



Full wwPDB EM Validation Report ⓘ

Jun 11, 2026 – 05:51 pm BST

PDB ID : 9SJB / pdb_00009sjb
EMDB ID : EMD-54942
Title : Solution structure of Clostridioides difficile CspB oligomer determined by Cryo-EM
Authors : Alcorlo, M.; Lazaro, M.; Valle, M.; Hermoso, J.
Deposited on : 2025-08-31
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

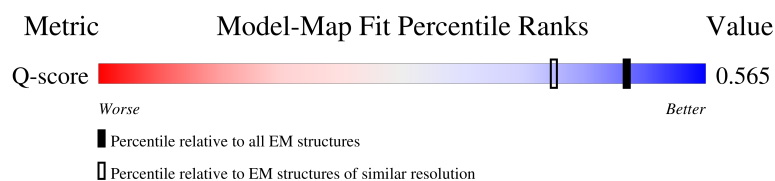
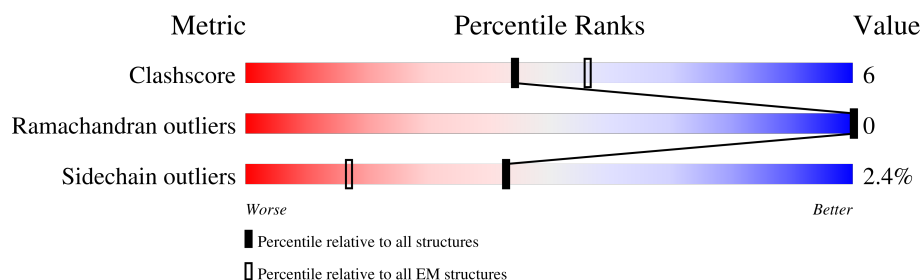
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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	10570 (2.25 - 3.25)

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	68	<div> <div>21%</div> <div>72%</div> <div>16%</div> <div>10%</div> </div>
1	AA	68	<div> <div>56%</div> <div>65%</div> <div>24%</div> <div>10%</div> </div>
1	B	68	<div> <div>22%</div> <div>72%</div> <div>16%</div> <div>10%</div> </div>
1	BB	68	<div> <div>56%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	68	
1	EE	68	
1	F	68	
1	FF	68	
1	I	68	
1	J	68	
1	LL	68	
1	M	68	
1	P	68	
1	Q	68	
1	T	68	
1	V	68	
1	Y	68	
1	Z	68	
2	C	492	
2	CC	492	
2	D	492	
2	G	492	
2	GG	492	
2	H	492	
2	K	492	
2	L	492	
2	N	492	
2	O	492	
2	R	492	

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Mol	Chain	Length	Quality of chain
2	S	492	<div><div>43%</div><div>79%</div><div>16%</div><div></div></div>
2	W	492	<div><div>21%</div><div>83%</div><div>13%</div><div></div></div>
2	X	492	<div><div>36%</div><div>78%</div><div>17%</div><div></div></div>
2	YY	492	<div><div>59%</div><div>79%</div><div>16%</div><div></div></div>
2	ZZ	492	<div><div>29%</div><div>81%</div><div>14%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 67110 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 Subtilisin-like serine germination related protease.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	61	Total	C	N	O	0	0
			496	321	72	103		
1	B	61	Total	C	N	O	0	0
			496	321	72	103		
1	E	61	Total	C	N	O	0	0
			496	321	72	103		
1	F	61	Total	C	N	O	0	0
			496	321	72	103		
1	I	61	Total	C	N	O	0	0
			496	321	72	103		
1	J	61	Total	C	N	O	0	0
			496	321	72	103		
1	LL	61	Total	C	N	O	0	0
			496	321	72	103		
1	M	61	Total	C	N	O	0	0
			496	321	72	103		
1	P	61	Total	C	N	O	0	0
			496	321	72	103		
1	Q	61	Total	C	N	O	0	0
			496	321	72	103		
1	T	61	Total	C	N	O	0	0
			496	321	72	103		
1	V	61	Total	C	N	O	0	0
			496	321	72	103		
1	Y	61	Total	C	N	O	0	0
			496	321	72	103		
1	Z	61	Total	C	N	O	0	0
			496	321	72	103		
1	AA	61	Total	C	N	O	0	0
			496	321	72	103		
1	BB	61	Total	C	N	O	0	0
			496	321	72	103		
1	EE	59	Total	C	N	O	0	0
			480	312	69	99		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	FF	61	Total 496	C 321	N 72	O 103	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CYS	-	expression tag	UNP A0AB74Q767
A	67	SER	-	expression tag	UNP A0AB74Q767
A	68	PRO	-	expression tag	UNP A0AB74Q767
B	66	CYS	-	expression tag	UNP A0AB74Q767
B	67	SER	-	expression tag	UNP A0AB74Q767
B	68	PRO	-	expression tag	UNP A0AB74Q767
E	66	CYS	-	expression tag	UNP A0AB74Q767
E	67	SER	-	expression tag	UNP A0AB74Q767
E	68	PRO	-	expression tag	UNP A0AB74Q767
F	66	CYS	-	expression tag	UNP A0AB74Q767
F	67	SER	-	expression tag	UNP A0AB74Q767
F	68	PRO	-	expression tag	UNP A0AB74Q767
I	66	CYS	-	expression tag	UNP A0AB74Q767
I	67	SER	-	expression tag	UNP A0AB74Q767
I	68	PRO	-	expression tag	UNP A0AB74Q767
J	66	CYS	-	expression tag	UNP A0AB74Q767
J	67	SER	-	expression tag	UNP A0AB74Q767
J	68	PRO	-	expression tag	UNP A0AB74Q767
LL	66	CYS	-	expression tag	UNP A0AB74Q767
LL	67	SER	-	expression tag	UNP A0AB74Q767
LL	68	PRO	-	expression tag	UNP A0AB74Q767
M	66	CYS	-	expression tag	UNP A0AB74Q767
M	67	SER	-	expression tag	UNP A0AB74Q767
M	68	PRO	-	expression tag	UNP A0AB74Q767
P	66	CYS	-	expression tag	UNP A0AB74Q767
P	67	SER	-	expression tag	UNP A0AB74Q767
P	68	PRO	-	expression tag	UNP A0AB74Q767
Q	66	CYS	-	expression tag	UNP A0AB74Q767
Q	67	SER	-	expression tag	UNP A0AB74Q767
Q	68	PRO	-	expression tag	UNP A0AB74Q767
T	66	CYS	-	expression tag	UNP A0AB74Q767
T	67	SER	-	expression tag	UNP A0AB74Q767
T	68	PRO	-	expression tag	UNP A0AB74Q767
V	66	CYS	-	expression tag	UNP A0AB74Q767
V	67	SER	-	expression tag	UNP A0AB74Q767
V	68	PRO	-	expression tag	UNP A0AB74Q767

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	66	CYS	-	expression tag	UNP A0AB74Q767
Y	67	SER	-	expression tag	UNP A0AB74Q767
Y	68	PRO	-	expression tag	UNP A0AB74Q767
Z	66	CYS	-	expression tag	UNP A0AB74Q767
Z	67	SER	-	expression tag	UNP A0AB74Q767
Z	68	PRO	-	expression tag	UNP A0AB74Q767
AA	66	CYS	-	expression tag	UNP A0AB74Q767
AA	67	SER	-	expression tag	UNP A0AB74Q767
AA	68	PRO	-	expression tag	UNP A0AB74Q767
BB	66	CYS	-	expression tag	UNP A0AB74Q767
BB	67	SER	-	expression tag	UNP A0AB74Q767
BB	68	PRO	-	expression tag	UNP A0AB74Q767
EE	66	CYS	-	expression tag	UNP A0AB74Q767
EE	67	SER	-	expression tag	UNP A0AB74Q767
EE	68	PRO	-	expression tag	UNP A0AB74Q767
FF	66	CYS	-	expression tag	UNP A0AB74Q767
FF	67	SER	-	expression tag	UNP A0AB74Q767
FF	68	PRO	-	expression tag	UNP A0AB74Q767

- Molecule 2 is a protein called Subtilisin-like serine germination related protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	D	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		
2	G	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	H	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		
2	K	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	L	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		
2	N	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	O	469	Total	C	N	O	S	0	0
			3631	2293	621	708	9		
2	R	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	S	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	X	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		
2	YY	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	ZZ	470	Total	C	N	O	S	0	0
			3639	2297	622	711	9		
2	CC	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		
2	GG	470	Total	C	N	O	S	0	0
			3637	2297	622	709	9		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	65	MET	-	initiating methionine	UNP A0AB74Q767
C	549	LEU	-	expression tag	UNP A0AB74Q767
C	550	GLU	-	expression tag	UNP A0AB74Q767
C	551	HIS	-	expression tag	UNP A0AB74Q767
C	552	HIS	-	expression tag	UNP A0AB74Q767
C	553	HIS	-	expression tag	UNP A0AB74Q767
C	554	HIS	-	expression tag	UNP A0AB74Q767
C	555	HIS	-	expression tag	UNP A0AB74Q767
C	556	HIS	-	expression tag	UNP A0AB74Q767
D	65	MET	-	initiating methionine	UNP A0AB74Q767
D	549	LEU	-	expression tag	UNP A0AB74Q767
D	550	GLU	-	expression tag	UNP A0AB74Q767
D	551	HIS	-	expression tag	UNP A0AB74Q767
D	552	HIS	-	expression tag	UNP A0AB74Q767
D	553	HIS	-	expression tag	UNP A0AB74Q767
D	554	HIS	-	expression tag	UNP A0AB74Q767
D	555	HIS	-	expression tag	UNP A0AB74Q767
D	556	HIS	-	expression tag	UNP A0AB74Q767
G	65	MET	-	initiating methionine	UNP A0AB74Q767
G	549	LEU	-	expression tag	UNP A0AB74Q767
G	550	GLU	-	expression tag	UNP A0AB74Q767
G	551	HIS	-	expression tag	UNP A0AB74Q767
G	552	HIS	-	expression tag	UNP A0AB74Q767
G	553	HIS	-	expression tag	UNP A0AB74Q767
G	554	HIS	-	expression tag	UNP A0AB74Q767
G	555	HIS	-	expression tag	UNP A0AB74Q767
G	556	HIS	-	expression tag	UNP A0AB74Q767

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Chain	Residue	Modelled	Actual	Comment	Reference
H	65	MET	-	initiating methionine	UNP A0AB74Q767
H	549	LEU	-	expression tag	UNP A0AB74Q767
H	550	GLU	-	expression tag	UNP A0AB74Q767
H	551	HIS	-	expression tag	UNP A0AB74Q767
H	552	HIS	-	expression tag	UNP A0AB74Q767
H	553	HIS	-	expression tag	UNP A0AB74Q767
H	554	HIS	-	expression tag	UNP A0AB74Q767
H	555	HIS	-	expression tag	UNP A0AB74Q767
H	556	HIS	-	expression tag	UNP A0AB74Q767
K	65	MET	-	initiating methionine	UNP A0AB74Q767
K	549	LEU	-	expression tag	UNP A0AB74Q767
K	550	GLU	-	expression tag	UNP A0AB74Q767
K	551	HIS	-	expression tag	UNP A0AB74Q767
K	552	HIS	-	expression tag	UNP A0AB74Q767
K	553	HIS	-	expression tag	UNP A0AB74Q767
K	554	HIS	-	expression tag	UNP A0AB74Q767
K	555	HIS	-	expression tag	UNP A0AB74Q767
K	556	HIS	-	expression tag	UNP A0AB74Q767
L	65	MET	-	initiating methionine	UNP A0AB74Q767
L	549	LEU	-	expression tag	UNP A0AB74Q767
L	550	GLU	-	expression tag	UNP A0AB74Q767
L	551	HIS	-	expression tag	UNP A0AB74Q767
L	552	HIS	-	expression tag	UNP A0AB74Q767
L	553	HIS	-	expression tag	UNP A0AB74Q767
L	554	HIS	-	expression tag	UNP A0AB74Q767
L	555	HIS	-	expression tag	UNP A0AB74Q767
L	556	HIS	-	expression tag	UNP A0AB74Q767
N	65	MET	-	initiating methionine	UNP A0AB74Q767
N	549	LEU	-	expression tag	UNP A0AB74Q767
N	550	GLU	-	expression tag	UNP A0AB74Q767
N	551	HIS	-	expression tag	UNP A0AB74Q767
N	552	HIS	-	expression tag	UNP A0AB74Q767
N	553	HIS	-	expression tag	UNP A0AB74Q767
N	554	HIS	-	expression tag	UNP A0AB74Q767
N	555	HIS	-	expression tag	UNP A0AB74Q767
N	556	HIS	-	expression tag	UNP A0AB74Q767
O	65	MET	-	initiating methionine	UNP A0AB74Q767
O	549	LEU	-	expression tag	UNP A0AB74Q767
O	550	GLU	-	expression tag	UNP A0AB74Q767
O	551	HIS	-	expression tag	UNP A0AB74Q767
O	552	HIS	-	expression tag	UNP A0AB74Q767
O	553	HIS	-	expression tag	UNP A0AB74Q767

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Chain	Residue	Modelled	Actual	Comment	Reference
O	554	HIS	-	expression tag	UNP A0AB74Q767
O	555	HIS	-	expression tag	UNP A0AB74Q767
O	556	HIS	-	expression tag	UNP A0AB74Q767
R	65	MET	-	initiating methionine	UNP A0AB74Q767
R	549	LEU	-	expression tag	UNP A0AB74Q767
R	550	GLU	-	expression tag	UNP A0AB74Q767
R	551	HIS	-	expression tag	UNP A0AB74Q767
R	552	HIS	-	expression tag	UNP A0AB74Q767
R	553	HIS	-	expression tag	UNP A0AB74Q767
R	554	HIS	-	expression tag	UNP A0AB74Q767
R	555	HIS	-	expression tag	UNP A0AB74Q767
R	556	HIS	-	expression tag	UNP A0AB74Q767
S	65	MET	-	initiating methionine	UNP A0AB74Q767
S	549	LEU	-	expression tag	UNP A0AB74Q767
S	550	GLU	-	expression tag	UNP A0AB74Q767
S	551	HIS	-	expression tag	UNP A0AB74Q767
S	552	HIS	-	expression tag	UNP A0AB74Q767
S	553	HIS	-	expression tag	UNP A0AB74Q767
S	554	HIS	-	expression tag	UNP A0AB74Q767
S	555	HIS	-	expression tag	UNP A0AB74Q767
S	556	HIS	-	expression tag	UNP A0AB74Q767
W	65	MET	-	initiating methionine	UNP A0AB74Q767
W	549	LEU	-	expression tag	UNP A0AB74Q767
W	550	GLU	-	expression tag	UNP A0AB74Q767
W	551	HIS	-	expression tag	UNP A0AB74Q767
W	552	HIS	-	expression tag	UNP A0AB74Q767
W	553	HIS	-	expression tag	UNP A0AB74Q767
W	554	HIS	-	expression tag	UNP A0AB74Q767
W	555	HIS	-	expression tag	UNP A0AB74Q767
W	556	HIS	-	expression tag	UNP A0AB74Q767
X	65	MET	-	initiating methionine	UNP A0AB74Q767
X	549	LEU	-	expression tag	UNP A0AB74Q767
X	550	GLU	-	expression tag	UNP A0AB74Q767
X	551	HIS	-	expression tag	UNP A0AB74Q767
X	552	HIS	-	expression tag	UNP A0AB74Q767
X	553	HIS	-	expression tag	UNP A0AB74Q767
X	554	HIS	-	expression tag	UNP A0AB74Q767
X	555	HIS	-	expression tag	UNP A0AB74Q767
X	556	HIS	-	expression tag	UNP A0AB74Q767
YY	65	MET	-	initiating methionine	UNP A0AB74Q767
YY	549	LEU	-	expression tag	UNP A0AB74Q767
YY	550	GLU	-	expression tag	UNP A0AB74Q767

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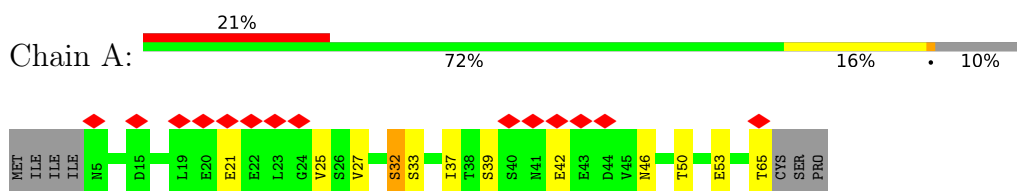
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Chain	Residue	Modelled	Actual	Comment	Reference
YY	551	HIS	-	expression tag	UNP A0AB74Q767
YY	552	HIS	-	expression tag	UNP A0AB74Q767
YY	553	HIS	-	expression tag	UNP A0AB74Q767
YY	554	HIS	-	expression tag	UNP A0AB74Q767
YY	555	HIS	-	expression tag	UNP A0AB74Q767
YY	556	HIS	-	expression tag	UNP A0AB74Q767
ZZ	65	MET	-	initiating methionine	UNP A0AB74Q767
ZZ	549	LEU	-	expression tag	UNP A0AB74Q767
ZZ	550	GLU	-	expression tag	UNP A0AB74Q767
ZZ	551	HIS	-	expression tag	UNP A0AB74Q767
ZZ	552	HIS	-	expression tag	UNP A0AB74Q767
ZZ	553	HIS	-	expression tag	UNP A0AB74Q767
ZZ	554	HIS	-	expression tag	UNP A0AB74Q767
ZZ	555	HIS	-	expression tag	UNP A0AB74Q767
ZZ	556	HIS	-	expression tag	UNP A0AB74Q767
CC	65	MET	-	initiating methionine	UNP A0AB74Q767
CC	549	LEU	-	expression tag	UNP A0AB74Q767
CC	550	GLU	-	expression tag	UNP A0AB74Q767
CC	551	HIS	-	expression tag	UNP A0AB74Q767
CC	552	HIS	-	expression tag	UNP A0AB74Q767
CC	553	HIS	-	expression tag	UNP A0AB74Q767
CC	554	HIS	-	expression tag	UNP A0AB74Q767
CC	555	HIS	-	expression tag	UNP A0AB74Q767
CC	556	HIS	-	expression tag	UNP A0AB74Q767
GG	65	MET	-	initiating methionine	UNP A0AB74Q767
GG	549	LEU	-	expression tag	UNP A0AB74Q767
GG	550	GLU	-	expression tag	UNP A0AB74Q767
GG	551	HIS	-	expression tag	UNP A0AB74Q767
GG	552	HIS	-	expression tag	UNP A0AB74Q767
GG	553	HIS	-	expression tag	UNP A0AB74Q767
GG	554	HIS	-	expression tag	UNP A0AB74Q767
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GG	556	HIS	-	expression tag	UNP A0AB74Q767

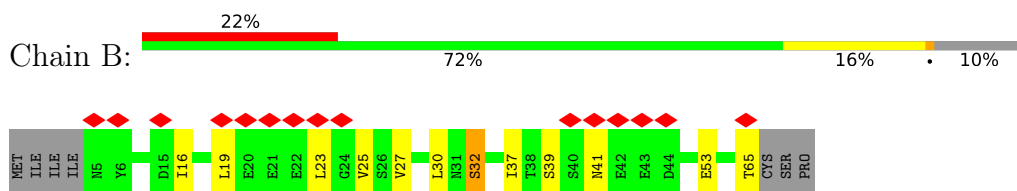
3 Residue-property plots [i](#)

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.

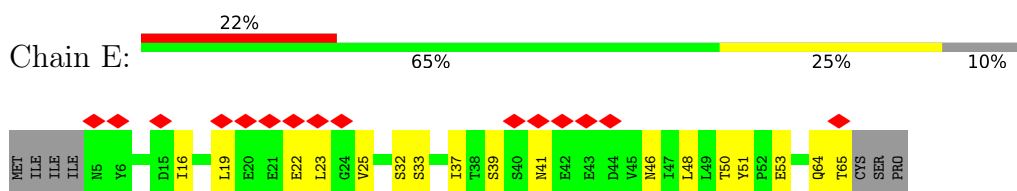
- Molecule 1: Subtilisin-like serine germination related protease



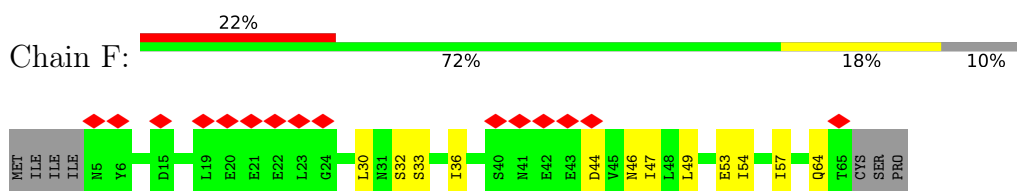
- Molecule 1: Subtilisin-like serine germination related protease



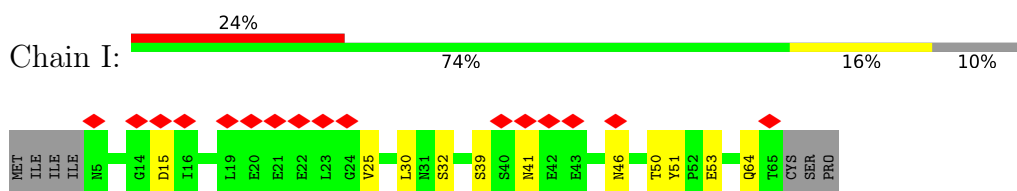
- Molecule 1: Subtilisin-like serine germination related protease



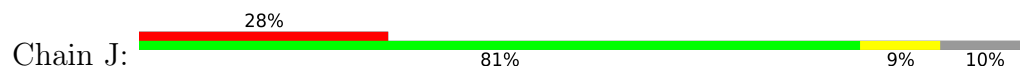
- Molecule 1: Subtilisin-like serine germination related protease



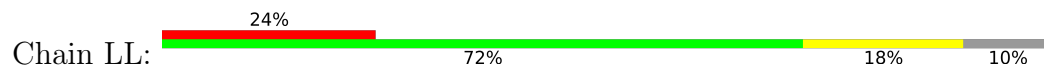
- Molecule 1: Subtilisin-like serine germination related protease



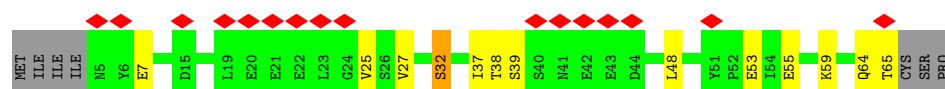
- Molecule 1: Subtilisin-like serine germination related protease



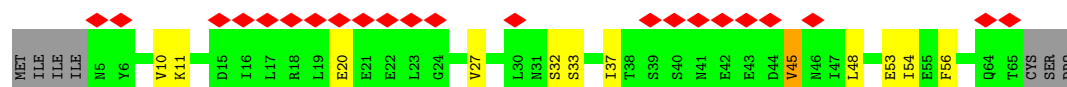
- Molecule 1: Subtilisin-like serine germination related protease



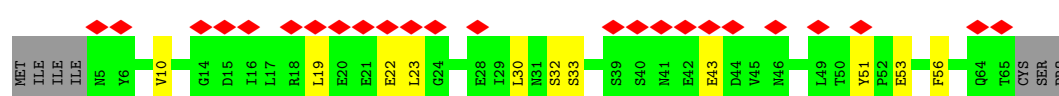
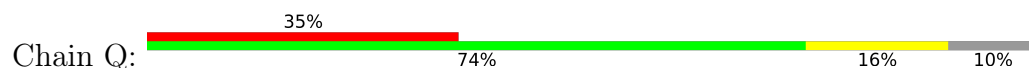
- Molecule 1: Subtilisin-like serine germination related protease



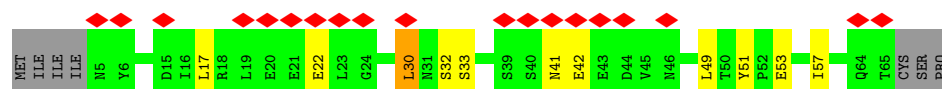
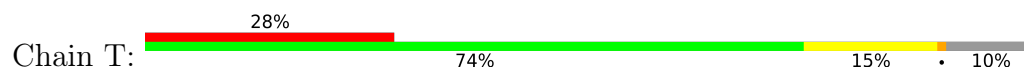
- Molecule 1: Subtilisin-like serine germination related protease



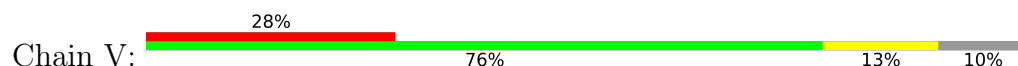
- Molecule 1: Subtilisin-like serine germination related protease



- Molecule 1: Subtilisin-like serine germination related protease

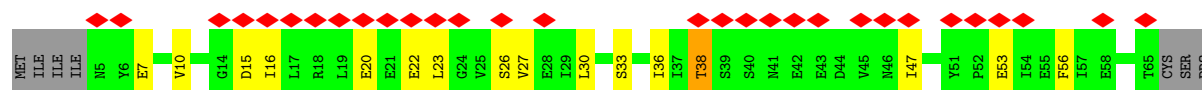
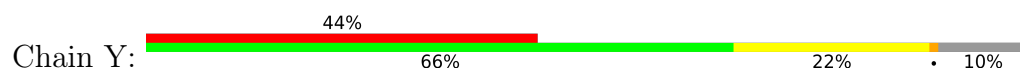


