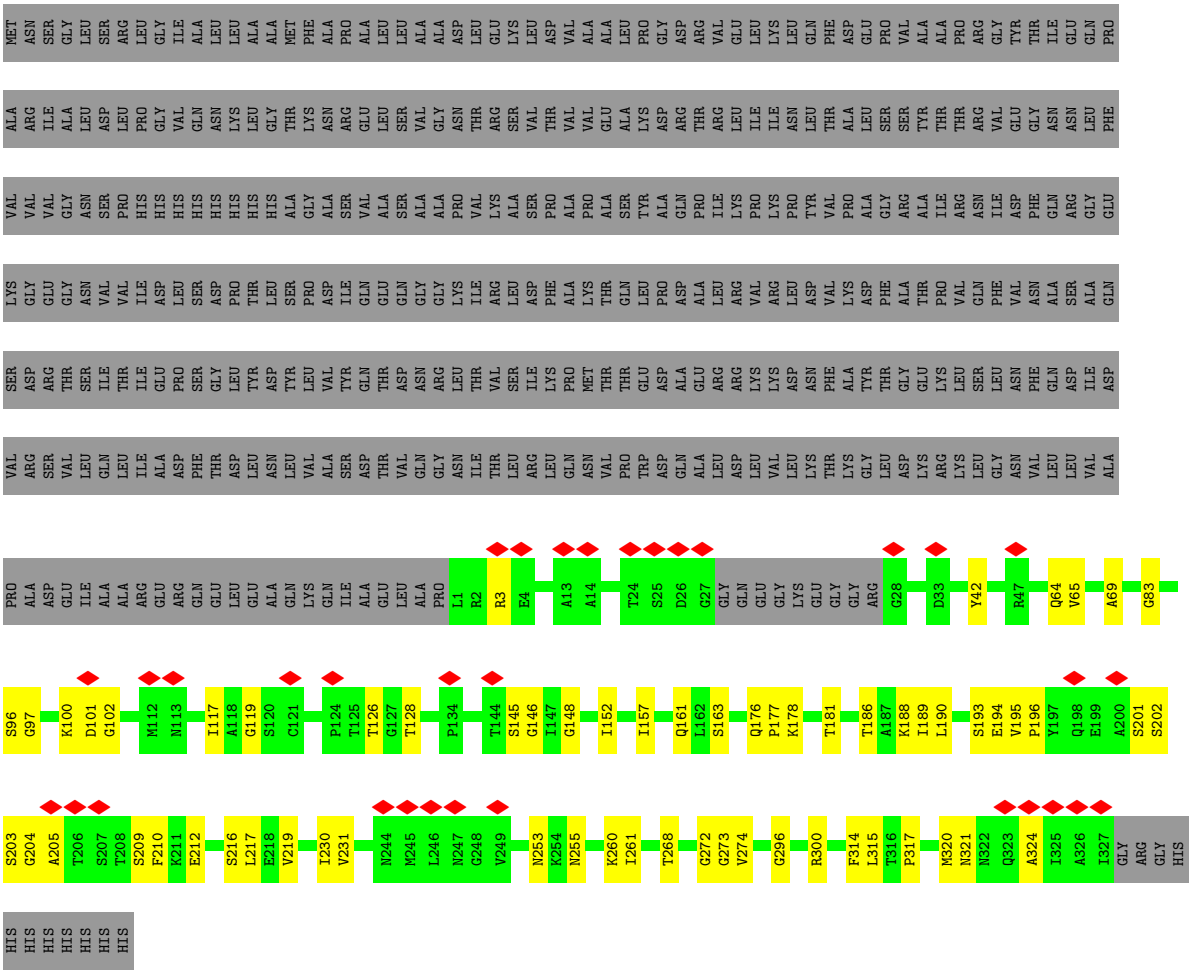
Chain K:





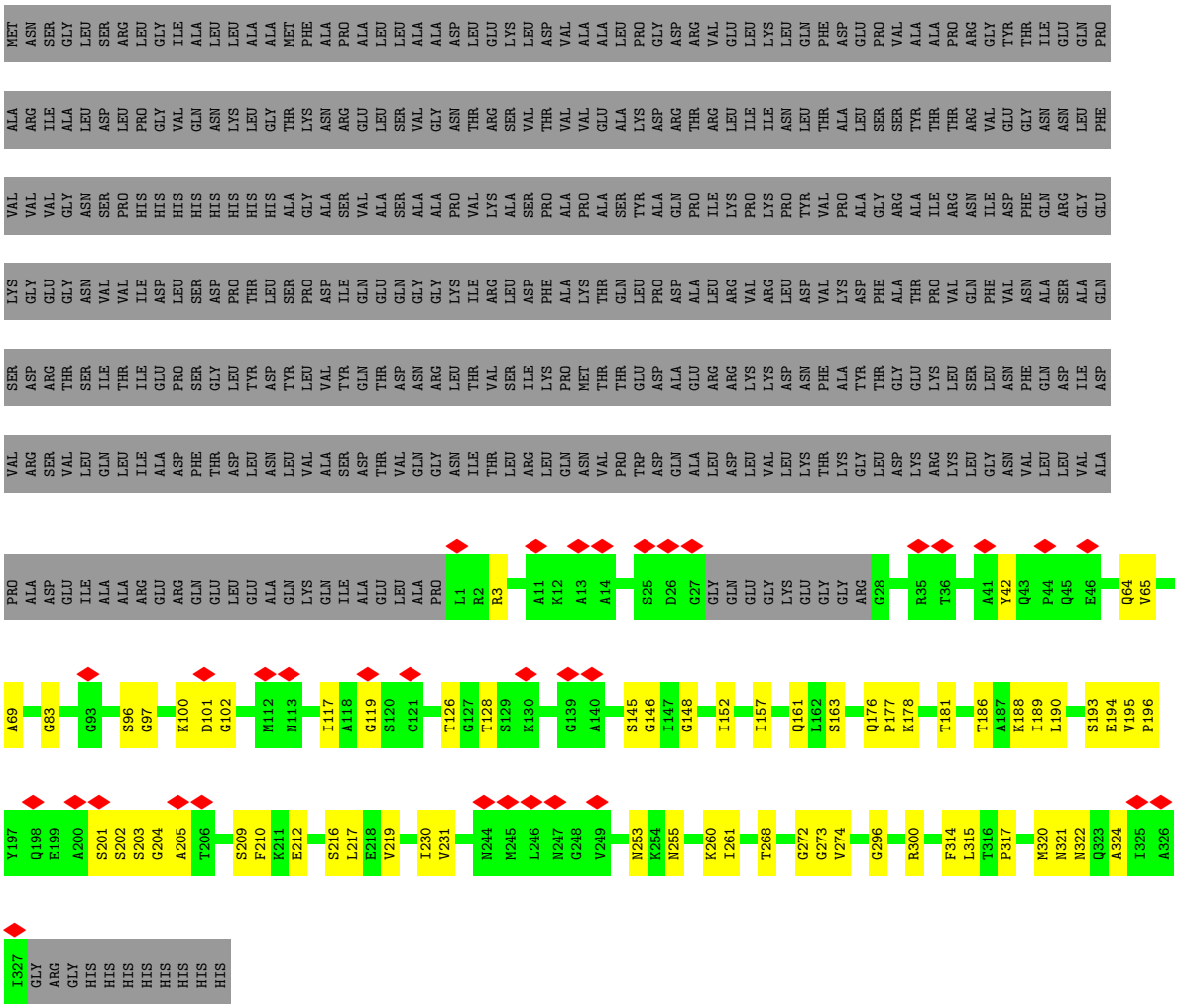
• Molecule 1: Fimbrial assembly protein PilQ

Chain L:



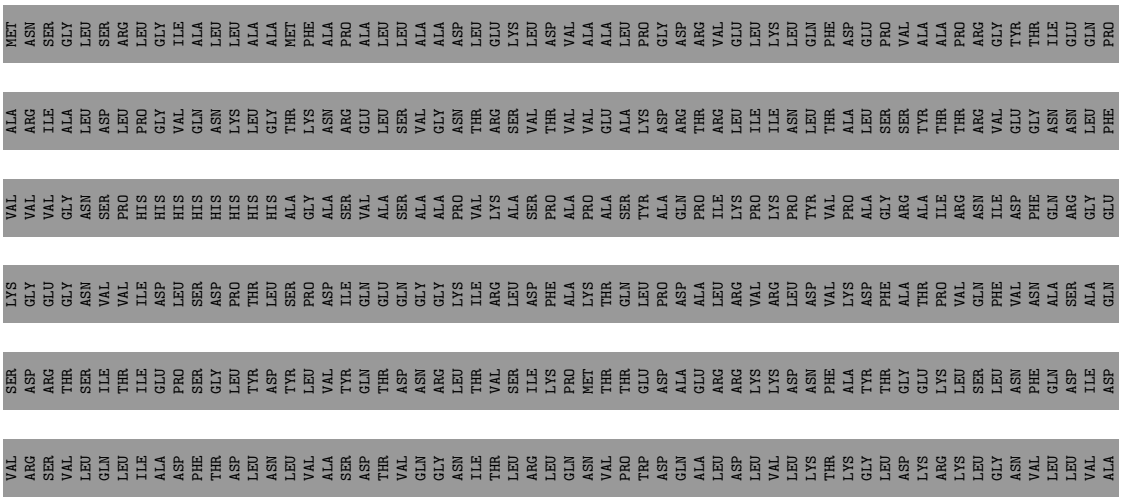
• Molecule 1: Fimbrial assembly protein PilQ

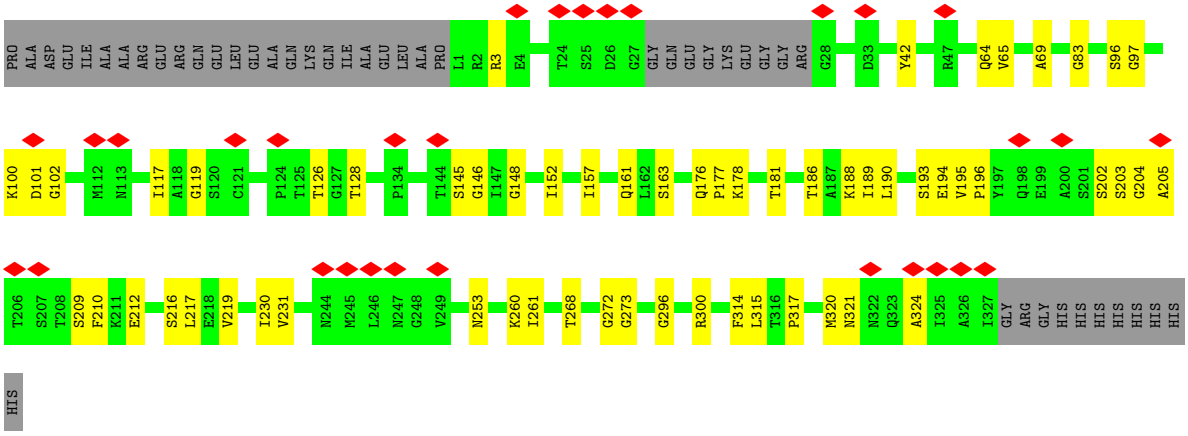
Chain M:



• Molecule 1: Fimbrial assembly protein PilQ

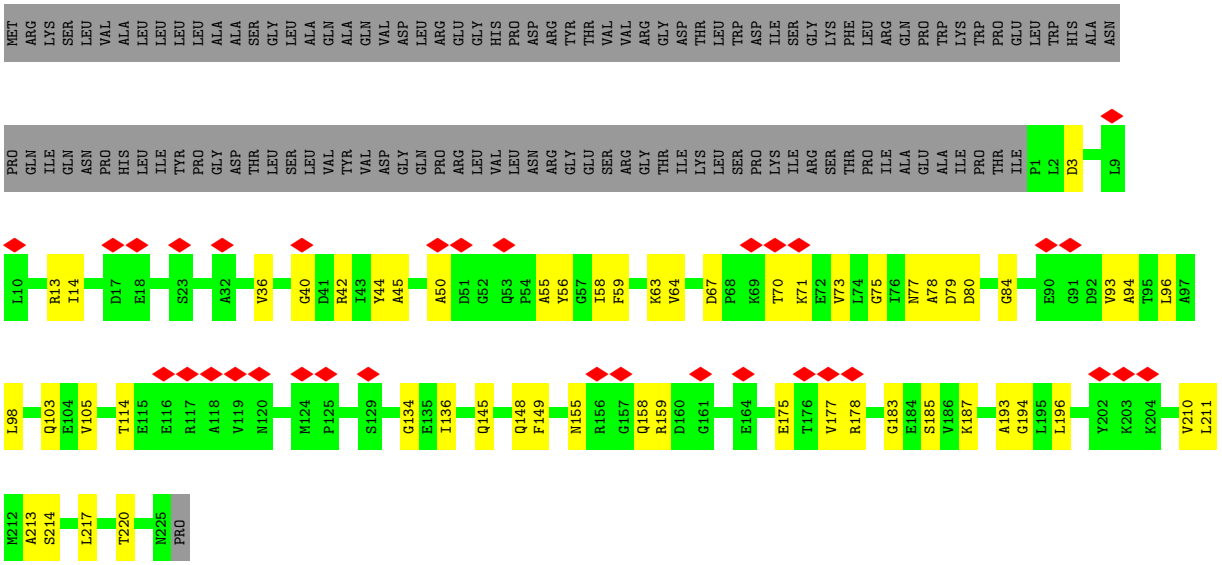
Chain N:





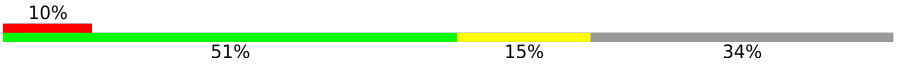
• Molecule 2: LysM domain-containing protein

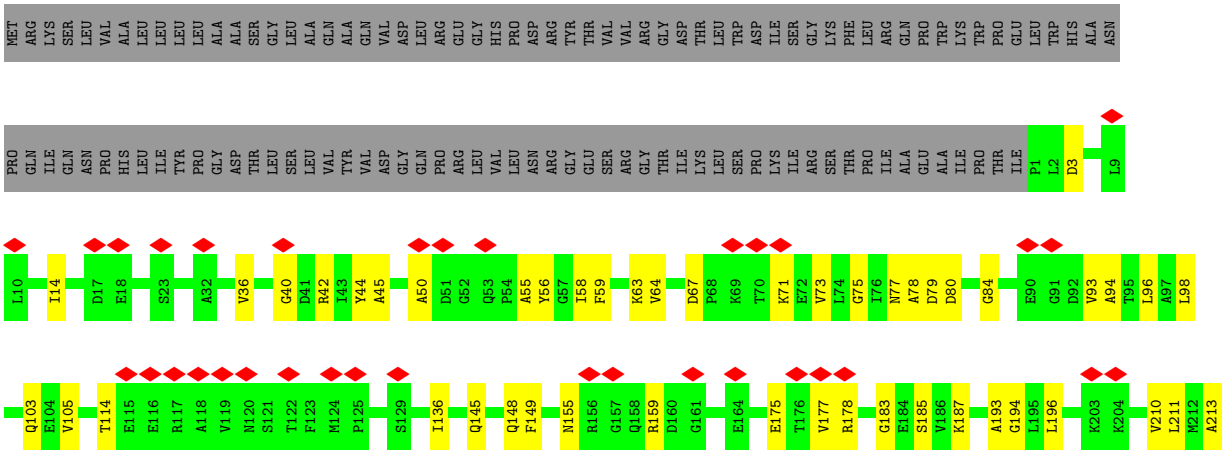
Chain O:

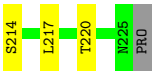


• Molecule 2: LysM domain-containing protein

Chain P:

