



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:10 PM UTC

PDB ID : 9MLG / pdb_00009mlg
EMDB ID : EMD-48371
Title : Xenorhabdus nematophilus XptA2 State 2, 1181insYWK1183, D1182T mutant
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 4.30 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

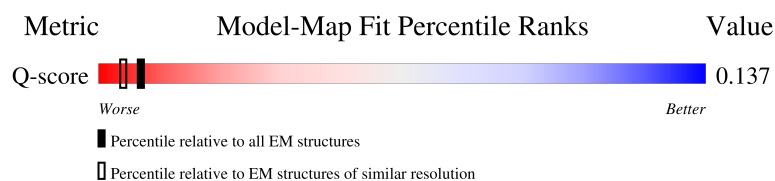
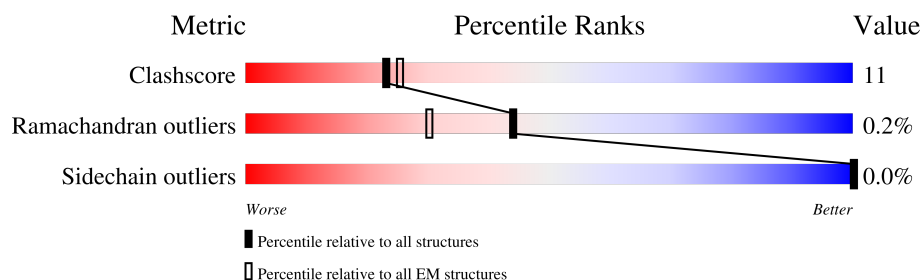
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	2540	18% 76% 24%
1	B	2540	19% 76% 24%
1	C	2540	19% 75% 25%
1	D	2540	21% 75% 25%

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Mol	Chain	Length	Quality of chain
1	E	2540	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100205 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	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	B	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	C	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	D	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0
1	E	2540	Total 20041	C 12651	N 3420	O 3897	S 73	0	0

There are 625 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	1182	TYR	-	insertion	UNP Q93RN7
A	1183	TRP	-	insertion	UNP Q93RN7
A	1184	LYS	-	insertion	UNP Q93RN7
A	1185	THR	ASP	engineered mutation	UNP Q93RN7
A	1253	LYS	VAL	conflict	UNP Q93RN7
A	1256	SER	PRO	conflict	UNP Q93RN7
A	1260	GLY	ASP	conflict	UNP Q93RN7
A	1261	SER	ASN	conflict	UNP Q93RN7
A	1517	ILE	VAL	conflict	UNP Q93RN7
A	1522	MET	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1880	ASN	TYR	conflict	UNP Q93RN7
A	1883	MET	THR	conflict	UNP Q93RN7
A	1887	ILE	VAL	conflict	UNP Q93RN7
A	1923	THR	ALA	conflict	UNP Q93RN7
A	1946	GLY	VAL	conflict	UNP Q93RN7
A	1950	GLN	HIS	conflict	UNP Q93RN7
A	1962	MET	ALA	conflict	UNP Q93RN7
A	1964	GLY	ASP	conflict	UNP Q93RN7
A	1965	ARG	ASN	conflict	UNP Q93RN7
A	1967	GLY	GLU	conflict	UNP Q93RN7
A	1969	SER	ALA	conflict	UNP Q93RN7
A	1970	LYS	THR	conflict	UNP Q93RN7
A	1971	ASN	GLN	conflict	UNP Q93RN7
A	1972	LEU	PRO	conflict	UNP Q93RN7
A	2031	THR	PRO	conflict	UNP Q93RN7
A	2060	THR	ALA	conflict	UNP Q93RN7
A	2152	LEU	PHE	conflict	UNP Q93RN7
A	2164	VAL	ALA	conflict	UNP Q93RN7
A	2167	ILE	VAL	conflict	UNP Q93RN7
A	2181	LEU	PHE	conflict	UNP Q93RN7
A	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
B	1183	TRP	-	insertion	UNP Q93RN7
B	1184	LYS	-	insertion	UNP Q93RN7
B	1185	THR	ASP	engineered mutation	UNP Q93RN7
B	1253	LYS	VAL	conflict	UNP Q93RN7
B	1256	SER	PRO	conflict	UNP Q93RN7
B	1260	GLY	ASP	conflict	UNP Q93RN7
B	1261	SER	ASN	conflict	UNP Q93RN7
B	1517	ILE	VAL	conflict	UNP Q93RN7
B	1522	MET	VAL	conflict	UNP Q93RN7
B	1880	ASN	TYR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1883	MET	THR	conflict	UNP Q93RN7
B	1887	ILE	VAL	conflict	UNP Q93RN7
B	1923	THR	ALA	conflict	UNP Q93RN7
B	1946	GLY	VAL	conflict	UNP Q93RN7
B	1950	GLN	HIS	conflict	UNP Q93RN7
B	1962	MET	ALA	conflict	UNP Q93RN7
B	1964	GLY	ASP	conflict	UNP Q93RN7
B	1965	ARG	ASN	conflict	UNP Q93RN7
B	1967	GLY	GLU	conflict	UNP Q93RN7
B	1969	SER	ALA	conflict	UNP Q93RN7
B	1970	LYS	THR	conflict	UNP Q93RN7
B	1971	ASN	GLN	conflict	UNP Q93RN7
B	1972	LEU	PRO	conflict	UNP Q93RN7
B	2031	THR	PRO	conflict	UNP Q93RN7
B	2060	THR	ALA	conflict	UNP Q93RN7
B	2152	LEU	PHE	conflict	UNP Q93RN7
B	2164	VAL	ALA	conflict	UNP Q93RN7
B	2167	ILE	VAL	conflict	UNP Q93RN7
B	2181	LEU	PHE	conflict	UNP Q93RN7
B	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
C	1183	TRP	-	insertion	UNP Q93RN7
C	1184	LYS	-	insertion	UNP Q93RN7
C	1185	THR	ASP	engineered mutation	UNP Q93RN7
C	1253	LYS	VAL	conflict	UNP Q93RN7
C	1256	SER	PRO	conflict	UNP Q93RN7
C	1260	GLY	ASP	conflict	UNP Q93RN7
C	1261	SER	ASN	conflict	UNP Q93RN7
C	1517	ILE	VAL	conflict	UNP Q93RN7
C	1522	MET	VAL	conflict	UNP Q93RN7
C	1880	ASN	TYR	conflict	UNP Q93RN7
C	1883	MET	THR	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1887	ILE	VAL	conflict	UNP Q93RN7
C	1923	THR	ALA	conflict	UNP Q93RN7
C	1946	GLY	VAL	conflict	UNP Q93RN7
C	1950	GLN	HIS	conflict	UNP Q93RN7
C	1962	MET	ALA	conflict	UNP Q93RN7
C	1964	GLY	ASP	conflict	UNP Q93RN7
C	1965	ARG	ASN	conflict	UNP Q93RN7
C	1967	GLY	GLU	conflict	UNP Q93RN7
C	1969	SER	ALA	conflict	UNP Q93RN7
C	1970	LYS	THR	conflict	UNP Q93RN7
C	1971	ASN	GLN	conflict	UNP Q93RN7
C	1972	LEU	PRO	conflict	UNP Q93RN7
C	2031	THR	PRO	conflict	UNP Q93RN7
C	2060	THR	ALA	conflict	UNP Q93RN7
C	2152	LEU	PHE	conflict	UNP Q93RN7
C	2164	VAL	ALA	conflict	UNP Q93RN7
C	2167	ILE	VAL	conflict	UNP Q93RN7
C	2181	LEU	PHE	conflict	UNP Q93RN7
C	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
D	1183	TRP	-	insertion	UNP Q93RN7
D	1184	LYS	-	insertion	UNP Q93RN7
D	1185	THR	ASP	engineered mutation	UNP Q93RN7
D	1253	LYS	VAL	conflict	UNP Q93RN7
D	1256	SER	PRO	conflict	UNP Q93RN7
D	1260	GLY	ASP	conflict	UNP Q93RN7
D	1261	SER	ASN	conflict	UNP Q93RN7
D	1517	ILE	VAL	conflict	UNP Q93RN7
D	1522	MET	VAL	conflict	UNP Q93RN7
D	1880	ASN	TYR	conflict	UNP Q93RN7
D	1883	MET	THR	conflict	UNP Q93RN7
D	1887	ILE	VAL	conflict	UNP Q93RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1923	THR	ALA	conflict	UNP Q93RN7
D	1946	GLY	VAL	conflict	UNP Q93RN7
D	1950	GLN	HIS	conflict	UNP Q93RN7
D	1962	MET	ALA	conflict	UNP Q93RN7
D	1964	GLY	ASP	conflict	UNP Q93RN7
D	1965	ARG	ASN	conflict	UNP Q93RN7
D	1967	GLY	GLU	conflict	UNP Q93RN7
D	1969	SER	ALA	conflict	UNP Q93RN7
D	1970	LYS	THR	conflict	UNP Q93RN7
D	1971	ASN	GLN	conflict	UNP Q93RN7
D	1972	LEU	PRO	conflict	UNP Q93RN7
D	2031	THR	PRO	conflict	UNP Q93RN7
D	2060	THR	ALA	conflict	UNP Q93RN7
D	2152	LEU	PHE	conflict	UNP Q93RN7
D	2164	VAL	ALA	conflict	UNP Q93RN7
D	2167	ILE	VAL	conflict	UNP Q93RN7
D	2181	LEU	PHE	conflict	UNP Q93RN7
D	2433	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1182	TYR	-	insertion	UNP Q93RN7
E	1183	TRP	-	insertion	UNP Q93RN7
E	1184	LYS	-	insertion	UNP Q93RN7
E	1185	THR	ASP	engineered mutation	UNP Q93RN7
E	1253	LYS	VAL	conflict	UNP Q93RN7
E	1256	SER	PRO	conflict	UNP Q93RN7
E	1260	GLY	ASP	conflict	UNP Q93RN7
E	1261	SER	ASN	conflict	UNP Q93RN7
E	1517	ILE	VAL	conflict	UNP Q93RN7
E	1522	MET	VAL	conflict	UNP Q93RN7
E	1880	ASN	TYR	conflict	UNP Q93RN7
E	1883	MET	THR	conflict	UNP Q93RN7
E	1887	ILE	VAL	conflict	UNP Q93RN7
E	1923	THR	ALA	conflict	UNP Q93RN7

