Full wwPDB EM Validation Report ⓘ

Nov 3, 2026 – 07:40 pm GMT

PDB ID	:	31QH / pdb_000031qh
EMDB ID	:	EMD-58628
Title	:	Photorhabdus luminescens TcdA1 inverted pore state
Authors	:	Ng'ang'a, P.N.; Raunser, S.; Bader, R.; Sitsel, O.
Deposited on	:	2026-06-17
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

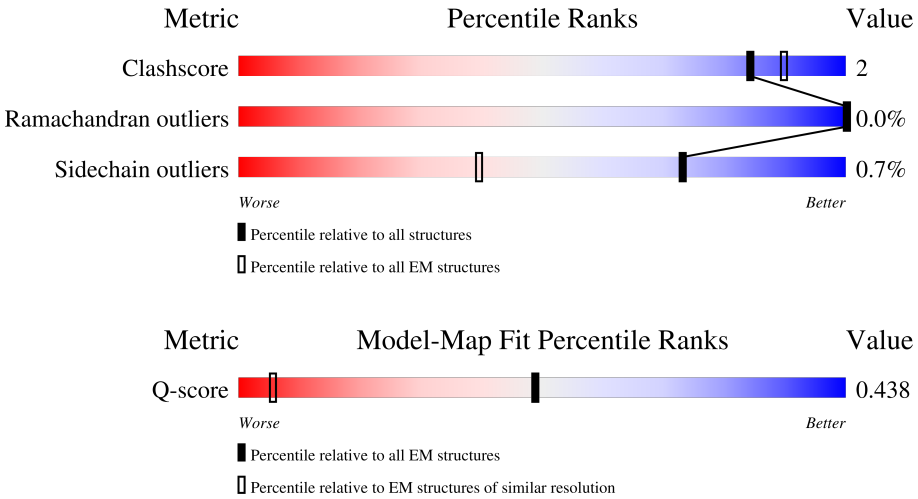
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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.



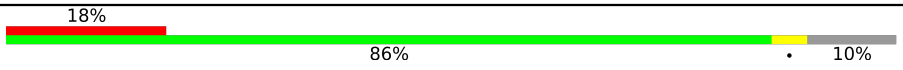
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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 <=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	2535	19% 86% • 10%
1	B	2535	18% 86% • 10%
1	C	2535	19% 85% 5% 10%
1	D	2535	19% 85% • • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	2535	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 179975 atoms, of which 88985 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 Virulence plasmid A protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	2292	Total	C	H	N	O	S	0	0
			35995	11530	17797	3083	3526	59		
1	E	2292	Total	C	H	N	O	S	0	0
			35995	11530	17797	3083	3526	59		
1	C	2292	Total	C	H	N	O	S	0	0
			35995	11530	17797	3083	3526	59		
1	A	2292	Total	C	H	N	O	S	0	0
			35995	11530	17797	3083	3526	59		
1	B	2292	Total	C	H	N	O	S	0	0
			35995	11530	17797	3083	3526	59		

