



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2024 – 03:24 pm GMT

PDB ID : 6GY6
EMDB ID : EMD-0088
Title : XaxAB pore complex from Xenorhabdus nematophila
Authors : Schubert, E.; Raunser, S.
Deposited on : 2018-06-28
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

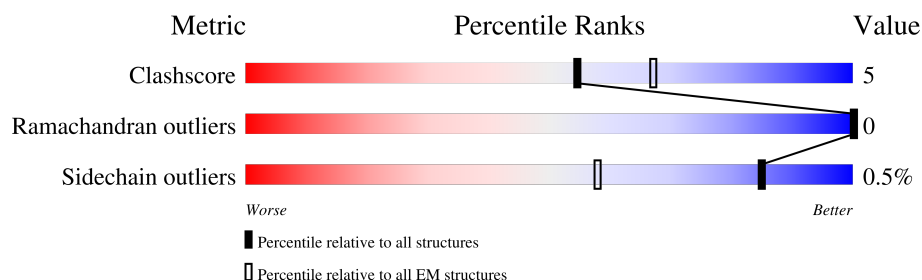
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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





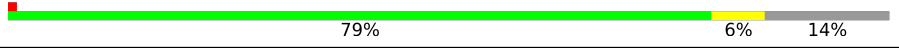



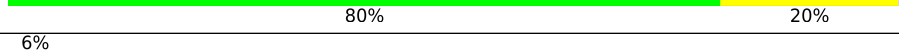
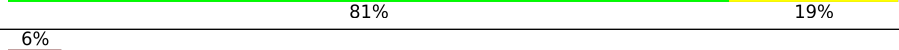
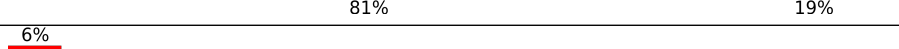
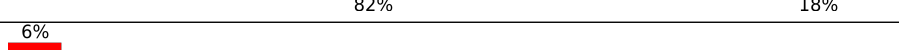




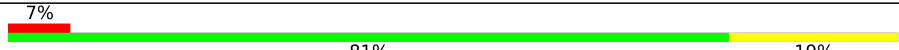



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	424	
1	C	424	
1	D	424	
1	E	424	
1	F	424	
1	I	424	
1	J	424	
1	M	424	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	424	
1	Q	424	
1	R	424	
1	S	424	
1	T	424	
2	B	338	
2	G	338	
2	H	338	
2	K	338	
2	L	338	
2	N	338	
2	O	338	
2	U	338	
2	V	338	
2	W	338	
2	X	338	
2	Y	338	
2	Z	338	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 72462 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 XaxA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	C	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	D	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	E	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	F	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	I	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	J	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	M	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	P	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	Q	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	R	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	S	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		
1	T	365	Total	C	N	O	S	0	0
			2875	1819	477	571	8		

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP D3VB22
A	410	THR	-	expression tag	UNP D3VB22
A	411	LEU	-	expression tag	UNP D3VB22
A	412	GLU	-	expression tag	UNP D3VB22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	VAL	-	expression tag	UNP D3VB22
A	414	LEU	-	expression tag	UNP D3VB22
A	415	PHE	-	expression tag	UNP D3VB22
A	416	GLN	-	expression tag	UNP D3VB22
A	417	GLY	-	expression tag	UNP D3VB22
A	418	PRO	-	expression tag	UNP D3VB22
A	419	HIS	-	expression tag	UNP D3VB22
A	420	HIS	-	expression tag	UNP D3VB22
A	421	HIS	-	expression tag	UNP D3VB22
A	422	HIS	-	expression tag	UNP D3VB22
A	423	HIS	-	expression tag	UNP D3VB22
A	424	HIS	-	expression tag	UNP D3VB22
C	409	GLY	-	expression tag	UNP D3VB22
C	410	THR	-	expression tag	UNP D3VB22
C	411	LEU	-	expression tag	UNP D3VB22
C	412	GLU	-	expression tag	UNP D3VB22
C	413	VAL	-	expression tag	UNP D3VB22
C	414	LEU	-	expression tag	UNP D3VB22
C	415	PHE	-	expression tag	UNP D3VB22
C	416	GLN	-	expression tag	UNP D3VB22
C	417	GLY	-	expression tag	UNP D3VB22
C	418	PRO	-	expression tag	UNP D3VB22
C	419	HIS	-	expression tag	UNP D3VB22
C	420	HIS	-	expression tag	UNP D3VB22
C	421	HIS	-	expression tag	UNP D3VB22
C	422	HIS	-	expression tag	UNP D3VB22
C	423	HIS	-	expression tag	UNP D3VB22
C	424	HIS	-	expression tag	UNP D3VB22
D	409	GLY	-	expression tag	UNP D3VB22
D	410	THR	-	expression tag	UNP D3VB22
D	411	LEU	-	expression tag	UNP D3VB22
D	412	GLU	-	expression tag	UNP D3VB22
D	413	VAL	-	expression tag	UNP D3VB22
D	414	LEU	-	expression tag	UNP D3VB22
D	415	PHE	-	expression tag	UNP D3VB22
D	416	GLN	-	expression tag	UNP D3VB22
D	417	GLY	-	expression tag	UNP D3VB22
D	418	PRO	-	expression tag	UNP D3VB22
D	419	HIS	-	expression tag	UNP D3VB22
D	420	HIS	-	expression tag	UNP D3VB22
D	421	HIS	-	expression tag	UNP D3VB22
D	422	HIS	-	expression tag	UNP D3VB22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	423	HIS	-	expression tag	UNP D3VB22
D	424	HIS	-	expression tag	UNP D3VB22
E	409	GLY	-	expression tag	UNP D3VB22
E	410	THR	-	expression tag	UNP D3VB22
E	411	LEU	-	expression tag	UNP D3VB22
E	412	GLU	-	expression tag	UNP D3VB22
E	413	VAL	-	expression tag	UNP D3VB22
E	414	LEU	-	expression tag	UNP D3VB22
E	415	PHE	-	expression tag	UNP D3VB22
E	416	GLN	-	expression tag	UNP D3VB22
E	417	GLY	-	expression tag	UNP D3VB22
E	418	PRO	-	expression tag	UNP D3VB22
E	419	HIS	-	expression tag	UNP D3VB22
E	420	HIS	-	expression tag	UNP D3VB22
E	421	HIS	-	expression tag	UNP D3VB22
E	422	HIS	-	expression tag	UNP D3VB22
E	423	HIS	-	expression tag	UNP D3VB22
E	424	HIS	-	expression tag	UNP D3VB22
F	409	GLY	-	expression tag	UNP D3VB22
F	410	THR	-	expression tag	UNP D3VB22
F	411	LEU	-	expression tag	UNP D3VB22
F	412	GLU	-	expression tag	UNP D3VB22
F	413	VAL	-	expression tag	UNP D3VB22
F	414	LEU	-	expression tag	UNP D3VB22
F	415	PHE	-	expression tag	UNP D3VB22
F	416	GLN	-	expression tag	UNP D3VB22
F	417	GLY	-	expression tag	UNP D3VB22
F	418	PRO	-	expression tag	UNP D3VB22
F	419	HIS	-	expression tag	UNP D3VB22
F	420	HIS	-	expression tag	UNP D3VB22
F	421	HIS	-	expression tag	UNP D3VB22
F	422	HIS	-	expression tag	UNP D3VB22
F	423	HIS	-	expression tag	UNP D3VB22
F	424	HIS	-	expression tag	UNP D3VB22
I	409	GLY	-	expression tag	UNP D3VB22
I	410	THR	-	expression tag	UNP D3VB22
I	411	LEU	-	expression tag	UNP D3VB22
I	412	GLU	-	expression tag	UNP D3VB22
I	413	VAL	-	expression tag	UNP D3VB22
I	414	LEU	-	expression tag	UNP D3VB22
I	415	PHE	-	expression tag	UNP D3VB22
I	416	GLN	-	expression tag	UNP D3VB22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	417	GLY	-	expression tag	UNP D3VB22
I	418	PRO	-	expression tag	UNP D3VB22
I	419	HIS	-	expression tag	UNP D3VB22
I	420	HIS	-	expression tag	UNP D3VB22
I	421	HIS	-	expression tag	UNP D3VB22
I	422	HIS	-	expression tag	UNP D3VB22
I	423	HIS	-	expression tag	UNP D3VB22
I	424	HIS	-	expression tag	UNP D3VB22
J	409	GLY	-	expression tag	UNP D3VB22
J	410	THR	-	expression tag	UNP D3VB22
J	411	LEU	-	expression tag	UNP D3VB22
J	412	GLU	-	expression tag	UNP D3VB22
J	413	VAL	-	expression tag	UNP D3VB22
J	414	LEU	-	expression tag	UNP D3VB22
J	415	PHE	-	expression tag	UNP D3VB22
J	416	GLN	-	expression tag	UNP D3VB22
J	417	GLY	-	expression tag	UNP D3VB22
J	418	PRO	-	expression tag	UNP D3VB22
J	419	HIS	-	expression tag	UNP D3VB22
J	420	HIS	-	expression tag	UNP D3VB22
J	421	HIS	-	expression tag	UNP D3VB22
J	422	HIS	-	expression tag	UNP D3VB22
J	423	HIS	-	expression tag	UNP D3VB22
J	424	HIS	-	expression tag	UNP D3VB22
M	409	GLY	-	expression tag	UNP D3VB22
M	410	THR	-	expression tag	UNP D3VB22
M	411	LEU	-	expression tag	UNP D3VB22
M	412	GLU	-	expression tag	UNP D3VB22
M	413	VAL	-	expression tag	UNP D3VB22
M	414	LEU	-	expression tag	UNP D3VB22
M	415	PHE	-	expression tag	UNP D3VB22
M	416	GLN	-	expression tag	UNP D3VB22
M	417	GLY	-	expression tag	UNP D3VB22
M	418	PRO	-	expression tag	UNP D3VB22
M	419	HIS	-	expression tag	UNP D3VB22
M	420	HIS	-	expression tag	UNP D3VB22
M	421	HIS	-	expression tag	UNP D3VB22
M	422	HIS	-	expression tag	UNP D3VB22
M	423	HIS	-	expression tag	UNP D3VB22
M	424	HIS	-	expression tag	UNP D3VB22
P	409	GLY	-	expression tag	UNP D3VB22
P	410	THR	-	expression tag	UNP D3VB22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	411	LEU	-	expression tag	UNP D3VB22
P	412	GLU	-	expression tag	UNP D3VB22
P	413	VAL	-	expression tag	UNP D3VB22
P	414	LEU	-	expression tag	UNP D3VB22
P	415	PHE	-	expression tag	UNP D3VB22
P	416	GLN	-	expression tag	UNP D3VB22
P	417	GLY	-	expression tag	UNP D3VB22
P	418	PRO	-	expression tag	UNP D3VB22
P	419	HIS	-	expression tag	UNP D3VB22
P	420	HIS	-	expression tag	UNP D3VB22
P	421	HIS	-	expression tag	UNP D3VB22
P	422	HIS	-	expression tag	UNP D3VB22
P	423	HIS	-	expression tag	UNP D3VB22
P	424	HIS	-	expression tag	UNP D3VB22
Q	409	GLY	-	expression tag	UNP D3VB22
Q	410	THR	-	expression tag	UNP D3VB22
Q	411	LEU	-	expression tag	UNP D3VB22
Q	412	GLU	-	expression tag	UNP D3VB22
Q	413	VAL	-	expression tag	UNP D3VB22
Q	414	LEU	-	expression tag	UNP D3VB22
Q	415	PHE	-	expression tag	UNP D3VB22
Q	416	GLN	-	expression tag	UNP D3VB22
Q	417	GLY	-	expression tag	UNP D3VB22
Q	418	PRO	-	expression tag	UNP D3VB22
Q	419	HIS	-	expression tag	UNP D3VB22
Q	420	HIS	-	expression tag	UNP D3VB22
Q	421	HIS	-	expression tag	UNP D3VB22
Q	422	HIS	-	expression tag	UNP D3VB22
Q	423	HIS	-	expression tag	UNP D3VB22
Q	424	HIS	-	expression tag	UNP D3VB22
R	409	GLY	-	expression tag	UNP D3VB22
R	410	THR	-	expression tag	UNP D3VB22
R	411	LEU	-	expression tag	UNP D3VB22
R	412	GLU	-	expression tag	UNP D3VB22
R	413	VAL	-	expression tag	UNP D3VB22
R	414	LEU	-	expression tag	UNP D3VB22
R	415	PHE	-	expression tag	UNP D3VB22
R	416	GLN	-	expression tag	UNP D3VB22
R	417	GLY	-	expression tag	UNP D3VB22
R	418	PRO	-	expression tag	UNP D3VB22
R	419	HIS	-	expression tag	UNP D3VB22
R	420	HIS	-	expression tag	UNP D3VB22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	421	HIS	-	expression tag	UNP D3VB22
R	422	HIS	-	expression tag	UNP D3VB22
R	423	HIS	-	expression tag	UNP D3VB22
R	424	HIS	-	expression tag	UNP D3VB22
S	409	GLY	-	expression tag	UNP D3VB22
S	410	THR	-	expression tag	UNP D3VB22
S	411	LEU	-	expression tag	UNP D3VB22
S	412	GLU	-	expression tag	UNP D3VB22
S	413	VAL	-	expression tag	UNP D3VB22
S	414	LEU	-	expression tag	UNP D3VB22
S	415	PHE	-	expression tag	UNP D3VB22
S	416	GLN	-	expression tag	UNP D3VB22
S	417	GLY	-	expression tag	UNP D3VB22
S	418	PRO	-	expression tag	UNP D3VB22
S	419	HIS	-	expression tag	UNP D3VB22
S	420	HIS	-	expression tag	UNP D3VB22
S	421	HIS	-	expression tag	UNP D3VB22
S	422	HIS	-	expression tag	UNP D3VB22
S	423	HIS	-	expression tag	UNP D3VB22
S	424	HIS	-	expression tag	UNP D3VB22
T	409	GLY	-	expression tag	UNP D3VB22
T	410	THR	-	expression tag	UNP D3VB22
T	411	LEU	-	expression tag	UNP D3VB22
T	412	GLU	-	expression tag	UNP D3VB22
T	413	VAL	-	expression tag	UNP D3VB22
T	414	LEU	-	expression tag	UNP D3VB22
T	415	PHE	-	expression tag	UNP D3VB22
T	416	GLN	-	expression tag	UNP D3VB22
T	417	GLY	-	expression tag	UNP D3VB22
T	418	PRO	-	expression tag	UNP D3VB22
T	419	HIS	-	expression tag	UNP D3VB22
T	420	HIS	-	expression tag	UNP D3VB22
T	421	HIS	-	expression tag	UNP D3VB22
T	422	HIS	-	expression tag	UNP D3VB22
T	423	HIS	-	expression tag	UNP D3VB22
T	424	HIS	-	expression tag	UNP D3VB22