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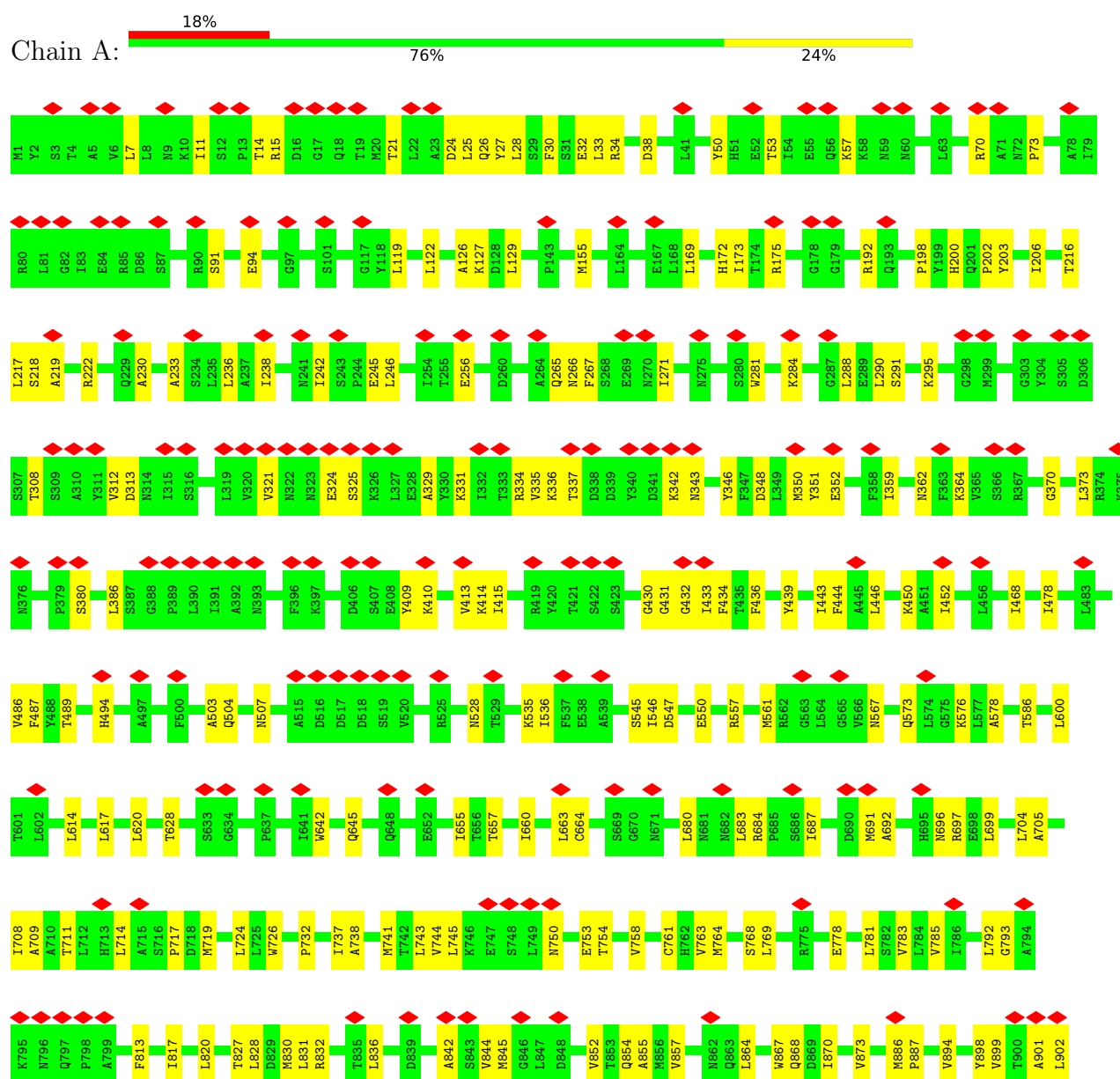
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Chain	Residue	Modelled	Actual	Comment	Reference
E	1946	GLY	VAL	conflict	UNP Q93RN7
E	1950	GLN	HIS	conflict	UNP Q93RN7
E	1962	MET	ALA	conflict	UNP Q93RN7
E	1964	GLY	ASP	conflict	UNP Q93RN7
E	1965	ARG	ASN	conflict	UNP Q93RN7
E	1967	GLY	GLU	conflict	UNP Q93RN7
E	1969	SER	ALA	conflict	UNP Q93RN7
E	1970	LYS	THR	conflict	UNP Q93RN7
E	1971	ASN	GLN	conflict	UNP Q93RN7
E	1972	LEU	PRO	conflict	UNP Q93RN7
E	2031	THR	PRO	conflict	UNP Q93RN7
E	2060	THR	ALA	conflict	UNP Q93RN7
E	2152	LEU	PHE	conflict	UNP Q93RN7
E	2164	VAL	ALA	conflict	UNP Q93RN7
E	2167	ILE	VAL	conflict	UNP Q93RN7
E	2181	LEU	PHE	conflict	UNP Q93RN7
E	2433	LEU	PHE	conflict	UNP Q93RN7

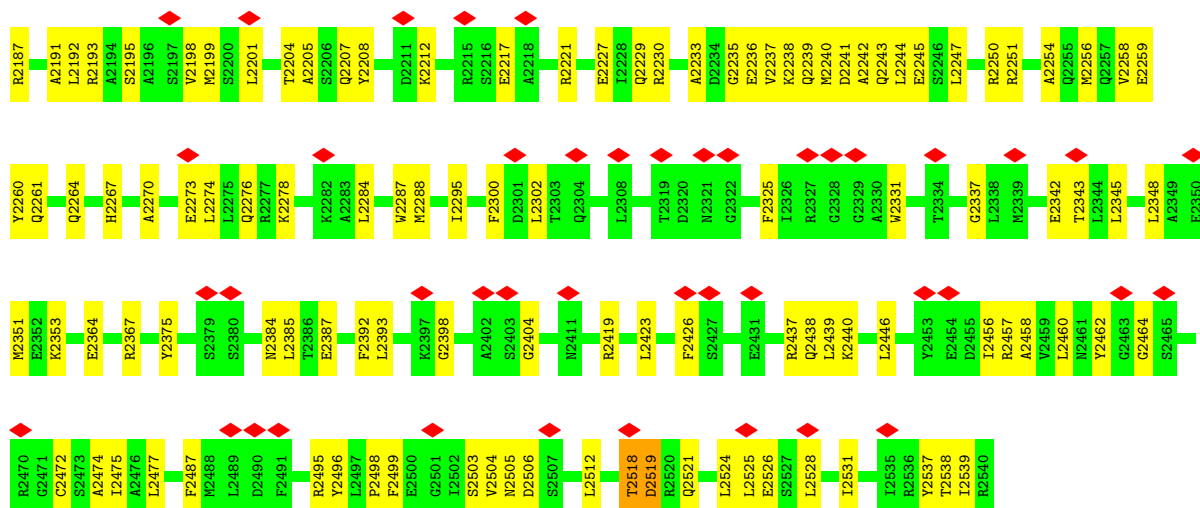
3 Residue-property plots

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.

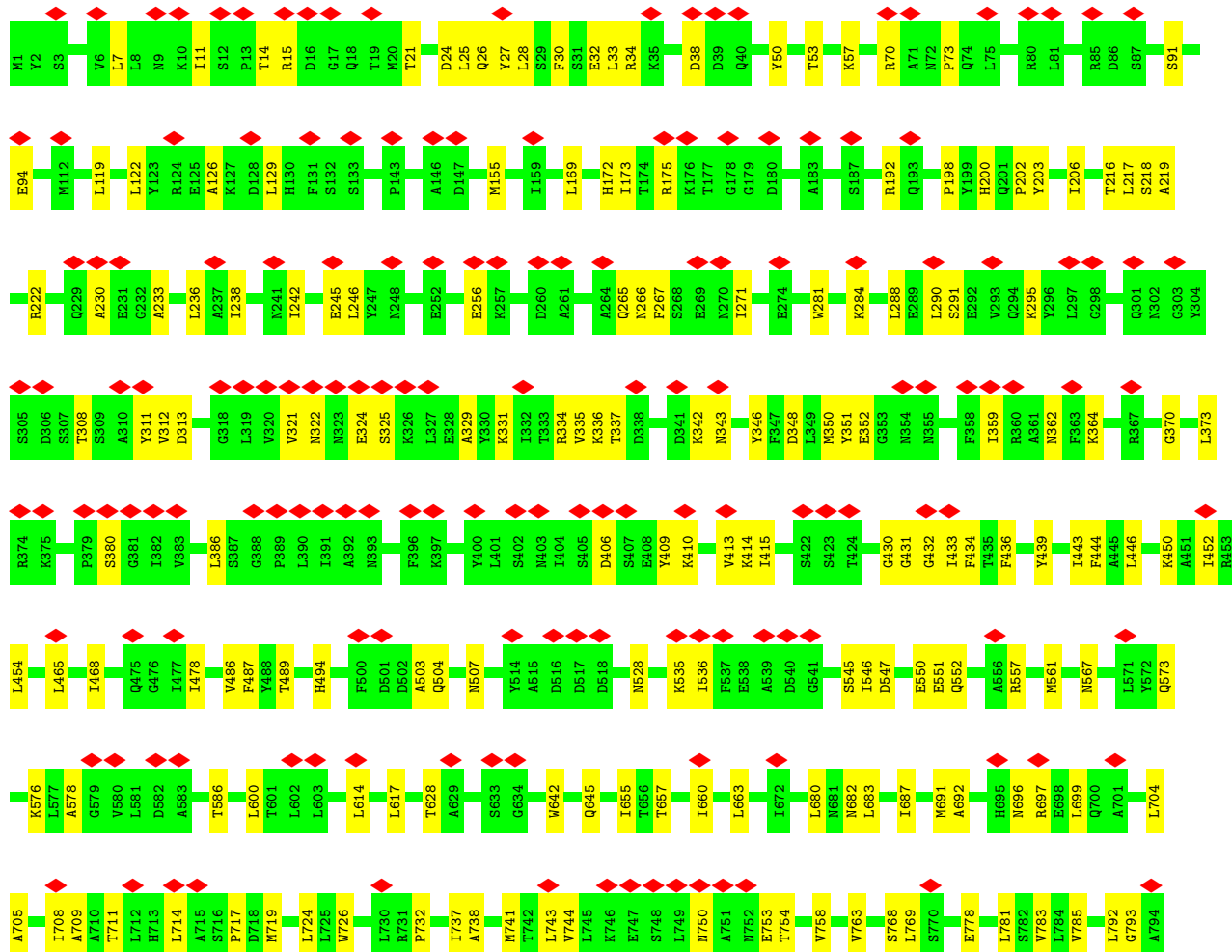
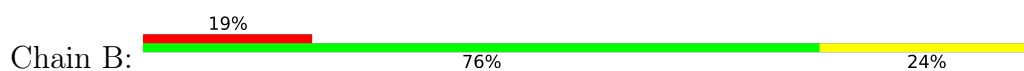
• Molecule 1: XptA2 protein