There are 990 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP A0A1G5RA58
D	-17	ALA	-	expression tag	UNP A0A1G5RA58
D	-16	HIS	-	expression tag	UNP A0A1G5RA58
D	-15	HIS	-	expression tag	UNP A0A1G5RA58
D	-14	HIS	-	expression tag	UNP A0A1G5RA58
D	-13	HIS	-	expression tag	UNP A0A1G5RA58
D	-12	HIS	-	expression tag	UNP A0A1G5RA58
D	-11	HIS	-	expression tag	UNP A0A1G5RA58
D	-10	SER	-	expression tag	UNP A0A1G5RA58
D	-9	SER	-	expression tag	UNP A0A1G5RA58
D	-8	GLY	-	expression tag	UNP A0A1G5RA58
D	-7	LEU	-	expression tag	UNP A0A1G5RA58
D	-6	GLU	-	expression tag	UNP A0A1G5RA58
D	-5	VAL	-	expression tag	UNP A0A1G5RA58
D	-4	LEU	-	expression tag	UNP A0A1G5RA58
D	-3	PHE	-	expression tag	UNP A0A1G5RA58
D	-2	GLN	-	expression tag	UNP A0A1G5RA58
D	-1	GLY	-	expression tag	UNP A0A1G5RA58
D	0	PRO	-	expression tag	UNP A0A1G5RA58
D	3	GLU	SER	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	PRO	conflict	UNP A0A1G5RA58
D	14	SER	ILE	conflict	UNP A0A1G5RA58
D	19	ASN	GLN	conflict	UNP A0A1G5RA58
D	33	ARG	HIS	conflict	UNP A0A1G5RA58
D	45	THR	ALA	conflict	UNP A0A1G5RA58
D	70	ALA	THR	conflict	UNP A0A1G5RA58
D	83	LEU	VAL	conflict	UNP A0A1G5RA58
D	137	TYR	ARG	conflict	UNP A0A1G5RA58
D	157	ILE	THR	conflict	UNP A0A1G5RA58
D	180	GLU	ASP	conflict	UNP A0A1G5RA58
D	184	LYS	GLN	conflict	UNP A0A1G5RA58
D	191	THR	ALA	conflict	UNP A0A1G5RA58
D	209	GLU	LYS	conflict	UNP A0A1G5RA58
D	283	LYS	ARG	conflict	UNP A0A1G5RA58
D	317	VAL	ILE	conflict	UNP A0A1G5RA58
D	321	SER	ASN	conflict	UNP A0A1G5RA58
D	339	TYR	ASN	conflict	UNP A0A1G5RA58
D	341	MET	VAL	conflict	UNP A0A1G5RA58
D	348	PHE	TYR	conflict	UNP A0A1G5RA58
D	354	ARG	GLN	conflict	UNP A0A1G5RA58
D	356	ASP	ASN	conflict	UNP A0A1G5RA58
D	361	ASN	ASP	conflict	UNP A0A1G5RA58
D	362	PHE	SER	conflict	UNP A0A1G5RA58
D	363	TYR	ARG	conflict	UNP A0A1G5RA58
D	?	-	GLN	deletion	UNP A0A1G5RA58
D	364	ASN	ASP	conflict	UNP A0A1G5RA58
D	365	ALA	VAL	conflict	UNP A0A1G5RA58
D	379	VAL	ILE	conflict	UNP A0A1G5RA58
D	381	THR	ILE	conflict	UNP A0A1G5RA58
D	393	ALA	GLU	conflict	UNP A0A1G5RA58
D	394	ASN	HIS	conflict	UNP A0A1G5RA58
D	398	ASN	SER	conflict	UNP A0A1G5RA58
D	400	ALA	THR	conflict	UNP A0A1G5RA58
D	414	LEU	TYR	conflict	UNP A0A1G5RA58
D	417	GLY	SER	conflict	UNP A0A1G5RA58
D	428	VAL	ILE	conflict	UNP A0A1G5RA58
D	459	GLY	SER	conflict	UNP A0A1G5RA58
D	466	LEU	GLN	conflict	UNP A0A1G5RA58
D	472	THR	ALA	conflict	UNP A0A1G5RA58
D	473	ASP	GLU	conflict	UNP A0A1G5RA58
D	491	HIS	ASN	conflict	UNP A0A1G5RA58
D	502	PRO	LEU	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	540	SER	PRO	conflict	UNP A0A1G5RA58
D	549	THR	SER	conflict	UNP A0A1G5RA58
D	550	ILE	VAL	conflict	UNP A0A1G5RA58
D	560	VAL	ILE	conflict	UNP A0A1G5RA58
D	563	PHE	TYR	conflict	UNP A0A1G5RA58
D	570	ASP	ASN	conflict	UNP A0A1G5RA58
D	572	ASP	ASN	conflict	UNP A0A1G5RA58
D	574	LYS	GLN	conflict	UNP A0A1G5RA58
D	583	LYS	ASN	conflict	UNP A0A1G5RA58
D	587	ASN	ASP	conflict	UNP A0A1G5RA58
D	596	ASP	GLU	conflict	UNP A0A1G5RA58
D	610	ILE	VAL	conflict	UNP A0A1G5RA58
D	616	LYS	GLU	conflict	UNP A0A1G5RA58
D	629	THR	ALA	conflict	UNP A0A1G5RA58
D	639	SER	VAL	conflict	UNP A0A1G5RA58
D	642	HIS	GLN	conflict	UNP A0A1G5RA58
D	648	VAL	ALA	conflict	UNP A0A1G5RA58
D	653	ILE	VAL	conflict	UNP A0A1G5RA58
D	687	ASP	ASN	conflict	UNP A0A1G5RA58
D	719	GLN	LYS	conflict	UNP A0A1G5RA58
D	737	LYS	GLN	conflict	UNP A0A1G5RA58
D	741	GLY	ASP	conflict	UNP A0A1G5RA58
D	745	ALA	VAL	conflict	UNP A0A1G5RA58
D	746	VAL	LEU	conflict	UNP A0A1G5RA58
D	747	GLU	ALA	conflict	UNP A0A1G5RA58
D	788	ALA	SER	conflict	UNP A0A1G5RA58
D	789	ALA	SER	conflict	UNP A0A1G5RA58
D	791	GLY	GLU	conflict	UNP A0A1G5RA58
D	793	ALA	VAL	conflict	UNP A0A1G5RA58
D	851	ILE	THR	conflict	UNP A0A1G5RA58
D	864	PRO	GLN	conflict	UNP A0A1G5RA58
D	865	GLU	LYS	conflict	UNP A0A1G5RA58
D	875	ASN	ASP	conflict	UNP A0A1G5RA58
D	904	GLU	GLN	conflict	UNP A0A1G5RA58
D	905	SER	LEU	conflict	UNP A0A1G5RA58
D	906	MET	ASN	conflict	UNP A0A1G5RA58
D	907	LYS	GLN	conflict	UNP A0A1G5RA58
D	908	GLU	LYS	conflict	UNP A0A1G5RA58
D	909	THR	ILE	conflict	UNP A0A1G5RA58
D	917	ASN	SER	conflict	UNP A0A1G5RA58
D	919	ALA	GLY	conflict	UNP A0A1G5RA58
D	920	GLY	GLU	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	921	VAL	ILE	conflict	UNP A0A1G5RA58
D	932	ASN	ASP	conflict	UNP A0A1G5RA58
D	933	THR	ILE	conflict	UNP A0A1G5RA58
D	957	ALA	PRO	conflict	UNP A0A1G5RA58
D	1000	ALA	THR	conflict	UNP A0A1G5RA58
D	1009	ASN	HIS	conflict	UNP A0A1G5RA58
D	1118	ALA	THR	conflict	UNP A0A1G5RA58
D	1132	ASN	SER	conflict	UNP A0A1G5RA58
D	1155	LYS	ARG	conflict	UNP A0A1G5RA58
D	1162	ILE	MET	conflict	UNP A0A1G5RA58
D	1219	LYS	GLU	conflict	UNP A0A1G5RA58
D	1223	GLU	LYS	conflict	UNP A0A1G5RA58
D	1225	LYS	GLU	conflict	UNP A0A1G5RA58
D	1227	GLU	ALA	conflict	UNP A0A1G5RA58
D	1230	ARG	LYS	conflict	UNP A0A1G5RA58
D	1261	ASN	THR	conflict	UNP A0A1G5RA58
D	1274	ALA	GLU	conflict	UNP A0A1G5RA58
D	1275	SER	TYR	conflict	UNP A0A1G5RA58
D	1280	PRO	ASP	conflict	UNP A0A1G5RA58
D	1281	GLU	GLY	conflict	UNP A0A1G5RA58
D	1283	SER	TYR	conflict	UNP A0A1G5RA58
D	1284	ASN	LYS	conflict	UNP A0A1G5RA58
D	1285	VAL	SER	conflict	UNP A0A1G5RA58
D	1292	GLN	LYS	conflict	UNP A0A1G5RA58
D	1298	ASN	SER	conflict	UNP A0A1G5RA58
D	1317	SER	ASN	conflict	UNP A0A1G5RA58
D	1321	ASP	GLY	conflict	UNP A0A1G5RA58
D	1323	GLY	ASP	conflict	UNP A0A1G5RA58
D	1341	ASN	SER	conflict	UNP A0A1G5RA58
D	1345	ALA	THR	conflict	UNP A0A1G5RA58
D	1368	LYS	GLN	conflict	UNP A0A1G5RA58
D	1411	SER	ASN	conflict	UNP A0A1G5RA58
D	1414	THR	VAL	conflict	UNP A0A1G5RA58
D	1418	ASN	SER	conflict	UNP A0A1G5RA58
D	1429	THR	ASN	conflict	UNP A0A1G5RA58
D	1431	PRO	SER	conflict	UNP A0A1G5RA58
D	1442	LYS	GLY	conflict	UNP A0A1G5RA58
D	1448	GLN	PRO	conflict	UNP A0A1G5RA58
D	1465	ASP	ASN	conflict	UNP A0A1G5RA58
D	1471	ILE	VAL	conflict	UNP A0A1G5RA58
D	1472	PHE	TYR	conflict	UNP A0A1G5RA58
D	1488	GLU	ASP	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1500	ILE	VAL	conflict	UNP A0A1G5RA58
D	1501	ILE	THR	conflict	UNP A0A1G5RA58
D	1506	GLY	SER	conflict	UNP A0A1G5RA58
D	1516	ASP	ASN	conflict	UNP A0A1G5RA58
D	1541	GLY	SER	conflict	UNP A0A1G5RA58
D	1545	ILE	THR	conflict	UNP A0A1G5RA58
D	1553	VAL	ILE	conflict	UNP A0A1G5RA58
D	1574	VAL	ILE	conflict	UNP A0A1G5RA58
D	1576	LEU	ARG	conflict	UNP A0A1G5RA58
D	1583	ALA	SER	conflict	UNP A0A1G5RA58
D	1587	HIS	ARG	conflict	UNP A0A1G5RA58
D	1599	GLN	GLY	conflict	UNP A0A1G5RA58
D	1600	SER	VAL	conflict	UNP A0A1G5RA58
D	1603	THR	ILE	conflict	UNP A0A1G5RA58
D	1652	LEU	PRO	conflict	UNP A0A1G5RA58
D	1682	THR	LYS	conflict	UNP A0A1G5RA58
D	1687	ASN	SER	conflict	UNP A0A1G5RA58
D	1688	ILE	THR	conflict	UNP A0A1G5RA58
D	1704	HIS	SER	conflict	UNP A0A1G5RA58
D	1903	SER	ASN	conflict	UNP A0A1G5RA58
D	1909	ARG	LYS	conflict	UNP A0A1G5RA58
D	1917	ASN	SER	conflict	UNP A0A1G5RA58
D	1920	ASP	SER	conflict	UNP A0A1G5RA58
D	1922	ALA	SER	conflict	UNP A0A1G5RA58
D	1929	ASN	SER	conflict	UNP A0A1G5RA58
D	1930	ILE	-	insertion	UNP A0A1G5RA58
D	1931	PRO	-	insertion	UNP A0A1G5RA58
D	1935	PRO	LEU	conflict	UNP A0A1G5RA58
D	2028	GLY	SER	conflict	UNP A0A1G5RA58
D	2100	GLY	SER	conflict	UNP A0A1G5RA58
D	2103	TYR	HIS	conflict	UNP A0A1G5RA58
D	2206	ILE	LEU	conflict	UNP A0A1G5RA58
D	2236	SER	ALA	conflict	UNP A0A1G5RA58
D	2270	VAL	ILE	conflict	UNP A0A1G5RA58
D	2284	LEU	ILE	conflict	UNP A0A1G5RA58
D	2285	ASN	SER	conflict	UNP A0A1G5RA58
D	2323	LYS	ARG	conflict	UNP A0A1G5RA58
D	2340	VAL	ILE	conflict	UNP A0A1G5RA58
D	2346	LYS	GLN	conflict	UNP A0A1G5RA58
D	2348	ASN	LYS	conflict	UNP A0A1G5RA58
D	2354	ALA	THR	conflict	UNP A0A1G5RA58
D	2358	ASP	GLU	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2362	SER	ASN	conflict	UNP A0A1G5RA58
D	2363	GLN	ALA	conflict	UNP A0A1G5RA58
D	2391	VAL	ILE	conflict	UNP A0A1G5RA58
D	2393	PHE	LEU	conflict	UNP A0A1G5RA58
D	2404	ALA	GLU	conflict	UNP A0A1G5RA58
D	2406	LEU	ILE	conflict	UNP A0A1G5RA58
D	2446	GLU	ALA	conflict	UNP A0A1G5RA58
D	2454	MET	THR	conflict	UNP A0A1G5RA58
D	2491	MET	THR	conflict	UNP A0A1G5RA58
D	2493	GLU	ALA	conflict	UNP A0A1G5RA58
E	-18	MET	-	initiating methionine	UNP A0A1G5RA58
E	-17	ALA	-	expression tag	UNP A0A1G5RA58
E	-16	HIS	-	expression tag	UNP A0A1G5RA58
E	-15	HIS	-	expression tag	UNP A0A1G5RA58
E	-14	HIS	-	expression tag	UNP A0A1G5RA58
E	-13	HIS	-	expression tag	UNP A0A1G5RA58
E	-12	HIS	-	expression tag	UNP A0A1G5RA58
E	-11	HIS	-	expression tag	UNP A0A1G5RA58
E	-10	SER	-	expression tag	UNP A0A1G5RA58
E	-9	SER	-	expression tag	UNP A0A1G5RA58
E	-8	GLY	-	expression tag	UNP A0A1G5RA58
E	-7	LEU	-	expression tag	UNP A0A1G5RA58
E	-6	GLU	-	expression tag	UNP A0A1G5RA58
E	-5	VAL	-	expression tag	UNP A0A1G5RA58
E	-4	LEU	-	expression tag	UNP A0A1G5RA58
E	-3	PHE	-	expression tag	UNP A0A1G5RA58
E	-2	GLN	-	expression tag	UNP A0A1G5RA58
E	-1	GLY	-	expression tag	UNP A0A1G5RA58
E	0	PRO	-	expression tag	UNP A0A1G5RA58
E	3	GLU	SER	conflict	UNP A0A1G5RA58
E	4	SER	PRO	conflict	UNP A0A1G5RA58
E	14	SER	ILE	conflict	UNP A0A1G5RA58
E	19	ASN	GLN	conflict	UNP A0A1G5RA58
E	33	ARG	HIS	conflict	UNP A0A1G5RA58
E	45	THR	ALA	conflict	UNP A0A1G5RA58
E	70	ALA	THR	conflict	UNP A0A1G5RA58
E	83	LEU	VAL	conflict	UNP A0A1G5RA58
E	137	TYR	ARG	conflict	UNP A0A1G5RA58
E	157	ILE	THR	conflict	UNP A0A1G5RA58
E	180	GLU	ASP	conflict	UNP A0A1G5RA58
E	184	LYS	GLN	conflict	UNP A0A1G5RA58
E	191	THR	ALA	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	209	GLU	LYS	conflict	UNP A0A1G5RA58
E	283	LYS	ARG	conflict	UNP A0A1G5RA58
E	317	VAL	ILE	conflict	UNP A0A1G5RA58
E	321	SER	ASN	conflict	UNP A0A1G5RA58
E	339	TYR	ASN	conflict	UNP A0A1G5RA58
E	341	MET	VAL	conflict	UNP A0A1G5RA58
E	348	PHE	TYR	conflict	UNP A0A1G5RA58
E	354	ARG	GLN	conflict	UNP A0A1G5RA58
E	356	ASP	ASN	conflict	UNP A0A1G5RA58
E	361	ASN	ASP	conflict	UNP A0A1G5RA58
E	362	PHE	SER	conflict	UNP A0A1G5RA58
E	363	TYR	ARG	conflict	UNP A0A1G5RA58
E	?	-	GLN	deletion	UNP A0A1G5RA58
E	364	ASN	ASP	conflict	UNP A0A1G5RA58
E	365	ALA	VAL	conflict	UNP A0A1G5RA58
E	379	VAL	ILE	conflict	UNP A0A1G5RA58
E	381	THR	ILE	conflict	UNP A0A1G5RA58
E	393	ALA	GLU	conflict	UNP A0A1G5RA58
E	394	ASN	HIS	conflict	UNP A0A1G5RA58
E	398	ASN	SER	conflict	UNP A0A1G5RA58
E	400	ALA	THR	conflict	UNP A0A1G5RA58
E	414	LEU	TYR	conflict	UNP A0A1G5RA58
E	417	GLY	SER	conflict	UNP A0A1G5RA58
E	428	VAL	ILE	conflict	UNP A0A1G5RA58
E	459	GLY	SER	conflict	UNP A0A1G5RA58
E	466	LEU	GLN	conflict	UNP A0A1G5RA58
E	472	THR	ALA	conflict	UNP A0A1G5RA58
E	473	ASP	GLU	conflict	UNP A0A1G5RA58
E	491	HIS	ASN	conflict	UNP A0A1G5RA58
E	502	PRO	LEU	conflict	UNP A0A1G5RA58
E	540	SER	PRO	conflict	UNP A0A1G5RA58
E	549	THR	SER	conflict	UNP A0A1G5RA58
E	550	ILE	VAL	conflict	UNP A0A1G5RA58
E	560	VAL	ILE	conflict	UNP A0A1G5RA58
E	563	PHE	TYR	conflict	UNP A0A1G5RA58
E	570	ASP	ASN	conflict	UNP A0A1G5RA58
E	572	ASP	ASN	conflict	UNP A0A1G5RA58
E	574	LYS	GLN	conflict	UNP A0A1G5RA58
E	583	LYS	ASN	conflict	UNP A0A1G5RA58
E	587	ASN	ASP	conflict	UNP A0A1G5RA58
E	596	ASP	GLU	conflict	UNP A0A1G5RA58
E	610	ILE	VAL	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	616	LYS	GLU	conflict	UNP A0A1G5RA58
E	629	THR	ALA	conflict	UNP A0A1G5RA58
E	639	SER	VAL	conflict	UNP A0A1G5RA58
E	642	HIS	GLN	conflict	UNP A0A1G5RA58
E	648	VAL	ALA	conflict	UNP A0A1G5RA58
E	653	ILE	VAL	conflict	UNP A0A1G5RA58
E	687	ASP	ASN	conflict	UNP A0A1G5RA58
E	719	GLN	LYS	conflict	UNP A0A1G5RA58
E	737	LYS	GLN	conflict	UNP A0A1G5RA58
E	741	GLY	ASP	conflict	UNP A0A1G5RA58
E	745	ALA	VAL	conflict	UNP A0A1G5RA58
E	746	VAL	LEU	conflict	UNP A0A1G5RA58
E	747	GLU	ALA	conflict	UNP A0A1G5RA58
E	788	ALA	SER	conflict	UNP A0A1G5RA58
E	789	ALA	SER	conflict	UNP A0A1G5RA58
E	791	GLY	GLU	conflict	UNP A0A1G5RA58
E	793	ALA	VAL	conflict	UNP A0A1G5RA58
E	851	ILE	THR	conflict	UNP A0A1G5RA58
E	864	PRO	GLN	conflict	UNP A0A1G5RA58
E	865	GLU	LYS	conflict	UNP A0A1G5RA58
E	875	ASN	ASP	conflict	UNP A0A1G5RA58
E	904	GLU	GLN	conflict	UNP A0A1G5RA58
E	905	SER	LEU	conflict	UNP A0A1G5RA58
E	906	MET	ASN	conflict	UNP A0A1G5RA58
E	907	LYS	GLN	conflict	UNP A0A1G5RA58
E	908	GLU	LYS	conflict	UNP A0A1G5RA58
E	909	THR	ILE	conflict	UNP A0A1G5RA58
E	917	ASN	SER	conflict	UNP A0A1G5RA58
E	919	ALA	GLY	conflict	UNP A0A1G5RA58
E	920	GLY	GLU	conflict	UNP A0A1G5RA58
E	921	VAL	ILE	conflict	UNP A0A1G5RA58
E	932	ASN	ASP	conflict	UNP A0A1G5RA58
E	933	THR	ILE	conflict	UNP A0A1G5RA58
E	957	ALA	PRO	conflict	UNP A0A1G5RA58
E	1000	ALA	THR	conflict	UNP A0A1G5RA58
E	1009	ASN	HIS	conflict	UNP A0A1G5RA58
E	1118	ALA	THR	conflict	UNP A0A1G5RA58
E	1132	ASN	SER	conflict	UNP A0A1G5RA58
E	1155	LYS	ARG	conflict	UNP A0A1G5RA58
E	1162	ILE	MET	conflict	UNP A0A1G5RA58
E	1219	LYS	GLU	conflict	UNP A0A1G5RA58
E	1223	GLU	LYS	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1225	LYS	GLU	conflict	UNP A0A1G5RA58
E	1227	GLU	ALA	conflict	UNP A0A1G5RA58
E	1230	ARG	LYS	conflict	UNP A0A1G5RA58
E	1261	ASN	THR	conflict	UNP A0A1G5RA58
E	1274	ALA	GLU	conflict	UNP A0A1G5RA58
E	1275	SER	TYR	conflict	UNP A0A1G5RA58
E	1280	PRO	ASP	conflict	UNP A0A1G5RA58
E	1281	GLU	GLY	conflict	UNP A0A1G5RA58
E	1283	SER	TYR	conflict	UNP A0A1G5RA58
E	1284	ASN	LYS	conflict	UNP A0A1G5RA58
E	1285	VAL	SER	conflict	UNP A0A1G5RA58
E	1292	GLN	LYS	conflict	UNP A0A1G5RA58
E	1298	ASN	SER	conflict	UNP A0A1G5RA58
E	1317	SER	ASN	conflict	UNP A0A1G5RA58