- Molecule 2 is a protein called XaxB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	H	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	K	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	L	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	N	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	O	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	U	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	V	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	W	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	X	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	Y	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		
2	Z	338	Total	C	N	O	S	0	0
			2699	1682	467	543	7		

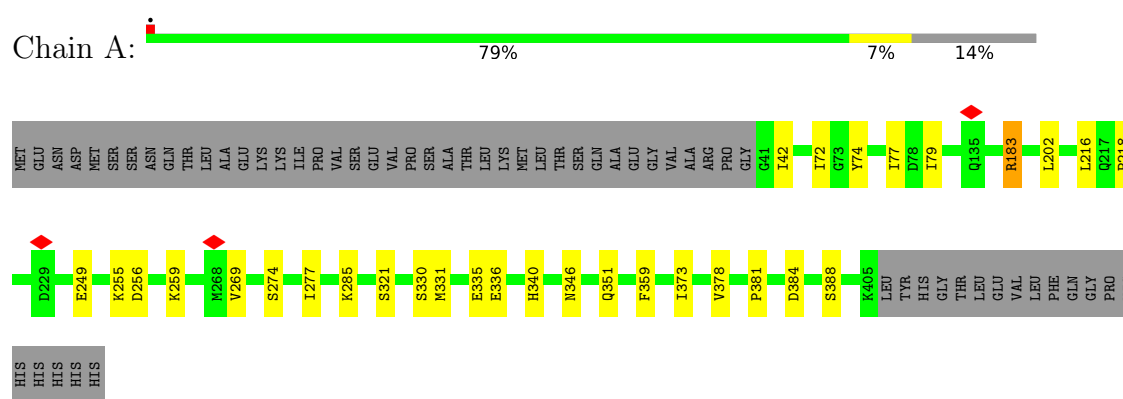
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	51	ALA	LEU	conflict	UNP D3VB23
G	51	ALA	LEU	conflict	UNP D3VB23
H	51	ALA	LEU	conflict	UNP D3VB23
K	51	ALA	LEU	conflict	UNP D3VB23
L	51	ALA	LEU	conflict	UNP D3VB23
N	51	ALA	LEU	conflict	UNP D3VB23
O	51	ALA	LEU	conflict	UNP D3VB23
U	51	ALA	LEU	conflict	UNP D3VB23
V	51	ALA	LEU	conflict	UNP D3VB23
W	51	ALA	LEU	conflict	UNP D3VB23
X	51	ALA	LEU	conflict	UNP D3VB23
Y	51	ALA	LEU	conflict	UNP D3VB23
Z	51	ALA	LEU	conflict	UNP D3VB23

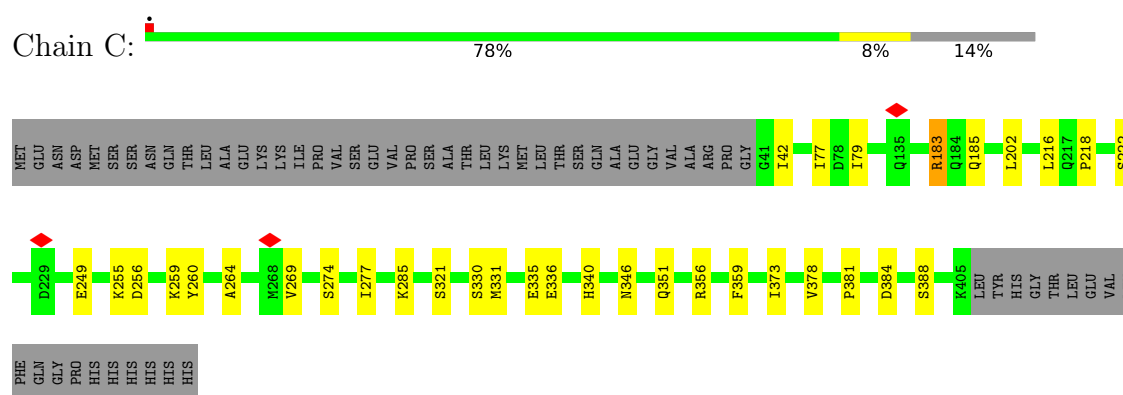
3 Residue-property plots

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

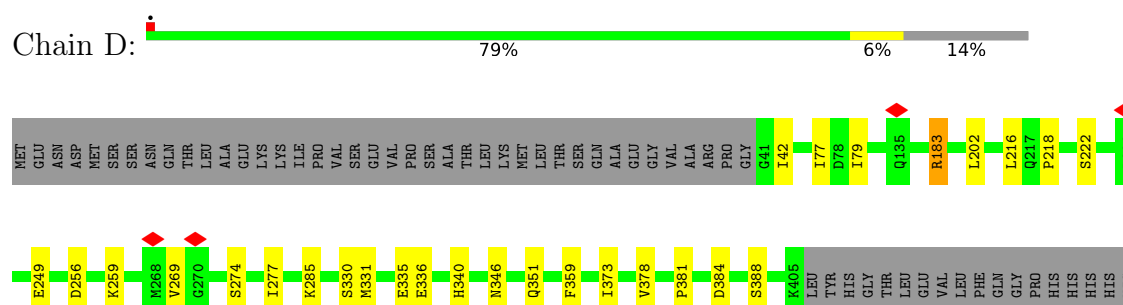
• Molecule 1: XaxA



• Molecule 1: XaxA

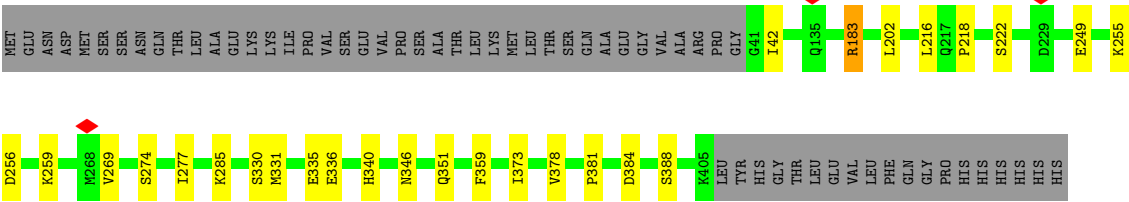
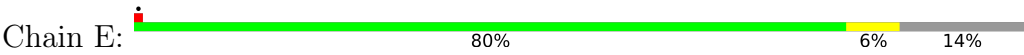