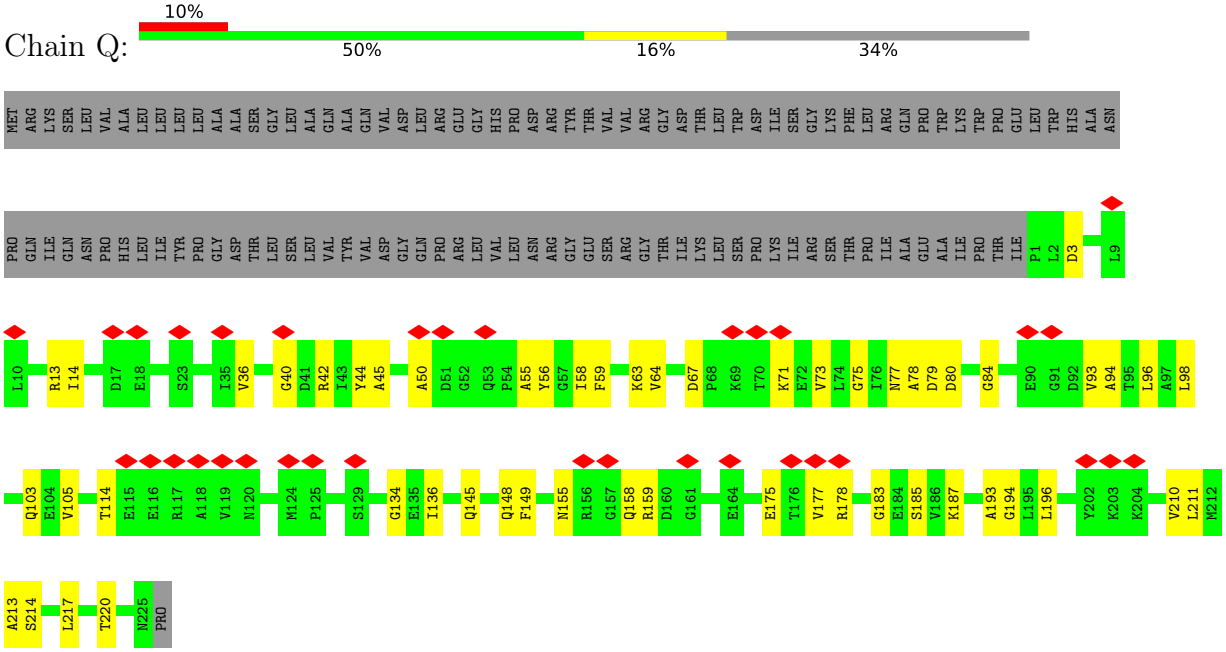






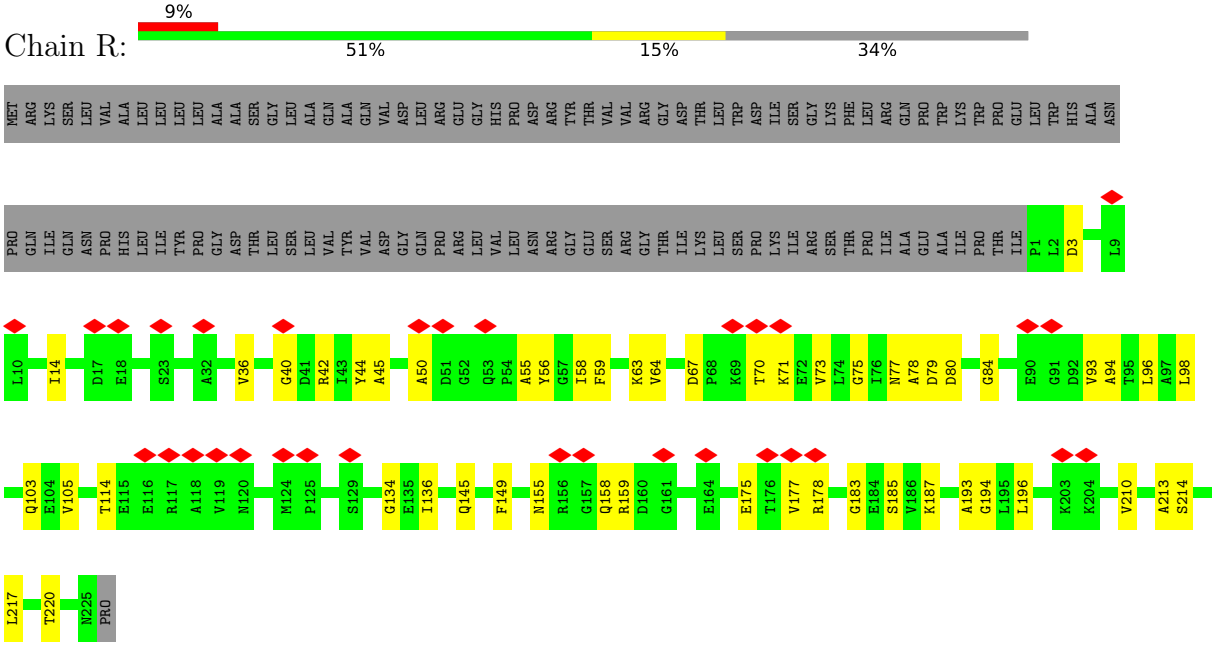
• Molecule 2: LysM domain-containing protein

Chain Q:



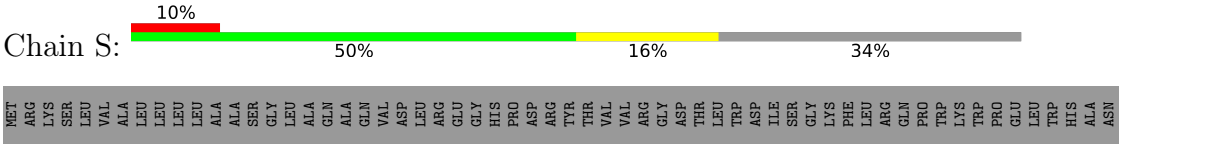
• Molecule 2: LysM domain-containing protein

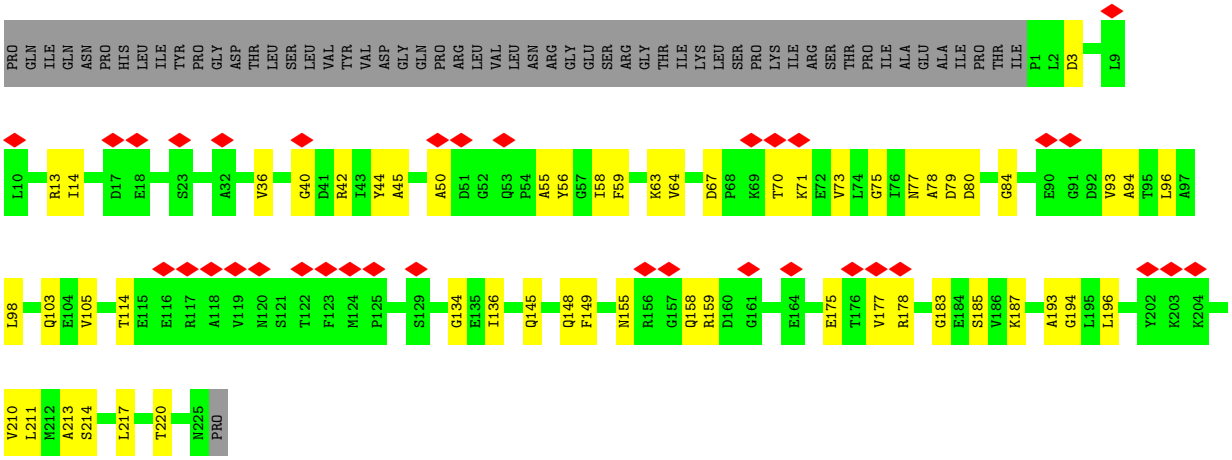
Chain R:



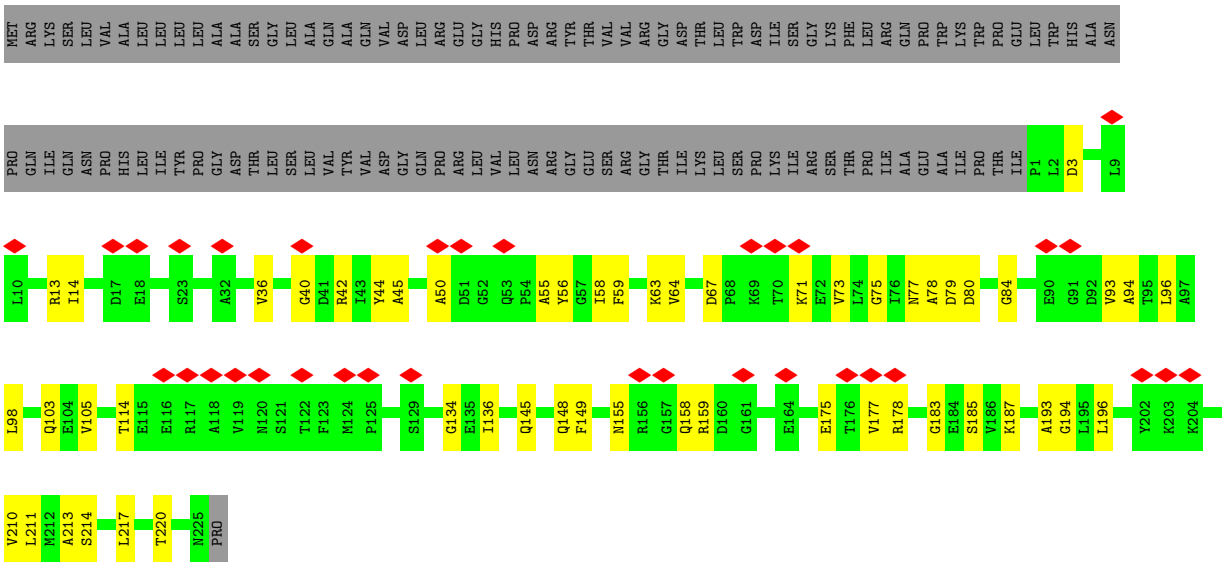
• Molecule 2: LysM domain-containing protein

Chain S:

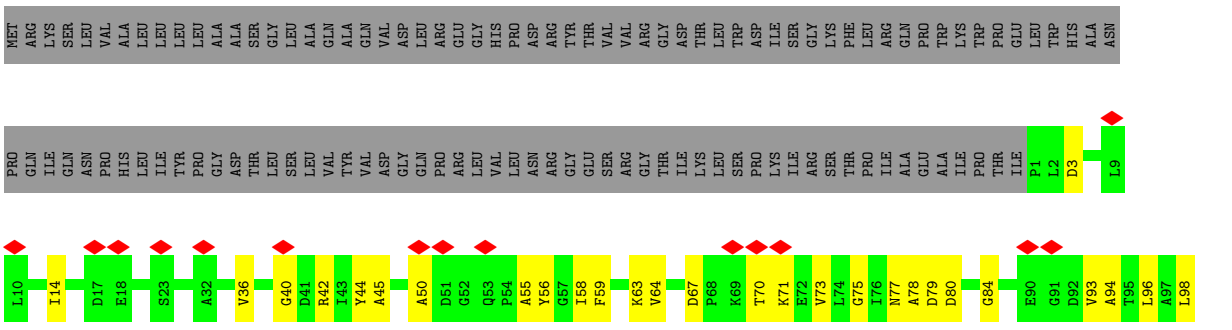


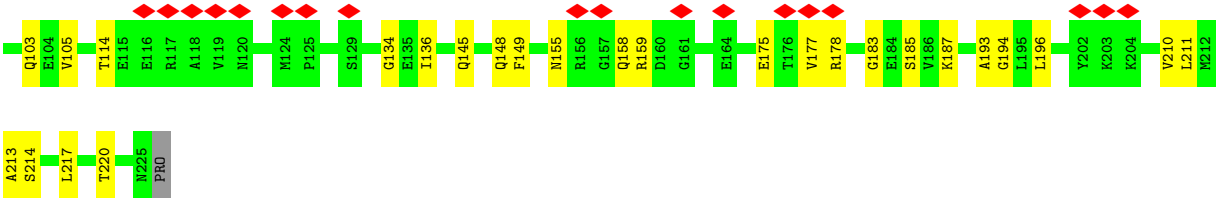


• Molecule 2: LysM domain-containing protein



• Molecule 2: LysM domain-containing protein




Q103
E104
V105
T114
E115
E116
R117
A118
V119
N120
M124
P125
S129
G134
E135
I136
Q145
Q148
F149
N155
R156
G157
Q158
R159
D160
G161
E164
E175
T176
V177
R178
G183
E184
S185
V186
K187
A193
G194
L195
L196
Y202
K203
K204
V210
L211
M212

A213
S214
L217
T220
N225
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	47468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	35.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.116	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	A	0.39	0/1604	0.65	0/2225
1	B	0.39	0/1604	0.65	0/2225
1	C	0.39	0/1604	0.65	0/2225
1	D	0.39	0/1604	0.65	0/2225
1	E	0.39	0/1604	0.65	0/2225
1	F	0.39	0/1604	0.65	0/2225
1	G	0.39	0/1604	0.65	0/2225
1	H	0.39	0/1604	0.65	0/2225
1	I	0.39	0/1604	0.65	0/2225
1	J	0.39	0/1604	0.65	0/2225
1	K	0.39	0/1604	0.65	0/2225
1	L	0.39	0/1604	0.65	0/2225
1	M	0.39	0/1604	0.65	0/2225
1	N	0.39	0/1604	0.65	0/2225
2	O	0.36	0/1101	0.67	0/1526
2	P	0.36	0/1101	0.67	0/1526
2	Q	0.36	0/1101	0.67	0/1526
2	R	0.36	0/1101	0.67	0/1526
2	S	0.36	0/1101	0.67	0/1526
2	T	0.36	0/1101	0.67	0/1526
2	U	0.36	0/1101	0.67	0/1526
All	All	0.38	0/30163	0.65	0/41832

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1606	0	731	46	0
1	B	1606	0	731	56	0
1	C	1606	0	731	51	0
1	D	1606	0	731	45	0
1	E	1606	0	731	47	0
1	F	1606	0	731	50	0
1	G	1606	0	731	49	0
1	H	1606	0	731	46	0
1	I	1606	0	731	44	0
1	J	1606	0	731	41	0
1	K	1606	0	731	43	0
1	L	1606	0	731	51	0
1	M	1606	0	731	51	0
1	N	1606	0	731	44	0
2	O	1102	0	514	34	0
2	P	1102	0	514	32	0
2	Q	1102	0	514	33	0
2	R	1102	0	514	34	0
2	S	1102	0	514	34	0
2	T	1102	0	514	34	0
2	U	1102	0	514	34	0
All	All	30198	0	13832	727	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 17.

