



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2025 – 01:33 PM EST

PDB ID : 9MLH
EMDB ID : EMD-48372
Title : Xenorhabdus nematophilus XptA2, wild type State 2
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 3.90 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.dev117
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) : 2.41.4

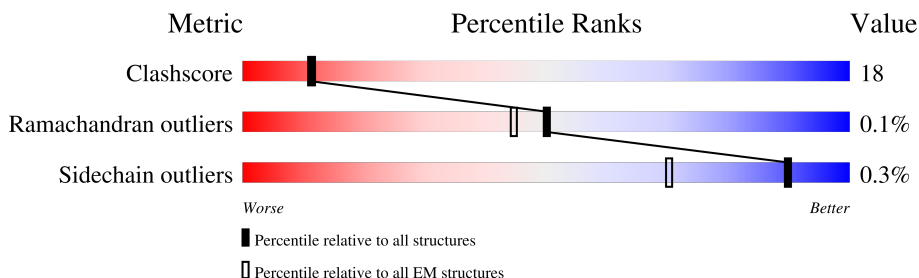
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	2538	
1	B	2538	
1	C	2538	
1	D	2538	
1	E	2538	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100034 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 XptA2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2537	Total 20006	C 12625	N 3414	O 3894	S 73	0	0
1	B	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	C	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	D	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0
1	E	2537	Total 20007	C 12625	N 3415	O 3894	S 73	0	0