E	1321	ASP	GLY	conflict	UNP A0A1G5RA58
E	1323	GLY	ASP	conflict	UNP A0A1G5RA58
E	1341	ASN	SER	conflict	UNP A0A1G5RA58
E	1345	ALA	THR	conflict	UNP A0A1G5RA58
E	1368	LYS	GLN	conflict	UNP A0A1G5RA58
E	1411	SER	ASN	conflict	UNP A0A1G5RA58
E	1414	THR	VAL	conflict	UNP A0A1G5RA58
E	1418	ASN	SER	conflict	UNP A0A1G5RA58
E	1429	THR	ASN	conflict	UNP A0A1G5RA58
E	1431	PRO	SER	conflict	UNP A0A1G5RA58
E	1442	LYS	GLY	conflict	UNP A0A1G5RA58
E	1448	GLN	PRO	conflict	UNP A0A1G5RA58
E	1465	ASP	ASN	conflict	UNP A0A1G5RA58
E	1471	ILE	VAL	conflict	UNP A0A1G5RA58
E	1472	PHE	TYR	conflict	UNP A0A1G5RA58
E	1488	GLU	ASP	conflict	UNP A0A1G5RA58
E	1500	ILE	VAL	conflict	UNP A0A1G5RA58
E	1501	ILE	THR	conflict	UNP A0A1G5RA58
E	1506	GLY	SER	conflict	UNP A0A1G5RA58
E	1516	ASP	ASN	conflict	UNP A0A1G5RA58
E	1541	GLY	SER	conflict	UNP A0A1G5RA58
E	1545	ILE	THR	conflict	UNP A0A1G5RA58
E	1553	VAL	ILE	conflict	UNP A0A1G5RA58
E	1574	VAL	ILE	conflict	UNP A0A1G5RA58
E	1576	LEU	ARG	conflict	UNP A0A1G5RA58
E	1583	ALA	SER	conflict	UNP A0A1G5RA58
E	1587	HIS	ARG	conflict	UNP A0A1G5RA58
E	1599	GLN	GLY	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1600	SER	VAL	conflict	UNP A0A1G5RA58
E	1603	THR	ILE	conflict	UNP A0A1G5RA58
E	1652	LEU	PRO	conflict	UNP A0A1G5RA58
E	1682	THR	LYS	conflict	UNP A0A1G5RA58
E	1687	ASN	SER	conflict	UNP A0A1G5RA58
E	1688	ILE	THR	conflict	UNP A0A1G5RA58
E	1704	HIS	SER	conflict	UNP A0A1G5RA58
E	1903	SER	ASN	conflict	UNP A0A1G5RA58
E	1909	ARG	LYS	conflict	UNP A0A1G5RA58
E	1917	ASN	SER	conflict	UNP A0A1G5RA58
E	1920	ASP	SER	conflict	UNP A0A1G5RA58
E	1922	ALA	SER	conflict	UNP A0A1G5RA58
E	1929	ASN	SER	conflict	UNP A0A1G5RA58
E	1930	ILE	-	insertion	UNP A0A1G5RA58
E	1931	PRO	-	insertion	UNP A0A1G5RA58
E	1935	PRO	LEU	conflict	UNP A0A1G5RA58
E	2028	GLY	SER	conflict	UNP A0A1G5RA58
E	2100	GLY	SER	conflict	UNP A0A1G5RA58
E	2103	TYR	HIS	conflict	UNP A0A1G5RA58
E	2206	ILE	LEU	conflict	UNP A0A1G5RA58
E	2236	SER	ALA	conflict	UNP A0A1G5RA58
E	2270	VAL	ILE	conflict	UNP A0A1G5RA58
E	2284	LEU	ILE	conflict	UNP A0A1G5RA58
E	2285	ASN	SER	conflict	UNP A0A1G5RA58
E	2323	LYS	ARG	conflict	UNP A0A1G5RA58
E	2340	VAL	ILE	conflict	UNP A0A1G5RA58
E	2346	LYS	GLN	conflict	UNP A0A1G5RA58
E	2348	ASN	LYS	conflict	UNP A0A1G5RA58
E	2354	ALA	THR	conflict	UNP A0A1G5RA58
E	2358	ASP	GLU	conflict	UNP A0A1G5RA58
E	2362	SER	ASN	conflict	UNP A0A1G5RA58
E	2363	GLN	ALA	conflict	UNP A0A1G5RA58
E	2391	VAL	ILE	conflict	UNP A0A1G5RA58
E	2393	PHE	LEU	conflict	UNP A0A1G5RA58
E	2404	ALA	GLU	conflict	UNP A0A1G5RA58
E	2406	LEU	ILE	conflict	UNP A0A1G5RA58
E	2446	GLU	ALA	conflict	UNP A0A1G5RA58
E	2454	MET	THR	conflict	UNP A0A1G5RA58
E	2491	MET	THR	conflict	UNP A0A1G5RA58
E	2493	GLU	ALA	conflict	UNP A0A1G5RA58
C	-18	MET	-	initiating methionine	UNP A0A1G5RA58
C	-17	ALA	-	expression tag	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP A0A1G5RA58
C	-15	HIS	-	expression tag	UNP A0A1G5RA58
C	-14	HIS	-	expression tag	UNP A0A1G5RA58
C	-13	HIS	-	expression tag	UNP A0A1G5RA58
C	-12	HIS	-	expression tag	UNP A0A1G5RA58
C	-11	HIS	-	expression tag	UNP A0A1G5RA58
C	-10	SER	-	expression tag	UNP A0A1G5RA58
C	-9	SER	-	expression tag	UNP A0A1G5RA58
C	-8	GLY	-	expression tag	UNP A0A1G5RA58
C	-7	LEU	-	expression tag	UNP A0A1G5RA58
C	-6	GLU	-	expression tag	UNP A0A1G5RA58
C	-5	VAL	-	expression tag	UNP A0A1G5RA58
C	-4	LEU	-	expression tag	UNP A0A1G5RA58
C	-3	PHE	-	expression tag	UNP A0A1G5RA58
C	-2	GLN	-	expression tag	UNP A0A1G5RA58
C	-1	GLY	-	expression tag	UNP A0A1G5RA58
C	0	PRO	-	expression tag	UNP A0A1G5RA58
C	3	GLU	SER	conflict	UNP A0A1G5RA58
C	4	SER	PRO	conflict	UNP A0A1G5RA58
C	14	SER	ILE	conflict	UNP A0A1G5RA58
C	19	ASN	GLN	conflict	UNP A0A1G5RA58
C	33	ARG	HIS	conflict	UNP A0A1G5RA58
C	45	THR	ALA	conflict	UNP A0A1G5RA58
C	70	ALA	THR	conflict	UNP A0A1G5RA58
C	83	LEU	VAL	conflict	UNP A0A1G5RA58
C	137	TYR	ARG	conflict	UNP A0A1G5RA58
C	157	ILE	THR	conflict	UNP A0A1G5RA58
C	180	GLU	ASP	conflict	UNP A0A1G5RA58
C	184	LYS	GLN	conflict	UNP A0A1G5RA58
C	191	THR	ALA	conflict	UNP A0A1G5RA58
C	209	GLU	LYS	conflict	UNP A0A1G5RA58
C	283	LYS	ARG	conflict	UNP A0A1G5RA58
C	317	VAL	ILE	conflict	UNP A0A1G5RA58
C	321	SER	ASN	conflict	UNP A0A1G5RA58
C	339	TYR	ASN	conflict	UNP A0A1G5RA58
C	341	MET	VAL	conflict	UNP A0A1G5RA58
C	348	PHE	TYR	conflict	UNP A0A1G5RA58
C	354	ARG	GLN	conflict	UNP A0A1G5RA58
C	356	ASP	ASN	conflict	UNP A0A1G5RA58
C	361	ASN	ASP	conflict	UNP A0A1G5RA58
C	362	PHE	SER	conflict	UNP A0A1G5RA58
C	363	TYR	ARG	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLN	deletion	UNP A0A1G5RA58
C	364	ASN	ASP	conflict	UNP A0A1G5RA58
C	365	ALA	VAL	conflict	UNP A0A1G5RA58
C	379	VAL	ILE	conflict	UNP A0A1G5RA58
C	381	THR	ILE	conflict	UNP A0A1G5RA58
C	393	ALA	GLU	conflict	UNP A0A1G5RA58
C	394	ASN	HIS	conflict	UNP A0A1G5RA58
C	398	ASN	SER	conflict	UNP A0A1G5RA58
C	400	ALA	THR	conflict	UNP A0A1G5RA58
C	414	LEU	TYR	conflict	UNP A0A1G5RA58
C	417	GLY	SER	conflict	UNP A0A1G5RA58
C	428	VAL	ILE	conflict	UNP A0A1G5RA58
C	459	GLY	SER	conflict	UNP A0A1G5RA58
C	466	LEU	GLN	conflict	UNP A0A1G5RA58
C	472	THR	ALA	conflict	UNP A0A1G5RA58
C	473	ASP	GLU	conflict	UNP A0A1G5RA58
C	491	HIS	ASN	conflict	UNP A0A1G5RA58
C	502	PRO	LEU	conflict	UNP A0A1G5RA58
C	540	SER	PRO	conflict	UNP A0A1G5RA58
C	549	THR	SER	conflict	UNP A0A1G5RA58
C	550	ILE	VAL	conflict	UNP A0A1G5RA58
C	560	VAL	ILE	conflict	UNP A0A1G5RA58
C	563	PHE	TYR	conflict	UNP A0A1G5RA58
C	570	ASP	ASN	conflict	UNP A0A1G5RA58
C	572	ASP	ASN	conflict	UNP A0A1G5RA58
C	574	LYS	GLN	conflict	UNP A0A1G5RA58
C	583	LYS	ASN	conflict	UNP A0A1G5RA58
C	587	ASN	ASP	conflict	UNP A0A1G5RA58
C	596	ASP	GLU	conflict	UNP A0A1G5RA58
C	610	ILE	VAL	conflict	UNP A0A1G5RA58
C	616	LYS	GLU	conflict	UNP A0A1G5RA58
C	629	THR	ALA	conflict	UNP A0A1G5RA58
C	639	SER	VAL	conflict	UNP A0A1G5RA58
C	642	HIS	GLN	conflict	UNP A0A1G5RA58
C	648	VAL	ALA	conflict	UNP A0A1G5RA58
C	653	ILE	VAL	conflict	UNP A0A1G5RA58
C	687	ASP	ASN	conflict	UNP A0A1G5RA58
C	719	GLN	LYS	conflict	UNP A0A1G5RA58
C	737	LYS	GLN	conflict	UNP A0A1G5RA58
C	741	GLY	ASP	conflict	UNP A0A1G5RA58
C	745	ALA	VAL	conflict	UNP A0A1G5RA58
C	746	VAL	LEU	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	747	GLU	ALA	conflict	UNP A0A1G5RA58
C	788	ALA	SER	conflict	UNP A0A1G5RA58
C	789	ALA	SER	conflict	UNP A0A1G5RA58
C	791	GLY	GLU	conflict	UNP A0A1G5RA58
C	793	ALA	VAL	conflict	UNP A0A1G5RA58
C	851	ILE	THR	conflict	UNP A0A1G5RA58
C	864	PRO	GLN	conflict	UNP A0A1G5RA58
C	865	GLU	LYS	conflict	UNP A0A1G5RA58
C	875	ASN	ASP	conflict	UNP A0A1G5RA58
C	904	GLU	GLN	conflict	UNP A0A1G5RA58
C	905	SER	LEU	conflict	UNP A0A1G5RA58
C	906	MET	ASN	conflict	UNP A0A1G5RA58
C	907	LYS	GLN	conflict	UNP A0A1G5RA58
C	908	GLU	LYS	conflict	UNP A0A1G5RA58
C	909	THR	ILE	conflict	UNP A0A1G5RA58
C	917	ASN	SER	conflict	UNP A0A1G5RA58
C	919	ALA	GLY	conflict	UNP A0A1G5RA58
C	920	GLY	GLU	conflict	UNP A0A1G5RA58
C	921	VAL	ILE	conflict	UNP A0A1G5RA58
C	932	ASN	ASP	conflict	UNP A0A1G5RA58
C	933	THR	ILE	conflict	UNP A0A1G5RA58
C	957	ALA	PRO	conflict	UNP A0A1G5RA58
C	1000	ALA	THR	conflict	UNP A0A1G5RA58
C	1009	ASN	HIS	conflict	UNP A0A1G5RA58
C	1118	ALA	THR	conflict	UNP A0A1G5RA58
C	1132	ASN	SER	conflict	UNP A0A1G5RA58
C	1155	LYS	ARG	conflict	UNP A0A1G5RA58
C	1162	ILE	MET	conflict	UNP A0A1G5RA58
C	1219	LYS	GLU	conflict	UNP A0A1G5RA58
C	1223	GLU	LYS	conflict	UNP A0A1G5RA58
C	1225	LYS	GLU	conflict	UNP A0A1G5RA58
C	1227	GLU	ALA	conflict	UNP A0A1G5RA58
C	1230	ARG	LYS	conflict	UNP A0A1G5RA58
C	1261	ASN	THR	conflict	UNP A0A1G5RA58
C	1274	ALA	GLU	conflict	UNP A0A1G5RA58
C	1275	SER	TYR	conflict	UNP A0A1G5RA58
C	1280	PRO	ASP	conflict	UNP A0A1G5RA58
C	1281	GLU	GLY	conflict	UNP A0A1G5RA58
C	1283	SER	TYR	conflict	UNP A0A1G5RA58
C	1284	ASN	LYS	conflict	UNP A0A1G5RA58
C	1285	VAL	SER	conflict	UNP A0A1G5RA58
C	1292	GLN	LYS	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1298	ASN	SER	conflict	UNP A0A1G5RA58
C	1317	SER	ASN	conflict	UNP A0A1G5RA58
C	1321	ASP	GLY	conflict	UNP A0A1G5RA58
C	1323	GLY	ASP	conflict	UNP A0A1G5RA58
C	1341	ASN	SER	conflict	UNP A0A1G5RA58
C	1345	ALA	THR	conflict	UNP A0A1G5RA58
C	1368	LYS	GLN	conflict	UNP A0A1G5RA58
C	1411	SER	ASN	conflict	UNP A0A1G5RA58
C	1414	THR	VAL	conflict	UNP A0A1G5RA58
C	1418	ASN	SER	conflict	UNP A0A1G5RA58
C	1429	THR	ASN	conflict	UNP A0A1G5RA58
C	1431	PRO	SER	conflict	UNP A0A1G5RA58
C	1442	LYS	GLY	conflict	UNP A0A1G5RA58
C	1448	GLN	PRO	conflict	UNP A0A1G5RA58
C	1465	ASP	ASN	conflict	UNP A0A1G5RA58
C	1471	ILE	VAL	conflict	UNP A0A1G5RA58
C	1472	PHE	TYR	conflict	UNP A0A1G5RA58
C	1488	GLU	ASP	conflict	UNP A0A1G5RA58
C	1500	ILE	VAL	conflict	UNP A0A1G5RA58
C	1501	ILE	THR	conflict	UNP A0A1G5RA58
C	1506	GLY	SER	conflict	UNP A0A1G5RA58
C	1516	ASP	ASN	conflict	UNP A0A1G5RA58
C	1541	GLY	SER	conflict	UNP A0A1G5RA58
C	1545	ILE	THR	conflict	UNP A0A1G5RA58
C	1553	VAL	ILE	conflict	UNP A0A1G5RA58
C	1574	VAL	ILE	conflict	UNP A0A1G5RA58
C	1576	LEU	ARG	conflict	UNP A0A1G5RA58
C	1583	ALA	SER	conflict	UNP A0A1G5RA58
C	1587	HIS	ARG	conflict	UNP A0A1G5RA58
C	1599	GLN	GLY	conflict	UNP A0A1G5RA58
C	1600	SER	VAL	conflict	UNP A0A1G5RA58
C	1603	THR	ILE	conflict	UNP A0A1G5RA58
C	1652	LEU	PRO	conflict	UNP A0A1G5RA58
C	1682	THR	LYS	conflict	UNP A0A1G5RA58
C	1687	ASN	SER	conflict	UNP A0A1G5RA58
C	1688	ILE	THR	conflict	UNP A0A1G5RA58
C	1704	HIS	SER	conflict	UNP A0A1G5RA58
C	1903	SER	ASN	conflict	UNP A0A1G5RA58
C	1909	ARG	LYS	conflict	UNP A0A1G5RA58
C	1917	ASN	SER	conflict	UNP A0A1G5RA58
C	1920	ASP	SER	conflict	UNP A0A1G5RA58
C	1922	ALA	SER	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1929	ASN	SER	conflict	UNP A0A1G5RA58
C	1930	ILE	-	insertion	UNP A0A1G5RA58
C	1931	PRO	-	insertion	UNP A0A1G5RA58
C	1935	PRO	LEU	conflict	UNP A0A1G5RA58
C	2028	GLY	SER	conflict	UNP A0A1G5RA58
C	2100	GLY	SER	conflict	UNP A0A1G5RA58
C	2103	TYR	HIS	conflict	UNP A0A1G5RA58
C	2206	ILE	LEU	conflict	UNP A0A1G5RA58
C	2236	SER	ALA	conflict	UNP A0A1G5RA58
C	2270	VAL	ILE	conflict	UNP A0A1G5RA58
C	2284	LEU	ILE	conflict	UNP A0A1G5RA58
C	2285	ASN	SER	conflict	UNP A0A1G5RA58
C	2323	LYS	ARG	conflict	UNP A0A1G5RA58
C	2340	VAL	ILE	conflict	UNP A0A1G5RA58
C	2346	LYS	GLN	conflict	UNP A0A1G5RA58
C	2348	ASN	LYS	conflict	UNP A0A1G5RA58
C	2354	ALA	THR	conflict	UNP A0A1G5RA58
C	2358	ASP	GLU	conflict	UNP A0A1G5RA58
C	2362	SER	ASN	conflict	UNP A0A1G5RA58
C	2363	GLN	ALA	conflict	UNP A0A1G5RA58
C	2391	VAL	ILE	conflict	UNP A0A1G5RA58
C	2393	PHE	LEU	conflict	UNP A0A1G5RA58
C	2404	ALA	GLU	conflict	UNP A0A1G5RA58
C	2406	LEU	ILE	conflict	UNP A0A1G5RA58
C	2446	GLU	ALA	conflict	UNP A0A1G5RA58
C	2454	MET	THR	conflict	UNP A0A1G5RA58
C	2491	MET	THR	conflict	UNP A0A1G5RA58
C	2493	GLU	ALA	conflict	UNP A0A1G5RA58
A	-18	MET	-	initiating methionine	UNP A0A1G5RA58
A	-17	ALA	-	expression tag	UNP A0A1G5RA58
A	-16	HIS	-	expression tag	UNP A0A1G5RA58
A	-15	HIS	-	expression tag	UNP A0A1G5RA58
A	-14	HIS	-	expression tag	UNP A0A1G5RA58
A	-13	HIS	-	expression tag	UNP A0A1G5RA58
A	-12	HIS	-	expression tag	UNP A0A1G5RA58
A	-11	HIS	-	expression tag	UNP A0A1G5RA58
A	-10	SER	-	expression tag	UNP A0A1G5RA58
A	-9	SER	-	expression tag	UNP A0A1G5RA58
A	-8	GLY	-	expression tag	UNP A0A1G5RA58
A	-7	LEU	-	expression tag	UNP A0A1G5RA58
A	-6	GLU	-	expression tag	UNP A0A1G5RA58
A	-5	VAL	-	expression tag	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP A0A1G5RA58
A	-3	PHE	-	expression tag	UNP A0A1G5RA58
A	-2	GLN	-	expression tag	UNP A0A1G5RA58
A	-1	GLY	-	expression tag	UNP A0A1G5RA58
A	0	PRO	-	expression tag	UNP A0A1G5RA58
A	3	GLU	SER	conflict	UNP A0A1G5RA58
A	4	SER	PRO	conflict	UNP A0A1G5RA58
A	14	SER	ILE	conflict	UNP A0A1G5RA58
A	19	ASN	GLN	conflict	UNP A0A1G5RA58
A	33	ARG	HIS	conflict	UNP A0A1G5RA58
A	45	THR	ALA	conflict	UNP A0A1G5RA58
A	70	ALA	THR	conflict	UNP A0A1G5RA58
A	83	LEU	VAL	conflict	UNP A0A1G5RA58
A	137	TYR	ARG	conflict	UNP A0A1G5RA58
A	157	ILE	THR	conflict	UNP A0A1G5RA58
A	180	GLU	ASP	conflict	UNP A0A1G5RA58
A	184	LYS	GLN	conflict	UNP A0A1G5RA58
A	191	THR	ALA	conflict	UNP A0A1G5RA58
A	209	GLU	LYS	conflict	UNP A0A1G5RA58
A	283	LYS	ARG	conflict	UNP A0A1G5RA58
A	317	VAL	ILE	conflict	UNP A0A1G5RA58
A	321	SER	ASN	conflict	UNP A0A1G5RA58
A	339	TYR	ASN	conflict	UNP A0A1G5RA58
A	341	MET	VAL	conflict	UNP A0A1G5RA58
A	348	PHE	TYR	conflict	UNP A0A1G5RA58
A	354	ARG	GLN	conflict	UNP A0A1G5RA58
A	356	ASP	ASN	conflict	UNP A0A1G5RA58
A	361	ASN	ASP	conflict	UNP A0A1G5RA58
A	362	PHE	SER	conflict	UNP A0A1G5RA58
A	363	TYR	ARG	conflict	UNP A0A1G5RA58
A	?	-	GLN	deletion	UNP A0A1G5RA58
A	364	ASN	ASP	conflict	UNP A0A1G5RA58
A	365	ALA	VAL	conflict	UNP A0A1G5RA58
A	379	VAL	ILE	conflict	UNP A0A1G5RA58
A	381	THR	ILE	conflict	UNP A0A1G5RA58
A	393	ALA	GLU	conflict	UNP A0A1G5RA58
A	394	ASN	HIS	conflict	UNP A0A1G5RA58
A	398	ASN	SER	conflict	UNP A0A1G5RA58
A	400	ALA	THR	conflict	UNP A0A1G5RA58
A	414	LEU	TYR	conflict	UNP A0A1G5RA58
A	417	GLY	SER	conflict	UNP A0A1G5RA58
A	428	VAL	ILE	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLY	SER	conflict	UNP A0A1G5RA58
A	466	LEU	GLN	conflict	UNP A0A1G5RA58
A	472	THR	ALA	conflict	UNP A0A1G5RA58
A	473	ASP	GLU	conflict	UNP A0A1G5RA58
A	491	HIS	ASN	conflict	UNP A0A1G5RA58
A	502	PRO	LEU	conflict	UNP A0A1G5RA58
A	540	SER	PRO	conflict	UNP A0A1G5RA58