All (727) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:149:PHE:HA	2:S:210:VAL:O	1.60	1.02
2:P:149:PHE:HA	2:P:210:VAL:O	1.60	1.01
2:O:149:PHE:HA	2:O:210:VAL:O	1.61	1.01
2:R:149:PHE:HA	2:R:210:VAL:O	1.61	1.01
2:T:149:PHE:HA	2:T:210:VAL:O	1.61	1.01
2:U:149:PHE:HA	2:U:210:VAL:O	1.60	1.01
2:Q:149:PHE:HA	2:Q:210:VAL:O	1.61	1.01
1:L:203:SER:CB	1:M:203:SER:HA	1.98	0.93
1:D:203:SER:CB	1:E:203:SER:HA	1.99	0.93
1:B:205:ALA:HB2	1:C:204:GLY:HA2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:ALA:HB2	1:M:204:GLY:HA2	1.52	0.92
1:F:203:SER:CB	1:G:203:SER:HA	2.00	0.90
1:B:203:SER:CB	1:C:203:SER:HA	2.03	0.89
1:B:205:ALA:CB	1:C:204:GLY:HA2	2.03	0.88
1:H:205:ALA:HB2	1:I:204:GLY:HA2	1.56	0.87
1:A:203:SER:HA	1:N:203:SER:CB	2.04	0.87
1:H:203:SER:CB	1:I:203:SER:HA	2.05	0.85
2:P:44:TYR:HA	2:P:94:ALA:O	1.77	0.85
2:O:44:TYR:HA	2:O:94:ALA:O	1.77	0.84
1:D:205:ALA:HB2	1:E:204:GLY:HA2	1.59	0.84
2:Q:44:TYR:HA	2:Q:94:ALA:O	1.77	0.84
2:U:44:TYR:HA	2:U:94:ALA:O	1.77	0.84
1:L:205:ALA:CB	1:M:204:GLY:HA2	2.07	0.84
1:J:203:SER:CB	1:K:203:SER:HA	2.08	0.83
2:R:44:TYR:HA	2:R:94:ALA:O	1.77	0.83
2:T:44:TYR:HA	2:T:94:ALA:O	1.77	0.83
1:A:204:GLY:HA2	1:N:205:ALA:HB2	1.61	0.83
2:S:44:TYR:HA	2:S:94:ALA:O	1.77	0.83
1:F:205:ALA:HB2	1:G:204:GLY:HA2	1.61	0.82
1:E:203:SER:CB	1:F:203:SER:HA	2.10	0.81
1:I:203:SER:CB	1:J:203:SER:HA	2.11	0.81
1:M:152:ILE:O	1:M:157:ILE:HA	1.81	0.80
1:F:152:ILE:O	1:F:157:ILE:HA	1.81	0.80
1:A:152:ILE:O	1:A:157:ILE:HA	1.81	0.80
1:E:152:ILE:O	1:E:157:ILE:HA	1.81	0.80
1:K:203:SER:CB	1:L:203:SER:HA	2.12	0.80
1:N:152:ILE:O	1:N:157:ILE:HA	1.81	0.80
1:B:152:ILE:O	1:B:157:ILE:HA	1.81	0.79
1:D:152:ILE:O	1:D:157:ILE:HA	1.81	0.79
1:K:152:ILE:O	1:K:157:ILE:HA	1.81	0.79
1:G:152:ILE:O	1:G:157:ILE:HA	1.81	0.79
1:G:203:SER:CB	1:H:203:SER:HA	2.11	0.79
1:C:152:ILE:O	1:C:157:ILE:HA	1.81	0.79
1:M:203:SER:CB	1:N:203:SER:HA	2.13	0.79
1:H:152:ILE:O	1:H:157:ILE:HA	1.81	0.79
1:L:152:ILE:O	1:L:157:ILE:HA	1.81	0.79
1:H:205:ALA:CB	1:I:204:GLY:HA2	2.12	0.78
1:I:152:ILE:O	1:I:157:ILE:HA	1.81	0.78
1:J:205:ALA:HB2	1:K:204:GLY:HA2	1.66	0.78
1:J:152:ILE:O	1:J:157:ILE:HA	1.81	0.77
1:L:203:SER:N	1:M:202:SER:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:CB	1:B:203:SER:HA	2.15	0.77
1:A:204:GLY:HA2	1:N:205:ALA:CB	2.15	0.76
1:D:205:ALA:CB	1:E:204:GLY:HA2	2.15	0.76
1:I:205:ALA:HB2	1:J:204:GLY:HA2	1.68	0.76
1:F:205:ALA:CB	1:G:204:GLY:HA2	2.15	0.76
1:F:203:SER:N	1:G:202:SER:O	2.18	0.75
1:D:194:GLU:HA	1:D:212:GLU:HA	1.68	0.74
1:D:203:SER:N	1:E:202:SER:O	2.19	0.74
1:E:194:GLU:HA	1:E:212:GLU:HA	1.68	0.74
1:K:194:GLU:HA	1:K:212:GLU:HA	1.68	0.74
1:F:194:GLU:HA	1:F:212:GLU:HA	1.68	0.74
1:I:194:GLU:HA	1:I:212:GLU:HA	1.68	0.74
1:J:194:GLU:HA	1:J:212:GLU:HA	1.68	0.74
1:B:194:GLU:HA	1:B:212:GLU:HA	1.68	0.74
1:C:194:GLU:HA	1:C:212:GLU:HA	1.68	0.74
1:L:194:GLU:HA	1:L:212:GLU:HA	1.68	0.74
1:G:194:GLU:HA	1:G:212:GLU:HA	1.68	0.73
1:H:194:GLU:HA	1:H:212:GLU:HA	1.68	0.73
1:A:194:GLU:HA	1:A:212:GLU:HA	1.68	0.73
2:U:59:PHE:HA	2:U:78:ALA:O	1.88	0.73
2:P:59:PHE:HA	2:P:78:ALA:O	1.89	0.73
2:S:59:PHE:HA	2:S:78:ALA:O	1.89	0.73
2:R:59:PHE:HA	2:R:78:ALA:O	1.89	0.73
1:N:194:GLU:HA	1:N:212:GLU:HA	1.68	0.73
2:Q:59:PHE:HA	2:Q:78:ALA:O	1.89	0.73
1:B:203:SER:N	1:C:202:SER:O	2.21	0.73
1:M:194:GLU:HA	1:M:212:GLU:HA	1.68	0.73
2:T:59:PHE:HA	2:T:78:ALA:O	1.89	0.73
1:G:205:ALA:HB2	1:H:204:GLY:HA2	1.71	0.73
1:C:203:SER:CB	1:D:203:SER:HA	2.19	0.72
1:N:321:ASN:HA	1:N:324:ALA:HB3	1.71	0.72
1:I:321:ASN:HA	1:I:324:ALA:HB3	1.72	0.72
1:M:321:ASN:HA	1:M:324:ALA:HB3	1.72	0.72
1:A:321:ASN:HA	1:A:324:ALA:HB3	1.72	0.72
1:B:321:ASN:HA	1:B:324:ALA:HB3	1.72	0.72
1:G:321:ASN:HA	1:G:324:ALA:HB3	1.72	0.72
1:H:321:ASN:HA	1:H:324:ALA:HB3	1.72	0.72
1:J:321:ASN:HA	1:J:324:ALA:HB3	1.72	0.72
1:K:321:ASN:HA	1:K:324:ALA:HB3	1.72	0.72
1:C:321:ASN:HA	1:C:324:ALA:HB3	1.72	0.72
1:D:321:ASN:HA	1:D:324:ALA:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:ASN:HA	1:E:324:ALA:HB3	1.72	0.72
1:F:321:ASN:HA	1:F:324:ALA:HB3	1.71	0.72
1:L:321:ASN:HA	1:L:324:ALA:HB3	1.72	0.72
2:O:59:PHE:HA	2:O:78:ALA:O	1.89	0.71
1:A:202:SER:O	1:N:203:SER:N	2.23	0.71
1:A:205:ALA:HB2	1:B:204:GLY:HA2	1.73	0.71
1:M:205:ALA:HB2	1:N:204:GLY:HA2	1.75	0.69
2:U:67:ASP:O	2:U:71:LYS:N	2.24	0.68
1:H:203:SER:N	1:I:202:SER:O	2.25	0.68
1:J:205:ALA:CB	1:K:204:GLY:HA2	2.24	0.68
2:O:67:ASP:O	2:O:71:LYS:N	2.24	0.68
2:T:67:ASP:O	2:T:71:LYS:N	2.24	0.68
2:U:155:ASN:O	2:U:159:ARG:N	2.27	0.68
1:E:205:ALA:HB2	1:F:204:GLY:HA2	1.75	0.67
1:G:205:ALA:CB	1:H:204:GLY:HA2	2.24	0.67
2:S:67:ASP:O	2:S:71:LYS:N	2.24	0.67
2:T:155:ASN:O	2:T:159:ARG:N	2.27	0.67
2:P:67:ASP:O	2:P:71:LYS:N	2.24	0.67
2:P:155:ASN:O	2:P:159:ARG:N	2.27	0.67
2:Q:67:ASP:O	2:Q:71:LYS:N	2.24	0.67
2:S:155:ASN:O	2:S:159:ARG:N	2.27	0.67
2:R:155:ASN:O	2:R:159:ARG:N	2.28	0.67
1:I:205:ALA:CB	1:J:204:GLY:HA2	2.25	0.66
2:O:155:ASN:O	2:O:159:ARG:N	2.28	0.66
2:R:67:ASP:O	2:R:71:LYS:N	2.24	0.66
1:M:322:ASN:CB	2:Q:3:ASP:CB	2.73	0.66
1:J:203:SER:N	1:K:202:SER:O	2.28	0.66
1:B:268:THR:CB	2:O:214:SER:HA	2.25	0.66
1:J:268:THR:CB	2:R:214:SER:HA	2.26	0.66
2:Q:155:ASN:O	2:Q:159:ARG:N	2.28	0.66
2:R:177:VAL:HA	2:R:185:SER:HA	1.78	0.65
2:Q:177:VAL:HA	2:Q:185:SER:HA	1.78	0.65
1:L:268:THR:CB	2:Q:214:SER:HA	2.27	0.65
1:C:64:GLN:HA	1:C:181:THR:O	1.97	0.65
1:F:268:THR:CB	2:T:214:SER:HA	2.27	0.65
1:B:64:GLN:HA	1:B:181:THR:O	1.97	0.65
1:F:64:GLN:HA	1:F:181:THR:O	1.97	0.65
1:K:64:GLN:HA	1:K:181:THR:O	1.97	0.65
1:G:64:GLN:HA	1:G:181:THR:O	1.97	0.65
1:J:64:GLN:HA	1:J:181:THR:O	1.97	0.65
1:A:205:ALA:CB	1:B:204:GLY:HA2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:SER:N	1:H:202:SER:O	2.28	0.64
2:S:177:VAL:HA	2:S:185:SER:HA	1.79	0.64
1:B:96:SER:HA	1:B:102:GLY:O	1.98	0.64
1:E:64:GLN:HA	1:E:181:THR:O	1.97	0.64
1:L:96:SER:HA	1:L:102:GLY:O	1.98	0.64
1:A:64:GLN:HA	1:A:181:THR:O	1.97	0.64
1:K:96:SER:HA	1:K:102:GLY:O	1.98	0.64
1:A:96:SER:HA	1:A:102:GLY:O	1.98	0.64
1:I:64:GLN:HA	1:I:181:THR:O	1.97	0.64
1:H:64:GLN:HA	1:H:181:THR:O	1.97	0.64
1:L:64:GLN:HA	1:L:181:THR:O	1.97	0.64
1:B:117:ILE:O	1:B:128:THR:HA	1.98	0.64
1:D:117:ILE:O	1:D:128:THR:HA	1.98	0.64
1:F:96:SER:HA	1:F:102:GLY:O	1.98	0.64
1:M:96:SER:HA	1:M:102:GLY:O	1.98	0.64
2:P:177:VAL:HA	2:P:185:SER:HA	1.78	0.64
1:D:64:GLN:HA	1:D:181:THR:O	1.97	0.63
1:E:96:SER:HA	1:E:102:GLY:O	1.98	0.63
1:G:196:PRO:HA	1:G:209:SER:O	1.99	0.63
1:K:203:SER:N	1:L:202:SER:O	2.29	0.63
1:N:117:ILE:O	1:N:128:THR:HA	1.98	0.63
2:T:177:VAL:HA	2:T:185:SER:HA	1.79	0.63
2:U:177:VAL:HA	2:U:185:SER:HA	1.78	0.63
1:C:96:SER:HA	1:C:102:GLY:O	1.98	0.63
1:G:96:SER:HA	1:G:102:GLY:O	1.98	0.63
1:H:96:SER:HA	1:H:102:GLY:O	1.98	0.63
1:M:196:PRO:HA	1:M:209:SER:O	1.98	0.63
1:C:196:PRO:HA	1:C:209:SER:O	1.99	0.63
1:L:196:PRO:HA	1:L:209:SER:O	1.98	0.63
1:N:96:SER:HA	1:N:102:GLY:O	1.98	0.63
1:A:117:ILE:O	1:A:128:THR:HA	1.98	0.63
1:F:117:ILE:O	1:F:128:THR:HA	1.98	0.63
1:M:117:ILE:O	1:M:128:THR:HA	1.98	0.63
1:N:64:GLN:HA	1:N:181:THR:O	1.97	0.63
1:D:196:PRO:HA	1:D:209:SER:O	1.98	0.63
1:F:196:PRO:HA	1:F:209:SER:O	1.99	0.63
1:H:196:PRO:HA	1:H:209:SER:O	1.99	0.63
1:I:96:SER:HA	1:I:102:GLY:O	1.98	0.63
1:N:196:PRO:HA	1:N:209:SER:O	1.98	0.63
2:O:177:VAL:HA	2:O:185:SER:HA	1.79	0.63
1:G:117:ILE:O	1:G:128:THR:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:SER:HA	1:J:102:GLY:O	1.98	0.63
1:K:196:PRO:HA	1:K:209:SER:O	1.98	0.63
1:M:64:GLN:HA	1:M:181:THR:O	1.97	0.63
1:D:96:SER:HA	1:D:102:GLY:O	1.98	0.63
1:E:117:ILE:O	1:E:128:THR:HA	1.98	0.63
1:J:117:ILE:O	1:J:128:THR:HA	1.98	0.63
1:K:117:ILE:O	1:K:128:THR:HA	1.98	0.63
1:L:117:ILE:O	1:L:128:THR:HA	1.98	0.63
1:E:196:PRO:HA	1:E:209:SER:O	1.99	0.63
1:H:117:ILE:O	1:H:128:THR:HA	1.98	0.63
1:B:196:PRO:HA	1:B:209:SER:O	1.99	0.63
1:C:117:ILE:O	1:C:128:THR:HA	1.98	0.63
1:I:117:ILE:O	1:I:128:THR:HA	1.98	0.63
1:J:196:PRO:HA	1:J:209:SER:O	1.99	0.62
1:A:196:PRO:HA	1:A:209:SER:O	1.98	0.62
1:C:322:ASN:CB	2:O:3:ASP:CB	2.77	0.62
1:I:196:PRO:HA	1:I:209:SER:O	1.98	0.62
1:K:205:ALA:HB2	1:L:204:GLY:HA2	1.82	0.62
1:A:203:SER:N	1:B:202:SER:O	2.33	0.61
1:I:203:SER:N	1:J:202:SER:O	2.31	0.61
1:C:148:GLY:O	1:C:161:GLN:HA	2.02	0.60
1:H:83:GLY:HA3	1:H:100:LYS:H	1.67	0.60
1:H:148:GLY:O	1:H:161:GLN:HA	2.02	0.60
1:I:148:GLY:O	1:I:161:GLN:HA	2.02	0.60
1:E:148:GLY:O	1:E:161:GLN:HA	2.02	0.60
1:G:148:GLY:O	1:G:161:GLN:HA	2.02	0.60
1:J:148:GLY:O	1:J:161:GLN:HA	2.02	0.60
1:M:205:ALA:CB	1:N:204:GLY:HA2	2.32	0.60
1:L:83:GLY:HA3	1:L:100:LYS:H	1.67	0.60
1:E:203:SER:N	1:F:202:SER:O	2.29	0.60
1:K:322:ASN:CB	2:R:3:ASP:CB	2.80	0.60
1:E:296:GLY:O	1:E:300:ARG:N	2.35	0.60
1:J:83:GLY:HA3	1:J:100:LYS:H	1.67	0.60
1:K:148:GLY:O	1:K:161:GLN:HA	2.02	0.60
1:B:296:GLY:O	1:B:300:ARG:N	2.35	0.60
1:C:296:GLY:O	1:C:300:ARG:N	2.35	0.60
1:D:83:GLY:HA3	1:D:100:LYS:H	1.67	0.60
1:E:83:GLY:HA3	1:E:100:LYS:H	1.67	0.60
1:F:148:GLY:O	1:F:161:GLN:HA	2.02	0.60
1:N:83:GLY:HA3	1:N:100:LYS:H	1.67	0.60
1:E:205:ALA:CB	1:F:204:GLY:HA2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:148:GLY:O	1:L:161:GLN:HA	2.02	0.60
1:N:296:GLY:O	1:N:300:ARG:N	2.35	0.60
1:G:296:GLY:O	1:G:300:ARG:N	2.35	0.59
1:A:148:GLY:O	1:A:161:GLN:HA	2.02	0.59
1:F:83:GLY:HA3	1:F:100:LYS:H	1.67	0.59
1:C:83:GLY:HA3	1:C:100:LYS:H	1.67	0.59
1:J:195:VAL:O	1:J:210:PHE:HA	2.03	0.59
1:K:195:VAL:O	1:K:210:PHE:HA	2.03	0.59
1:A:83:GLY:HA3	1:A:100:LYS:H	1.67	0.59
1:A:195:VAL:O	1:A:210:PHE:HA	2.03	0.59
1:N:148:GLY:O	1:N:161:GLN:HA	2.02	0.59
1:B:148:GLY:O	1:B:161:GLN:HA	2.01	0.59
1:D:296:GLY:O	1:D:300:ARG:N	2.35	0.59
1:M:83:GLY:HA3	1:M:100:LYS:H	1.67	0.59
1:F:296:GLY:O	1:F:300:ARG:N	2.35	0.59
1:G:195:VAL:O	1:G:210:PHE:HA	2.02	0.59
1:M:148:GLY:O	1:M:161:GLN:HA	2.02	0.59
1:A:296:GLY:O	1:A:300:ARG:N	2.35	0.59
1:D:148:GLY:O	1:D:161:GLN:HA	2.02	0.59
1:H:296:GLY:O	1:H:300:ARG:N	2.35	0.59
1:K:296:GLY:O	1:K:300:ARG:N	2.35	0.59
1:N:195:VAL:O	1:N:210:PHE:HA	2.03	0.59
1:L:296:GLY:O	1:L:300:ARG:N	2.35	0.59
1:B:83:GLY:HA3	1:B:100:LYS:H	1.67	0.59
1:I:195:VAL:O	1:I:210:PHE:HA	2.02	0.59
1:I:296:GLY:O	1:I:300:ARG:N	2.35	0.59
1:K:83:GLY:HA3	1:K:100:LYS:H	1.67	0.59
1:L:195:VAL:O	1:L:210:PHE:HA	2.03	0.59
1:D:268:THR:CB	2:U:214:SER:HA	2.32	0.59
1:I:83:GLY:HA3	1:I:100:LYS:H	1.67	0.59
1:M:195:VAL:O	1:M:210:PHE:HA	2.03	0.58
1:B:195:VAL:O	1:B:210:PHE:HA	2.02	0.58
1:F:195:VAL:O	1:F:210:PHE:HA	2.02	0.58
1:J:296:GLY:O	1:J:300:ARG:N	2.35	0.58
