



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 11:18 PM UTC

PDB ID : 9MLH / pdb_00009mlh
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

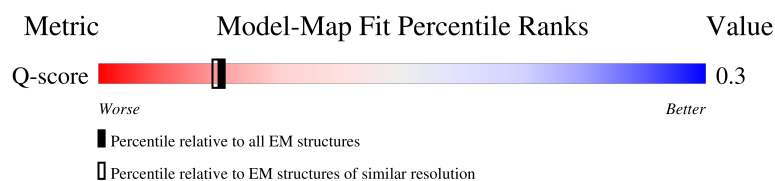
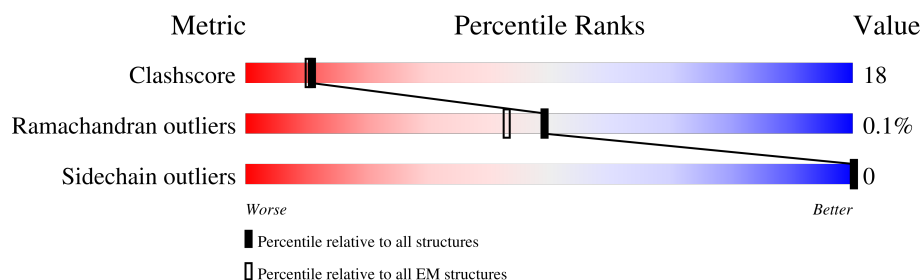
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	

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Mol	Chain	Length	Quality of chain
1	E	2538	 A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment on the left representing 64% and a yellow segment on the right representing 35%. A small red dot is visible at the beginning of the green segment.

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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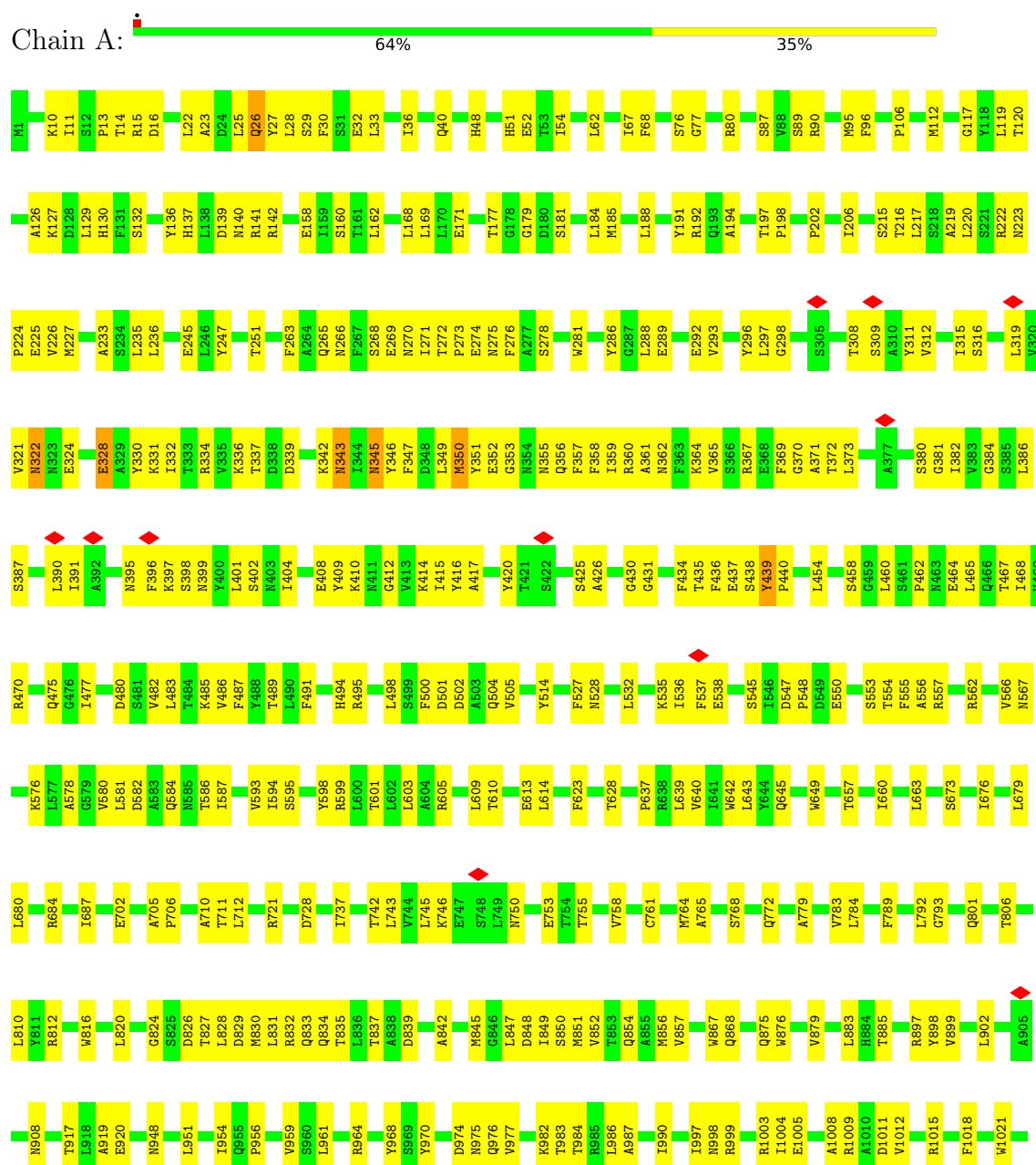
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Chain	Residue	Modelled	Actual	Comment	Reference
E	855	ALA	GLY	conflict	UNP Q93RN7
E	856	MET	HIS	conflict	UNP Q93RN7
E	857	VAL	GLY	conflict	UNP Q93RN7
E	872	THR	PRO	conflict	UNP Q93RN7
E	878	ASP	HIS	conflict	UNP Q93RN7
E	884	HIS	ILE	conflict	UNP Q93RN7
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

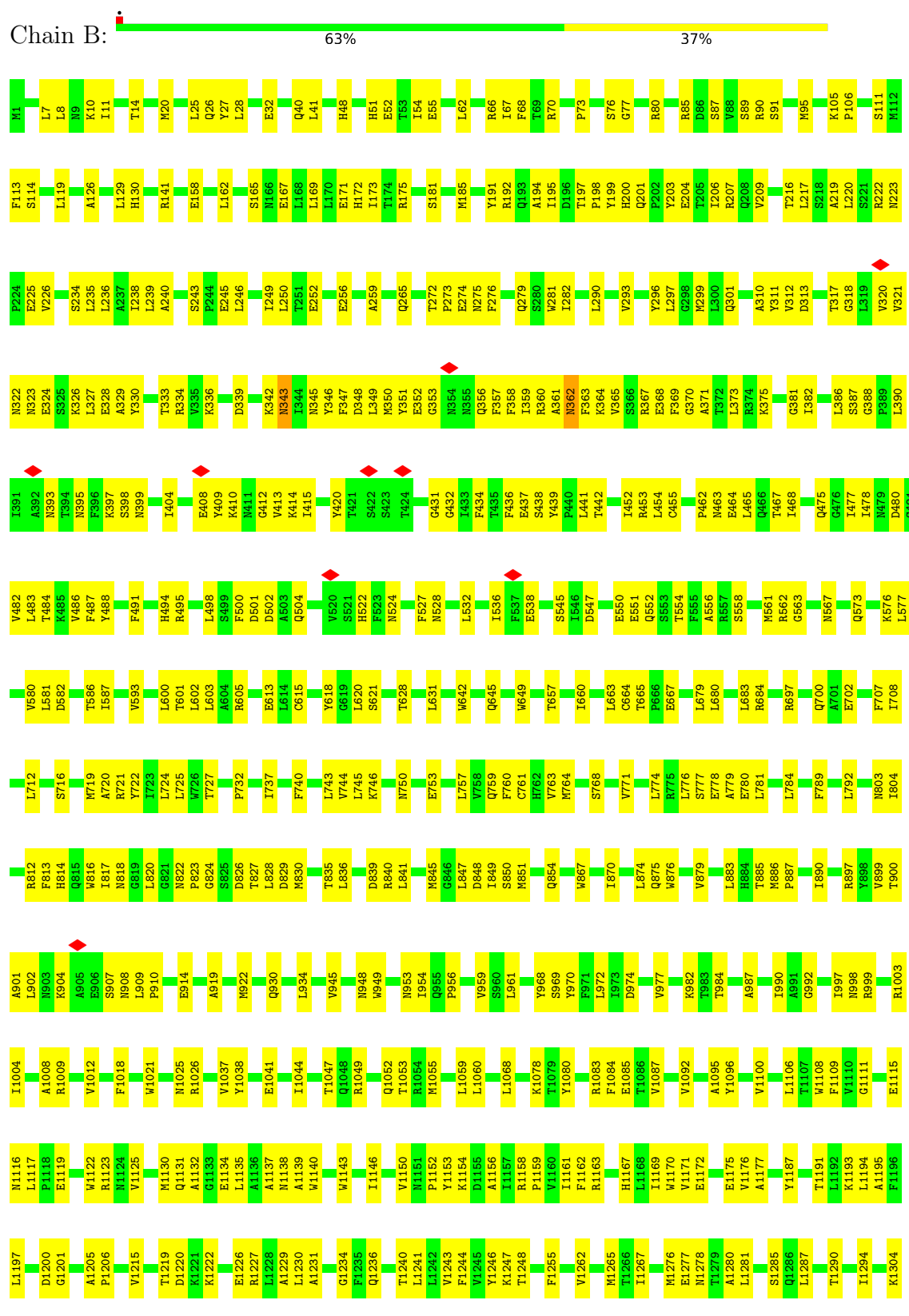
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