- Molecule 1: Subtilisin-like serine germination related protease

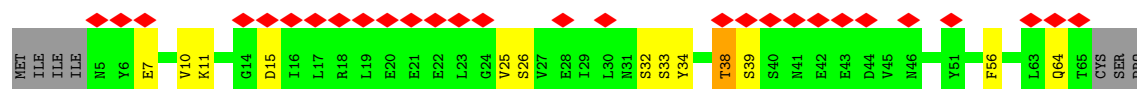




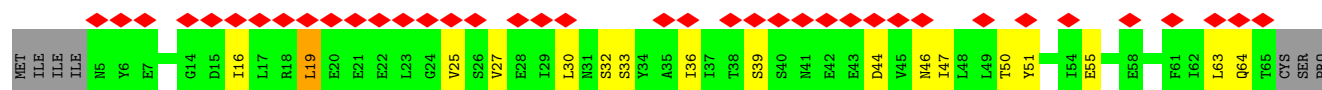
- Molecule 1: Subtilisin-like serine germination related protease



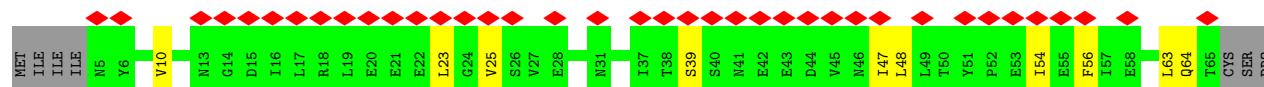
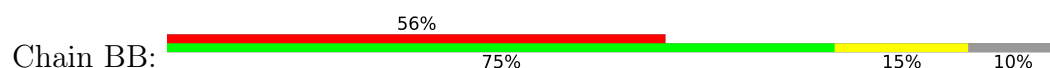
- Molecule 1: Subtilisin-like serine germination related protease



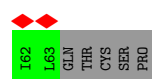
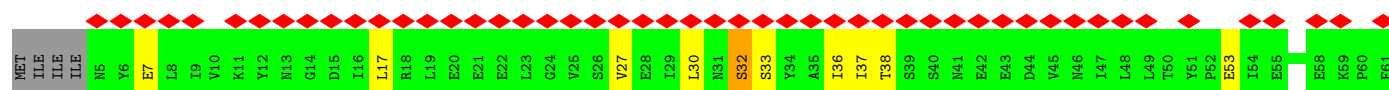
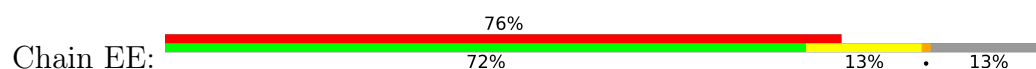
- Molecule 1: Subtilisin-like serine germination related protease



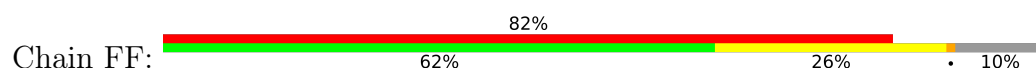
- Molecule 1: Subtilisin-like serine germination related protease



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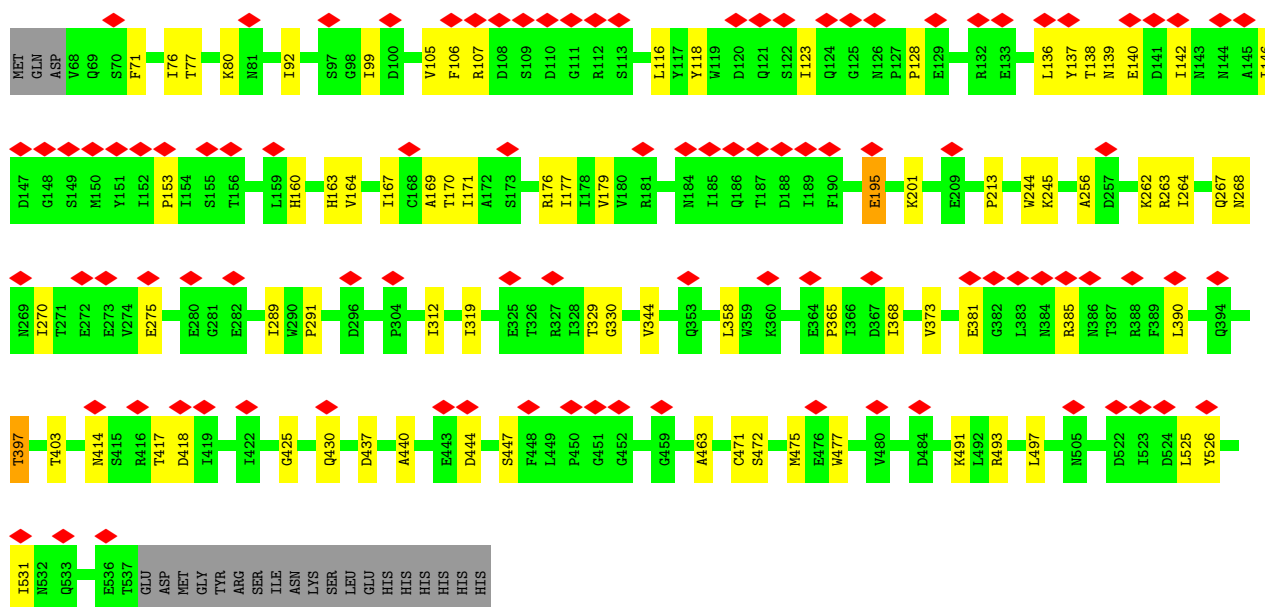
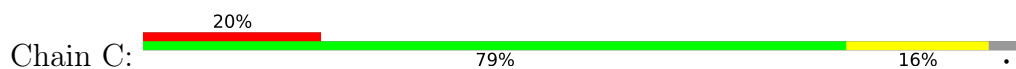


- Molecule 1: Subtilisin-like serine germination related protease

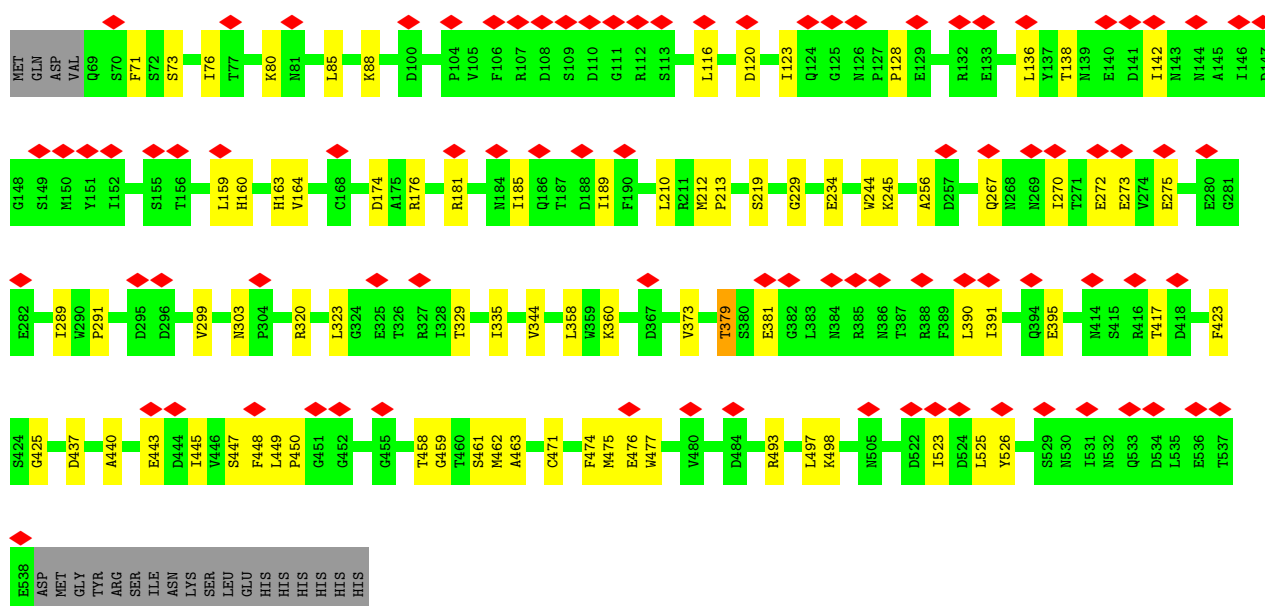
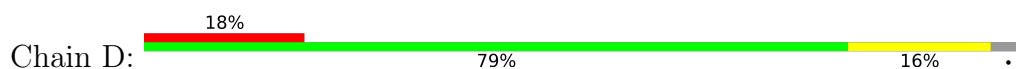




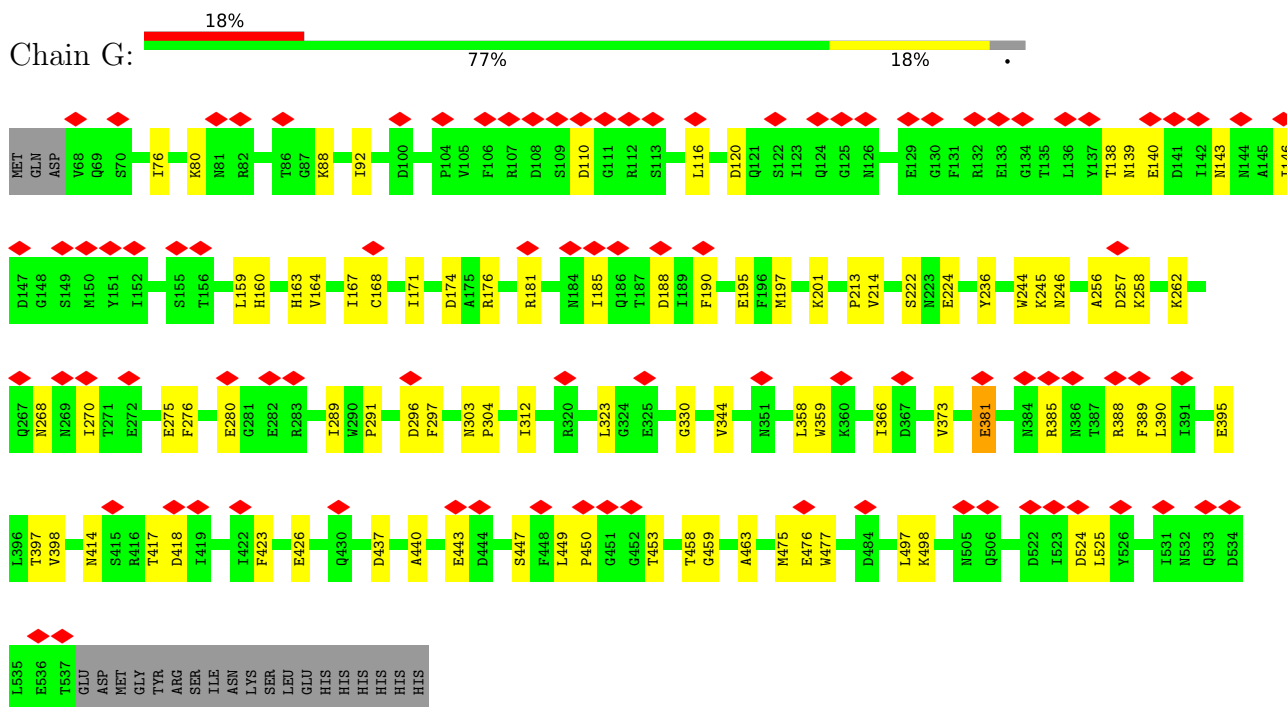
- Molecule 2: Subtilisin-like serine germination related protease



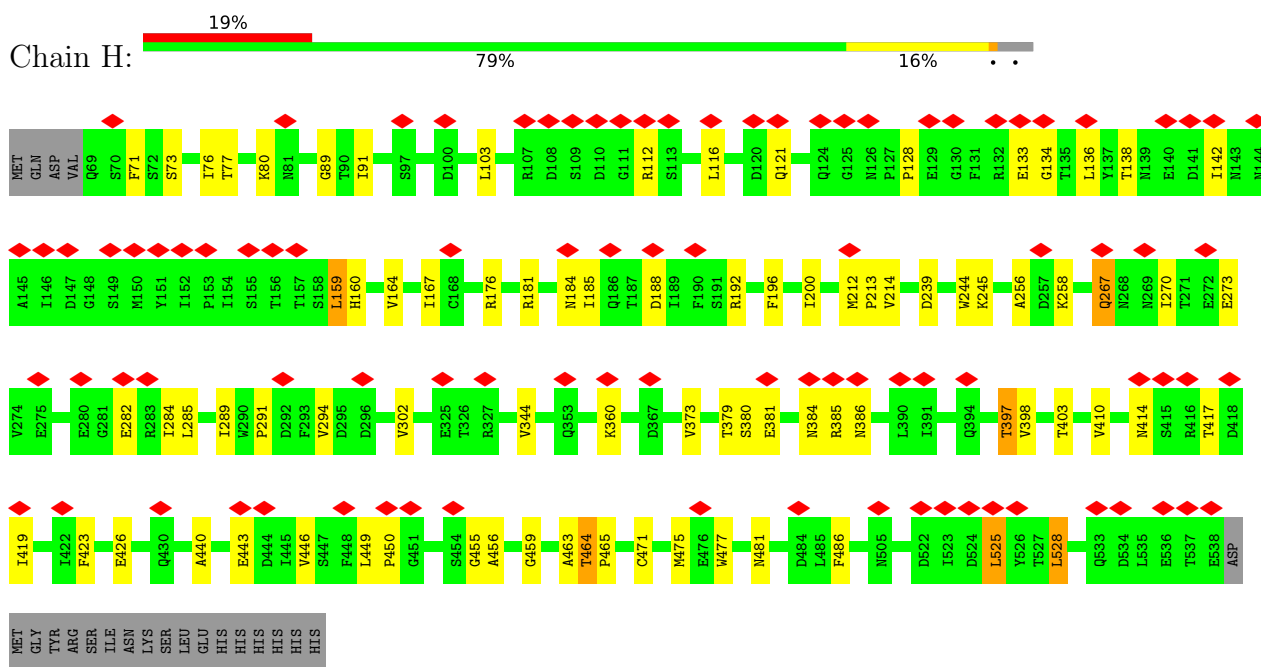
- Molecule 2: Subtilisin-like serine germination related protease



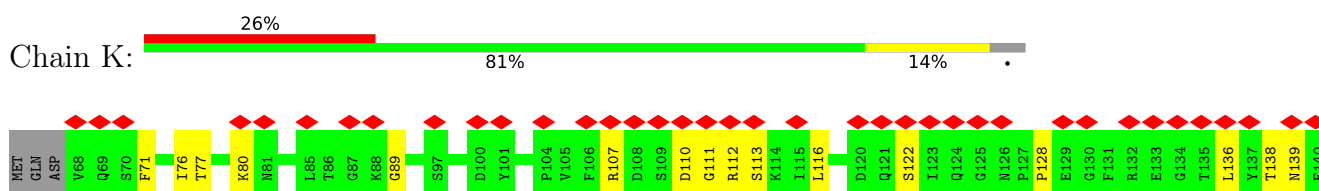
- Molecule 2: Subtilisin-like serine germination related protease

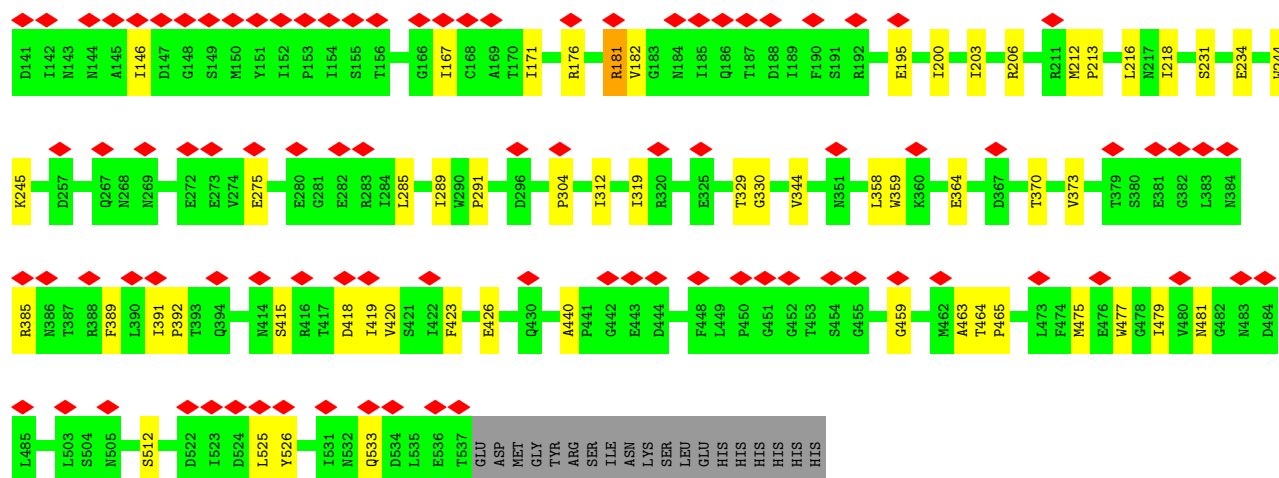


- Molecule 2: Subtilisin-like serine germination related protease

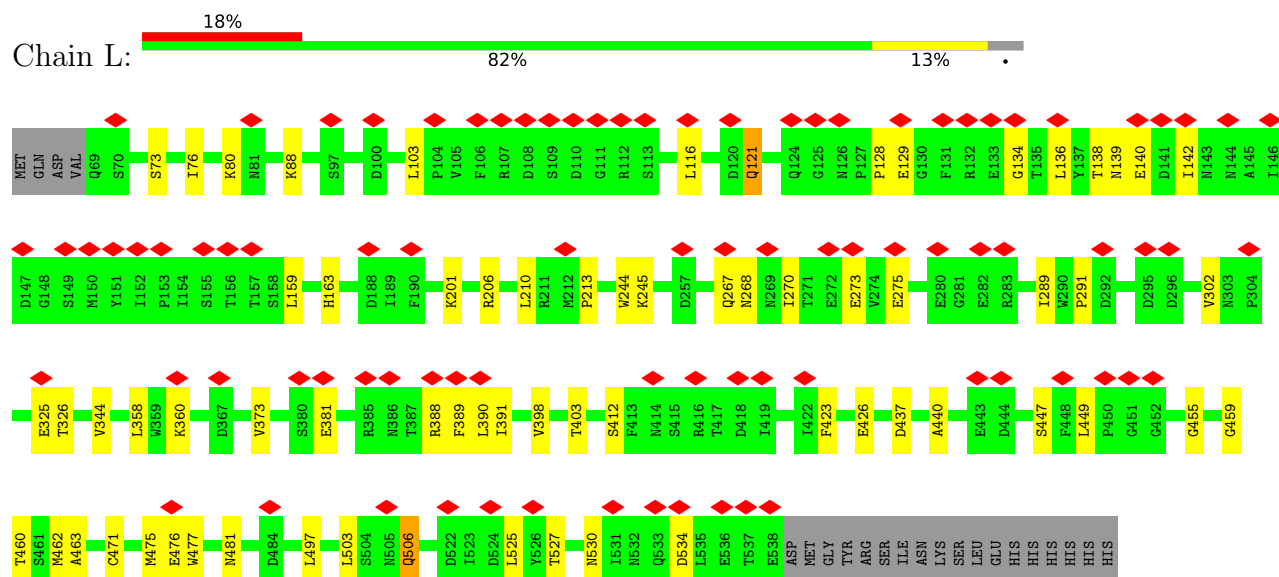


- Molecule 2: Subtilisin-like serine germination related protease

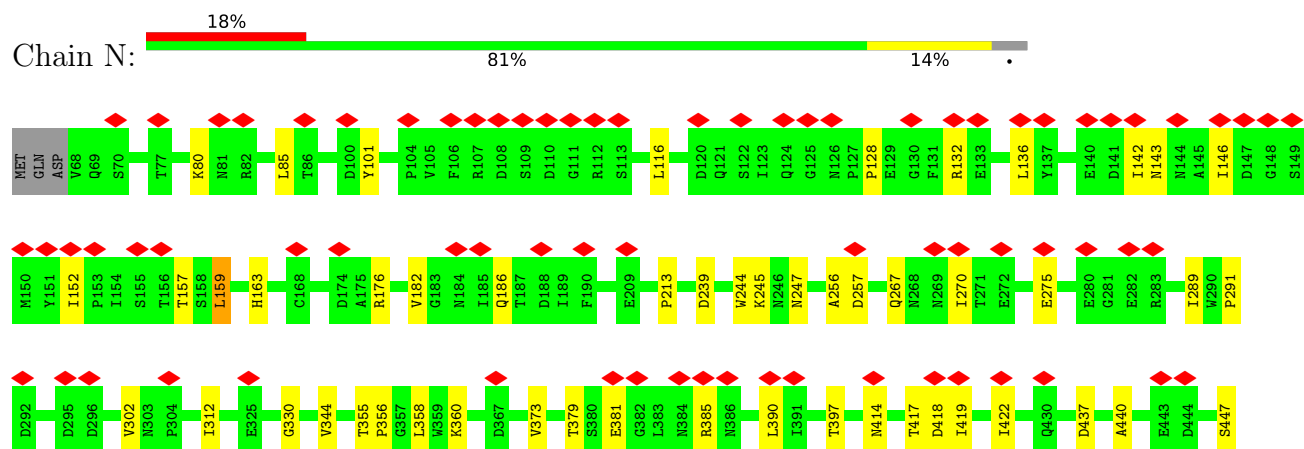


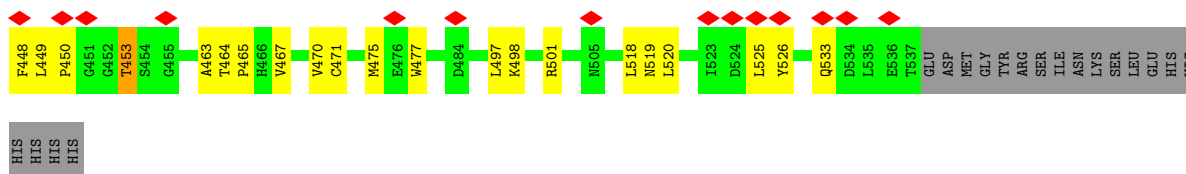


- Molecule 2: Subtilisin-like serine germination related protease

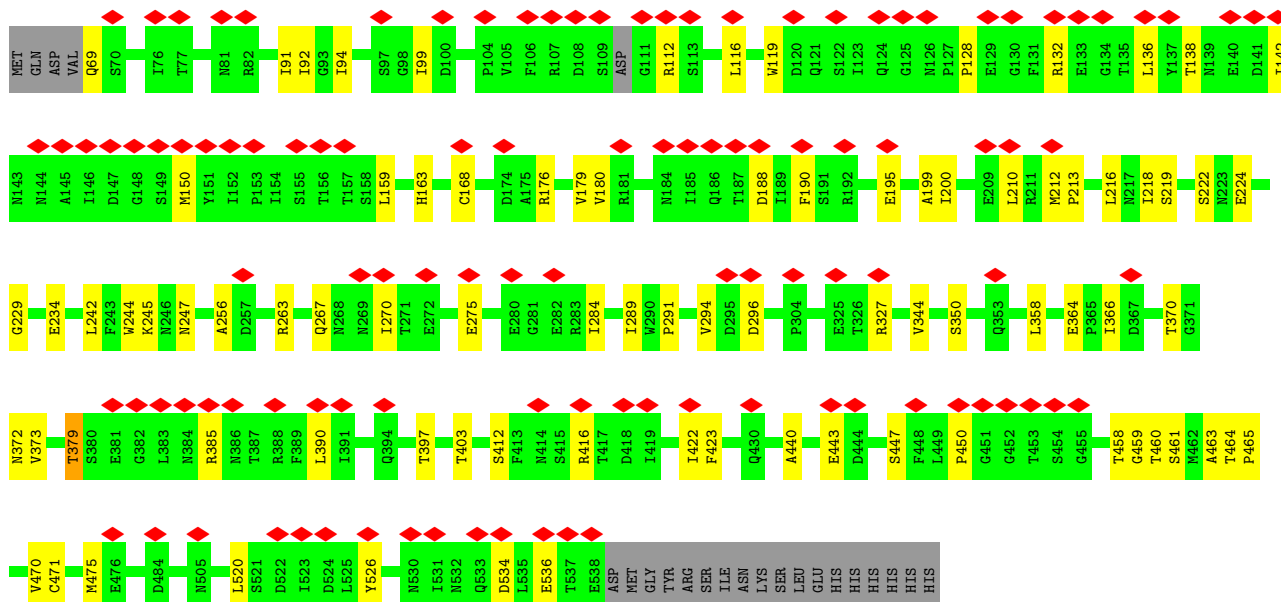
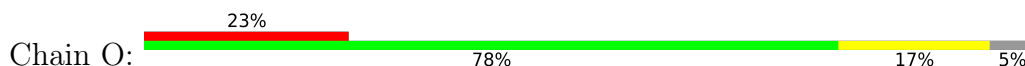