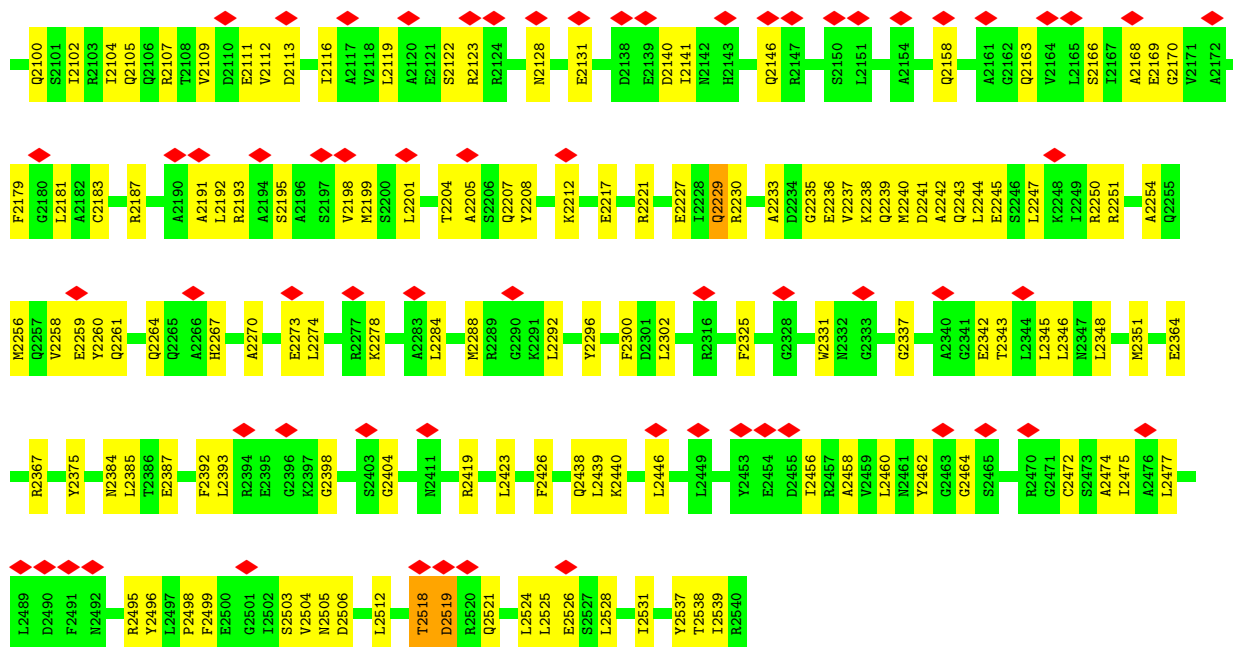




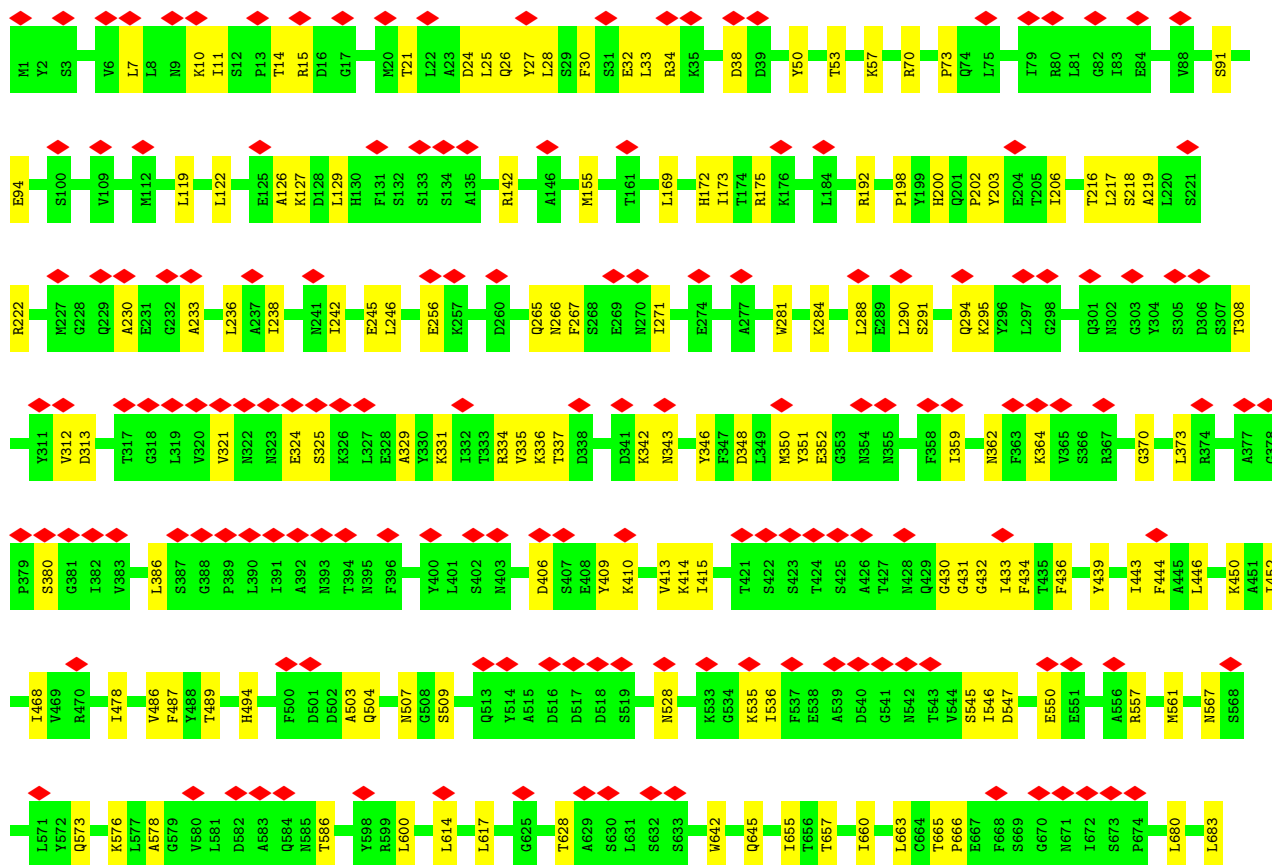
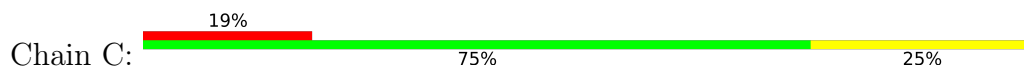
• Molecule 1: XptA2 protein