V2366	F2494	Q2262	V2161	Q2063	L1969	F1847	G1726	R1604	I1514	H1428	I1338	K1221	W1122	R1025
S2367	F2498	A2263	L2162	Q2066	R1970	W1848	V1727	Y1618	K1515	L1429	I1339	K1222	R1123	R1026
L2368	A2369	H2265	L2163	Q2066	L1975	N1851	G1728	Y1729	T1516	M1430	Q1340	E1226	M1124	T1029
Q2370	L2494	Q2266	S2163	Q2066	L1976	R1852	K1730	L1626	T1517	R1436	T1126	E1226	W1125	
P2495	P2495	A2267	A2164	T2069	V1976	R1853	K1731	L1626	M1518	R1437	D1126	A1229	I1127	V1037
		Q2268	A2165	T2069	F1979	P1854	I1732	Q1629	M1519	L1438	I1127	L1230	Y1038	
		L2269	N2174	M2074	L1980	L1855	T1733	Q1629	K1523	L1439	M1130	A1231		
L2375	T2499	E2270	L2178	D2079	P1981	P1865	F1742	R1633	F1527	L1440	Q1131	Q1236	E1041	
L2382	S2501	L2272	W2185	L2088	E1982	P1870	Y1743	I1638	S1530	L1441	A1132	Q1236		
F2389	D2503	K2275	R2184	L2088	N1984	D1870	Y1744	D1639	S1530	L1442	G1133	T1240	D1045	
L2390			W2185	A2095		D1871	F1745	T1640	H1531	L1451	W1140	T1241	T1047	
K2391	L2507	N2278	G2186	A2095	L1987	D1872	D1746	L1641	H1532			F1244	Q1048	
E2392		K2279		T2096	W1991	A1873	E1747	L1642	I1533	L1452	W1143	Y1245	R1049	
E2392		K2279		S2097	Q1992	A1874	T1748	L1643	I1533	E1453		F1245	I1050	
P2511	F2511	M2285	R2190	S2098	T1993	A1875	T1748	M1644	S1535	E1454	T1148	Y1246	G1051	
P2512	P2512	R2286	S2192	R2100	L1994	H1881	I1755	E1645	S1536	P1455	A1149	K1247	Q1052	
D2513	D2513	T2101	R1995	R2101	L1995	Y1882	M1764	T1646	N1539	F1456	V1150	F1255	T1053	
A2514	A2514	Q2102	L1996	Q2102	L1996	Y1883	T1765	Q1647	S1540	S1457	M1151		R1054	
T2515	T2515	Q2103	Y1997	L1997	R1997	X1884	Q1766	L1649	F1541	P1488	P1152		M1055	
D2516	D2516	R2104	L1998	A1885	L1998	A1885	I1769	P1650	M1544	T1461	A1156	M1265	M1056	
K2519	K2519	L2108	S2197	L2198	F1999	M1888	I1769	E1651		L1462	A1157	I1267	L1059	
		E2109				R1889	K1777	P1652	T1547	M1463	R1158	I1267	L1060	
V2415	L2522	V2109			R2002	R1890			F1548	F1466	P1159	K1274		
R2416	E2523	D2110			H2003	R1897	L1780	F1662	K1549	T1467	V1160	R1275	I1063	
L2417	S2524	A2111				R1897		F1662	P1550	V1468	I1161	E1277	S1064	
L2420	L2525	D2112			I2007	Y1902	Y1801		L1551		R1162		R1163	
K2421	L2528	L2113						K1666	E1552	F1476	E1164	L1281	L1068	
I2422		A2114			S2013	E1912	E1804		I1553	K1477		S1285	A1076	
Q2434	T2532	V2115			L2014	A1913	L1805	H1672	D1554		H1167	Q1286	F1077	
L2436	Y2534	A2117			A2015	K1914	F1806		A1555	Y1481	L1168	K1287	K1078	
K2437	T2535	E2118			L2016	M1915	Y1807	F1678	S1556	V1483	I1169	K1288	T1079	
Q2438	I2536	S2119			Y2017	Y1916	Y1808			V1484	W1170		Y1080	
V2439	SER	R2120			A2018	Y1917	C1813	R1691	D1568	G1485	V1171	F1291	L1081	
					E2019	V1918	F1814	Q1692	I1569	G1486	E1172	D1292	T1082	
					P2020	R1919	Q1815	P1693	V1570	N1487	K1173	I1293	R1083	
					T2021	L1921	R1816	L1699	E1572	S1488	E1174		F1084	
					D2022	L1817	L1817		T1573	Q1489	E1175	V1302	E1085	
						G1925	K1821	S1703	K1574	F1491	V1176	R1303	T1086	
					A2025	E1927	Q1822	E1704	A1575	Q1492		K1304	V1087	
					L2026	G1932	F1823	M1707	K1576	I1493	R1189	F1309	V1092	
					L2027	G1932	T1827	F1710	L1581	F1494	T1191	R1308	A1095	
					V2031	Q1935	W1829	A1714	I1584	Y1497	K1193	F1313	Y1096	
					G2043	L1941	N1831		L1588	Q1498	L1197	P1316	H1097	
					R2049	Q1955	Y1832	Y1717	K1591	S1499	R1198	L1319	V1100	
					P2050	L1960	Y1833	Y1718	R1592	M1502	W1203	L1319	L1106	
					P2051	L1960	Y1834	H1720	V1593	G1508	W1203	I1325	T1107	
					V2052	G1964	Y1834	E1721	I1600	T1509	I1211	I1325	F1108	
					M2053	G1964	G1838	G1722	I1600	N1510	I1211	V1332	F1109	
					L2054	Y1839	Y1839	V1723	L1601	M1511	V1215	M1333	W1116	
					R2056	K1967	R1724	R1724	F1602	T1512	Q1426	E1334	L1117	
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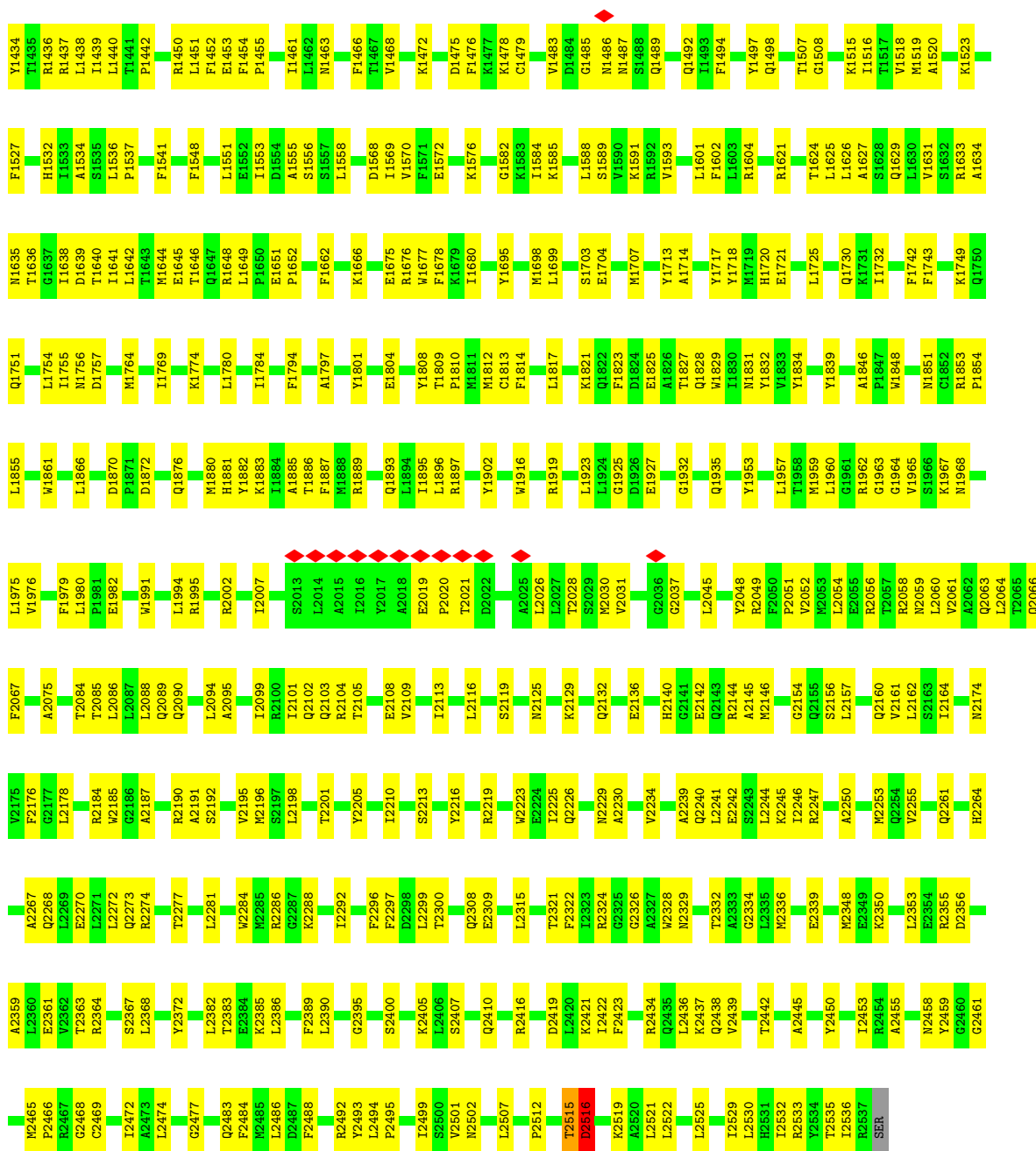
● Molecule 1: XptA2 protein