There are 605 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	HIS	PRO	conflict	UNP Q93RN7
A	343	ASN	HIS	conflict	UNP Q93RN7
A	344	ILE	VAL	conflict	UNP Q93RN7
A	360	ARG	CYS	conflict	UNP Q93RN7
A	365	VAL	ILE	conflict	UNP Q93RN7
A	377	ALA	SER	conflict	UNP Q93RN7
A	379	PRO	THR	conflict	UNP Q93RN7
A	391	ILE	VAL	conflict	UNP Q93RN7
A	407	SER	ASN	conflict	UNP Q93RN7
A	410	LYS	ARG	conflict	UNP Q93RN7
A	566	VAL	ILE	conflict	UNP Q93RN7
A	583	ALA	THR	conflict	UNP Q93RN7
A	586	THR	ILE	conflict	UNP Q93RN7
A	587	ILE	LEU	conflict	UNP Q93RN7
A	592	PHE	PRO	conflict	UNP Q93RN7
A	606	VAL	ALA	conflict	UNP Q93RN7
A	620	LEU	PHE	conflict	UNP Q93RN7
A	637	PRO	SER	conflict	UNP Q93RN7
A	682	ASN	THR	conflict	UNP Q93RN7
A	686	SER	ARG	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	695	HIS	SER	conflict	UNP Q93RN7
A	696	ASN	ASP	conflict	UNP Q93RN7
A	736	ASP	ASN	conflict	UNP Q93RN7
A	742	THR	MET	conflict	UNP Q93RN7
A	748	SER	THR	conflict	UNP Q93RN7
A	750	ASN	SER	conflict	UNP Q93RN7
A	751	ALA	ASP	conflict	UNP Q93RN7
A	752	ASN	GLU	conflict	UNP Q93RN7
A	788	GLY	ASP	conflict	UNP Q93RN7
A	790	ALA	VAL	conflict	UNP Q93RN7
A	795	LYS	ARG	conflict	UNP Q93RN7
A	796	ASN	SER	conflict	UNP Q93RN7
A	799	ALA	PRO	conflict	UNP Q93RN7
A	800	GLY	ASP	conflict	UNP Q93RN7
A	801	GLN	ASN	conflict	UNP Q93RN7
A	?	-	THR	deletion	UNP Q93RN7
A	?	-	ILE	deletion	UNP Q93RN7
A	?	-	LEU	deletion	UNP Q93RN7
A	?	-	ILE	deletion	UNP Q93RN7
A	?	-	LEU	deletion	UNP Q93RN7
A	?	-	CYS	deletion	UNP Q93RN7
A	?	-	SER	deletion	UNP Q93RN7
A	803	ASN	SER	conflict	UNP Q93RN7
A	804	ILE	THR	conflict	UNP Q93RN7
A	806	THR	SER	conflict	UNP Q93RN7
A	807	LEU	THR	conflict	UNP Q93RN7
A	808	PHE	SER	conflict	UNP Q93RN7
A	809	SER	GLY	conflict	UNP Q93RN7
A	811	TYR	MET	conflict	UNP Q93RN7
A	812	ARG	-	insertion	UNP Q93RN7
A	813	PHE	-	insertion	UNP Q93RN7
A	814	HIS	-	insertion	UNP Q93RN7
A	815	GLN	-	insertion	UNP Q93RN7
A	816	TRP	-	insertion	UNP Q93RN7
A	817	ILE	-	insertion	UNP Q93RN7
A	818	ASN	-	insertion	UNP Q93RN7
A	820	LEU	TRP	conflict	UNP Q93RN7
A	821	GLY	GLU	conflict	UNP Q93RN7
A	822	ASN	ILE	conflict	UNP Q93RN7
A	824	GLY	ALA	conflict	UNP Q93RN7
A	825	SER	LEU	conflict	UNP Q93RN7
A	826	ASP	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	827	THR	ARG	conflict	UNP Q93RN7
A	828	LEU	TRP	conflict	UNP Q93RN7
A	829	ASP	ILE	conflict	UNP Q93RN7
A	830	MET	CYS	conflict	UNP Q93RN7
A	831	LEU	CYS	conflict	UNP Q93RN7
A	832	ARG	ALA	conflict	UNP Q93RN7
A	833	GLN	LYS	conflict	UNP Q93RN7
A	838	ALA	GLY	conflict	UNP Q93RN7
A	842	ALA	GLY	conflict	UNP Q93RN7
A	843	SER	LEU	conflict	UNP Q93RN7
A	844	VAL	ARG	conflict	UNP Q93RN7
A	845	MET	ASP	conflict	UNP Q93RN7
A	847	LEU	ALA	conflict	UNP Q93RN7
A	848	ASP	GLY	conflict	UNP Q93RN7
A	849	ILE	HIS	conflict	UNP Q93RN7
A	850	SER	GLN	conflict	UNP Q93RN7
A	851	MET	TYR	conflict	UNP Q93RN7
A	852	VAL	GLY	conflict	UNP Q93RN7
A	853	THR	ASN	conflict	UNP Q93RN7
A	854	GLN	ALA	conflict	UNP Q93RN7
A	855	ALA	GLY	conflict	UNP Q93RN7
A	856	MET	HIS	conflict	UNP Q93RN7
A	857	VAL	GLY	conflict	UNP Q93RN7
A	872	THR	PRO	conflict	UNP Q93RN7
A	878	ASP	HIS	conflict	UNP Q93RN7
A	884	HIS	ILE	conflict	UNP Q93RN7
A	911	SER	ALA	conflict	UNP Q93RN7
A	914	GLU	LYS	conflict	UNP Q93RN7
A	923	GLU	ALA	conflict	UNP Q93RN7
A	1067	LYS	GLN	conflict	UNP Q93RN7
A	1075	ASP	GLU	conflict	UNP Q93RN7
A	1126	ASP	ASN	conflict	UNP Q93RN7
A	1250	LYS	VAL	conflict	UNP Q93RN7
A	1253	SER	PRO	conflict	UNP Q93RN7
A	1257	GLY	ASP	conflict	UNP Q93RN7
A	1258	SER	ASN	conflict	UNP Q93RN7
A	1514	ILE	VAL	conflict	UNP Q93RN7
A	1519	MET	VAL	conflict	UNP Q93RN7
A	1877	ASN	TYR	conflict	UNP Q93RN7
A	1880	MET	THR	conflict	UNP Q93RN7
A	1884	ILE	VAL	conflict	UNP Q93RN7
A	1920	THR	ALA	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1943	GLY	VAL	conflict	UNP Q93RN7
A	1947	GLN	HIS	conflict	UNP Q93RN7
A	1959	MET	ALA	conflict	UNP Q93RN7
A	1961	GLY	ASP	conflict	UNP Q93RN7
A	1962	ARG	ASN	conflict	UNP Q93RN7
A	1964	GLY	GLU	conflict	UNP Q93RN7
A	1966	SER	ALA	conflict	UNP Q93RN7
A	1967	LYS	THR	conflict	UNP Q93RN7
A	1968	ASN	GLN	conflict	UNP Q93RN7
A	1969	LEU	PRO	conflict	UNP Q93RN7
A	2028	THR	PRO	conflict	UNP Q93RN7
A	2057	THR	ALA	conflict	UNP Q93RN7
A	2149	LEU	PHE	conflict	UNP Q93RN7
A	2161	VAL	ALA	conflict	UNP Q93RN7
A	2164	ILE	VAL	conflict	UNP Q93RN7
A	2178	LEU	PHE	conflict	UNP Q93RN7
A	2430	LEU	PHE	conflict	UNP Q93RN7
B	172	HIS	PRO	conflict	UNP Q93RN7
B	343	ASN	HIS	conflict	UNP Q93RN7
B	344	ILE	VAL	conflict	UNP Q93RN7
B	360	ARG	CYS	conflict	UNP Q93RN7
B	365	VAL	ILE	conflict	UNP Q93RN7
B	377	ALA	SER	conflict	UNP Q93RN7
B	379	PRO	THR	conflict	UNP Q93RN7
B	391	ILE	VAL	conflict	UNP Q93RN7
B	407	SER	ASN	conflict	UNP Q93RN7
B	410	LYS	ARG	conflict	UNP Q93RN7
B	566	VAL	ILE	conflict	UNP Q93RN7
B	583	ALA	THR	conflict	UNP Q93RN7
B	586	THR	ILE	conflict	UNP Q93RN7
B	587	ILE	LEU	conflict	UNP Q93RN7
B	592	PHE	PRO	conflict	UNP Q93RN7
B	606	VAL	ALA	conflict	UNP Q93RN7
B	620	LEU	PHE	conflict	UNP Q93RN7
B	637	PRO	SER	conflict	UNP Q93RN7
B	682	ASN	THR	conflict	UNP Q93RN7
B	686	SER	ARG	conflict	UNP Q93RN7
B	695	HIS	SER	conflict	UNP Q93RN7
B	696	ASN	ASP	conflict	UNP Q93RN7
B	736	ASP	ASN	conflict	UNP Q93RN7
B	742	THR	MET	conflict	UNP Q93RN7
B	748	SER	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	750	ASN	SER	conflict	UNP Q93RN7
B	751	ALA	ASP	conflict	UNP Q93RN7
B	752	ASN	GLU	conflict	UNP Q93RN7
B	788	GLY	ASP	conflict	UNP Q93RN7
B	790	ALA	VAL	conflict	UNP Q93RN7
B	795	LYS	ARG	conflict	UNP Q93RN7
B	796	ASN	SER	conflict	UNP Q93RN7
B	799	ALA	PRO	conflict	UNP Q93RN7
B	800	GLY	ASP	conflict	UNP Q93RN7
B	801	GLN	ASN	conflict	UNP Q93RN7
B	?	-	THR	deletion	UNP Q93RN7
B	?	-	ILE	deletion	UNP Q93RN7
B	?	-	LEU	deletion	UNP Q93RN7
B	?	-	ILE	deletion	UNP Q93RN7
B	?	-	LEU	deletion	UNP Q93RN7
B	?	-	CYS	deletion	UNP Q93RN7
B	?	-	SER	deletion	UNP Q93RN7
B	803	ASN	SER	conflict	UNP Q93RN7
B	804	ILE	THR	conflict	UNP Q93RN7
B	806	THR	SER	conflict	UNP Q93RN7
B	807	LEU	THR	conflict	UNP Q93RN7
B	808	PHE	SER	conflict	UNP Q93RN7
B	809	SER	GLY	conflict	UNP Q93RN7
B	811	TYR	MET	conflict	UNP Q93RN7
B	812	ARG	-	insertion	UNP Q93RN7
B	813	PHE	-	insertion	UNP Q93RN7
B	814	HIS	-	insertion	UNP Q93RN7
B	815	GLN	-	insertion	UNP Q93RN7
B	816	TRP	-	insertion	UNP Q93RN7
B	817	ILE	-	insertion	UNP Q93RN7
B	818	ASN	-	insertion	UNP Q93RN7
B	820	LEU	TRP	conflict	UNP Q93RN7
B	821	GLY	GLU	conflict	UNP Q93RN7
B	822	ASN	ILE	conflict	UNP Q93RN7
B	824	GLY	ALA	conflict	UNP Q93RN7
B	825	SER	LEU	conflict	UNP Q93RN7
B	826	ASP	THR	conflict	UNP Q93RN7
B	827	THR	ARG	conflict	UNP Q93RN7
B	828	LEU	TRP	conflict	UNP Q93RN7
B	829	ASP	ILE	conflict	UNP Q93RN7
B	830	MET	CYS	conflict	UNP Q93RN7
B	831	LEU	CYS	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	832	ARG	ALA	conflict	UNP Q93RN7
B	833	GLN	LYS	conflict	UNP Q93RN7
B	838	ALA	GLY	conflict	UNP Q93RN7
B	842	ALA	GLY	conflict	UNP Q93RN7
B	843	SER	LEU	conflict	UNP Q93RN7
B	844	VAL	ARG	conflict	UNP Q93RN7
B	845	MET	ASP	conflict	UNP Q93RN7
B	847	LEU	ALA	conflict	UNP Q93RN7
B	848	ASP	GLY	conflict	UNP Q93RN7
B	849	ILE	HIS	conflict	UNP Q93RN7
B	850	SER	GLN	conflict	UNP Q93RN7
B	851	MET	TYR	conflict	UNP Q93RN7
B	852	VAL	GLY	conflict	UNP Q93RN7
B	853	THR	ASN	conflict	UNP Q93RN7
B	854	GLN	ALA	conflict	UNP Q93RN7
B	855	ALA	GLY	conflict	UNP Q93RN7
B	856	MET	HIS	conflict	UNP Q93RN7
B	857	VAL	GLY	conflict	UNP Q93RN7
B	872	THR	PRO	conflict	UNP Q93RN7
B	878	ASP	HIS	conflict	UNP Q93RN7
B	884	HIS	ILE	conflict	UNP Q93RN7
B	911	SER	ALA	conflict	UNP Q93RN7
B	914	GLU	LYS	conflict	UNP Q93RN7
B	923	GLU	ALA	conflict	UNP Q93RN7
B	1067	LYS	GLN	conflict	UNP Q93RN7
B	1075	ASP	GLU	conflict	UNP Q93RN7
B	1126	ASP	ASN	conflict	UNP Q93RN7
B	1250	LYS	VAL	conflict	UNP Q93RN7
B	1253	SER	PRO	conflict	UNP Q93RN7
B	1257	GLY	ASP	conflict	UNP Q93RN7
B	1258	SER	ASN	conflict	UNP Q93RN7
B	1514	ILE	VAL	conflict	UNP Q93RN7
B	1519	MET	VAL	conflict	UNP Q93RN7
B	1877	ASN	TYR	conflict	UNP Q93RN7
B	1880	MET	THR	conflict	UNP Q93RN7
B	1884	ILE	VAL	conflict	UNP Q93RN7
B	1920	THR	ALA	conflict	UNP Q93RN7
B	1943	GLY	VAL	conflict	UNP Q93RN7
B	1947	GLN	HIS	conflict	UNP Q93RN7
B	1959	MET	ALA	conflict	UNP Q93RN7
B	1961	GLY	ASP	conflict	UNP Q93RN7
B	1962	ARG	ASN	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1964	GLY	GLU	conflict	UNP Q93RN7
B	1966	SER	ALA	conflict	UNP Q93RN7
B	1967	LYS	THR	conflict	UNP Q93RN7
B	1968	ASN	GLN	conflict	UNP Q93RN7
B	1969	LEU	PRO	conflict	UNP Q93RN7
B	2028	THR	PRO	conflict	UNP Q93RN7
B	2057	THR	ALA	conflict	UNP Q93RN7
B	2149	LEU	PHE	conflict	UNP Q93RN7
B	2161	VAL	ALA	conflict	UNP Q93RN7
B	2164	ILE	VAL	conflict	UNP Q93RN7
B	2178	LEU	PHE	conflict	UNP Q93RN7
B	2430	LEU	PHE	conflict	UNP Q93RN7
C	172	HIS	PRO	conflict	UNP Q93RN7
C	343	ASN	HIS	conflict	UNP Q93RN7
C	344	ILE	VAL	conflict	UNP Q93RN7
C	360	ARG	CYS	conflict	UNP Q93RN7
C	365	VAL	ILE	conflict	UNP Q93RN7
C	377	ALA	SER	conflict	UNP Q93RN7
C	379	PRO	THR	conflict	UNP Q93RN7
C	391	ILE	VAL	conflict	UNP Q93RN7
C	407	SER	ASN	conflict	UNP Q93RN7
C	410	LYS	ARG	conflict	UNP Q93RN7
C	566	VAL	ILE	conflict	UNP Q93RN7
C	583	ALA	THR	conflict	UNP Q93RN7
C	586	THR	ILE	conflict	UNP Q93RN7
C	587	ILE	LEU	conflict	UNP Q93RN7
C	592	PHE	PRO	conflict	UNP Q93RN7
C	606	VAL	ALA	conflict	UNP Q93RN7
C	620	LEU	PHE	conflict	UNP Q93RN7
C	637	PRO	SER	conflict	UNP Q93RN7
C	682	ASN	THR	conflict	UNP Q93RN7
C	686	SER	ARG	conflict	UNP Q93RN7
C	695	HIS	SER	conflict	UNP Q93RN7
C	696	ASN	ASP	conflict	UNP Q93RN7
C	736	ASP	ASN	conflict	UNP Q93RN7
C	742	THR	MET	conflict	UNP Q93RN7
C	748	SER	THR	conflict	UNP Q93RN7
C	750	ASN	SER	conflict	UNP Q93RN7
C	751	ALA	ASP	conflict	UNP Q93RN7
C	752	ASN	GLU	conflict	UNP Q93RN7
C	788	GLY	ASP	conflict	UNP Q93RN7
C	790	ALA	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	795	LYS	ARG	conflict	UNP Q93RN7
C	796	ASN	SER	conflict	UNP Q93RN7
C	799	ALA	PRO	conflict	UNP Q93RN7
C	800	GLY	ASP	conflict	UNP Q93RN7
C	801	GLN	ASN	conflict	UNP Q93RN7
C	?	-	THR	deletion	UNP Q93RN7
C	?	-	ILE	deletion	UNP Q93RN7
C	?	-	LEU	deletion	UNP Q93RN7
C	?	-	ILE	deletion	UNP Q93RN7
C	?	-	LEU	deletion	UNP Q93RN7
C	?	-	CYS	deletion	UNP Q93RN7
C	?	-	SER	deletion	UNP Q93RN7
C	803	ASN	SER	conflict	UNP Q93RN7
C	804	ILE	THR	conflict	UNP Q93RN7
C	806	THR	SER	conflict	UNP Q93RN7
C	807	LEU	THR	conflict	UNP Q93RN7
C	808	PHE	SER	conflict	UNP Q93RN7
C	809	SER	GLY	conflict	UNP Q93RN7
C	811	TYR	MET	conflict	UNP Q93RN7
C	812	ARG	-	insertion	UNP Q93RN7
C	813	PHE	-	insertion	UNP Q93RN7
C	814	HIS	-	insertion	UNP Q93RN7
C	815	GLN	-	insertion	UNP Q93RN7
C	816	TRP	-	insertion	UNP Q93RN7
C	817	ILE	-	insertion	UNP Q93RN7
C	818	ASN	-	insertion	UNP Q93RN7
C	820	LEU	TRP	conflict	UNP Q93RN7
C	821	GLY	GLU	conflict	UNP Q93RN7
C	822	ASN	ILE	conflict	UNP Q93RN7
C	824	GLY	ALA	conflict	UNP Q93RN7
C	825	SER	LEU	conflict	UNP Q93RN7
C	826	ASP	THR	conflict	UNP Q93RN7
C	827	THR	ARG	conflict	UNP Q93RN7
C	828	LEU	TRP	conflict	UNP Q93RN7
C	829	ASP	ILE	conflict	UNP Q93RN7
C	830	MET	CYS	conflict	UNP Q93RN7
C	831	LEU	CYS	conflict	UNP Q93RN7
C	832	ARG	ALA	conflict	UNP Q93RN7
C	833	GLN	LYS	conflict	UNP Q93RN7
C	838	ALA	GLY	conflict	UNP Q93RN7
C	842	ALA	GLY	conflict	UNP Q93RN7
C	843	SER	LEU	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	844	VAL	ARG	conflict	UNP Q93RN7
C	845	MET	ASP	conflict	UNP Q93RN7
C	847	LEU	ALA	conflict	UNP Q93RN7
C	848	ASP	GLY	conflict	UNP Q93RN7
C	849	ILE	HIS	conflict	UNP Q93RN7
C	850	SER	GLN	conflict	UNP Q93RN7
C	851	MET	TYR	conflict	UNP Q93RN7
C	852	VAL	GLY	conflict	UNP Q93RN7
C	853	THR	ASN	conflict	UNP Q93RN7
C	854	GLN	ALA	conflict	UNP Q93RN7
C	855	ALA	GLY	conflict	UNP Q93RN7
C	856	MET	HIS	conflict	UNP Q93RN7
C	857	VAL	GLY	conflict	UNP Q93RN7
C	872	THR	PRO	conflict	UNP Q93RN7
C	878	ASP	HIS	conflict	UNP Q93RN7
C	884	HIS	ILE	conflict	UNP Q93RN7
C	911	SER	ALA	conflict	UNP Q93RN7
C	914	GLU	LYS	conflict	UNP Q93RN7
C	923	GLU	ALA	conflict	UNP Q93RN7
C	1067	LYS	GLN	conflict	UNP Q93RN7
C	1075	ASP	GLU	conflict	UNP Q93RN7
C	1126	ASP	ASN	conflict	UNP Q93RN7
C	1250	LYS	VAL	conflict	UNP Q93RN7
C	1253	SER	PRO	conflict	UNP Q93RN7
C	1257	GLY	ASP	conflict	UNP Q93RN7
C	1258	SER	ASN	conflict	UNP Q93RN7
C	1514	ILE	VAL	conflict	UNP Q93RN7
C	1519	MET	VAL	conflict	UNP Q93RN7
C	1877	ASN	TYR	conflict	UNP Q93RN7
C	1880	MET	THR	conflict	UNP Q93RN7
C	1884	ILE	VAL	conflict	UNP Q93RN7
C	1920	THR	ALA	conflict	UNP Q93RN7
C	1943	GLY	VAL	conflict	UNP Q93RN7
C	1947	GLN	HIS	conflict	UNP Q93RN7
C	1959	MET	ALA	conflict	UNP Q93RN7
C	1961	GLY	ASP	conflict	UNP Q93RN7
C	1962	ARG	ASN	conflict	UNP Q93RN7
C	1964	GLY	GLU	conflict	UNP Q93RN7
C	1966	SER	ALA	conflict	UNP Q93RN7
C	1967	LYS	THR	conflict	UNP Q93RN7
C	1968	ASN	GLN	conflict	UNP Q93RN7
C	1969	LEU	PRO	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2028	THR	PRO	conflict	UNP Q93RN7
C	2057	THR	ALA	conflict	UNP Q93RN7
C	2149	LEU	PHE	conflict	UNP Q93RN7
C	2161	VAL	ALA	conflict	UNP Q93RN7
C	2164	ILE	VAL	conflict	UNP Q93RN7
C	2178	LEU	PHE	conflict	UNP Q93RN7
C	2430	LEU	PHE	conflict	UNP Q93RN7
D	172	HIS	PRO	conflict	UNP Q93RN7
D	343	ASN	HIS	conflict	UNP Q93RN7
D	344	ILE	VAL	conflict	UNP Q93RN7
D	360	ARG	CYS	conflict	UNP Q93RN7
D	365	VAL	ILE	conflict	UNP Q93RN7
D	377	ALA	SER	conflict	UNP Q93RN7
D	379	PRO	THR	conflict	UNP Q93RN7
D	391	ILE	VAL	conflict	UNP Q93RN7
D	407	SER	ASN	conflict	UNP Q93RN7
D	410	LYS	ARG	conflict	UNP Q93RN7
D	566	VAL	ILE	conflict	UNP Q93RN7
D	583	ALA	THR	conflict	UNP Q93RN7
D	586	THR	ILE	conflict	UNP Q93RN7
D	587	ILE	LEU	conflict	UNP Q93RN7
D	592	PHE	PRO	conflict	UNP Q93RN7
D	606	VAL	ALA	conflict	UNP Q93RN7
D	620	LEU	PHE	conflict	UNP Q93RN7
D	637	PRO	SER	conflict	UNP Q93RN7
D	682	ASN	THR	conflict	UNP Q93RN7
D	686	SER	ARG	conflict	UNP Q93RN7
D	695	HIS	SER	conflict	UNP Q93RN7
D	696	ASN	ASP	conflict	UNP Q93RN7
D	736	ASP	ASN	conflict	UNP Q93RN7
D	742	THR	MET	conflict	UNP Q93RN7
D	748	SER	THR	conflict	UNP Q93RN7
D	750	ASN	SER	conflict	UNP Q93RN7
D	751	ALA	ASP	conflict	UNP Q93RN7
D	752	ASN	GLU	conflict	UNP Q93RN7
D	788	GLY	ASP	conflict	UNP Q93RN7
D	790	ALA	VAL	conflict	UNP Q93RN7
D	795	LYS	ARG	conflict	UNP Q93RN7
D	796	ASN	SER	conflict	UNP Q93RN7
D	799	ALA	PRO	conflict	UNP Q93RN7
D	800	GLY	ASP	conflict	UNP Q93RN7
D	801	GLN	ASN	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	THR	deletion	UNP Q93RN7
D	?	-	ILE	deletion	UNP Q93RN7
D	?	-	LEU	deletion	UNP Q93RN7
D	?	-	ILE	deletion	UNP Q93RN7
D	?	-	LEU	deletion	UNP Q93RN7
D	?	-	CYS	deletion	UNP Q93RN7
D	?	-	SER	deletion	UNP Q93RN7
D	803	ASN	SER	conflict	UNP Q93RN7
D	804	ILE	THR	conflict	UNP Q93RN7
D	806	THR	SER	conflict	UNP Q93RN7
D	807	LEU	THR	conflict	UNP Q93RN7
D	808	PHE	SER	conflict	UNP Q93RN7
D	809	SER	GLY	conflict	UNP Q93RN7
D	811	TYR	MET	conflict	UNP Q93RN7
D	812	ARG	-	insertion	UNP Q93RN7
D	813	PHE	-	insertion	UNP Q93RN7
D	814	HIS	-	insertion	UNP Q93RN7
D	815	GLN	-	insertion	UNP Q93RN7
D	816	TRP	-	insertion	UNP Q93RN7
D	817	ILE	-	insertion	UNP Q93RN7
D	818	ASN	-	insertion	UNP Q93RN7
D	820	LEU	TRP	conflict	UNP Q93RN7
D	821	GLY	GLU	conflict	UNP Q93RN7
D	822	ASN	ILE	conflict	UNP Q93RN7
D	824	GLY	ALA	conflict	UNP Q93RN7
D	825	SER	LEU	conflict	UNP Q93RN7
D	826	ASP	THR	conflict	UNP Q93RN7
D	827	THR	ARG	conflict	UNP Q93RN7
D	828	LEU	TRP	conflict	UNP Q93RN7
D	829	ASP	ILE	conflict	UNP Q93RN7
D	830	MET	CYS	conflict	UNP Q93RN7
D	831	LEU	CYS	conflict	UNP Q93RN7
D	832	ARG	ALA	conflict	UNP Q93RN7
D	833	GLN	LYS	conflict	UNP Q93RN7
D	838	ALA	GLY	conflict	UNP Q93RN7
D	842	ALA	GLY	conflict	UNP Q93RN7
D	843	SER	LEU	conflict	UNP Q93RN7
D	844	VAL	ARG	conflict	UNP Q93RN7
D	845	MET	ASP	conflict	UNP Q93RN7
D	847	LEU	ALA	conflict	UNP Q93RN7
D	848	ASP	GLY	conflict	UNP Q93RN7
D	849	ILE	HIS	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	850	SER	GLN	conflict	UNP Q93RN7
D	851	MET	TYR	conflict	UNP Q93RN7
D	852	VAL	GLY	conflict	UNP Q93RN7
D	853	THR	ASN	conflict	UNP Q93RN7
D	854	GLN	ALA	conflict	UNP Q93RN7
D	855	ALA	GLY	conflict	UNP Q93RN7
D	856	MET	HIS	conflict	UNP Q93RN7
D	857	VAL	GLY	conflict	UNP Q93RN7
D	872	THR	PRO	conflict	UNP Q93RN7
D	878	ASP	HIS	conflict	UNP Q93RN7
D	884	HIS	ILE	conflict	UNP Q93RN7
D	911	SER	ALA	conflict	UNP Q93RN7
D	914	GLU	LYS	conflict	UNP Q93RN7
D	923	GLU	ALA	conflict	UNP Q93RN7
D	1067	LYS	GLN	conflict	UNP Q93RN7
D	1075	ASP	GLU	conflict	UNP Q93RN7
D	1126	ASP	ASN	conflict	UNP Q93RN7
D	1250	LYS	VAL	conflict	UNP Q93RN7
D	1253	SER	PRO	conflict	UNP Q93RN7
D	1257	GLY	ASP	conflict	UNP Q93RN7
D	1258	SER	ASN	conflict	UNP Q93RN7
D	1514	ILE	VAL	conflict	UNP Q93RN7
D	1519	MET	VAL	conflict	UNP Q93RN7
D	1877	ASN	TYR	conflict	UNP Q93RN7
D	1880	MET	THR	conflict	UNP Q93RN7
D	1884	ILE	VAL	conflict	UNP Q93RN7
D	1920	THR	ALA	conflict	UNP Q93RN7
D	1943	GLY	VAL	conflict	UNP Q93RN7
D	1947	GLN	HIS	conflict	UNP Q93RN7
D	1959	MET	ALA	conflict	UNP Q93RN7
D	1961	GLY	ASP	conflict	UNP Q93RN7
D	1962	ARG	ASN	conflict	UNP Q93RN7
D	1964	GLY	GLU	conflict	UNP Q93RN7
D	1966	SER	ALA	conflict	UNP Q93RN7
D	1967	LYS	THR	conflict	UNP Q93RN7
D	1968	ASN	GLN	conflict	UNP Q93RN7
D	1969	LEU	PRO	conflict	UNP Q93RN7
D	2028	THR	PRO	conflict	UNP Q93RN7
D	2057	THR	ALA	conflict	UNP Q93RN7
D	2149	LEU	PHE	conflict	UNP Q93RN7
D	2161	VAL	ALA	conflict	UNP Q93RN7
D	2164	ILE	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2178	LEU	PHE	conflict	UNP Q93RN7
D	2430	LEU	PHE	conflict	UNP Q93RN7
E	172	HIS	PRO	conflict	UNP Q93RN7
E	343	ASN	HIS	conflict	UNP Q93RN7
E	344	ILE	VAL	conflict	UNP Q93RN7
E	360	ARG	CYS	conflict	UNP Q93RN7
E	365	VAL	ILE	conflict	UNP Q93RN7
E	377	ALA	SER	conflict	UNP Q93RN7
E	379	PRO	THR	conflict	UNP Q93RN7
E	391	ILE	VAL	conflict	UNP Q93RN7
E	407	SER	ASN	conflict	UNP Q93RN7
E	410	LYS	ARG	conflict	UNP Q93RN7
E	566	VAL	ILE	conflict	UNP Q93RN7
E	583	ALA	THR	conflict	UNP Q93RN7
E	586	THR	ILE	conflict	UNP Q93RN7
E	587	ILE	LEU	conflict	UNP Q93RN7
E	592	PHE	PRO	conflict	UNP Q93RN7
E	606	VAL	ALA	conflict	UNP Q93RN7
E	620	LEU	PHE	conflict	UNP Q93RN7
E	637	PRO	SER	conflict	UNP Q93RN7
E	682	ASN	THR	conflict	UNP Q93RN7
E	686	SER	ARG	conflict	UNP Q93RN7
E	695	HIS	SER	conflict	UNP Q93RN7
E	696	ASN	ASP	conflict	UNP Q93RN7
E	736	ASP	ASN	conflict	UNP Q93RN7
E	742	THR	MET	conflict	UNP Q93RN7
E	748	SER	THR	conflict	UNP Q93RN7
E	750	ASN	SER	conflict	UNP Q93RN7
E	751	ALA	ASP	conflict	UNP Q93RN7
E	752	ASN	GLU	conflict	UNP Q93RN7
E	788	GLY	ASP	conflict	UNP Q93RN7
E	790	ALA	VAL	conflict	UNP Q93RN7
E	795	LYS	ARG	conflict	UNP Q93RN7
E	796	ASN	SER	conflict	UNP Q93RN7
E	799	ALA	PRO	conflict	UNP Q93RN7
E	800	GLY	ASP	conflict	UNP Q93RN7
E	801	GLN	ASN	conflict	UNP Q93RN7
E	?	-	THR	deletion	UNP Q93RN7
E	?	-	ILE	deletion	UNP Q93RN7
E	?	-	LEU	deletion	UNP Q93RN7
E	?	-	ILE	deletion	UNP Q93RN7
E	?	-	LEU	deletion	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	CYS	deletion	UNP Q93RN7
E	?	-	SER	deletion	UNP Q93RN7
E	803	ASN	SER	conflict	UNP Q93RN7
E	804	ILE	THR	conflict	UNP Q93RN7
E	806	THR	SER	conflict	UNP Q93RN7
E	807	LEU	THR	conflict	UNP Q93RN7
E	808	PHE	SER	conflict	UNP Q93RN7
E	809	SER	GLY	conflict	UNP Q93RN7
E	811	TYR	MET	conflict	UNP Q93RN7
E	812	ARG	-	insertion	UNP Q93RN7
E	813	PHE	-	insertion	UNP Q93RN7
E	814	HIS	-	insertion	UNP Q93RN7
E	815	GLN	-	insertion	UNP Q93RN7
E	816	TRP	-	insertion	UNP Q93RN7
E	817	ILE	-	insertion	UNP Q93RN7
E	818	ASN	-	insertion	UNP Q93RN7
E	820	LEU	TRP	conflict	UNP Q93RN7
E	821	GLY	GLU	conflict	UNP Q93RN7
E	822	ASN	ILE	conflict	UNP Q93RN7
E	824	GLY	ALA	conflict	UNP Q93RN7
E	825	SER	LEU	conflict	UNP Q93RN7
E	826	ASP	THR	conflict	UNP Q93RN7
E	827	THR	ARG	conflict	UNP Q93RN7
E	828	LEU	TRP	conflict	UNP Q93RN7
E	829	ASP	ILE	conflict	UNP Q93RN7
E	830	MET	CYS	conflict	UNP Q93RN7
E	831	LEU	CYS	conflict	UNP Q93RN7
E	832	ARG	ALA	conflict	UNP Q93RN7
E	833	GLN	LYS	conflict	UNP Q93RN7
E	838	ALA	GLY	conflict	UNP Q93RN7
E	842	ALA	GLY	conflict	UNP Q93RN7
E	843	SER	LEU	conflict	UNP Q93RN7
E	844	VAL	ARG	conflict	UNP Q93RN7
E	845	MET	ASP	conflict	UNP Q93RN7
E	847	LEU	ALA	conflict	UNP Q93RN7
E	848	ASP	GLY	conflict	UNP Q93RN7
E	849	ILE	HIS	conflict	UNP Q93RN7
E	850	SER	GLN	conflict	UNP Q93RN7
E	851	MET	TYR	conflict	UNP Q93RN7
E	852	VAL	GLY	conflict	UNP Q93RN7
E	853	THR	ASN	conflict	UNP Q93RN7
E	854	GLN	ALA	conflict	UNP Q93RN7