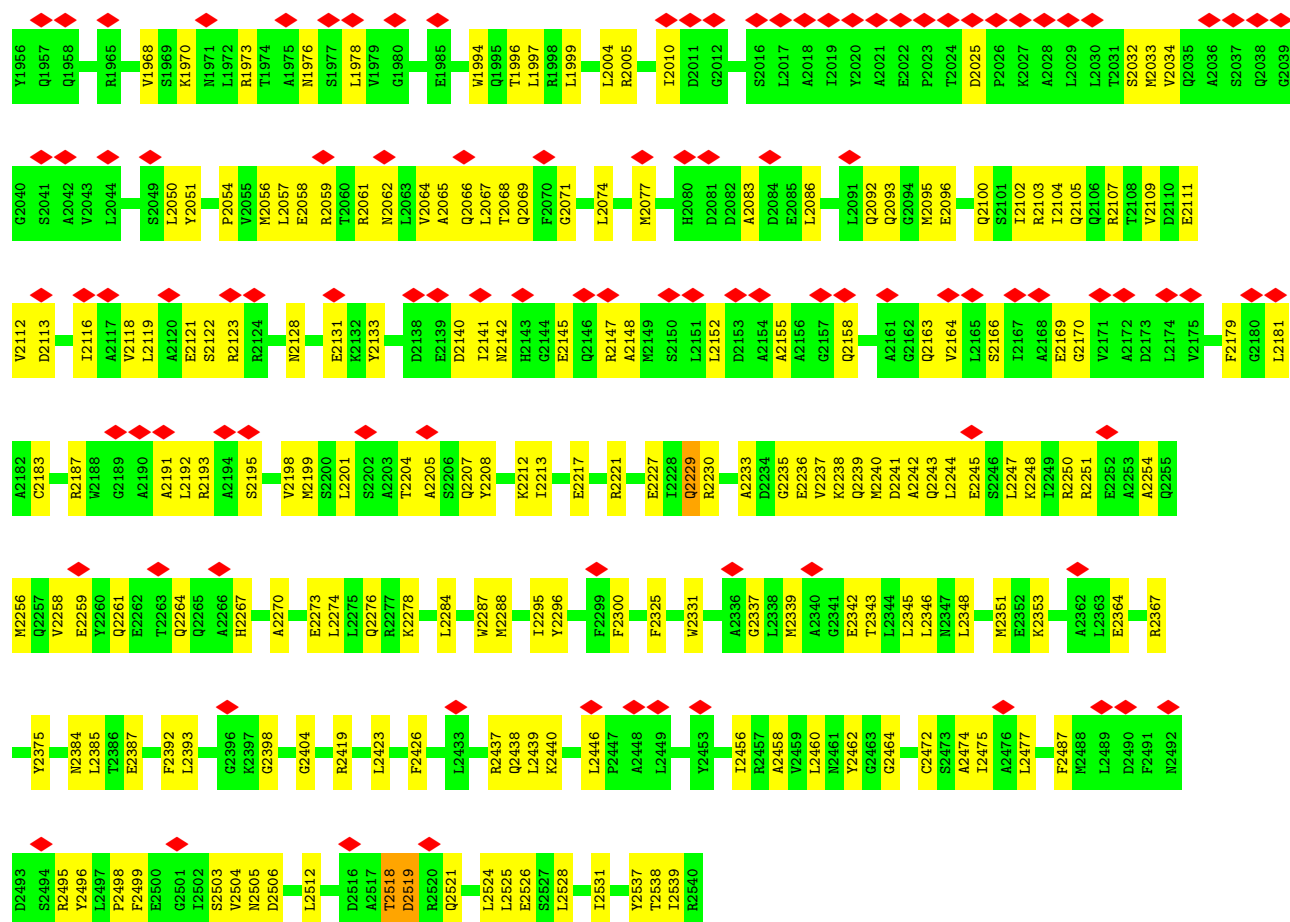




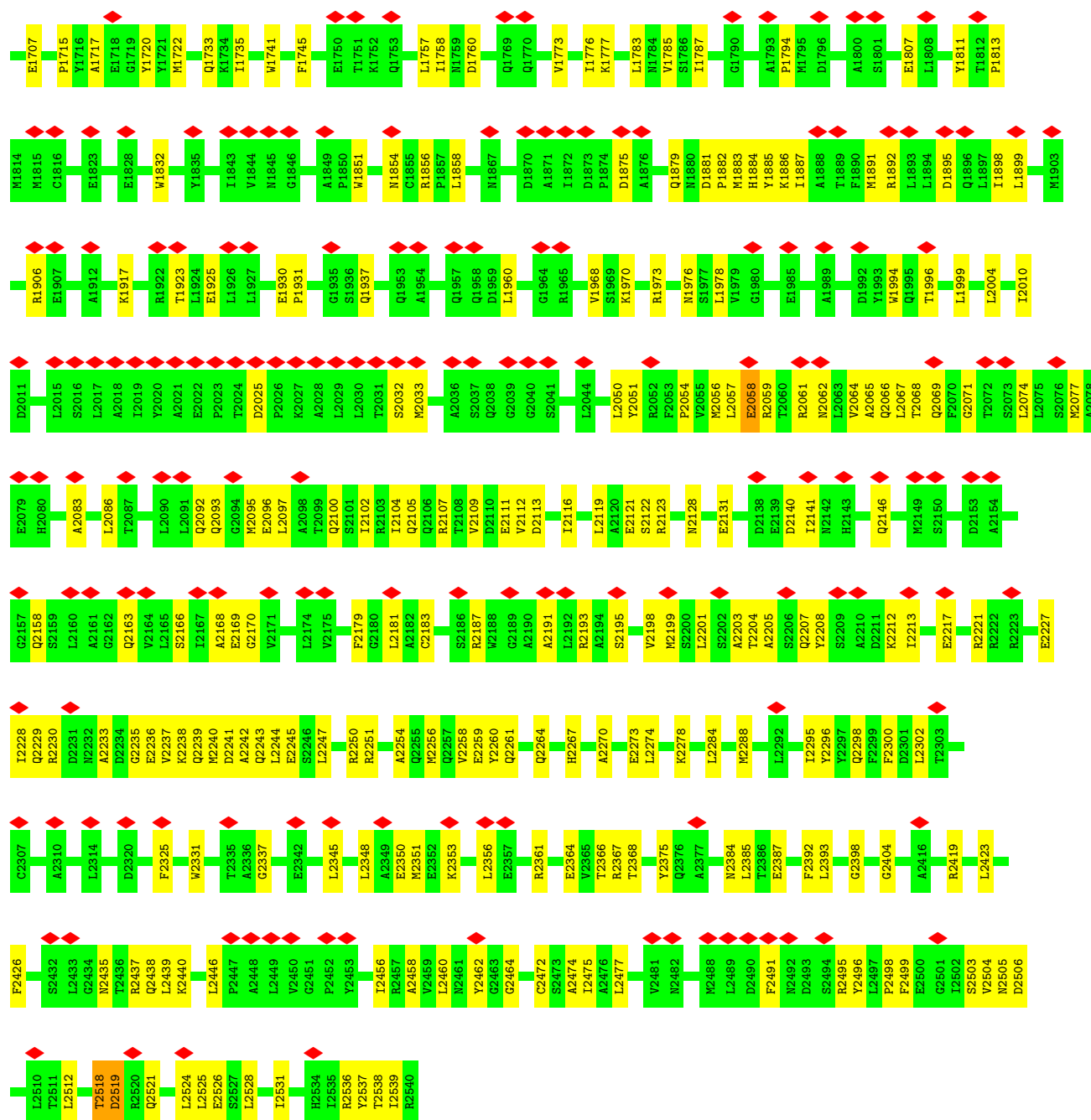
• Molecule 1: XptA2 protein



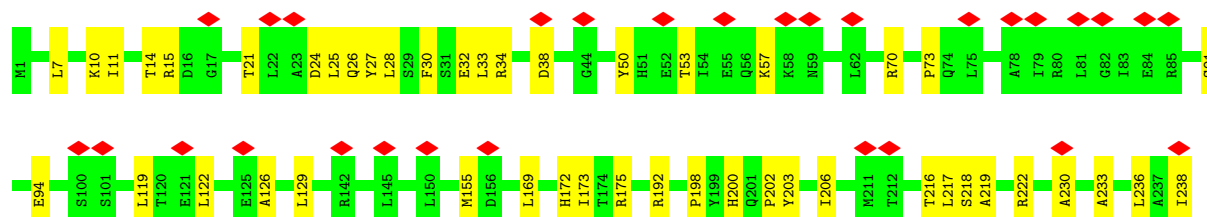
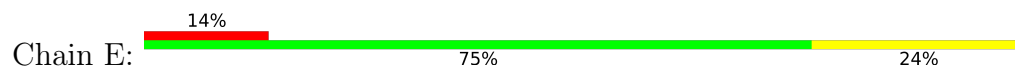
L1858	E1859	E1860	A1866	N1867	D1870	A1871	I1872	P1874	D1875	A1876	Q1879	N1880	P1881	M1882	H1883	H1884	Y1885	K1886	I1887	M1891	R1892	D1895	Q1896	L1897	I1898	L1899	R1906	K1917	V1921	R1922	T1923	L1924	E1925	L1926	G1928	D1929	E1930	P1931	G1935	S1936	Q1937	S1945	N1945	I1951	A1954	A1955						
W1741	F1745	E1750	L1757	N1758	D1760	Q1770	G1771	I1772	V1773	K1774	N1775	I1776	K1777	L1783	N1784	V1785	S1786	I1787	A1793	P1794	M1795	D1796	L1803	E1807	Y1811	T1812	P1813	M1814	Q1825	A1829	W1832	Y1835	V1836	G1841	V1844	N1845	W1851	N1854	C1855	P1856	P1857											
M1638	T1639	G1640	I1641	D1642	T1643	I1644	M1647	E1648	R1651	L1657	A1663	N1664	F1665	P1668	R1669	Y1670	D1671	E1674	R1679	W1680	F1681	K1682	N1687	G1690	N1691	T1692	G1693	R1694	L1702	E1707	M1710	P1715	Y1716	A1717	E1718	G1719	Y1720	M1721	M1722	H1723	Q1733	K1734	I1735	T1740								
S1543	A1546	M1547	P1548	E1555	I1556	D1557	S1560	A1568	V1573	F1574	E1575	T1576	K1577	A1578	K1579	D1580	G1581	T1587	K1588	L1591	S1592	V1593	V1596	N1599	P1600	I1603	L1604	E1608	Q1614	Q1617	L1618	G1619	R1622	I1623	R1624	L1625	A1630	S1631	Q1632	L1633	V1634	S1635	R1636	A1637								
T1467	V1468	F1469	T1470	V1471	G1472	S1473	N1474	K1475	T1476	S1477	D1478	K1480	S1481	C1482	Y1484	A1485	N1490	S1491	F1493	Q1495	I1496	S1499	D1507	G1511	N1512	M1513	N1514	I1517	K1518	I1519	T1520	V1521	M1522	A1523	G1524	S1525	K1526	T1529	S1533	D1534	H1535	I1536	A1537	S1538	L1539	P1540	A1541	N1542				
G1393	V1402	Y1408	G1412	G1413	T1414	I1415	V1417	Y1418	N1419	K1420	T1421	K1422	N1423	Y1424	I1425	A1426	G1430	H1431	L1432	M1433	N1434	A1435	D1436	Y1437	T1438	R1439	L1440	L1441	L1442	L1443	T1444	V1445	V1446	E1447	N1448	N1449	Y1450	Y1451	A1452	R1453	L1454	F1455	F1457	P1458	F1459	S1460	P1461	N1462	T1463	I1464	N1465	N1466
K1278	T1282	A1283	L1284	S1285	R1286	M1292	I1296	T1299	N1302	Y1310	P1319	A1320	M1324	D1331	M1336	E1337	N1338	L1341	P1342	Q1343	K1347	Y1348	S1349	S1350	D1351	N1352	L1353	A1354	I1355	T1356	L1357	H1358	V1364	R1374	K1376	K1382	G1385	V1386	D1387	G1388	K1389	S1390										
V1187	E1188	L1195	K1196	L1197	A1198	F1199	L1200	R1201	H1202	P1209	D1213	L1214	T1215	Q1217	V1218	E1219	A1220	V1221	T1222	D1223	K1224	E1229	G1237	F1238	Q1239	G1240	E1241	T1242	L1243	L1244	L1245	Y1249	Y1255	S1256	D1257	F1258	G1259	Q1260	S1261	V1265	A1266	G1267	M1268	L1270	T1271	G1272	F1276	K1277				
T1086	V1087	V1100	L1106	R1114	E1115	N1116	L1117	P1118	E1119	Y1120	Y1121	Y1122	Y1123	N1124	S1128	A1132	L1135	W1140	T1144	K1145	I1146	D1147	T1148	A1149	V1150	M1151	P1152	Y1153	A1156	I1157	F1162	R1163	E1164	H1167	W1170	A1177	K1178	N1179	G1180	Y1181	Y1182	V1183	K1184	T1185	P1186							
L986	T990	I993	G994	L995	T996	N998	R999	A1000	R1003	I1004	N1007	A1010	D1011	T1014	F1018	T1019	D1020	W1021	N1024	L1036	P1040	E1041	N1042	Y1043	E923	L926	Q930	L934	N948	Q955	P956	E957	Q958	V959	S960	D966	Y970	T971	L972	T983												
C761	H762	V763	M764	S768	L769	E778	L781	S782	L783	V785	A790	L791	G792	A794	N795	N796	Q797	P798	R812	F813	I817	L820	T827	L828	D829	M830	L831	R832	L836	T837	A838	D839	R840	L841	S842	V844	M845	D848	I849	S850	M851	V852	T853	Q854	F855	M856						
I687	M691	A692	Q693	S694	H695	N696	R697	E698	L699	Q700	A701	A705	I708	A709	A710	T711	L714	A715	S716	P717	D718	M719	L724	L725	W726	L730	R731	P732	G733	G734	I737	A738	G739	F740	M741	T742	L743	V744	L745	K746	E747	S748	L749	N750	A751	N752	E753	T754	V758			