- Molecule 1: XptA2 protein

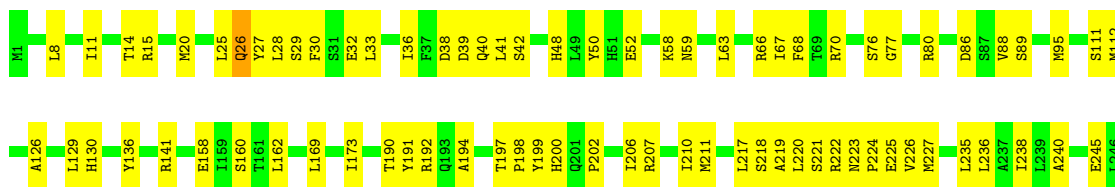


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L1135	L1136	W1140	W1143	W1150	M1151	P1152	Y1153	K1154	R1158	P1159	V1160	I1161	F1162	R1163	E1164	H1167	L1168	I1169	W1170	K1173	E1174	R1189	F1190	T1191	L1192	L1193	L1194	A1195	F1196	L1197	G1201	S1202	W1203	S1204	A1205	P1206	W1207	I1211	W1215	R1227	L1228	A1229	L1230	A1231	G1234	F1235	Q1236		
T1240	L1241	V1243	F1244	Y1245	Y1246	F1255	V1262	M1265	T1266	I1267	M1276	A1280	L1281	S1285	Q1286	L1287	T1290	K1304	A1305	S1306	Y1307	R1308	F1309	F1313	E1314	V1315	P1316	S1317	L1318	S1319	A1323	A1324	I1325	M1333	E1334	T1338	P1339	Q1340	T1341	V1342	S1343	K1344	Y1345	S1346					
T1029	E1041	T1044	D1045	P1046	R1049	T1050	G1051	Q1052	M1056	D1057	E1058	L1059	L1060	E1061	L1068	V1073	E1074	K1078	T1079	Y1080	T1081	T1082	L1083	F1084	E1085	A1086	V1087	V1092	A1095	Y1096	V1100	W1108	F1109	T1113	R1114	E1115	N1116	L1117	W1122	L1123	N1124	V1125	M1130	G1133					
G824	S825	D826	T827	L828	D829	M830	Q833	Q834	T835	L836	T837	A838	D839	R840	D848	T849	S850	M851	Q854	A855	M856	V857	S858	V861	L864	W867	L870	Q875	W876	M886	P887	I890	R891	R897	Y898	T899	A901	L902	N903	K904	F1018	S907	N908	L909	P910	W915			
A919	M922	V945	L946	C947	N948	W949	N953	L954	Q955	P956	V959	S960	L961	Y968	S969	F971	M972	T973	D974	T984	R985	L986	A987	E988	A989	T990	A991	C992	T997	N998	R999	R1003	L1004	E1005	R1009	A1010	D1011	V1012	R1015	F1018	W1021	M1025	R1026	G1133					
T1029	E1041	T1044	D1045	P1046	R1049	T1050	G1051	Q1052	M1056	D1057	E1058	L1059	L1060	E1061	L1068	V1073	E1074	K1078	T1079	Y1080	T1081	T1082	L1083	F1084	E1085	A1086	V1087	V1092	A1095	Y1096	V1100	W1108	F1109	T1113	R1114	E1115	N1116	L1117	W1122	L1123	N1124	V1125	M1130	G1133					
E1134	L1135	W1140	W1143	W1150	M1151	P1152	Y1153	K1154	R1158	P1159	V1160	I1161	F1162	R1163	E1164	H1167	L1168	I1169	W1170	K1173	E1174	R1189	F1190	T1191	L1192	L1193	L1194	A1195	F1196	L1197	G1201	S1202	W1203	S1204	A1205	P1206	W1207	I1211	W1215	R1227	L1228	A1229	L1230	A1231	G1234	F1235	Q1236		
T1240	L1241	V1243	F1244	Y1245	Y1246	F1255	V1262	M1265	T1266	I1267	M1276	A1280	L1281	S1285	Q1286	L1287	T1290	K1304	A1305	S1306	Y1307	R1308	F1309	F1313	E1314	V1315	P1316	S1317	L1318	S1319	A1323	A1324	I1325	M1333	E1334	T1338	P1339	Q1340	T1341	V1342	S1343	K1344	Y1345	S1346					
M1349	M1350	T1353	L1354	H1355	Y1363	D1364	G1365	S1366	G1367	T1370	R1371	M1372	K1373	Q1374	T1375	S1376	A1377	M1378	K1379	T1380	T1381	K1386	S1387	A1392	F1393	H1394	I1395	V1399	Y1405	G1410	F1411	T1412	T1413	V1414	V1415	M1416	T1417	T1418	K1419	N1420	V1421	I1422	S1423	V1424	Q1425	Q1426	L1429	M1430	M1431

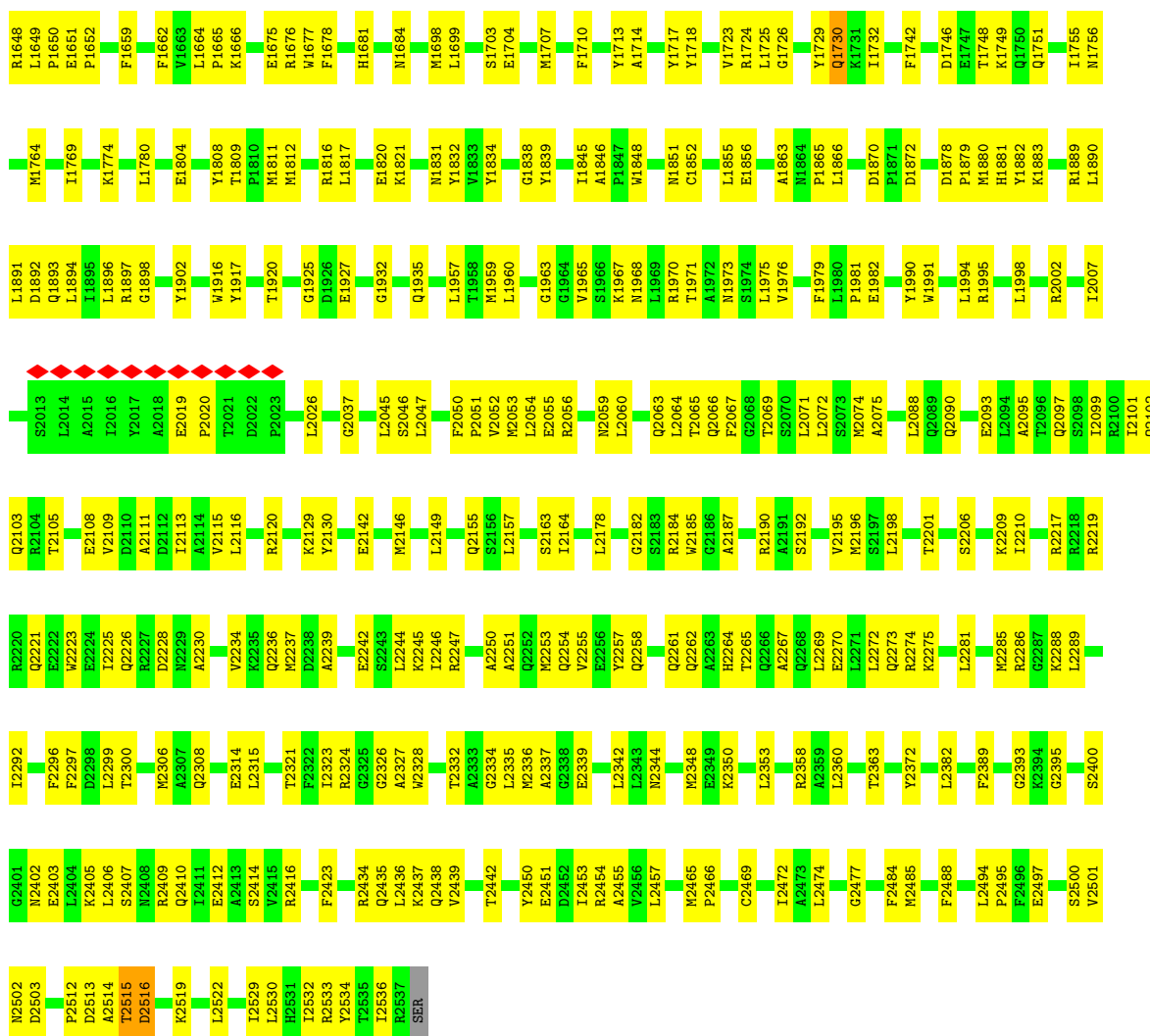


• Molecule 1: XptA2 protein

Chain D:

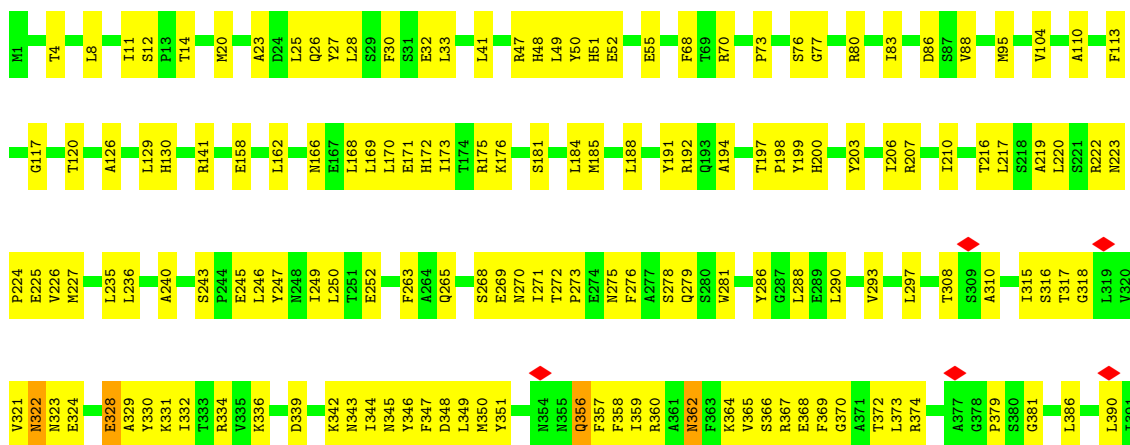


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H1533	V1443	Y1363	V1243	W1021	A919	N818	F707	I587	D406	D406	A329	R248
A1534	N1444	G1367	F1244	W1143	E920	G819	I708	T588	Y409	Y409	K330	I249
N1539	N1446	N1368	Y1246	N1024	N921	G824	T711	E920	N411	N411	K331	L250
S1540	Y1447	V1369	K1250	N1025	N922	S825	L712	V593	G412	G412	L251	T251
F1541	R1450	I1371	K1250	W1030	E923	D826	L713	S596	W413	W413	T333	E252
M1544	L1451	N1372	F1255	P1040	V945	T827	L714	S596	K414	K414	R334	E256
F1548	E1452	Q1374	M1285	P1040	V945	D829	R721	R599	I415	I415	K342	K257
X1549	F1454	I1375	T1266	I1044	W949	N830	L725	L602	Y416	Y416	A259	N258
P1550	F1456	A1377	I1267	P1046	F950	L831	D728	R605	Y420	Y420	N344	Q265
L1551	S1457	M1378	M1276	P1046	F950	R832	P732	V606	T421	T421	N345	Q266
A1555	P1458	K1379	M1276	P1046	F950	R832	P732	V606	S422	S422	Y346	R267
S1556	I1461	S1387	A1280	R1049	N953	D839	T742	R605	G431	G431	N350	E269
Q1557	L1462	Q1388	A1281	R1049	N953	R840	L743	V606	I432	I432	Y351	N270
L1558	N1463	Y1389	L1281	I1050	Q955	R841	V744	H607	F434	F434	E352	T272
D1568	F1466	G1390	S1285	M1055	V959	N845	L745	L620	L525	L525	G353	T273
I1569	T1467	F1393	Q1286	T1063	S960	G846	L746	T628	N524	N524	N354	E274
V1570	V1468	I1394	K1288	S1066	L961	D848	K746	L631	L532	L532	N355	N275
F1571	V1468	I1395	N1289	K1067	R964	I849	L757	L631	K533	K533	Q356	F276
K1576	K1472	I1395	F1291	L1068	L967	S850	L757	W642	I536	I536	F357	A277
G1582	T1473	V1399	H1295	K1078	Y968	N856	F760	L943	F537	F537	R358	S278
K1583	D1475	K1400	H1295	T1079	S969	Y861	F760	Q645	S545	S545	R360	Q279
I1584	F1476	Y1405	K1304	Y1080	Y970	V861	M764	Q645	I546	I546	Y281	W281
K1585	K1477	Y1405	K1304	Y1081	F971	W867	M764	Q645	D547	D547	A361	I282
Q1586	K1478	G1409	S1306	R1083	T973	I870	S768	A653	P548	P548	S366	Y286
V1593	S1480	G1410	T1307	E1085	N975	I870	L769	A653	E550	E550	R367	E289
I1600	A1482	N1416	M1321	Y1086	Q976	V873	S770	T657	Q552	Q552	E368	L290
L1601	G1485	V1414	S1318	A1088	I981	Q875	R775	I660	S553	S553	E369	S291
F1602	N1486	N1416	L1319	D1089	K962	W876	L776	W661	T554	T554	G370	E292
A1610	S1488	K1417	M1321	Y1096	T983	D878	S777	L663	F555	F555	A371	V293
Y1618	Q1489	N1420	V1332	V1100	T984	V879	E778	C664	A556	A556	L373	Q294
L1626	F1491	I1422	M1333	V1100	R985	V879	E780	P666	M561	M561	G381	Y296
A1627	Q1492	A1423	E1334	L1106	A987	T885	E780	E667	R562	R562	L386	L297
S1628	F1494	V1425	G1336	T1107	E988	N886	V783	E667	M463	M463	S387	T308
Q1629	Y1497	Q1426	G1336	W1108	A989	I890	L784	I676	E464	E464	G388	S309
V1631	Q1498	G1427	T1341	L1117	A991	V894	F789	L680	I468	I468	P389	A310
S1632	W1502	N1431	T1342	L1117	G932	V899	L792	R684	M473	M473	A392	Y312
R1633	T1507	Y1434	L1350	W1122	I997	T900	A799	R684	A474	A474	N395	T317
I1638	F1507	T1436	T1353	N1124	N998	A901	N903	N696	Q475	Q475	F396	G318
T1640	I1516	R1436	Q1236	V1125	R1009	L902	I804	G575	G476	G476	K397	L319
I1641	K1523	L1438	H1355	Q1131	D1011	N903	I804	K576	I477	I477	S398	V320
M1644	F1527	L1439	F1359	Q1133	R1015	A905	F813	L577	K486	K486	N399	V321
		L1440	F1359	G1133	R1015	E906	Q815	V580	Y488	Y488	Y400	N322
		T1441	F1359	G1133	R1015	S907	Q815	L581	F487	F487	N323	E324
						N908	Q815	D582	Y488	Y488	S402	S325
						L909	W816		T489	T489	K326	K327
											I404	



• Molecule 1: XptA2 protein

Chain E: 64% 35%



A1846	A1847	A1714	I1620	G1508	K1417	A1317	A1205	R1114	T983	W867	E778	R684	K576	Q475	A392
P1847	W1848	Y1717	R1621	I1509	M1420	S1318	P1206	R1115	T994	Q868	A779	R684	K576	G476	N396
M1851	Y1718	L1718	N1623	K1515	Y1421	L1319	W1207	N1116	A987	D869	E780	E689	V580	I477	N395
C1852	H1720	H1719	L1626	T1516	I1422	A1324	D1220	L1117	A987	D870	L784	A692	D582	V482	K397
R1853	E1721	H1721	A1627	T1517	A1423	L1330	K1221	P1118	G992	N871	L785	Q700	T586	F487	N399
P1854	G1722	G1722	S1628	M1519	S1424	L1331	K1222	E1119	I997	L874	F789	I708	T587	Y488	N398
L1855	L1725	L1725	L1629	K1523	G1427	V1332	E1226	W1122	R998	Q875	A790	I703	I587	Y489	Y400
E1856	L1726	L1726	L1630	M1523	M1431	M1333	R1227	N1124	R999	W876	V791	T703	V593	Y492	M401
D1870	Q1730	Q1730	V1631	A1534	M1431	I1338	A1229	V1125	R1003	V879	G793	I708	Y598	H494	M403
H1881	D1735	D1735	R1633	P1537	R1436	P1339	G1234	I1127	I1004	M886	A799	T711	R599	H495	I404
Y1882	F1742	F1742	T1636	F1541	R1437	Q1340	F1235	M1130	R1009	P887	G800	L712	L600	R495	S405
A1885	F1743	F1743	D1639	D1542	I1438	I1341	F1235	W1130	R1015	Q801	H713	H713	A804	Y496	S407
T1886	D1746	D1746	T1640	M1544	L1440	L1350	L1244	L1135	R1015	H802	L714	L714	V606	L498	E408
R1889	K1749	K1749	L1641	F1545	P1442	A1351	L1242	A1139	F1018	N897	T806	M719	F500	F500	Y409
L1890	I1755	I1755	L1642	F1546	Y1447	H1355	V1243	W1140	W1021	Y898	L810	R720	D501	D501	G412
D1892	Q1766	Q1766	T1643	F1548	R1450	V1361	F1244	W1143	N1024	A905	L810	R722	D502	D502	Y413
Q1893	Q1767	Q1767	M1644	F1548	F1452	Y1363	V1245	W1143	N1025	N908	F813	I723	A503	A503	K414
L1896	A1768	A1768	R1648	E1552	F1453	G1367	K1247	I1146	W1030	P910	H814	L730	L620	Q504	I415
R1897	D1769	D1769	L1649	I1553	F1454	G1367	T1248	D1147	Y1038	E914	Q815	R731	L616	V505	Y416
L1897	H1760	H1760	P1650	D1554	F1455	R1371	F1255	A1149	Y1038	W915	N818	R732	C615	L506	A417
Y1902	Q1766	Q1766	P1652	S1556	F1456	K1372	V1262	N1151	E1041	A919	G819	D736	M616	Y420	Y420
A1913	Q1767	Q1767	F1659	S1557	P1458	Q1374	V1262	P1152	E1041	A919	L820	I737	F623	S422	S422
R1914	I1784	I1784	L1664	D1568	I1461	I1375	M1265	R1158	P1046	M922	G824	A738	K626	S521	A426
W1916	M1792	M1792	P1666	I1569	F1466	K1379	I1267	P1159	I1050	E923	S825	G739	T627	H522	G432
Y1917	Y1801	Y1801	Y1667	E1572	T1467	L1380	F1273	F1162	T1053	L926	T827	E747	L631	F523	I433
R1918	Y1801	Y1801	D1668	T1573	V1468	T1381	K1274	H1167	M1055	S927	L828	S748	L636	N528	F434
T1920	E1804	E1804	E1671	K1574	T1473	K1386	K1275	L1168	M1056	Q930	M830	L749	L636	Y439	Y439
L1921	Y1808	Y1808	E1675	A1575	F1476	S1387	M1276	W1170	L1059	L934	T835	N750	I641	P440	P440
G1925	T1809	T1809	E1675	K1576	C1479	Q1388	M1276	K1173	L1060	Y945	D839	N752	W642	L441	L441
G1932	P1810	P1810	R1676	L1581	G1479	Y1389	D1292	E1174	T1079	I954	R840	E753	Q645	T442	T442
S1933	M1811	M1811	F1677	G1582	A1482	G1390	D1293	E1175	Y1080	Q955	L841	T754	L650	I443	I443
Q1934	M1812	M1812	K1679	I1584	G1485	F1393	I1293	D1182	T1082	P956	S843	T755	L650	L446	L446
Q1935	L1817	L1817	V1685	L1588	G1485	I1395	I1294	P1183	R1083	Y968	D848	V758	I655	M449	M449
Q1955	K1821	K1821	R1691	S1589	Q1489	V1399	I1294	L1192	R1084	Y969	D848	Q759	I655	K450	K450
D1956	W1829	W1829	M1698	V1593	F1490	K1400	L1301	L1193	F1084	S969	I849	F760	T554	A451	A451
L1957	I1830	I1830	L1699	L1601	F1491	H1401	L1301	L1194	E1085	Y970	I849	C761	F555	I452	I452
L1960	Y1831	Y1831	F1602	F1602	Q1492	G1409	K1304	L1197	T1086	F971	S850	H762	A556	R453	R453
G1963	Y1832	Y1832	S1703	E1605	F1494	G1410	A1305	L1197	D1089	L972	M851	V763	R557	P462	P462
G1964	Y1833	Y1833	E1704	E1605	F1494	I1411	S1306	L1197	D1089	L973	T853	M764	L560	M463	M463
Y1965	T1705	T1705	T1705	Q1611	Y1497	I1412	Y1307	D1200	Y1096	D974	Q854	L769	C664	E464	E464
S1966	Q1838	Q1838	F1710	Y1612	Q1498	T1413	R1308	G1201	G1201	V977	A855	S770	I676	L465	L465
L1967	Y1839	Y1839	M1613	M1613	S1499	Y1414	F1309	W1203	W1203	T981	M856	L776	V666	Q466	Q466
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S2491	L2390	G2186	L1975	L2028	L2045	L2064
R2492	L2393	A2187	V1976	S2029	L2046	
Y2493	G2393	A2188		S2030	L2047	
L2494	G2394	L2189	P1981	H2140	Y2048	
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D2503	E2412	A2200	R2100	S2156	F2050	
	R2416	T2201	I2101	L2157	P2051	
L2507	L2417	E2222	Q2102	S2163	V2052	
P2512	D2419	Q2226	Q2103	I2164	M2053	
D2513	T2422	A2230	R2104	L2178	L2054	
A2514	F2423	E2233	V2109	R2184	R2056	
T2515	R2434	V2234	L2116	W2185	L2060	
D2516	G2325	W2237	A2117		V2061	
R2517	Q2435	D2238	E2118			
Q2518	L2436	A2239	S2119			
K2519	R2437	Q2240	R2120			
A2520	Q2438	E2241	R2121			
L2521	V2447	E2242	S2122			
L2522	Y2450	L2244	E2019			
L2523	E2451	K2245	P2020			
S2524	L2452	R2246	T2021			
L2525	L2453	R2247	S2022			
	R2454	K2350	P2023			
L2526	A2455	L2353	Y2024			
R2533	V2456	E2339	A2025			
Y2534	L2457	T2340				
T2535	W2458	L2341				
I2536	Y2459	K2350				
R2537	G2461	L2363				
SER	P2466	R2364				
	C2469	S2367				
	L2472	L2368				
	A2473	Y2372				
	L2474	L2375				
	G2477	N2379				
	D2480	F2380				
	Q2483	N2381				
	F2484	E2384				
	W2485	T2387				