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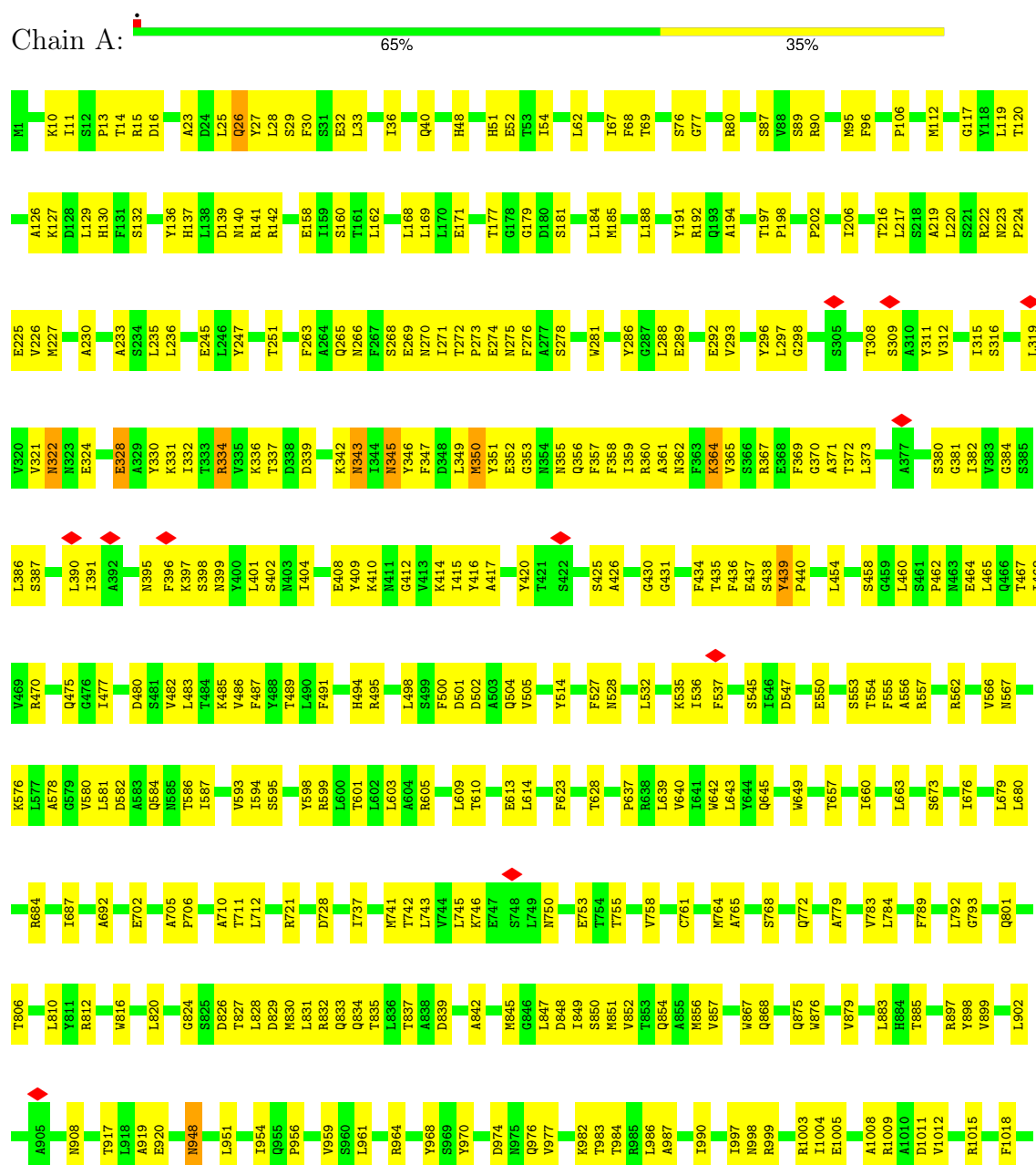
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Chain	Residue	Modelled	Actual	Comment	Reference
E	855	ALA	GLY	conflict	UNP Q93RN7
E	856	MET	HIS	conflict	UNP Q93RN7
E	857	VAL	GLY	conflict	UNP Q93RN7
E	872	THR	PRO	conflict	UNP Q93RN7
E	878	ASP	HIS	conflict	UNP Q93RN7
E	884	HIS	ILE	conflict	UNP Q93RN7
E	911	SER	ALA	conflict	UNP Q93RN7
E	914	GLU	LYS	conflict	UNP Q93RN7
E	923	GLU	ALA	conflict	UNP Q93RN7
E	1067	LYS	GLN	conflict	UNP Q93RN7
E	1075	ASP	GLU	conflict	UNP Q93RN7
E	1126	ASP	ASN	conflict	UNP Q93RN7
E	1250	LYS	VAL	conflict	UNP Q93RN7
E	1253	SER	PRO	conflict	UNP Q93RN7
E	1257	GLY	ASP	conflict	UNP Q93RN7
E	1258	SER	ASN	conflict	UNP Q93RN7
E	1514	ILE	VAL	conflict	UNP Q93RN7
E	1519	MET	VAL	conflict	UNP Q93RN7
E	1877	ASN	TYR	conflict	UNP Q93RN7
E	1880	MET	THR	conflict	UNP Q93RN7
E	1884	ILE	VAL	conflict	UNP Q93RN7
E	1920	THR	ALA	conflict	UNP Q93RN7
E	1943	GLY	VAL	conflict	UNP Q93RN7
E	1947	GLN	HIS	conflict	UNP Q93RN7
E	1959	MET	ALA	conflict	UNP Q93RN7
E	1961	GLY	ASP	conflict	UNP Q93RN7
E	1962	ARG	ASN	conflict	UNP Q93RN7
E	1964	GLY	GLU	conflict	UNP Q93RN7
E	1966	SER	ALA	conflict	UNP Q93RN7
E	1967	LYS	THR	conflict	UNP Q93RN7
E	1968	ASN	GLN	conflict	UNP Q93RN7
E	1969	LEU	PRO	conflict	UNP Q93RN7
E	2028	THR	PRO	conflict	UNP Q93RN7
E	2057	THR	ALA	conflict	UNP Q93RN7
E	2149	LEU	PHE	conflict	UNP Q93RN7
E	2161	VAL	ALA	conflict	UNP Q93RN7
E	2164	ILE	VAL	conflict	UNP Q93RN7
E	2178	LEU	PHE	conflict	UNP Q93RN7
E	2430	LEU	PHE	conflict	UNP Q93RN7