- Molecule 2: Subtilisin-like serine germination related protease

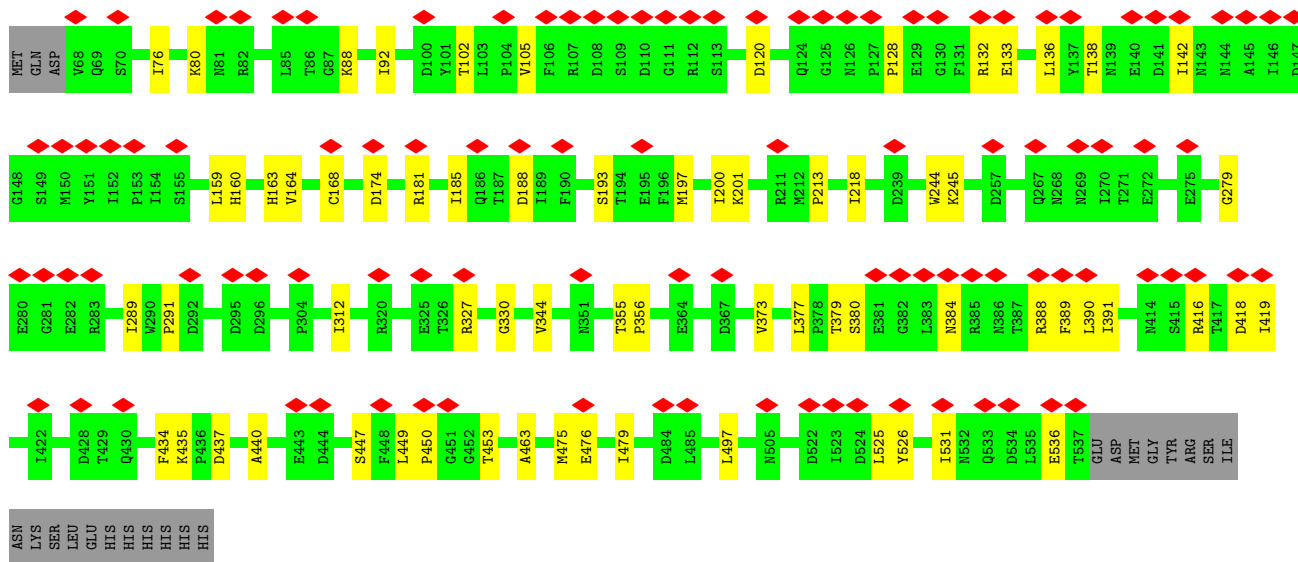
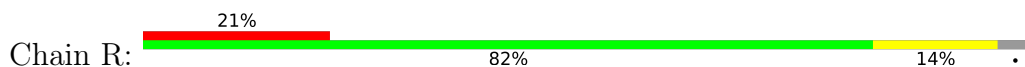





- Molecule 2: Subtilisin-like serine germination related protease

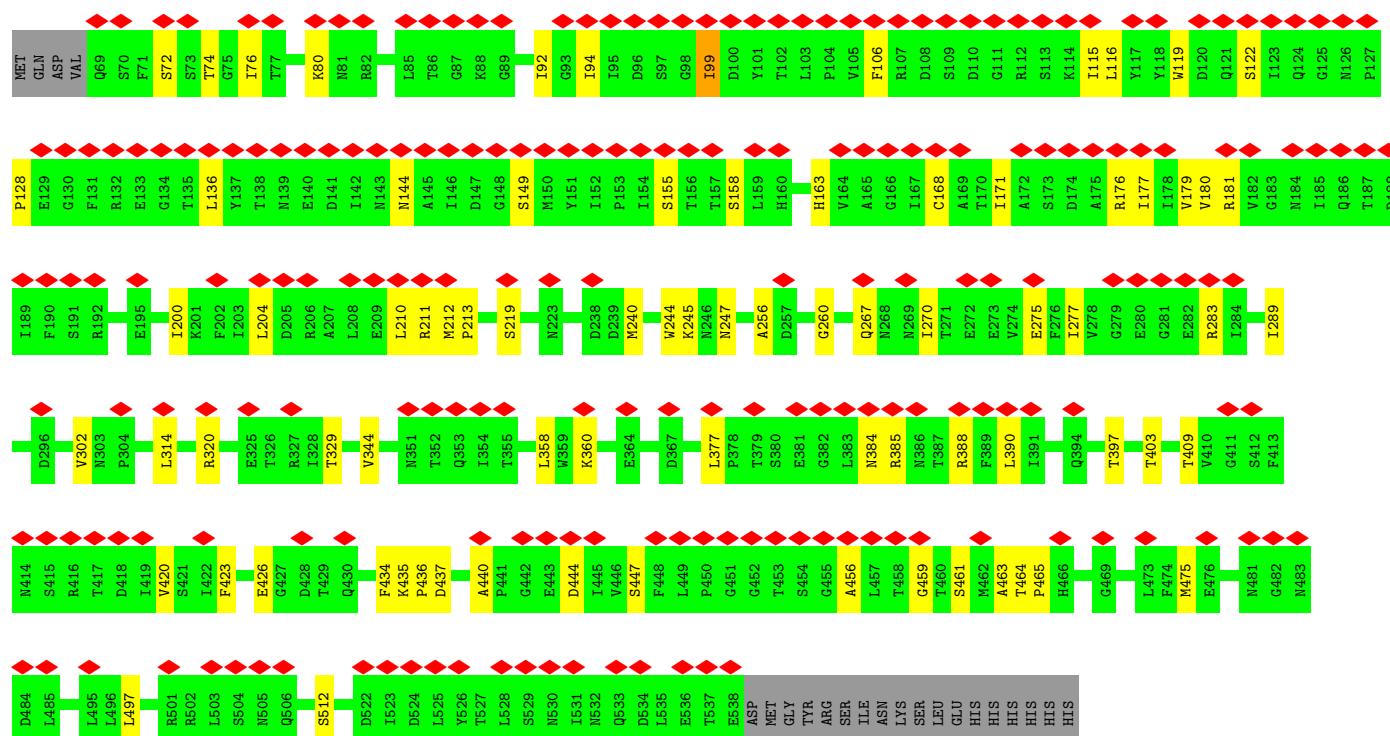


- Molecule 2: Subtilisin-like serine germination related protease




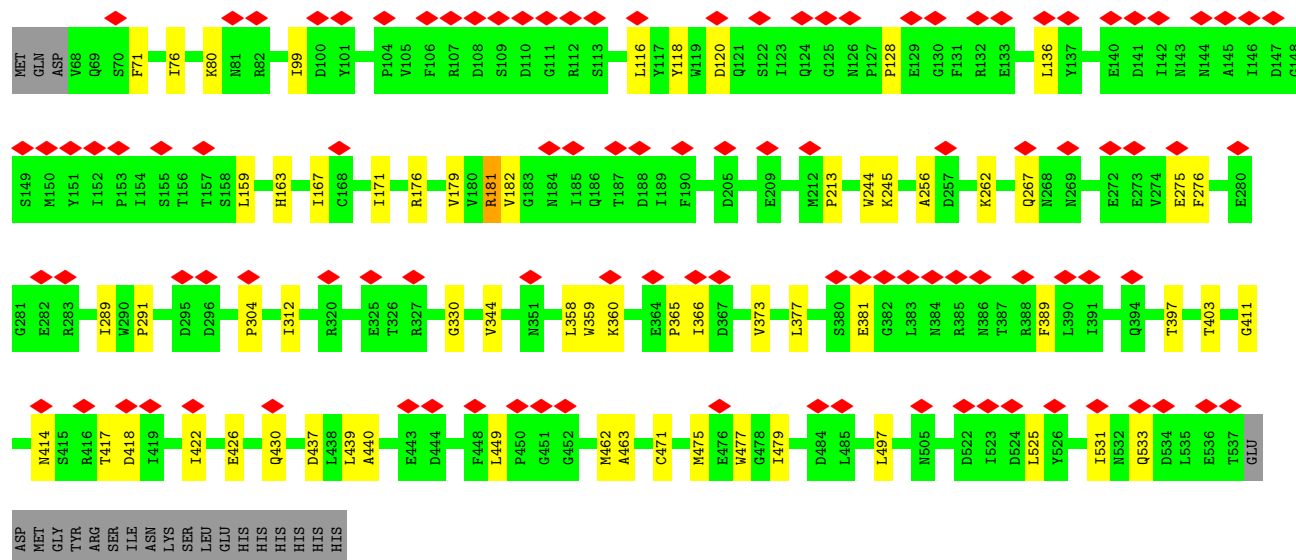
- Molecule 2: Subtilisin-like serine germination related protease

Chain S: 




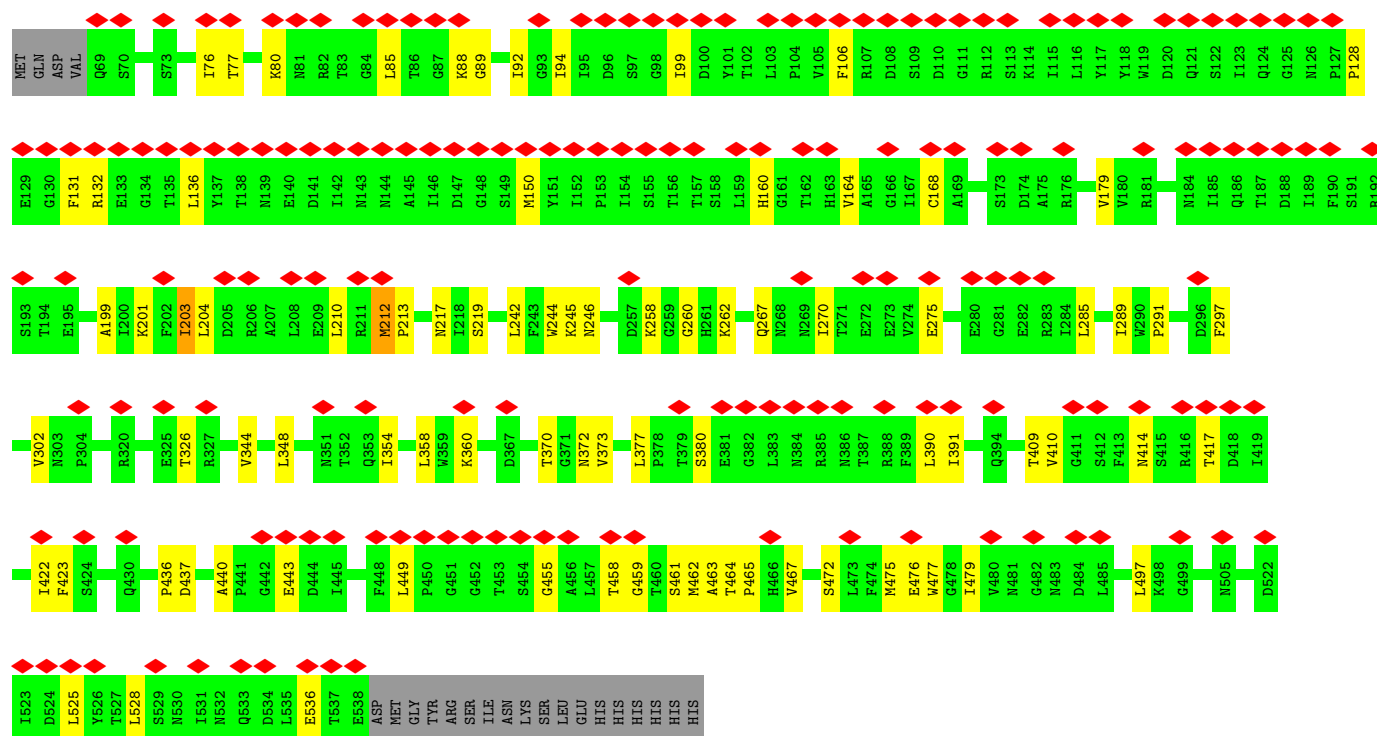
- Molecule 2: Subtilisin-like serine germination related protease

Chain W: 

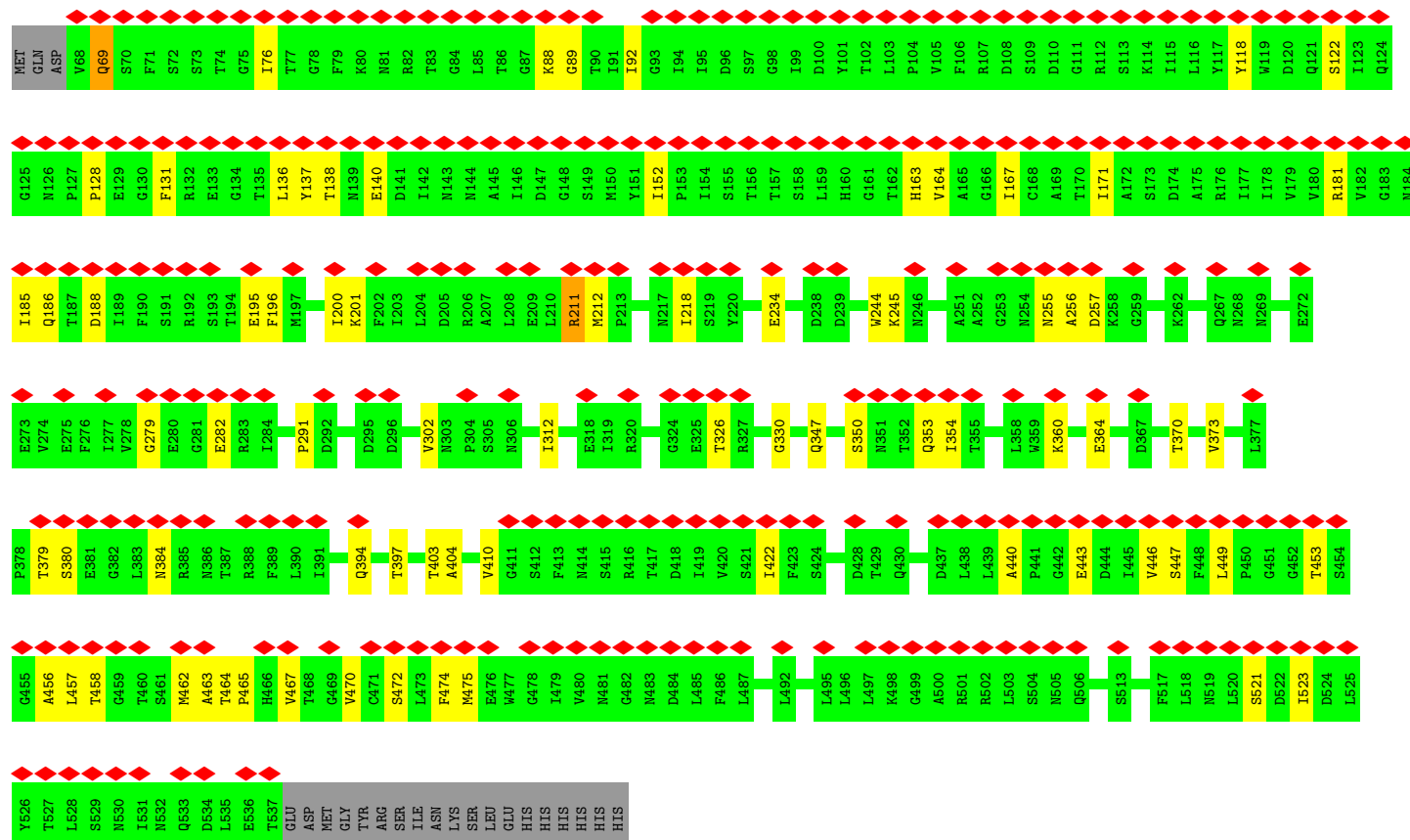
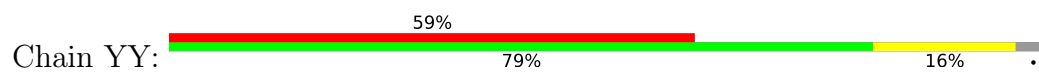


- Molecule 2: Subtilisin-like serine germination related protease

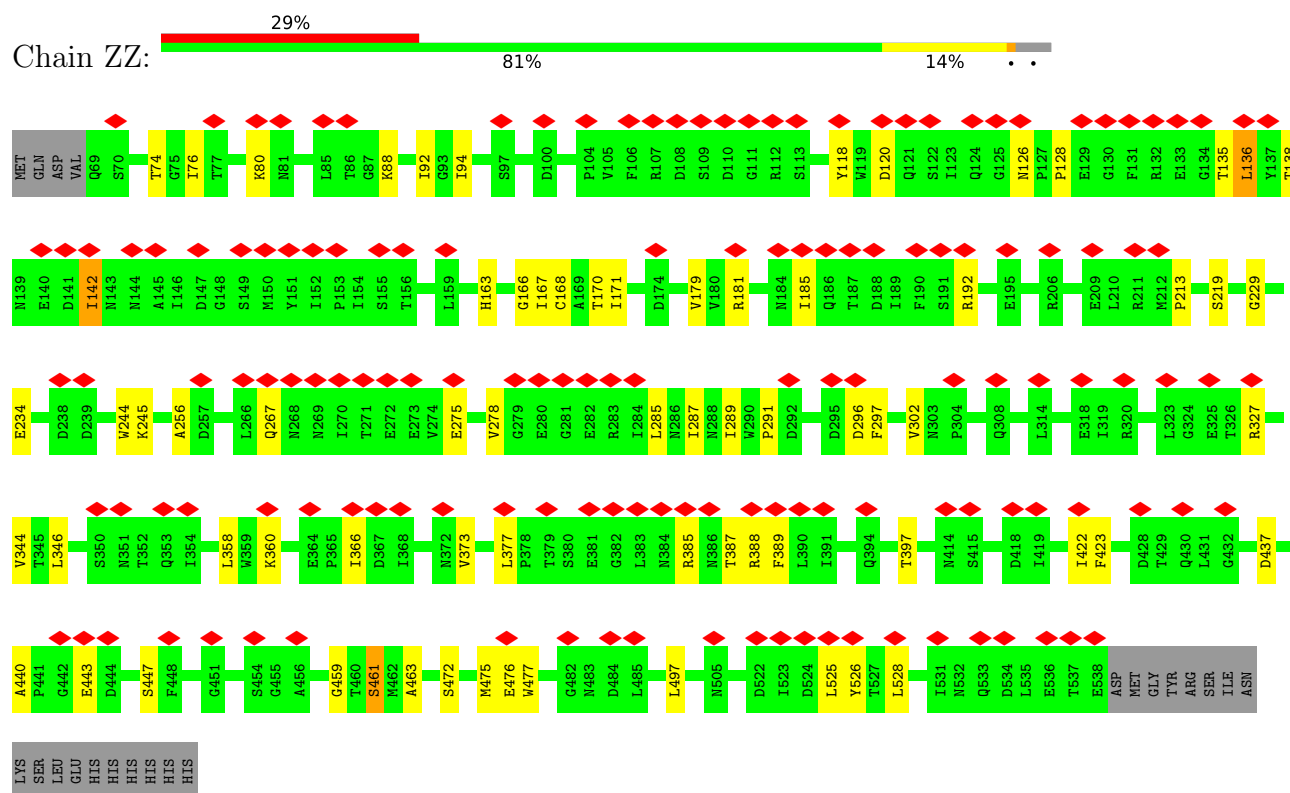
Chain X: 



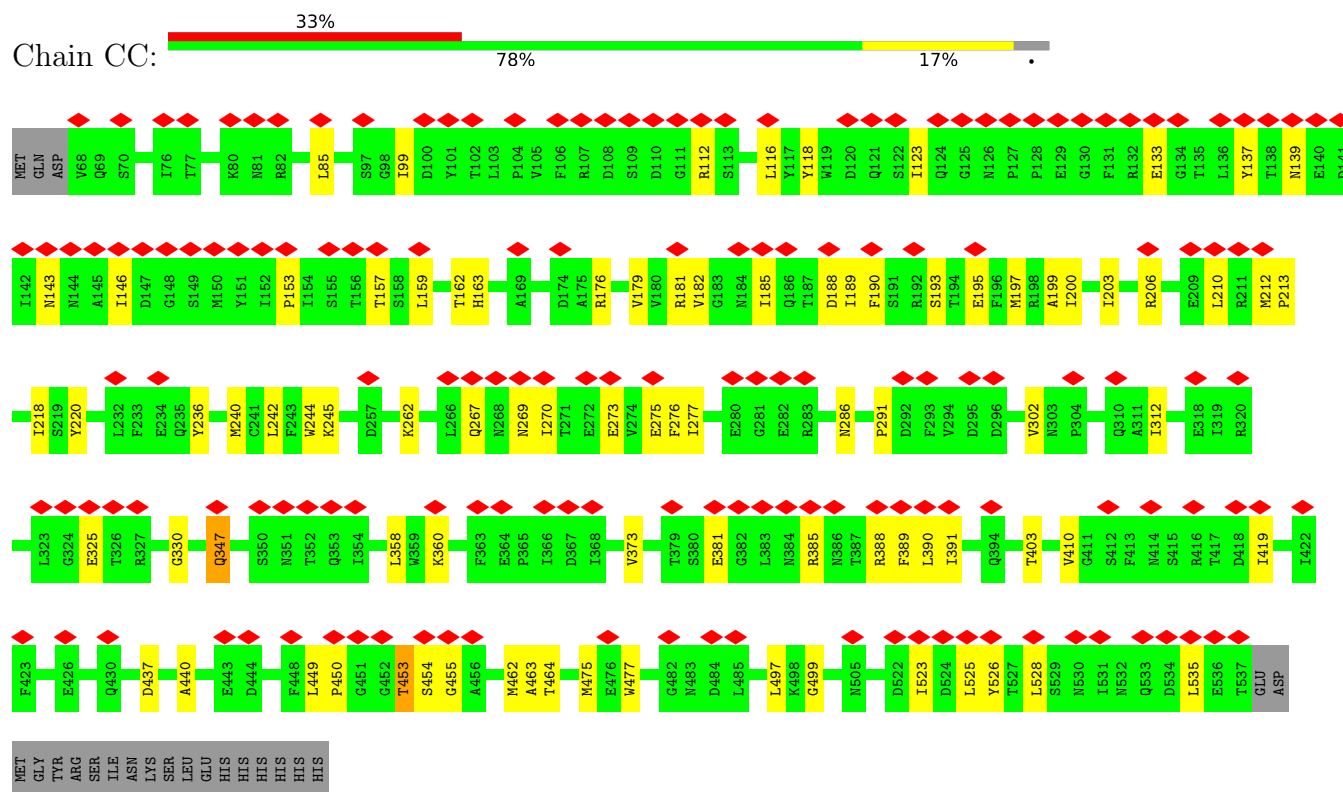
• Molecule 2: Subtilisin-like serine germination related protease



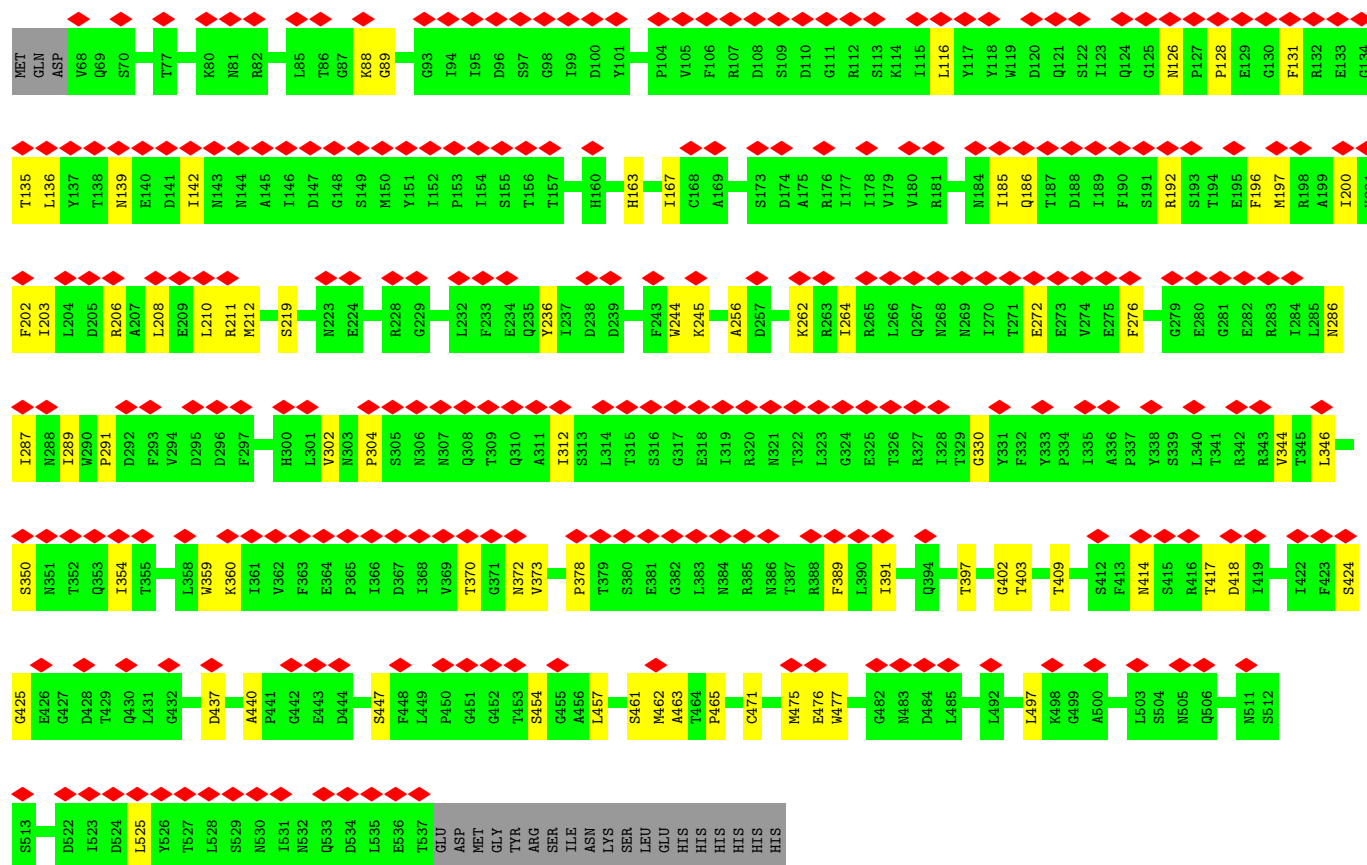
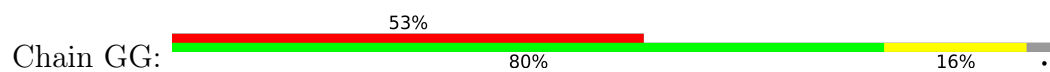
- Molecule 2: Subtilisin-like serine germination related protease



- Molecule 2: Subtilisin-like serine germination related protease



- Molecule 2: Subtilisin-like serine germination related protease



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=135.9°, rise=24.7 Å, axial sym=C1	Depositor
Number of segments used	200	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.03	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	266.802, 266.802, 266.802	wwPDB
Map dimensions	318, 318, 318	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	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	0.16	0/503	0.41	0/684
1	AA	0.15	0/503	0.39	0/684
1	B	0.16	0/503	0.35	0/684
1	BB	0.17	0/503	0.42	0/684
1	E	0.19	0/503	0.49	0/684
1	EE	0.18	0/487	0.49	0/662
1	F	0.16	0/503	0.40	0/684
1	FF	0.17	0/503	0.48	0/684
1	I	0.20	0/503	0.48	0/684
1	J	0.18	0/503	0.43	0/684
1	LL	0.18	0/503	0.38	0/684
1	M	0.17	0/503	0.37	0/684
1	P	0.16	0/503	0.44	0/684
1	Q	0.17	0/503	0.41	0/684
1	T	0.17	0/503	0.41	0/684
1	V	0.17	0/503	0.41	0/684
1	Y	0.16	0/503	0.43	0/684
1	Z	0.18	0/503	0.49	0/684
2	C	0.15	0/3708	0.31	0/5043
2	CC	0.15	0/3708	0.33	0/5043
2	D	0.16	0/3710	0.32	0/5045
2	G	0.16	0/3708	0.34	0/5043
2	GG	0.13	0/3708	0.33	0/5043
2	H	0.16	0/3710	0.31	0/5045
2	K	0.15	0/3708	0.31	0/5043
2	L	0.16	0/3710	0.34	0/5045
2	N	0.16	0/3708	0.32	0/5043
2	O	0.15	0/3701	0.32	0/5031
2	R	0.15	0/3708	0.32	0/5043
2	S	0.14	0/3710	0.30	0/5045
2	W	0.15	0/3708	0.31	0/5043
2	X	0.14	0/3710	0.31	0/5045
2	YY	0.13	0/3708	0.33	0/5043
2	ZZ	0.14	0/3710	0.33	0/5045

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/68371	0.34	0/92978

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	496	0	492	7	0
1	AA	496	0	492	11	0
1	B	496	0	492	9	0
1	BB	496	0	492	8	0
1	E	496	0	492	10	0
1	EE	480	0	477	7	0
1	F	496	0	492	10	0
1	FF	496	0	492	11	0
1	I	496	0	492	8	0
1	J	496	0	492	3	0
1	LL	496	0	492	9	0
1	M	496	0	492	9	0
1	P	496	0	492	5	0
1	Q	496	0	492	7	0
1	T	496	0	492	8	0
1	V	496	0	492	6	0
1	Y	496	0	492	9	0
1	Z	496	0	492	6	0
2	C	3637	0	3595	51	0
2	CC	3637	0	3595	57	0
2	D	3639	0	3592	47	0
2	G	3637	0	3595	59	0
2	GG	3637	0	3595	43	0
2	H	3639	0	3592	53	0
2	K	3637	0	3595	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	3639	0	3592	40	0
2	N	3637	0	3595	44	0
2	O	3631	0	3587	53	0
2	R	3637	0	3595	40	0
2	S	3639	0	3592	45	0
2	W	3637	0	3595	36	0
2	X	3639	0	3592	55	0
2	YY	3637	0	3595	47	0
2	ZZ	3639	0	3592	47	0
All	All	67110	0	66335	858	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 6.