A	549	THR	SER	conflict	UNP A0A1G5RA58
A	550	ILE	VAL	conflict	UNP A0A1G5RA58
A	560	VAL	ILE	conflict	UNP A0A1G5RA58
A	563	PHE	TYR	conflict	UNP A0A1G5RA58
A	570	ASP	ASN	conflict	UNP A0A1G5RA58
A	572	ASP	ASN	conflict	UNP A0A1G5RA58
A	574	LYS	GLN	conflict	UNP A0A1G5RA58
A	583	LYS	ASN	conflict	UNP A0A1G5RA58
A	587	ASN	ASP	conflict	UNP A0A1G5RA58
A	596	ASP	GLU	conflict	UNP A0A1G5RA58
A	610	ILE	VAL	conflict	UNP A0A1G5RA58
A	616	LYS	GLU	conflict	UNP A0A1G5RA58
A	629	THR	ALA	conflict	UNP A0A1G5RA58
A	639	SER	VAL	conflict	UNP A0A1G5RA58
A	642	HIS	GLN	conflict	UNP A0A1G5RA58
A	648	VAL	ALA	conflict	UNP A0A1G5RA58
A	653	ILE	VAL	conflict	UNP A0A1G5RA58
A	687	ASP	ASN	conflict	UNP A0A1G5RA58
A	719	GLN	LYS	conflict	UNP A0A1G5RA58
A	737	LYS	GLN	conflict	UNP A0A1G5RA58
A	741	GLY	ASP	conflict	UNP A0A1G5RA58
A	745	ALA	VAL	conflict	UNP A0A1G5RA58
A	746	VAL	LEU	conflict	UNP A0A1G5RA58
A	747	GLU	ALA	conflict	UNP A0A1G5RA58
A	788	ALA	SER	conflict	UNP A0A1G5RA58
A	789	ALA	SER	conflict	UNP A0A1G5RA58
A	791	GLY	GLU	conflict	UNP A0A1G5RA58
A	793	ALA	VAL	conflict	UNP A0A1G5RA58
A	851	ILE	THR	conflict	UNP A0A1G5RA58
A	864	PRO	GLN	conflict	UNP A0A1G5RA58
A	865	GLU	LYS	conflict	UNP A0A1G5RA58
A	875	ASN	ASP	conflict	UNP A0A1G5RA58
A	904	GLU	GLN	conflict	UNP A0A1G5RA58
A	905	SER	LEU	conflict	UNP A0A1G5RA58
A	906	MET	ASN	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	907	LYS	GLN	conflict	UNP A0A1G5RA58
A	908	GLU	LYS	conflict	UNP A0A1G5RA58
A	909	THR	ILE	conflict	UNP A0A1G5RA58
A	917	ASN	SER	conflict	UNP A0A1G5RA58
A	919	ALA	GLY	conflict	UNP A0A1G5RA58
A	920	GLY	GLU	conflict	UNP A0A1G5RA58
A	921	VAL	ILE	conflict	UNP A0A1G5RA58
A	932	ASN	ASP	conflict	UNP A0A1G5RA58
A	933	THR	ILE	conflict	UNP A0A1G5RA58
A	957	ALA	PRO	conflict	UNP A0A1G5RA58
A	1000	ALA	THR	conflict	UNP A0A1G5RA58
A	1009	ASN	HIS	conflict	UNP A0A1G5RA58
A	1118	ALA	THR	conflict	UNP A0A1G5RA58
A	1132	ASN	SER	conflict	UNP A0A1G5RA58
A	1155	LYS	ARG	conflict	UNP A0A1G5RA58
A	1162	ILE	MET	conflict	UNP A0A1G5RA58
A	1219	LYS	GLU	conflict	UNP A0A1G5RA58
A	1223	GLU	LYS	conflict	UNP A0A1G5RA58
A	1225	LYS	GLU	conflict	UNP A0A1G5RA58
A	1227	GLU	ALA	conflict	UNP A0A1G5RA58
A	1230	ARG	LYS	conflict	UNP A0A1G5RA58
A	1261	ASN	THR	conflict	UNP A0A1G5RA58
A	1274	ALA	GLU	conflict	UNP A0A1G5RA58
A	1275	SER	TYR	conflict	UNP A0A1G5RA58
A	1280	PRO	ASP	conflict	UNP A0A1G5RA58
A	1281	GLU	GLY	conflict	UNP A0A1G5RA58
A	1283	SER	TYR	conflict	UNP A0A1G5RA58
A	1284	ASN	LYS	conflict	UNP A0A1G5RA58
A	1285	VAL	SER	conflict	UNP A0A1G5RA58
A	1292	GLN	LYS	conflict	UNP A0A1G5RA58
A	1298	ASN	SER	conflict	UNP A0A1G5RA58
A	1317	SER	ASN	conflict	UNP A0A1G5RA58
A	1321	ASP	GLY	conflict	UNP A0A1G5RA58
A	1323	GLY	ASP	conflict	UNP A0A1G5RA58
A	1341	ASN	SER	conflict	UNP A0A1G5RA58
A	1345	ALA	THR	conflict	UNP A0A1G5RA58
A	1368	LYS	GLN	conflict	UNP A0A1G5RA58
A	1411	SER	ASN	conflict	UNP A0A1G5RA58
A	1414	THR	VAL	conflict	UNP A0A1G5RA58
A	1418	ASN	SER	conflict	UNP A0A1G5RA58
A	1429	THR	ASN	conflict	UNP A0A1G5RA58
A	1431	PRO	SER	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1442	LYS	GLY	conflict	UNP A0A1G5RA58
A	1448	GLN	PRO	conflict	UNP A0A1G5RA58
A	1465	ASP	ASN	conflict	UNP A0A1G5RA58
A	1471	ILE	VAL	conflict	UNP A0A1G5RA58
A	1472	PHE	TYR	conflict	UNP A0A1G5RA58
A	1488	GLU	ASP	conflict	UNP A0A1G5RA58
A	1500	ILE	VAL	conflict	UNP A0A1G5RA58
A	1501	ILE	THR	conflict	UNP A0A1G5RA58
A	1506	GLY	SER	conflict	UNP A0A1G5RA58
A	1516	ASP	ASN	conflict	UNP A0A1G5RA58
A	1541	GLY	SER	conflict	UNP A0A1G5RA58
A	1545	ILE	THR	conflict	UNP A0A1G5RA58
A	1553	VAL	ILE	conflict	UNP A0A1G5RA58
A	1574	VAL	ILE	conflict	UNP A0A1G5RA58
A	1576	LEU	ARG	conflict	UNP A0A1G5RA58
A	1583	ALA	SER	conflict	UNP A0A1G5RA58
A	1587	HIS	ARG	conflict	UNP A0A1G5RA58
A	1599	GLN	GLY	conflict	UNP A0A1G5RA58
A	1600	SER	VAL	conflict	UNP A0A1G5RA58
A	1603	THR	ILE	conflict	UNP A0A1G5RA58
A	1652	LEU	PRO	conflict	UNP A0A1G5RA58
A	1682	THR	LYS	conflict	UNP A0A1G5RA58
A	1687	ASN	SER	conflict	UNP A0A1G5RA58
A	1688	ILE	THR	conflict	UNP A0A1G5RA58
A	1704	HIS	SER	conflict	UNP A0A1G5RA58
A	1903	SER	ASN	conflict	UNP A0A1G5RA58
A	1909	ARG	LYS	conflict	UNP A0A1G5RA58
A	1917	ASN	SER	conflict	UNP A0A1G5RA58
A	1920	ASP	SER	conflict	UNP A0A1G5RA58
A	1922	ALA	SER	conflict	UNP A0A1G5RA58
A	1929	ASN	SER	conflict	UNP A0A1G5RA58
A	1930	ILE	-	insertion	UNP A0A1G5RA58
A	1931	PRO	-	insertion	UNP A0A1G5RA58
A	1935	PRO	LEU	conflict	UNP A0A1G5RA58
A	2028	GLY	SER	conflict	UNP A0A1G5RA58
A	2100	GLY	SER	conflict	UNP A0A1G5RA58
A	2103	TYR	HIS	conflict	UNP A0A1G5RA58
A	2206	ILE	LEU	conflict	UNP A0A1G5RA58
A	2236	SER	ALA	conflict	UNP A0A1G5RA58
A	2270	VAL	ILE	conflict	UNP A0A1G5RA58
A	2284	LEU	ILE	conflict	UNP A0A1G5RA58
A	2285	ASN	SER	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2323	LYS	ARG	conflict	UNP A0A1G5RA58
A	2340	VAL	ILE	conflict	UNP A0A1G5RA58
A	2346	LYS	GLN	conflict	UNP A0A1G5RA58
A	2348	ASN	LYS	conflict	UNP A0A1G5RA58
A	2354	ALA	THR	conflict	UNP A0A1G5RA58
A	2358	ASP	GLU	conflict	UNP A0A1G5RA58
A	2362	SER	ASN	conflict	UNP A0A1G5RA58
A	2363	GLN	ALA	conflict	UNP A0A1G5RA58
A	2391	VAL	ILE	conflict	UNP A0A1G5RA58
A	2393	PHE	LEU	conflict	UNP A0A1G5RA58
A	2404	ALA	GLU	conflict	UNP A0A1G5RA58
A	2406	LEU	ILE	conflict	UNP A0A1G5RA58
A	2446	GLU	ALA	conflict	UNP A0A1G5RA58
A	2454	MET	THR	conflict	UNP A0A1G5RA58
A	2491	MET	THR	conflict	UNP A0A1G5RA58
A	2493	GLU	ALA	conflict	UNP A0A1G5RA58
B	-18	MET	-	initiating methionine	UNP A0A1G5RA58
B	-17	ALA	-	expression tag	UNP A0A1G5RA58
B	-16	HIS	-	expression tag	UNP A0A1G5RA58
B	-15	HIS	-	expression tag	UNP A0A1G5RA58
B	-14	HIS	-	expression tag	UNP A0A1G5RA58
B	-13	HIS	-	expression tag	UNP A0A1G5RA58
B	-12	HIS	-	expression tag	UNP A0A1G5RA58
B	-11	HIS	-	expression tag	UNP A0A1G5RA58
B	-10	SER	-	expression tag	UNP A0A1G5RA58
B	-9	SER	-	expression tag	UNP A0A1G5RA58
B	-8	GLY	-	expression tag	UNP A0A1G5RA58
B	-7	LEU	-	expression tag	UNP A0A1G5RA58
B	-6	GLU	-	expression tag	UNP A0A1G5RA58
B	-5	VAL	-	expression tag	UNP A0A1G5RA58
B	-4	LEU	-	expression tag	UNP A0A1G5RA58
B	-3	PHE	-	expression tag	UNP A0A1G5RA58
B	-2	GLN	-	expression tag	UNP A0A1G5RA58
B	-1	GLY	-	expression tag	UNP A0A1G5RA58
B	0	PRO	-	expression tag	UNP A0A1G5RA58
B	3	GLU	SER	conflict	UNP A0A1G5RA58
B	4	SER	PRO	conflict	UNP A0A1G5RA58
B	14	SER	ILE	conflict	UNP A0A1G5RA58
B	19	ASN	GLN	conflict	UNP A0A1G5RA58
B	33	ARG	HIS	conflict	UNP A0A1G5RA58
B	45	THR	ALA	conflict	UNP A0A1G5RA58
B	70	ALA	THR	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	83	LEU	VAL	conflict	UNP A0A1G5RA58
B	137	TYR	ARG	conflict	UNP A0A1G5RA58
B	157	ILE	THR	conflict	UNP A0A1G5RA58
B	180	GLU	ASP	conflict	UNP A0A1G5RA58
B	184	LYS	GLN	conflict	UNP A0A1G5RA58
B	191	THR	ALA	conflict	UNP A0A1G5RA58
B	209	GLU	LYS	conflict	UNP A0A1G5RA58
B	283	LYS	ARG	conflict	UNP A0A1G5RA58
B	317	VAL	ILE	conflict	UNP A0A1G5RA58
B	321	SER	ASN	conflict	UNP A0A1G5RA58
B	339	TYR	ASN	conflict	UNP A0A1G5RA58
B	341	MET	VAL	conflict	UNP A0A1G5RA58
B	348	PHE	TYR	conflict	UNP A0A1G5RA58
B	354	ARG	GLN	conflict	UNP A0A1G5RA58
B	356	ASP	ASN	conflict	UNP A0A1G5RA58
B	361	ASN	ASP	conflict	UNP A0A1G5RA58
B	362	PHE	SER	conflict	UNP A0A1G5RA58
B	363	TYR	ARG	conflict	UNP A0A1G5RA58
B	?	-	GLN	deletion	UNP A0A1G5RA58
B	364	ASN	ASP	conflict	UNP A0A1G5RA58
B	365	ALA	VAL	conflict	UNP A0A1G5RA58
B	379	VAL	ILE	conflict	UNP A0A1G5RA58
B	381	THR	ILE	conflict	UNP A0A1G5RA58
B	393	ALA	GLU	conflict	UNP A0A1G5RA58
B	394	ASN	HIS	conflict	UNP A0A1G5RA58
B	398	ASN	SER	conflict	UNP A0A1G5RA58
B	400	ALA	THR	conflict	UNP A0A1G5RA58
B	414	LEU	TYR	conflict	UNP A0A1G5RA58
B	417	GLY	SER	conflict	UNP A0A1G5RA58
B	428	VAL	ILE	conflict	UNP A0A1G5RA58
B	459	GLY	SER	conflict	UNP A0A1G5RA58
B	466	LEU	GLN	conflict	UNP A0A1G5RA58
B	472	THR	ALA	conflict	UNP A0A1G5RA58
B	473	ASP	GLU	conflict	UNP A0A1G5RA58
B	491	HIS	ASN	conflict	UNP A0A1G5RA58
B	502	PRO	LEU	conflict	UNP A0A1G5RA58
B	540	SER	PRO	conflict	UNP A0A1G5RA58
B	549	THR	SER	conflict	UNP A0A1G5RA58
B	550	ILE	VAL	conflict	UNP A0A1G5RA58
B	560	VAL	ILE	conflict	UNP A0A1G5RA58
B	563	PHE	TYR	conflict	UNP A0A1G5RA58
B	570	ASP	ASN	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	572	ASP	ASN	conflict	UNP A0A1G5RA58
B	574	LYS	GLN	conflict	UNP A0A1G5RA58
B	583	LYS	ASN	conflict	UNP A0A1G5RA58
B	587	ASN	ASP	conflict	UNP A0A1G5RA58
B	596	ASP	GLU	conflict	UNP A0A1G5RA58
B	610	ILE	VAL	conflict	UNP A0A1G5RA58
B	616	LYS	GLU	conflict	UNP A0A1G5RA58
B	629	THR	ALA	conflict	UNP A0A1G5RA58
B	639	SER	VAL	conflict	UNP A0A1G5RA58
B	642	HIS	GLN	conflict	UNP A0A1G5RA58
B	648	VAL	ALA	conflict	UNP A0A1G5RA58
B	653	ILE	VAL	conflict	UNP A0A1G5RA58
B	687	ASP	ASN	conflict	UNP A0A1G5RA58
B	719	GLN	LYS	conflict	UNP A0A1G5RA58
B	737	LYS	GLN	conflict	UNP A0A1G5RA58
B	741	GLY	ASP	conflict	UNP A0A1G5RA58
B	745	ALA	VAL	conflict	UNP A0A1G5RA58
B	746	VAL	LEU	conflict	UNP A0A1G5RA58
B	747	GLU	ALA	conflict	UNP A0A1G5RA58
B	788	ALA	SER	conflict	UNP A0A1G5RA58
B	789	ALA	SER	conflict	UNP A0A1G5RA58
B	791	GLY	GLU	conflict	UNP A0A1G5RA58
B	793	ALA	VAL	conflict	UNP A0A1G5RA58
B	851	ILE	THR	conflict	UNP A0A1G5RA58
B	864	PRO	GLN	conflict	UNP A0A1G5RA58
B	865	GLU	LYS	conflict	UNP A0A1G5RA58
B	875	ASN	ASP	conflict	UNP A0A1G5RA58
B	904	GLU	GLN	conflict	UNP A0A1G5RA58
B	905	SER	LEU	conflict	UNP A0A1G5RA58
B	906	MET	ASN	conflict	UNP A0A1G5RA58
B	907	LYS	GLN	conflict	UNP A0A1G5RA58
B	908	GLU	LYS	conflict	UNP A0A1G5RA58
B	909	THR	ILE	conflict	UNP A0A1G5RA58
B	917	ASN	SER	conflict	UNP A0A1G5RA58
B	919	ALA	GLY	conflict	UNP A0A1G5RA58
B	920	GLY	GLU	conflict	UNP A0A1G5RA58
B	921	VAL	ILE	conflict	UNP A0A1G5RA58
B	932	ASN	ASP	conflict	UNP A0A1G5RA58
B	933	THR	ILE	conflict	UNP A0A1G5RA58
B	957	ALA	PRO	conflict	UNP A0A1G5RA58
B	1000	ALA	THR	conflict	UNP A0A1G5RA58
B	1009	ASN	HIS	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1118	ALA	THR	conflict	UNP A0A1G5RA58
B	1132	ASN	SER	conflict	UNP A0A1G5RA58
B	1155	LYS	ARG	conflict	UNP A0A1G5RA58
B	1162	ILE	MET	conflict	UNP A0A1G5RA58
B	1219	LYS	GLU	conflict	UNP A0A1G5RA58
B	1223	GLU	LYS	conflict	UNP A0A1G5RA58
B	1225	LYS	GLU	conflict	UNP A0A1G5RA58
B	1227	GLU	ALA	conflict	UNP A0A1G5RA58
B	1230	ARG	LYS	conflict	UNP A0A1G5RA58
B	1261	ASN	THR	conflict	UNP A0A1G5RA58
B	1274	ALA	GLU	conflict	UNP A0A1G5RA58
B	1275	SER	TYR	conflict	UNP A0A1G5RA58
B	1280	PRO	ASP	conflict	UNP A0A1G5RA58
B	1281	GLU	GLY	conflict	UNP A0A1G5RA58
B	1283	SER	TYR	conflict	UNP A0A1G5RA58
B	1284	ASN	LYS	conflict	UNP A0A1G5RA58
B	1285	VAL	SER	conflict	UNP A0A1G5RA58
B	1292	GLN	LYS	conflict	UNP A0A1G5RA58
B	1298	ASN	SER	conflict	UNP A0A1G5RA58
B	1317	SER	ASN	conflict	UNP A0A1G5RA58
B	1321	ASP	GLY	conflict	UNP A0A1G5RA58
B	1323	GLY	ASP	conflict	UNP A0A1G5RA58
B	1341	ASN	SER	conflict	UNP A0A1G5RA58
B	1345	ALA	THR	conflict	UNP A0A1G5RA58
B	1368	LYS	GLN	conflict	UNP A0A1G5RA58
B	1411	SER	ASN	conflict	UNP A0A1G5RA58
B	1414	THR	VAL	conflict	UNP A0A1G5RA58
B	1418	ASN	SER	conflict	UNP A0A1G5RA58
B	1429	THR	ASN	conflict	UNP A0A1G5RA58
B	1431	PRO	SER	conflict	UNP A0A1G5RA58
B	1442	LYS	GLY	conflict	UNP A0A1G5RA58
B	1448	GLN	PRO	conflict	UNP A0A1G5RA58
B	1465	ASP	ASN	conflict	UNP A0A1G5RA58
B	1471	ILE	VAL	conflict	UNP A0A1G5RA58
B	1472	PHE	TYR	conflict	UNP A0A1G5RA58
B	1488	GLU	ASP	conflict	UNP A0A1G5RA58
B	1500	ILE	VAL	conflict	UNP A0A1G5RA58
B	1501	ILE	THR	conflict	UNP A0A1G5RA58
B	1506	GLY	SER	conflict	UNP A0A1G5RA58
B	1516	ASP	ASN	conflict	UNP A0A1G5RA58
B	1541	GLY	SER	conflict	UNP A0A1G5RA58
B	1545	ILE	THR	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1553	VAL	ILE	conflict	UNP A0A1G5RA58
B	1574	VAL	ILE	conflict	UNP A0A1G5RA58
B	1576	LEU	ARG	conflict	UNP A0A1G5RA58
B	1583	ALA	SER	conflict	UNP A0A1G5RA58
B	1587	HIS	ARG	conflict	UNP A0A1G5RA58
B	1599	GLN	GLY	conflict	UNP A0A1G5RA58
B	1600	SER	VAL	conflict	UNP A0A1G5RA58
B	1603	THR	ILE	conflict	UNP A0A1G5RA58
B	1652	LEU	PRO	conflict	UNP A0A1G5RA58
B	1682	THR	LYS	conflict	UNP A0A1G5RA58
B	1687	ASN	SER	conflict	UNP A0A1G5RA58
B	1688	ILE	THR	conflict	UNP A0A1G5RA58
B	1704	HIS	SER	conflict	UNP A0A1G5RA58
B	1903	SER	ASN	conflict	UNP A0A1G5RA58
B	1909	ARG	LYS	conflict	UNP A0A1G5RA58
B	1917	ASN	SER	conflict	UNP A0A1G5RA58
B	1920	ASP	SER	conflict	UNP A0A1G5RA58
B	1922	ALA	SER	conflict	UNP A0A1G5RA58
B	1929	ASN	SER	conflict	UNP A0A1G5RA58
B	1930	ILE	-	insertion	UNP A0A1G5RA58
B	1931	PRO	-	insertion	UNP A0A1G5RA58
B	1935	PRO	LEU	conflict	UNP A0A1G5RA58
B	2028	GLY	SER	conflict	UNP A0A1G5RA58
B	2100	GLY	SER	conflict	UNP A0A1G5RA58
B	2103	TYR	HIS	conflict	UNP A0A1G5RA58
B	2206	ILE	LEU	conflict	UNP A0A1G5RA58
B	2236	SER	ALA	conflict	UNP A0A1G5RA58
B	2270	VAL	ILE	conflict	UNP A0A1G5RA58
B	2284	LEU	ILE	conflict	UNP A0A1G5RA58
B	2285	ASN	SER	conflict	UNP A0A1G5RA58
B	2323	LYS	ARG	conflict	UNP A0A1G5RA58
B	2340	VAL	ILE	conflict	UNP A0A1G5RA58
B	2346	LYS	GLN	conflict	UNP A0A1G5RA58
B	2348	ASN	LYS	conflict	UNP A0A1G5RA58
B	2354	ALA	THR	conflict	UNP A0A1G5RA58
B	2358	ASP	GLU	conflict	UNP A0A1G5RA58
B	2362	SER	ASN	conflict	UNP A0A1G5RA58
B	2363	GLN	ALA	conflict	UNP A0A1G5RA58
B	2391	VAL	ILE	conflict	UNP A0A1G5RA58
B	2393	PHE	LEU	conflict	UNP A0A1G5RA58
B	2404	ALA	GLU	conflict	UNP A0A1G5RA58
B	2406	LEU	ILE	conflict	UNP A0A1G5RA58