1:D:195:VAL:O	1:D:210:PHE:HA	2.02	0.58
1:H:195:VAL:O	1:H:210:PHE:HA	2.02	0.58
1:M:203:SER:N	1:N:202:SER:O	2.31	0.58
1:M:296:GLY:O	1:M:300:ARG:N	2.35	0.58
1:N:268:THR:CB	2:P:214:SER:HA	2.33	0.58
1:C:195:VAL:O	1:C:210:PHE:HA	2.03	0.58
1:G:83:GLY:HA3	1:G:100:LYS:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:VAL:O	1:E:210:PHE:HA	2.03	0.58
2:T:58:ILE:O	2:T:80:ASP:N	2.33	0.57
1:B:253:ASN:HA	1:C:193:SER:HA	1.85	0.57
1:H:268:THR:CB	2:S:214:SER:HA	2.35	0.57
1:E:322:ASN:CB	2:U:3:ASP:CB	2.82	0.56
1:L:253:ASN:HA	1:M:193:SER:HA	1.86	0.56
1:B:205:ALA:HB2	1:C:204:GLY:CA	2.31	0.56
2:S:45:ALA:O	2:S:93:VAL:HA	2.06	0.56
2:T:175:GLU:HA	2:T:187:LYS:HA	1.89	0.55
2:U:175:GLU:HA	2:U:187:LYS:HA	1.88	0.55
1:B:203:SER:CB	1:C:203:SER:CA	2.82	0.55
2:T:45:ALA:O	2:T:93:VAL:HA	2.06	0.55
2:O:175:GLU:HA	2:O:187:LYS:HA	1.88	0.55
2:P:175:GLU:HA	2:P:187:LYS:HA	1.89	0.55
2:S:175:GLU:HA	2:S:187:LYS:HA	1.89	0.55
2:U:45:ALA:O	2:U:93:VAL:HA	2.06	0.55
1:F:253:ASN:HA	1:G:193:SER:HA	1.88	0.55
2:P:58:ILE:O	2:P:80:ASP:N	2.33	0.55
1:B:268:THR:HA	1:B:315:LEU:O	2.07	0.55
1:C:268:THR:HA	1:C:315:LEU:O	2.07	0.55
1:D:268:THR:HA	1:D:315:LEU:O	2.07	0.55
2:Q:58:ILE:O	2:Q:80:ASP:N	2.33	0.55
2:Q:175:GLU:HA	2:Q:187:LYS:HA	1.89	0.55
2:R:45:ALA:O	2:R:93:VAL:HA	2.06	0.55
1:F:268:THR:HA	1:F:315:LEU:O	2.07	0.55
2:R:175:GLU:HA	2:R:187:LYS:HA	1.89	0.55
1:A:268:THR:HA	1:A:315:LEU:O	2.07	0.55
2:O:45:ALA:O	2:O:93:VAL:HA	2.06	0.55
1:D:253:ASN:HA	1:E:193:SER:HA	1.88	0.55
1:N:268:THR:HA	1:N:315:LEU:O	2.07	0.55
1:C:205:ALA:HB2	1:D:204:GLY:HA2	1.88	0.54
1:E:268:THR:HA	1:E:315:LEU:O	2.07	0.54
1:G:188:LYS:HA	1:G:217:LEU:O	2.07	0.54
1:H:268:THR:HA	1:H:315:LEU:O	2.07	0.54
2:Q:45:ALA:O	2:Q:93:VAL:HA	2.06	0.54
1:A:188:LYS:HA	1:A:217:LEU:O	2.08	0.54
1:B:188:LYS:HA	1:B:217:LEU:O	2.07	0.54
1:F:188:LYS:HA	1:F:217:LEU:O	2.08	0.54
1:K:188:LYS:HA	1:K:217:LEU:O	2.07	0.54
1:G:268:THR:HA	1:G:315:LEU:O	2.07	0.54
1:H:253:ASN:HA	1:I:193:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:268:THR:HA	1:M:315:LEU:O	2.07	0.54
2:P:45:ALA:O	2:P:93:VAL:HA	2.06	0.54
1:L:188:LYS:HA	1:L:217:LEU:O	2.07	0.54
1:H:188:LYS:HA	1:H:217:LEU:O	2.08	0.54
1:J:188:LYS:HA	1:J:217:LEU:O	2.07	0.54
1:L:203:SER:CB	1:M:203:SER:CA	2.79	0.54
1:N:188:LYS:HA	1:N:217:LEU:O	2.08	0.54
1:C:188:LYS:HA	1:C:217:LEU:O	2.08	0.54
1:E:188:LYS:HA	1:E:217:LEU:O	2.07	0.54
2:P:196:LEU:HA	2:P:210:VAL:HA	1.90	0.54
1:M:188:LYS:HA	1:M:217:LEU:O	2.08	0.54
2:Q:196:LEU:HA	2:Q:210:VAL:HA	1.90	0.54
1:J:268:THR:HA	1:J:315:LEU:O	2.07	0.53
2:U:36:VAL:O	2:U:105:VAL:N	2.42	0.53
1:L:268:THR:HA	1:L:315:LEU:O	2.07	0.53
2:S:36:VAL:O	2:S:105:VAL:N	2.42	0.53
2:T:36:VAL:O	2:T:105:VAL:N	2.42	0.53
1:G:322:ASN:CB	2:T:3:ASP:CB	2.86	0.53
1:I:188:LYS:HA	1:I:217:LEU:O	2.08	0.53
2:O:196:LEU:HA	2:O:210:VAL:HA	1.90	0.53
1:D:203:SER:CB	1:E:203:SER:CA	2.82	0.53
2:R:196:LEU:HA	2:R:210:VAL:HA	1.91	0.53
2:S:196:LEU:HA	2:S:210:VAL:HA	1.90	0.53
1:D:188:LYS:HA	1:D:217:LEU:O	2.08	0.53
1:K:205:ALA:CB	1:L:204:GLY:HA2	2.39	0.53
1:K:268:THR:HA	1:K:315:LEU:O	2.07	0.53
2:O:36:VAL:O	2:O:105:VAL:N	2.42	0.53
1:I:268:THR:HA	1:I:315:LEU:O	2.07	0.53
2:U:58:ILE:O	2:U:80:ASP:N	2.33	0.53
1:I:322:ASN:CB	2:S:3:ASP:CB	2.87	0.53
1:L:203:SER:H	1:M:202:SER:C	2.12	0.52
2:T:196:LEU:HA	2:T:210:VAL:HA	1.90	0.52
2:U:196:LEU:HA	2:U:210:VAL:HA	1.90	0.52
1:L:202:SER:H	1:M:202:SER:HA	1.74	0.52
2:P:36:VAL:O	2:P:105:VAL:N	2.42	0.52
2:Q:36:VAL:O	2:Q:105:VAL:N	2.42	0.52
2:R:36:VAL:O	2:R:105:VAL:N	2.42	0.52
2:O:136:ILE:O	2:O:220:THR:HA	2.10	0.52
2:P:55:ALA:HA	2:P:84:GLY:O	2.10	0.52
1:A:193:SER:HA	1:N:253:ASN:HA	1.91	0.52
2:P:136:ILE:O	2:P:220:THR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:55:ALA:HA	2:U:84:GLY:O	2.10	0.52
2:U:136:ILE:O	2:U:220:THR:HA	2.10	0.52
2:O:55:ALA:HA	2:O:84:GLY:O	2.10	0.52
2:T:50:ALA:CB	2:T:94:ALA:HB2	2.40	0.51
2:Q:55:ALA:HA	2:Q:84:GLY:O	2.10	0.51
2:S:55:ALA:HA	2:S:84:GLY:O	2.10	0.51
2:T:55:ALA:HA	2:T:84:GLY:O	2.10	0.51
1:B:202:SER:H	1:C:202:SER:HA	1.75	0.51
1:F:203:SER:CB	1:G:203:SER:CA	2.82	0.51
2:U:50:ALA:CB	2:U:94:ALA:HB2	2.41	0.51
1:H:3:ARG:HA	1:H:42:TYR:HA	1.93	0.51
2:Q:42:ARG:HA	2:Q:96:LEU:O	2.11	0.51
1:E:3:ARG:HA	1:E:42:TYR:HA	1.93	0.51
1:F:3:ARG:HA	1:F:42:TYR:HA	1.93	0.51
1:I:3:ARG:HA	1:I:42:TYR:HA	1.93	0.51
2:P:42:ARG:HA	2:P:96:LEU:O	2.11	0.51
2:Q:136:ILE:O	2:Q:220:THR:HA	2.10	0.51
2:R:50:ALA:CB	2:R:94:ALA:HB2	2.41	0.51
2:S:58:ILE:O	2:S:80:ASP:N	2.33	0.51
1:D:230:ILE:HA	1:D:261:ILE:O	2.11	0.51
1:I:230:ILE:HA	1:I:261:ILE:O	2.11	0.51
1:L:230:ILE:HA	1:L:261:ILE:O	2.11	0.51
2:O:40:GLY:N	2:O:98:LEU:O	2.36	0.51
2:O:42:ARG:HA	2:O:96:LEU:O	2.11	0.51
2:R:42:ARG:HA	2:R:96:LEU:O	2.11	0.51
1:A:230:ILE:HA	1:A:261:ILE:O	2.11	0.51
1:G:3:ARG:HA	1:G:42:TYR:HA	1.93	0.51
1:J:230:ILE:HA	1:J:261:ILE:O	2.11	0.51
2:P:50:ALA:CB	2:P:94:ALA:HB2	2.40	0.51
2:R:136:ILE:O	2:R:220:THR:HA	2.10	0.51
2:T:136:ILE:O	2:T:220:THR:HA	2.10	0.51
1:C:230:ILE:HA	1:C:261:ILE:O	2.11	0.50
1:D:3:ARG:HA	1:D:42:TYR:HA	1.93	0.50
1:H:230:ILE:HA	1:H:261:ILE:O	2.11	0.50
2:S:136:ILE:O	2:S:220:THR:HA	2.10	0.50
1:C:3:ARG:HA	1:C:42:TYR:HA	1.93	0.50
2:Q:50:ALA:CB	2:Q:94:ALA:HB2	2.41	0.50
2:R:40:GLY:N	2:R:98:LEU:O	2.36	0.50
2:R:55:ALA:HA	2:R:84:GLY:O	2.10	0.50
1:E:230:ILE:HA	1:E:261:ILE:O	2.11	0.50
1:K:231:VAL:O	1:K:260:LYS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:VAL:O	1:L:260:LYS:HA	2.12	0.50
1:A:231:VAL:O	1:A:260:LYS:HA	2.12	0.50
1:J:3:ARG:HA	1:J:42:TYR:HA	1.93	0.50
1:K:3:ARG:HA	1:K:42:TYR:HA	1.93	0.50
1:K:230:ILE:HA	1:K:261:ILE:O	2.11	0.50
1:M:230:ILE:HA	1:M:261:ILE:O	2.11	0.50
1:M:231:VAL:O	1:M:260:LYS:HA	2.12	0.50
1:N:231:VAL:O	1:N:260:LYS:HA	2.12	0.50
2:O:50:ALA:CB	2:O:94:ALA:HB2	2.40	0.50
2:U:40:GLY:N	2:U:98:LEU:O	2.36	0.50
1:B:231:VAL:O	1:B:260:LYS:HA	2.12	0.50
1:N:230:ILE:HA	1:N:261:ILE:O	2.11	0.50
2:Q:64:VAL:O	2:Q:73:VAL:HA	2.12	0.50
1:D:231:VAL:O	1:D:260:LYS:HA	2.12	0.50
1:L:202:SER:N	1:M:202:SER:HA	2.27	0.50
2:T:64:VAL:O	2:T:73:VAL:HA	2.12	0.50
2:O:64:VAL:O	2:O:73:VAL:HA	2.12	0.50
2:S:42:ARG:HA	2:S:96:LEU:O	2.11	0.50
2:S:40:GLY:N	2:S:98:LEU:O	2.36	0.50
2:S:50:ALA:CB	2:S:94:ALA:HB2	2.41	0.50
2:U:42:ARG:HA	2:U:96:LEU:O	2.11	0.50
1:A:3:ARG:HA	1:A:42:TYR:HA	1.93	0.49
1:B:230:ILE:HA	1:B:261:ILE:O	2.11	0.49
1:G:230:ILE:HA	1:G:261:ILE:O	2.11	0.49
1:M:3:ARG:HA	1:M:42:TYR:HA	1.93	0.49
1:N:3:ARG:HA	1:N:42:TYR:HA	1.93	0.49
1:F:231:VAL:O	1:F:260:LYS:HA	2.12	0.49
1:I:231:VAL:O	1:I:260:LYS:HA	2.12	0.49
1:J:231:VAL:O	1:J:260:LYS:HA	2.12	0.49
2:O:58:ILE:O	2:O:80:ASP:N	2.33	0.49
1:A:253:ASN:HA	1:B:193:SER:HA	1.95	0.49
1:C:231:VAL:O	1:C:260:LYS:HA	2.12	0.49
1:F:230:ILE:HA	1:F:261:ILE:O	2.11	0.49
1:L:3:ARG:HA	1:L:42:TYR:HA	1.93	0.49
1:B:3:ARG:HA	1:B:42:TYR:HA	1.93	0.49
1:L:205:ALA:HB2	1:M:204:GLY:CA	2.32	0.49
2:P:64:VAL:O	2:P:73:VAL:HA	2.12	0.49
2:R:145:GLN:HA	2:R:217:LEU:N	2.28	0.49
2:O:145:GLN:HA	2:O:217:LEU:N	2.28	0.49
2:P:145:GLN:HA	2:P:217:LEU:N	2.28	0.49
1:B:205:ALA:HB3	1:C:204:GLY:HA2	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:178:ARG:O	2:Q:183:GLY:N	2.32	0.49
2:U:64:VAL:O	2:U:73:VAL:HA	2.12	0.49
1:H:231:VAL:O	1:H:260:LYS:HA	2.12	0.49
1:J:253:ASN:HA	1:K:193:SER:HA	1.94	0.49
2:S:64:VAL:O	2:S:73:VAL:HA	2.12	0.49
2:T:42:ARG:HA	2:T:96:LEU:O	2.11	0.49
2:T:50:ALA:HB1	2:T:94:ALA:HB2	1.95	0.49
2:U:145:GLN:HA	2:U:217:LEU:N	2.28	0.49
2:Q:40:GLY:N	2:Q:98:LEU:O	2.36	0.49
2:R:64:VAL:O	2:R:73:VAL:HA	2.12	0.49
2:P:50:ALA:HB1	2:P:94:ALA:HB2	1.95	0.49
2:T:145:GLN:HA	2:T:217:LEU:N	2.28	0.49
1:A:322:ASN:CB	2:P:3:ASP:CB	2.90	0.48
1:G:231:VAL:O	1:G:260:LYS:HA	2.12	0.48
2:Q:145:GLN:HA	2:Q:217:LEU:N	2.28	0.48
2:S:50:ALA:HB1	2:S:94:ALA:HB2	1.95	0.48
2:U:50:ALA:HB1	2:U:94:ALA:HB2	1.95	0.48
2:R:58:ILE:O	2:R:80:ASP:N	2.33	0.48
1:G:253:ASN:HA	1:H:193:SER:HA	1.94	0.48
2:O:50:ALA:HB1	2:O:94:ALA:HB2	1.95	0.48
1:E:231:VAL:O	1:E:260:LYS:HA	2.12	0.48
2:Q:50:ALA:HB1	2:Q:94:ALA:HB2	1.95	0.48
1:F:202:SER:H	1:G:202:SER:HA	1.77	0.48
1:I:97:GLY:H	1:I:102:GLY:H	1.62	0.48
2:R:50:ALA:HB1	2:R:94:ALA:HB2	1.95	0.48
1:F:97:GLY:H	1:F:102:GLY:H	1.62	0.48
1:G:97:GLY:H	1:G:102:GLY:H	1.62	0.48
1:I:253:ASN:HA	1:J:193:SER:HA	1.95	0.48
1:D:203:SER:H	1:E:202:SER:C	2.16	0.48
1:K:274:VAL:HA	1:L:176:GLN:O	2.14	0.48
1:L:97:GLY:H	1:L:102:GLY:H	1.62	0.48
1:L:201:SER:CB	1:M:201:SER:O	2.62	0.48
2:S:14:ILE:HA	2:S:77:ASN:O	2.14	0.48
2:S:145:GLN:HA	2:S:217:LEU:N	2.28	0.48
1:B:202:SER:N	1:C:202:SER:HA	2.29	0.48
1:B:201:SER:CB	1:C:201:SER:O	2.61	0.47
1:J:97:GLY:H	1:J:102:GLY:H	1.62	0.47
1:K:97:GLY:H	1:K:102:GLY:H	1.62	0.47
1:B:201:SER:CA	1:C:202:SER:HA	2.45	0.47
1:H:97:GLY:H	1:H:102:GLY:H	1.62	0.47
1:E:97:GLY:H	1:E:102:GLY:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:97:GLY:H	1:M:102:GLY:H	1.62	0.47
1:D:97:GLY:H	1:D:102:GLY:H	1.62	0.47
1:D:272:GLY:HA2	1:E:178:LYS:O	2.14	0.47
1:N:97:GLY:H	1:N:102:GLY:H	1.62	0.47
1:H:203:SER:CB	1:I:203:SER:CA	2.88	0.47
2:U:14:ILE:HA	2:U:77:ASN:O	2.14	0.47
2:P:40:GLY:N	2:P:98:LEU:O	2.36	0.47
1:B:97:GLY:H	1:B:102:GLY:H	1.62	0.47
2:Q:14:ILE:HA	2:Q:77:ASN:O	2.14	0.47
2:R:194:GLY:HA3	2:R:213:ALA:H	1.80	0.47
1:C:97:GLY:H	1:C:102:GLY:H	1.62	0.47
2:R:14:ILE:HA	2:R:77:ASN:O	2.14	0.47
1:L:201:SER:CA	1:M:202:SER:HA	2.45	0.47
1:M:253:ASN:HA	1:N:193:SER:HA	1.97	0.47
2:T:14:ILE:HA	2:T:77:ASN:O	2.14	0.47
1:A:97:GLY:H	1:A:102:GLY:H	1.62	0.46
2:P:194:GLY:HA3	2:P:213:ALA:H	1.80	0.46
1:D:202:SER:H	1:E:202:SER:HA	1.79	0.46
2:O:14:ILE:HA	2:O:77:ASN:O	2.14	0.46
1:F:146:GLY:O	1:F:163:SER:HA	2.15	0.46
1:H:146:GLY:O	1:H:163:SER:HA	2.15	0.46
2:T:194:GLY:HA3	2:T:213:ALA:H	1.80	0.46
1:F:255:ASN:HA	1:G:190:LEU:O	2.16	0.46
1:G:146:GLY:O	1:G:163:SER:HA	2.15	0.46
1:M:119:GLY:O	1:M:126:THR:HA	2.16	0.46
2:P:14:ILE:HA	2:P:77:ASN:O	2.14	0.46
2:Q:56:TYR:HA	2:Q:114:THR:N	2.31	0.46
1:D:273:GLY:O	1:E:177:PRO:HA	2.15	0.46
1:E:119:GLY:O	1:E:126:THR:HA	2.16	0.46
1:G:119:GLY:O	1:G:126:THR:HA	2.16	0.46
1:J:119:GLY:O	1:J:126:THR:HA	2.16	0.46
1:K:119:GLY:O	1:K:126:THR:HA	2.16	0.46
2:P:56:TYR:HA	2:P:114:THR:N	2.31	0.46
2:S:194:GLY:HA3	2:S:213:ALA:H	1.80	0.46
1:A:146:GLY:O	1:A:163:SER:HA	2.15	0.46
1:I:272:GLY:HA2	1:J:178:LYS:O	2.15	0.46
1:K:272:GLY:HA2	1:L:178:LYS:O	2.15	0.46
2:R:56:TYR:HA	2:R:114:THR:N	2.31	0.46
1:B:119:GLY:O	1:B:126:THR:HA	2.16	0.46
1:I:119:GLY:O	1:I:126:THR:HA	2.16	0.46
1:I:146:GLY:O	1:I:163:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:GLY:O	1:L:126:THR:HA	2.16	0.46