• Molecule 1: XaxA

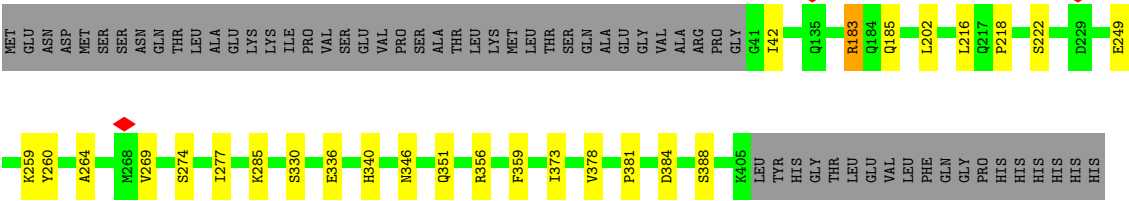
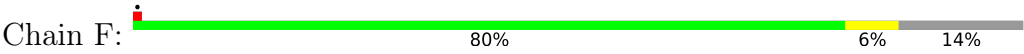


HIS

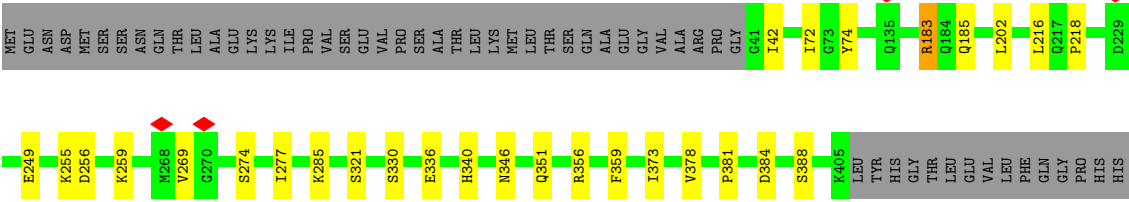
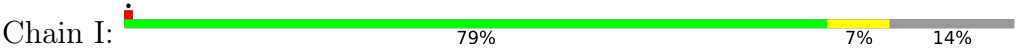
• Molecule 1: XaxA



• Molecule 1: XaxA

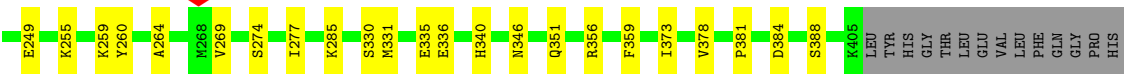
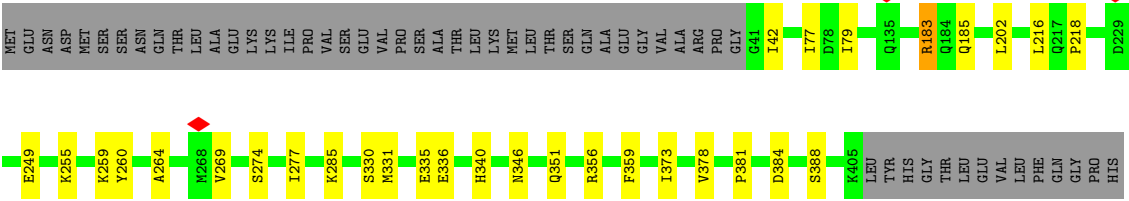
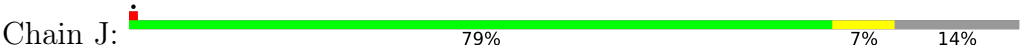


• Molecule 1: XaxA




HIS
HIS
HIS

• Molecule 1: XaxA



HIS
HIS
HIS
HIS
HIS

• Molecule 1: XaxA


Chain M: 

MET GLU ASN ASP MET SER SER ASN THR LEU ALA GLU LYS LYS ILE PRO VAL SER GLU VAL PRO SER THR LEU LYS MET LEU THR SER GLN ALA GLU GLY VAL ARG PRO GLY G41 I42 I77 D78 I79 Q135 R183 L202 L216 Q217 P218 S222 D229

E249 K255 D256 K259 Y260 A264 M268 V269 G270 S274 I277 K285 S321 S330 E336 H340 N346 Q351 F359 I373 V378 P381 D384 S388 K405 LEU TYR HIS GLY THR LEU VAL PHE LEU GLN PRO HIS

HIS
HIS
HIS
HIS

• Molecule 1: XaxA


Chain P: 

MET GLU ASN ASP MET SER SER ASN THR LEU ALA GLU LYS LYS ILE PRO VAL SER GLU VAL PRO SER THR LEU LYS MET LEU THR SER GLN ALA GLU GLY VAL ARG PRO GLY G41 I42 Q135 R183 Q184 Q185 L202 L216 Q217 P218 S222 D229 E249

K255 D256 K259 M268 V269 G270 S274 I277 K285 S330 M331 E335 E336 H340 N346 Q351 R356 F359 I373 V378 P381 D384 S388 K405 LEU TYR HIS GLY THR LEU VAL PHE LEU GLN PRO HIS HIS HIS

HIS
HIS

• Molecule 1: XaxA


Chain Q: 

MET GLU ASN ASP MET SER SER ASN THR LEU ALA GLU LYS LYS ILE PRO VAL SER GLU VAL PRO SER THR LEU LYS MET LEU THR SER GLN ALA GLU GLY VAL ARG PRO GLY G41 I42 I77 D78 I79 D80 G81 Q135 R183 L202 L216 Q217 P218 S222

K223 D229 E249 K255 K259 Y260 A264 M268 V269 S274 I277 K285 S330 E336 H340 N346 Q351 F359 I373 V378 P381 D384 S388 K405 LEU TYR HIS GLY THR LEU VAL PHE LEU GLN PRO HIS HIS

HIS
HIS
HIS

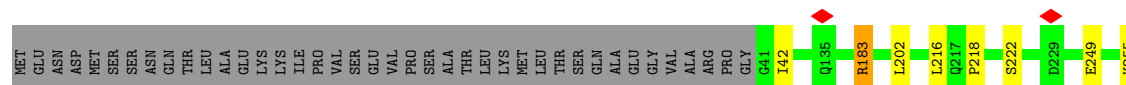
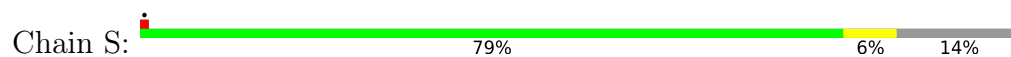
• Molecule 1: XaxA

Chain R: 

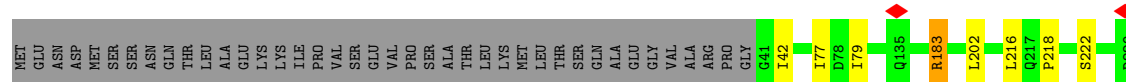
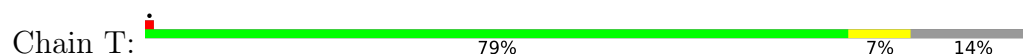
MET GLU ASN ASP MET SER SER ASN THR LEU ALA GLU LYS LYS ILE VAL SER GLU VAL PRO SER THR LEU LYS MET LEU THR SER GLN ALA GLU GLY VAL ARG PRO GLY G41 I42 G81 Q135 R183 L202 L216 Q217 P218 S222 K223 D229



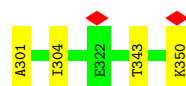
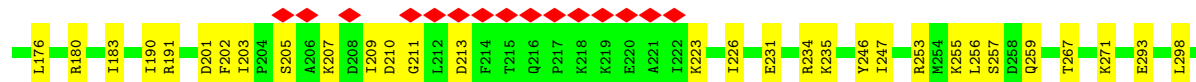
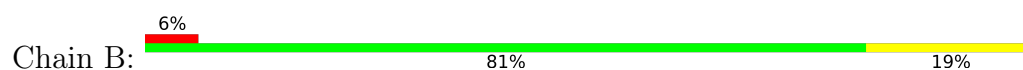
- Molecule 1: XaxA



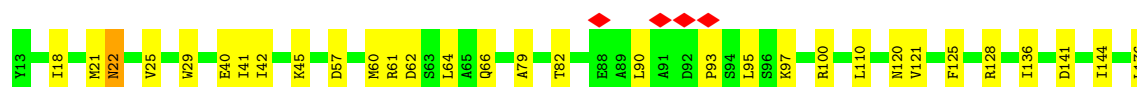
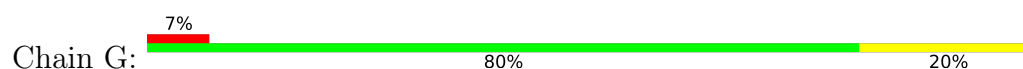
- Molecule 1: XaxA