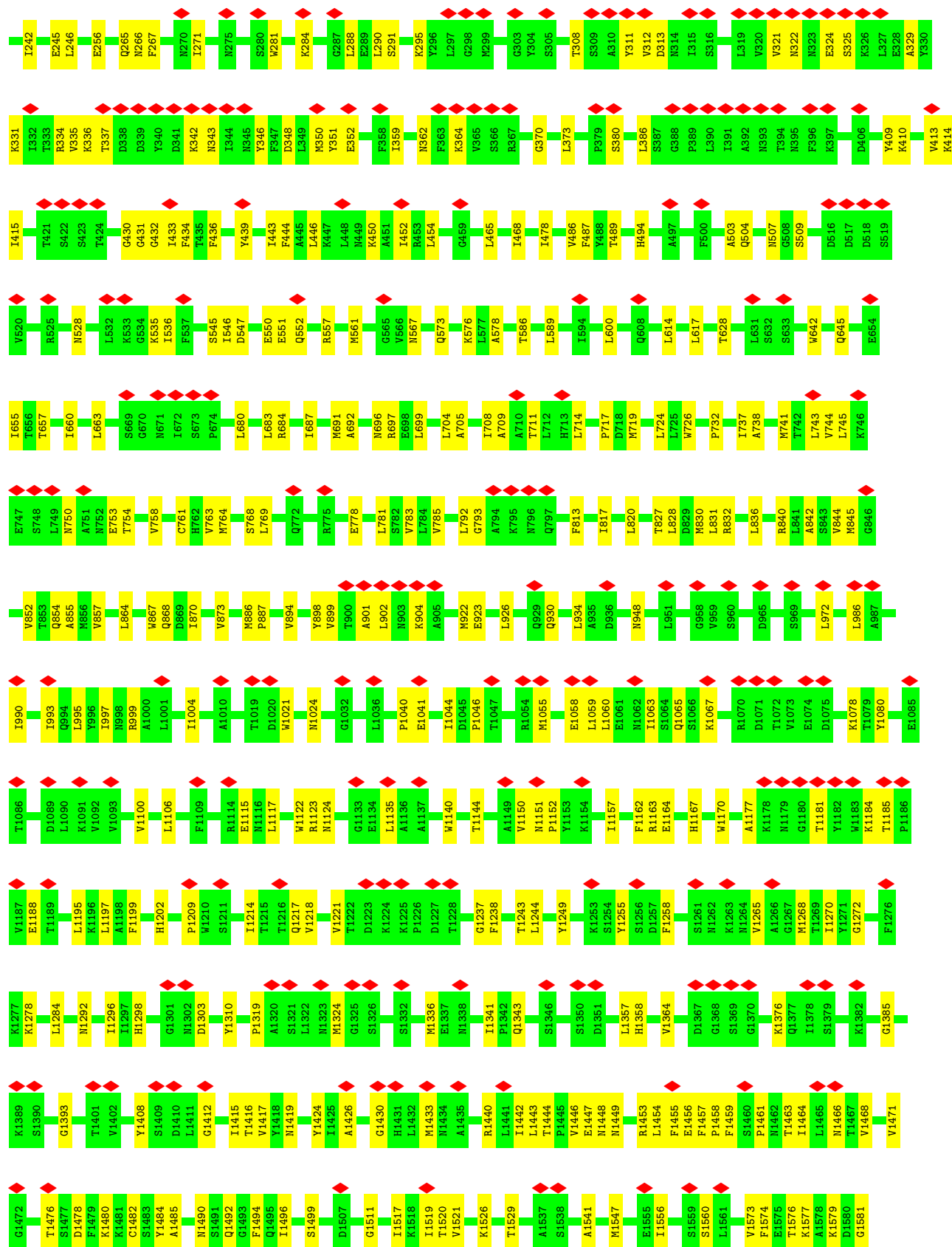






• Molecule 1: XptA2 protein





V2504	G2398	A2270	S1915	L2091	L2017	A1888	S1765	D1671	I1587
N2505	G2404	E2273	V2198	Q2092	A2018	T1889	I1787	E1674	K1588
D2506	M2199	L2274	M2199	Q2093	I2019	F1890	G1790	R1679	L1591
L2512	R2419	K2278	S2200	W2095	Y2020	M1891	Y1791	F1681	V1596
T2518	L2423	L2284	L2201	L2097	E2021	L1892	S1792	K1682	M1599
D2519	F2426	L2296	T2204	Q2100	P2023	D1895	P1794	N1687	P1600
R2520	S2427	M2288	A2205	S2101	T2024	I1898	S1801	M1701	E1601
Q2521	D2428	Y2296	S2206	I2102	D2025	L1899	Y1804	L1702	D1602
L2524	L2433	F2300	Y2208	R2103	P2026	M1903	E1807	E1707	I1603
L2525	Q2438	D2301	A2210	T2104	K2027	A1904	L1908	T1708	L1604
S2527	L2439	L2302	D2211	Q2105	A2028	Y1905	L1909	T1609	E1608
L2528	K2440	G2322	K2212	R2107	L2029	R1906	Y1811	S1709	H1610
L2531	L2446	E2325	L2213	V2109	L2030	E1907	T1812	P1715	Q1614
Y2537	V2450	F2326	S2214	D2110	T2031	D1911	P1813	A1717	Q1617
T2538	R2327	L2326	E2217	E2111	S2032	K1917	G1816	E1718	R1622
T2539	R2327	R2327	R2221	D2112	M2033	I1923	R1819	Y1720	I1623
R2540	W2331	G2337	E2227	D2113	V2034	T1924	E1828	M1722	R1624
		L2338	L2228	L2116	Q2035	E1925	W1832	Q1733	L1628
		M2339	R2230	R2123	A2036	L1926	I1833	K1734	L1629
		E2342	A2233	D2140	S2037	D1929	M1834	I1735	A1630
		T2343	D2234	T2141	G2041	E1930	E1847	W1741	Q1632
		L2345	E2235	R2147	A2042	P1931	I1843	F1745	L1633
		L2346	G2236	Q2158	G2046	Q1937	V1844	E1750	V1634
		W2347	E2237	Q2163	L2050	A1947	N1845	T1751	S1635
		L2348	L2228	S2166	Y2051	V1968	G1846	K1752	A1637
		M2351	R2240	E2169	P2054	S1989	I1848	Q1753	M1638
		E2352	A2242	G2170	M2055	N1970	W1851	L1757	T1639
		K2353	Q2243	L2174	M2056	N1971	N1854	N1758	G1640
		L2356	L2244	F2179	L2057	L1972	C1855	D1760	M1647
		F2357	E2245	Q2180	E2058	R1973	R1856	E1648	R1651
		E2364	L2247	L2181	R2059	N1976	P1857	S1765	L1652
		R2367	R2250	A2182	T2060	L1977	L1858	M1767	P1653
		Y2375	R2251	C2183	N2062	Q1995	D1870	T1768	L1657
		S2379	A2254	R2187	R2063	T1996	A1871	Q1769	G1658
		N2384	Q2255	W2188	V2064	L1997	D1875	I1772	E1659
		L2385	M2256	Q2189	A2065	R1998	Q1879	V1773	F1665
		T2386	Q2257	A2190	Q2066	L1999	N1880	K1777	P1668
		E2387	E2258	A2191	L2067	L2004	P1882	L1783	K1669
		F2392	E2259	L2192	T2068	I2010	M1884	Y1785	V1670
		L2393	Q2261	R2193	Q2069	L2015	Y1885		
			Q2264	A2194	F2070	S2016	K1886		
			H2267	R2194	G2071		I1887		
					L2074				
					M2077				
					A2083				
					L2086				
					L2090				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.069	Depositor
Minimum map value	-0.470	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	473.796, 473.796, 473.796	wwPDB
Map dimensions	246, 246, 246	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.926, 1.926, 1.926	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	0.14	0/20450	0.40	2/27765 (0.0%)
1	B	0.14	0/20450	0.40	4/27765 (0.0%)
1	C	0.14	0/20450	0.40	2/27765 (0.0%)
1	D	0.14	0/20450	0.40	4/27765 (0.0%)
1	E	0.14	0/20450	0.40	2/27765 (0.0%)
All	All	0.14	0/102250	0.40	14/138825 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2518	THR	CA-C-N	9.52	138.83	121.70
1	D	2518	THR	C-N-CA	9.52	138.83	121.70
1	B	2518	THR	CA-C-N	9.50	138.80	121.70
1	B	2518	THR	C-N-CA	9.50	138.80	121.70
1	C	2518	THR	CA-C-N	9.49	138.79	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	20041	0	19627	443	0
1	B	20041	0	19627	454	0
1	C	20041	0	19627	493	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	20041	0	19627	509	0
1	E	20041	0	19627	463	0
All	All	100205	0	98135	2194	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 11.

The worst 5 of 2194 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:2518:THR:H	1:C:2519:ASP:HB2	1.22	1.04
1:D:2518:THR:H	1:D:2519:ASP:HB2	1.22	1.04
1:B:2518:THR:H	1:B:2519:ASP:HB2	1.22	1.00
1:A:2518:THR:H	1:A:2519:ASP:HB2	1.22	0.99
1:E:2518:THR:H	1:E:2519:ASP:HB2	1.22	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	43	77
1	B	2538/2540 (100%)	2375 (94%)	159 (6%)	4 (0%)	43	77
1	C	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
1	D	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
1	E	2538/2540 (100%)	2374 (94%)	160 (6%)	4 (0%)	43	77
All	All	12690/12700 (100%)	11872 (94%)	798 (6%)	20 (0%)	44	77

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2519	ASP
1	B	2519	ASP
1	C	2519	ASP
1	D	2519	ASP
1	E	2519	ASP

5.3.2 Protein sidechains [i](#)

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	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	B	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	C	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	D	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
1	E	2175/2177 (100%)	2174 (100%)	1 (0%)	100	100
All	All	10875/10885 (100%)	10870 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2229	GLN
1	B	2229	GLN
1	C	2229	GLN
1	D	2229	GLN
1	E	2229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	801	GLN
1	E	1733	GLN
1	D	40	GLN
1	E	1687	ASN
1	E	2391	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

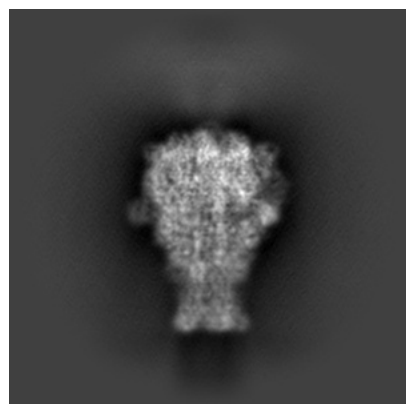
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48371. These allow visual inspection of the internal detail of the map and identification of artifacts.

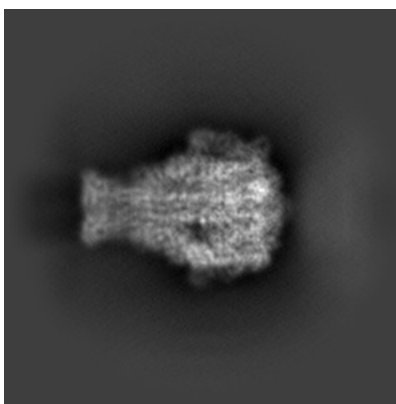
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

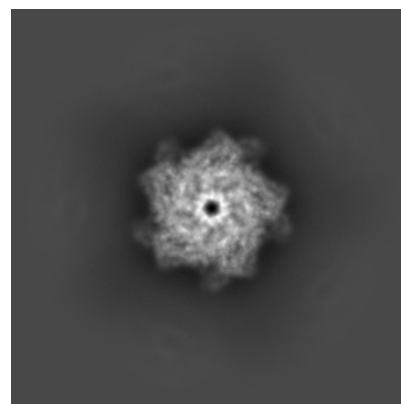
6.1.1 Primary map



X

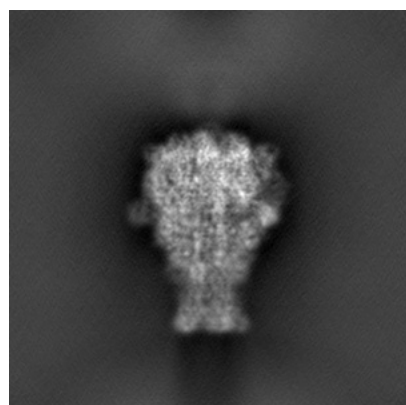


Y

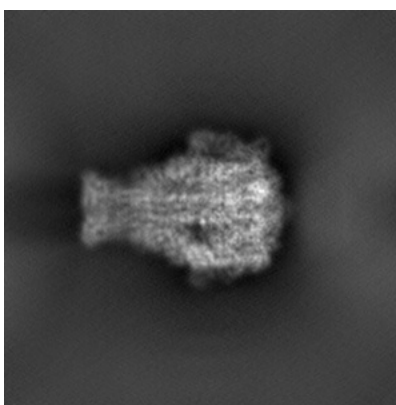


Z

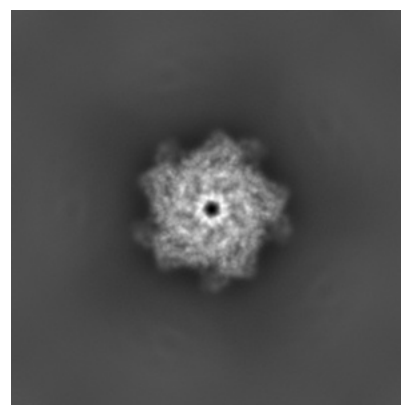
6.1.2 Raw map



X



Y

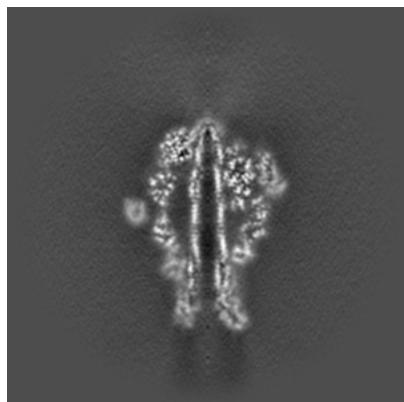


Z

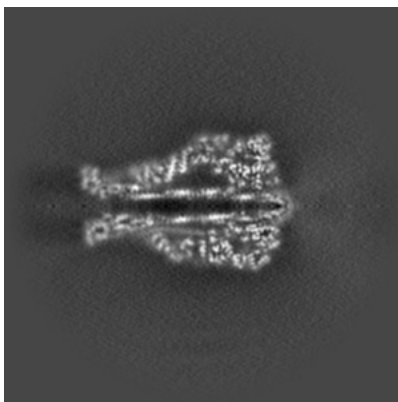
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