All (858) 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:C:116:LEU:HD21	2:C:176:ARG:HB3	1.48	0.95
2:N:213:PRO:HB2	2:N:475:MET:HE3	1.50	0.94
2:H:213:PRO:HB2	2:H:475:MET:HE3	1.53	0.89
2:W:213:PRO:HB2	2:W:475:MET:HE3	1.52	0.89
2:G:213:PRO:HB2	2:G:475:MET:HE3	1.58	0.85
2:O:213:PRO:HB2	2:O:475:MET:HE3	1.60	0.83
2:S:213:PRO:HB2	2:S:475:MET:HE3	1.61	0.83
2:S:99:ILE:HD11	2:S:106:PHE:HE1	1.42	0.83
2:L:213:PRO:HB2	2:L:475:MET:HE3	1.62	0.81
2:C:213:PRO:HB2	2:C:475:MET:HE3	1.61	0.81
2:CC:116:LEU:HD21	2:CC:176:ARG:HB3	1.64	0.80
2:D:213:PRO:HB2	2:D:475:MET:HE3	1.64	0.77
2:X:99:ILE:HD11	2:X:106:PHE:HE1	1.49	0.77
2:CC:213:PRO:HB2	2:CC:475:MET:HE3	1.65	0.76
2:ZZ:213:PRO:HB2	2:ZZ:475:MET:HE3	1.68	0.75
2:H:159:LEU:HD22	2:H:450:PRO:HD2	1.68	0.74
2:H:302:VAL:HB	2:H:360:LYS:HB2	1.69	0.74
2:CC:159:LEU:HD22	2:CC:450:PRO:HD2	1.70	0.74
2:S:210:LEU:HB3	2:S:212:MET:HG3	1.70	0.72
1:LL:64:GLN:HE21	2:O:379:THR:HG22	1.55	0.72
2:X:213:PRO:HB2	2:X:475:MET:HE3	1.71	0.71
2:O:219:SER:HB3	2:O:461:SER:HB2	1.73	0.70
2:G:414:ASN:HB3	2:G:417:THR:HG22	1.73	0.70
2:YY:138:THR:HG22	2:YY:140:GLU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZZ:219:SER:HB2	2:ZZ:461:SER:HB2	1.75	0.69
2:W:163:HIS:HD2	2:W:462:MET:HE2	1.57	0.68
2:C:99:ILE:HB	2:C:179:VAL:HG11	1.76	0.68
2:R:132:ARG:NH1	2:R:132:ARG:HB2	2.09	0.68
2:D:390:LEU:HD23	2:D:391:ILE:HG13	1.76	0.68
2:R:391:ILE:HG13	2:R:391:ILE:O	1.94	0.68
2:W:128:PRO:HG3	2:W:136:LEU:HB2	1.76	0.68
2:L:503:LEU:HD12	2:L:506:GLN:HE21	1.59	0.66
2:X:219:SER:HB2	2:X:461:SER:HB2	1.77	0.66
2:C:275:GLU:HB3	2:C:358:LEU:HD11	1.78	0.66
2:O:385:ARG:H	2:O:385:ARG:HD3	1.60	0.66
1:FF:9:ILE:HD12	2:GG:197:MET:HE1	1.78	0.66
2:C:138:THR:HG22	2:C:140:GLU:H	1.62	0.65
2:GG:262:LYS:HE2	2:GG:391:ILE:HG23	1.77	0.65
2:S:275:GLU:HB2	2:S:390:LEU:HD22	1.79	0.65
2:G:262:LYS:HB2	2:G:389:PHE:CD2	2.31	0.65
2:R:244:TRP:CG	2:R:245:LYS:H	2.15	0.65
2:G:138:THR:HG22	2:G:140:GLU:H	1.62	0.65
1:I:64:GLN:HG3	2:L:381:GLU:OE2	1.96	0.65
2:X:132:ARG:HG3	2:X:132:ARG:HH11	1.62	0.64
2:C:244:TRP:CG	2:C:245:LYS:H	2.16	0.64
2:YY:302:VAL:HB	2:YY:360:LYS:HB2	1.80	0.64
2:L:302:VAL:HB	2:L:360:LYS:HB2	1.80	0.64
2:K:128:PRO:HG3	2:K:136:LEU:HB2	1.80	0.63
2:D:219:SER:HB2	2:D:461:SER:HB2	1.79	0.63
2:W:275:GLU:HB3	2:W:358:LEU:HD11	1.80	0.63
2:GG:440:ALA:HB3	2:GG:463:ALA:HB1	1.80	0.63
2:C:471:CYS:O	2:C:475:MET:HB2	1.99	0.63
2:YY:244:TRP:CG	2:YY:245:LYS:H	2.17	0.63
1:Z:25:VAL:HG13	1:Z:39:SER:HB2	1.80	0.63
1:FF:8:LEU:HD11	1:FF:43:GLU:HG3	1.81	0.63
2:GG:163:HIS:HD2	2:GG:462:MET:HE2	1.62	0.63
1:E:25:VAL:HG12	1:E:39:SER:HB2	1.79	0.63
2:O:119:TRP:HB3	2:O:180:VAL:HG23	1.81	0.63
2:S:99:ILE:HB	2:S:179:VAL:HG11	1.81	0.63
2:G:120:ASP:HA	2:G:181:ARG:HB3	1.81	0.63
2:GG:244:TRP:CG	2:GG:245:LYS:H	2.16	0.63
1:V:59:LYS:HE3	2:X:536:GLU:HG3	1.80	0.62
2:CC:244:TRP:CG	2:CC:245:LYS:H	2.17	0.62
1:A:25:VAL:HG12	1:A:39:SER:HB2	1.81	0.62
2:ZZ:192:ARG:HG3	2:ZZ:192:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YY:128:PRO:HG3	2:YY:136:LEU:HB2	1.82	0.62
2:X:302:VAL:HB	2:X:360:LYS:HB2	1.81	0.62
2:L:477:TRP:CE2	2:L:525:LEU:HD22	2.35	0.61
2:O:200:ILE:HD11	2:O:218:ILE:HD11	1.82	0.61
2:H:164:VAL:HA	2:H:167:ILE:HD12	1.82	0.61
2:N:244:TRP:CG	2:N:245:LYS:H	2.18	0.61
1:I:25:VAL:HG12	1:I:39:SER:HB2	1.83	0.61
2:GG:219:SER:HB2	2:GG:461:SER:HB2	1.82	0.61
2:G:244:TRP:CG	2:G:245:LYS:H	2.18	0.61
2:L:390:LEU:HD23	2:L:391:ILE:HG13	1.83	0.61
2:N:128:PRO:HG3	2:N:136:LEU:HB2	1.82	0.60
2:W:256:ALA:HA	2:W:397:THR:HG21	1.84	0.60
2:CC:200:ILE:HD11	2:CC:218:ILE:HD11	1.83	0.60
2:CC:163:HIS:HD2	2:CC:462:MET:HE2	1.65	0.60
2:CC:302:VAL:HB	2:CC:360:LYS:HB2	1.84	0.60
2:D:244:TRP:CG	2:D:245:LYS:H	2.19	0.60
1:E:64:GLN:HG3	2:H:381:GLU:OE2	2.02	0.60
1:J:30:LEU:HD11	1:J:36:ILE:HG13	1.83	0.60
2:CC:210:LEU:HB3	2:CC:212:MET:HE3	1.82	0.60
2:K:275:GLU:HB3	2:K:358:LEU:HD11	1.82	0.60
2:C:92:ILE:HD11	2:C:472:SER:HB2	1.85	0.59
2:GG:414:ASN:HB3	2:GG:417:THR:HG22	1.83	0.59
2:O:94:ILE:HB	2:O:179:VAL:HG12	1.82	0.59
2:W:244:TRP:CG	2:W:245:LYS:H	2.21	0.59
2:YY:457:LEU:HB2	2:YY:462:MET:HE3	1.84	0.59
1:BB:64:GLN:NE2	2:CC:381:GLU:HB3	2.18	0.59
2:K:116:LEU:HA	2:K:139:ASN:HB2	1.85	0.59
2:R:440:ALA:HB3	2:R:463:ALA:HB1	1.83	0.59
2:CC:185:ILE:HB	2:CC:188:ASP:HB3	1.85	0.59
2:G:275:GLU:HB3	2:G:358:LEU:HD11	1.85	0.59
2:X:260:GLY:HA2	2:X:377:LEU:HD12	1.85	0.59
2:O:526:TYR:HE1	2:ZZ:526:TYR:HE1	1.49	0.58
2:YY:92:ILE:HD11	2:YY:472:SER:HB2	1.85	0.58
2:CC:391:ILE:HG13	2:CC:391:ILE:O	2.04	0.58
2:GG:350:SER:HB3	2:GG:354:ILE:HD12	1.86	0.58
2:G:423:PHE:HE2	2:G:459:GLY:HA2	1.68	0.58
2:L:159:LEU:HD22	2:N:453:THR:HG21	1.85	0.58
2:N:471:CYS:O	2:N:475:MET:HB2	2.03	0.58
2:K:244:TRP:CG	2:K:245:LYS:H	2.22	0.57
2:D:275:GLU:HB3	2:D:358:LEU:HD11	1.85	0.57
2:G:440:ALA:HB3	2:G:463:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CC:440:ALA:HB3	2:CC:463:ALA:HB1	1.85	0.57
2:D:303:ASN:HB3	2:D:323:LEU:HD23	1.86	0.57
2:G:116:LEU:HA	2:G:139:ASN:HB2	1.84	0.57
2:GG:302:VAL:HB	2:GG:360:LYS:HB2	1.86	0.57
2:W:414:ASN:HB3	2:W:417:THR:HG22	1.85	0.57
2:S:99:ILE:HD11	2:S:106:PHE:CE1	2.33	0.57
1:FF:22:GLU:OE1	1:FF:23:LEU:HD13	2.04	0.57
2:C:160:HIS:O	2:C:164:VAL:HG23	2.04	0.57
2:H:267:GLN:HG3	2:H:270:ILE:HB	1.87	0.57
2:S:171:ILE:HD12	2:S:171:ILE:H	1.70	0.57
2:H:289:ILE:HB	2:H:344:VAL:HB	1.86	0.57
2:GG:203:ILE:HD12	2:GG:203:ILE:H	1.69	0.57
2:D:160:HIS:O	2:D:164:VAL:HG22	2.05	0.56
2:H:273:GLU:OE2	2:H:360:LYS:HE3	2.05	0.56
2:S:92:ILE:HD12	2:S:168:CYS:HB3	1.87	0.56
2:W:245:LYS:HD3	2:W:479:ILE:HD13	1.85	0.56
2:X:289:ILE:HB	2:X:344:VAL:HB	1.87	0.56
2:L:128:PRO:HG3	2:L:136:LEU:HB2	1.87	0.56
1:Q:19:LEU:HD12	1:Q:23:LEU:HG	1.88	0.56
2:C:116:LEU:H	2:C:116:LEU:HD22	1.71	0.56
2:G:477:TRP:NE1	2:G:525:LEU:HD11	2.21	0.56
2:GG:276:PHE:HB3	2:GG:389:PHE:CD2	2.41	0.56
2:H:440:ALA:HB3	2:H:463:ALA:HB1	1.88	0.56
2:X:244:TRP:CG	2:X:245:LYS:H	2.23	0.56
1:LL:16:ILE:HD12	1:LL:19:LEU:HD23	1.88	0.56
2:R:128:PRO:HG3	2:R:136:LEU:HB2	1.88	0.56
2:S:128:PRO:HG3	2:S:136:LEU:HB2	1.88	0.56
2:D:440:ALA:HB3	2:D:463:ALA:HB1	1.88	0.56
2:H:410:VAL:HG21	2:H:464:THR:HA	1.87	0.56
2:R:159:LEU:HD22	2:R:450:PRO:HD2	1.87	0.56
2:CC:275:GLU:HB3	2:CC:358:LEU:HD11	1.87	0.56
2:GG:287:ILE:HB	2:GG:346:LEU:HB2	1.87	0.56
2:H:423:PHE:HE2	2:H:459:GLY:HA2	1.71	0.56
2:N:275:GLU:HB3	2:N:358:LEU:HD11	1.87	0.56
2:O:116:LEU:HD23	2:O:176:ARG:HB3	1.88	0.55
1:A:27:VAL:HG22	1:A:37:ILE:HG12	1.87	0.55
2:D:471:CYS:O	2:D:475:MET:HB2	2.06	0.55
2:H:471:CYS:O	2:H:475:MET:HB2	2.06	0.55
1:LL:64:GLN:HE21	2:O:379:THR:CG2	2.17	0.55
2:N:302:VAL:HB	2:N:360:LYS:HB2	1.88	0.55
2:W:471:CYS:O	2:W:475:MET:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:26:SER:HB3	1:Y:38:THR:HG23	1.88	0.55
1:V:30:LEU:HD11	1:V:36:ILE:HG13	1.88	0.55
1:BB:25:VAL:HG12	1:BB:39:SER:HB2	1.88	0.55
2:H:291:PRO:HB3	2:H:373:VAL:HG22	1.89	0.55
2:H:414:ASN:HB3	2:H:417:THR:HG22	1.89	0.55
2:N:159:LEU:HD22	2:N:450:PRO:HD2	1.88	0.55
2:O:244:TRP:CG	2:O:245:LYS:H	2.25	0.55
2:R:200:ILE:HD11	2:R:218:ILE:HD11	1.89	0.55
2:R:245:LYS:HD3	2:R:479:ILE:HD13	1.88	0.55
2:R:291:PRO:HB3	2:R:373:VAL:HG22	1.89	0.55
2:YY:164:VAL:HG13	2:YY:465:PRO:HG3	1.88	0.55
2:K:440:ALA:HB3	2:K:463:ALA:HB1	1.89	0.55
1:M:55:GLU:HB3	2:O:242:LEU:HB3	1.89	0.54
2:ZZ:244:TRP:CG	2:ZZ:245:LYS:H	2.25	0.54
2:H:477:TRP:NE1	2:H:525:LEU:HD11	2.23	0.54
2:L:244:TRP:CG	2:L:245:LYS:H	2.26	0.54
2:L:273:GLU:HB3	2:L:360:LYS:NZ	2.21	0.54
2:G:185:ILE:HB	2:G:188:ASP:OD2	2.08	0.54
2:G:289:ILE:HB	2:G:344:VAL:HB	1.90	0.54
2:CC:244:TRP:CG	2:CC:245:LYS:N	2.76	0.54
2:CC:453:THR:HG22	2:CC:454:SER:H	1.73	0.54
2:D:128:PRO:HG3	2:D:136:LEU:HB2	1.89	0.54
2:W:262:LYS:HB2	2:W:389:PHE:CD2	2.42	0.54
2:N:477:TRP:NE1	2:N:525:LEU:HD11	2.23	0.54
2:X:440:ALA:HB3	2:X:463:ALA:HB1	1.89	0.54
1:M:64:GLN:HE21	2:N:379:THR:CG2	2.21	0.54
1:AA:16:ILE:HD12	1:AA:19:LEU:HD23	1.90	0.54
2:CC:199:ALA:O	2:CC:203:ILE:HD12	2.08	0.54
2:C:244:TRP:CG	2:C:245:LYS:N	2.76	0.53
2:X:94:ILE:HB	2:X:179:VAL:HG12	1.89	0.53
2:K:423:PHE:HE2	2:K:459:GLY:HA2	1.73	0.53
2:R:244:TRP:CG	2:R:245:LYS:N	2.77	0.53
1:T:49:LEU:HD13	1:T:57:ILE:HD12	1.89	0.53
2:W:437:ASP:HB3	2:W:497:LEU:HD21	1.90	0.53
2:H:244:TRP:CG	2:H:245:LYS:H	2.26	0.53
2:K:200:ILE:HD11	2:K:218:ILE:HD11	1.90	0.53
1:LL:27:VAL:HG22	1:LL:37:ILE:HG12	1.91	0.53
2:YY:118:TYR:HB3	2:YY:137:TYR:HB2	1.91	0.53
2:YY:185:ILE:HD13	2:YY:188:ASP:H	1.74	0.53
2:O:99:ILE:HD12	2:O:179:VAL:HG11	1.91	0.53
2:G:160:HIS:O	2:G:164:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:THR:O	2:D:142:ILE:HD12	2.09	0.53
2:R:132:ARG:HB2	2:R:132:ARG:HH11	1.72	0.53
2:S:444:ASP:HA	2:S:456:ALA:HB1	1.90	0.53
1:B:16:ILE:HD12	1:B:19:LEU:HD23	1.92	0.52
2:S:219:SER:HB2	2:S:461:SER:HB2	1.91	0.52
2:W:440:ALA:HB3	2:W:463:ALA:HB1	1.91	0.52
2:X:414:ASN:OD1	2:X:417:THR:HG22	2.09	0.52
1:E:22:GLU:OE1	1:E:23:LEU:HD23	2.09	0.52
2:H:128:PRO:HG3	2:H:136:LEU:HB2	1.90	0.52
2:H:192:ARG:HH11	2:H:192:ARG:HB2	1.74	0.52
1:AA:19:LEU:HD11	1:AA:51:TYR:HD1	1.73	0.52
2:C:116:LEU:HA	2:C:139:ASN:HB2	1.90	0.52
2:X:370:THR:HG22	2:X:372:ASN:H	1.75	0.52
2:YY:137:TYR:CE2	2:YY:152:ILE:HG23	2.44	0.52
2:GG:286:ASN:O	2:GG:378:PRO:HD3	2.09	0.52
2:R:185:ILE:HB	2:R:188:ASP:OD2	2.10	0.52
2:GG:276:PHE:HB3	2:GG:389:PHE:HD2	1.75	0.52
2:C:291:PRO:HB3	2:C:373:VAL:HG22	1.92	0.52
2:K:291:PRO:HB3	2:K:373:VAL:HG22	1.92	0.52
2:N:159:LEU:HD21	2:N:449:LEU:HD23	1.92	0.52
2:X:99:ILE:HD11	2:X:106:PHE:CE1	2.38	0.52
2:CC:477:TRP:HE1	2:CC:525:LEU:HD11	1.75	0.52
2:C:526:TYR:CE1	2:R:526:TYR:HE1	2.27	0.52
2:K:426:GLU:HG2	2:K:512:SER:HA	1.91	0.52
2:L:449:LEU:HD11	2:L:455:GLY:HA3	1.91	0.52
2:L:289:ILE:HB	2:L:344:VAL:HB	1.92	0.52
2:YY:122:SER:HB3	2:YY:181:ARG:NH1	2.25	0.52
2:GG:402:GLY:O	2:GG:409:THR:HG21	2.10	0.52
2:S:384:ASN:HA	2:S:385:ARG:NH1	2.25	0.52
2:X:275:GLU:HB2	2:X:390:LEU:HD22	1.92	0.52
2:O:180:VAL:HG11	2:O:199:ALA:HB1	1.91	0.51
2:X:267:GLN:HG3	2:X:270:ILE:HB	1.91	0.51
2:GG:289:ILE:HB	2:GG:344:VAL:HB	1.92	0.51
2:D:244:TRP:CG	2:D:245:LYS:N	2.79	0.51
2:O:128:PRO:HG3	2:O:136:LEU:HB2	1.92	0.51
2:S:426:GLU:HG2	2:S:512:SER:HA	1.92	0.51
2:YY:446:VAL:HG22	2:YY:456:ALA:HB2	1.91	0.51
2:GG:196:PHE:O	2:GG:200:ILE:HG13	2.11	0.51
2:C:430:GLN:HA	2:C:430:GLN:OE1	2.10	0.51
2:D:123:ILE:HD12	2:D:123:ILE:H	1.75	0.51
2:K:312:ILE:HD13	2:K:330:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:27:VAL:HG22	1:M:37:ILE:HG12	1.91	0.51
2:D:116:LEU:HD13	2:D:176:ARG:HB3	1.92	0.51
2:H:477:TRP:HE1	2:H:525:LEU:HD11	1.74	0.51
2:K:112:ARG:HD2	2:K:112:ARG:N	2.26	0.51
2:O:412:SER:HB2	2:O:460:THR:HG22	1.92	0.51
2:W:244:TRP:CG	2:W:245:LYS:N	2.79	0.51
2:K:71:PHE:HB3	2:K:77:THR:HG23	1.93	0.51
2:X:443:GLU:HA	2:X:458:THR:HG23	1.93	0.51
2:C:256:ALA:HA	2:C:397:THR:HG21	1.93	0.51
2:C:526:TYR:HE1	2:R:526:TYR:HE1	1.57	0.51
2:D:256:ALA:HB2	2:D:425:GLY:HA2	1.91	0.51
2:D:267:GLN:HG3	2:D:270:ILE:HB	1.92	0.51
2:N:244:TRP:CG	2:N:245:LYS:N	2.77	0.51
2:R:437:ASP:HB3	2:R:497:LEU:HD21	1.93	0.51
2:ZZ:94:ILE:HB	2:ZZ:179:VAL:HG12	1.91	0.51
2:ZZ:423:PHE:HE2	2:ZZ:459:GLY:HA2	1.76	0.51
2:L:423:PHE:HE2	2:L:459:GLY:HA2	1.74	0.51
2:O:275:GLU:HB3	2:O:358:LEU:HD21	1.92	0.51
2:S:302:VAL:HB	2:S:360:LYS:HB2	1.92	0.51
1:Y:7:GLU:HG2	1:Y:38:THR:HB	1.93	0.51
2:YY:196:PHE:O	2:YY:200:ILE:HG12	2.11	0.51
2:O:327:ARG:HH12	2:O:350:SER:HA	1.74	0.51
2:X:437:ASP:HB3	2:X:497:LEU:HD21	1.92	0.51
2:YY:350:SER:HB3	2:YY:354:ILE:HD13	1.93	0.51
2:ZZ:377:LEU:HG	2:ZZ:389:PHE:HE1	1.76	0.51
2:ZZ:477:TRP:NE1	2:ZZ:525:LEU:HD11	2.25	0.51
2:C:414:ASN:HB3	2:C:417:THR:HG22	1.93	0.51
2:G:244:TRP:CG	2:G:245:LYS:N	2.79	0.51
2:N:291:PRO:HB3	2:N:373:VAL:HG22	1.92	0.51
2:C:163:HIS:CD2	2:C:447:SER:HB3	2.47	0.50
2:G:275:GLU:HB2	2:G:390:LEU:HD22	1.92	0.50
2:H:192:ARG:HB2	2:H:192:ARG:NH1	2.26	0.50
2:CC:210:LEU:HB3	2:CC:212:MET:CE	2.41	0.50
2:K:203:ILE:HG21	2:K:216:LEU:HD21	1.93	0.50
2:ZZ:213:PRO:HB2	2:ZZ:475:MET:CE	2.39	0.50
2:D:291:PRO:HB3	2:D:373:VAL:HG22	1.94	0.50
2:K:245:LYS:HD3	2:K:479:ILE:HD13	1.93	0.50
2:GG:163:HIS:CE1	2:GG:447:SER:HB3	2.47	0.50
2:X:160:HIS:O	2:X:164:VAL:HG22	2.11	0.50
2:CC:276:PHE:HB3	2:CC:389:PHE:CD1	2.46	0.50
2:K:122:SER:HB3	2:K:181:ARG:HE	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:138:THR:HG22	2:K:139:ASN:H	1.76	0.50
2:L:244:TRP:CG	2:L:245:LYS:N	2.80	0.50
1:LL:49:LEU:HD13	1:LL:57:ILE:HD12	1.94	0.50
2:O:289:ILE:HB	2:O:344:VAL:HB	1.92	0.50
2:S:155:SER:HB3	2:S:158:SER:HB3	1.94	0.50
2:K:244:TRP:CG	2:K:245:LYS:N	2.79	0.50
2:K:289:ILE:HB	2:K:344:VAL:HB	1.94	0.50
2:O:132:ARG:HB2	2:O:132:ARG:CZ	2.41	0.50
2:O:200:ILE:HD13	2:O:216:LEU:HD22	1.94	0.50
2:D:210:LEU:HB2	2:D:212:MET:HG3	1.93	0.50
1:AA:25:VAL:HG12	1:AA:39:SER:HB2	1.94	0.50
2:CC:99:ILE:HB	2:CC:179:VAL:HG11	1.94	0.50
2:K:477:TRP:HE1	2:K:525:LEU:HD11	1.76	0.50
1:LL:64:GLN:OE1	2:O:190:PHE:HE2	1.94	0.50
2:N:275:GLU:HB2	2:N:390:LEU:HD22	1.93	0.50
2:D:437:ASP:HB3	2:D:497:LEU:HD21	1.92	0.49
2:H:121:GLN:HA	2:H:134:GLY:HA3	1.94	0.49
2:K:213:PRO:HB2	2:K:475:MET:SD	2.52	0.49
2:C:256:ALA:HB2	2:C:425:GLY:HA2	1.93	0.49
2:L:437:ASP:HB3	2:L:497:LEU:HD21	1.93	0.49
2:O:92:ILE:HD12	2:O:168:CYS:HB3	1.94	0.49
2:G:437:ASP:HB3	2:G:497:LEU:HD21	1.94	0.49
2:W:291:PRO:HB3	2:W:373:VAL:HG22	1.94	0.49
2:X:291:PRO:HB3	2:X:373:VAL:HG22	1.95	0.49
1:AA:19:LEU:HD11	1:AA:51:TYR:CD1	2.46	0.49
2:YY:279:GLY:HA3	2:YY:384:ASN:HD22	1.78	0.49
2:G:296:ASP:HB3	2:G:366:ILE:HB	1.94	0.49
2:CC:286:ASN:OD1	2:CC:347:GLN:NE2	2.44	0.49
1:FF:47:ILE:HD12	1:FF:48:LEU:N	2.27	0.49
2:GG:128:PRO:HB3	2:GG:136:LEU:HD22	1.92	0.49
2:G:159:LEU:HD22	2:G:450:PRO:HD2	1.94	0.49
2:H:384:ASN:HA	2:H:385:ARG:NH1	2.27	0.49
2:R:289:ILE:HB	2:R:344:VAL:HB	1.94	0.49
2:YY:196:PHE:HE2	2:YY:218:ILE:HD12	1.77	0.49
2:ZZ:291:PRO:HB3	2:ZZ:373:VAL:HG22	1.94	0.49
2:C:76:ILE:O	2:C:80:LYS:HG3	2.12	0.49
2:K:167:ILE:O	2:K:171:ILE:HD12	2.13	0.49
2:GG:262:LYS:HB2	2:GG:389:PHE:CD1	2.48	0.49
2:G:213:PRO:HB2	2:G:475:MET:CE	2.37	0.49
2:H:112:ARG:HH11	2:H:112:ARG:HG2	1.78	0.49
2:L:471:CYS:O	2:L:475:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:92:ILE:HG21	2:R:168:CYS:HB3	1.95	0.49
2:W:289:ILE:HB	2:W:344:VAL:HB	1.94	0.49
2:R:531:ILE:HD12	2:S:314:LEU:HB3	1.94	0.49
1:AA:64:GLN:OE1	1:AA:64:GLN:HA	2.12	0.49
2:C:71:PHE:HE2	2:C:170:THR:HG22	1.77	0.49
2:G:498:LYS:HA	2:H:294:VAL:HG23	1.94	0.49
1:V:64:GLN:HG3	2:W:381:GLU:OE2	2.12	0.49
2:YY:326:THR:HG23	2:YY:354:ILE:HD12	1.95	0.49
2:H:121:GLN:HG3	2:H:181:ARG:O	2.12	0.48
2:O:244:TRP:CG	2:O:245:LYS:N	2.81	0.48
2:R:434:PHE:O	2:R:435:LYS:HD3	2.13	0.48
2:ZZ:437:ASP:HB3	2:ZZ:497:LEU:HD21	1.94	0.48
2:K:231:SER:HG	2:K:234:GLU:HG3	1.78	0.48
2:L:140:GLU:OE2	2:L:140:GLU:HA	2.12	0.48
2:N:312:ILE:HD13	2:N:330:GLY:HA3	1.95	0.48
2:N:437:ASP:HB3	2:N:497:LEU:HD21	1.94	0.48
2:H:258:LYS:HG2	2:H:380:SER:OG	2.13	0.48
2:YY:443:GLU:HA	2:YY:458:THR:HG23	1.95	0.48
2:GG:116:LEU:HA	2:GG:139:ASN:HB2	1.95	0.48
2:K:89:GLY:O	2:K:212:MET:HB3	2.14	0.48
2:O:291:PRO:HB3	2:O:373:VAL:HG22	1.95	0.48
2:O:440:ALA:HB3	2:O:463:ALA:HB1	1.94	0.48
2:YY:163:HIS:CE1	2:YY:447:SER:HB3	2.49	0.48
1:Z:11:LYS:HG3	1:Z:34:TYR:CE1	2.48	0.48
2:H:449:LEU:HD11	2:H:455:GLY:HA3	1.95	0.48
2:L:267:GLN:HG3	2:L:270:ILE:HB	1.95	0.48
2:X:449:LEU:HD11	2:X:455:GLY:HA3	1.96	0.48
2:D:423:PHE:HE2	2:D:459:GLY:HA2	1.78	0.48
2:H:244:TRP:CG	2:H:245:LYS:N	2.82	0.48
2:YY:257:ASP:HA	2:YY:394:GLN:HE22	1.78	0.48
1:EE:7:GLU:HB3	1:EE:38:THR:HG22	1.96	0.48
2:S:163:HIS:NE2	2:S:447:SER:HB3	2.29	0.48
2:X:128:PRO:HG3	2:X:136:LEU:HB2	1.95	0.48
2:CC:477:TRP:NE1	2:CC:525:LEU:HD11	2.29	0.48
2:GG:291:PRO:HB3	2:GG:373:VAL:HG22	1.95	0.48
2:C:107:ARG:HD3	2:C:146:ILE:HD13	1.95	0.48
2:G:256:ALA:HA	2:G:397:THR:HG21	1.96	0.48
2:G:312:ILE:HD13	2:G:330:GLY:HA3	1.96	0.48
1:M:65:THR:O	2:N:381:GLU:HG3	2.14	0.48
2:N:132:ARG:CZ	2:N:132:ARG:HB2	2.44	0.48
2:X:199:ALA:O	2:X:203:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:GLY:O	2:H:212:MET:HB3	2.14	0.47
2:S:358:LEU:HD12	2:CC:277:ILE:HD12	1.96	0.47
1:Z:10:VAL:HA	1:Z:56:PHE:O	2.14	0.47
2:GG:244:TRP:CG	2:GG:245:LYS:N	2.81	0.47
2:GG:370:THR:HG22	2:GG:372:ASN:H	1.79	0.47
2:C:136:LEU:HD12	2:C:137:TYR:N	2.29	0.47
2:D:474:PHE:HZ	2:D:523:ILE:HG21	1.80	0.47
2:G:291:PRO:HB3	2:G:373:VAL:HG22	1.95	0.47
1:Q:30:LEU:HA	2:R:201:LYS:HE2	1.96	0.47
1:Z:26:SER:HB2	1:Z:38:THR:HG23	1.95	0.47
2:K:113:SER:HB3	2:K:146:ILE:HD11	1.95	0.47
2:R:138:THR:O	2:R:142:ILE:HD12	2.13	0.47
2:ZZ:244:TRP:CG	2:ZZ:245:LYS:N	2.81	0.47
2:D:213:PRO:HB2	2:D:475:MET:CE	2.40	0.47
2:K:391:ILE:HG13	2:K:391:ILE:O	2.15	0.47
2:O:112:ARG:HH11	2:O:112:ARG:HG2	1.78	0.47
2:S:116:LEU:HD23	2:S:176:ARG:HB3	1.96	0.47
2:S:320:ARG:HG2	2:S:329:THR:HG22	1.97	0.47
1:V:55:GLU:HB3	2:X:242:LEU:HB3	1.96	0.47
2:X:150:MET:HA	2:X:150:MET:HE2	1.96	0.47
2:X:244:TRP:CG	2:X:245:LYS:N	2.81	0.47
2:YY:467:VAL:HA	2:YY:470:VAL:HG12	1.96	0.47
2:GG:197:MET:HG2	2:GG:236:TYR:CD2	2.49	0.47
2:L:138:THR:O	2:L:142:ILE:HD12	2.14	0.47
2:W:99:ILE:HD12	2:W:179:VAL:HG21	1.96	0.47
2:YY:474:PHE:HZ	2:YY:523:ILE:HG21	1.79	0.47
2:ZZ:440:ALA:HB3	2:ZZ:463:ALA:HB1	1.96	0.47
2:C:262:LYS:HE3	2:C:264:ILE:HG22	1.95	0.47
2:X:89:GLY:O	2:X:212:MET:HB3	2.15	0.47
2:C:105:VAL:HG13	2:C:106:PHE:CD1	2.50	0.47
2:D:185:ILE:HD12	2:D:185:ILE:O	2.14	0.47
2:H:381:GLU:H	2:H:381:GLU:HG3	1.54	0.47
1:I:46:ASN:O	1:I:50:THR:HG23	2.14	0.47
2:L:462:MET:HE2	2:L:462:MET:HB2	1.65	0.47
2:O:163:HIS:CD2	2:O:447:SER:HB3	2.50	0.47
2:O:256:ALA:HA	2:O:397:THR:HG21	1.95	0.47
2:O:471:CYS:O	2:O:475:MET:HB2	2.14	0.47
2:R:193:SER:O	2:R:197:MET:HG3	2.14	0.47
2:X:409:THR:HG23	2:X:436:PRO:HA	1.96	0.47
2:CC:143:ASN:HA	2:CC:146:ILE:HD12	1.95	0.47
2:CC:276:PHE:HB3	2:CC:389:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:126:ASN:H	2:GG:135:THR:HG23	1.80	0.47
2:X:88:LYS:O	2:X:476:GLU:HG3	2.15	0.47
1:A:46:ASN:O	1:A:50:THR:HG23	2.15	0.47
1:F:64:GLN:NE2	2:G:381:GLU:HB2	2.30	0.47
2:G:88:LYS:O	2:G:476:GLU:HG3	2.15	0.47
2:R:279:GLY:HA3	2:R:384:ASN:HD22	1.80	0.47
1:EE:17:LEU:HD22	1:EE:17:LEU:H	1.79	0.47
2:D:163:HIS:CD2	2:D:447:SER:HB3	2.50	0.47
2:D:474:PHE:CZ	2:D:523:ILE:HG21	2.50	0.47
2:G:163:HIS:CD2	2:G:447:SER:HB3	2.50	0.47
2:K:76:ILE:O	2:K:80:LYS:HG3	2.14	0.47
2:R:88:LYS:O	2:R:476:GLU:HG3	2.14	0.47
2:YY:122:SER:HB2	2:YY:186:GLN:HG3	1.95	0.47
1:B:19:LEU:HD12	1:B:23:LEU:HD12	1.96	0.46
2:R:213:PRO:HB2	2:R:475:MET:SD	2.55	0.46
2:C:289:ILE:HB	2:C:344:VAL:HB	1.96	0.46
2:L:275:GLU:HB3	2:L:358:LEU:HD11	1.97	0.46
1:M:59:LYS:HE3	2:O:536:GLU:HG3	1.96	0.46
1:T:17:LEU:HD22	1:T:17:LEU:H	1.79	0.46
2:YY:89:GLY:O	2:YY:212:MET:HB3	2.16	0.46
2:YY:137:TYR:HE2	2:YY:152:ILE:HG23	1.81	0.46
2:YY:244:TRP:CG	2:YY:245:LYS:N	2.81	0.46
2:ZZ:256:ALA:HA	2:ZZ:397:THR:HG21	1.97	0.46
2:ZZ:472:SER:HA	2:ZZ:475:MET:HB2	1.97	0.46
2:S:244:TRP:CG	2:S:245:LYS:N	2.82	0.46
2:W:312:ILE:HD13	2:W:330:GLY:HA3	1.97	0.46
2:ZZ:287:ILE:HB	2:ZZ:346:LEU:HB2	1.96	0.46
2:CC:262:LYS:HB2	2:CC:389:PHE:CD2	2.49	0.46
2:S:211:ARG:HA	2:S:211:ARG:HD3	1.60	0.46
2:X:94:ILE:HD13	2:X:217:ASN:HB3	1.98	0.46
2:YY:234:GLU:HG2	2:YY:404:ALA:HB2	1.96	0.46
2:ZZ:278:VAL:HA	2:ZZ:387:THR:HG23	1.97	0.46
2:G:116:LEU:CD2	2:G:176:ARG:HB3	2.46	0.46
2:O:526:TYR:CE1	2:ZZ:526:TYR:HE1	2.32	0.46
1:V:16:ILE:HD12	1:V:19:LEU:HG	1.98	0.46
2:X:132:ARG:HG3	2:X:132:ARG:NH1	2.30	0.46
2:G:388:ARG:HH22	2:N:390:LEU:HD23	1.80	0.46
2:X:245:LYS:HE2	2:X:479:ILE:HD13	1.97	0.46
2:YY:211:ARG:HD3	2:YY:244:TRP:CH2	2.51	0.46
2:CC:116:LEU:HA	2:CC:139:ASN:HB2	1.96	0.46
2:GG:163:HIS:CD2	2:GG:457:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:76:ILE:O	2:G:80:LYS:HG3	2.15	0.46
2:G:385:ARG:NE	2:G:385:ARG:H	2.13	0.46
2:N:440:ALA:HB3	2:N:463:ALA:HB1	1.98	0.46
2:S:144:ASN:HB3	2:S:149:SER:HB2	1.96	0.46
2:GG:437:ASP:HB3	2:GG:497:LEU:HD21	1.97	0.46
2:C:268:ASN:O	2:C:270:ILE:HD12	2.16	0.46
2:D:229:GLY:HA2	2:D:234:GLU:OE1	2.16	0.46
2:R:160:HIS:O	2:R:164:VAL:HG22	2.15	0.46
1:F:64:GLN:HE21	2:G:381:GLU:HB2	1.81	0.45
2:H:185:ILE:HG13	2:H:188:ASP:OD2	2.16	0.45
2:L:76:ILE:O	2:L:80:LYS:HG3	2.16	0.45
2:O:229:GLY:HA2	2:O:234:GLU:OE1	2.16	0.45
1:T:41:ASN:OD1	1:T:41:ASN:C	2.59	0.45
2:CC:388:ARG:HG2	2:CC:389:PHE:O	2.17	0.45
1:E:37:ILE:HD12	1:E:48:LEU:HD21	1.99	0.45
2:G:222:SER:OG	2:G:224:GLU:HG3	2.17	0.45
2:G:423:PHE:CE2	2:G:459:GLY:HA2	2.51	0.45
2:ZZ:128:PRO:HA	2:ZZ:136:LEU:HD12	1.98	0.45
1:FF:16:ILE:HG23	1:FF:27:VAL:HG11	1.99	0.45
1:B:30:LEU:HA	2:C:201:LYS:HD2	1.98	0.45
2:K:116:LEU:HD11	2:K:176:ARG:HD3	1.98	0.45
2:L:423:PHE:CE2	2:L:459:GLY:HA2	2.51	0.45
2:N:289:ILE:HB	2:N:344:VAL:HB	1.98	0.45
2:N:498:LYS:HA	2:O:294:VAL:HG23	1.97	0.45
2:L:163:HIS:CE1	2:L:447:SER:HB3	2.51	0.45
1:P:53:GLU:OE1	1:P:53:GLU:N	2.49	0.45
2:S:115:ILE:HG13	2:S:177:ILE:HG22	1.98	0.45
2:ZZ:74:THR:OG1	2:ZZ:76:ILE:HG13	2.15	0.45
2:ZZ:377:LEU:HG	2:ZZ:389:PHE:CE1	2.52	0.45