Continued on next page...

Continued from previous page...

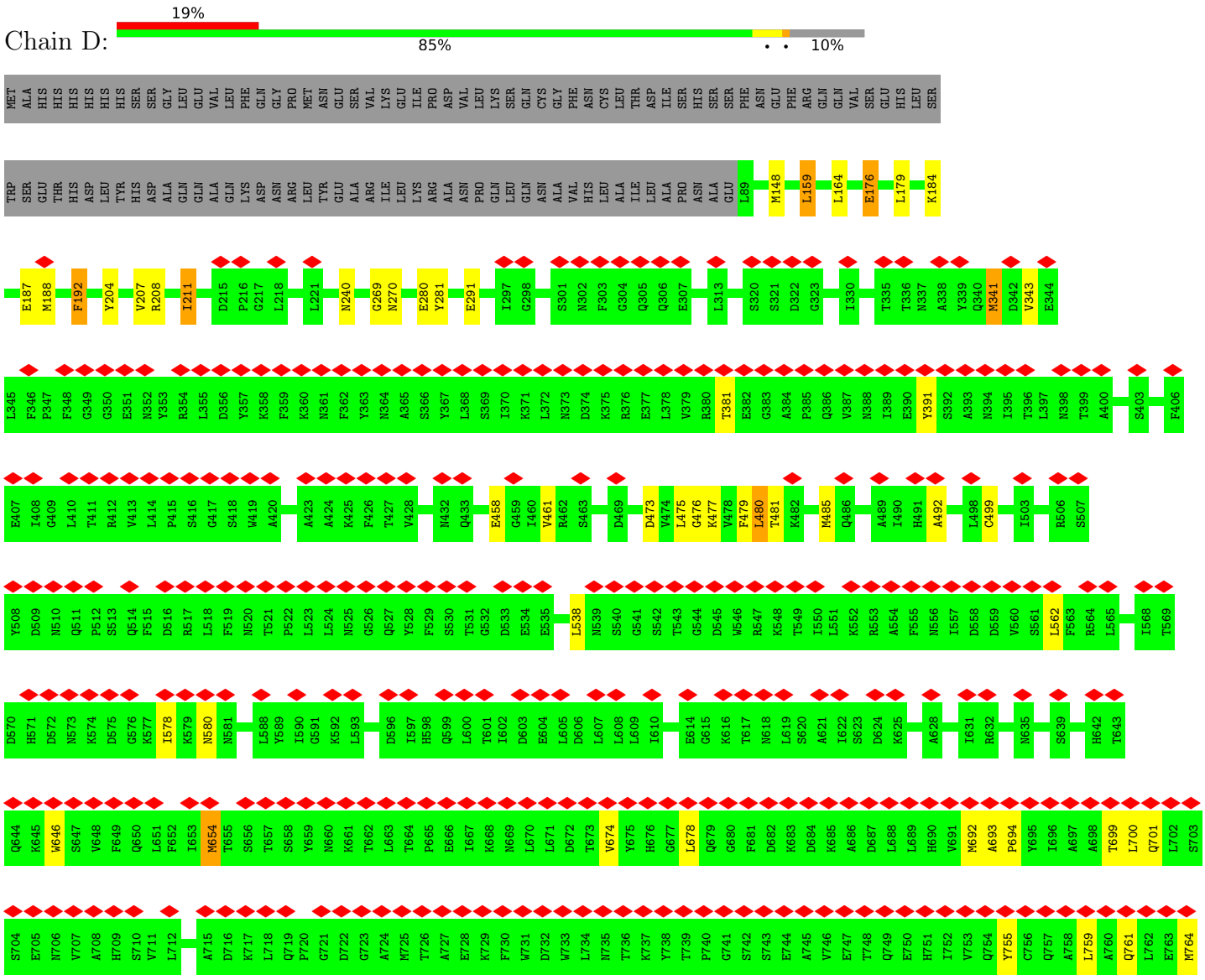
Chain	Residue	Modelled	Actual	Comment	Reference
B	2446	GLU	ALA	conflict	UNP A0A1G5RA58
B	2454	MET	THR	conflict	UNP A0A1G5RA58
B	2491	MET	THR	conflict	UNP A0A1G5RA58
B	2493	GLU	ALA	conflict	UNP A0A1G5RA58