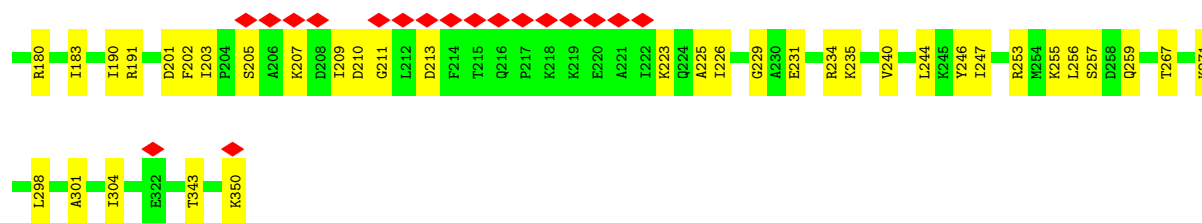


- Molecule 2: XaxB

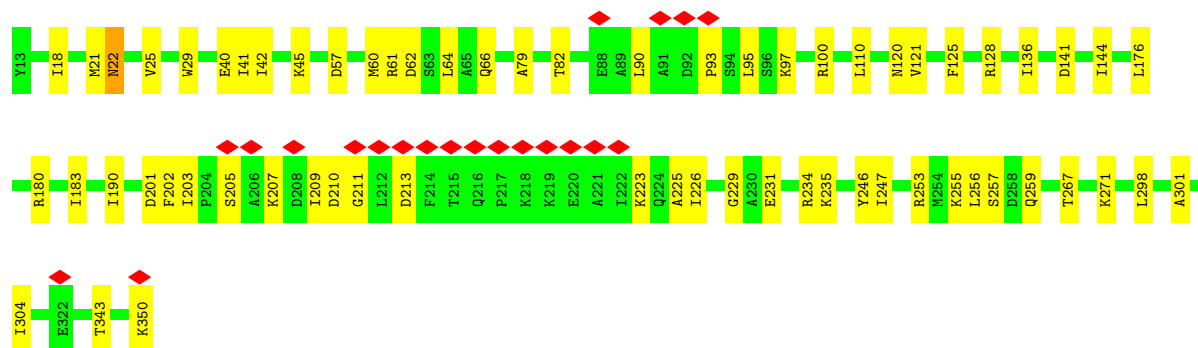
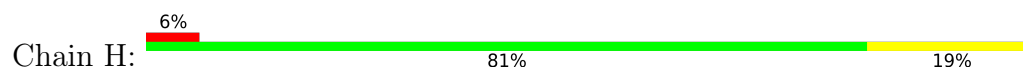


- Molecule 2: XaxB

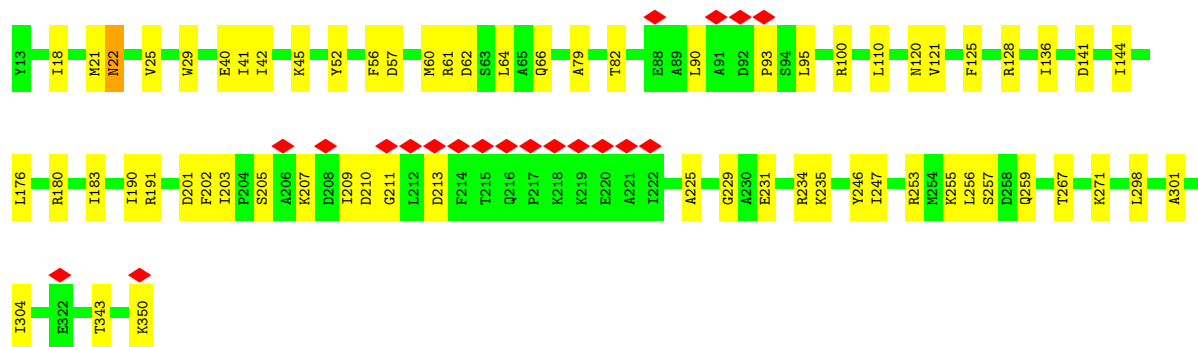
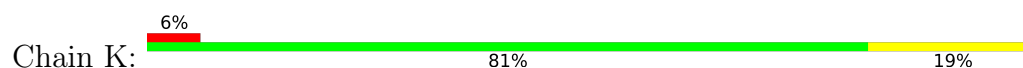




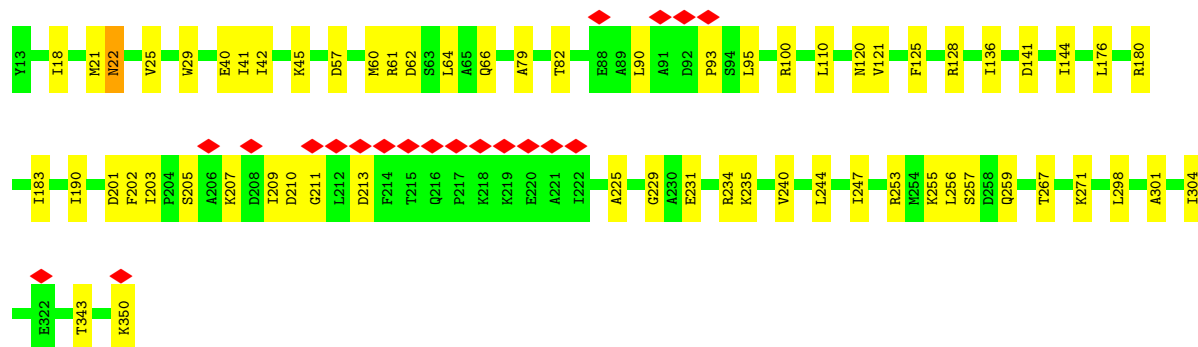
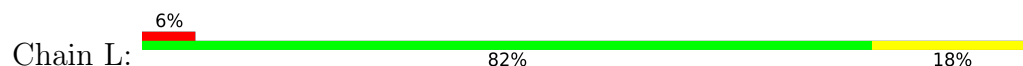
• Molecule 2: XaxB