2:CC:291:PRO:HB3	2:CC:373:VAL:HG22	1.99	0.45
2:D:120:ASP:HA	2:D:181:ARG:HB3	1.99	0.45
1:E:65:THR:HG21	2:H:160:HIS:CE1	2.51	0.45
2:S:440:ALA:HB3	2:S:463:ALA:HB1	1.97	0.45
1:FF:27:VAL:HG22	1:FF:37:ILE:HG13	1.98	0.45
2:GG:128:PRO:HB2	2:GG:131:PHE:HD2	1.81	0.45
2:G:291:PRO:HG3	2:G:297:PHE:HZ	1.81	0.45
1:A:65:THR:HG23	2:D:189:ILE:HD12	1.98	0.45
1:F:30:LEU:HD11	1:F:36:ILE:HG13	1.99	0.45
2:O:267:GLN:HG3	2:O:270:ILE:HB	1.98	0.45
2:G:477:TRP:HE1	2:G:525:LEU:HD11	1.81	0.45
2:H:116:LEU:HD13	2:H:176:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:304:PRO:HD3	2:K:359:TRP:CE2	2.52	0.45
2:O:423:PHE:HE2	2:O:459:GLY:HA2	1.80	0.45
2:S:76:ILE:O	2:S:80:LYS:HG3	2.16	0.45
2:C:312:ILE:HD13	2:C:330:GLY:HA3	1.97	0.45
2:D:289:ILE:HB	2:D:344:VAL:HB	1.99	0.45
2:H:71:PHE:HB3	2:H:77:THR:HG23	1.98	0.45
2:H:423:PHE:CE2	2:H:459:GLY:HA2	2.49	0.45
1:J:53:GLU:OE1	1:J:53:GLU:N	2.49	0.45
1:LL:41:ASN:C	1:LL:41:ASN:OD1	2.60	0.45
2:R:76:ILE:O	2:R:80:LYS:HG3	2.17	0.45
2:S:244:TRP:CG	2:S:245:LYS:H	2.34	0.45
2:W:276:PHE:HB3	2:W:389:PHE:CD1	2.52	0.45
2:YY:410:VAL:HG21	2:YY:464:THR:HA	1.99	0.45
1:AA:55:GLU:HB3	2:CC:242:LEU:HB3	1.99	0.45
2:CC:123:ILE:HD13	2:CC:153:PRO:HG2	1.99	0.45
2:D:379:THR:HG23	2:D:381:GLU:HG2	1.99	0.45
2:H:384:ASN:HA	2:H:385:ARG:HH11	1.82	0.45
2:GG:192:ARG:H	2:GG:192:ARG:HG2	1.58	0.45
2:G:116:LEU:HD21	2:G:176:ARG:HB3	1.97	0.44
2:K:80:LYS:HB3	2:K:80:LYS:HE2	1.76	0.44
2:L:325:GLU:OE2	2:L:325:GLU:N	2.50	0.44
2:C:440:ALA:HB3	2:C:463:ALA:HB1	1.99	0.44
1:F:64:GLN:OE1	2:G:190:PHE:HE2	1.99	0.44
2:K:231:SER:OG	2:K:234:GLU:HG3	2.17	0.44
2:N:163:HIS:CD2	2:N:447:SER:HB3	2.52	0.44
2:N:385:ARG:NE	2:N:385:ARG:H	2.15	0.44
2:N:519:ASN:C	2:N:519:ASN:OD1	2.60	0.44
2:O:443:GLU:HB3	2:O:458:THR:HG23	1.98	0.44
2:S:283:ARG:HB2	2:S:283:ARG:NH1	2.32	0.44
2:W:411:GLY:HA3	2:W:439:LEU:HD23	1.99	0.44
2:X:462:MET:HB2	2:X:462:MET:HE2	1.73	0.44
1:Z:7:GLU:N	1:Z:7:GLU:OE2	2.50	0.44
2:D:498:LYS:HZ2	2:D:498:LYS:HG2	1.68	0.44
1:I:41:ASN:OD1	1:I:41:ASN:C	2.60	0.44
2:L:527:THR:HA	2:L:530:ASN:HB2	1.99	0.44
2:N:256:ALA:HA	2:N:397:THR:HG21	1.98	0.44
2:W:159:LEU:HD22	2:W:449:LEU:HD12	2.00	0.44
2:X:464:THR:HG23	2:X:465:PRO:HD3	1.99	0.44
2:YY:167:ILE:O	2:YY:171:ILE:HD12	2.18	0.44
1:AA:30:LEU:HD21	1:AA:36:ILE:HG13	2.00	0.44
2:GG:208:LEU:O	2:GG:211:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:210:LEU:HB3	2:GG:212:MET:CE	2.47	0.44
2:O:296:ASP:HB3	2:O:366:ILE:HB	2.00	0.44
2:W:275:GLU:HG3	2:W:360:LYS:HG2	1.98	0.44
2:X:291:PRO:HG3	2:X:297:PHE:HZ	1.82	0.44
2:ZZ:120:ASP:HA	2:ZZ:181:ARG:HB3	1.98	0.44
2:ZZ:388:ARG:HG2	2:ZZ:389:PHE:O	2.17	0.44
2:CC:275:GLU:HB2	2:CC:390:LEU:HD22	1.99	0.44
2:C:385:ARG:H	2:C:385:ARG:NE	2.15	0.44
2:S:289:ILE:HB	2:S:344:VAL:HB	2.00	0.44
2:X:477:TRP:CZ3	2:X:528:LEU:HD23	2.52	0.44
2:YY:440:ALA:HB3	2:YY:463:ALA:HB1	1.99	0.44
2:C:195:GLU:H	2:C:195:GLU:HG2	1.58	0.44
2:C:477:TRP:NE1	2:C:525:LEU:HD13	2.33	0.44
2:L:412:SER:HB2	2:L:460:THR:HG22	2.00	0.44
1:LL:32:SER:HB2	1:M:32:SER:HB2	2.00	0.44
2:X:422:ILE:HD12	2:X:422:ILE:HA	1.85	0.44
2:CC:99:ILE:HD12	2:CC:162:THR:HA	2.00	0.44
2:CC:273:GLU:OE2	2:CC:360:LYS:HB3	2.17	0.44
1:EE:53:GLU:OE2	1:EE:53:GLU:N	2.49	0.44
2:G:443:GLU:HB3	2:G:458:THR:HG23	2.00	0.44
2:H:477:TRP:O	2:H:481:ASN:HB2	2.18	0.44
2:L:129:GLU:CD	2:L:129:GLU:H	2.26	0.44
2:N:470:VAL:HG13	2:N:520:LEU:HD21	2.00	0.44
2:YY:69:GLN:HA	2:YY:69:GLN:HE21	1.82	0.44
2:ZZ:76:ILE:O	2:ZZ:80:LYS:HG3	2.18	0.44
2:D:76:ILE:O	2:D:80:LYS:HG3	2.17	0.44
1:F:53:GLU:OE1	1:F:53:GLU:N	2.49	0.44
2:H:464:THR:HG23	2:H:465:PRO:HD3	1.99	0.44
2:O:370:THR:HG22	2:O:372:ASN:H	1.83	0.44
2:YY:69:GLN:HE21	2:YY:69:GLN:CA	2.31	0.44
2:ZZ:138:THR:O	2:ZZ:142:ILE:HG22	2.18	0.44
2:L:121:GLN:HA	2:L:134:GLY:HA3	1.99	0.44
2:R:120:ASP:OD1	2:R:181:ARG:HG2	2.18	0.44
2:S:94:ILE:HB	2:S:179:VAL:HG22	1.99	0.44
2:CC:526:TYR:CD1	2:CC:526:TYR:C	2.96	0.44
1:B:41:ASN:C	1:B:41:ASN:OD1	2.61	0.43
2:C:491:LYS:HG3	2:D:335:ILE:O	2.18	0.43
2:G:280:GLU:OE2	2:G:280:GLU:N	2.51	0.43
2:H:112:ARG:HG2	2:H:112:ARG:NH1	2.33	0.43
2:L:388:ARG:HG3	2:L:389:PHE:O	2.19	0.43
2:N:267:GLN:HG2	2:N:270:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:163:HIS:CD2	2:R:447:SER:HB3	2.53	0.43
2:YY:76:ILE:HG21	2:YY:171:ILE:HG12	2.01	0.43
2:ZZ:88:LYS:O	2:ZZ:476:GLU:HG3	2.18	0.43
2:CC:410:VAL:HG21	2:CC:464:THR:HA	2.00	0.43
1:B:27:VAL:HG22	1:B:37:ILE:HG12	2.00	0.43
2:D:88:LYS:O	2:D:476:GLU:HG3	2.18	0.43
1:I:15:ASP:O	1:I:15:ASP:OD2	2.36	0.43
2:K:385:ARG:CZ	2:K:385:ARG:H	2.31	0.43
2:O:69:GLN:HE21	2:O:416:ARG:HG2	1.83	0.43
2:R:327:ARG:NH1	2:R:327:ARG:HG3	2.33	0.43
2:W:80:LYS:HE2	2:W:80:LYS:HB3	1.71	0.43
1:AA:44:ASP:CG	1:AA:47:ILE:HD12	2.43	0.43
2:CC:116:LEU:CD2	2:CC:176:ARG:HB3	2.42	0.43
2:CC:236:TYR:O	2:CC:240:MET:HG2	2.18	0.43
2:CC:390:LEU:HD12	2:CC:390:LEU:HA	1.90	0.43
2:GG:312:ILE:HD13	2:GG:330:GLY:HA3	2.00	0.43
2:H:446:VAL:HG22	2:H:456:ALA:HB2	2.00	0.43
2:K:477:TRP:NE1	2:K:525:LEU:HD11	2.32	0.43
1:M:53:GLU:OE2	1:M:53:GLU:N	2.50	0.43
2:R:525:LEU:HD13	2:R:525:LEU:O	2.18	0.43
2:S:99:ILE:HD12	2:S:99:ILE:HA	1.72	0.43
2:ZZ:289:ILE:HB	2:ZZ:344:VAL:HB	2.00	0.43
2:CC:99:ILE:HG22	2:CC:118:TYR:CE2	2.52	0.43
2:D:443:GLU:HA	2:D:458:THR:HG23	1.98	0.43
2:D:448:PHE:N	2:D:448:PHE:CD1	2.85	0.43
2:N:275:GLU:OE1	2:N:275:GLU:N	2.51	0.43
1:T:22:GLU:HG2	1:T:51:TYR:HE1	1.82	0.43
2:W:167:ILE:O	2:W:171:ILE:HD12	2.18	0.43
1:Y:20:GLU:OE2	1:Y:26:SER:HA	2.18	0.43
1:EE:27:VAL:HG12	1:EE:37:ILE:HG12	2.00	0.43
2:G:163:HIS:O	2:G:167:ILE:HD12	2.19	0.43
2:G:449:LEU:HD12	2:G:453:THR:O	2.19	0.43
2:W:99:ILE:HB	2:W:179:VAL:HG11	2.01	0.43
2:YY:88:LYS:HE3	2:YY:88:LYS:HB2	1.78	0.43
2:CC:437:ASP:HB3	2:CC:497:LEU:HD21	2.00	0.43
1:E:41:ASN:C	1:E:41:ASN:OD1	2.62	0.43
1:I:30:LEU:HA	2:L:201:LYS:HE2	2.01	0.43
2:K:107:ARG:HG2	2:K:113:SER:HA	2.00	0.43
2:X:204:LEU:HD21	2:X:246:ASN:HD22	1.82	0.43
2:ZZ:275:GLU:HB3	2:ZZ:358:LEU:HD11	2.00	0.43
2:C:92:ILE:HD11	2:C:472:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:395:GLU:OE2	2:G:395:GLU:N	2.48	0.43
2:O:464:THR:N	2:O:465:PRO:HD2	2.34	0.43
2:W:422:ILE:HD12	2:W:422:ILE:HA	1.88	0.43
2:X:275:GLU:HB3	2:X:358:LEU:HD21	2.01	0.43
2:C:169:ALA:HB2	2:C:177:ILE:HD11	1.99	0.43
2:G:268:ASN:O	2:G:270:ILE:HD12	2.19	0.43
2:N:464:THR:N	2:N:465:PRO:HD2	2.34	0.43
1:P:27:VAL:HG22	1:P:37:ILE:HG12	2.01	0.43
2:ZZ:126:ASN:H	2:ZZ:135:THR:HG23	1.83	0.43
2:ZZ:185:ILE:HD12	2:ZZ:185:ILE:HA	1.82	0.43
2:CC:325:GLU:OE1	2:CC:325:GLU:N	2.46	0.43
1:FF:30:LEU:HD21	1:FF:36:ILE:HG13	2.01	0.43
2:C:128:PRO:HB3	2:C:136:LEU:HD22	1.99	0.43
2:H:76:ILE:O	2:H:80:LYS:HG3	2.18	0.43
2:K:206:ARG:HD3	2:K:206:ARG:HA	1.79	0.43
2:L:291:PRO:HB3	2:L:373:VAL:HG22	1.99	0.43
2:N:414:ASN:HB3	2:N:417:THR:HG22	2.00	0.43
2:O:159:LEU:HD22	2:O:450:PRO:HD2	2.00	0.43
2:S:119:TRP:HB3	2:S:180:VAL:HG13	2.00	0.43
1:FF:19:LEU:HD12	1:FF:23:LEU:HD21	2.01	0.43
2:C:477:TRP:CD1	2:C:525:LEU:HD13	2.54	0.43
2:H:196:PHE:O	2:H:200:ILE:HG13	2.18	0.43
1:Q:43:GLU:OE2	1:Q:43:GLU:HA	2.19	0.43
2:R:377:LEU:HD11	2:R:389:PHE:CE1	2.54	0.43
2:S:434:PHE:O	2:S:435:LYS:HD3	2.18	0.43
1:T:22:GLU:HG2	1:T:51:TYR:CE1	2.53	0.43
2:YY:282:GLU:O	2:YY:354:ILE:HG12	2.18	0.43
1:B:25:VAL:HG12	1:B:39:SER:HB2	2.01	0.42
2:D:526:TYR:HE1	2:N:526:TYR:CE2	2.37	0.42
1:E:51:TYR:N	1:E:51:TYR:CD1	2.87	0.42
2:H:256:ALA:HA	2:H:397:THR:HG21	2.01	0.42
2:K:167:ILE:HB	2:K:465:PRO:HB2	2.01	0.42
2:L:142:ILE:HD12	2:L:142:ILE:H	1.84	0.42
2:S:256:ALA:HA	2:S:397:THR:HG21	2.01	0.42
1:Z:15:ASP:O	1:Z:15:ASP:OD2	2.37	0.42
2:ZZ:302:VAL:HB	2:ZZ:360:LYS:HB2	2.00	0.42
1:AA:16:ILE:HG13	1:AA:27:VAL:HG11	2.00	0.42
1:B:53:GLU:OE2	1:B:53:GLU:N	2.52	0.42
1:F:30:LEU:HA	2:G:201:LYS:HD2	2.02	0.42
2:S:74:THR:OG1	2:S:76:ILE:HG13	2.18	0.42
1:Y:53:GLU:N	1:Y:53:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:N	1:A:21:GLU:OE2	2.52	0.42
2:G:92:ILE:HG21	2:G:168:CYS:HB3	2.01	0.42
2:L:206:ARG:O	2:L:210:LEU:HG	2.19	0.42
1:P:45:VAL:HG21	2:R:536:GLU:HG3	2.01	0.42
1:Q:22:GLU:OE1	1:Q:23:LEU:HD23	2.20	0.42
2:S:267:GLN:HG3	2:S:270:ILE:HB	2.01	0.42
2:X:348:LEU:HB2	2:X:354:ILE:HD13	2.02	0.42
1:Y:16:ILE:HG23	1:Y:27:VAL:HG11	2.01	0.42
2:GG:264:ILE:HD13	2:GG:272:GLU:HG2	2.01	0.42
2:C:123:ILE:HD13	2:C:153:PRO:HG2	2.01	0.42
2:D:273:GLU:OE1	2:D:360:LYS:HE3	2.20	0.42
2:G:143:ASN:HA	2:G:146:ILE:HD12	2.01	0.42
2:G:276:PHE:HB3	2:G:389:PHE:CD1	2.54	0.42
2:K:319:ILE:O	2:K:329:THR:HA	2.20	0.42
2:S:204:LEU:HD12	2:S:240:MET:HE3	2.01	0.42
2:S:409:THR:HG23	2:S:436:PRO:HA	2.02	0.42
2:X:128:PRO:HB2	2:X:131:PHE:HD2	1.85	0.42
2:X:210:LEU:HB2	2:X:212:MET:SD	2.59	0.42
2:ZZ:167:ILE:O	2:ZZ:171:ILE:HD12	2.19	0.42
2:CC:275:GLU:OE1	2:CC:275:GLU:N	2.52	0.42
2:GG:202:PHE:O	2:GG:206:ARG:HB2	2.20	0.42
2:GG:256:ALA:HB2	2:GG:425:GLY:HA2	1.99	0.42
2:L:268:ASN:O	2:L:270:ILE:HD12	2.19	0.42
2:N:448:PHE:N	2:N:448:PHE:CD2	2.86	0.42
2:O:188:ASP:OD2	2:O:190:PHE:HD1	2.01	0.42
2:W:99:ILE:HG22	2:W:118:TYR:CE2	2.54	0.42
2:YY:137:TYR:CE2	2:YY:152:ILE:HD12	2.54	0.42
2:D:71:PHE:N	2:D:71:PHE:CD1	2.88	0.42
2:D:395:GLU:OE2	2:D:395:GLU:N	2.52	0.42
2:H:133:GLU:OE2	2:H:184:ASN:HB3	2.20	0.42
2:H:398:VAL:HG23	2:H:426:GLU:O	2.20	0.42
2:K:477:TRP:O	2:K:481:ASN:HB2	2.19	0.42
2:L:88:LYS:O	2:L:476:GLU:HG3	2.20	0.42
2:L:477:TRP:O	2:L:481:ASN:HB2	2.20	0.42
2:N:116:LEU:CD2	2:N:176:ARG:HB3	2.49	0.42
2:N:501:ARG:HB2	2:N:519:ASN:ND2	2.35	0.42
2:O:91:ILE:HD11	2:O:212:MET:HE2	2.02	0.42
1:Y:22:GLU:OE2	1:Y:23:LEU:HD23	2.20	0.42
2:YY:256:ALA:HA	2:YY:397:THR:HG21	2.00	0.42
2:ZZ:327:ARG:HB3	2:ZZ:327:ARG:NH1	2.35	0.42
2:S:260:GLY:HA2	2:S:377:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YY:131:PHE:HZ	2:YY:201:LYS:HG2	1.84	0.42
2:C:99:ILE:HD12	2:C:99:ILE:HA	1.84	0.42
2:D:128:PRO:HB3	2:D:136:LEU:HD22	2.02	0.42
2:G:167:ILE:O	2:G:171:ILE:HD12	2.19	0.42
2:O:390:LEU:HA	2:O:390:LEU:HD12	1.75	0.42
2:X:258:LYS:HG2	2:X:380:SER:CB	2.50	0.42
1:Y:10:VAL:HA	1:Y:56:PHE:O	2.20	0.42
2:ZZ:422:ILE:HD12	2:ZZ:422:ILE:HA	1.85	0.42
2:CC:118:TYR:HD1	2:CC:137:TYR:HD2	1.68	0.42
1:FF:20:GLU:OE2	1:FF:20:GLU:HA	2.20	0.42
2:GG:167:ILE:HB	2:GG:465:PRO:HB2	2.01	0.42
2:G:257:ASP:OD1	2:G:258:LYS:HD2	2.19	0.42
2:X:76:ILE:O	2:X:80:LYS:HG3	2.20	0.42
2:YY:449:LEU:HB2	2:YY:453:THR:HG23	2.01	0.42
2:ZZ:92:ILE:HG21	2:ZZ:168:CYS:HB3	2.02	0.42
2:ZZ:118:TYR:HD1	2:ZZ:179:VAL:HG23	1.83	0.42
1:EE:32:SER:HB2	1:FF:32:SER:HB2	2.02	0.42
2:C:319:ILE:O	2:C:329:THR:HA	2.20	0.42
2:G:80:LYS:HB3	2:G:80:LYS:HE2	1.74	0.42
2:YY:312:ILE:HD13	2:YY:330:GLY:HA3	2.02	0.42
1:E:46:ASN:O	1:E:50:THR:HG23	2.20	0.41
1:F:49:LEU:HD13	1:F:57:ILE:HD12	2.02	0.41
2:H:285:LEU:HD12	2:H:285:LEU:HA	1.86	0.41
2:H:414:ASN:HB2	2:H:443:GLU:OE2	2.20	0.41
2:L:116:LEU:HA	2:L:139:ASN:HB2	2.01	0.41
2:N:467:VAL:HG22	2:N:518:LEU:HD22	2.01	0.41
2:O:422:ILE:HD12	2:O:422:ILE:HA	1.90	0.41
1:T:30:LEU:HA	2:X:201:LYS:HE3	2.02	0.41
2:X:262:LYS:HE2	2:X:391:ILE:HG23	2.02	0.41
1:BB:47:ILE:HD12	1:BB:48:LEU:N	2.35	0.41
1:BB:63:LEU:HB3	2:CC:220:TYR:HB3	2.01	0.41
1:E:16:ILE:HD12	1:E:19:LEU:HD23	2.01	0.41
2:O:138:THR:O	2:O:142:ILE:HD12	2.20	0.41
1:Q:53:GLU:OE1	1:Q:53:GLU:N	2.53	0.41
2:R:80:LYS:HB3	2:R:80:LYS:HE2	1.81	0.41
2:S:200:ILE:HD13	2:S:200:ILE:HA	1.87	0.41
2:ZZ:229:GLY:HA2	2:ZZ:234:GLU:OE1	2.19	0.41
2:CC:116:LEU:H	2:CC:116:LEU:HD22	1.83	0.41
1:EE:30:LEU:H	1:EE:30:LEU:HD22	1.85	0.41
1:FF:10:VAL:HA	1:FF:56:PHE:O	2.20	0.41
2:D:159:LEU:HD22	2:D:450:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:GLU:OE1	1:I:53:GLU:N	2.50	0.41
2:X:464:THR:N	2:X:465:PRO:HD2	2.35	0.41
2:C:71:PHE:HB3	2:C:77:THR:HG23	2.01	0.41
2:C:164:VAL:HA	2:C:167:ILE:HD12	2.02	0.41
2:C:493:ARG:O	2:C:497:LEU:HG	2.21	0.41
1:F:54:ILE:HD13	1:F:54:ILE:HA	1.90	0.41
2:H:214:VAL:C	2:H:475:MET:HE1	2.45	0.41
2:H:525:LEU:O	2:H:525:LEU:HD13	2.21	0.41
2:K:116:LEU:CD1	2:K:176:ARG:HB3	2.51	0.41
2:L:440:ALA:HB3	2:L:463:ALA:HB1	2.02	0.41
2:O:112:ARG:HG2	2:O:112:ARG:NH1	2.35	0.41
1:Q:19:LEU:HD11	1:Q:51:TYR:CD2	2.55	0.41
2:S:122:SER:HB3	2:S:181:ARG:NE	2.35	0.41
2:YY:474:PHE:CZ	2:YY:523:ILE:HG21	2.55	0.41
2:CC:449:LEU:HD11	2:CC:455:GLY:N	2.35	0.41
2:C:99:ILE:HG22	2:C:118:TYR:CZ	2.56	0.41
2:D:273:GLU:CD	2:D:360:LYS:HE3	2.44	0.41
1:F:44:ASP:OD2	1:F:44:ASP:C	2.64	0.41
2:G:214:VAL:O	2:G:246:ASN:HA	2.21	0.41
2:G:304:PRO:HD3	2:G:359:TRP:CE2	2.55	0.41
2:R:312:ILE:HD13	2:R:330:GLY:HA3	2.01	0.41
2:S:423:PHE:HE2	2:S:459:GLY:HA2	1.85	0.41
1:T:42:GLU:HA	1:T:42:GLU:OE2	2.20	0.41
1:V:53:GLU:OE2	1:V:53:GLU:N	2.51	0.41
2:X:410:VAL:HG11	2:X:467:VAL:HG21	2.02	0.41
2:YY:422:ILE:HD12	2:YY:422:ILE:HA	1.85	0.41
2:CC:312:ILE:HD13	2:CC:330:GLY:HA3	2.03	0.41
2:G:524:ASP:C	2:G:524:ASP:OD1	2.64	0.41
2:K:285:LEU:HD12	2:K:285:LEU:HA	1.93	0.41
1:LL:53:GLU:OE1	1:LL:53:GLU:N	2.53	0.41
2:N:143:ASN:HA	2:N:146:ILE:HD12	2.02	0.41
2:N:448:PHE:N	2:N:448:PHE:HD2	2.18	0.41
2:O:526:TYR:HE1	2:ZZ:526:TYR:CE1	2.35	0.41
2:R:355:THR:HA	2:R:356:PRO:HD3	1.93	0.41
2:X:462:MET:C	2:X:465:PRO:HD2	2.46	0.41
2:YY:185:ILE:O	2:YY:185:ILE:HD12	2.20	0.41
2:YY:475:MET:HE2	2:YY:475:MET:HB3	1.74	0.41
2:ZZ:163:HIS:CD2	2:ZZ:447:SER:HB3	2.56	0.41
1:BB:48:LEU:HD11	1:BB:54:ILE:HG13	2.02	0.41
2:CC:206:ARG:HA	2:CC:206:ARG:HD3	1.70	0.41
2:CC:535:LEU:HD23	2:CC:535:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:88:LYS:O	2:GG:476:GLU:HG3	2.21	0.41
2:GG:89:GLY:O	2:GG:212:MET:HB3	2.21	0.41
2:GG:471:CYS:O	2:GG:475:MET:HG3	2.21	0.41
1:A:32:SER:HB2	1:B:32:SER:HB2	2.03	0.41
2:H:138:THR:O	2:H:142:ILE:HD12	2.20	0.41
1:I:51:TYR:N	1:I:51:TYR:CD1	2.89	0.41
2:K:182:VAL:HG23	2:K:195:GLU:HB3	2.02	0.41
2:N:101:TYR:OH	2:N:152:ILE:HB	2.21	0.41
2:N:355:THR:HA	2:N:356:PRO:HD3	1.94	0.41
1:P:48:LEU:CD2	1:P:54:ILE:HG13	2.51	0.41
2:R:388:ARG:HG2	2:R:389:PHE:O	2.21	0.41
2:CC:385:ARG:H	2:CC:385:ARG:HG3	1.65	0.41
2:C:167:ILE:O	2:C:171:ILE:HG13	2.19	0.41
2:G:303:ASN:HB3	2:G:323:LEU:HD23	2.03	0.41
2:L:398:VAL:HG23	2:L:426:GLU:O	2.21	0.41
1:M:25:VAL:HG12	1:M:39:SER:HB2	2.03	0.41
2:N:477:TRP:HE1	2:N:525:LEU:HD11	1.85	0.41
2:S:464:THR:N	2:S:465:PRO:HD2	2.36	0.41
2:ZZ:296:ASP:HB3	2:ZZ:366:ILE:HB	2.02	0.41
1:AA:46:ASN:O	1:AA:50:THR:HG23	2.20	0.41
2:CC:99:ILE:HD12	2:CC:99:ILE:HA	1.94	0.41
1:A:53:GLU:OE2	1:A:53:GLU:N	2.53	0.41
2:C:437:ASP:HB3	2:C:497:LEU:HD21	2.03	0.41
2:C:531:ILE:HD13	2:C:531:ILE:HA	1.87	0.41
2:D:159:LEU:CD2	2:D:449:LEU:HD12	2.51	0.41
1:F:46:ASN:HD22	2:H:486:PHE:HE2	1.67	0.41
2:H:477:TRP:CZ3	2:H:528:LEU:HD23	2.56	0.41
2:O:210:LEU:HB2	2:O:212:MET:SD	2.61	0.41
2:O:470:VAL:HG11	2:O:520:LEU:HD11	2.03	0.41
1:Q:10:VAL:HA	1:Q:56:PHE:O	2.21	0.41
2:R:327:ARG:HG3	2:R:327:ARG:HH11	1.84	0.41
1:T:53:GLU:OE2	1:T:53:GLU:N	2.51	0.41
2:W:71:PHE:N	2:W:71:PHE:CD1	2.89	0.41
2:W:262:LYS:HB2	2:W:389:PHE:HD2	1.85	0.41
2:W:477:TRP:CD1	2:W:525:LEU:HD21	2.56	0.41
2:X:326:THR:HG21	2:X:354:ILE:HG23	2.03	0.41
1:Y:30:LEU:HD11	1:Y:36:ILE:HG13	2.03	0.41
2:ZZ:285:LEU:HA	2:ZZ:285:LEU:HD12	1.84	0.41
2:ZZ:385:ARG:CZ	2:ZZ:385:ARG:H	2.34	0.41
1:BB:64:GLN:OE1	2:CC:190:PHE:HE2	2.04	0.41
2:CC:193:SER:O	2:CC:197:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:304:PRO:HD3	2:GG:359:TRP:CE2	2.55	0.41
2:GG:477:TRP:NE1	2:GG:525:LEU:HD13	2.35	0.41
1:B:65:THR:O	2:C:381:GLU:HG3	2.21	0.41
2:K:526:TYR:CD2	2:K:526:TYR:C	2.98	0.41
2:N:80:LYS:HB3	2:N:80:LYS:HE2	1.83	0.41
2:S:277:ILE:HD13	2:S:388:ARG:NH1	2.35	0.41
2:S:437:ASP:HB3	2:S:497:LEU:HD21	2.03	0.41
2:X:85:LEU:HD12	2:X:476:GLU:HB3	2.03	0.41
2:ZZ:166:GLY:O	2:ZZ:170:THR:HG23	2.22	0.41
1:AA:19:LEU:HD13	1:AA:19:LEU:HA	1.86	0.41
2:CC:112:ARG:HB3	2:CC:143:ASN:HD21	1.86	0.41
2:CC:499:GLY:HA3	2:CC:523:ILE:HD11	2.03	0.41
2:D:493:ARG:O	2:D:497:LEU:HG	2.21	0.40
1:E:53:GLU:N	1:E:53:GLU:OE2	2.53	0.40
2:G:398:VAL:HG23	2:G:426:GLU:O	2.21	0.40
2:H:91:ILE:HD11	2:H:212:MET:HE3	2.03	0.40
2:K:111:GLY:C	2:K:112:ARG:HD2	2.46	0.40
2:W:76:ILE:O	2:W:80:LYS:HG3	2.21	0.40
2:W:116:LEU:HD13	2:W:176:ARG:HB3	2.04	0.40
2:W:304:PRO:HD3	2:W:359:TRP:CE2	2.56	0.40
2:W:365:PRO:O	2:W:366:ILE:HD13	2.21	0.40
2:X:477:TRP:NE1	2:X:525:LEU:HD13	2.36	0.40
2:C:365:PRO:HB3	2:C:368:ILE:HG13	2.04	0.40
2:D:320:ARG:HG2	2:D:329:THR:HG22	2.02	0.40
1:M:7:GLU:HG2	1:M:38:THR:HG23	2.03	0.40
2:N:257:ASP:OD2	2:N:422:ILE:HG23	2.22	0.40
2:O:222:SER:OG	2:O:224:GLU:HG3	2.20	0.40
1:P:10:VAL:HA	1:P:56:PHE:O	2.21	0.40
2:X:285:LEU:HD12	2:X:285:LEU:HA	1.95	0.40
1:Y:15:ASP:OD2	1:Y:15:ASP:C	2.64	0.40
2:ZZ:475:MET:HE2	2:ZZ:475:MET:HB3	1.91	0.40
2:G:388:ARG:HG2	2:G:389:PHE:O	2.21	0.40
2:R:418:ASP:OD2	2:R:418:ASP:C	2.65	0.40
2:X:92:ILE:HG21	2:X:168:CYS:HB3	2.03	0.40
2:YY:255:ASN:HD21	2:YY:379:THR:HG22	1.86	0.40
1:BB:48:LEU:O	1:BB:48:LEU:HD12	2.21	0.40
2:CC:269:ASN:C	2:CC:270:ILE:HD12	2.45	0.40
2:GG:185:ILE:HD13	2:GG:185:ILE:HA	1.92	0.40
2:D:477:TRP:CD1	2:D:525:LEU:HD13	2.57	0.40
2:G:197:MET:HE3	2:G:236:TYR:CG	2.57	0.40
1:J:51:TYR:CD1	1:J:51:TYR:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:422:ILE:HD12	2:N:422:ILE:HA	1.91	0.40
2:O:464:THR:H	2:O:464:THR:HG23	1.65	0.40
2:R:159:LEU:HD21	2:R:449:LEU:HD23	2.03	0.40
2:W:120:ASP:OD1	2:W:181:ARG:HD3	2.21	0.40
2:ZZ:377:LEU:HD23	2:ZZ:377:LEU:HA	1.97	0.40
1:BB:10:VAL:HA	1:BB:56:PHE:O	2.21	0.40
2:G:110:ASP:OD1	2:G:110:ASP:C	2.64	0.40
2:K:110:ASP:C	2:K:110:ASP:OD2	2.65	0.40
2:K:389:PHE:O	2:K:392:PRO:HD3	2.21	0.40
2:W:397:THR:HG22	2:W:426:GLU:H	1.87	0.40
2:X:423:PHE:HE2	2:X:459:GLY:HA2	1.86	0.40
2:YY:291:PRO:HB3	2:YY:373:VAL:HG22	2.03	0.40
2:ZZ:291:PRO:HG3	2:ZZ:297:PHE:HZ	1.87	0.40
1:EE:30:LEU:HD21	1:EE:36:ILE:HG13	2.04	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	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	AA	59/68 (87%)	59 (100%)	0	0	100	100
1	B	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	BB	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	E	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	EE	57/68 (84%)	57 (100%)	0	0	100	100
1	F	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	FF	59/68 (87%)	57 (97%)	2 (3%)	0	100	100
1	I	59/68 (87%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	LL	59/68 (87%)	59 (100%)	0	0	100	100
1	M	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	P	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	Q	59/68 (87%)	59 (100%)	0	0	100	100
1	T	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	V	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	Y	59/68 (87%)	59 (100%)	0	0	100	100
1	Z	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
2	C	468/492 (95%)	460 (98%)	8 (2%)	0	100	100
2	CC	468/492 (95%)	463 (99%)	5 (1%)	0	100	100
2	D	468/492 (95%)	454 (97%)	14 (3%)	0	100	100
2	G	468/492 (95%)	455 (97%)	13 (3%)	0	100	100
2	GG	468/492 (95%)	456 (97%)	12 (3%)	0	100	100
2	H	468/492 (95%)	457 (98%)	11 (2%)	0	100	100
2	K	468/492 (95%)	458 (98%)	10 (2%)	0	100	100
2	L	468/492 (95%)	453 (97%)	15 (3%)	0	100	100
2	N	468/492 (95%)	457 (98%)	11 (2%)	0	100	100
2	O	465/492 (94%)	453 (97%)	12 (3%)	0	100	100
2	R	468/492 (95%)	458 (98%)	10 (2%)	0	100	100
2	S	468/492 (95%)	459 (98%)	9 (2%)	0	100	100
2	W	468/492 (95%)	456 (97%)	12 (3%)	0	100	100
2	X	468/492 (95%)	460 (98%)	8 (2%)	0	100	100
2	YY	468/492 (95%)	458 (98%)	10 (2%)	0	100	100
2	ZZ	468/492 (95%)	458 (98%)	10 (2%)	0	100	100
All	All	8545/9096 (94%)	8361 (98%)	184 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/65 (89%)	55 (95%)	3 (5%)	21	39
1	AA	58/65 (89%)	54 (93%)	4 (7%)	14	26
1	B	58/65 (89%)	57 (98%)	1 (2%)	53	71
1	BB	58/65 (89%)	57 (98%)	1 (2%)	53	71
1	E	58/65 (89%)	56 (97%)	2 (3%)	32	57
1	EE	56/65 (86%)	54 (96%)	2 (4%)	31	55
1	F	58/65 (89%)	55 (95%)	3 (5%)	21	39
1	FF	58/65 (89%)	55 (95%)	3 (5%)	21	39
1	I	58/65 (89%)	57 (98%)	1 (2%)	53	71
1	J	58/65 (89%)	56 (97%)	2 (3%)	32	57
1	LL	58/65 (89%)	56 (97%)	2 (3%)	32	57
1	M	58/65 (89%)	56 (97%)	2 (3%)	32	57
1	P	58/65 (89%)	53 (91%)	5 (9%)	10	18
1	Q	58/65 (89%)	56 (97%)	2 (3%)	32	57
1	T	58/65 (89%)	55 (95%)	3 (5%)	21	39
1	V	58/65 (89%)	57 (98%)	1 (2%)	53	71
1	Y	58/65 (89%)	55 (95%)	3 (5%)	21	39
1	Z	58/65 (89%)	54 (93%)	4 (7%)	14	26
2	C	407/428 (95%)	398 (98%)	9 (2%)	45	67
2	CC	407/428 (95%)	394 (97%)	13 (3%)	34	58
2	D	407/428 (95%)	398 (98%)	9 (2%)	45	67
2	G	407/428 (95%)	403 (99%)	4 (1%)	68	81
2	GG	407/428 (95%)	400 (98%)	7 (2%)	53	71
2	H	407/428 (95%)	392 (96%)	15 (4%)	30	54
2	K	407/428 (95%)	398 (98%)	9 (2%)	45	67
2	L	407/428 (95%)	400 (98%)	7 (2%)	53	71
2	N	407/428 (95%)	395 (97%)	12 (3%)	37	61
2	O	406/428 (95%)	397 (98%)	9 (2%)	45	67
2	R	407/428 (95%)	397 (98%)	10 (2%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	407/428 (95%)	402 (99%)	5 (1%)	63	78
2	W	407/428 (95%)	398 (98%)	9 (2%)	45	67
2	X	407/428 (95%)	403 (99%)	4 (1%)	68	81
2	YY	407/428 (95%)	397 (98%)	10 (2%)	42	64
2	ZZ	407/428 (95%)	401 (98%)	6 (2%)	57	74
All	All	7553/8018 (94%)	7371 (98%)	182 (2%)	43	65