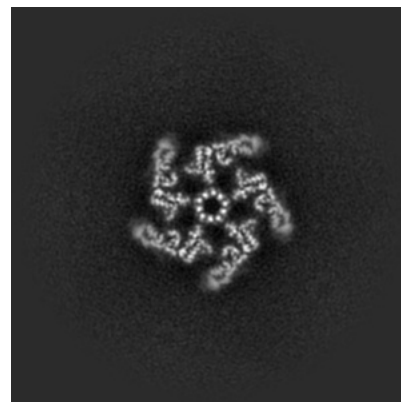
6.2.1 Primary map



X Index: 123

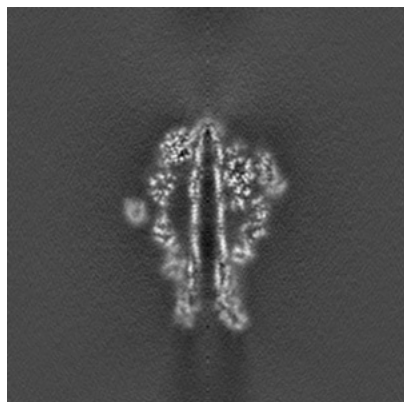


Y Index: 123

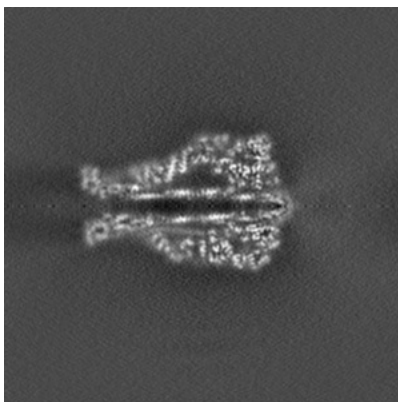


Z Index: 123

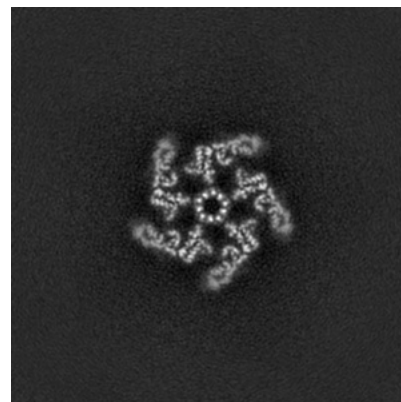
6.2.2 Raw map



X Index: 123



Y Index: 123

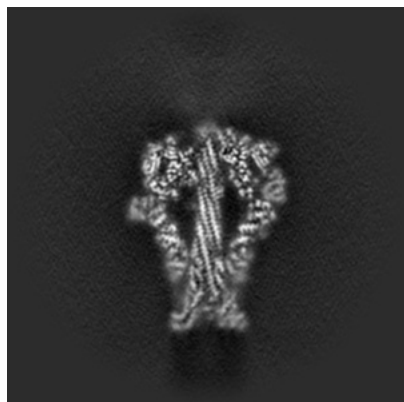


Z Index: 123

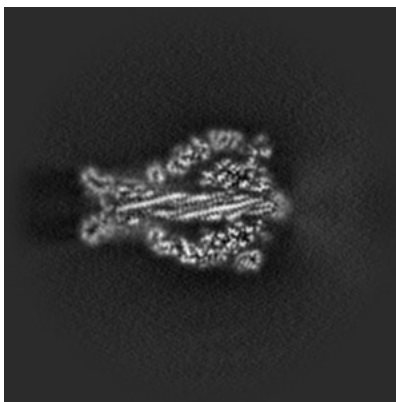
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

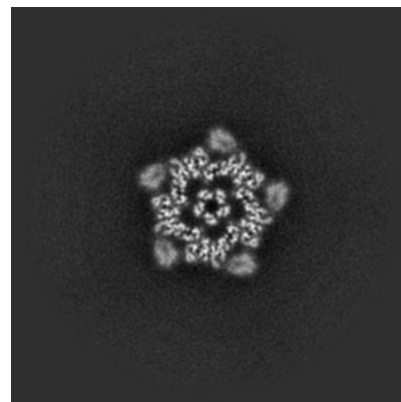
6.3.1 Primary map



X Index: 130

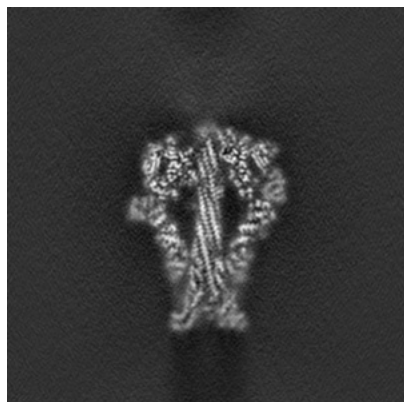


Y Index: 129

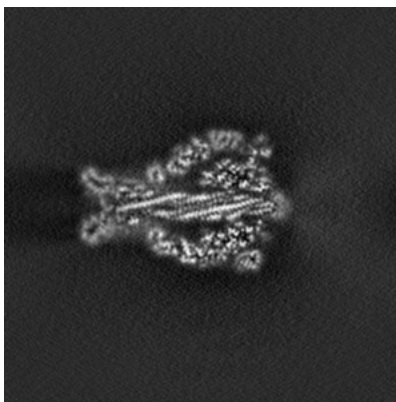


Z Index: 132

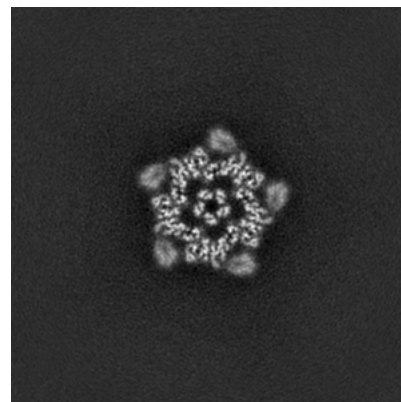
6.3.2 Raw map



X Index: 130



Y Index: 129

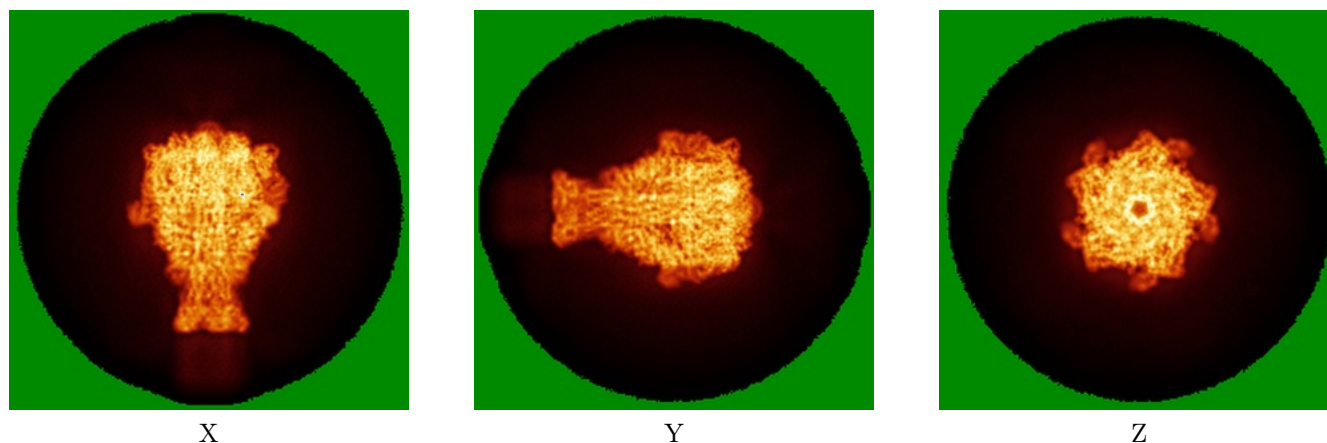


Z Index: 132

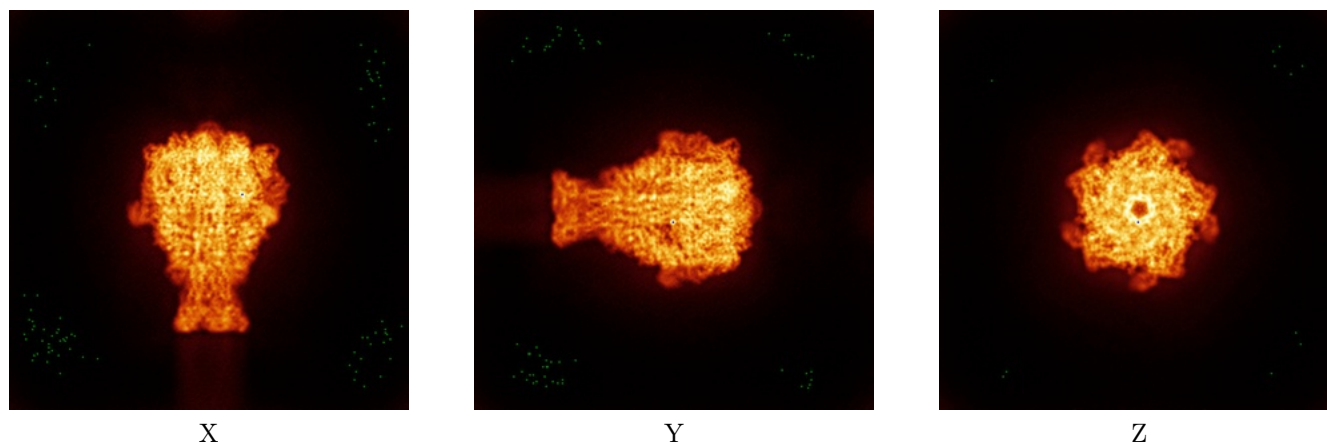
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