1:M:146:GLY:O	1:M:163:SER:HA	2.15	0.46
2:O:194:GLY:HA3	2:O:213:ALA:H	1.80	0.46
1:A:119:GLY:O	1:A:126:THR:HA	2.16	0.46
1:H:119:GLY:O	1:H:126:THR:HA	2.16	0.46
2:Q:194:GLY:HA3	2:Q:213:ALA:H	1.80	0.46
1:D:119:GLY:O	1:D:126:THR:HA	2.16	0.46
1:E:146:GLY:O	1:E:163:SER:HA	2.15	0.46
1:N:119:GLY:O	1:N:126:THR:HA	2.16	0.46
2:U:56:TYR:HA	2:U:114:THR:N	2.31	0.46
2:U:194:GLY:HA3	2:U:213:ALA:H	1.80	0.46
1:A:97:GLY:C	1:A:101:ASP:HA	2.36	0.45
1:C:97:GLY:C	1:C:101:ASP:HA	2.37	0.45
1:C:272:GLY:HA2	1:D:178:LYS:O	2.15	0.45
1:E:272:GLY:HA2	1:F:178:LYS:O	2.15	0.45
2:T:56:TYR:HA	2:T:114:THR:N	2.31	0.45
1:B:97:GLY:C	1:B:101:ASP:HA	2.36	0.45
1:C:146:GLY:O	1:C:163:SER:HA	2.15	0.45
1:J:146:GLY:O	1:J:163:SER:HA	2.15	0.45
1:N:97:GLY:C	1:N:101:ASP:HA	2.37	0.45
2:O:56:TYR:HA	2:O:114:THR:N	2.31	0.45
1:E:253:ASN:HA	1:F:193:SER:HA	1.97	0.45
1:F:119:GLY:O	1:F:126:THR:HA	2.16	0.45
1:M:97:GLY:C	1:M:101:ASP:HA	2.37	0.45
2:T:40:GLY:N	2:T:98:LEU:O	2.36	0.45
1:A:255:ASN:HA	1:B:190:LEU:O	2.16	0.45
1:G:97:GLY:C	1:G:101:ASP:HA	2.36	0.45
1:L:146:GLY:O	1:L:163:SER:HA	2.15	0.45
2:Q:80:ASP:HA	2:Q:103:GLN:CB	2.47	0.45
1:B:146:GLY:O	1:B:163:SER:HA	2.15	0.45
1:B:189:ILE:O	1:B:216:SER:HA	2.17	0.45
1:C:119:GLY:O	1:C:126:THR:HA	2.16	0.45
1:I:97:GLY:C	1:I:101:ASP:HA	2.37	0.45
1:L:97:GLY:C	1:L:101:ASP:HA	2.36	0.45
2:S:56:TYR:HA	2:S:114:THR:N	2.31	0.45
1:D:97:GLY:C	1:D:101:ASP:HA	2.36	0.45
1:K:146:GLY:O	1:K:163:SER:HA	2.15	0.45
1:L:272:GLY:HA2	1:M:178:LYS:O	2.16	0.45
1:N:146:GLY:O	1:N:163:SER:HA	2.15	0.45
1:A:189:ILE:O	1:A:216:SER:HA	2.17	0.45
1:J:97:GLY:C	1:J:101:ASP:HA	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:189:ILE:O	1:N:216:SER:HA	2.17	0.45
2:S:80:ASP:HA	2:S:103:GLN:CB	2.47	0.45
1:C:189:ILE:O	1:C:216:SER:HA	2.17	0.45
1:D:146:GLY:O	1:D:163:SER:HA	2.15	0.45
1:D:274:VAL:HA	1:E:176:GLN:O	2.17	0.45
1:H:65:VAL:HA	1:H:320:MET:H	1.82	0.45
1:H:97:GLY:C	1:H:101:ASP:HA	2.36	0.45
1:M:189:ILE:O	1:M:216:SER:HA	2.17	0.45
2:U:80:ASP:HA	2:U:103:GLN:CB	2.47	0.45
1:A:65:VAL:HA	1:A:320:MET:H	1.82	0.45
1:K:65:VAL:HA	1:K:320:MET:H	1.82	0.45
1:E:97:GLY:C	1:E:101:ASP:HA	2.37	0.45
1:K:97:GLY:C	1:K:101:ASP:HA	2.37	0.45
1:L:189:ILE:O	1:L:216:SER:HA	2.17	0.45
1:B:65:VAL:HA	1:B:320:MET:H	1.82	0.44
1:B:255:ASN:HA	1:C:190:LEU:O	2.18	0.44
1:D:189:ILE:O	1:D:216:SER:HA	2.17	0.44
1:E:65:VAL:HA	1:E:320:MET:H	1.82	0.44
1:G:189:ILE:O	1:G:216:SER:HA	2.17	0.44
1:L:273:GLY:O	1:M:177:PRO:HA	2.16	0.44
2:P:80:ASP:HA	2:P:103:GLN:CB	2.47	0.44
2:T:80:ASP:HA	2:T:103:GLN:CB	2.47	0.44
1:A:272:GLY:HA2	1:B:178:LYS:O	2.17	0.44
1:D:65:VAL:HA	1:D:320:MET:H	1.82	0.44
1:F:97:GLY:C	1:F:101:ASP:HA	2.36	0.44
1:J:189:ILE:O	1:J:216:SER:HA	2.17	0.44
1:K:255:ASN:HA	1:L:190:LEU:O	2.17	0.44
1:L:65:VAL:HA	1:L:320:MET:H	1.82	0.44
2:O:80:ASP:HA	2:O:103:GLN:CB	2.47	0.44
2:T:63:LYS:HA	2:T:75:GLY:HA2	2.00	0.44
1:E:189:ILE:O	1:E:216:SER:HA	2.17	0.44
1:F:189:ILE:O	1:F:216:SER:HA	2.17	0.44
1:I:189:ILE:O	1:I:216:SER:HA	2.17	0.44
1:K:189:ILE:O	1:K:216:SER:HA	2.17	0.44
1:C:203:SER:N	1:D:202:SER:O	2.40	0.44
1:F:272:GLY:HA2	1:G:178:LYS:O	2.17	0.44
1:F:274:VAL:HA	1:G:176:GLN:O	2.18	0.44
1:I:273:GLY:O	1:J:177:PRO:HA	2.17	0.44
2:S:145:GLN:HA	2:S:217:LEU:O	2.18	0.44
2:U:63:LYS:HA	2:U:75:GLY:HA2	2.00	0.44
1:A:203:SER:CA	1:N:203:SER:CB	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:VAL:HA	1:I:320:MET:H	1.82	0.44
1:M:255:ASN:HA	1:N:190:LEU:O	2.17	0.44
1:M:272:GLY:HA2	1:N:178:LYS:O	2.17	0.44
2:O:145:GLN:HA	2:O:217:LEU:O	2.18	0.44
2:P:145:GLN:HA	2:P:217:LEU:O	2.18	0.44
2:P:178:ARG:O	2:P:183:GLY:N	2.32	0.44
2:S:63:LYS:HA	2:S:75:GLY:HA2	2.00	0.44
2:O:63:LYS:HA	2:O:75:GLY:HA2	2.00	0.44
2:P:63:LYS:HA	2:P:75:GLY:HA2	2.00	0.44
2:U:145:GLN:HA	2:U:217:LEU:O	2.18	0.44
1:E:274:VAL:HA	1:F:176:GLN:O	2.17	0.44
1:G:65:VAL:HA	1:G:320:MET:H	1.82	0.44
1:G:255:ASN:HA	1:H:190:LEU:O	2.17	0.44
1:H:189:ILE:O	1:H:216:SER:HA	2.17	0.44
1:J:272:GLY:HA2	1:K:178:LYS:O	2.17	0.44
1:J:273:GLY:O	1:K:177:PRO:HA	2.17	0.44
2:R:80:ASP:HA	2:R:103:GLN:CB	2.47	0.44
2:R:145:GLN:HA	2:R:217:LEU:O	2.18	0.44
2:S:178:ARG:O	2:S:183:GLY:N	2.32	0.44
1:C:65:VAL:HA	1:C:320:MET:H	1.82	0.43
1:C:274:VAL:HA	1:D:176:GLN:O	2.17	0.43
1:F:69:ALA:HA	1:F:314:PHE:O	2.18	0.43
1:H:273:GLY:O	1:I:177:PRO:HA	2.18	0.43
1:M:274:VAL:HA	1:N:176:GLN:O	2.17	0.43
2:Q:58:ILE:O	2:Q:79:ASP:HA	2.18	0.43
2:T:58:ILE:O	2:T:79:ASP:HA	2.18	0.43
1:F:65:VAL:HA	1:F:320:MET:H	1.82	0.43
1:H:272:GLY:HA2	1:I:178:LYS:O	2.18	0.43
1:J:65:VAL:HA	1:J:320:MET:H	1.82	0.43
1:J:69:ALA:HA	1:J:314:PHE:O	2.18	0.43
1:K:69:ALA:HA	1:K:314:PHE:O	2.18	0.43
1:K:253:ASN:HA	1:L:193:SER:HA	1.99	0.43
1:N:65:VAL:HA	1:N:320:MET:H	1.83	0.43
2:O:58:ILE:O	2:O:79:ASP:HA	2.18	0.43
2:R:178:ARG:O	2:R:183:GLY:N	2.32	0.43
2:T:145:GLN:HA	2:T:217:LEU:O	2.18	0.43
1:D:255:ASN:HA	1:E:190:LEU:O	2.18	0.43
1:F:202:SER:N	1:G:202:SER:HA	2.32	0.43
1:G:272:GLY:HA2	1:H:178:LYS:O	2.17	0.43
1:H:69:ALA:HA	1:H:314:PHE:O	2.18	0.43
1:I:274:VAL:HA	1:J:176:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:VAL:HA	1:M:320:MET:H	1.82	0.43
1:C:205:ALA:CB	1:D:204:GLY:HA2	2.48	0.43
1:D:202:SER:N	1:E:202:SER:HA	2.32	0.43
1:I:69:ALA:HA	1:I:314:PHE:O	2.18	0.43
1:L:69:ALA:HA	1:L:314:PHE:O	2.18	0.43
1:L:205:ALA:HB3	1:M:204:GLY:HA2	1.96	0.43
1:M:69:ALA:HA	1:M:314:PHE:O	2.18	0.43
2:R:63:LYS:HA	2:R:75:GLY:HA2	2.00	0.43
2:U:58:ILE:O	2:U:79:ASP:HA	2.18	0.43
1:I:255:ASN:HA	1:J:190:LEU:O	2.18	0.43
2:S:58:ILE:O	2:S:79:ASP:HA	2.18	0.43
2:R:58:ILE:O	2:R:79:ASP:HA	2.18	0.43
2:U:178:ARG:O	2:U:183:GLY:N	2.32	0.43
1:B:203:SER:H	1:C:202:SER:C	2.16	0.43
1:E:255:ASN:HA	1:F:190:LEU:O	2.19	0.43
1:G:69:ALA:HA	1:G:314:PHE:O	2.18	0.43
2:Q:145:GLN:HA	2:Q:217:LEU:O	2.18	0.43
1:B:201:SER:HA	1:C:202:SER:HA	2.01	0.43
1:B:251:PRO:HA	1:C:194:GLU:O	2.19	0.43
2:Q:63:LYS:HA	2:Q:75:GLY:HA2	2.00	0.43
1:A:202:SER:HA	1:N:202:SER:H	1.82	0.42
1:D:69:ALA:HA	1:D:314:PHE:O	2.18	0.42
1:B:69:ALA:HA	1:B:314:PHE:O	2.18	0.42
1:E:273:GLY:O	1:F:177:PRO:HA	2.19	0.42
1:N:69:ALA:HA	1:N:314:PHE:O	2.19	0.42
2:P:58:ILE:O	2:P:79:ASP:HA	2.18	0.42
1:A:69:ALA:HA	1:A:314:PHE:O	2.18	0.42
1:B:273:GLY:O	1:C:177:PRO:HA	2.19	0.42
1:H:255:ASN:HA	1:I:190:LEU:O	2.20	0.42
2:Q:13:ARG:O	2:Q:79:ASP:N	2.52	0.42
1:G:274:VAL:HA	1:H:176:GLN:O	2.19	0.42
1:H:205:ALA:HB3	1:I:204:GLY:HA2	1.99	0.42
1:A:178:LYS:O	1:N:272:GLY:HA2	2.19	0.42
1:B:205:ALA:CB	1:C:204:GLY:CA	2.87	0.42
1:C:273:GLY:O	1:D:177:PRO:HA	2.19	0.42
1:F:203:SER:H	1:G:202:SER:C	2.17	0.42
1:F:273:GLY:O	1:G:177:PRO:HA	2.19	0.42
1:H:202:SER:H	1:I:202:SER:HA	1.85	0.42
1:A:273:GLY:O	1:B:177:PRO:HA	2.19	0.42
1:A:274:VAL:HA	1:B:176:GLN:O	2.19	0.42
1:C:69:ALA:HA	1:C:314:PHE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ALA:HA	1:E:314:PHE:O	2.18	0.42
1:M:273:GLY:O	1:N:177:PRO:HA	2.20	0.42
1:J:274:VAL:HA	1:K:176:GLN:O	2.20	0.42
1:L:274:VAL:HA	1:M:176:GLN:O	2.20	0.42
2:O:13:ARG:O	2:O:79:ASP:N	2.52	0.42
1:B:272:GLY:HA2	1:C:178:LYS:O	2.19	0.42
1:L:255:ASN:HA	1:M:190:LEU:O	2.19	0.42
1:F:251:PRO:HA	1:G:194:GLU:O	2.19	0.41
2:P:148:GLN:O	2:P:211:LEU:HA	2.21	0.41
2:T:13:ARG:O	2:T:79:ASP:N	2.52	0.41
2:T:148:GLN:O	2:T:211:LEU:HA	2.21	0.41
2:T:178:ARG:O	2:T:183:GLY:N	2.32	0.41
1:A:251:PRO:HA	1:B:194:GLU:O	2.21	0.41
1:G:273:GLY:O	1:H:177:PRO:HA	2.20	0.41
2:S:13:ARG:O	2:S:79:ASP:N	2.52	0.41
2:S:148:GLN:O	2:S:211:LEU:HA	2.21	0.41
1:K:273:GLY:O	1:L:177:PRO:HA	2.19	0.41
2:Q:193:ALA:HB3	2:Q:213:ALA:O	2.21	0.41
1:A:177:PRO:HA	1:N:273:GLY:O	2.20	0.41
1:G:251:PRO:HA	1:H:194:GLU:O	2.20	0.41
2:O:178:ARG:O	2:O:183:GLY:N	2.32	0.41
2:T:193:ALA:HB3	2:T:213:ALA:O	2.21	0.41
1:B:186:THR:HA	1:B:219:VAL:O	2.21	0.41
1:L:186:THR:HA	1:L:219:VAL:O	2.21	0.41
1:M:186:THR:HA	1:M:219:VAL:O	2.21	0.41
2:P:145:GLN:HA	2:P:217:LEU:C	2.42	0.41
2:P:193:ALA:HB3	2:P:213:ALA:O	2.21	0.41
2:T:134:GLY:HA3	2:T:158:GLN:CB	2.51	0.41
2:U:134:GLY:HA3	2:U:158:GLN:CB	2.51	0.41
2:U:193:ALA:HB3	2:U:213:ALA:O	2.20	0.41
1:A:274:VAL:HA	1:B:177:PRO:HA	2.03	0.41
1:N:186:THR:HA	1:N:219:VAL:O	2.21	0.41
2:Q:148:GLN:O	2:Q:211:LEU:HA	2.21	0.41
2:R:134:GLY:HA3	2:R:158:GLN:CB	2.51	0.41
2:R:145:GLN:HA	2:R:217:LEU:C	2.42	0.41
2:S:67:ASP:O	2:S:70:THR:N	2.55	0.40
2:S:193:ALA:HB3	2:S:213:ALA:O	2.21	0.40
2:T:145:GLN:HA	2:T:217:LEU:C	2.42	0.40
2:U:145:GLN:HA	2:U:217:LEU:C	2.41	0.40
1:B:201:SER:C	1:C:202:SER:O	2.60	0.40
1:D:186:THR:HA	1:D:219:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:THR:HA	1:E:219:VAL:O	2.21	0.40
2:O:148:GLN:O	2:O:211:LEU:HA	2.21	0.40
2:U:148:GLN:O	2:U:211:LEU:HA	2.21	0.40
1:F:201:SER:CB	1:G:201:SER:O	2.69	0.40
1:H:147:ILE:HA	1:H:162:LEU:O	2.22	0.40
1:K:147:ILE:HA	1:K:162:LEU:O	2.22	0.40
2:O:134:GLY:HA3	2:O:158:GLN:CB	2.51	0.40
2:O:193:ALA:HB3	2:O:213:ALA:O	2.21	0.40
2:R:145:GLN:N	2:R:217:LEU:O	2.54	0.40
2:S:134:GLY:HA3	2:S:158:GLN:CB	2.51	0.40
1:A:186:THR:HA	1:A:219:VAL:O	2.21	0.40
1:F:186:THR:HA	1:F:219:VAL:O	2.21	0.40
1:K:186:THR:HA	1:K:219:VAL:O	2.22	0.40
2:R:67:ASP:O	2:R:70:THR:N	2.55	0.40
1:A:202:SER:HA	1:N:202:SER:N	2.37	0.40
1:F:147:ILE:HA	1:F:162:LEU:O	2.22	0.40
2:O:67:ASP:O	2:O:70:THR:N	2.55	0.40
2:Q:134:GLY:HA3	2:Q:158:GLN:CB	2.51	0.40
2:R:193:ALA:HB3	2:R:213:ALA:O	2.21	0.40
2:U:67:ASP:O	2:U:70:THR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	B	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	C	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	D	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	F	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	G	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	H	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	I	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	J	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	K	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	L	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	M	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	N	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
2	O	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	P	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	Q	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	R	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	S	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	T	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	U	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
All	All	6083/12621 (48%)	5770 (95%)	285 (5%)	28 (0%)	32	68