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	33	SER
1	A	42	GLU
1	B	32	SER
2	C	142	ILE
2	C	195	GLU
2	C	263	ARG
2	C	267	GLN
2	C	390	LEU
2	C	397	THR
2	C	403	THR
2	C	418	ASP
2	C	444	ASP
2	D	73	SER
2	D	85	LEU
2	D	174	ASP
2	D	272	GLU
2	D	299	VAL
2	D	379	THR
2	D	417	THR
2	D	445	ILE
2	D	462	MET
1	E	32	SER
1	E	33	SER
1	F	32	SER
1	F	33	SER
1	F	47	ILE
2	G	174	ASP
2	G	195	GLU
2	G	381	GLU

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Mol	Chain	Res	Type
2	G	418	ASP
2	H	73	SER
2	H	103	LEU
2	H	159	LEU
2	H	239	ASP
2	H	267	GLN
2	H	282	GLU
2	H	284	ILE
2	H	379	THR
2	H	386	ASN
2	H	397	THR
2	H	403	THR
2	H	419	ILE
2	H	464	THR
2	H	525	LEU
2	H	528	LEU
1	I	32	SER
1	J	32	SER
1	J	33	SER
2	K	181	ARG
2	K	364	GLU
2	K	370	THR
2	K	415	SER
2	K	418	ASP
2	K	419	ILE
2	K	420	VAL
2	K	464	THR
2	K	533	GLN
2	L	73	SER
2	L	103	LEU
2	L	121	GLN
2	L	326	THR
2	L	403	THR
2	L	506	GLN
2	L	534	ASP
1	LL	17	LEU
1	LL	33	SER
1	M	32	SER
1	M	48	LEU
2	N	85	LEU
2	N	142	ILE
2	N	157	THR