3 Residue-property plots

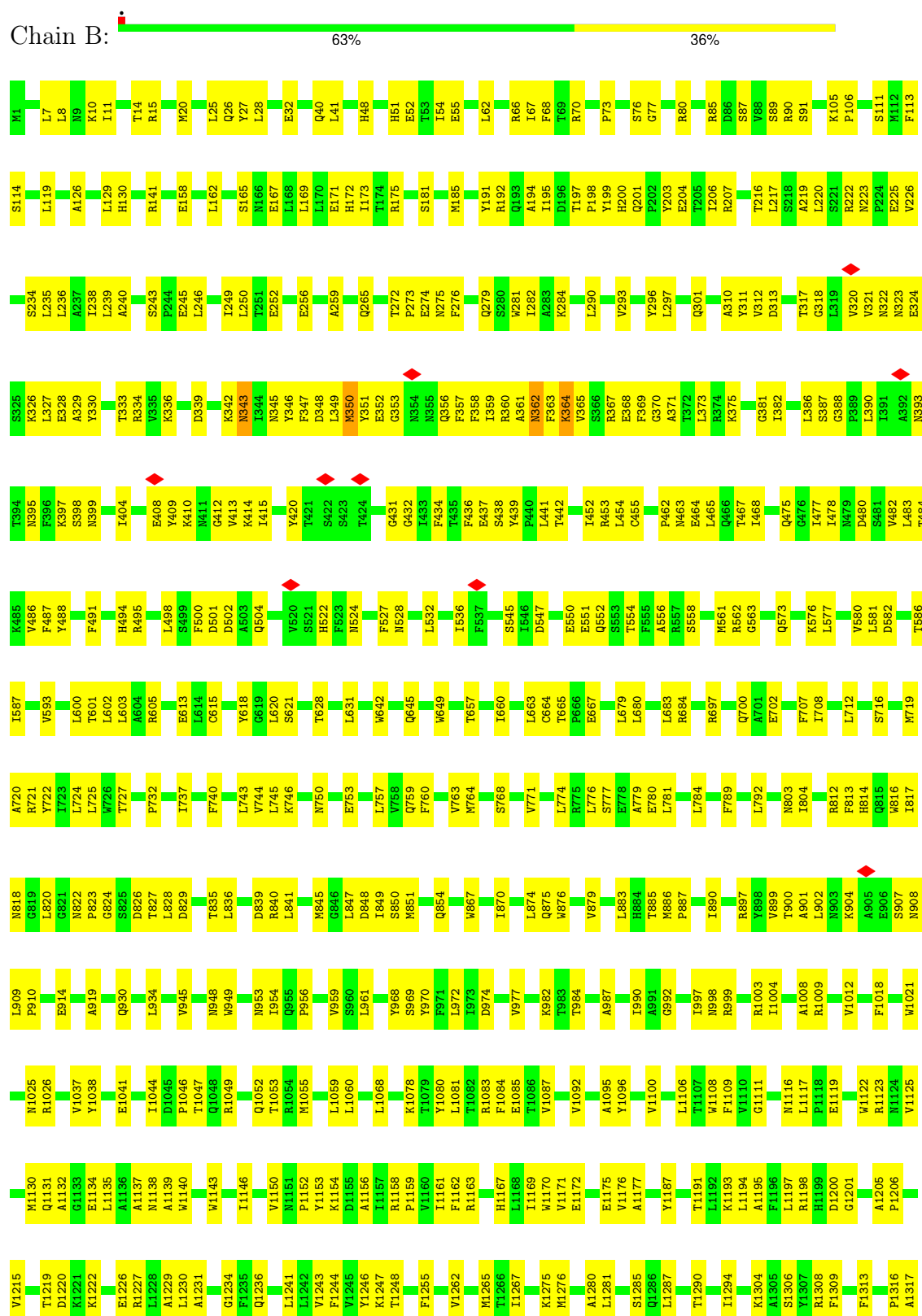
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: XptA2 protein





• Molecule 1: XptA2 protein



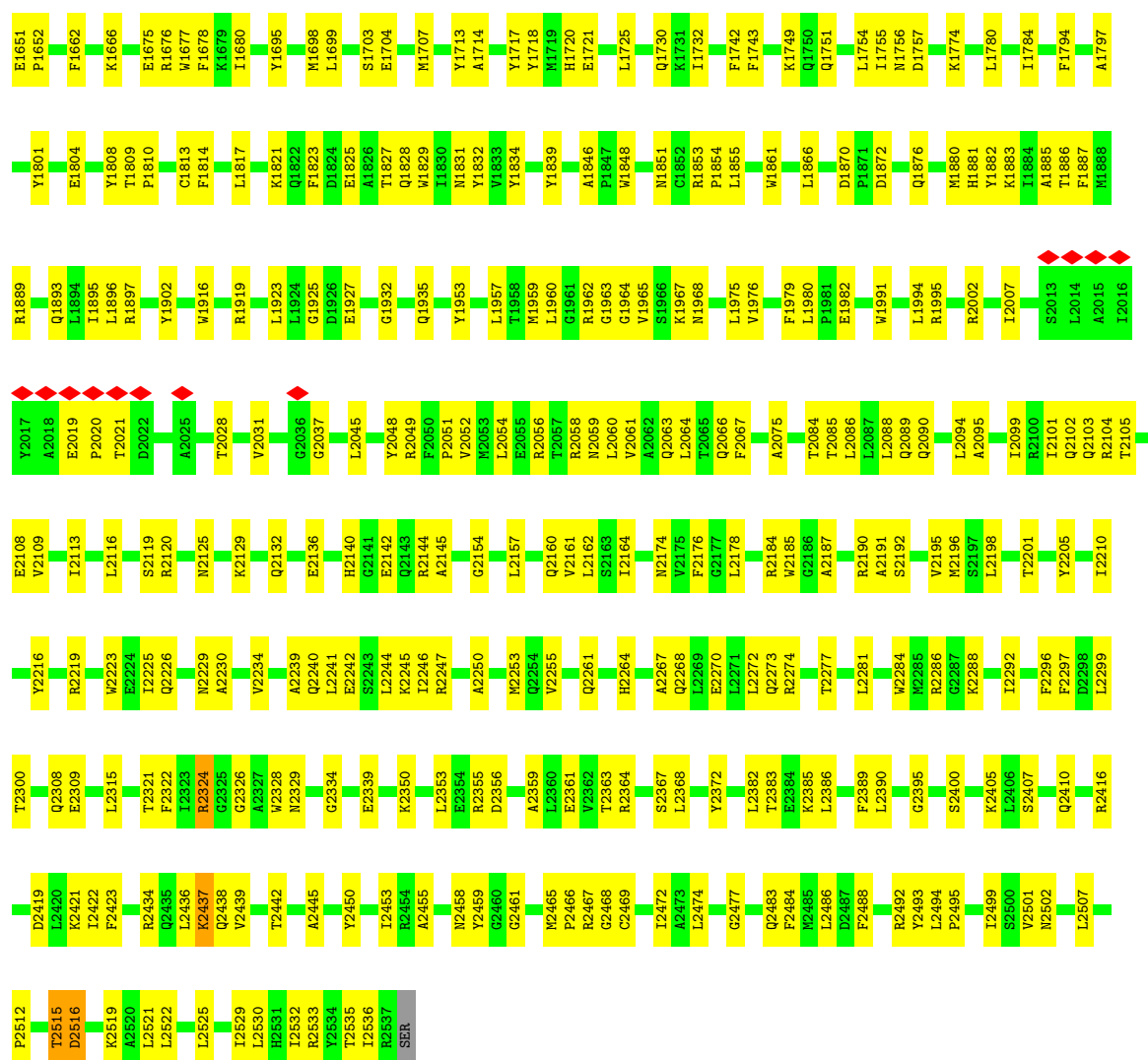
S1318	V1425	N1510	R1604	H1720	Q1828	L1960	E2055	S2163	E2249	E2347	V2456
L1319	N1431	N1511	A1610	E1721	W1829	L1960	R2056	I2164	A2250	W2348	L2457
M1320	T1434	T1514	Q1611	G1722	N1830	G1963	T2057	A2185	A2251	E2349	N2458
M1321	T1435	T1515	Q1612	L1725	N1831	G1964	R2058	E2166	K2252	K2351	Y2459
T1331	R1436	T1516	M1613	G1726	Y1832	N1965	N2059	N2174	Q2254	W2352	G2460
V1332	R1437	T1517	Q1614	V1727	Y1833	S1966	V2061	V2061	V2255	L2353	G2461
Q1340	L1438	V1518	Y1618	G1728	G1838	K1967	A2062	L2178	Q2258	R2388	N2465
I1341	L1440	V1519	T1624	Q1730	Y1839	T1970	Q2063	A2179	Q2261	T2363	P2466
T1342	T1441	T1520	L1625	Q1731	Y1840	T1971	L2064	G2182	Q2262	R2364	R2467
Y1345	V1442	F1527	L1626	T1732	A1846	L1975	Q2065	S2183	H2264	L2388	G2468
L1350	V1443	S1530	A1627	T1733	W1843	V1976	L2083	W2185	L2269	F2371	C2469
A1351	N1446	S1531	S1628	F1742	N1851	P1981	L2088	G2186	L2289	Y2372	T2472
I1352	R1450	T1532	Q1629	F1743	C1852	P1981	Q2089	A2187	K2274	L2389	A2473
T1353	R1451	T1533	L1630	K1749	R1853	W1991	Q2090	A2191	K2275	T2392	L2474
L1354	F1452	A1534	S1632	Q1750	P1854	R1995	A2095	S2192	R2276	L2376	G2477
H1355	E1453	F1541	R1633	Q1751	L1855	R1995	A2095	V2195	W2284	N2379	F2484
R1362	F1454	F1548	D1639	I1755	W1861	L1998	I2099	W2195	M2285	L2389	M2485
Y1363	F1455	F1548	I1641	S1762	N1862	F1999	R2100	L2198	K2288	L2389	Y2493
N1368	F1456	E1552	I1642	G1763	D1872	N2000	Q2102	T2201	L2289	T2393	L2494
V1369	P1458	T1553	T1643	Q1766	D1878	R2002	Q2103	A2202	I2292	L2386	P2495
M1459	M1459	D1554	M1644	Q1767	P1879	L1998	R2104	Y2205	F2297	Q2387	I2499
I1461	I1461	A1555	E1645	G1768	P1880	F1999	T2105	S2206	D2298	Q2389	S2500
Q1374	L1462	S1557	Q1647	I1769	H1881	I2007	V2109	A2207	T2299	F2390	V2501
I1375	M1463	L1558	R1648	V1770	H1882	D2008	D2110	D2268	T2300	R2391	M2502
S1376	F1466	L1558	L1649	K1771	K1883	D2008	A2111	K2269	T2300	G2395	D2503
A1377	T1467	N1563	P1650	E1651	I1894	S2013	D2112	Y2216	C2304	G2395	L2507
K1379	V1468	D1568	E1651	L1780	A1885	L2014	T2113	Q2221	M2306	R2409	T2508
S1387	T1473	I1569	F1658	Y1788	M1888	A2015	A2114	Q2222	A2307	Q2410	L2509
Q1388	F1476	F1571	F1659	P1791	R1889	L2016	V2115	W2223	Q2308	L2417	S2510
Y1389	C1479	E1572	L1664	M1792	L1891	V2017	L2116	E2224	L2311	L2420	P2511
I1394	C1479	K1574	E1675	A1797	D1892	A2018	R2120	Q2226	R2312	I2422	P2512
V1399	V1483	A1575	E1675	E1804	L1894	E2019	Q2124	Q2226	R2313	F2423	D2513
K1400	D1482	K1576	W1677	E1804	L1894	P2020	R2125	Q2226	T2321	L2436	T2515
G1410	G1485	L1581	F1678	Y1808	R1897	D2022	R2126	N2229	F2322	K2437	D2516
P1411	N1486	L1584	K1679	T1809	G1898	D2022	L2127	A2230	I2323	L2438	K2519
T1412	S1488	Q1586	L1699	M1812	Y1902	P2023	E2128	D2231	W2328	V2439	D2527
T1413	Q1489	T1587	E1704	C1813	R1907	L2026	K2129	D2231	Q2334	T2442	T2528
V1414	Q1492	T1587	T1705	L1818	L1910	L2027	Y2130	Q2236	Q2334	L2443	T2529
Y1415	T1493	L1588	F1710	Q1819	W1916	T2028	L2133	Q2236	Q2334	P2444	H2531
N1416	F1494	S1589	Y1713	E1820	Y1917	V2031	E2136	Q2236	Q2334	L2444	L2532
K1417	F1494	S1589	Y1713	E1820	Y1917	V2031	E2136	Q2236	Q2334	L2444	R2533
T1418	Y1497	V1592	A1714	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	R2537
K1419	Q1498	V1593	A1714	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	SER
N1420	S1499	T1600	Y1717	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	
Y1421	G1508	F1602	Y1718	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	
I1422	G1508	F1602	Y1718	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	
A1423	G1508	F1602	Y1718	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	
S1424	G1508	F1602	Y1718	Q1821	R1919	L2045	E2142	E2242	Q2334	G2448	