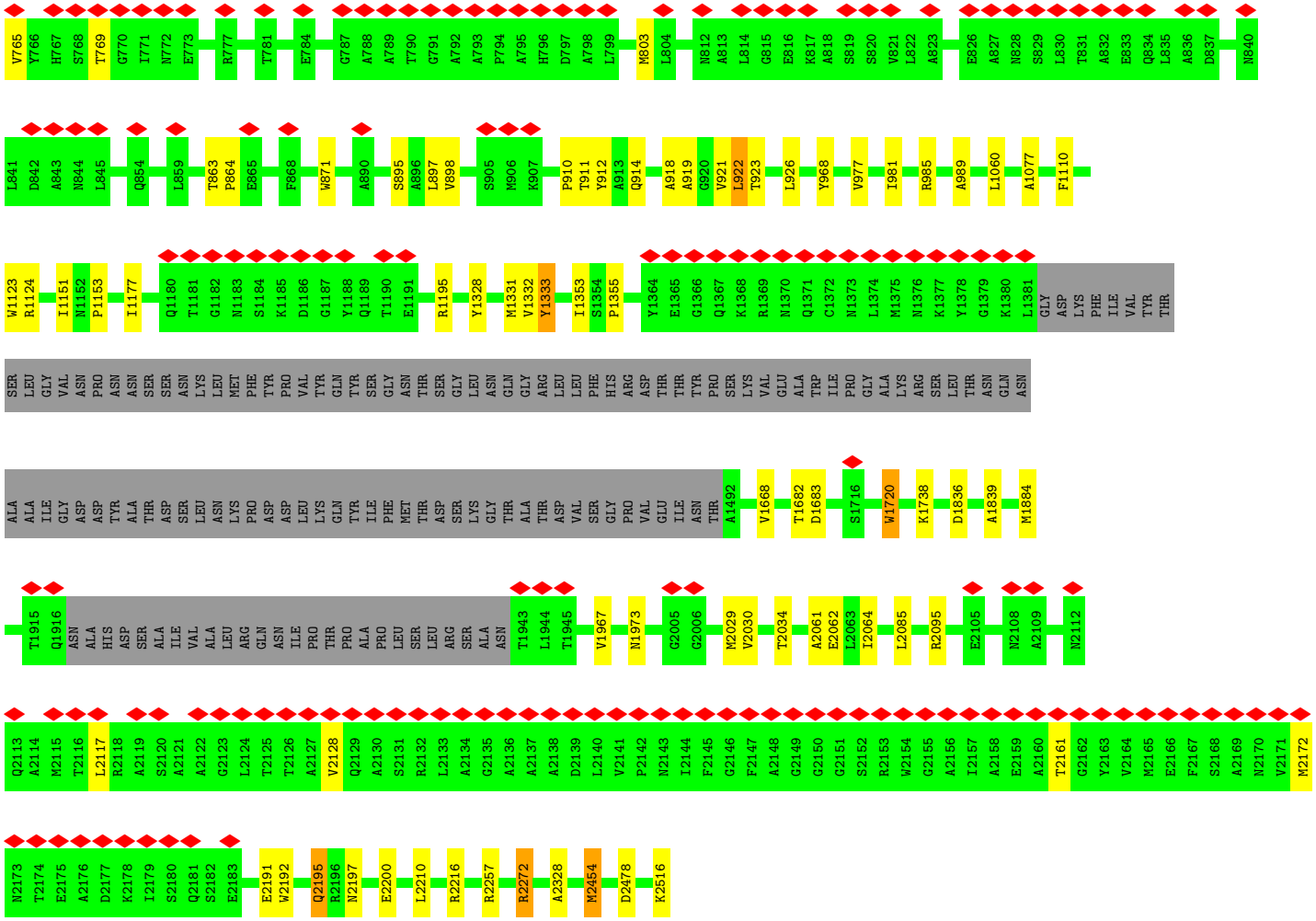
3 Residue-property plots (i)

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

- Molecule 1: Virulence plasmid A protein

Chain D:

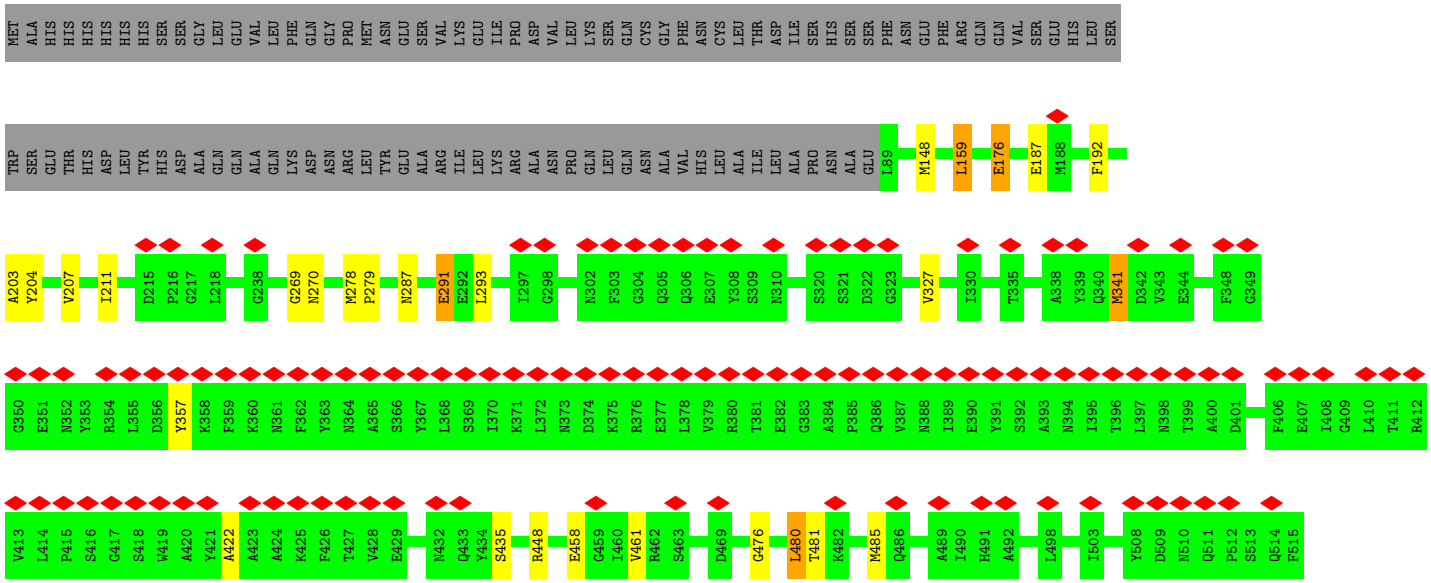


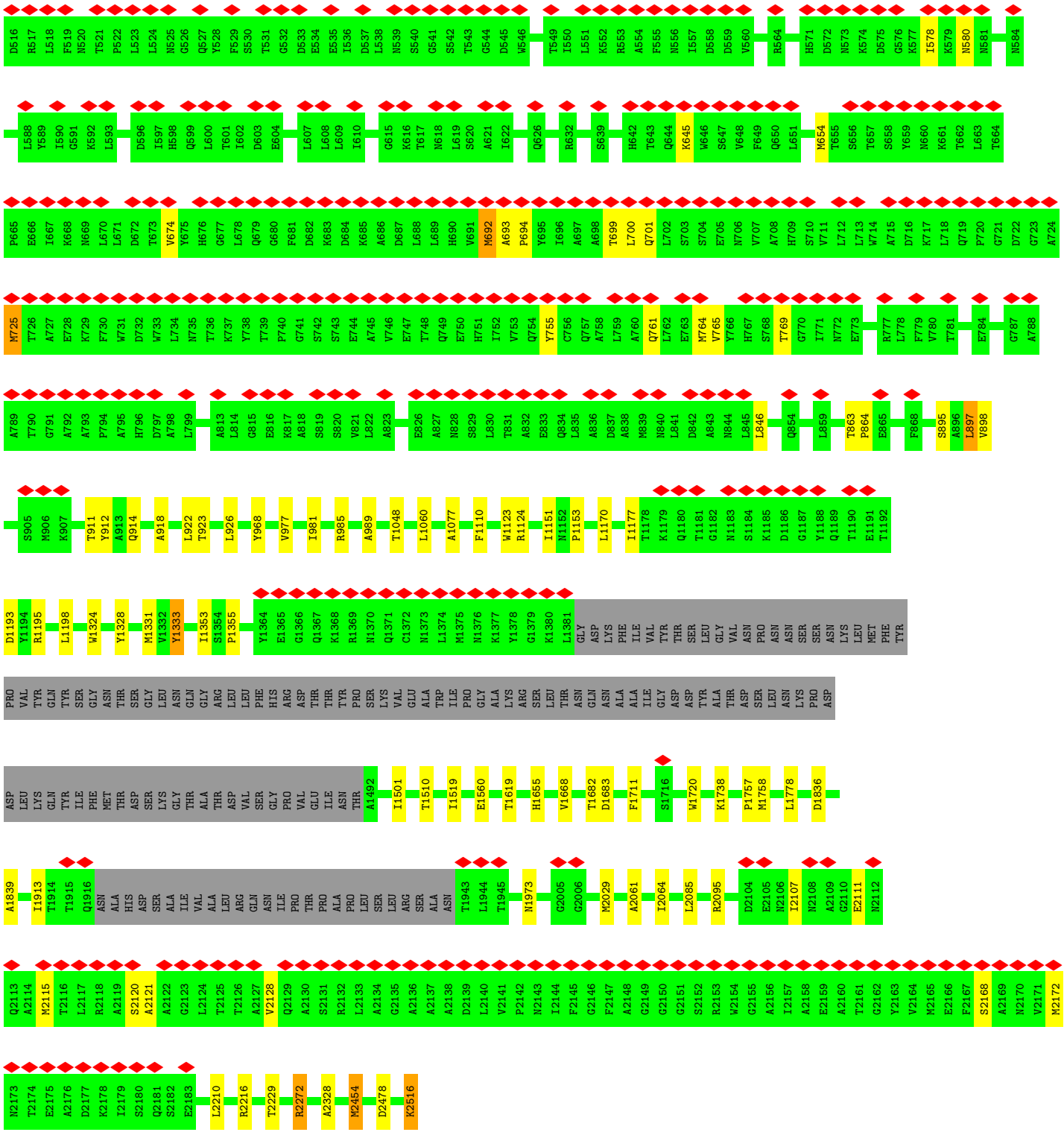


• Molecule 1: Virulence plasmid A protein

Chain E:





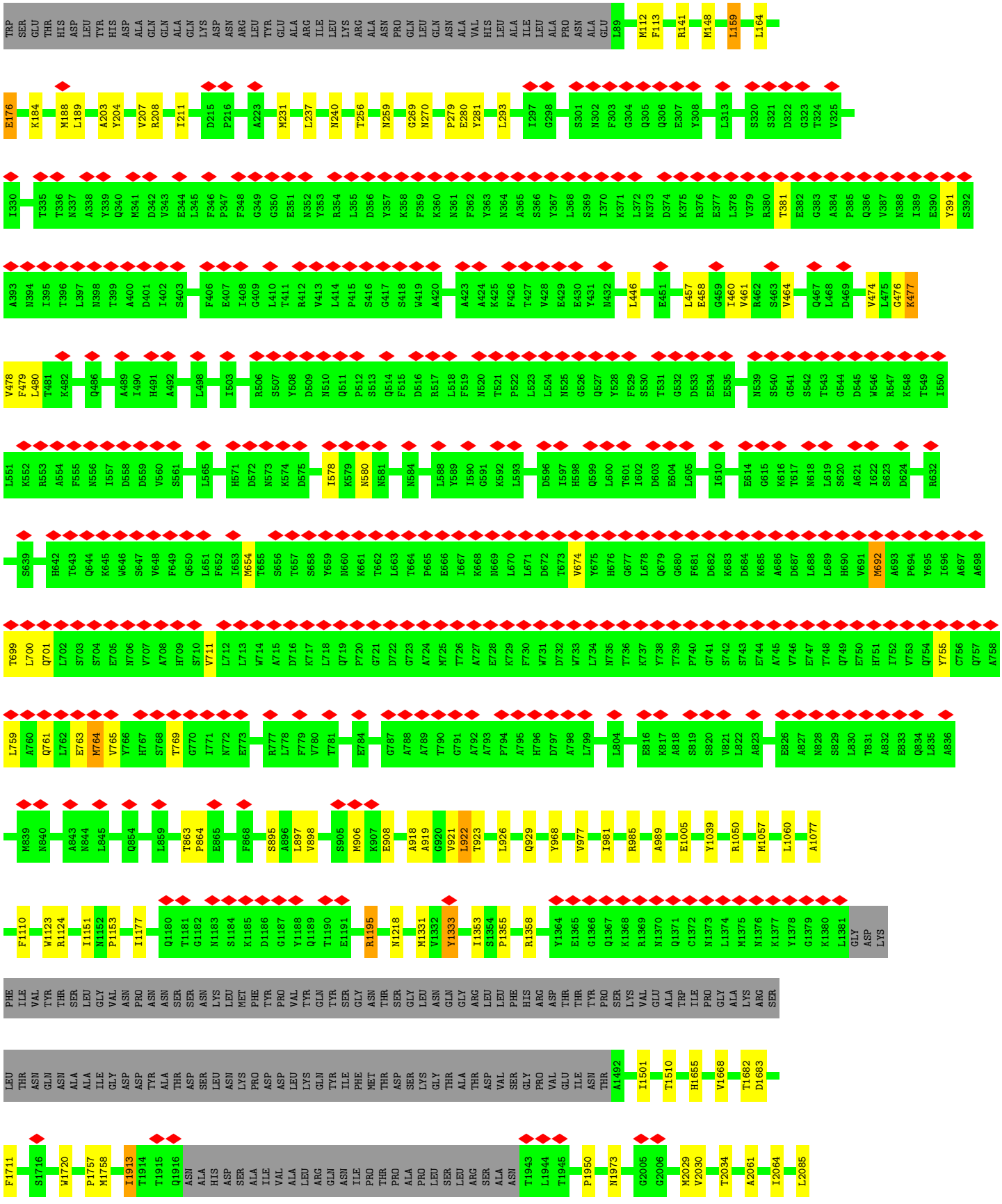


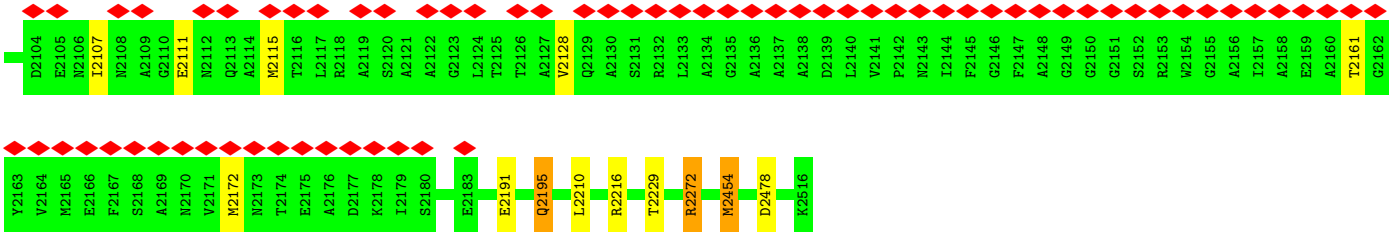
- Molecule 1: Virulence plasmid A protein