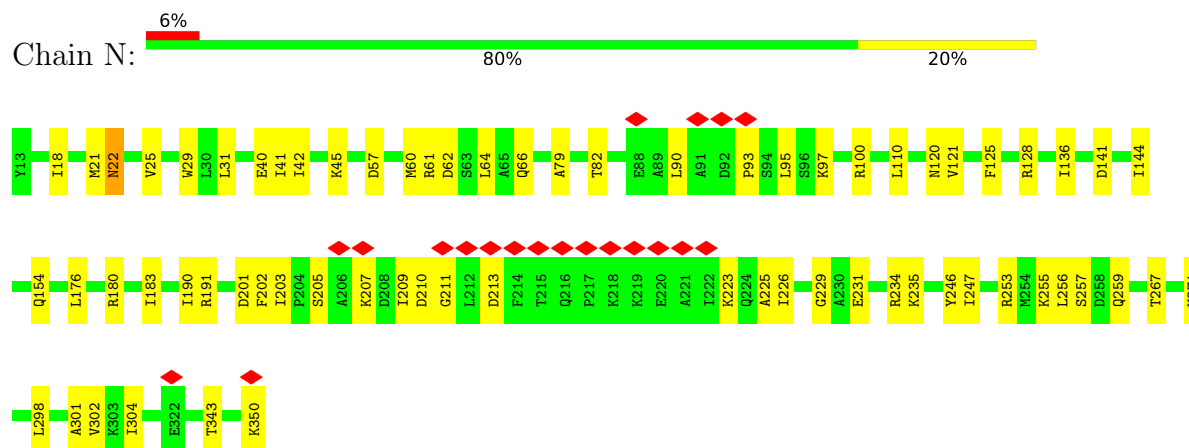
• Molecule 2: XaxB



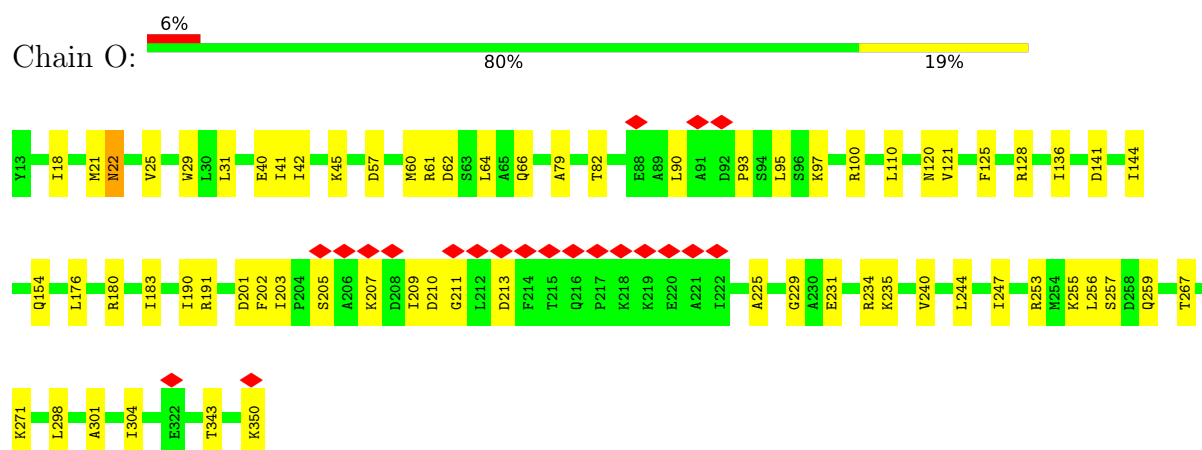
• Molecule 2: XaxB



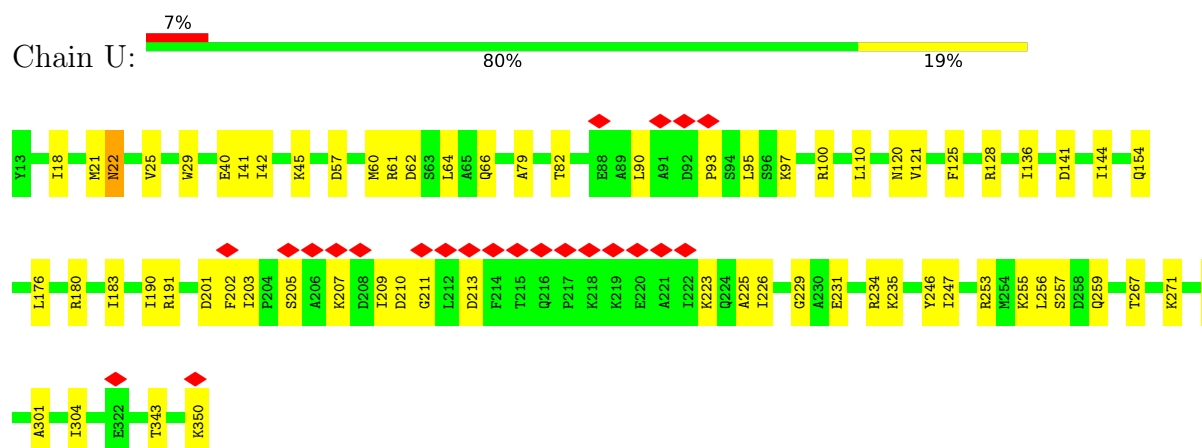
- Molecule 2: XaxB



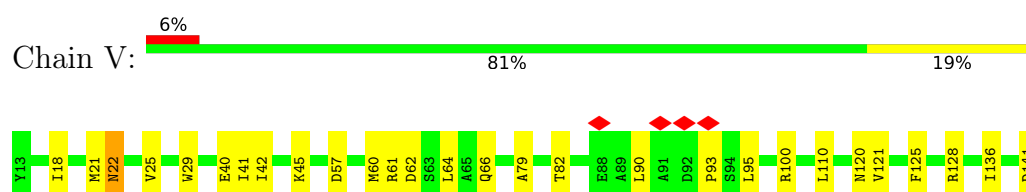
- Molecule 2: XaxB

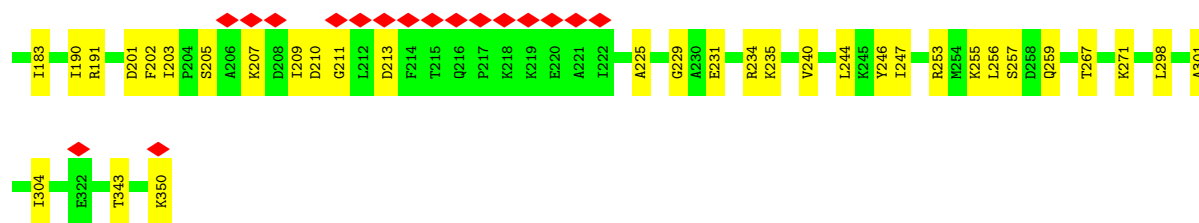


- Molecule 2: XaxB

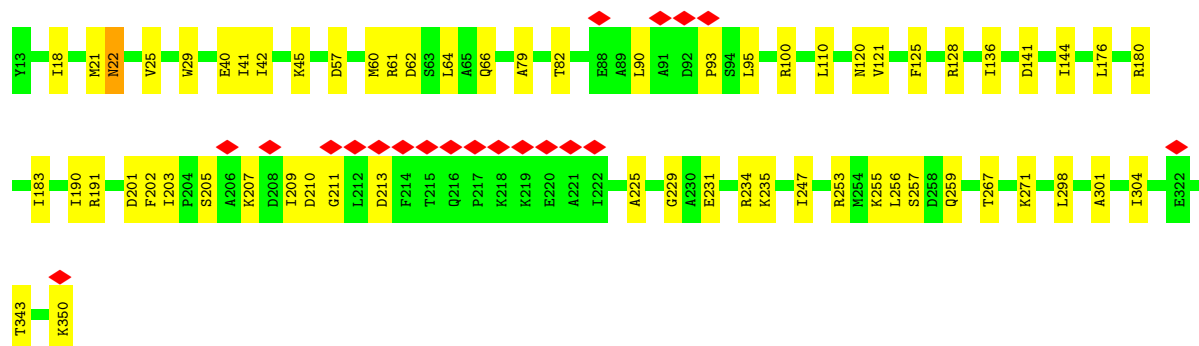
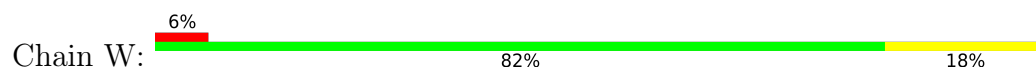


- Molecule 2: XaxB

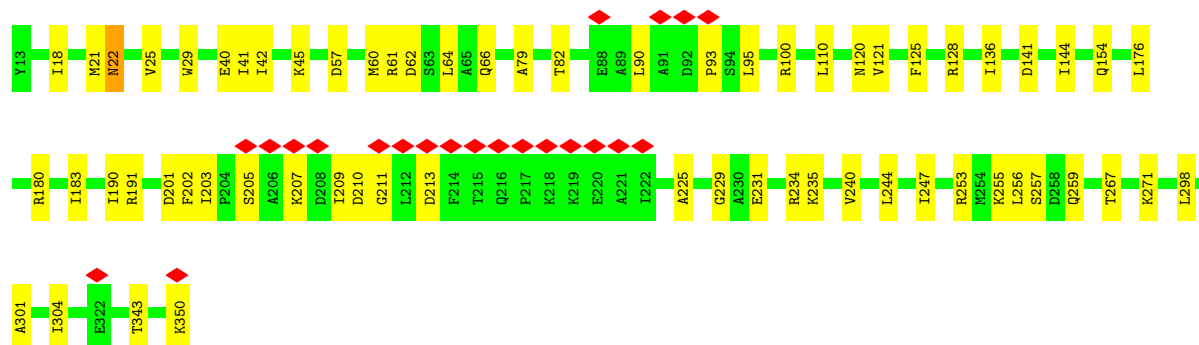
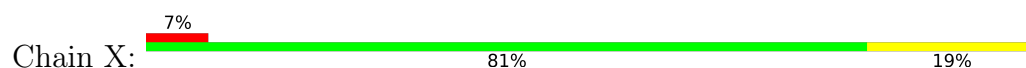




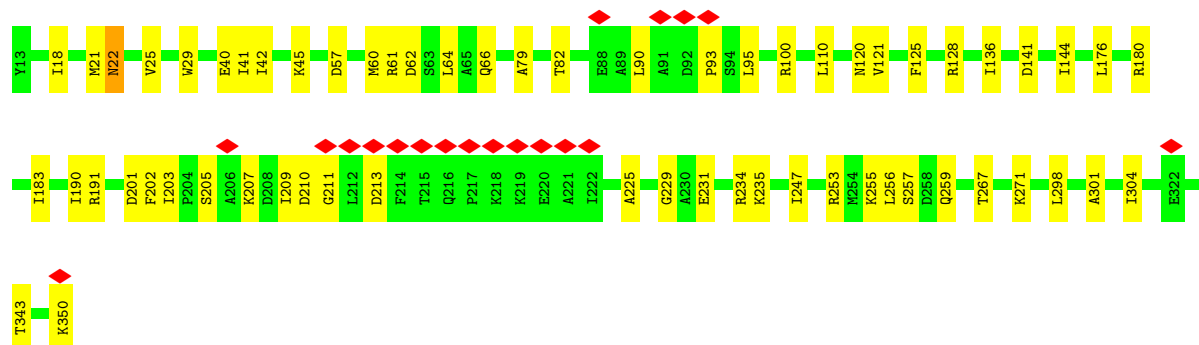
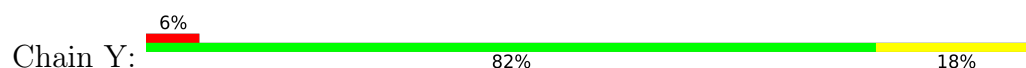
• Molecule 2: XaxB




• Molecule 2: XaxB

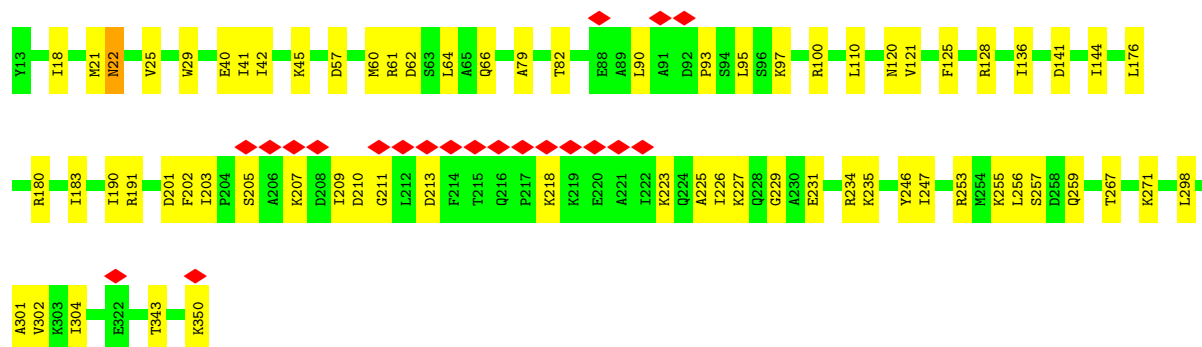


• Molecule 2: XaxB



● Molecule 2: XaxB

Chain Z:  6% 80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	43305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0192	Depositor
Map size (Å)	390.72, 390.72, 390.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/2912	0.47	0/3916
1	C	0.31	0/2912	0.47	0/3916
1	D	0.31	0/2912	0.47	0/3916
1	E	0.31	0/2912	0.47	0/3916
1	F	0.31	0/2912	0.47	0/3916
1	I	0.31	0/2912	0.47	0/3916
1	J	0.31	0/2912	0.47	0/3916
1	M	0.31	0/2912	0.47	0/3916
1	P	0.31	0/2912	0.47	0/3916
1	Q	0.31	0/2912	0.47	0/3916
1	R	0.31	0/2912	0.47	0/3916
1	S	0.31	0/2912	0.47	0/3916
1	T	0.31	0/2912	0.47	0/3916
2	B	0.32	0/2722	0.56	0/3666
2	G	0.32	0/2722	0.56	0/3666
2	H	0.32	0/2722	0.56	0/3666
2	K	0.32	0/2722	0.56	0/3666
2	L	0.32	0/2722	0.56	0/3666
2	N	0.32	0/2722	0.56	0/3666
2	O	0.32	0/2722	0.56	0/3666
2	U	0.32	0/2722	0.56	0/3666
2	V	0.32	0/2722	0.56	0/3666
2	W	0.32	0/2722	0.56	0/3666
2	X	0.32	0/2722	0.56	0/3666
2	Y	0.32	0/2722	0.56	0/3666
2	Z	0.32	0/2722	0.56	0/3666
All	All	0.32	0/73242	0.52	0/98566

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	2875	0	2923	26	0
1	C	2875	0	2923	27	0
1	D	2875	0	2923	23	0
1	E	2875	0	2923	22	0
1	F	2875	0	2923	23	0
1	I	2875	0	2923	24	0
1	J	2875	0	2923	24	0
1	M	2875	0	2923	25	0
1	P	2875	0	2923	25	0
1	Q	2875	0	2923	25	0
1	R	2875	0	2923	23	0
1	S	2875	0	2923	24	0
1	T	2875	0	2923	24	0
2	B	2699	0	2763	43	0
2	G	2699	0	2763	44	0
2	H	2699	0	2763	42	0
2	K	2699	0	2763	41	0
2	L	2699	0	2763	40	0
2	N	2699	0	2763	46	0
2	O	2699	0	2763	44	0
2	U	2699	0	2763	43	0
2	V	2699	0	2763	43	0
2	W	2699	0	2763	40	0
2	X	2699	0	2763	41	0
2	Y	2699	0	2763	40	0
2	Z	2699	0	2763	45	0
All	All	72462	0	73918	716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 716 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:183:ARG:HH11	1:S:183:ARG:HB2	1.12	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:ARG:HH11	1:M:183:ARG:HB2	1.12	1.14
1:P:183:ARG:HH11	1:P:183:ARG:HB2	1.12	1.13
1:F:183:ARG:HH11	1:F:183:ARG:HB2	1.12	1.12
1:R:183:ARG:HH11	1:R:183:ARG:HB2	1.12	1.12