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	B	145	SER
1	C	145	SER
1	D	145	SER
1	E	145	SER
1	F	145	SER
1	G	145	SER
1	H	145	SER
1	I	145	SER
1	J	145	SER
1	K	145	SER
1	L	145	SER
1	M	145	SER
1	N	145	SER

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Mol	Chain	Res	Type
1	J	317	PRO
1	A	317	PRO
1	B	317	PRO
1	C	317	PRO
1	D	317	PRO
1	E	317	PRO
1	F	317	PRO
1	G	317	PRO
1	H	317	PRO
1	I	317	PRO
1	K	317	PRO
1	L	317	PRO
1	M	317	PRO
1	N	317	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

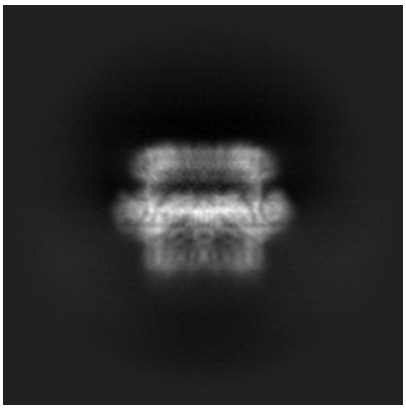
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21152. These allow visual inspection of the internal detail of the map and identification of artifacts.

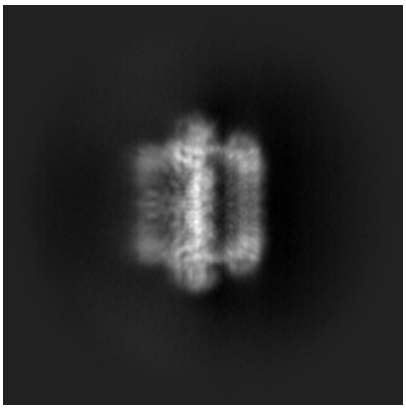
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

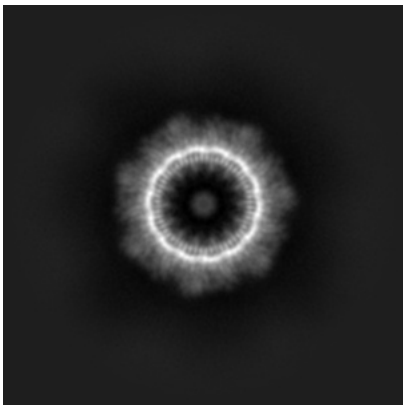
6.1.1 Primary map



X

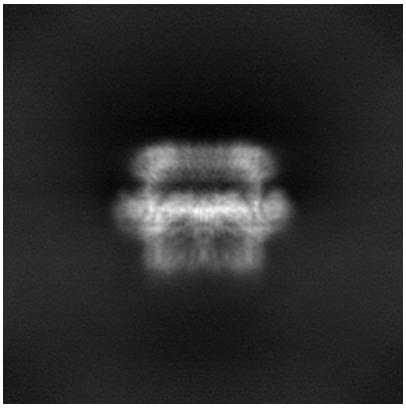


Y

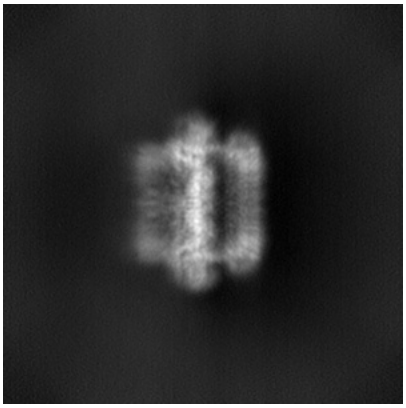


Z

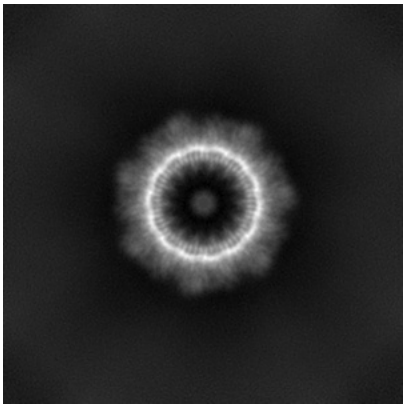
6.1.2 Raw map



X



Y

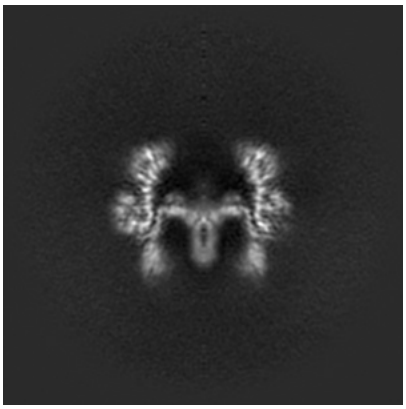


Z

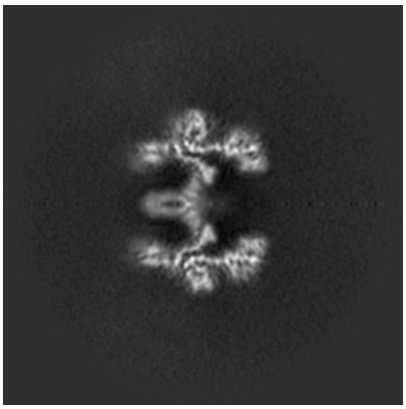
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