• Molecule 1: XptA2 protein

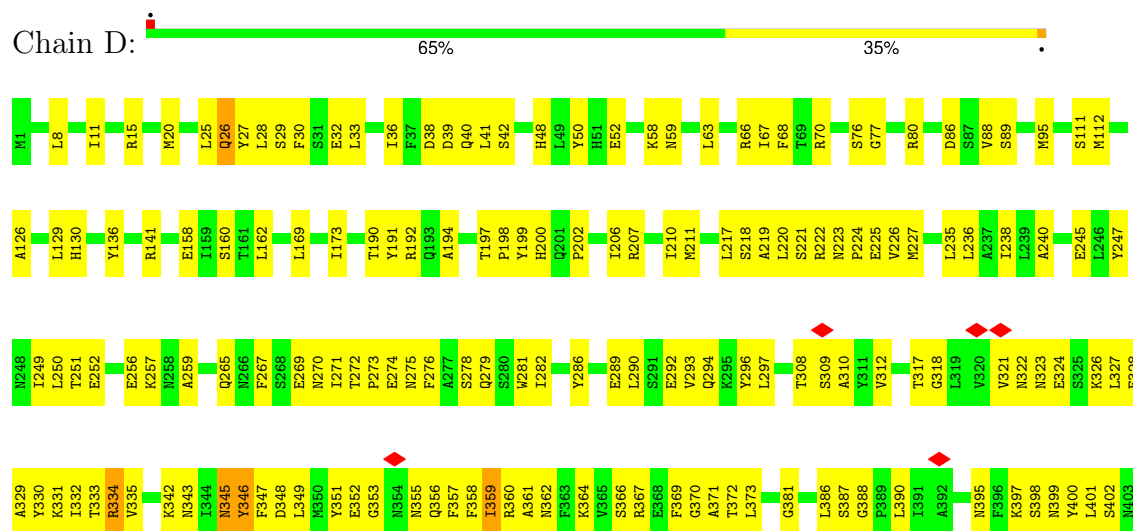
Chain C:  64% 35%

W1	V6	K10	I11	S12	P13	T14	R15	M20	L25	Q26	Y27	L28	S29	F30	S31	E32	L33	D38	S39	Q40	L41	L62	R66	167	R70	A71	T72	P73	Q74	L75	S76	G77	A78	I79	R80	S89	R90	S91	V104	A110	S111	M112	A126	L129	H130			
Y136	R141	R142	L168	E171	H172	I173	S181	L184	M185	L188	Y191	R192	Q193	A194	I195	D196	T197	P198	Y199	H200	Q201	P202	Y203	E204	T205	L206	R207	T208	V209	L210	M211	T212	L217	S218	A219	L220	S221	R222	N223	P224	E225	V226	M227	L236	A237	L238	L239	T245

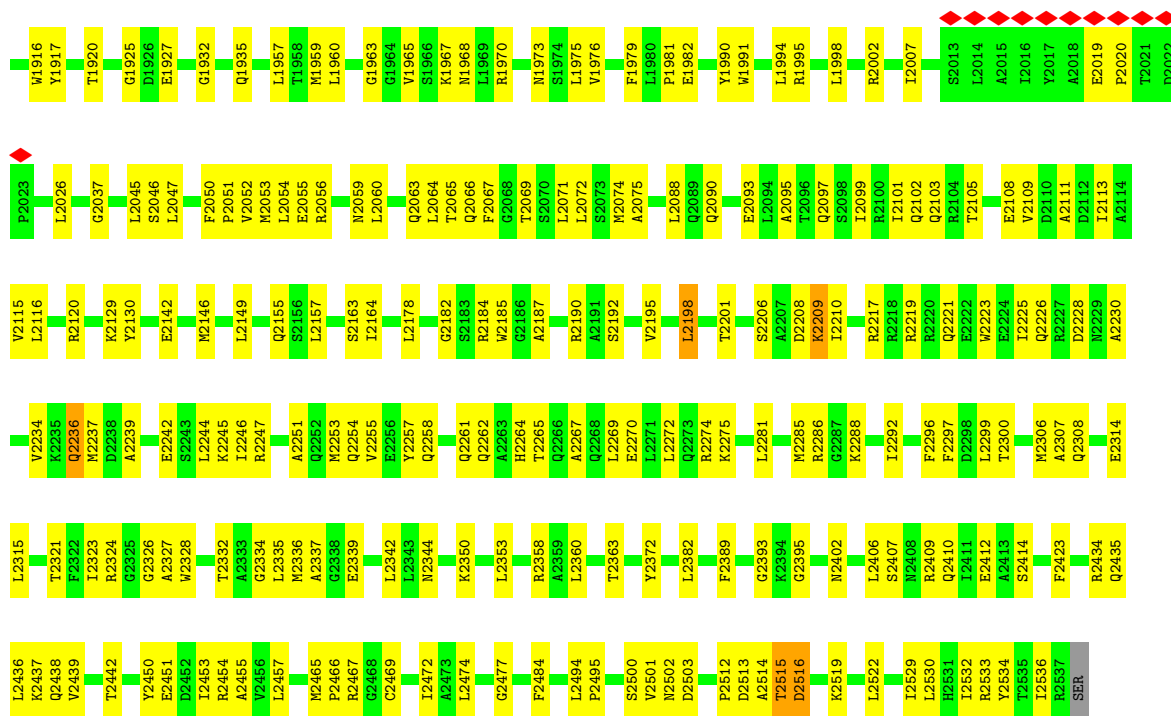




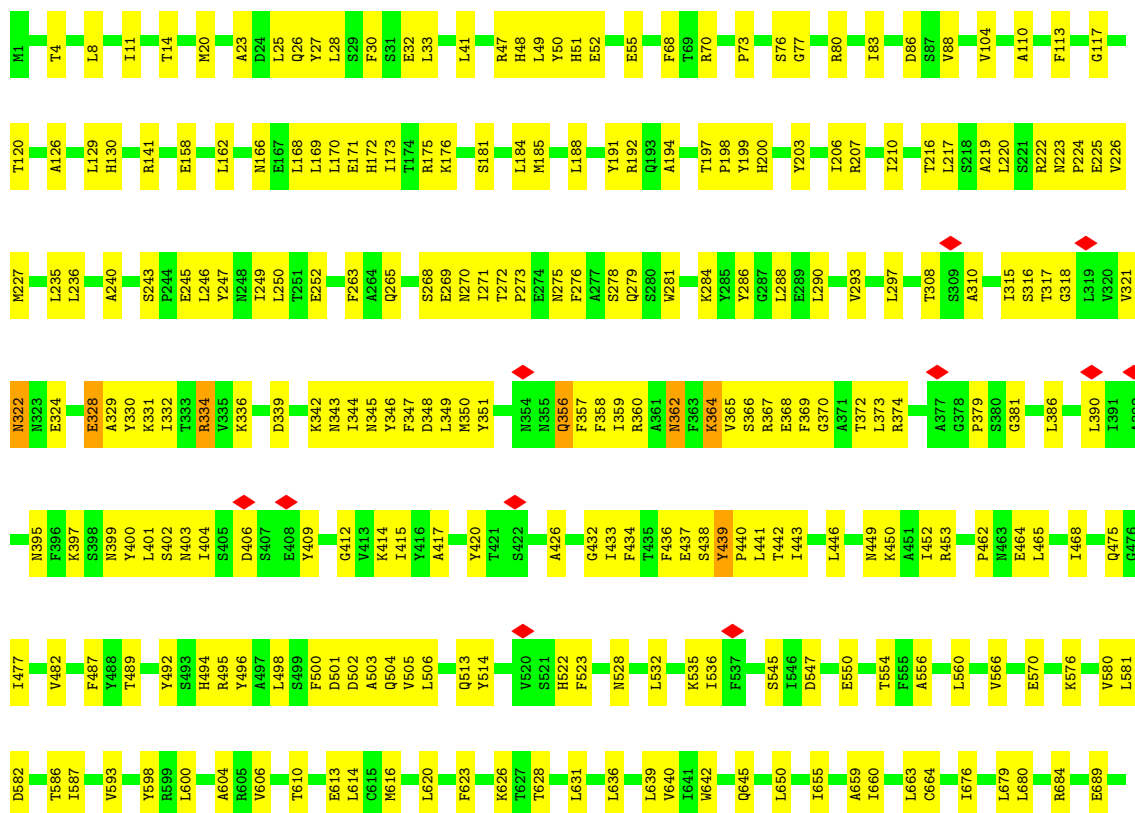
• Molecule 1: XptA2 protein







• Molecule 1: XptA2 protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	42561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00379	Depositor
Map size (Å)	438.728, 438.728, 438.728	wwPDB
Map dimensions	346, 346, 346	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	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	0.35	0/20412	0.58	3/27712 (0.0%)
1	B	0.36	0/20413	0.59	5/27714 (0.0%)
1	C	0.35	0/20413	0.57	2/27714 (0.0%)
1	D	0.35	0/20413	0.59	5/27714 (0.0%)
1	E	0.36	0/20413	0.59	3/27714 (0.0%)
All	All	0.35	0/102064	0.58	18/138568 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	7
All	All	0	21

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	ILE	CG1-CB-CG2	-8.84	91.96	111.40
1	C	2515	THR	C-N-CA	7.64	140.80	121.70
1	D	2515	THR	C-N-CA	7.38	140.14	121.70
1	B	2515	THR	C-N-CA	7.07	139.37	121.70
1	E	2515	THR	C-N-CA	6.60	138.21	121.70

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	GLN	Peptide
1	A	312	VAL	Peptide
1	A	322	ASN	Peptide
1	A	328	GLU	Peptide
1	A	345	ASN	Peptide

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	20006	0	19588	744	0
1	B	20007	0	19592	757	0
1	C	20007	0	19592	720	0
1	D	20007	0	19592	731	0
1	E	20007	0	19592	710	0
All	All	100034	0	97956	3503	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 18.

The worst 5 of 3503 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:C:316:SER:HA	1:C:331:LYS:HE3	1.37	1.03
1:D:2515:THR:H	1:D:2516:ASP:HB2	1.19	1.03
1:E:369:PHE:HA	1:E:386:LEU:O	1.56	1.03
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.19	1.02
1:C:2242:GLU:HA	1:C:2245:LYS:HD3	1.43	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2535/2538 (100%)	2328 (92%)	205 (8%)	2 (0%)	48	80
1	B	2535/2538 (100%)	2329 (92%)	202 (8%)	4 (0%)	44	75
1	C	2535/2538 (100%)	2332 (92%)	199 (8%)	4 (0%)	44	75
1	D	2535/2538 (100%)	2319 (92%)	212 (8%)	4 (0%)	44	75
1	E	2535/2538 (100%)	2329 (92%)	202 (8%)	4 (0%)	44	75
All	All	12675/12690 (100%)	11637 (92%)	1020 (8%)	18 (0%)	50	80

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	ASN
1	B	2516	ASP
1	C	343	ASN
1	C	2516	ASP
1	D	343	ASN

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	2171/2175 (100%)	2165 (100%)	6 (0%)	91	92
1	B	2172/2175 (100%)	2165 (100%)	7 (0%)	91	92
1	C	2172/2175 (100%)	2164 (100%)	8 (0%)	89	91
1	D	2172/2175 (100%)	2165 (100%)	7 (0%)	91	92
1	E	2172/2175 (100%)	2166 (100%)	6 (0%)	91	92
All	All	10859/10875 (100%)	10825 (100%)	34 (0%)	90	92

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	284	LYS
1	E	334	ARG
1	E	2329	ASN
1	B	2467	ARG
1	B	2437	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	275	ASN
1	D	1355	HIS
1	E	1766	GLN
1	D	528	ASN
1	D	998	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.

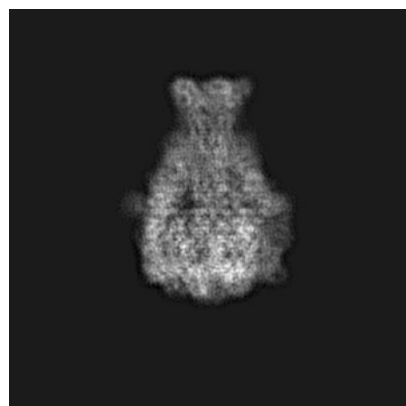
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48372. These allow visual inspection of the internal detail of the map and identification of artifacts.