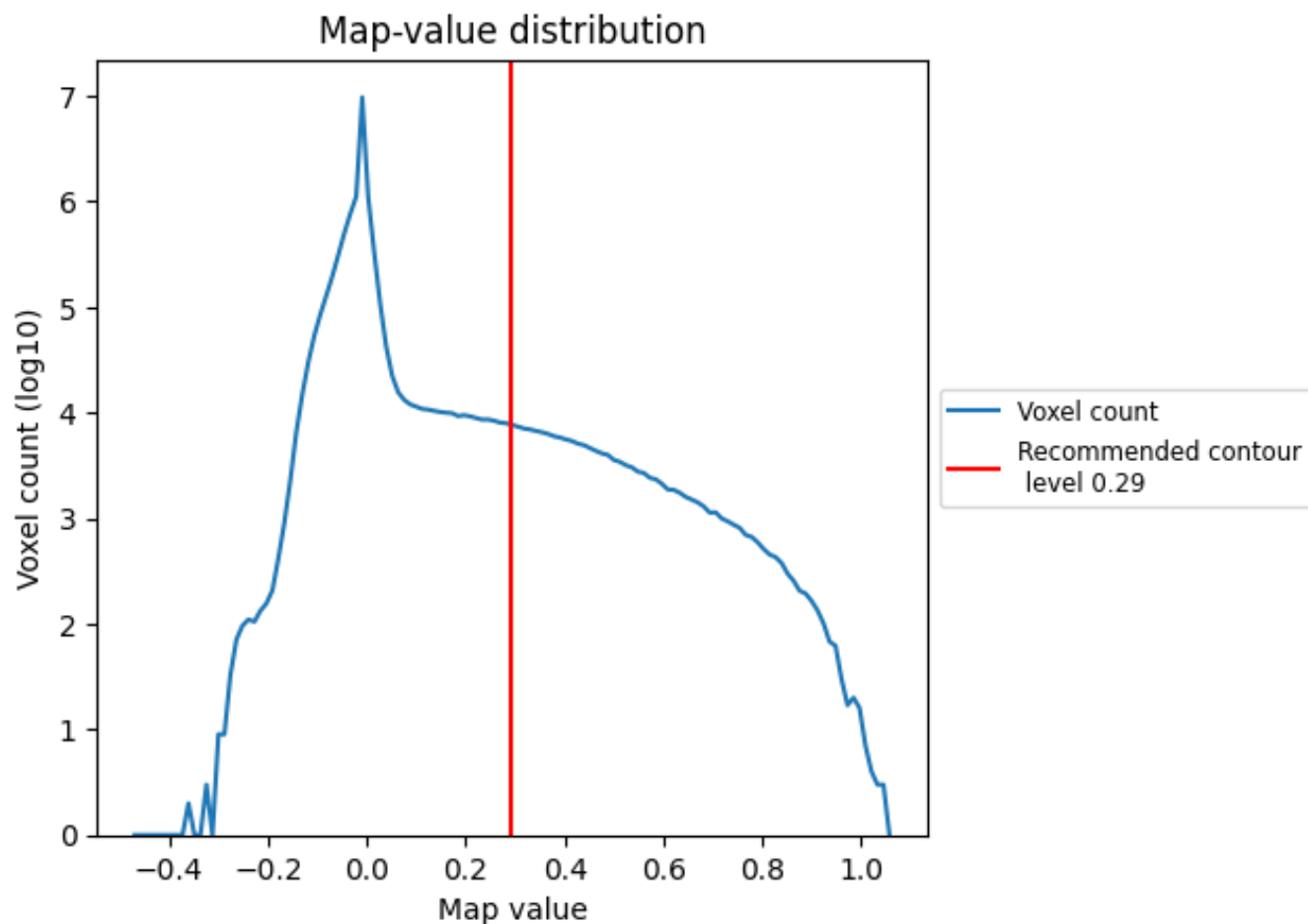
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

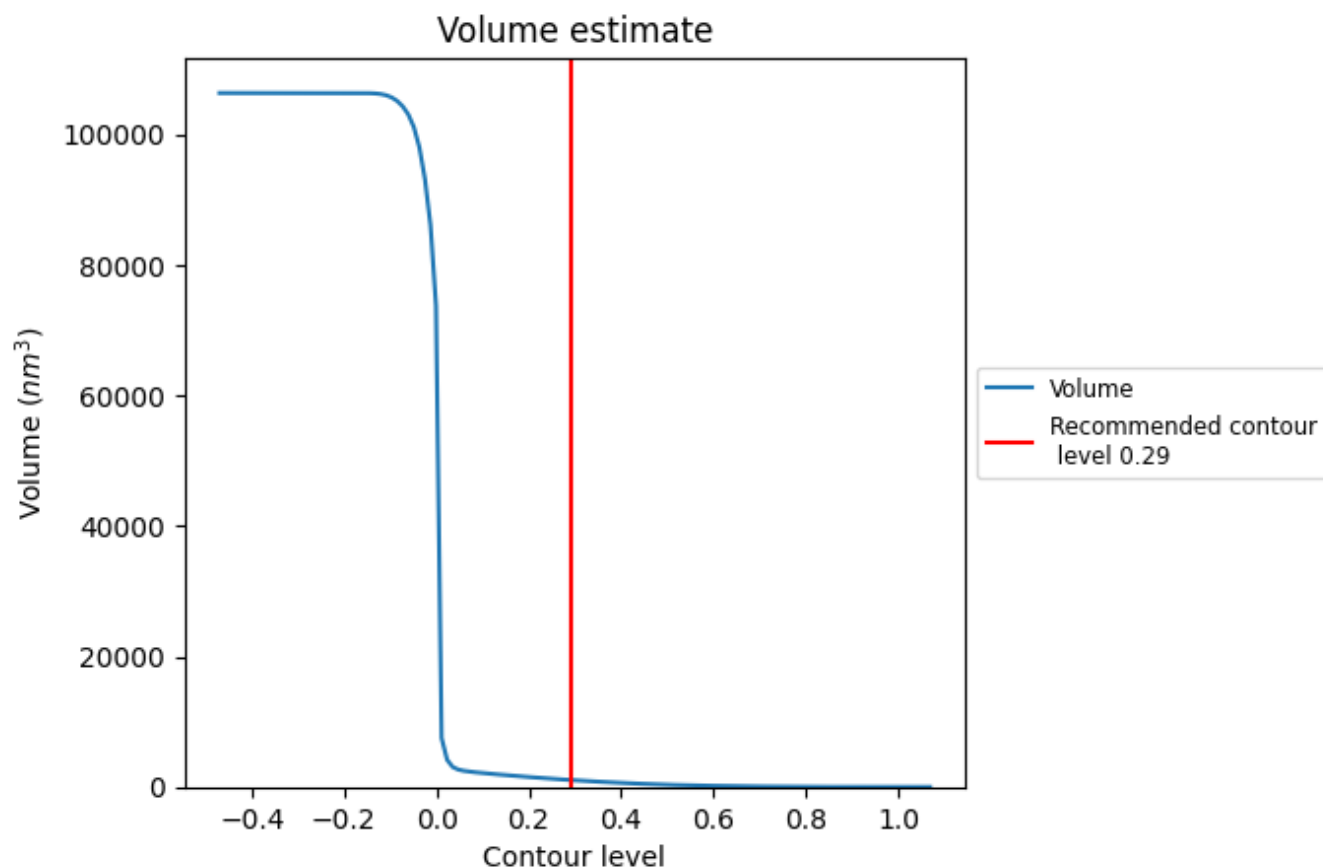
This section contains the results of statistical analysis of the map.

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.

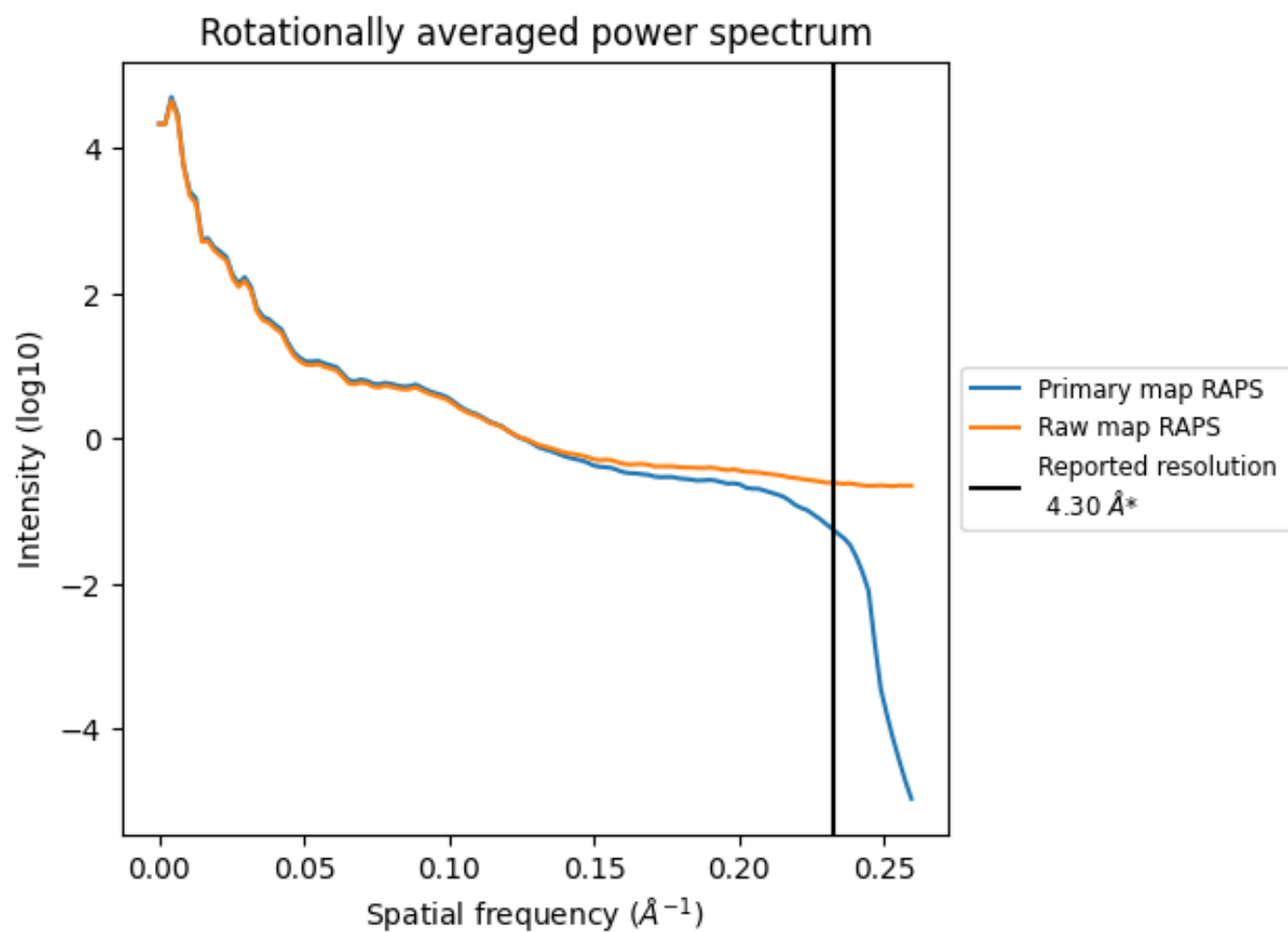
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1065 nm³; this corresponds to an approximate mass of 962 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 ⓘ