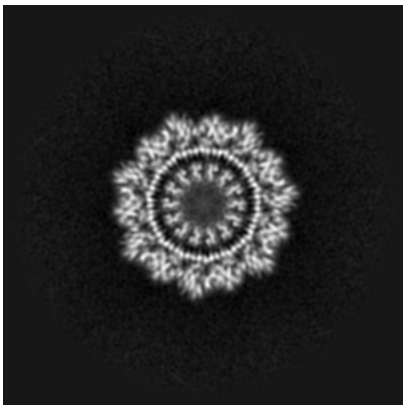
6.2.1 Primary map



X Index: 128

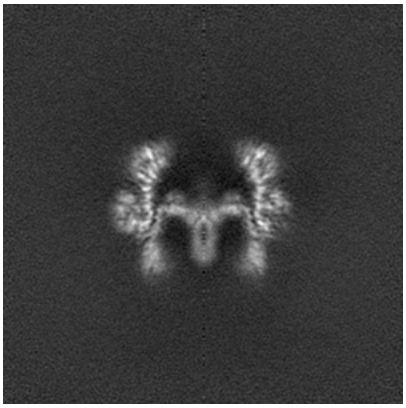


Y Index: 128

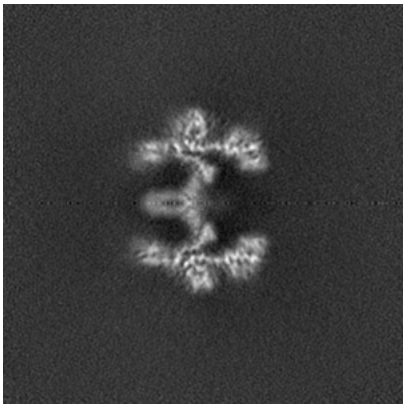


Z Index: 128

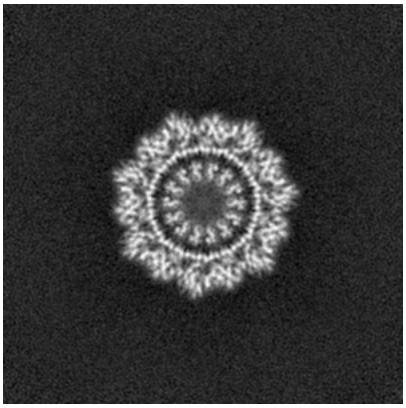
6.2.2 Raw map



X Index: 128



Y Index: 128

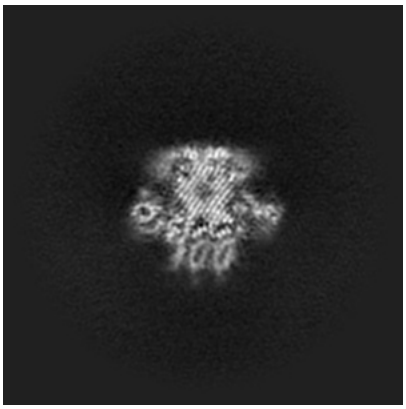


Z Index: 128

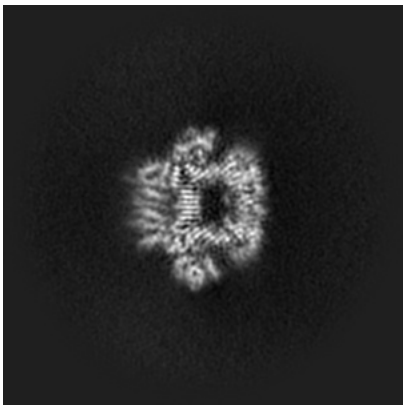
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

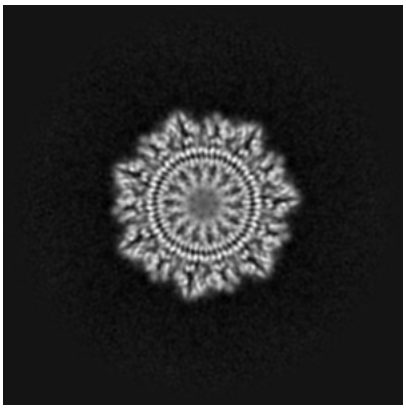
6.3.1 Primary map



X Index: 162

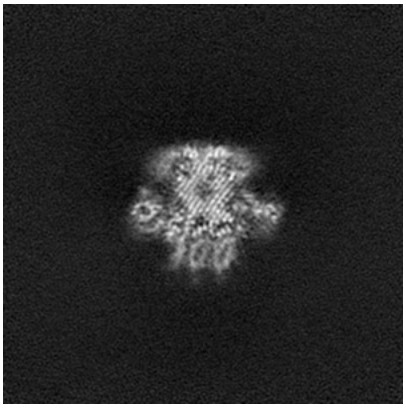


Y Index: 99

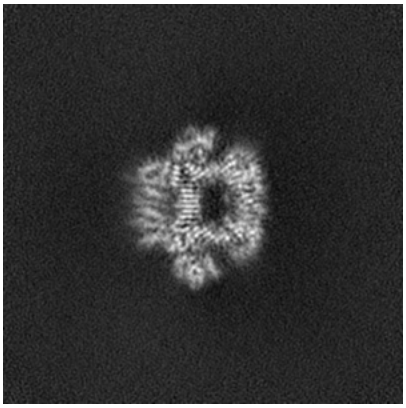


Z Index: 124

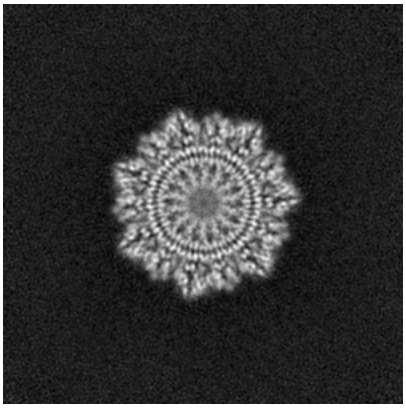
6.3.2 Raw map



X Index: 162



Y Index: 99

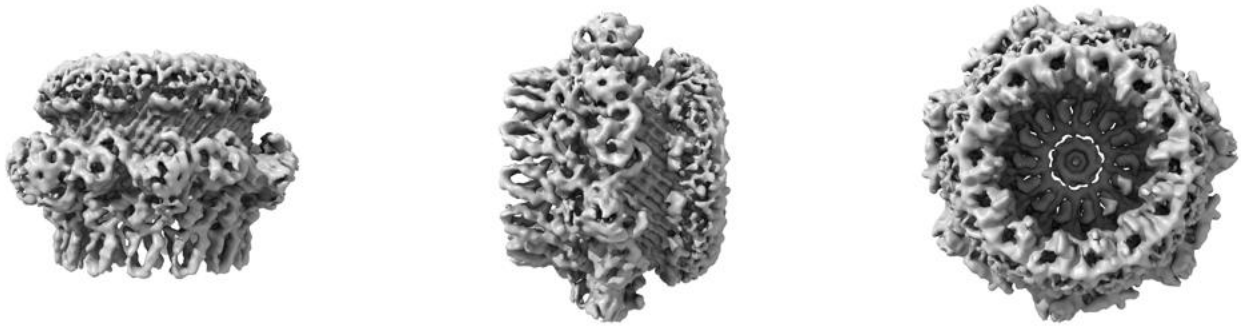


Z Index: 124

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

6.4 Orthogonal surface views (i)

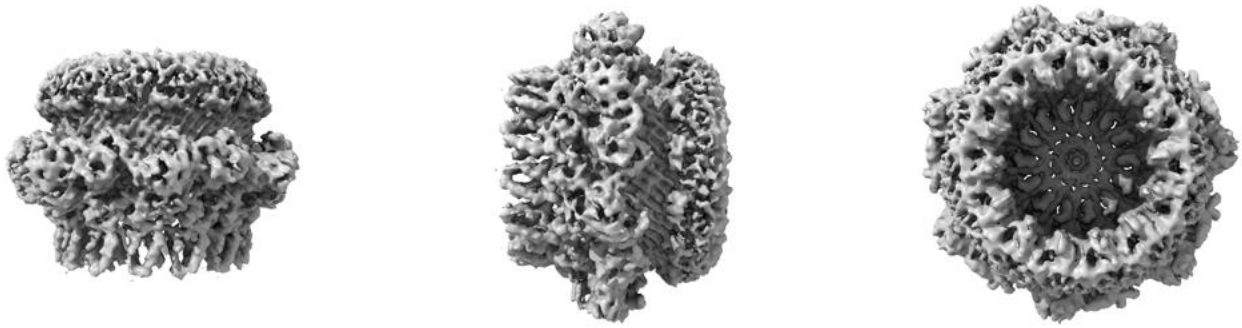
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

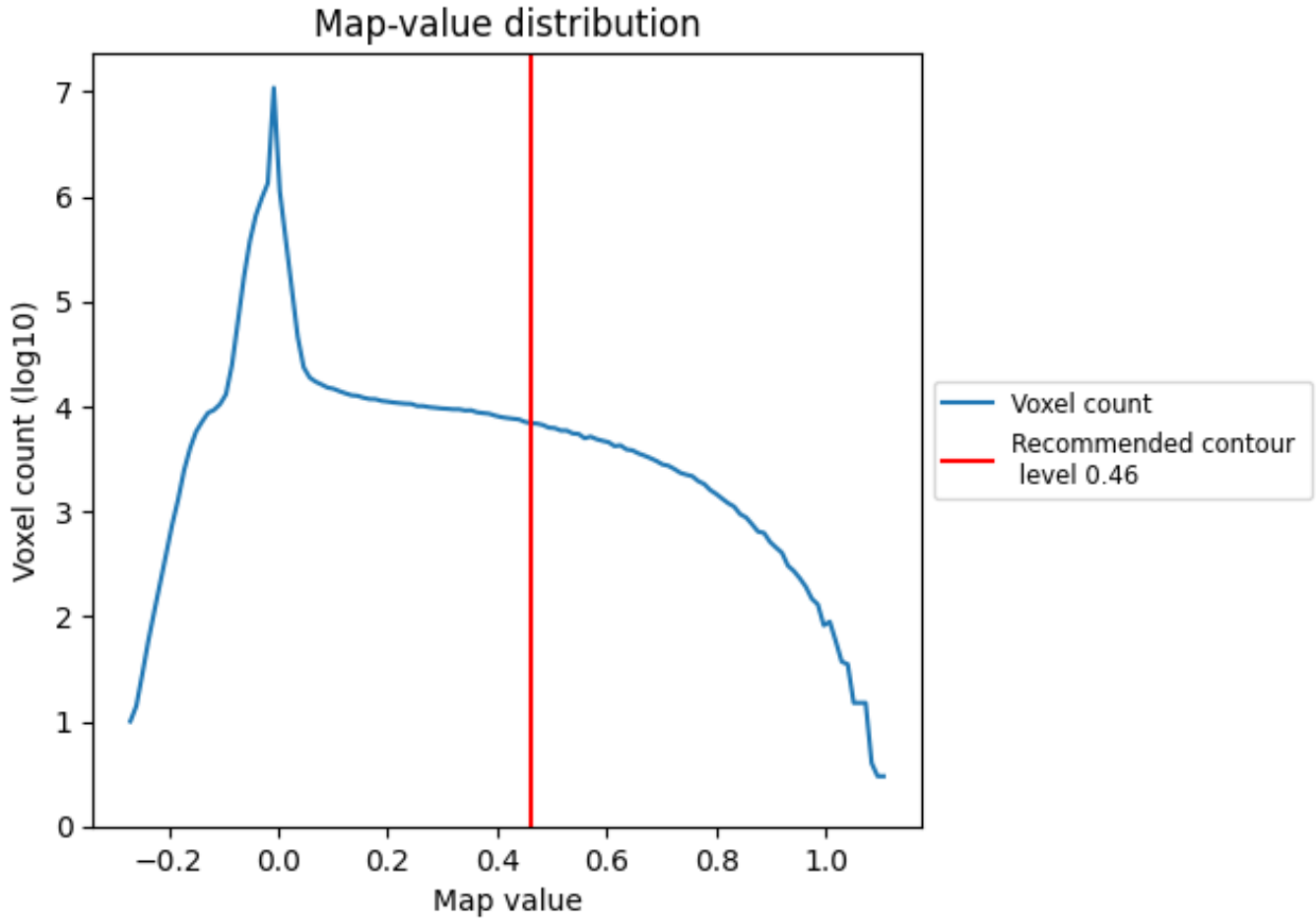
6.5 Mask visualisation (i)

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

7 Map analysis

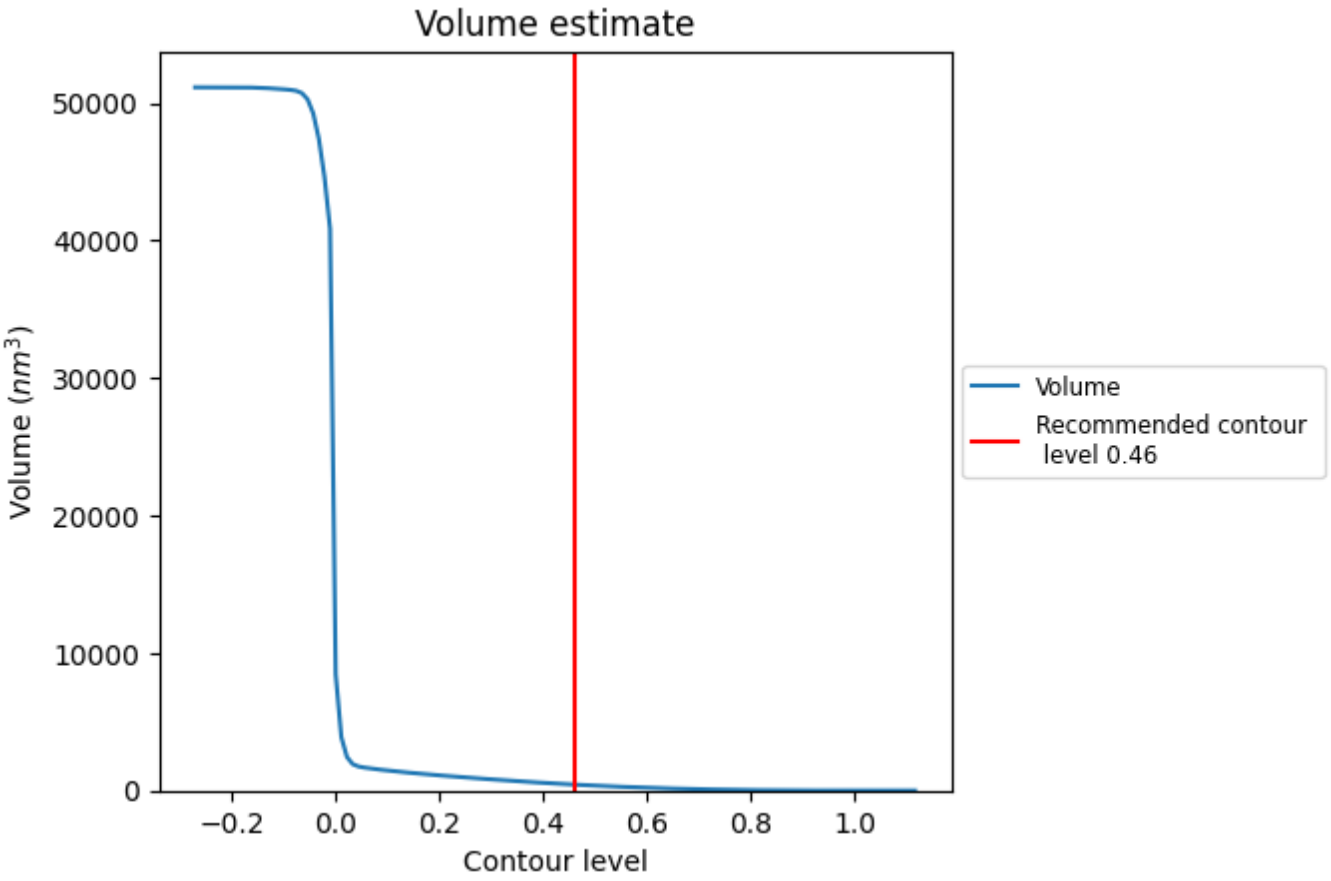
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