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	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	C	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	D	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	E	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	F	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	I	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	J	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	M	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	P	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	Q	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	R	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	S	363/424 (86%)	355 (98%)	8 (2%)	0	100	100
1	T	363/424 (86%)	356 (98%)	7 (2%)	0	100	100
2	B	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	G	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	H	336/338 (99%)	326 (97%)	10 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	L	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	N	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	O	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	U	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	V	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	W	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	X	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	Y	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
2	Z	336/338 (99%)	326 (97%)	10 (3%)	0	100	100
All	All	9087/9906 (92%)	8854 (97%)	233 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	C	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	D	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	E	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	F	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	I	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	J	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	M	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	P	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	Q	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	R	320/371 (86%)	319 (100%)	1 (0%)	91	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	320/371 (86%)	319 (100%)	1 (0%)	91	92
1	T	320/371 (86%)	319 (100%)	1 (0%)	91	92
2	B	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	G	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	H	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	K	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	L	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	N	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	O	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	U	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	V	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	W	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	X	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	Y	305/305 (100%)	303 (99%)	2 (1%)	81	86
2	Z	305/305 (100%)	303 (99%)	2 (1%)	81	86
All	All	8125/8788 (92%)	8086 (100%)	39 (0%)	85	89

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	183	ARG
1	Q	183	ARG
1	E	183	ARG
1	J	183	ARG
1	S	183	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	252	GLN
1	F	252	GLN
1	S	252	GLN
1	E	252	GLN
1	I	252	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

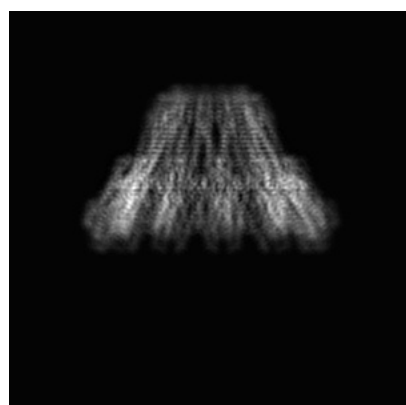
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0088. These allow visual inspection of the internal detail of the map and identification of artifacts.

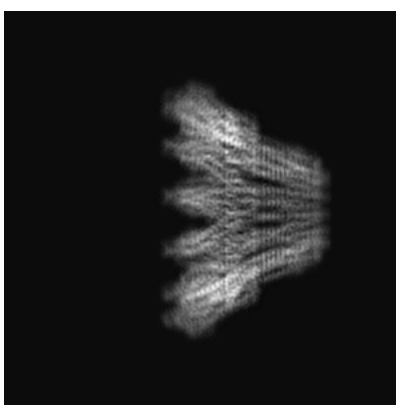
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

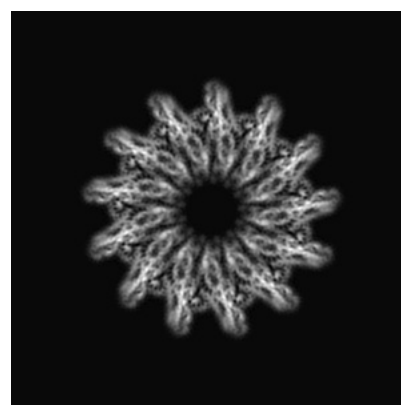
6.1.1 Primary map



X



Y

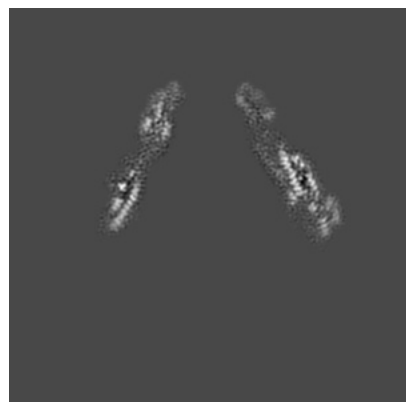


Z

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

6.2 Central slices [i](#)

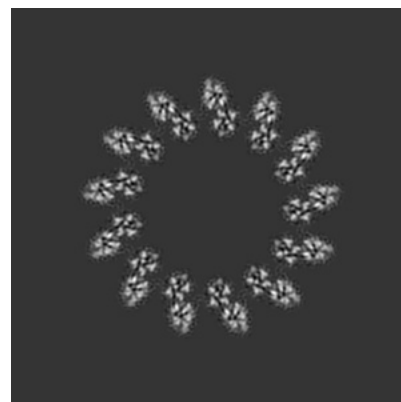
6.2.1 Primary map



X Index: 176



Y Index: 176



Z Index: 176

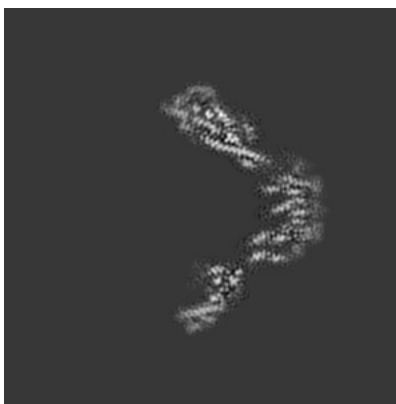
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

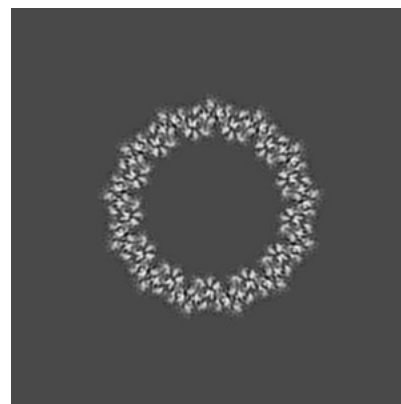
6.3.1 Primary map



X Index: 219



Y Index: 138

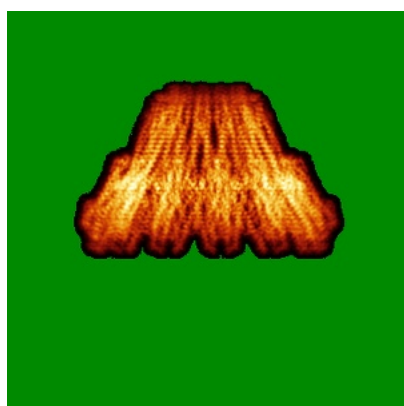


Z Index: 196

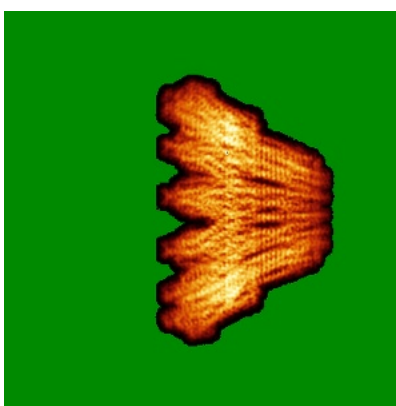
The images above show the largest variance slices of the map in three orthogonal directions.

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

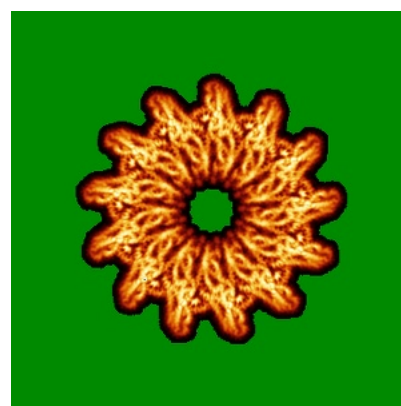
6.4.1 Primary map



X



Y

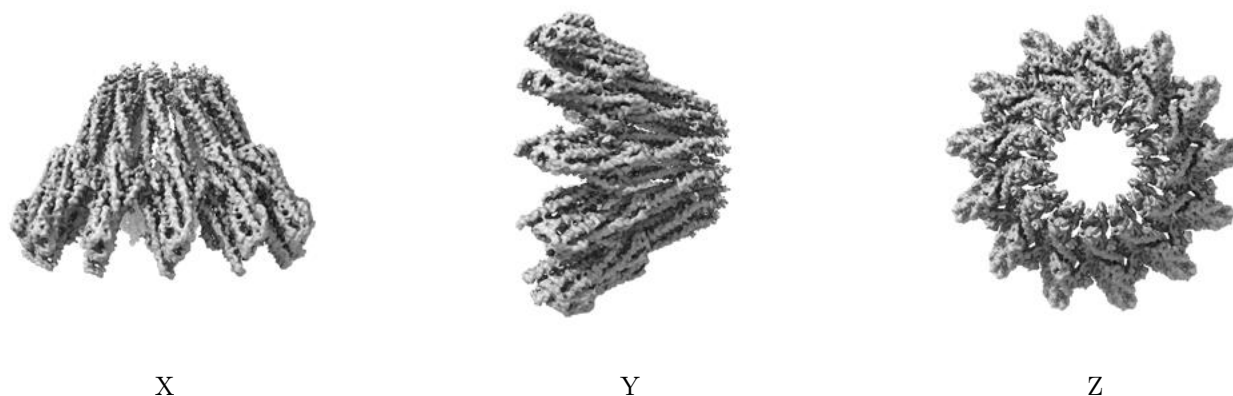


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0192. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