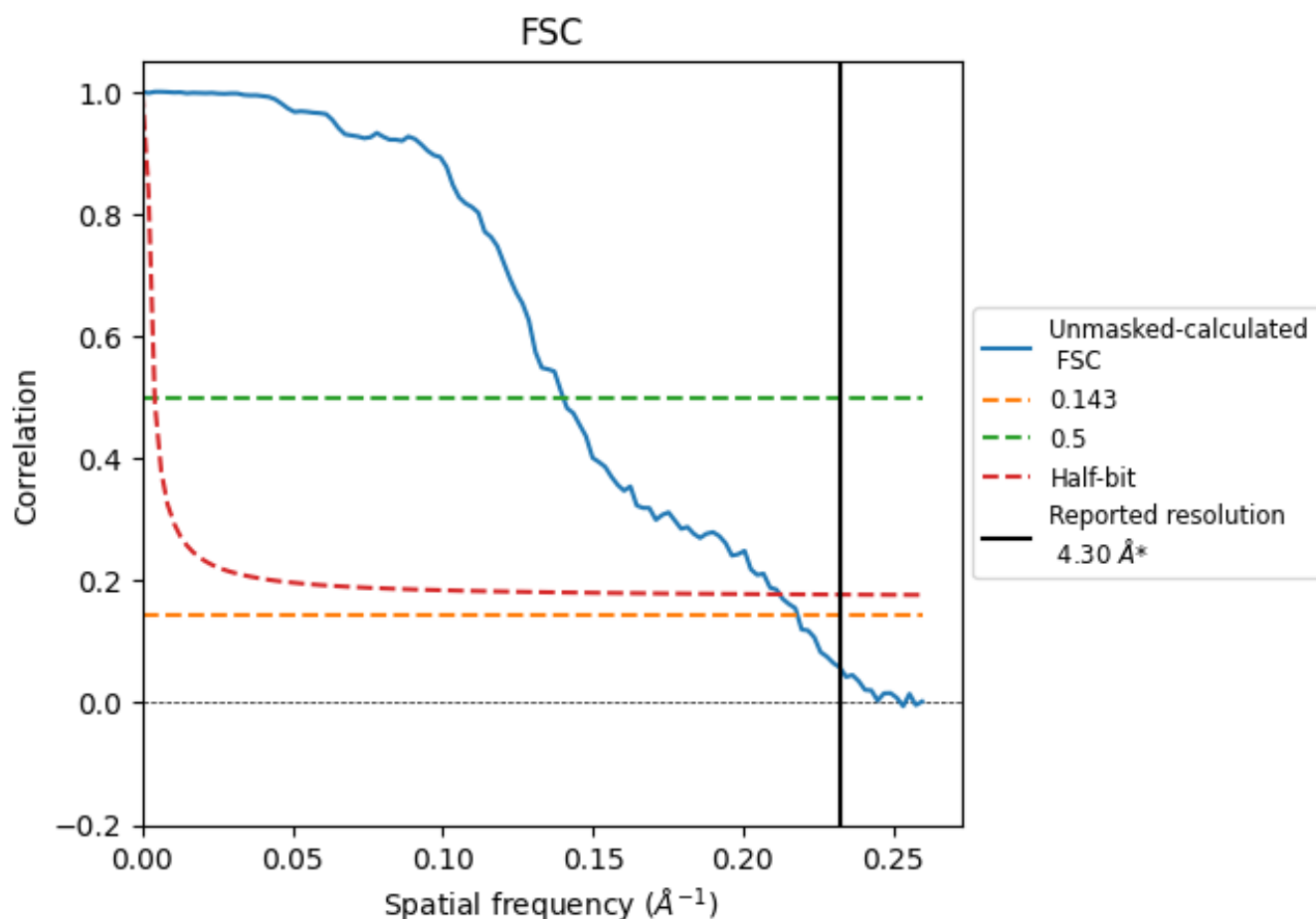


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

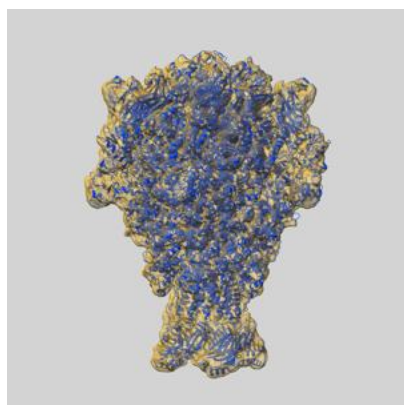
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.59	7.14	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

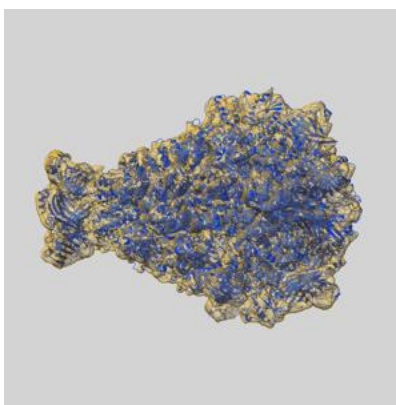
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48371 and PDB model 9MLG. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

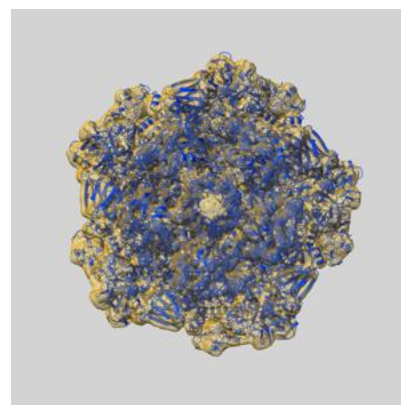
9.1 Map-model overlay [i](#)



X



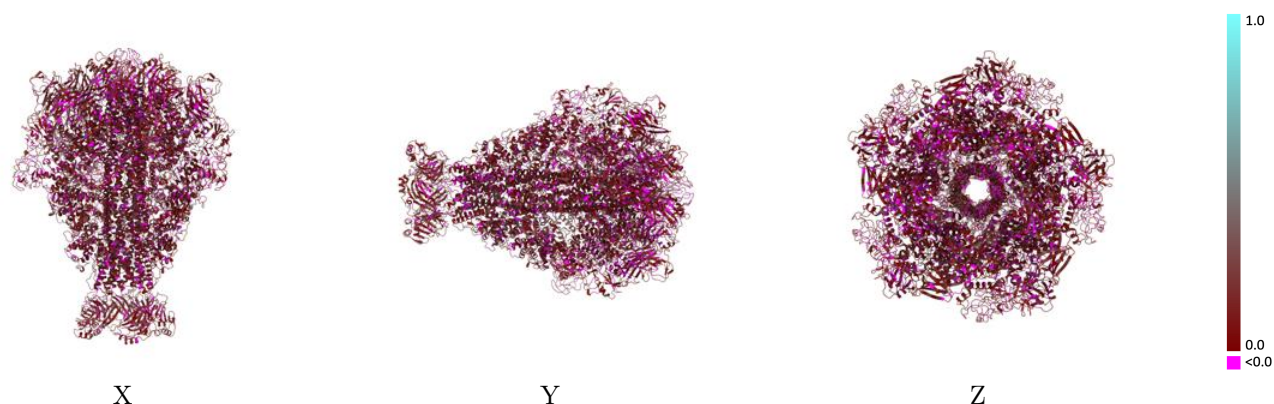
Y



Z

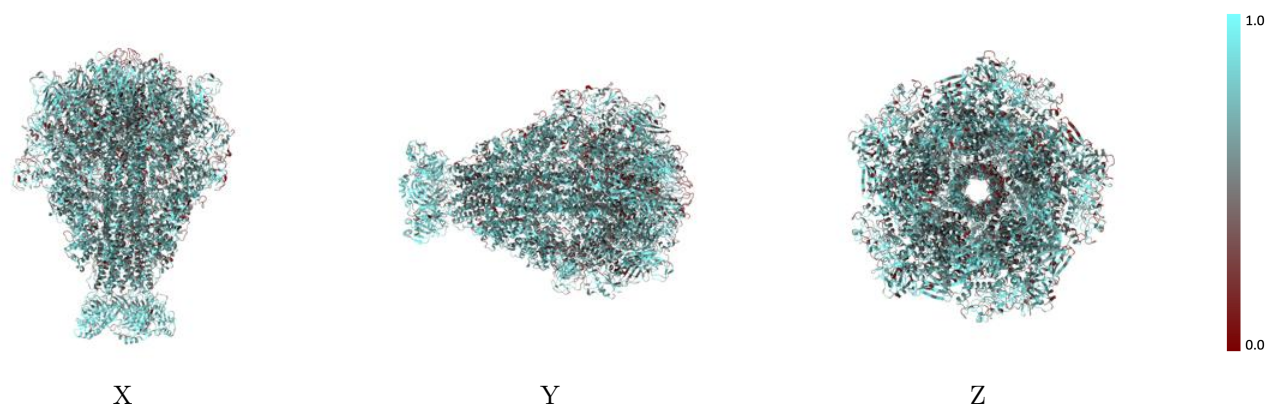
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



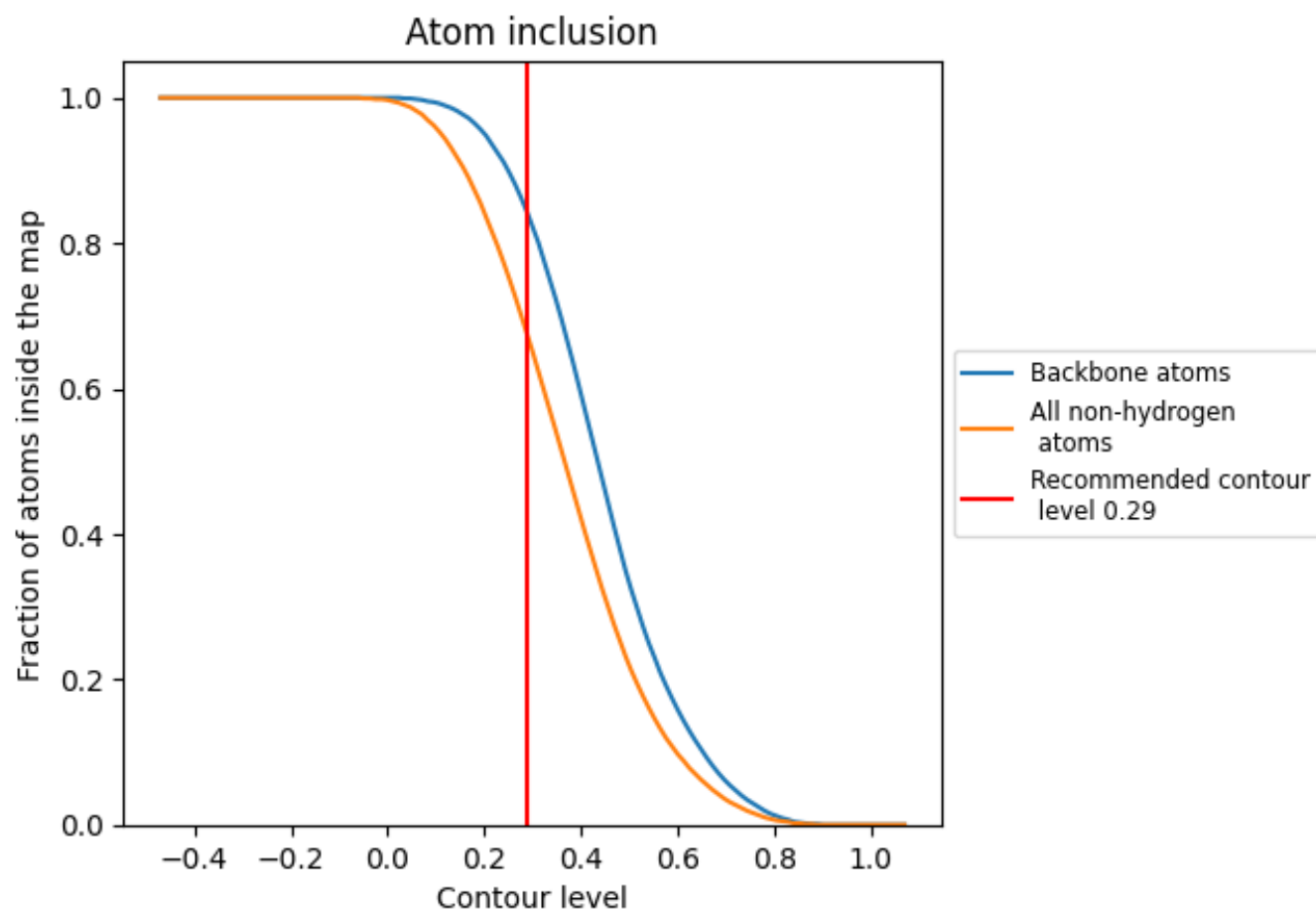
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.1370
A	0.6740	0.1390
B	0.6600	0.1280
C	0.6610	0.1250
D	0.6610	0.1310
E	0.7010	0.1610