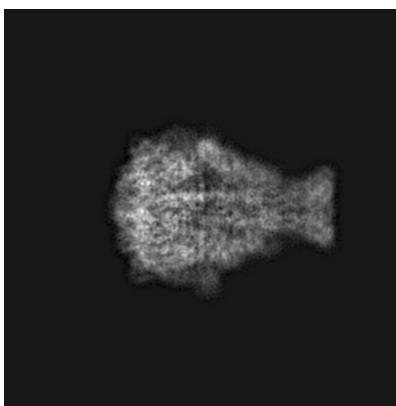
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

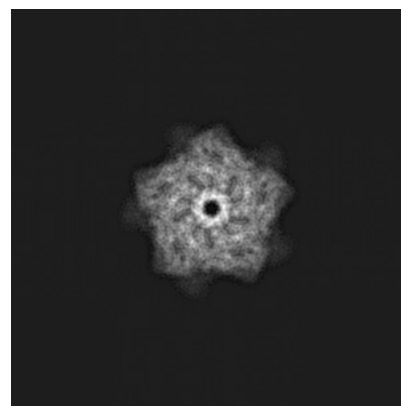
6.1.1 Primary map



X

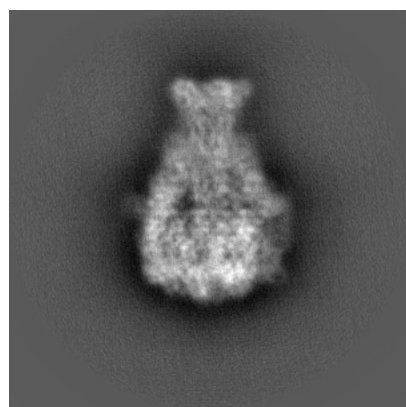


Y

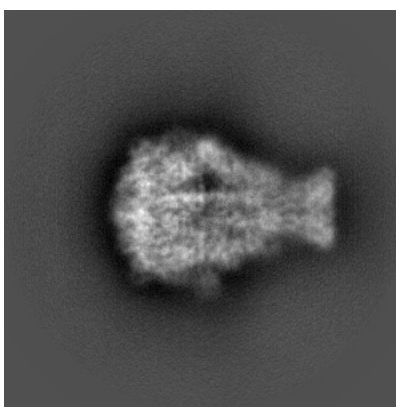


Z

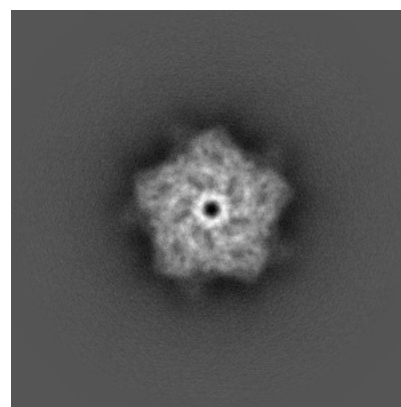
6.1.2 Raw map



X



Y

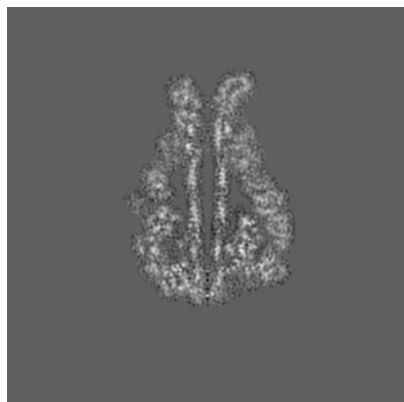


Z

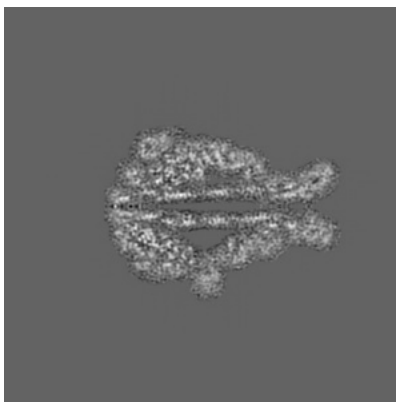
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

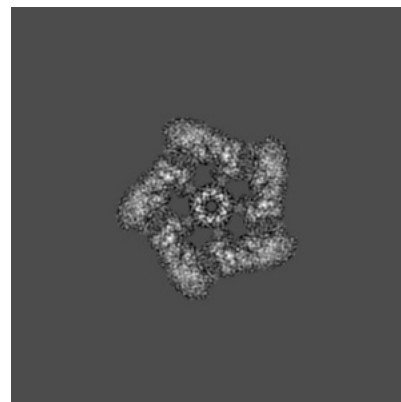
6.2.1 Primary map



X Index: 173

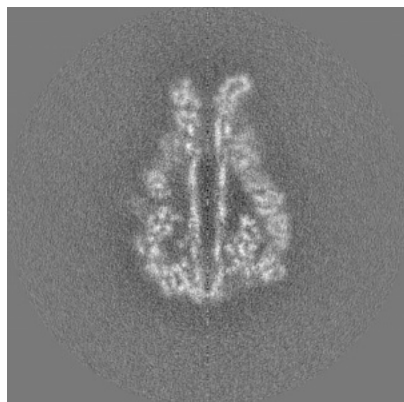


Y Index: 173

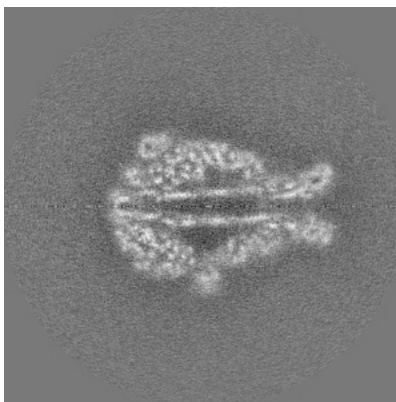


Z Index: 173

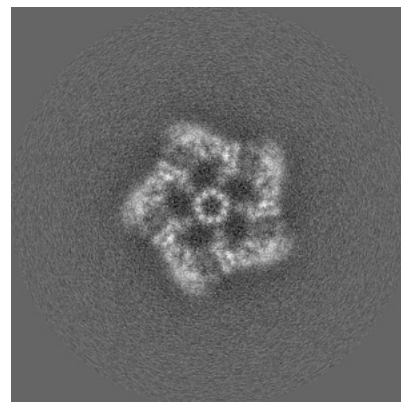
6.2.2 Raw map



X Index: 173



Y Index: 173

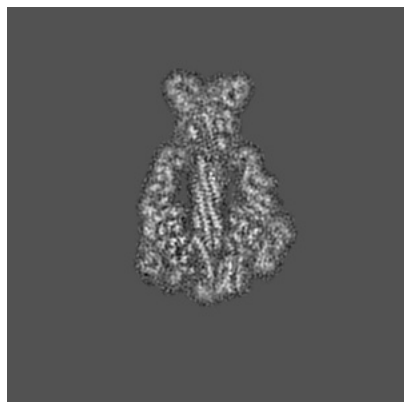


Z Index: 173

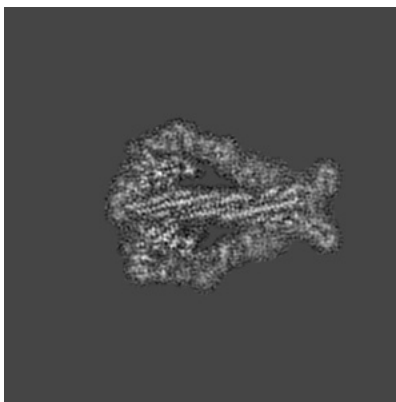
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

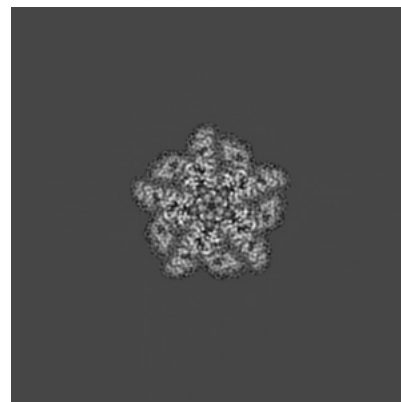
6.3.1 Primary map



X Index: 184

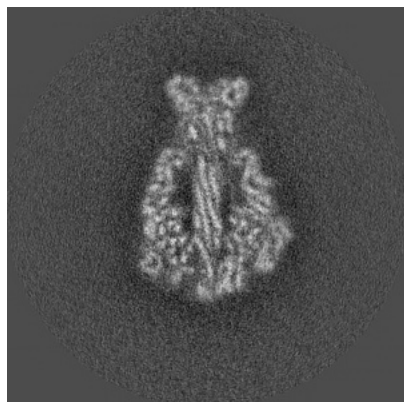


Y Index: 183

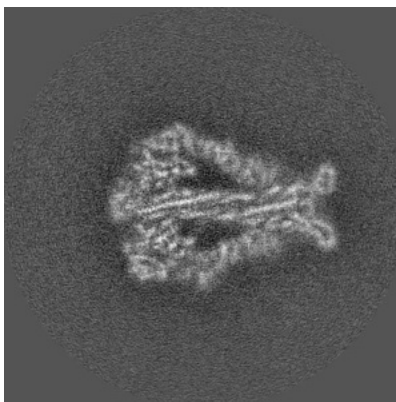


Z Index: 119

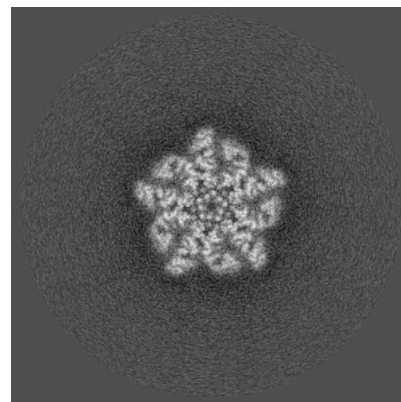
6.3.2 Raw map



X Index: 184



Y Index: 182

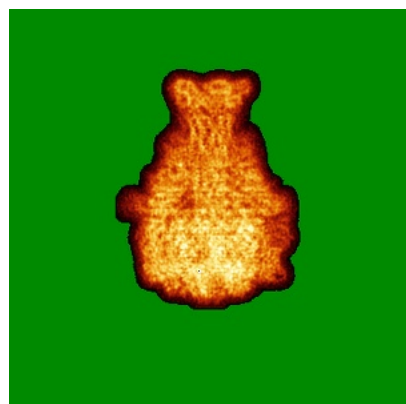


Z Index: 119

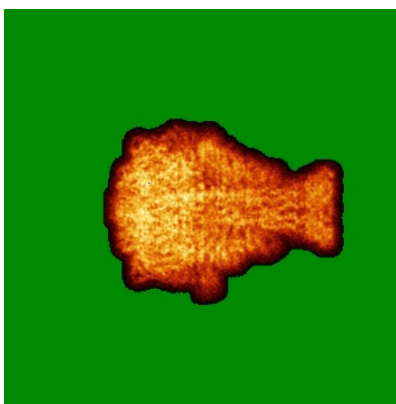
The images above show the largest variance slices of the map in three orthogonal directions.