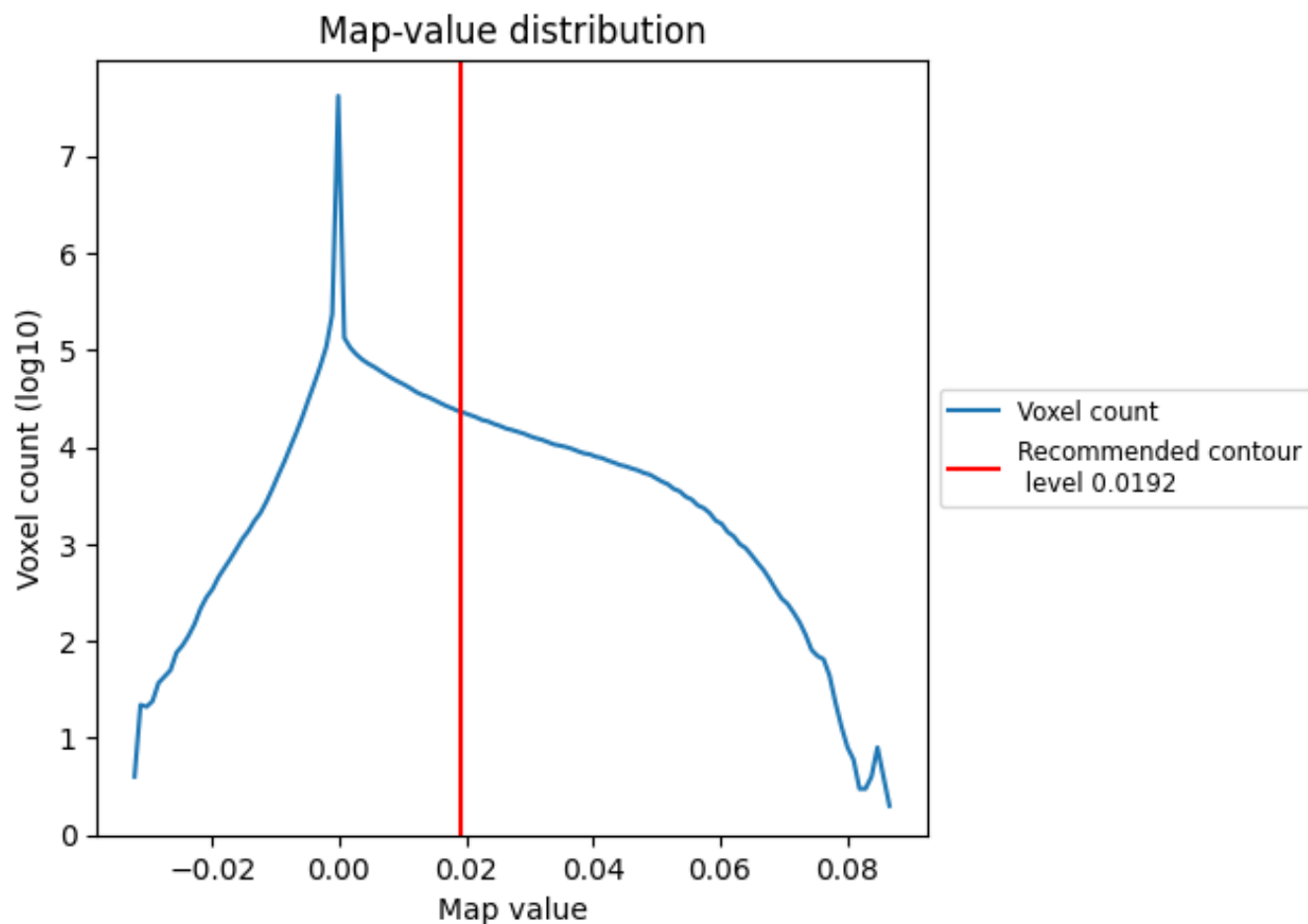
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

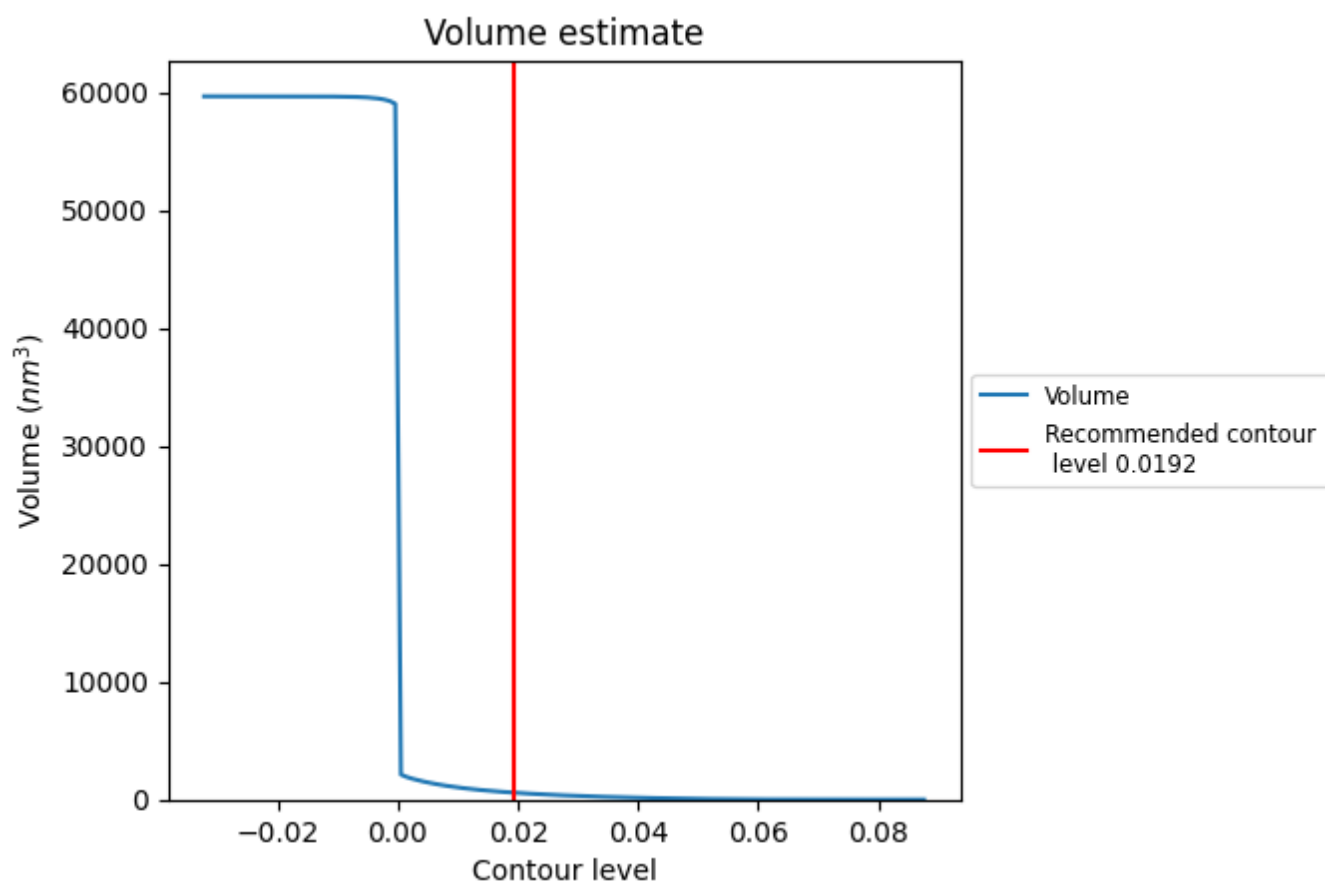
This section contains the results of statistical analysis of the map.

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.

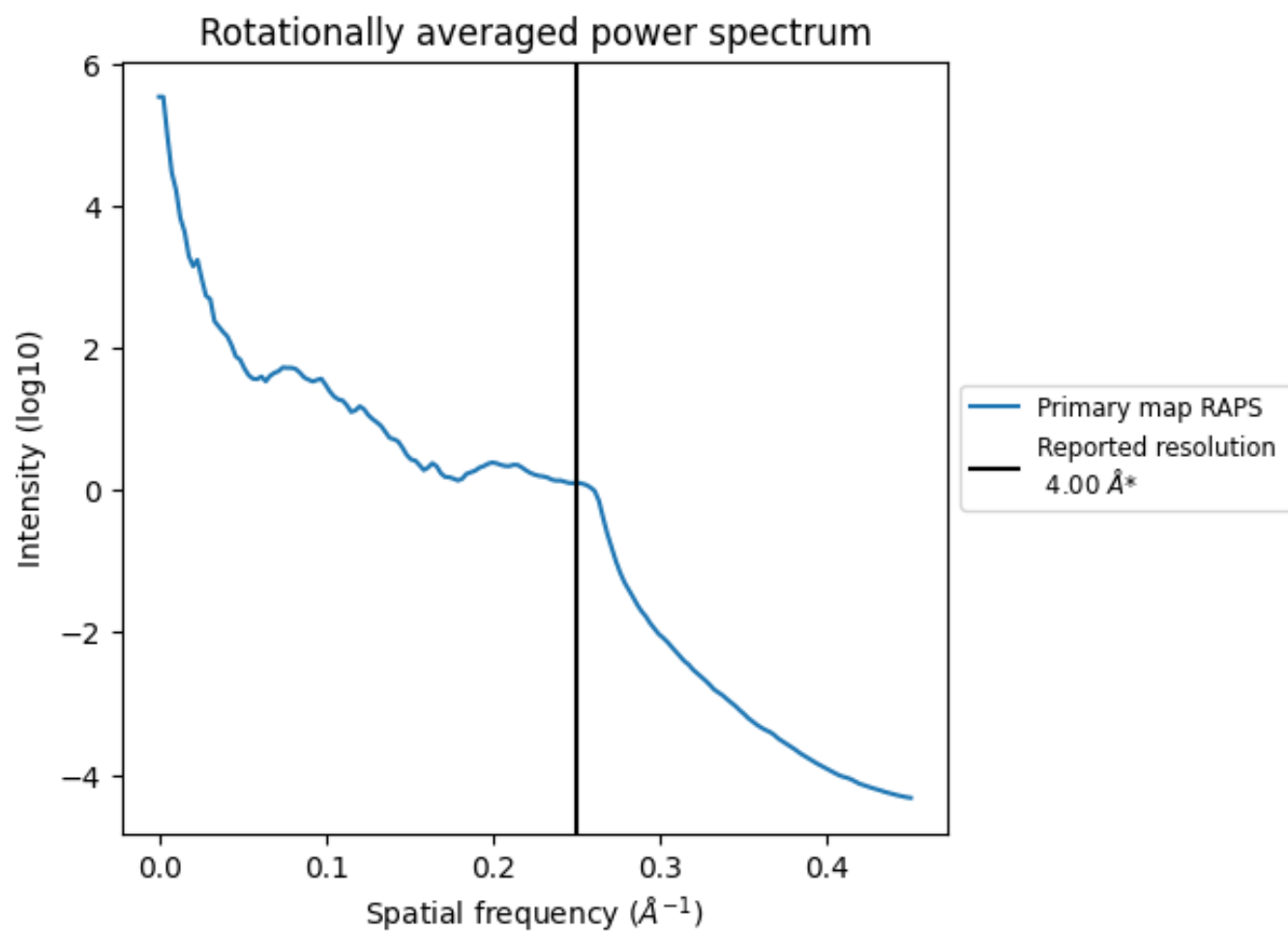
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 589 nm³; this corresponds to an approximate mass of 532 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 0.250 Å⁻¹

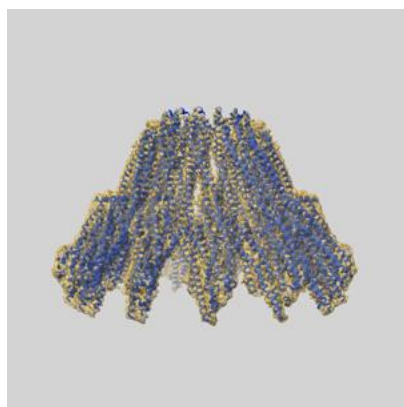
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

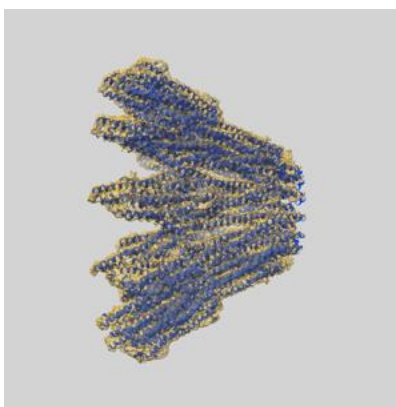
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0088 and PDB model 6GY6. Per-residue inclusion information can be found in section 3 on page 11.