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	0.27	0/20412	0.50	4/27712 (0.0%)
1	B	0.28	0/20413	0.52	5/27714 (0.0%)
1	C	0.27	0/20413	0.49	6/27714 (0.0%)
1	D	0.27	0/20413	0.51	5/27714 (0.0%)
1	E	0.28	0/20413	0.53	6/27714 (0.0%)
All	All	0.27	0/102064	0.51	26/138568 (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 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2515	THR	CA-C-N	10.61	140.80	121.70
1	C	2515	THR	C-N-CA	10.61	140.80	121.70
1	D	2515	THR	CA-C-N	10.24	140.14	121.70
1	D	2515	THR	C-N-CA	10.24	140.14	121.70
1	B	2515	THR	CA-C-N	9.82	139.37	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	771	0
1	B	20007	0	19592	781	0
1	C	20007	0	19592	756	0
1	D	20007	0	19592	766	0
1	E	20007	0	19592	737	0
All	All	100034	0	97956	3637	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 3637 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%)	43	74
1	C	2535/2538 (100%)	2332 (92%)	199 (8%)	4 (0%)	43	74
1	D	2535/2538 (100%)	2319 (92%)	212 (8%)	4 (0%)	43	74
1	E	2535/2538 (100%)	2329 (92%)	202 (8%)	4 (0%)	43	74
All	All	12675/12690 (100%)	11637 (92%)	1020 (8%)	18 (0%)	49	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%)	2171 (100%)	0	100	100
1	B	2172/2175 (100%)	2172 (100%)	0	100	100
1	C	2172/2175 (100%)	2172 (100%)	0	100	100
1	D	2172/2175 (100%)	2172 (100%)	0	100	100
1	E	2172/2175 (100%)	2172 (100%)	0	100	100
All	All	10859/10875 (100%)	10859 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1489	GLN
1	E	1335	ASN
1	D	1935	GLN
1	E	200	HIS
1	E	1862	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.

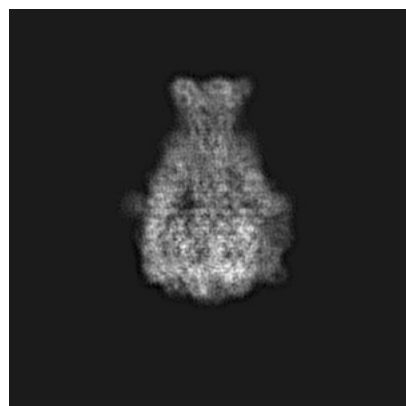
6 Map visualisation [i](#)

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.

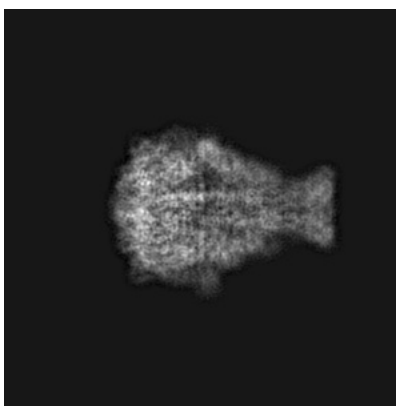
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

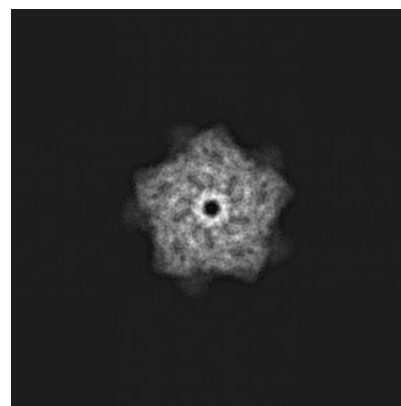
6.1.1 Primary map



X

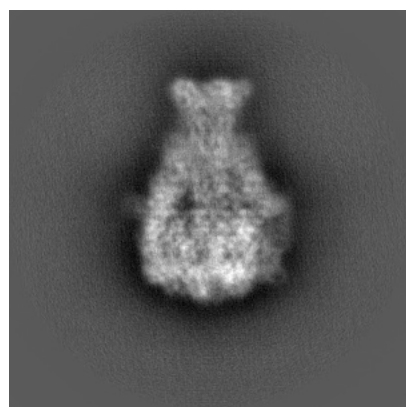


Y

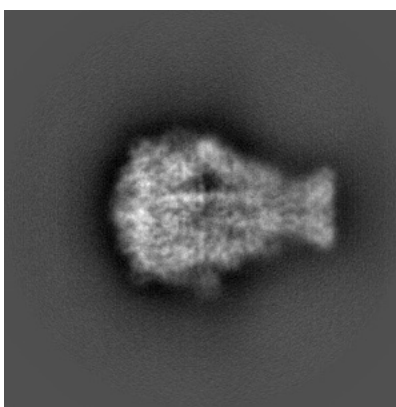


Z

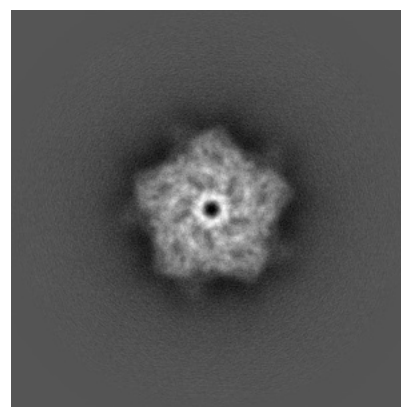
6.1.2 Raw map



X



Y

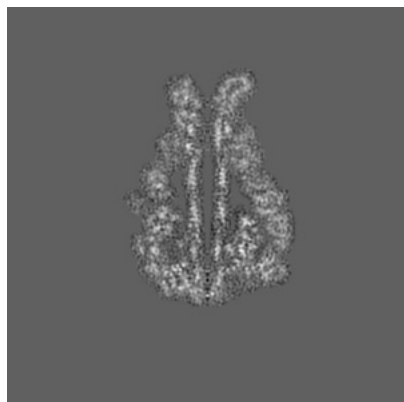


Z

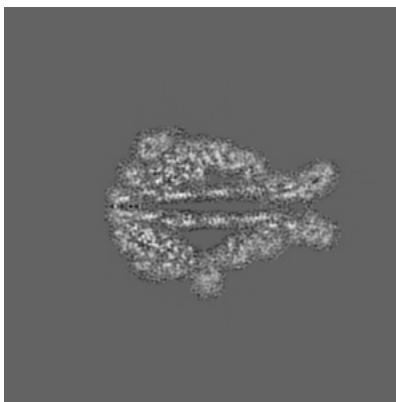
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

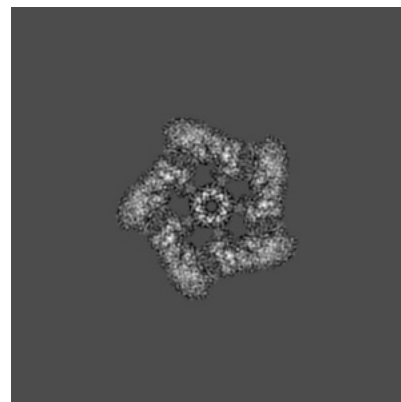
6.2.1 Primary map



X Index: 173

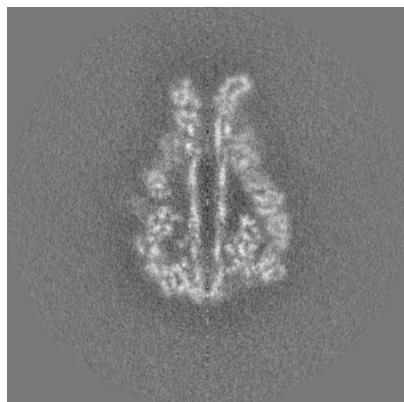


Y Index: 173

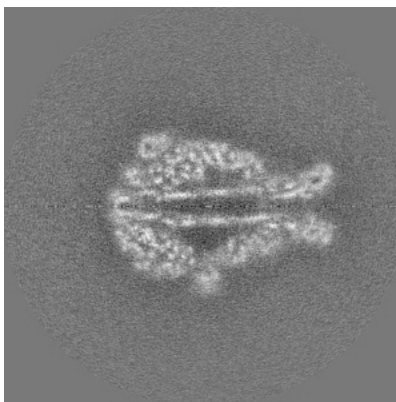


Z Index: 173

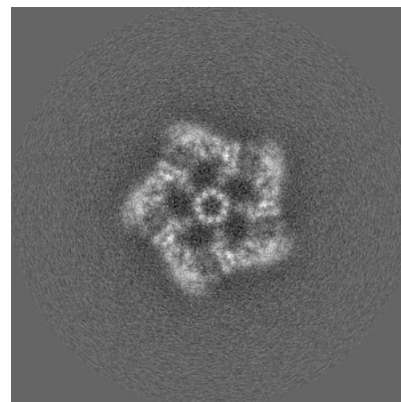
6.2.2 Raw map



X Index: 173



Y Index: 173

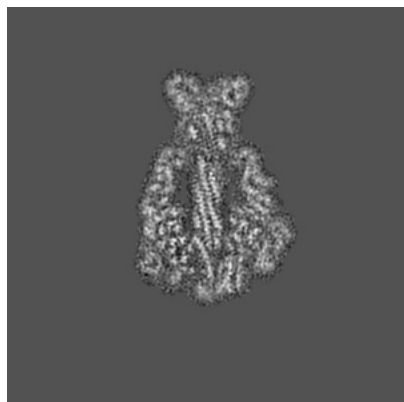


Z Index: 173

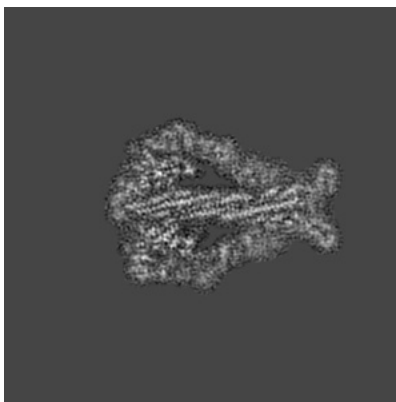
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