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

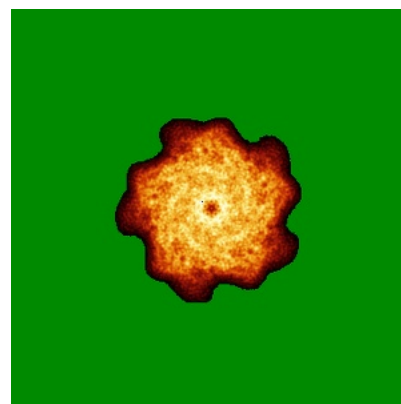
6.4.1 Primary map



X

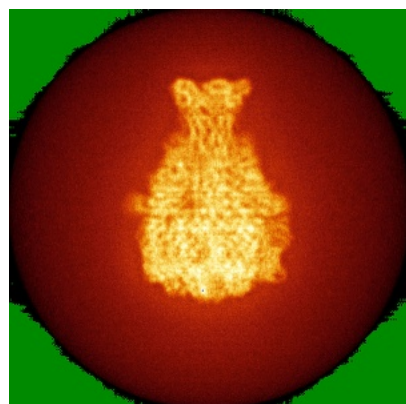


Y

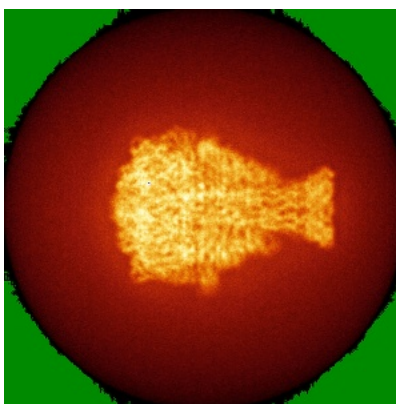


Z

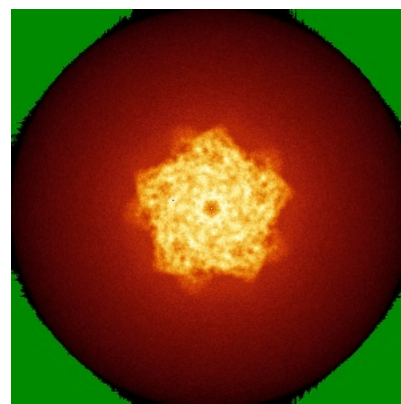
6.4.2 Raw map



X



Y

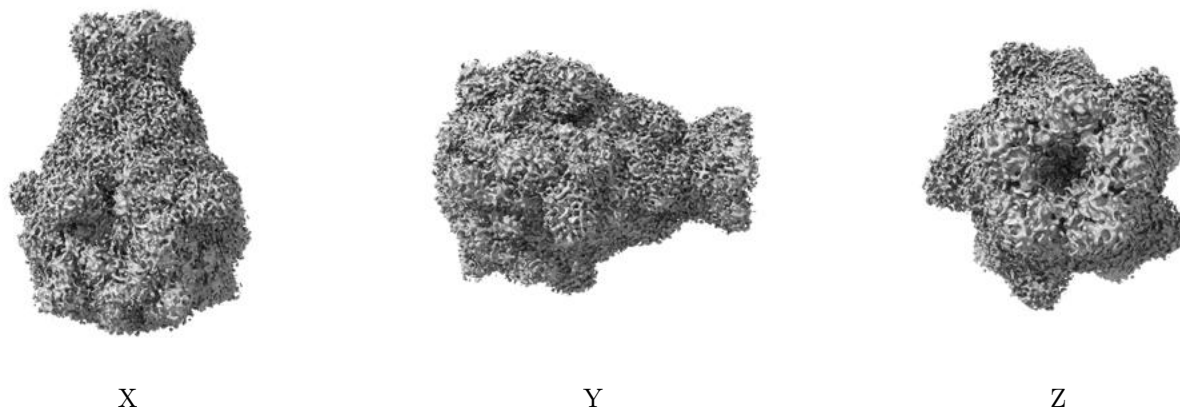


Z

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

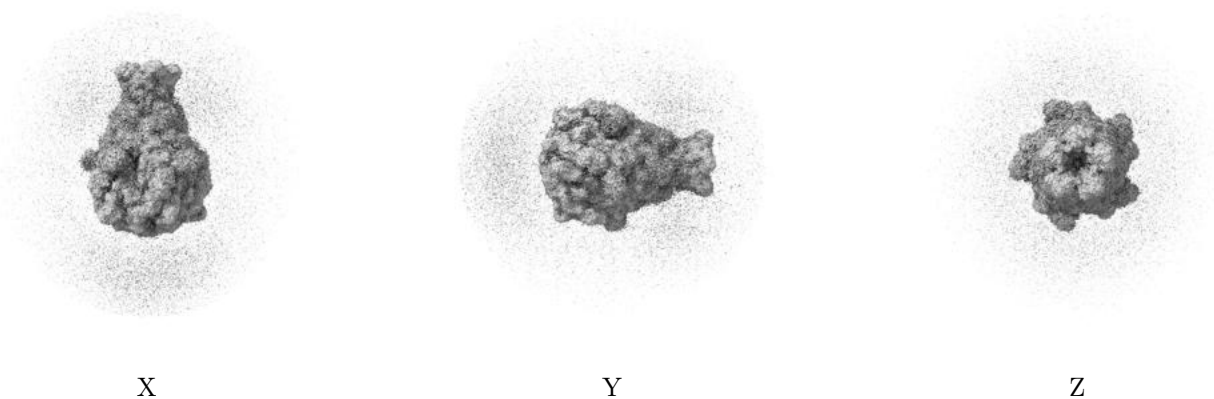
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00379. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

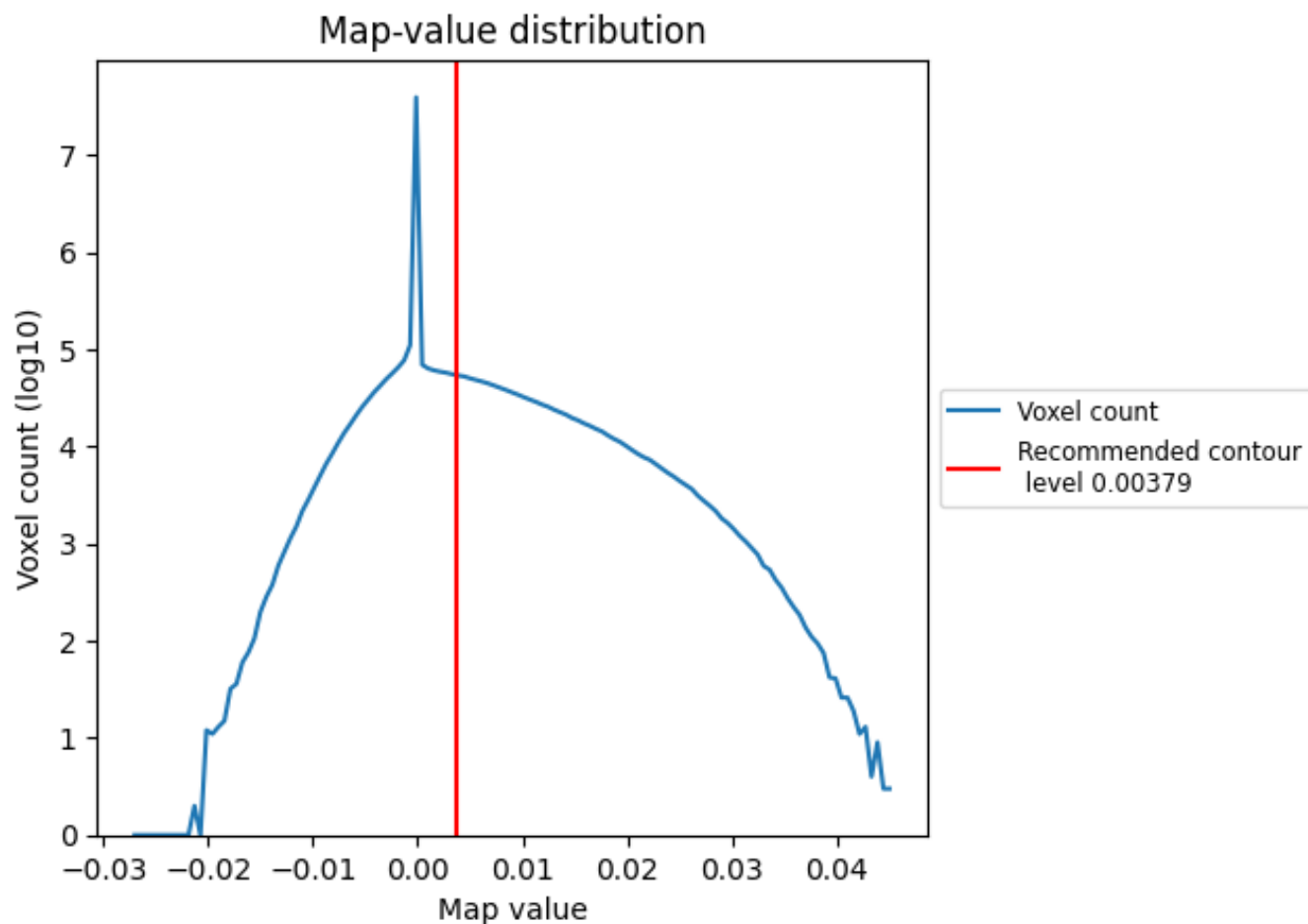
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

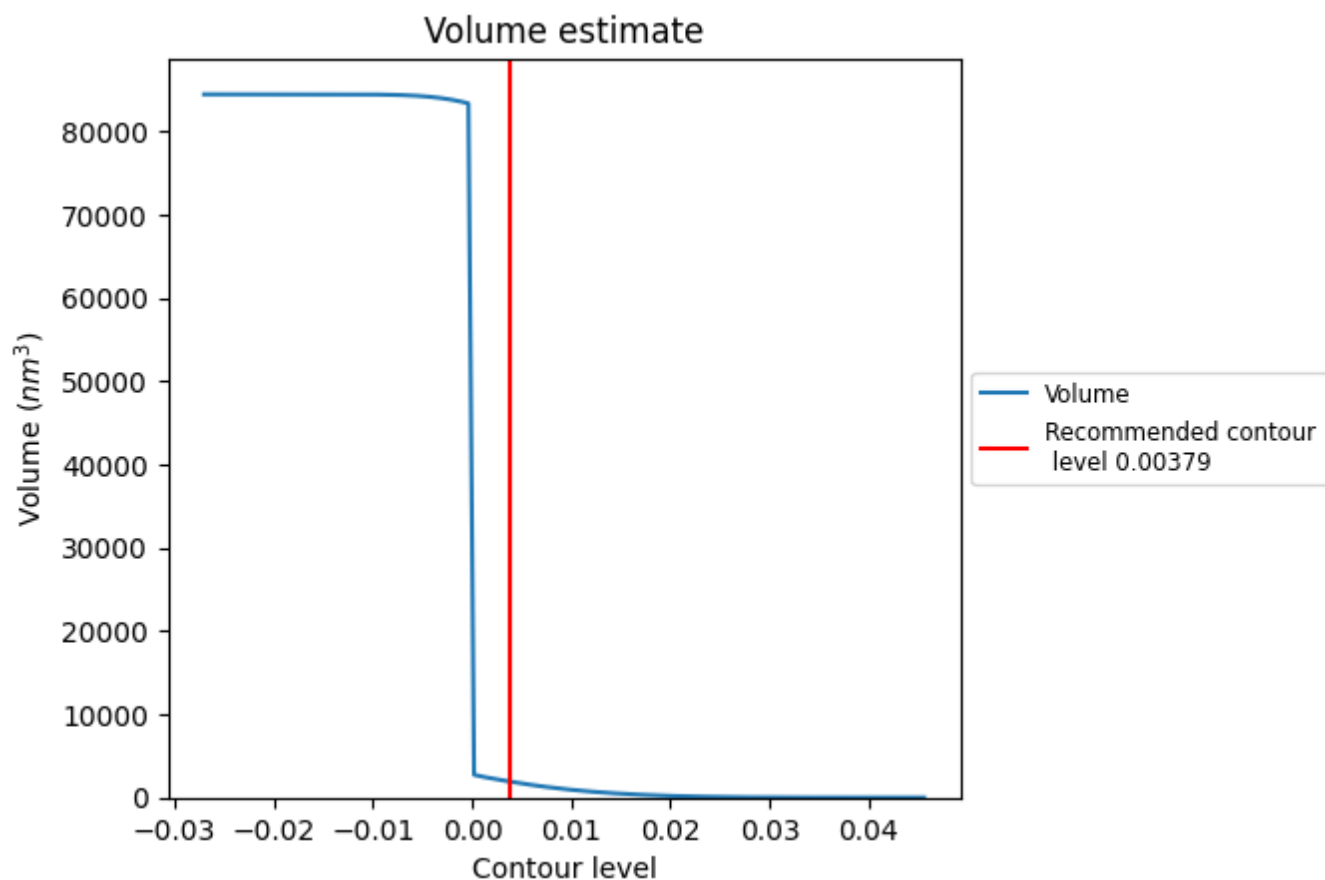
This section contains the results of statistical analysis of the map.

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.

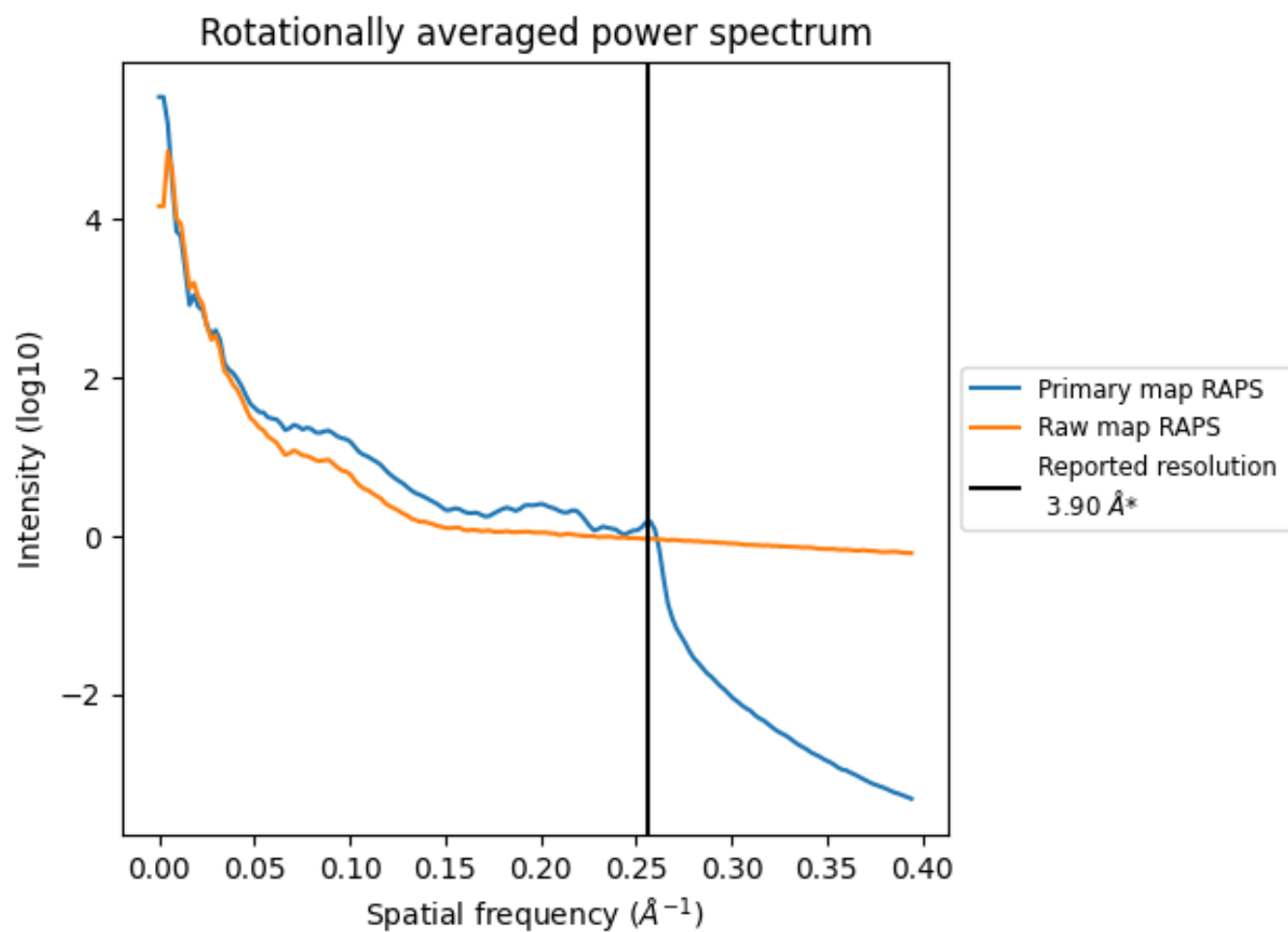
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1929 nm^3 ; this corresponds to an approximate mass of 1743 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 ⓘ