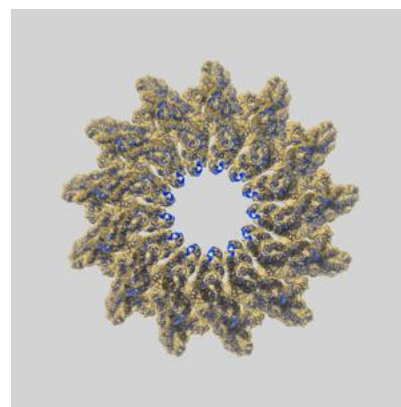
9.1 Map-model overlay [i](#)



X



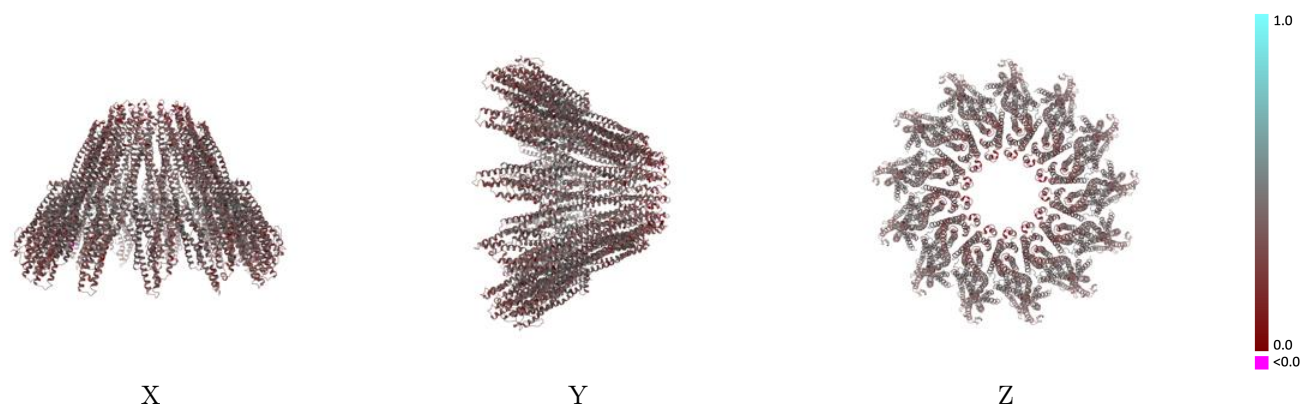
Y



Z

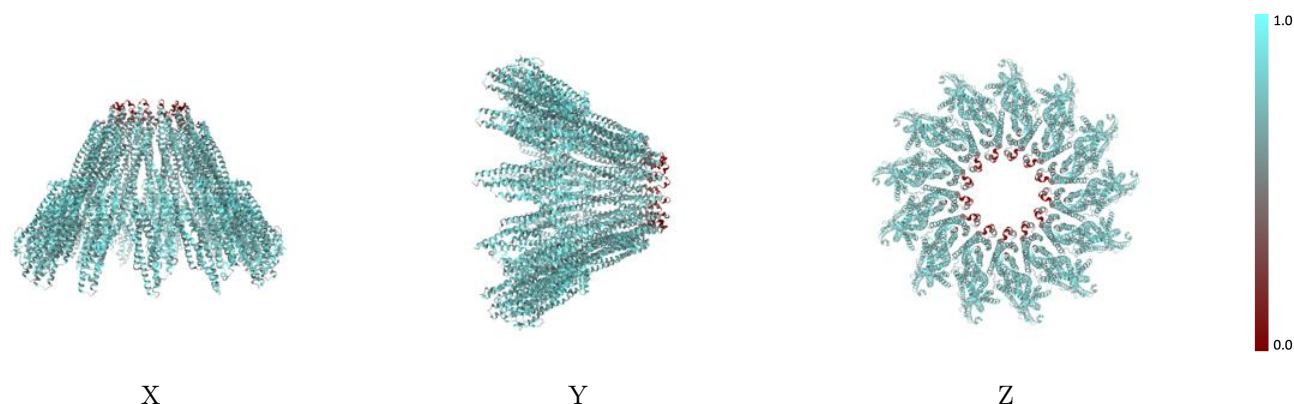
The images above show the 3D surface view of the map at the recommended contour level 0.0192 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



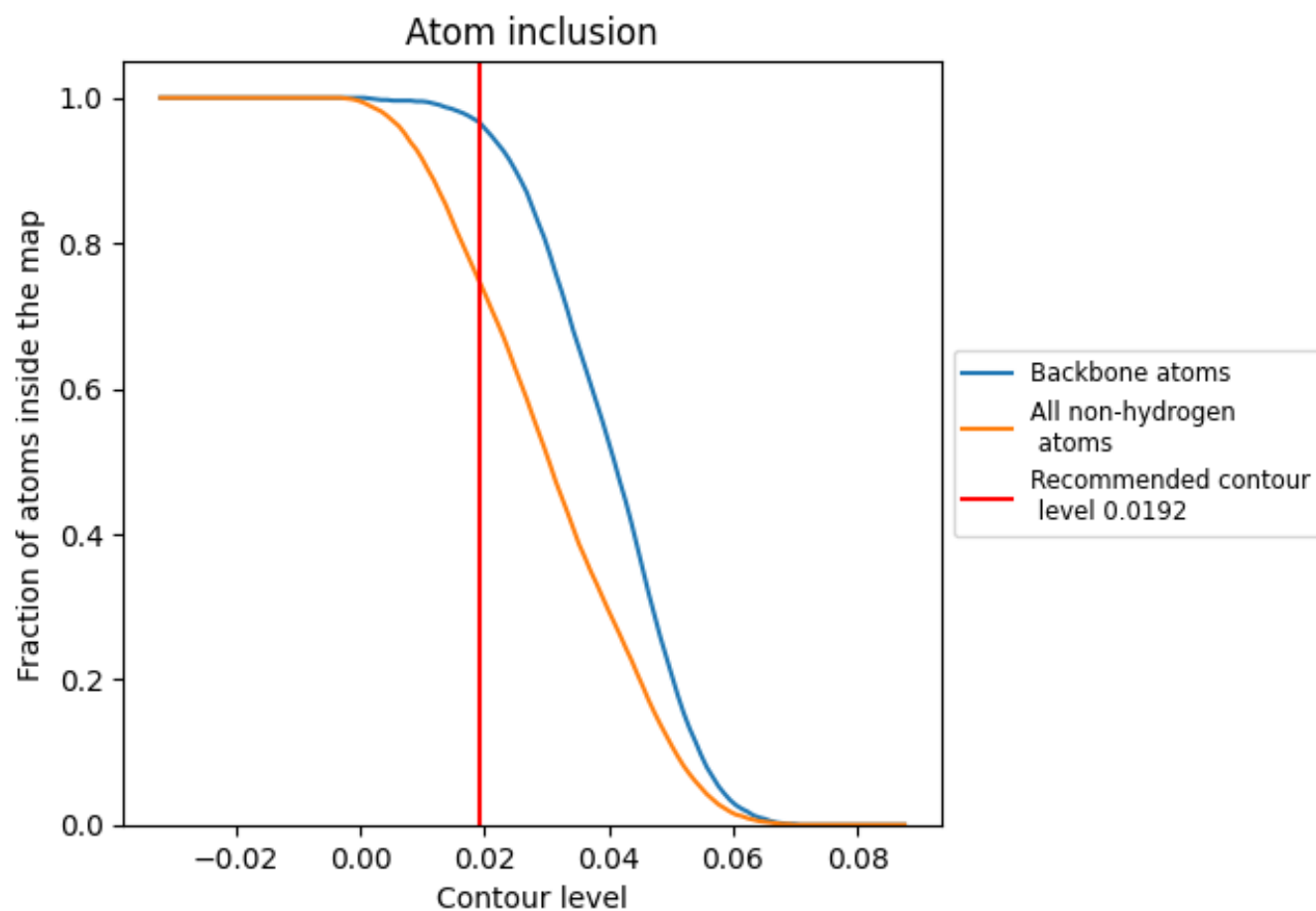
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0192).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.3600
A	 0.7740	 0.3680
B	 0.7160	 0.3540
C	 0.7750	 0.3660
D	 0.7750	 0.3680
E	 0.7750	 0.3660
F	 0.7760	 0.3690
G	 0.7180	 0.3540
H	 0.7200	 0.3530
I	 0.7720	 0.3670
J	 0.7790	 0.3670
K	 0.7160	 0.3530
L	 0.7150	 0.3520
M	 0.7730	 0.3660
N	 0.7150	 0.3550
O	 0.7190	 0.3550
P	 0.7720	 0.3660
Q	 0.7720	 0.3690
R	 0.7750	 0.3660
S	 0.7760	 0.3670
T	 0.7740	 0.3680
U	 0.7150	 0.3550
V	 0.7120	 0.3530
W	 0.7160	 0.3520
X	 0.7170	 0.3540
Y	 0.7170	 0.3510
Z	 0.7150	 0.3520