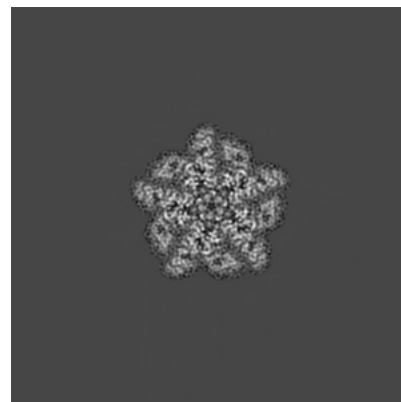
6.3.1 Primary map



X Index: 184

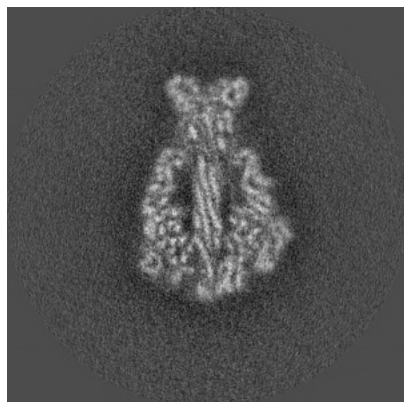


Y Index: 183

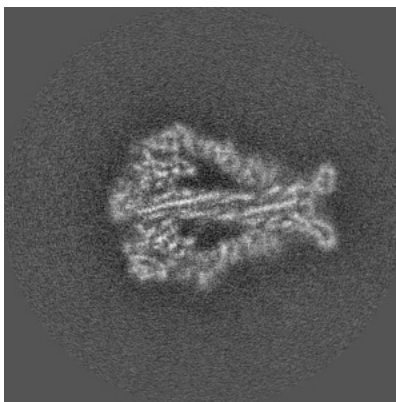


Z Index: 119

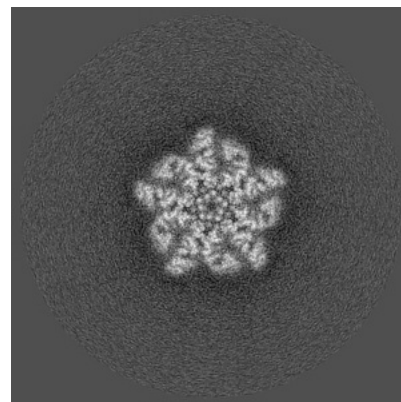
6.3.2 Raw map



X Index: 184



Y Index: 182

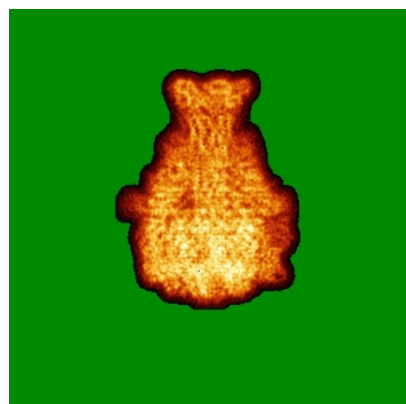


Z Index: 119

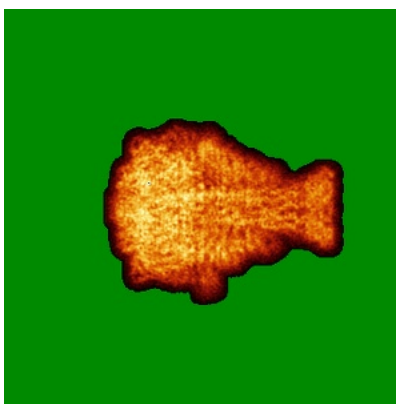
The images above show the largest variance slices of the map in three orthogonal directions.

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

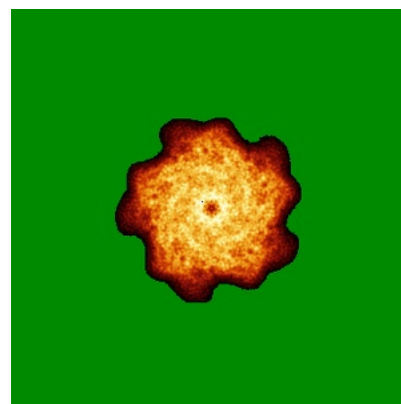
6.4.1 Primary map



X

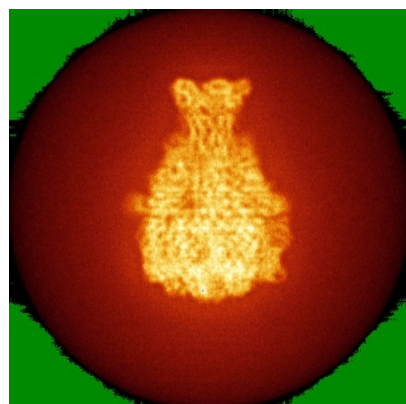


Y

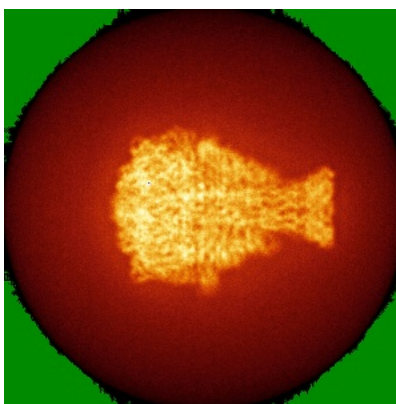


Z

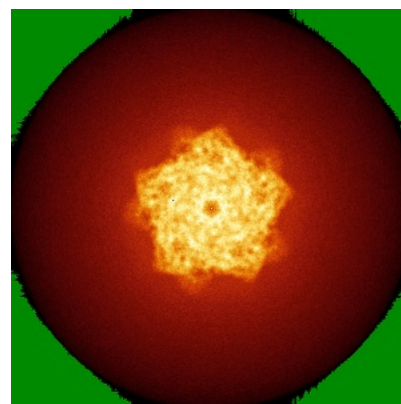
6.4.2 Raw map



X



Y



Z

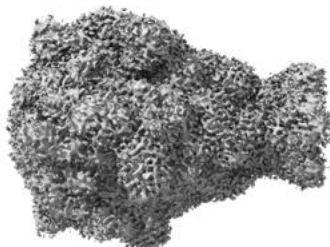
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

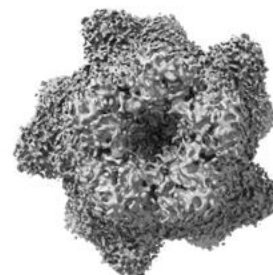
6.5.1 Primary map



X



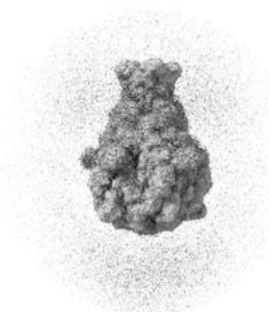
Y



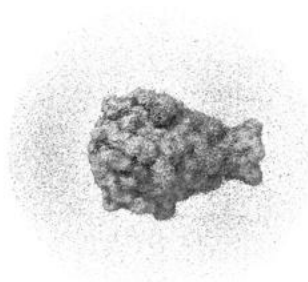
Z

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.

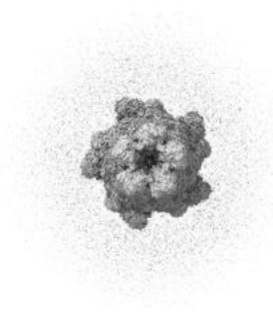
6.5.2 Raw map



X



Y



Z

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

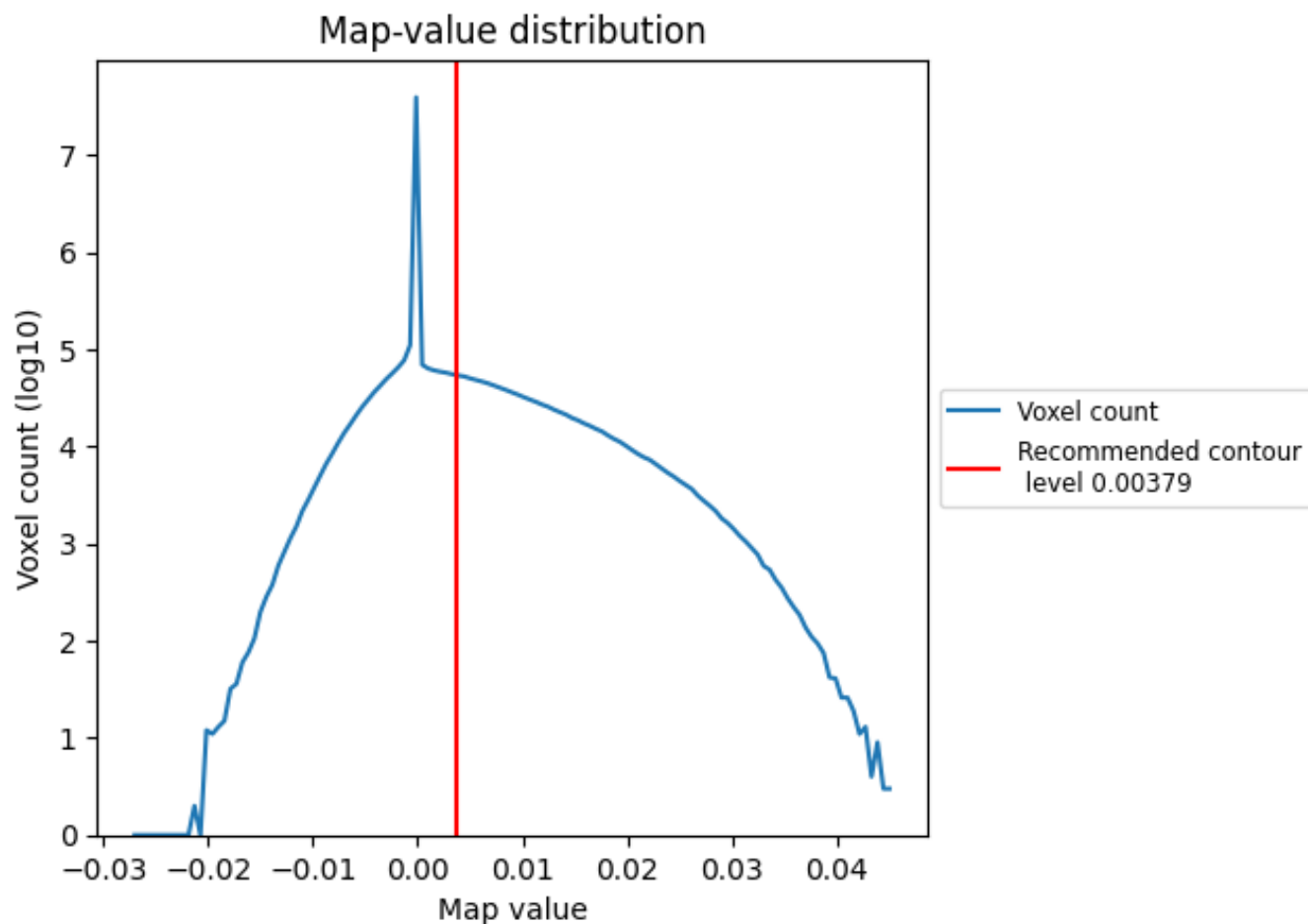
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