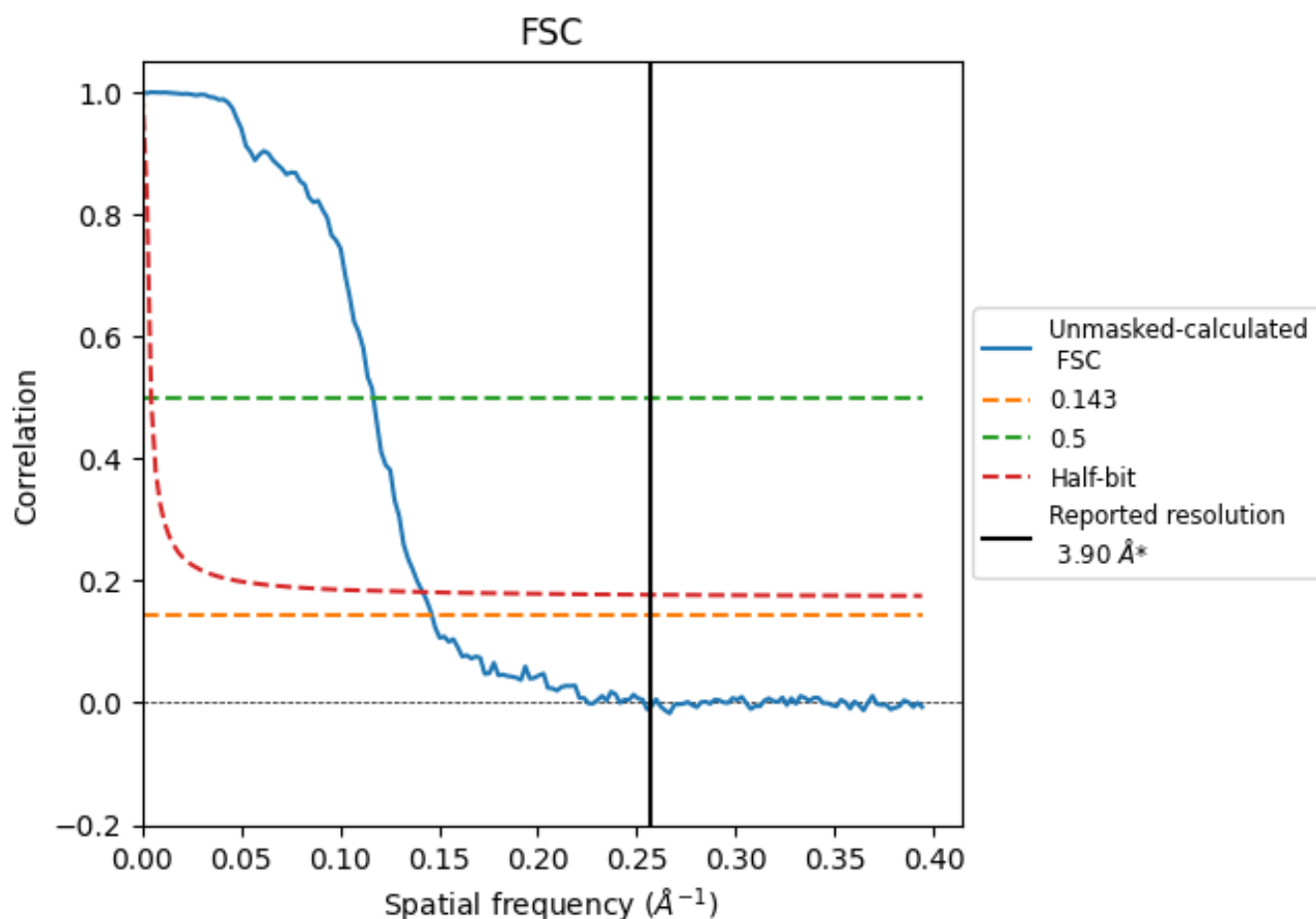


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

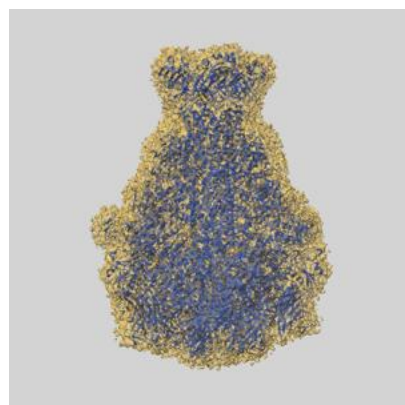
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.83	8.55	7.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.83 differs from the reported value 3.9 by more than 10 %

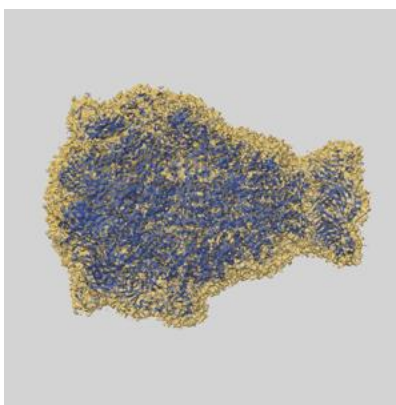
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48372 and PDB model 9MLH. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

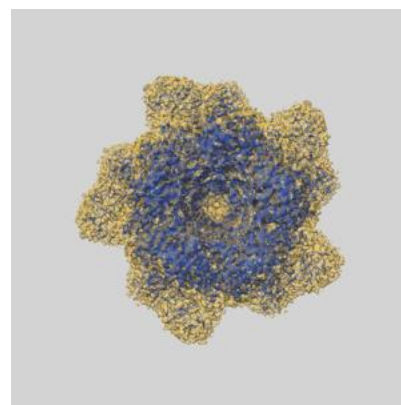
9.1 Map-model overlay [i](#)



X



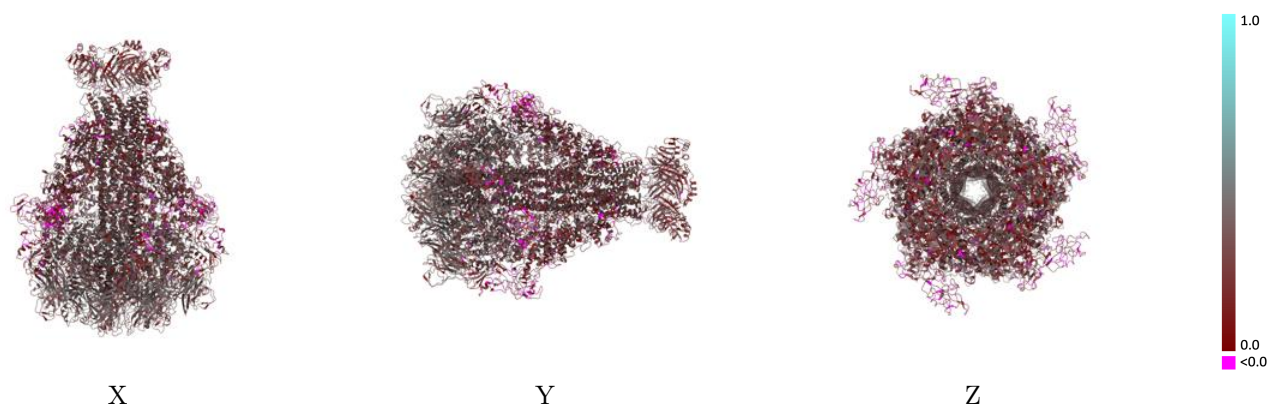
Y



Z

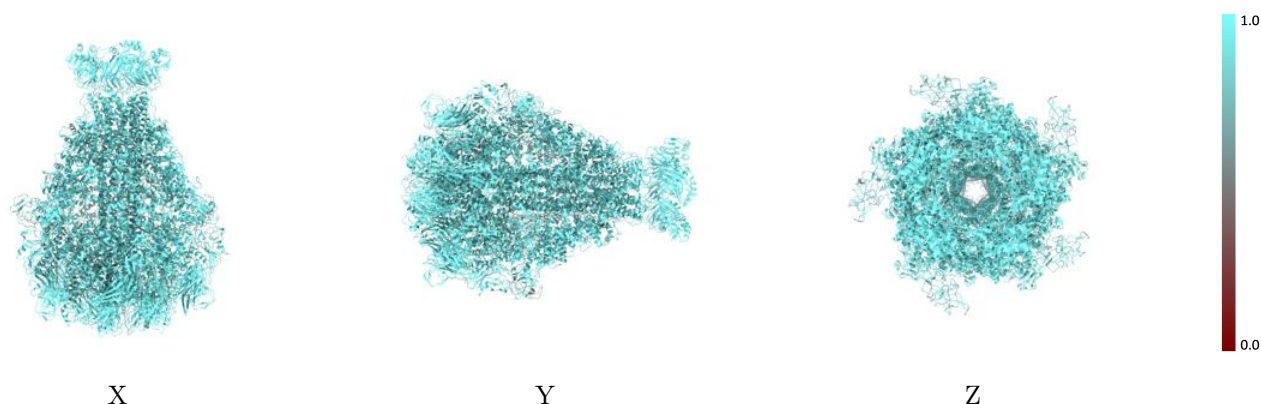
The images above show the 3D surface view of the map at the recommended contour level 0.00379 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



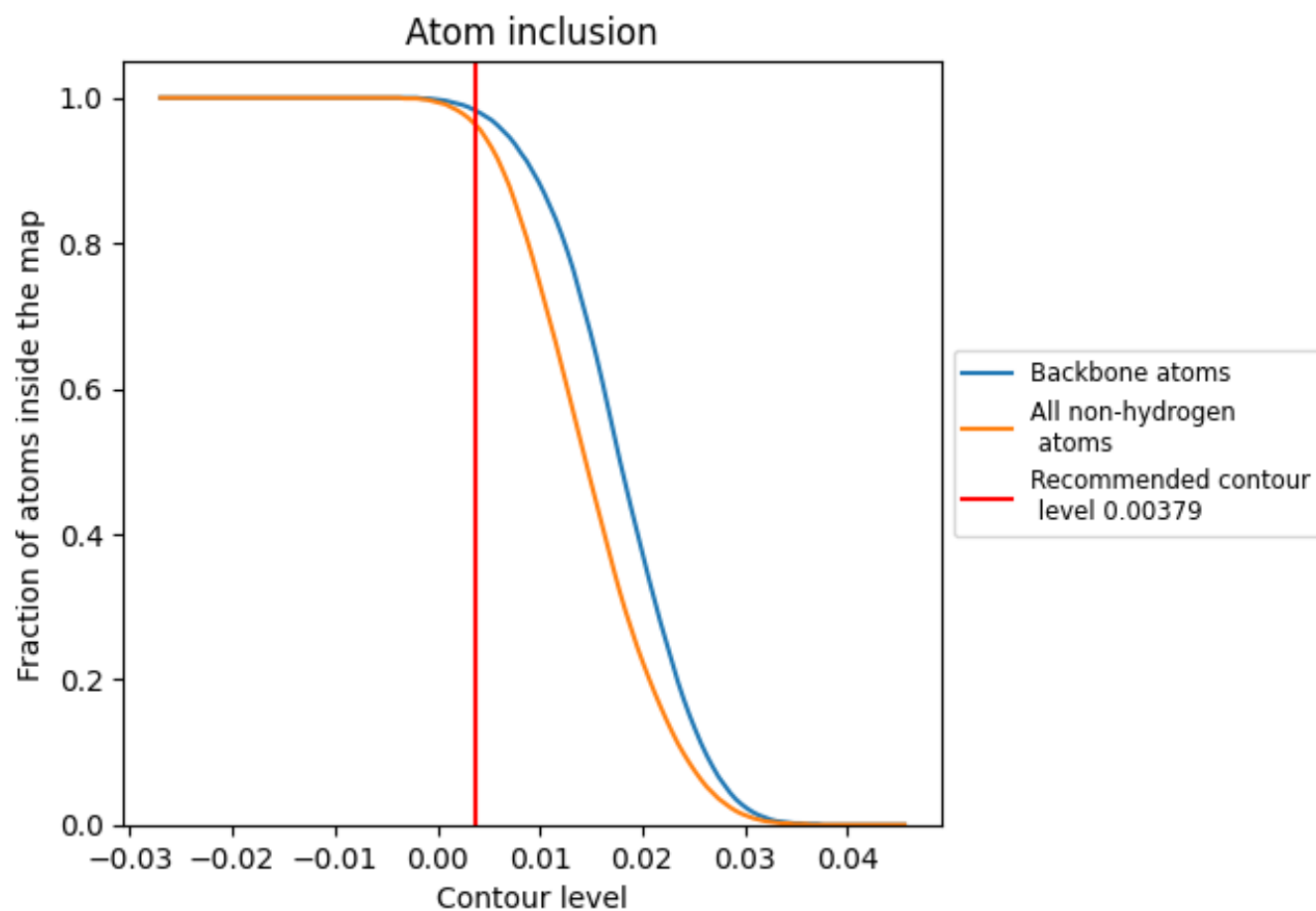
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00379).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.00379) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9620	<div></div> 0.3000
A	<div></div> 0.9610	<div></div> 0.2990
B	<div></div> 0.9630	<div></div> 0.2990
C	<div></div> 0.9620	<div></div> 0.3000
D	<div></div> 0.9630	<div></div> 0.3000
E	<div></div> 0.9630	<div></div> 0.3010