Chain C:

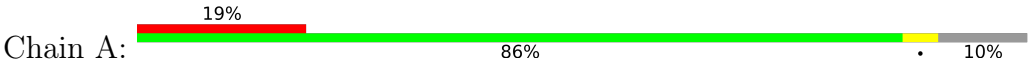


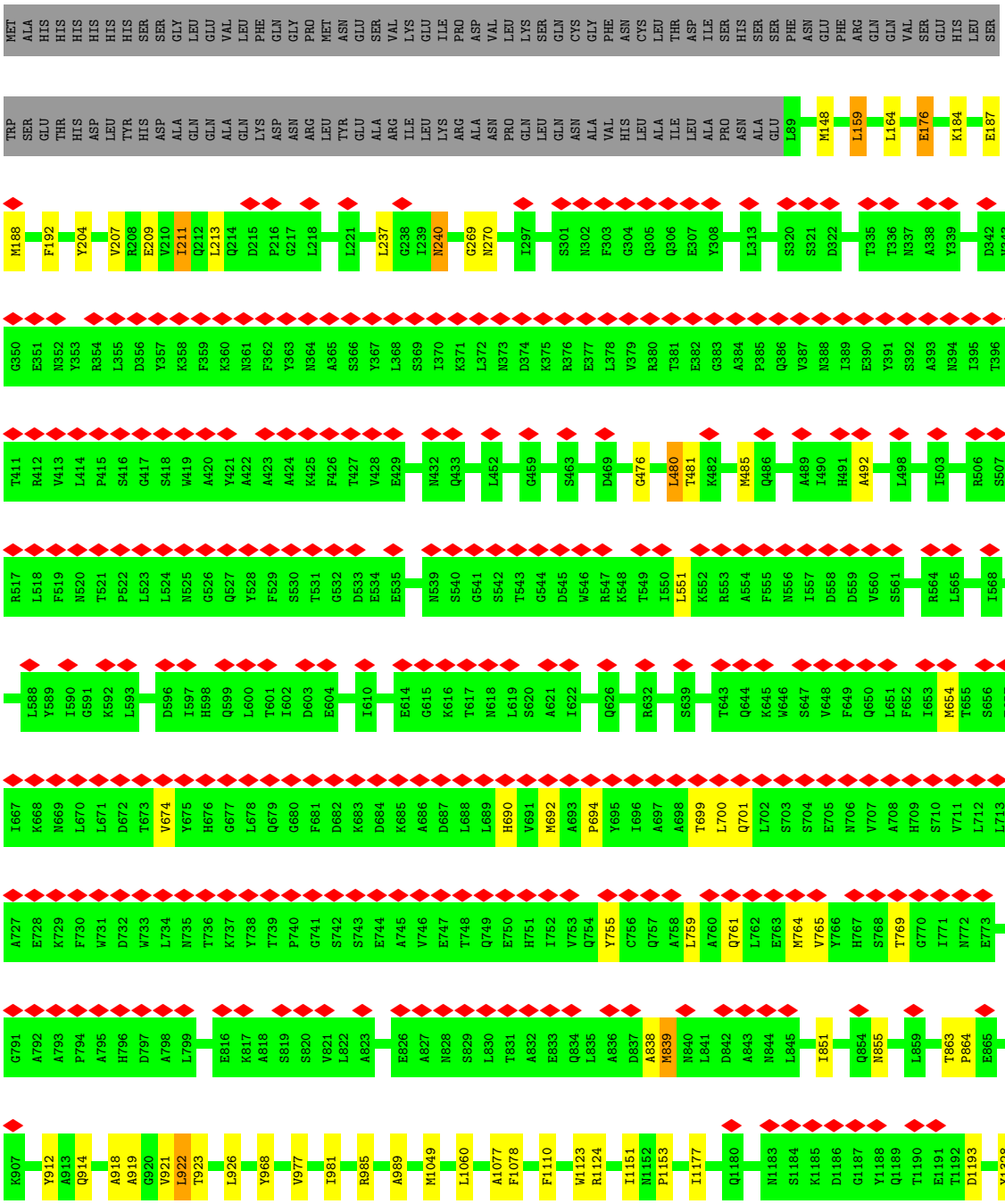


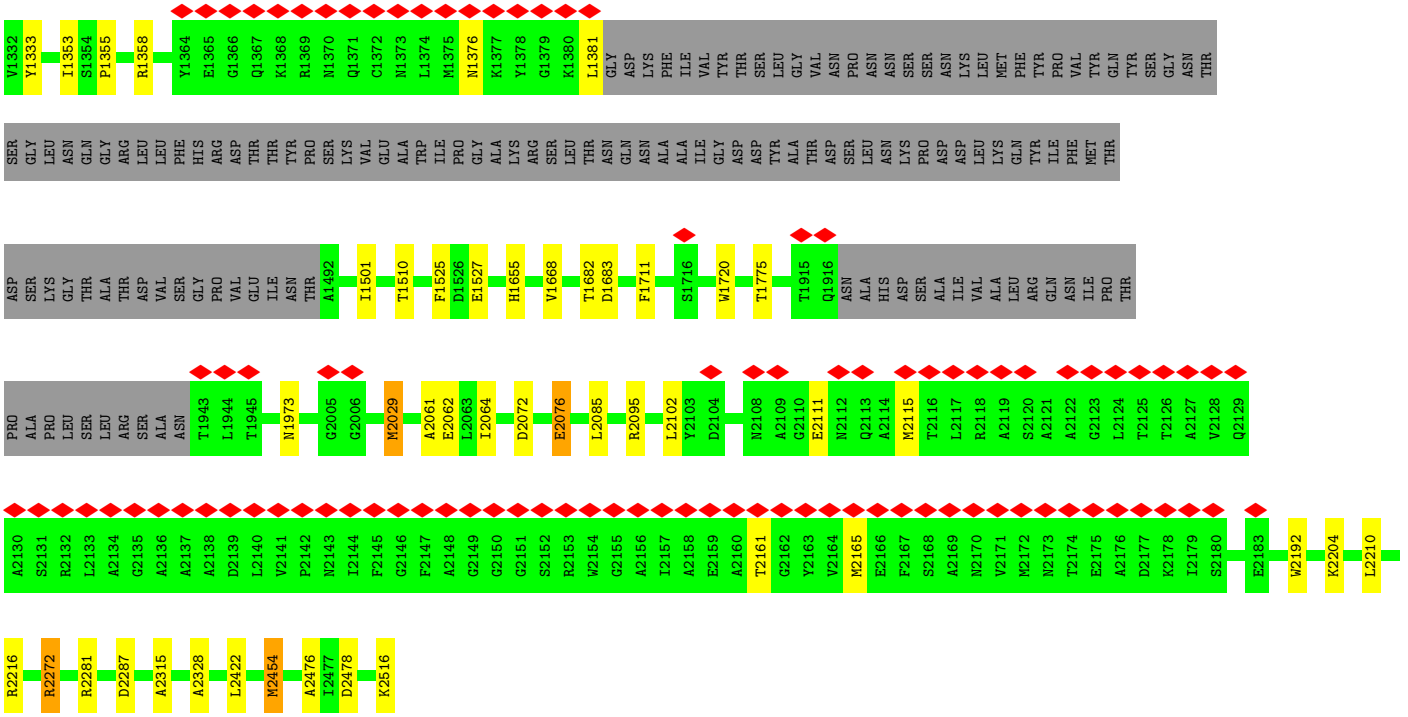

TRP SER GLU THR HIS ASP LEU TYR HIS ASP ALA GLN GLN ALA GLN LYS ASP ASN ARG LEU TYR GLU ALA ARG ILE LEU LYS ARG ALA ASN PRO GLN LEU GLN ASN ALA VAL HIS LEU ALA ILE LEU ALA PRO ASN ALA GLU L89 M112 F113 R141 M148 L159 L164
E176 K184 M188 L189 A203 Y204 V207 R208 I211 D215 P216 A223 M231 L237 N240 T256 N259 G269 N270 P279 E280 Y281 L293 I297 G298 S301 N302 F303 G304 Q305 Q306 E307 Y308 L313 S320 S321 D322 G323 T324 V325
I330 T335 T336 N337 A338 Y339 Q340 M341 D342 V343 E344 L345 F346 P347 F348 G349 G350 E351 N352 Y353 R354 L355 D356 Y357 K358 F359 K360 N361 F362 Y363 N364 A365 S366 Y367 L368 S369 I370 K371 L372 N373 D374 K375 R376 E377 L378 V379 R380 T381 E382 G383 A384 P385 Q386 V387 N388 I389 E390 Y391 S392
A393 N394 I395 T396 L397 N398 T399 A400 D401 I402 S403 F406 E407 I408 G409 L410 T411 R412 V413 L414 P415 S416 G417 S418 W419 A420 A423 A424 K425 F426 T427 V428 E429 E430 Y431 N432 L446 E451 L457 E458 G459 I460 V461 R462 S463 V464 Q467 L468 D469 V474 L475 G476 K477
V478 F479 L480 T481 K482 Q486 A489 I490 H491 A492 L498 I503 R506 S507 Y508 D509 N510 Q511 P512 S513 Q514 F515 D516 R517 L518 F519 N520 T521 P522 L523 L524 N525 G526 Q527 Y528 F529 S530 T531 G532 D533 E534 E535 N539 S540 G541 S542 T543 G544 D545 W546 R547 K548 T549 I550
L551 K552 R553 A554 F555 N556 I557 D558 D559 V560 S561 L565 H571 D572 N573 K574 D575 I578 K579 N580 N581 N584 L588 Y589 I590 G591 K592 L593 D596 I597 H598 Q599 L600 T601 I602 D603 E604 L605 I610 E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 D624 R632
S639 H642 T643 Q644 K645 W646 S647 V648 F649 Q650 L651 F652 I653 M654 T655 S656 T657 S658 Y659 N660 K661 T662 L663 T664 P665 E666 I667 K668 N669 L670 L671 D672 T673 V674 Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698
T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733 L734 N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 T752 V753 Q754 Y755 C756 Q757 A758
L759 A760 Q761 L762 E763 M764 V765 Y766 H767 S768 T769 G770 I771 N772 E773 R777 L778 F779 V780 T781 E784 G787 A788 A789 T790 G791 A792 A793 P794 A795 H796 D797 A798 L799 L804 E816 K817 A818 S819 S820 V821 L822 A823 E826 A827 N828 S829 L830 T831 A832 E833 Q834 L835 A836
M839 N840 A843 N844 L845 Q854 L859 T863 P864 E865 F868 S895 A896 L897 V898 S905 M906 K907 E908 A918 A919 G920 V921 L922 T923 L926 Q929 Y968 V977 I981 R985 A989 E1005 Y1039 R1050 M1057 L1060 A1077
F1110 W1123 R1124 I1151 N1152 P1153 I1177 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 R1196 N1218 M1331 Y1332 Y1333 I1353 S1354 P1355 R1358 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 GLY ASP LYS
PHE ILE VAL TYR THR SER LEU GLY VAL ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL TYR GLN TYR SER GLY ASN THR SER GLY LEU ASN GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ALA TRP ILE PRO GLY ALA LYS ARG SER
LEU THR ASN GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LYS GLN TYR ILE PHE MET THR ASP SER LYS GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR A1492 I1501 T1510 H1655 V1668 T1682 D1683
F1711 S1716 W1720 P1757 M1758 I1913 T1914 T1915 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN T1943 L1944 T1945 P1950 N1973 G2005 G2006 M2029 V2030 T2034 A2061 I2064 L2085