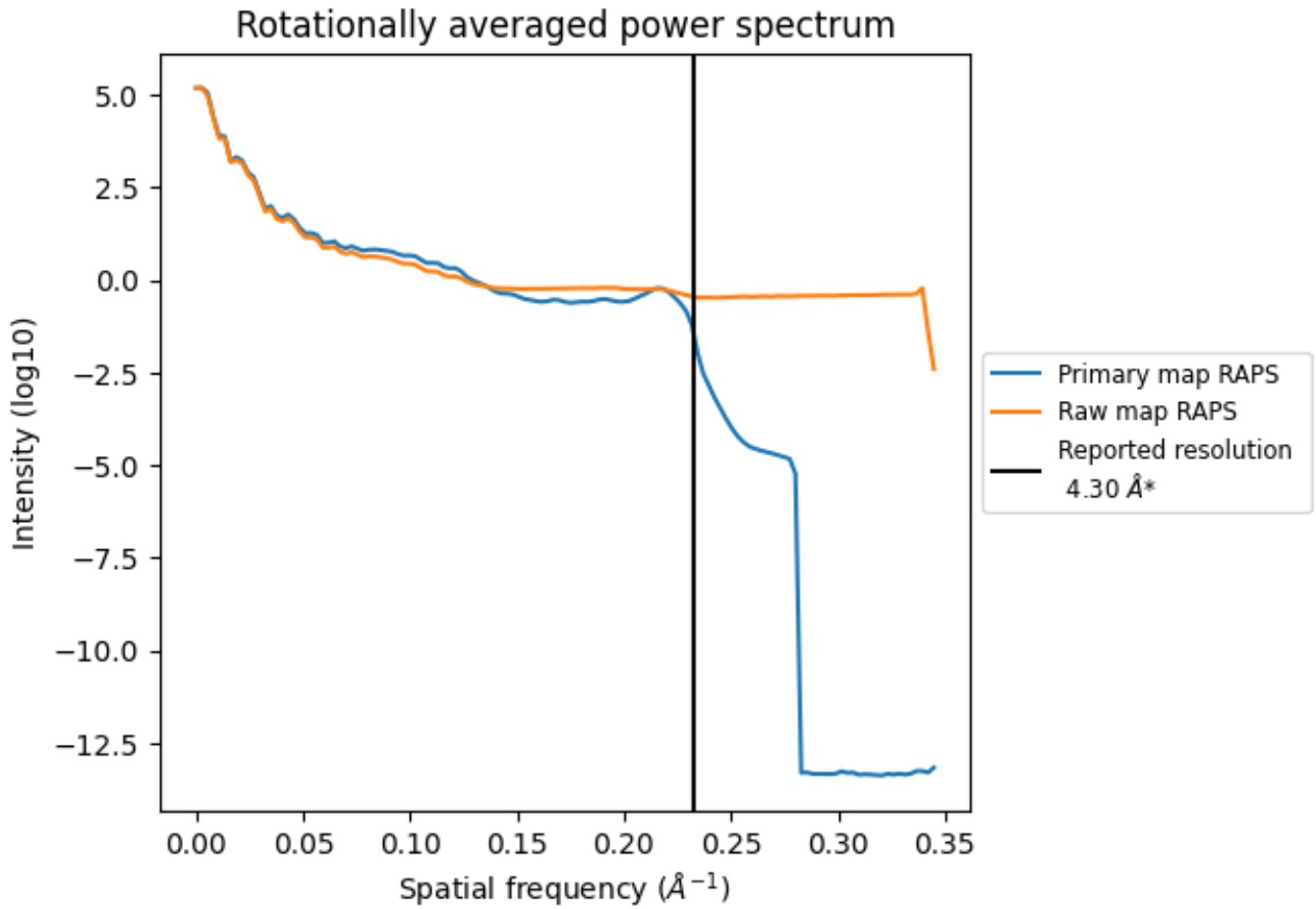
7.2 Volume estimate



The volume at the recommended contour level is 434 nm^3; this corresponds to an approximate mass of 392 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)

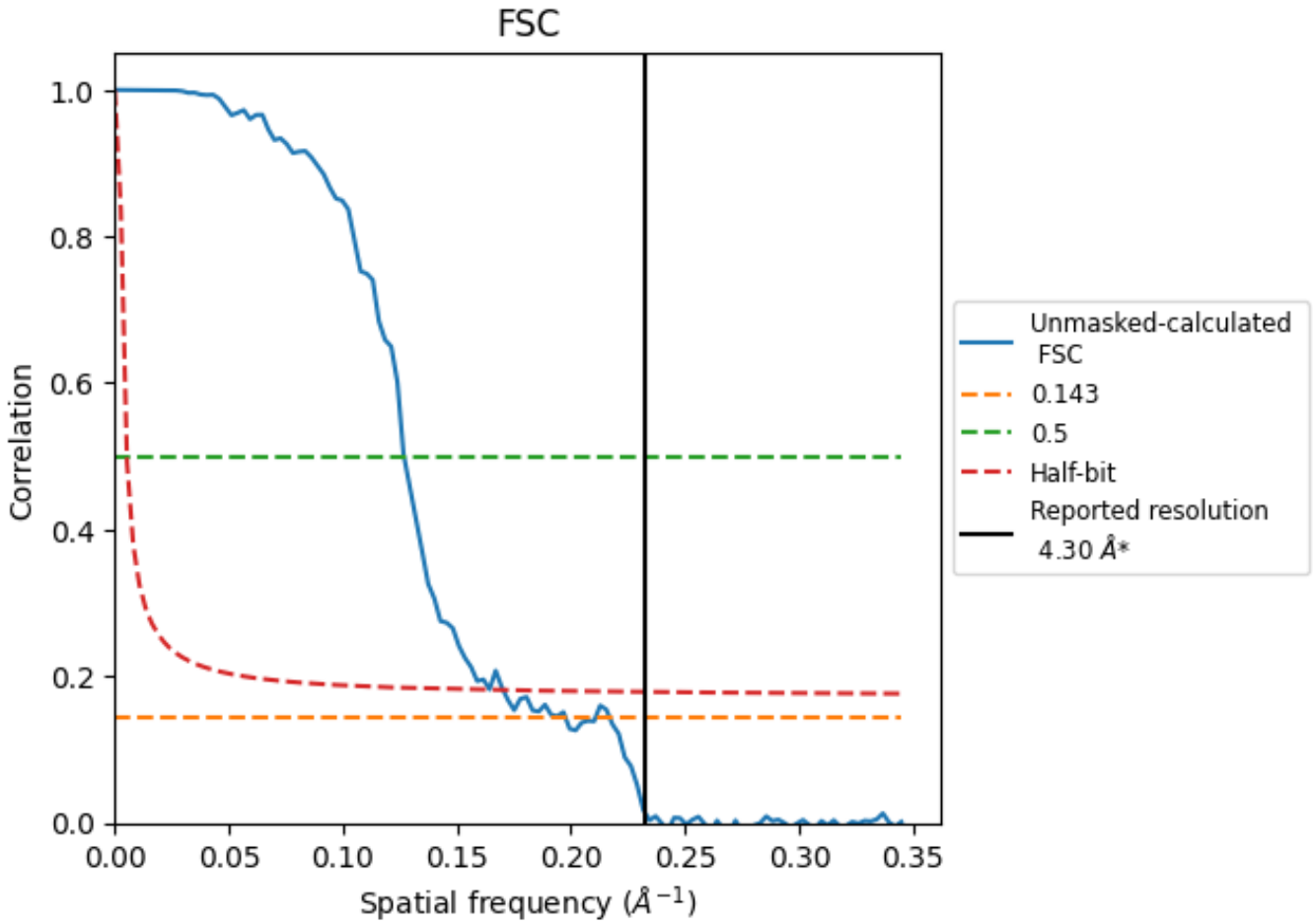


*Reported resolution corresponds to spatial frequency of 0.233 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

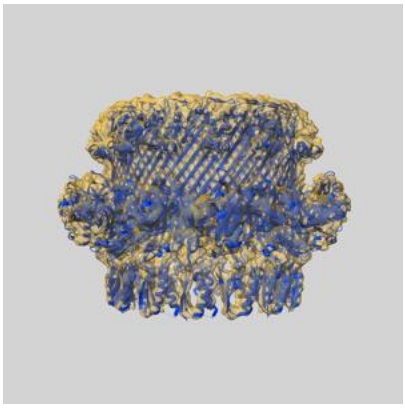
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.06	7.89	5.87

*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 5.06 differs from the reported value 4.3 by more than 10 %

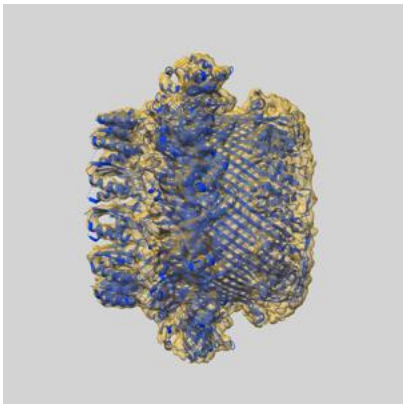
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21152 and PDB model 6VE2. Per-residue inclusion information can be found in section 3 on page 12.

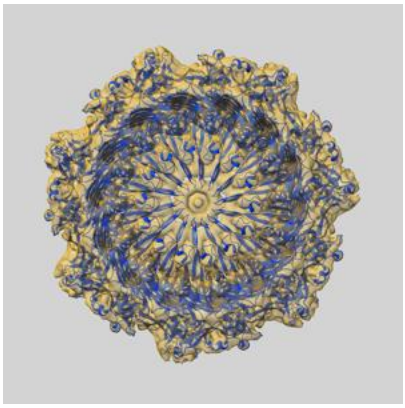
9.1 Map-model overlay



X



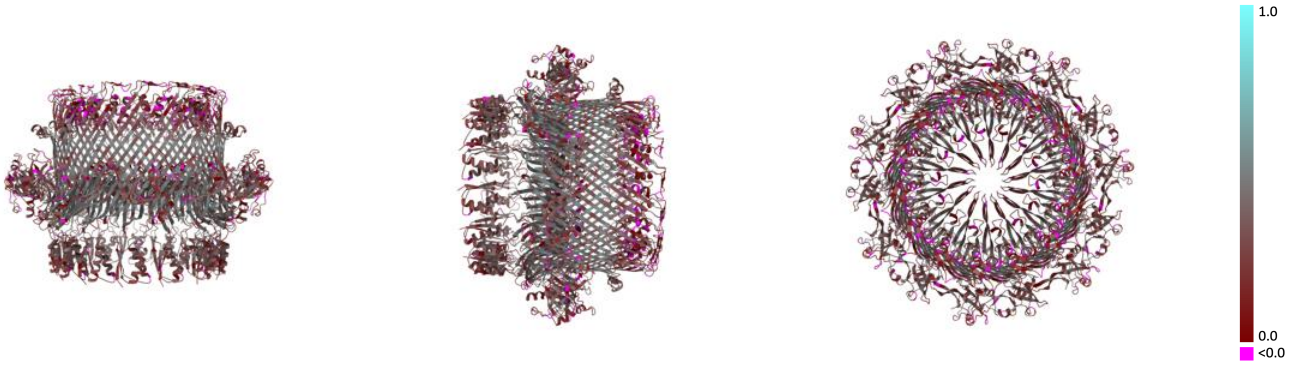
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.46 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.

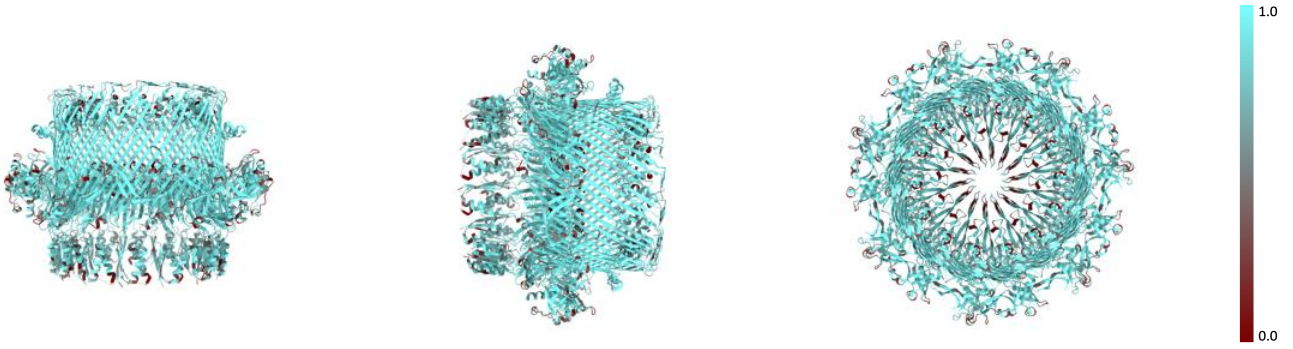
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

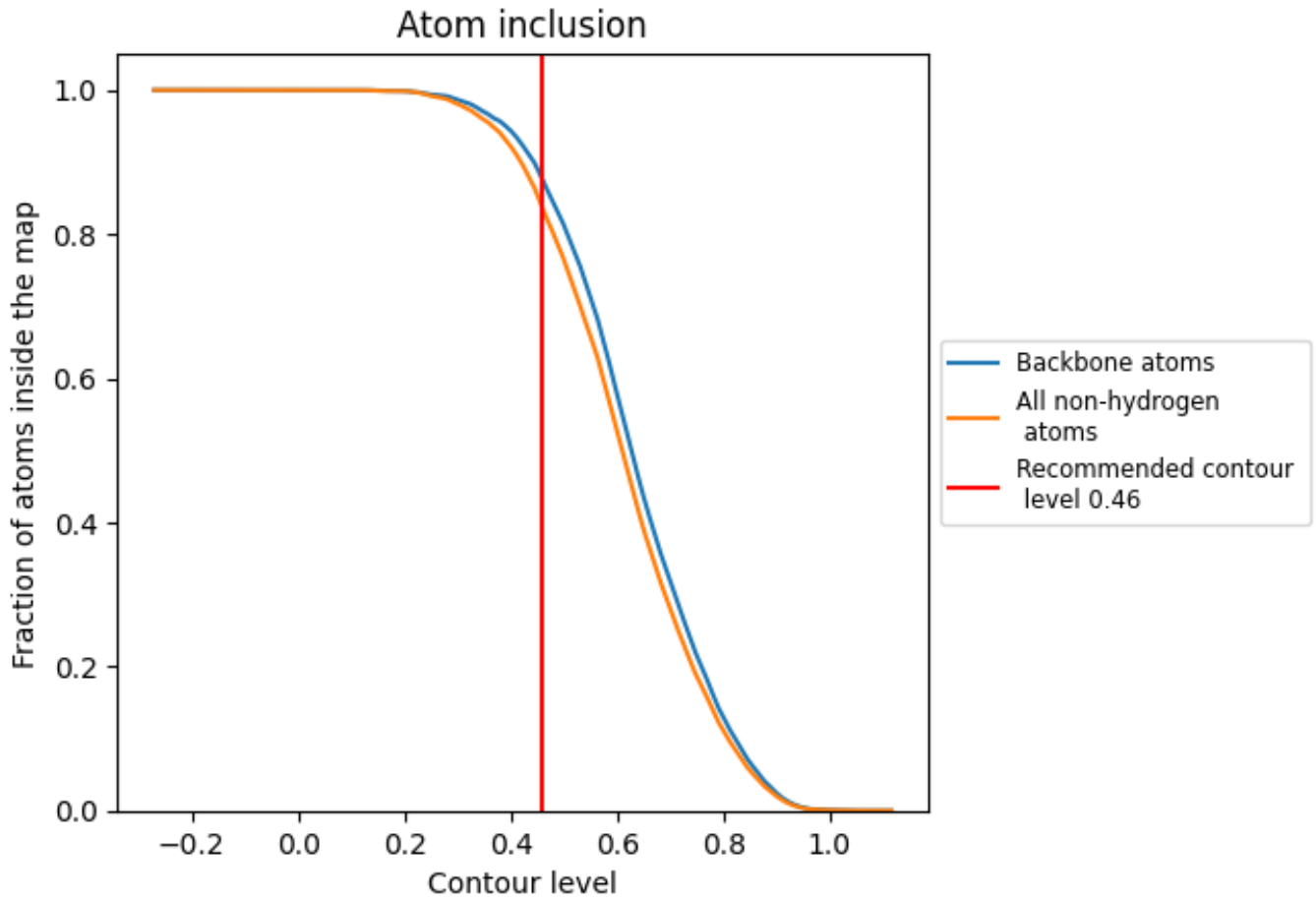
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.46).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8356	0.3020
A	0.8487	0.3140
B	0.8524	0.3160
C	0.8481	0.3160
D	0.8531	0.3160
E	0.8493	0.3140
F	0.8518	0.3150
G	0.8493	0.3180
H	0.8499	0.3170
I	0.8481	0.3180
J	0.8531	0.3190
K	0.8481	0.3150
L	0.8531	0.3160
M	0.8499	0.3140
N	0.8537	0.3170
O	0.7931	0.2630
P	0.7886	0.2620
Q	0.7913	0.2630
R	0.7958	0.2640
S	0.7904	0.2620
T	0.7940	0.2620
U	0.7904	0.2600