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Mol	Chain	Res	Type
2	N	159	LEU
2	N	182	VAL
2	N	186	GLN
2	N	239	ASP
2	N	247	ASN
2	N	418	ASP
2	N	419	ILE
2	N	453	THR
2	N	533	GLN
2	O	150	MET
2	O	195	GLU
2	O	247	ASN
2	O	263	ARG
2	O	284	ILE
2	O	364	GLU
2	O	379	THR
2	O	403	THR
2	O	534	ASP
1	P	11	LYS
1	P	20	GLU
1	P	32	SER
1	P	33	SER
1	P	45	VAL
1	Q	32	SER
1	Q	33	SER
2	R	102	THR
2	R	105	VAL
2	R	133	GLU
2	R	174	ASP
2	R	379	THR
2	R	380	SER
2	R	390	LEU
2	R	416	ARG
2	R	419	ILE
2	R	453	THR
2	S	72	SER
2	S	99	ILE
2	S	247	ASN
2	S	403	THR
2	S	420	VAL
1	T	30	LEU
1	T	32	SER

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Mol	Chain	Res	Type
1	T	33	SER
1	V	32	SER
2	W	181	ARG
2	W	182	VAL
2	W	267	GLN
2	W	377	LEU
2	W	403	THR
2	W	418	ASP
2	W	430	GLN
2	W	531	ILE
2	W	533	GLN
2	X	77	THR
2	X	203	ILE
2	X	212	MET
2	X	472	SER
1	Y	33	SER
1	Y	38	THR
1	Y	47	ILE
1	Z	32	SER
1	Z	33	SER
1	Z	38	THR
1	Z	64	GLN
2	YY	69	GLN
2	YY	195	GLU
2	YY	211	ARG
2	YY	347	GLN
2	YY	353	GLN
2	YY	364	GLU
2	YY	370	THR
2	YY	380	SER
2	YY	403	THR
2	YY	521	SER
2	ZZ	136	LEU
2	ZZ	142	ILE
2	ZZ	267	GLN
2	ZZ	443	GLU
2	ZZ	461	SER
2	ZZ	528	LEU
1	AA	19	LEU
1	AA	32	SER
1	AA	33	SER
1	AA	63	LEU

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Mol	Chain	Res	Type
1	BB	23	LEU
2	CC	85	LEU
2	CC	133	GLU
2	CC	157	THR
2	CC	181	ARG
2	CC	182	VAL
2	CC	189	ILE
2	CC	195	GLU
2	CC	267	GLN
2	CC	347	GLN
2	CC	403	THR
2	CC	419	ILE
2	CC	453	THR
2	CC	528	LEU
1	EE	32	SER
1	EE	33	SER
1	FF	6	TYR
1	FF	32	SER
1	FF	54	ILE
2	GG	142	ILE
2	GG	186	GLN
2	GG	397	THR
2	GG	403	THR
2	GG	418	ASP
2	GG	424	SER
2	GG	454	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
2	C	184	ASN
2	C	286	ASN
2	C	353	GLN
2	D	353	GLN
2	D	386	ASN
2	D	394	GLN
2	D	414	ASN
1	F	41	ASN
1	F	64	GLN
2	G	139	ASN
2	G	163	HIS

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Mol	Chain	Res	Type
2	G	286	ASN
2	H	306	ASN
2	H	310	GLN
2	H	351	ASN
2	H	430	GLN
1	I	46	ASN
1	J	64	GLN
2	K	184	ASN
2	K	286	ASN
2	K	530	ASN
2	L	217	ASN
2	L	286	ASN
2	L	347	GLN
2	L	506	GLN
2	L	519	ASN
1	LL	64	GLN
1	M	64	GLN
2	N	217	ASN
2	N	506	GLN
2	O	163	HIS
2	R	163	HIS
2	R	286	ASN
2	R	519	ASN
2	S	268	ASN
2	S	505	ASN
2	S	533	GLN
1	V	5	ASN
2	W	163	HIS
2	W	288	ASN
2	W	394	GLN
2	W	430	GLN
2	W	505	ASN
2	X	246	ASN
2	X	286	ASN
2	X	347	GLN
2	X	374	ASN
2	X	430	GLN
1	Z	64	GLN
2	YY	69	GLN
2	YY	246	ASN
2	YY	300	HIS
2	YY	394	GLN

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Mol	Chain	Res	Type
2	YY	505	ASN
2	YY	506	GLN
2	ZZ	163	HIS
2	ZZ	186	GLN
2	ZZ	288	ASN
2	ZZ	351	ASN
2	CC	163	HIS
2	CC	269	ASN
2	CC	533	GLN
2	GG	163	HIS
2	GG	269	ASN
2	GG	286	ASN
2	GG	372	ASN
2	GG	530	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

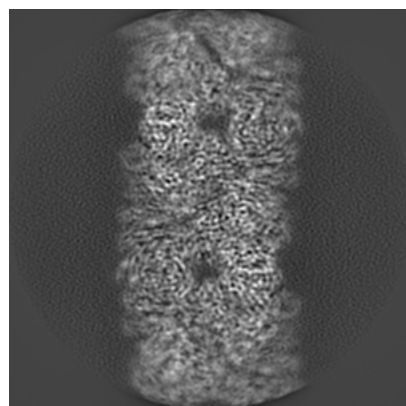
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54942. These allow visual inspection of the internal detail of the map and identification of artifacts.

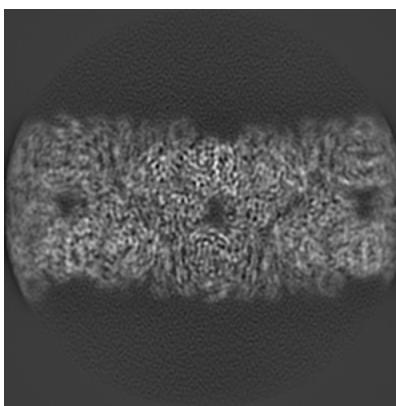
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

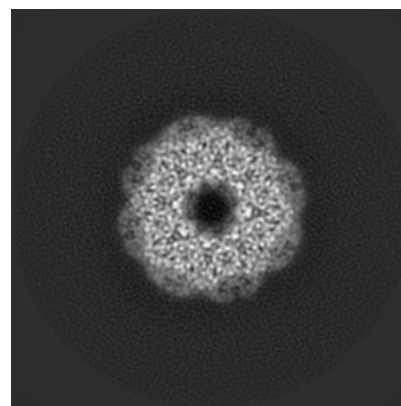
6.1.1 Primary map



X

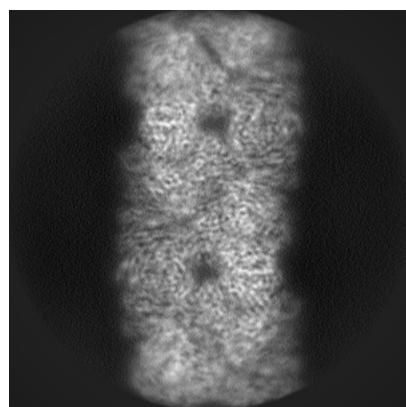


Y

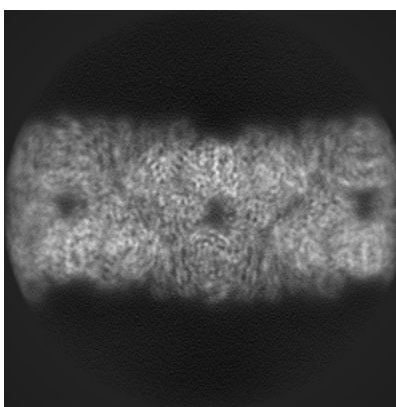


Z

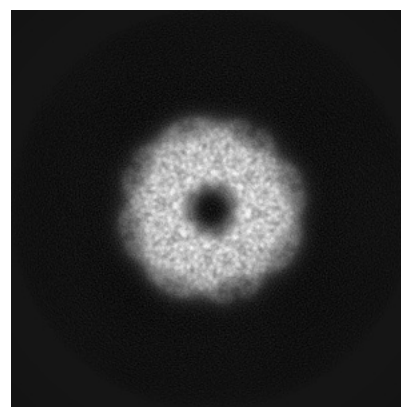
6.1.2 Raw map



X



Y

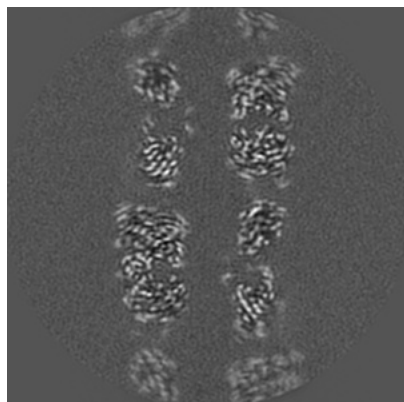


Z

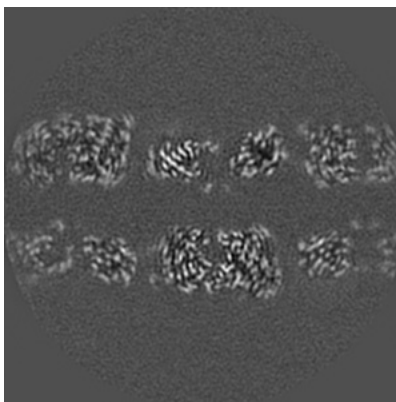
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

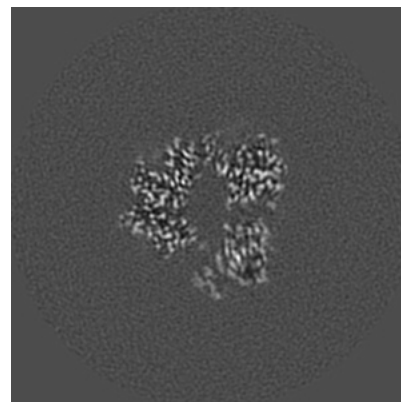
6.2.1 Primary map



X Index: 159

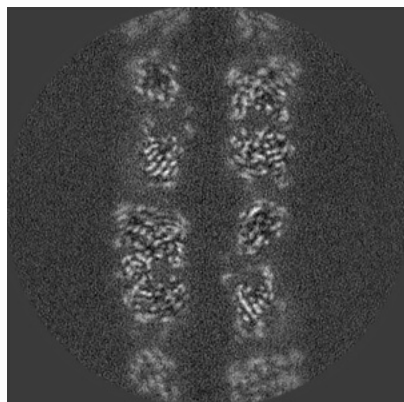


Y Index: 159

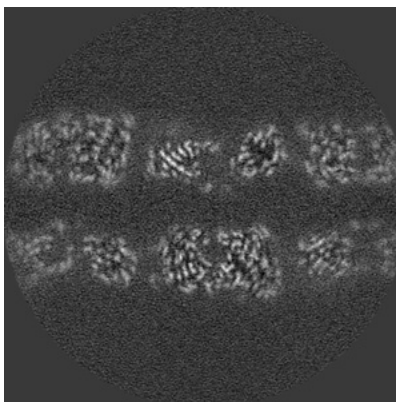


Z Index: 159

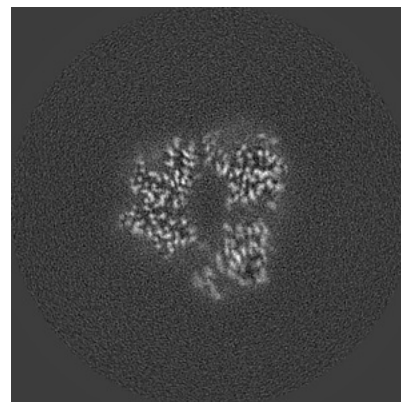
6.2.2 Raw map



X Index: 159



Y Index: 159

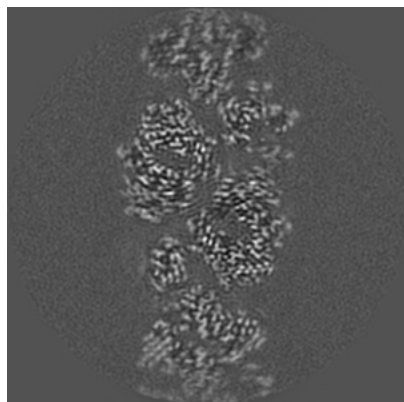


Z Index: 159

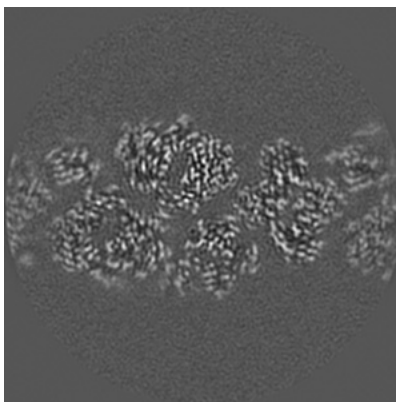
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

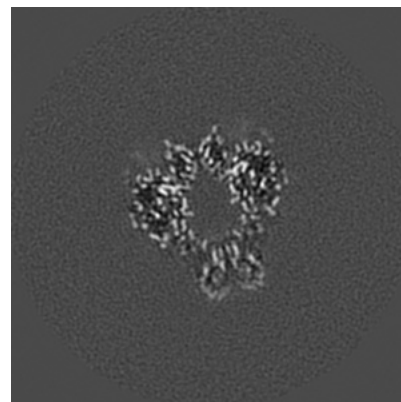
6.3.1 Primary map



X Index: 188

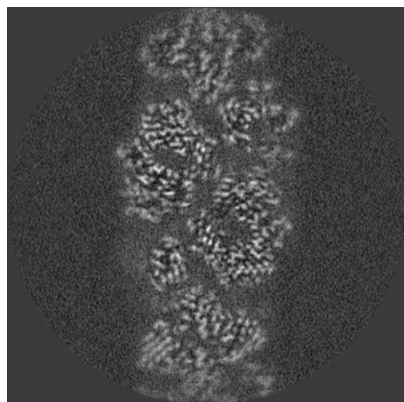


Y Index: 187

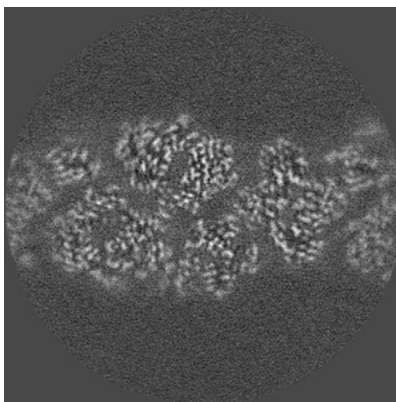


Z Index: 154

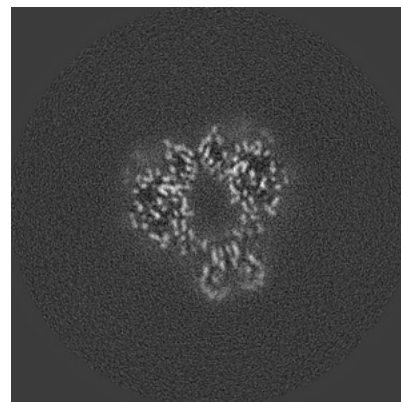
6.3.2 Raw map



X Index: 188



Y Index: 187

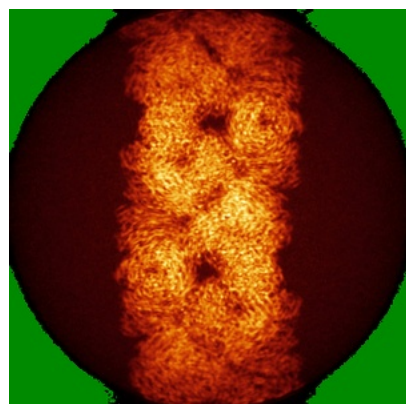


Z Index: 154

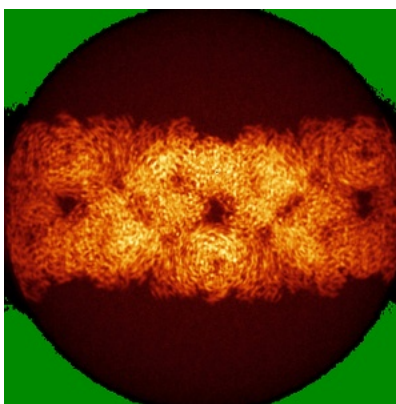
The images above show the largest variance slices of the map in three orthogonal directions.

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

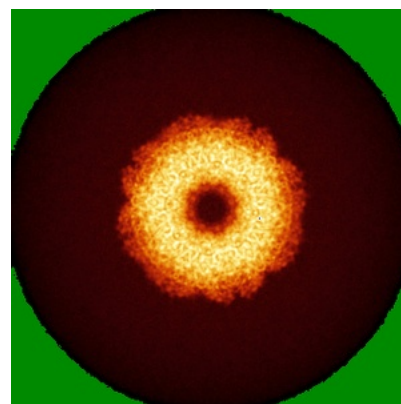
6.4.1 Primary map



X

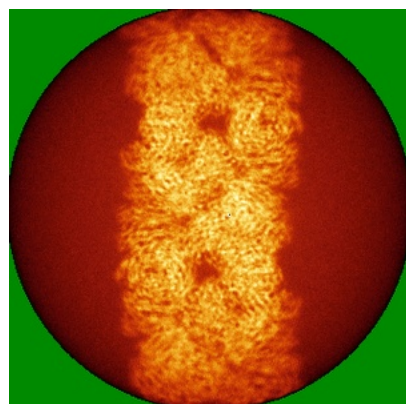


Y

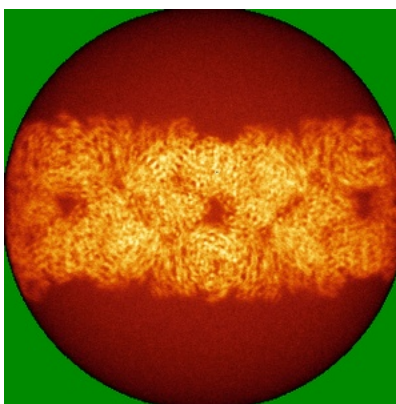


Z

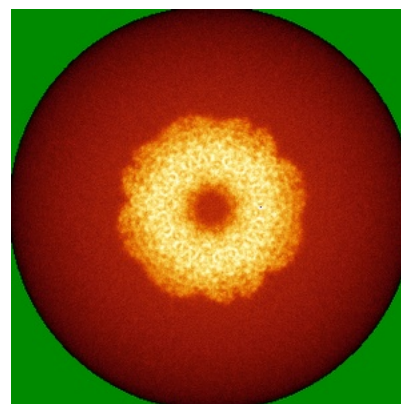
6.4.2 Raw map



X



Y

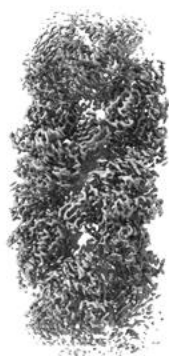


Z

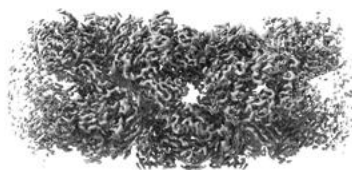
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



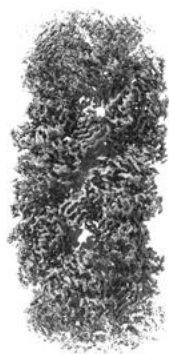
Y



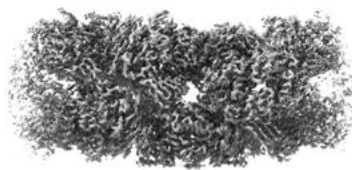
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. 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



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.