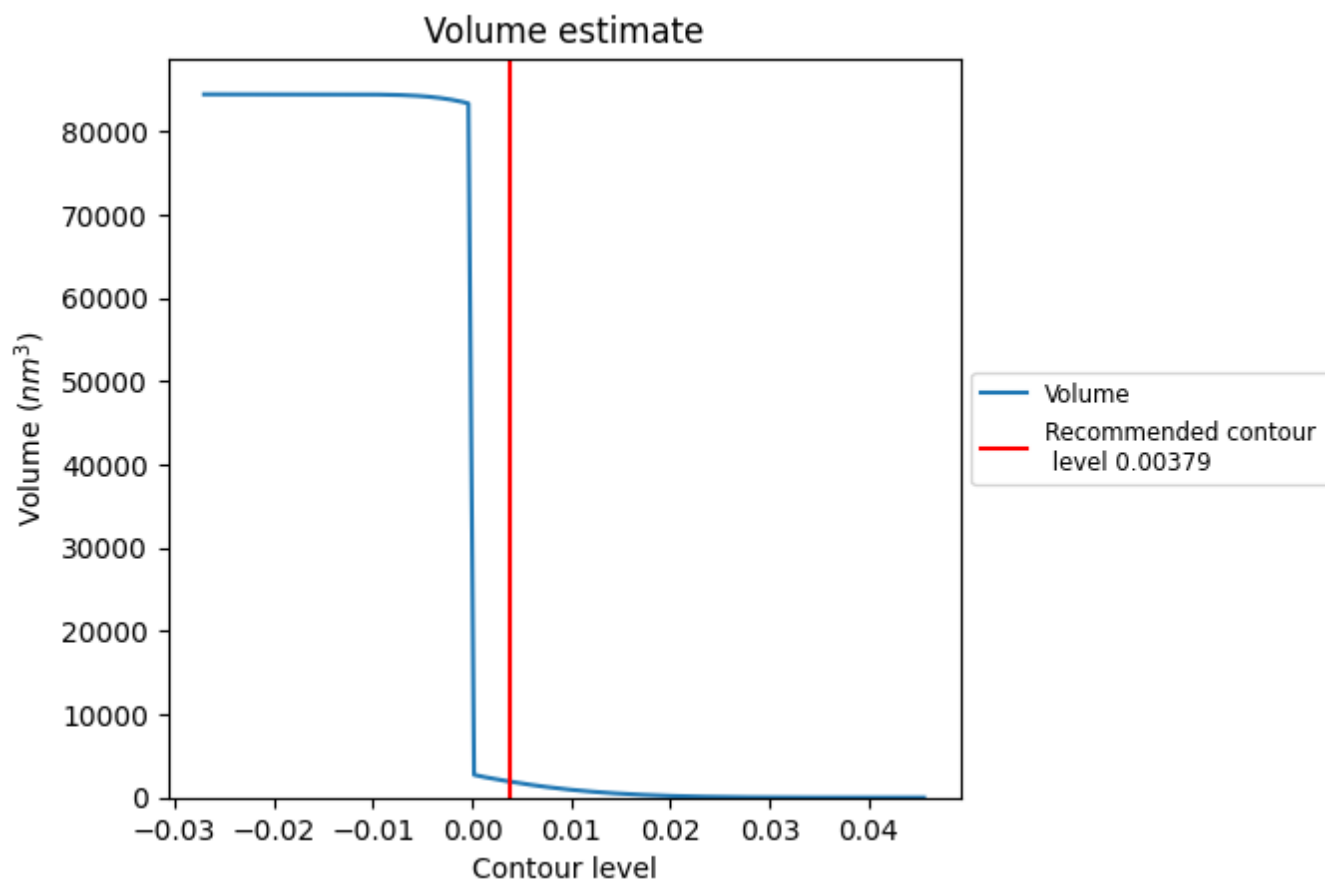
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

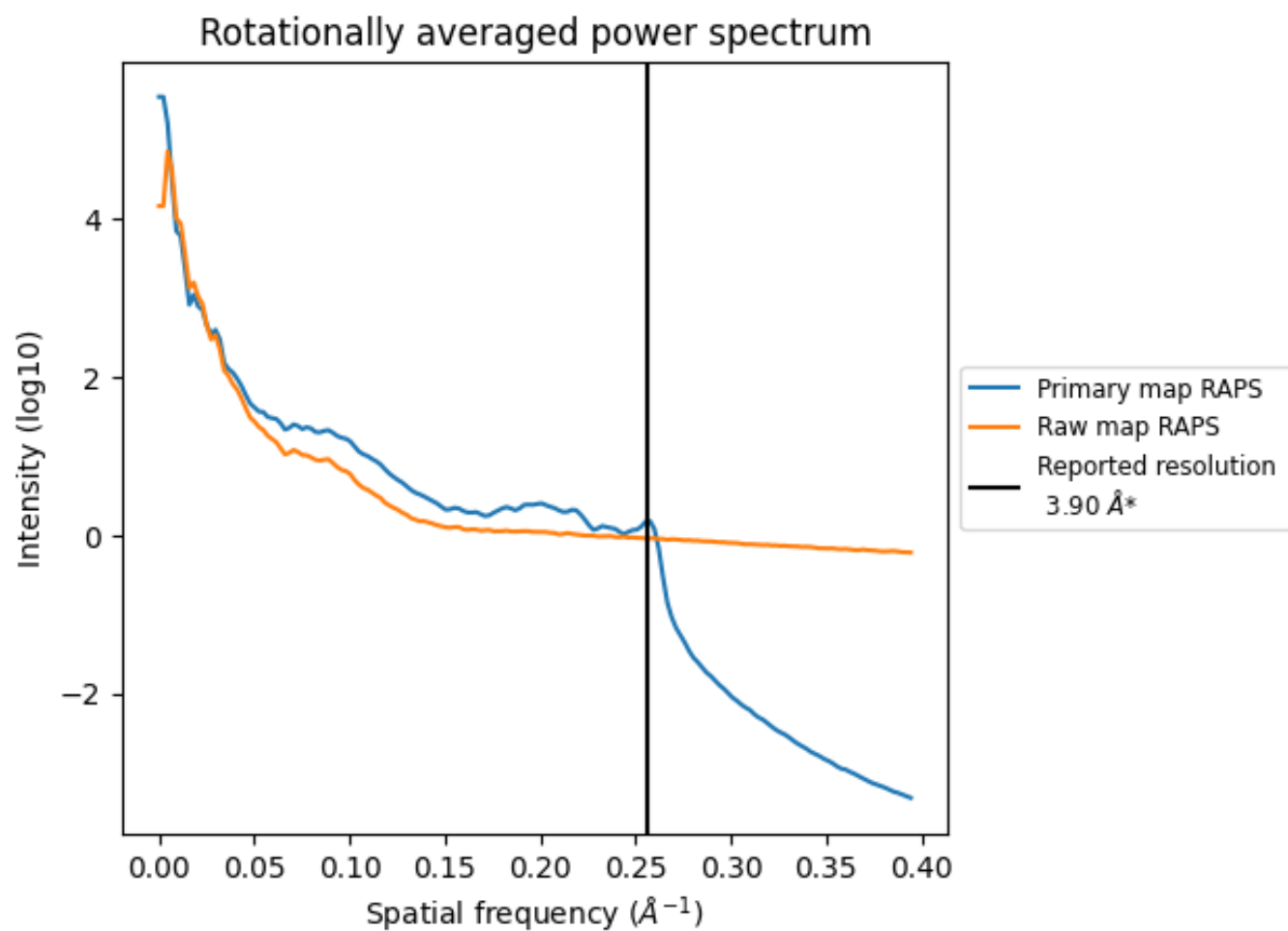
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

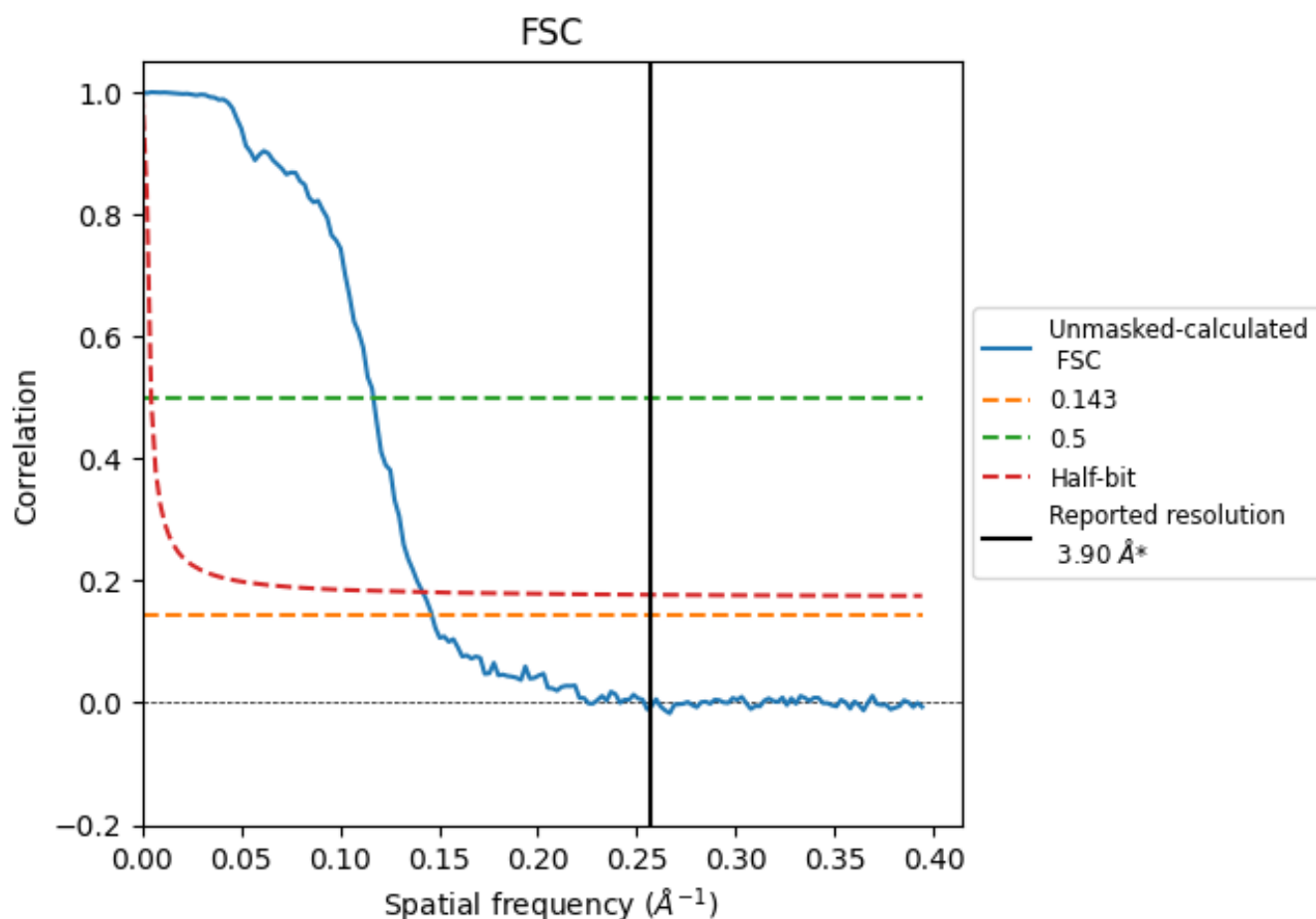


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

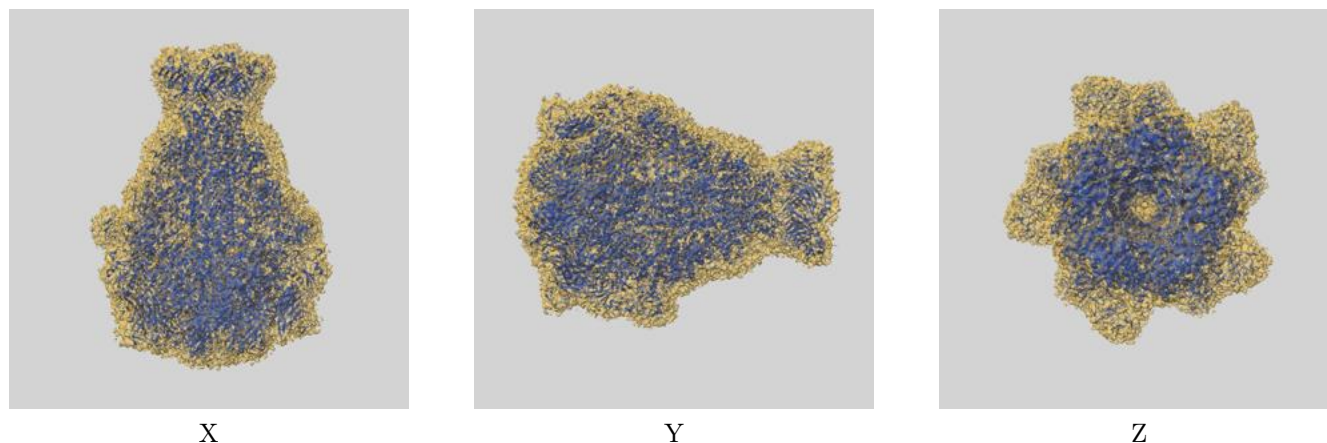
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.83	8.55	7.05

*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](#)

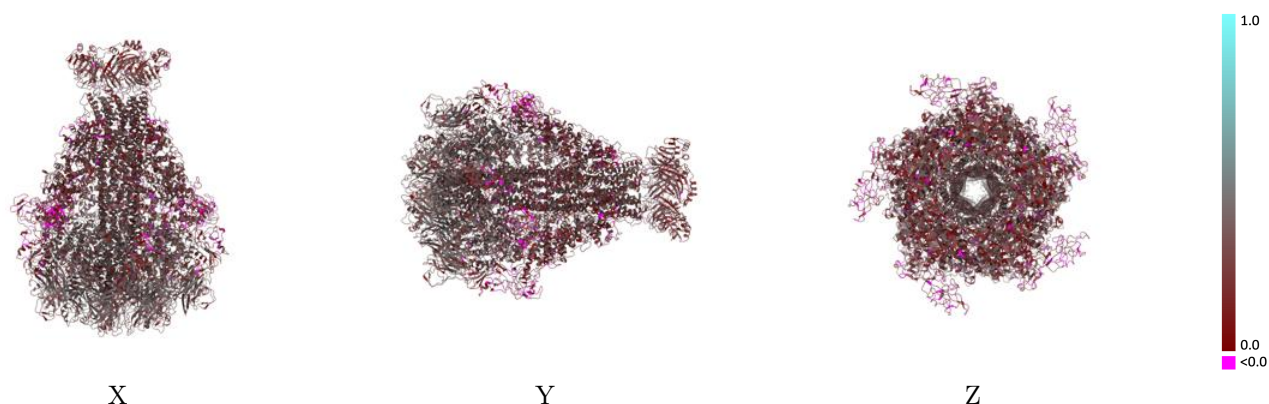
This section contains information regarding the fit between EMDB map EMD-48372 and PDB model 9MLH. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



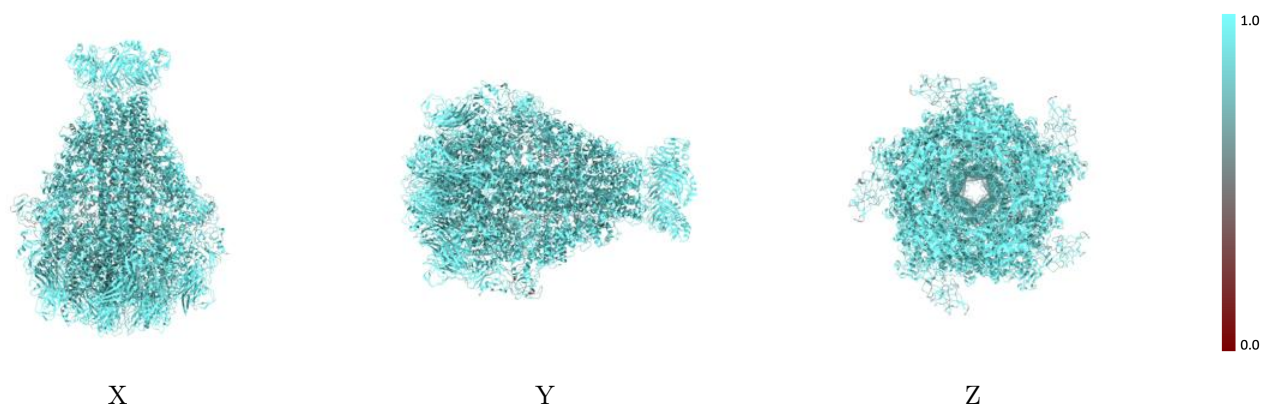
The images above show the 3D surface view of the map at the recommended contour level 0.00379 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



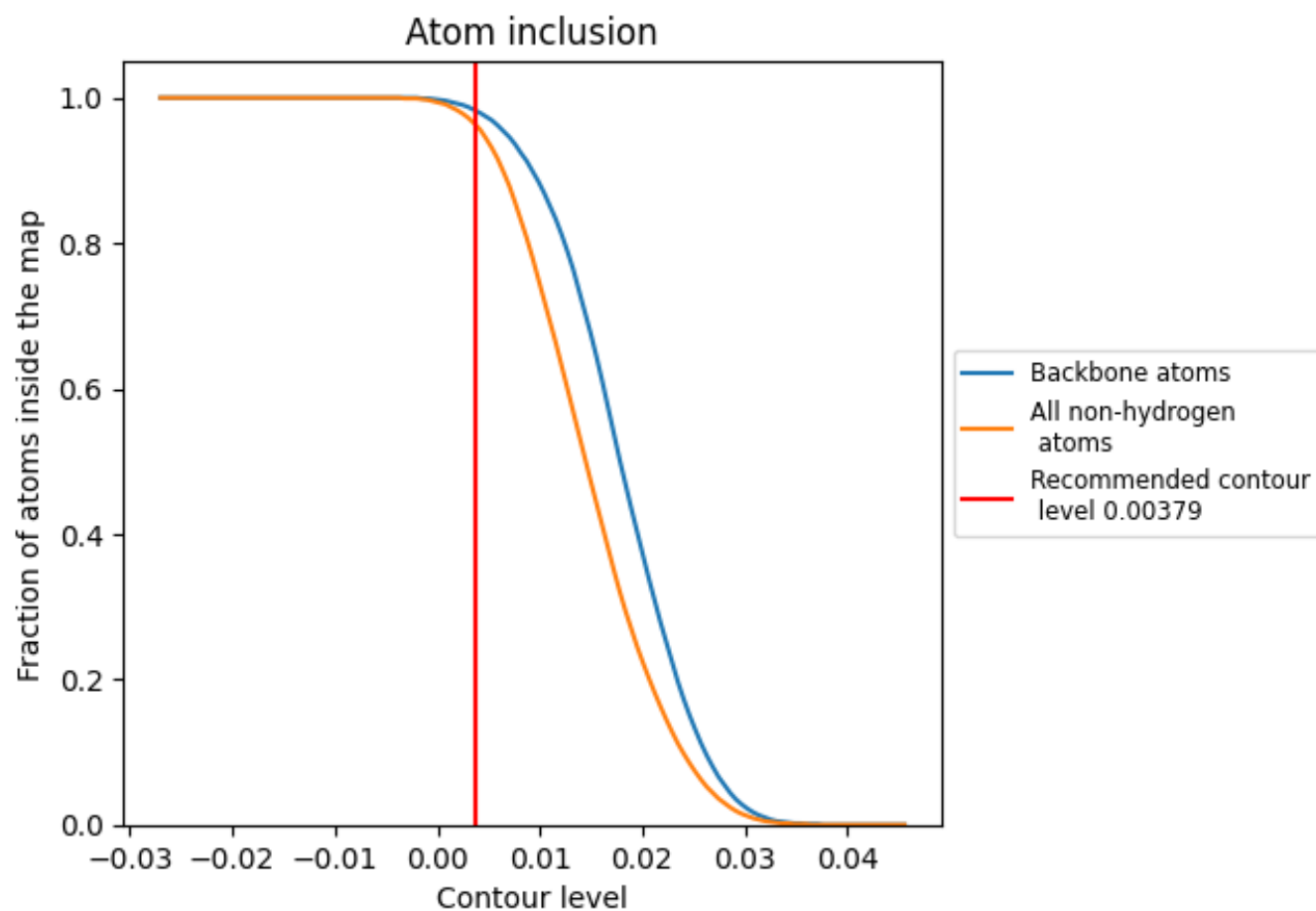
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.9620	0.3000
A	0.9610	0.2990
B	0.9630	0.2990
C	0.9620	0.3000
D	0.9630	0.3000
E	0.9630	0.3010