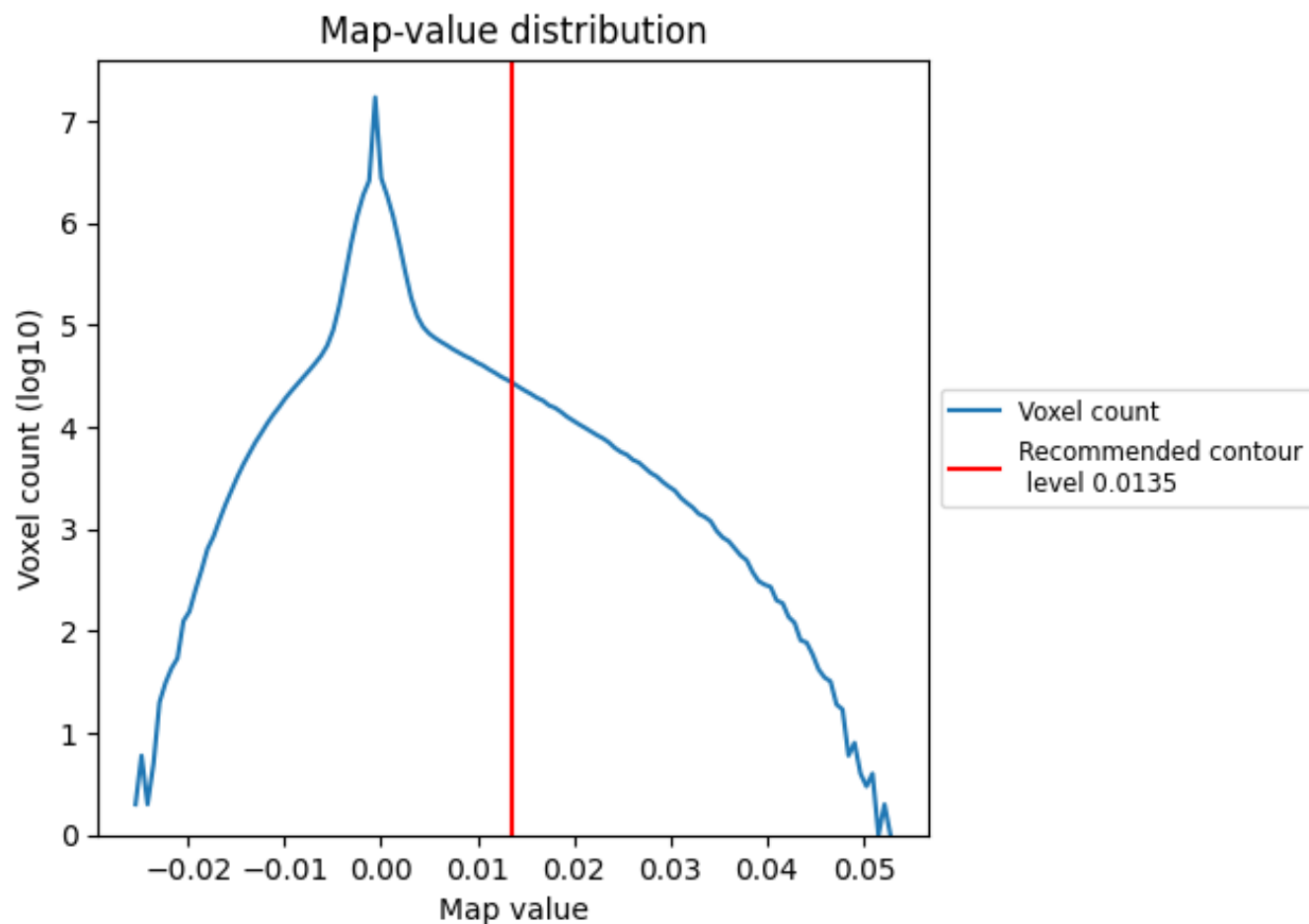
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

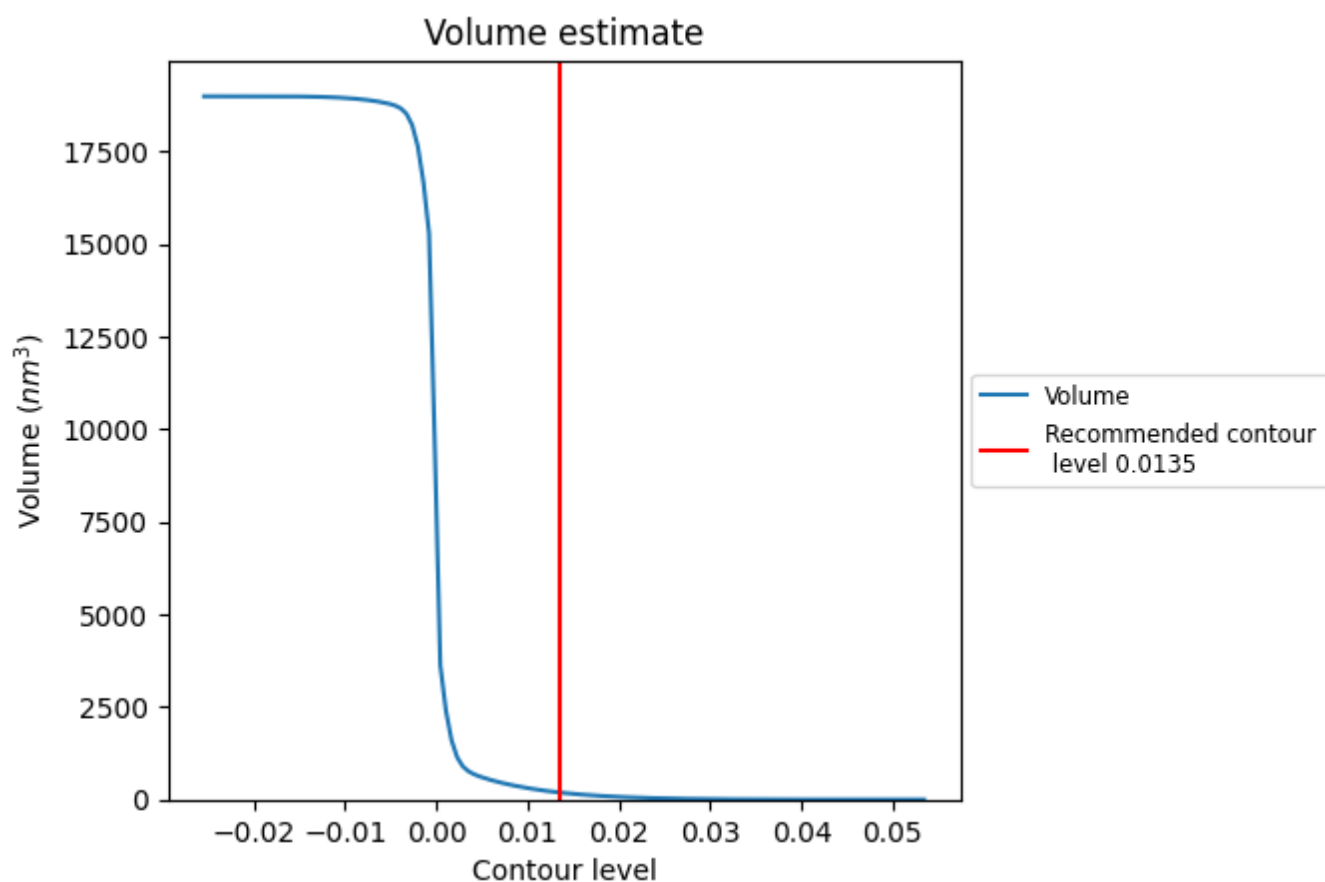
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

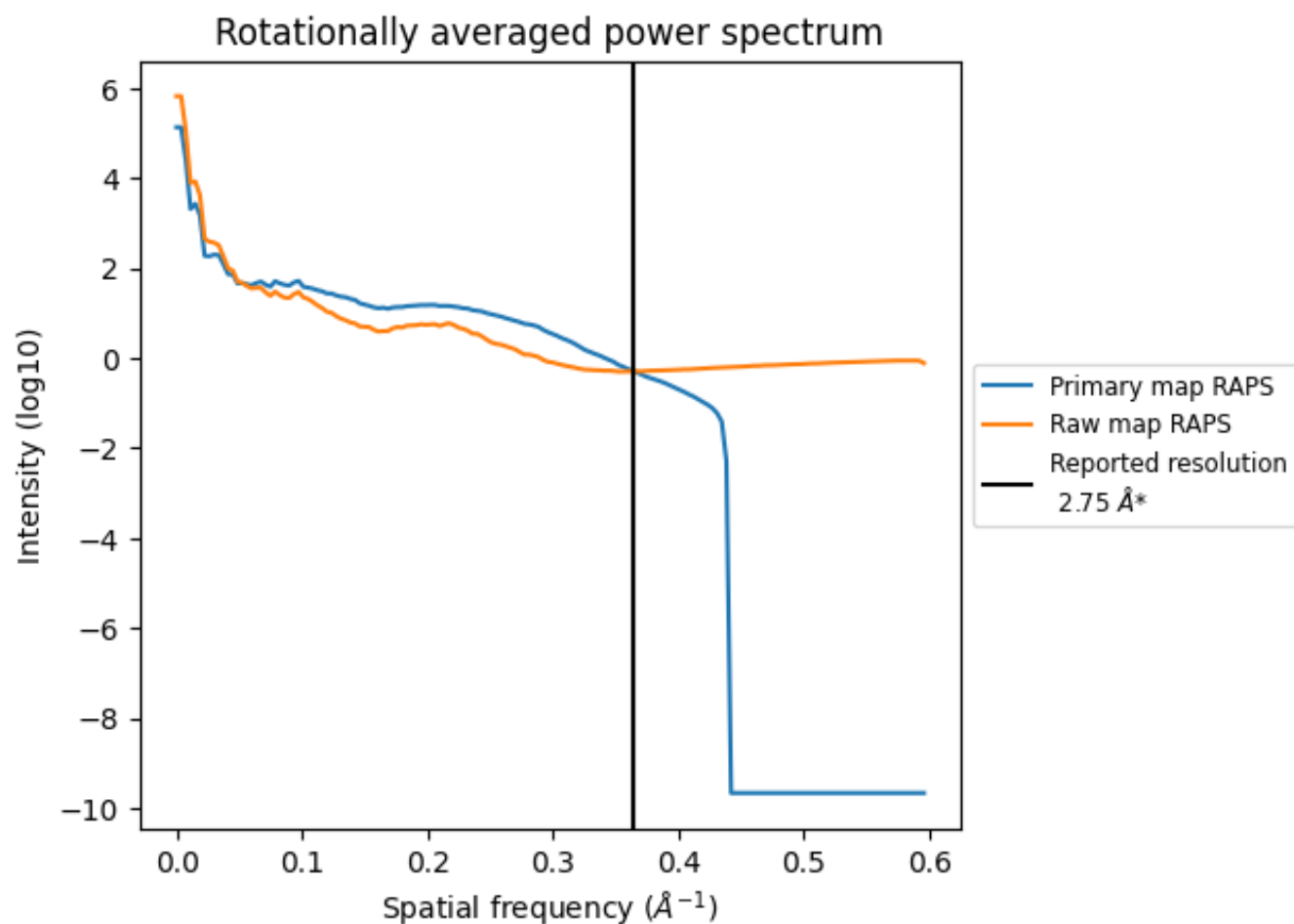
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

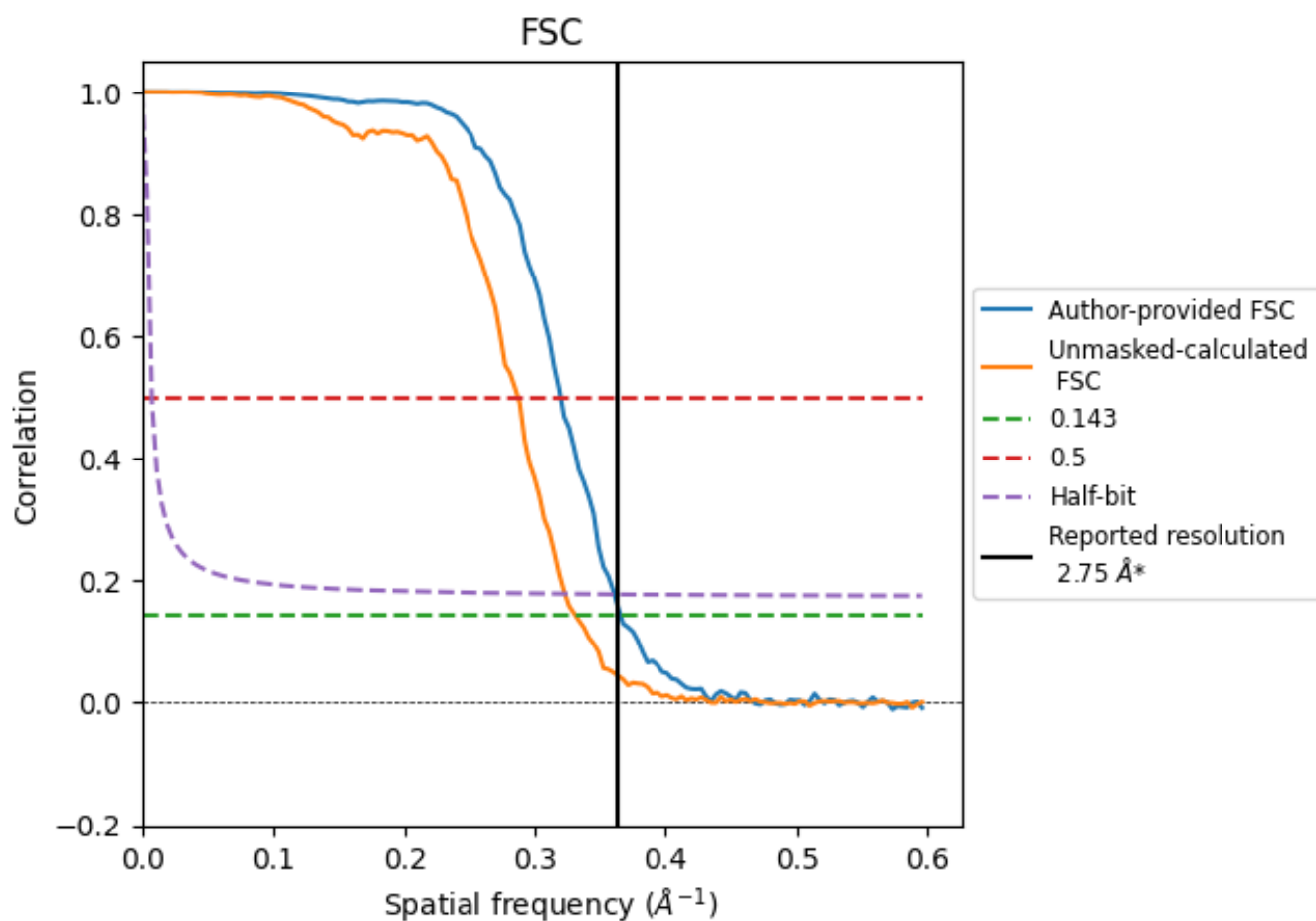


*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

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 0.364 \AA^{-1}

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.75	-
Author-provided FSC curve	2.74	3.13	2.77
Unmasked-calculated*	3.02	3.48	3.10

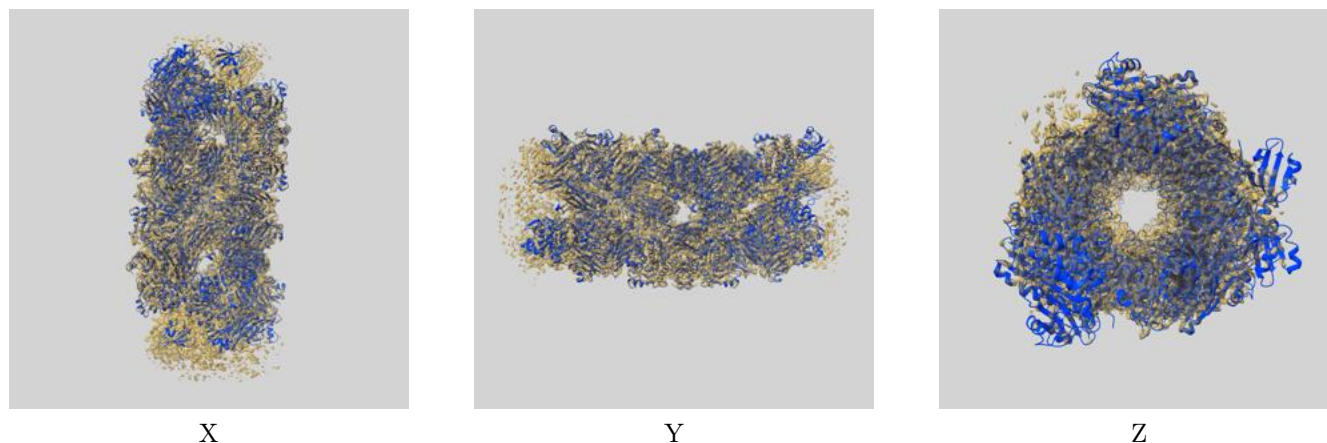
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.13 differs from the reported value 2.75 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 3.48 differs from the reported value 2.75 by more than 10 %

9 Map-model fit [i](#)

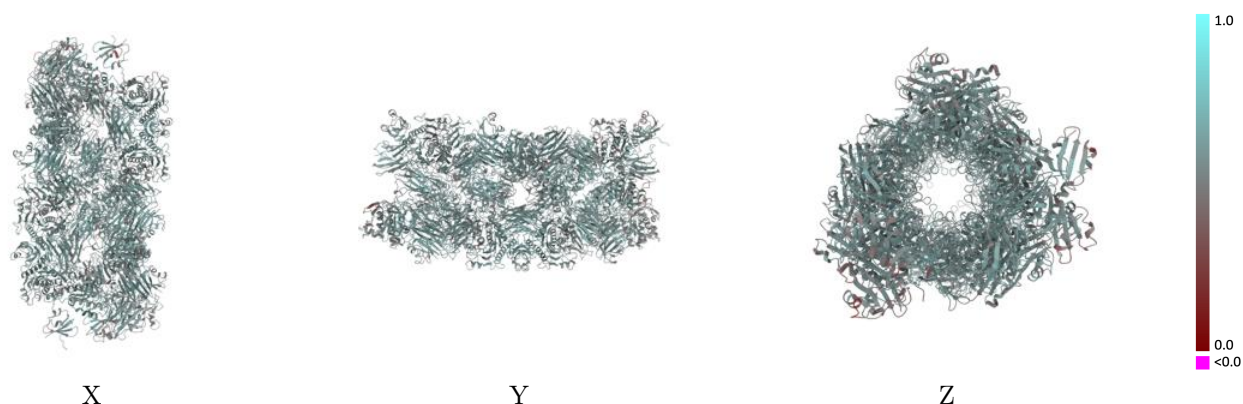
This section contains information regarding the fit between EMDB map EMD-54942 and PDB model 9SJB. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



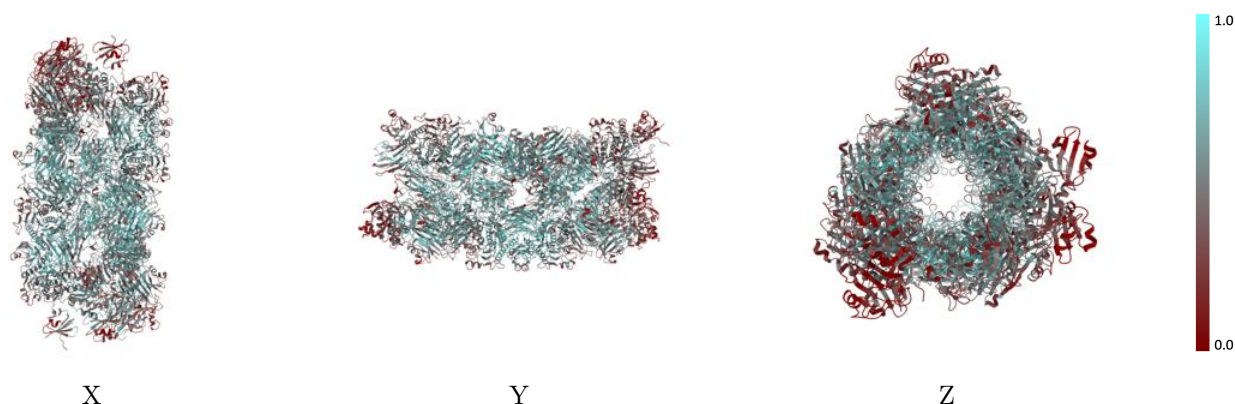
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



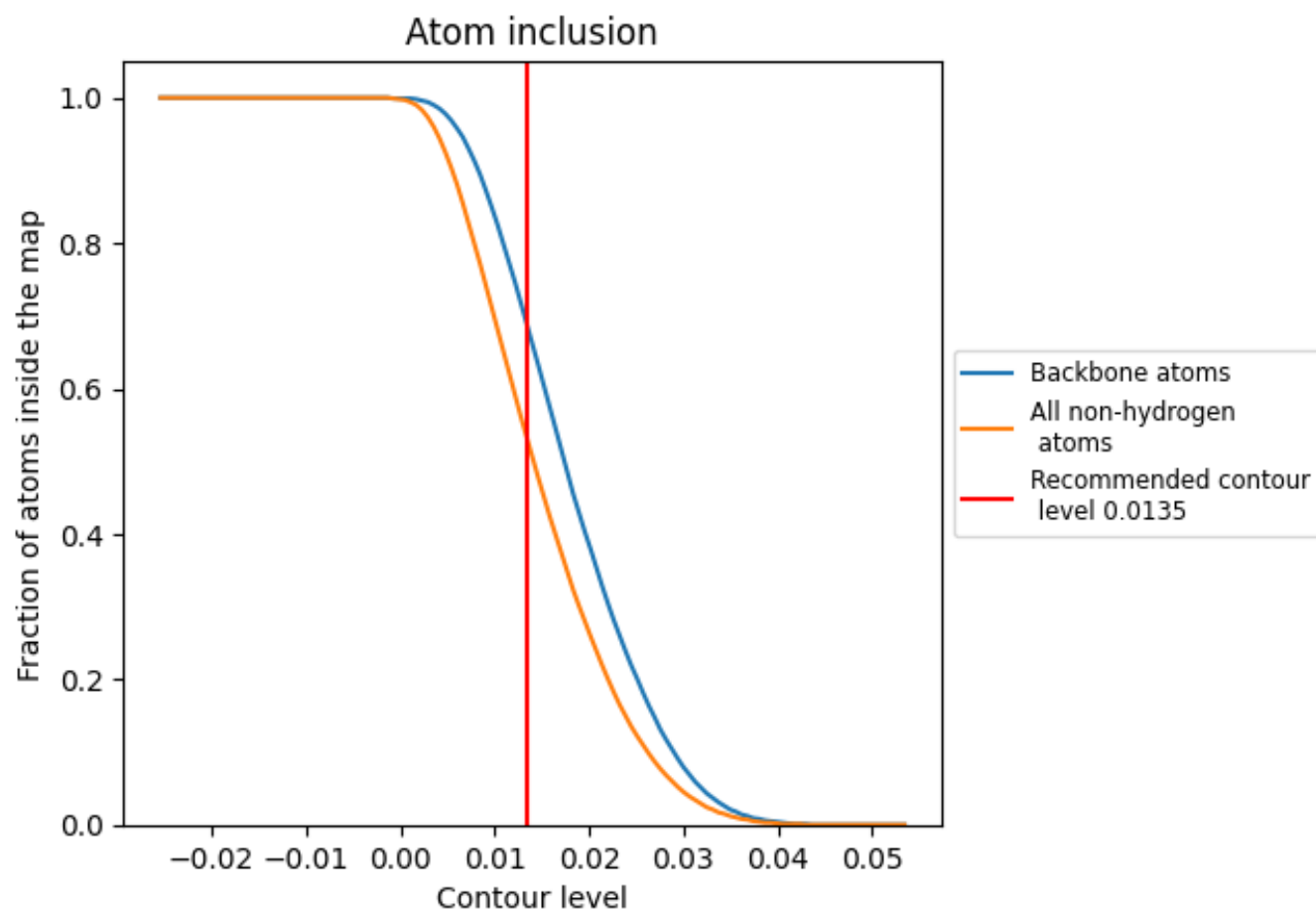
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 53% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5280	 0.5650
A	 0.5780	 0.5870
AA	 0.3290	 0.5430
B	 0.5650	 0.5830
BB	 0.3310	 0.5310
C	 0.6100	 0.5770
CC	 0.4850	 0.5560
D	 0.6200	 0.5780
E	 0.5630	 0.5790
EE	 0.1620	 0.5090
F	 0.5670	 0.5820
FF	 0.1610	 0.4970
G	 0.6200	 0.5790
GG	 0.3690	 0.5430
H	 0.6210	 0.5810
I	 0.5570	 0.5820
J	 0.5220	 0.5770
K	 0.5550	 0.5680
L	 0.6110	 0.5750
LL	 0.5470	 0.5850
M	 0.5530	 0.5840
N	 0.6140	 0.5760
O	 0.5810	 0.5750
P	 0.4610	 0.5580
Q	 0.4670	 0.5640
R	 0.5750	 0.5690
S	 0.4450	 0.5500
T	 0.4840	 0.5670
V	 0.5140	 0.5740
W	 0.5960	 0.5750
X	 0.4850	 0.5540
Y	 0.4080	 0.5540
YY	 0.3250	 0.5300
Z	 0.3800	 0.5380
ZZ	 0.5180	 0.5600