• Molecule 1: Virulence plasmid A protein



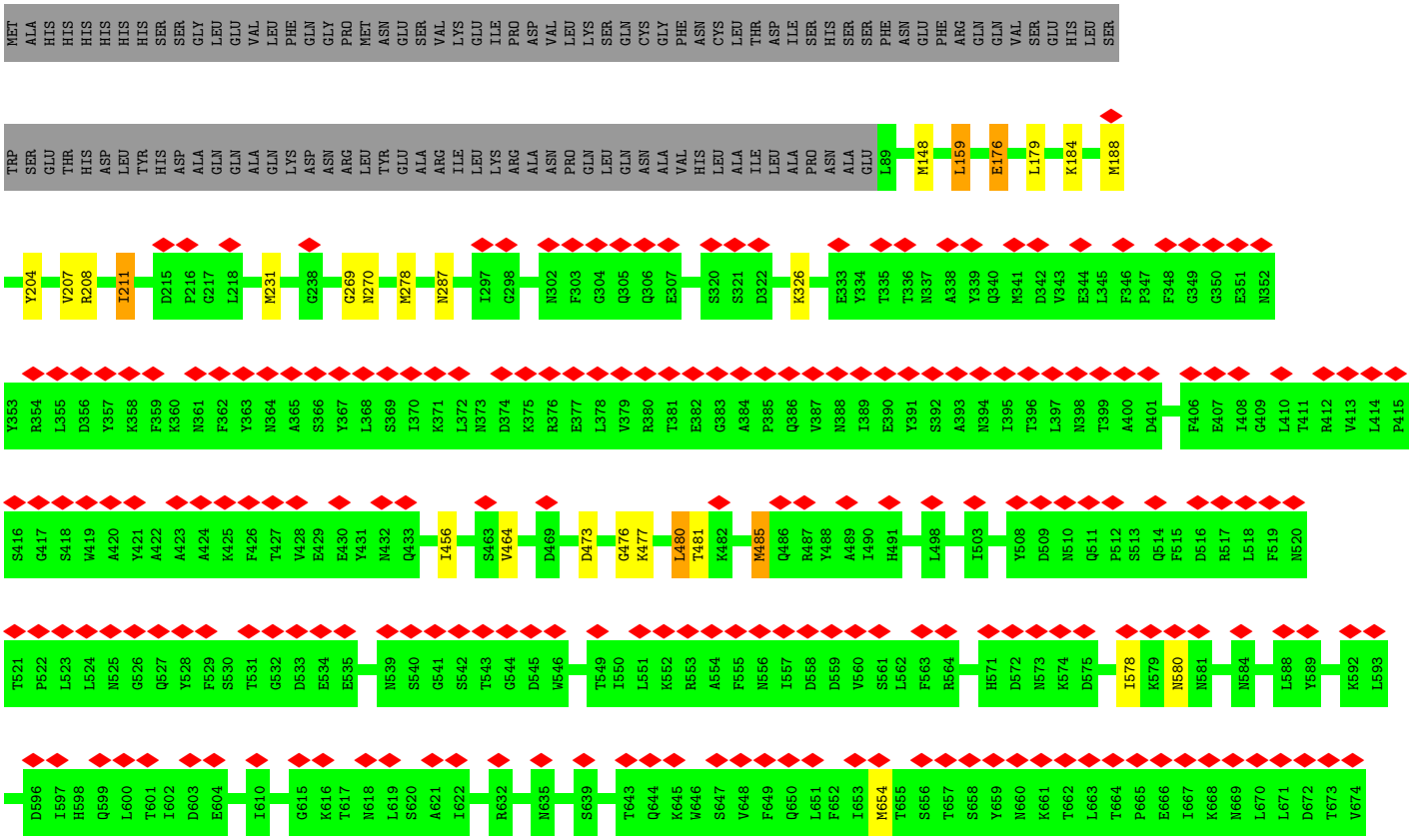


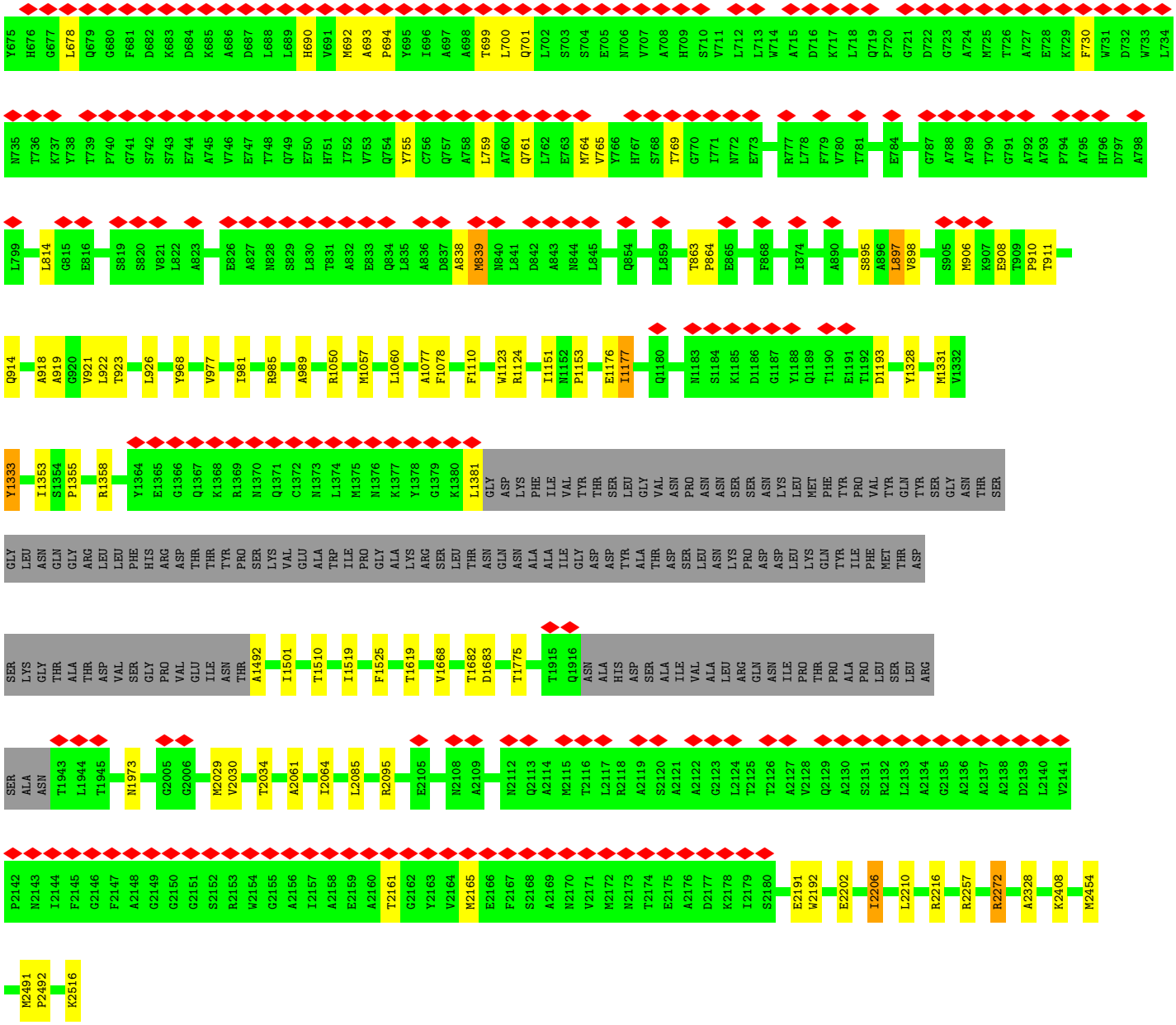


• Molecule 1: Virulence plasmid A protein

Chain B:






Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709 S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733 L734
N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 Y755 C756 Q757 A758 L759 A760 Q761 L762 E763 M764 V765 Y766 H767 S768 T769 G770 I771 N772 E773 R777 L778 F779 V780 T781 E784 G787 A788 A789 T790 G791 A792 A793 P794 A795 H796 D797 A798
L799 L814 G815 E816 S819 S820 V821 L822 A823 E826 A827 N828 S829 L830 T831 A832 E833 Q834 L835 A836 D837 A838 M839 N840 L841 D842 A843 N844 L845 Q854 L859 T863 P864 E865 F868 I874 A890 S895 A896 L897 V898 S905 M906 K907 E908 T909 P910 T911
Q914 A918 A919 G920 V921 L922 T923 L926 Y968 V977 I981 R985 A989 R1050 M1057 L1060 A1077 F1078 F1110 W1123 R1124 I1151 N1152 P1153 E1176 I1177 Q1180 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 T1192 D1193 Y1328 M1331 V1332
Y1333 I1353 S1354 P1355 R1358 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 GLY ASP LYS PHE ILE VAL TYR THR SER LEU GLY VAL ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL TYR GLN TYR SER GLY ASN THR SER
GLY LEU ASN GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ALA TRP ILE PRO GLY ALA LYS ARG SER LEU THR ASN GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LEU LYS GLN TYR ILE PHE MET THR ASP
SER LYS GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR A1492 I1501 T1510 I1519 F1525 T1619 V1668 T1682 D1683 T1775 T1915 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG
SER ALA ASN T1943 L1944 T1945 N1973 G2005 G2006 M2029 V2030 T2034 A2061 I2064 L2085 R2095 E2105 N2108 A2109 N2112 Q2113 A2114 M2115 T2116 L2117 R2118 A2119 S2120 A2121 A2122 G2123 L2124 T2125 T2126 A2127 V2128 Q2129 A2130 S2131 R2132 L2133 A2134 G2135 A2136 A2137 A2138 D2139 L2140 V2141
P2142 N2143 I2144 F2145 G2146 F2147 A2148 G2149 G2150 G2151 S2152 R2153 W2154 G2155 A2156 I2157 A2158 E2159 A2160 T2161 G2162 Y2163 V2164 M2165 E2166 F2167 S2168 A2169 N2170 V2171 M2172 N2173 T2174 E2175 A2176 D2177 K2178 I2179 S2180 E2191 W2192 E2202 I2206 L2210 R2216 R2257 R2272 A2328 K2408 M2454
M2491 P2492 K2516

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.229	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0262	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.68, 0.68, 0.68	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/18588	0.43	0/25239
1	B	0.15	0/18588	0.43	1/25239 (0.0%)
1	C	0.15	0/18588	0.44	2/25239 (0.0%)
1	D	0.15	0/18588	0.43	1/25239 (0.0%)
1	E	0.15	0/18588	0.44	4/25239 (0.0%)
All	All	0.15	0/92940	0.43	8/126195 (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	2
1	B	0	3
1	C	0	2
1	D	0	3
1	E	0	2
All	All	0	12

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	645	LYS	CA-C-N	7.46	134.82	122.07
1	E	645	LYS	C-N-CA	7.46	134.82	122.07
1	E	1333	TYR	CA-CB-CG	5.87	124.47	113.90
1	D	1333	TYR	CA-CB-CG	5.82	124.37	113.90
1	C	692	MET	CB-CG-SD	-5.73	95.50	112.70
1	B	1333	TYR	CA-CB-CG	5.65	124.06	113.90
1	C	1333	TYR	CA-CB-CG	5.59	123.97	113.90
1	E	692	MET	CB-CG-SD	-5.01	97.66	112.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1124	ARG	Sidechain
1	A	2272	ARG	Sidechain
1	B	1124	ARG	Sidechain
1	B	2257	ARG	Sidechain
1	B	2272	ARG	Sidechain
1	C	1124	ARG	Sidechain
1	C	2272	ARG	Sidechain
1	D	1124	ARG	Sidechain
1	D	2257	ARG	Sidechain
1	D	2272	ARG	Sidechain
1	E	1124	ARG	Sidechain
1	E	2272	ARG	Sidechain

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	18198	17797	17794	83	0
1	B	18198	17797	17794	83	0
1	C	18198	17797	17794	93	0
1	D	18198	17797	17794	92	0
1	E	18198	17797	17794	87	0
All	All	90990	88985	88970	422	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 2.

All (422) 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:E:918:ALA:O	1:E:922:LEU:HD12	1.77	0.84
1:C:1177:ILE:HD12	1:C:1177:ILE:O	1.84	0.78
1:E:1353:ILE:HG22	1:E:1355:PRO:HD3	1.71	0.73
1:D:481:THR:HG22	1:D:485:MET:HE3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HE2	1:C:1950:PRO:HA	1.71	0.72
1:D:1353:ILE:HG22	1:D:1355:PRO:HD3	1.72	0.71
1:C:1353:ILE:HG22	1:C:1355:PRO:HD3	1.72	0.71
1:B:476:GLY:O	1:B:480:LEU:HD23	1.91	0.71
1:A:1353:ILE:HG22	1:A:1355:PRO:HD3	1.73	0.71
1:B:918:ALA:O	1:B:922:LEU:HD13	1.91	0.71
1:D:485:MET:HE2	1:D:492:ALA:HB2	1.75	0.67
1:C:2128:VAL:HG11	1:B:2165:MET:HE1	1.77	0.67
1:A:654:MET:HE1	1:A:764:MET:SD	2.36	0.66
1:B:1353:ILE:HG22	1:B:1355:PRO:HD3	1.76	0.66
1:C:476:GLY:O	1:C:480:LEU:HD23	1.95	0.65
1:B:578:ILE:HG23	1:B:580:ASN:H	1.60	0.65
1:C:207:VAL:O	1:C:211:ILE:HD13	1.97	0.65
1:A:192:PHE:CG	1:A:192:PHE:O	2.50	0.65
1:C:148:MET:HE1	1:C:989:ALA:HB2	1.78	0.64
1:A:578:ILE:HG23	1:A:580:ASN:H	1.61	0.64
1:D:654:MET:SD	1:D:765:VAL:HG22	2.37	0.64
1:D:674:VAL:HG11	1:D:692:MET:HE1	1.79	0.63
1:D:192:PHE:CG	1:D:192:PHE:O	2.50	0.63
1:B:326:LYS:HB3	1:B:326:LYS:HZ3	1.63	0.63
1:E:192:PHE:CG	1:E:192:PHE:O	2.50	0.63
1:B:921:VAL:HG23	1:B:922:LEU:HD12	1.81	0.63
1:C:208:ARG:HG2	1:C:208:ARG:HH11	1.66	0.61
1:E:654:MET:HE1	1:E:764:MET:SD	2.41	0.60
1:E:1331:MET:SD	1:E:1333:TYR:CE2	2.94	0.60
1:A:674:VAL:HG11	1:A:692:MET:HE1	1.84	0.60
1:D:179:LEU:HD22	1:D:188:MET:HE1	1.84	0.60
1:C:1151:ILE:HG22	1:C:1153:PRO:HD3	1.82	0.60
1:E:578:ILE:HG23	1:E:580:ASN:H	1.66	0.59
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.66	0.59
1:A:2204:LYS:HE3	1:A:2204:LYS:HA	1.84	0.59
1:C:2191:GLU:O	1:C:2195:GLN:OE1	2.20	0.59
1:D:578:ILE:HG23	1:D:580:ASN:H	1.67	0.59
1:D:921:VAL:HG23	1:D:922:LEU:CD1	2.33	0.59
1:C:578:ILE:HG23	1:C:580:ASN:H	1.67	0.59
1:D:1151:ILE:HG22	1:D:1153:PRO:HD3	1.85	0.59
1:B:1331:MET:SD	1:B:1333:TYR:CE2	2.96	0.59
1:A:184:LYS:HG2	1:A:188:MET:HE2	1.84	0.58
1:B:207:VAL:O	1:B:211:ILE:HD13	2.02	0.58
1:E:1151:ILE:HG22	1:E:1153:PRO:HD3	1.86	0.58
1:B:2202:GLU:O	1:B:2206:ILE:HD13	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:GLU:O	1:A:2115:MET:SD	2.61	0.58
1:C:2216:ARG:HG3	1:C:2216:ARG:HH11	1.68	0.58
1:A:1151:ILE:HG22	1:A:1153:PRO:HD3	1.85	0.58
1:D:1177:ILE:HD12	1:D:1177:ILE:O	2.04	0.57
1:D:1331:MET:HE2	1:D:1332:VAL:O	2.03	0.57
1:D:485:MET:HE2	1:D:492:ALA:CB	2.34	0.57
1:B:1381:LEU:HD13	1:B:1525:PHE:HE1	1.68	0.57
1:D:2197:ASN:O	1:D:2200:GLU:HG2	2.05	0.57
1:A:839:MET:HE3	1:A:839:MET:N	2.19	0.57
1:B:179:LEU:HD22	1:B:188:MET:HE1	1.87	0.57
1:D:207:VAL:O	1:D:211:ILE:HD13	2.05	0.57
1:A:1358:ARG:HH11	1:A:1358:ARG:HG3	1.70	0.57
1:B:1151:ILE:HG22	1:B:1153:PRO:HD3	1.85	0.57
1:D:2191:GLU:O	1:D:2195:GLN:OE1	2.23	0.56
1:A:2328:ALA:HB2	1:A:2516:LYS:HG3	1.87	0.56
1:C:256:THR:O	1:C:259:ASN:OD1	2.24	0.56
1:C:921:VAL:HG13	1:C:922:LEU:HD12	1.88	0.56
1:A:207:VAL:O	1:A:211:ILE:HD13	2.05	0.56
1:C:906:MET:HE3	1:C:908:GLU:HB2	1.87	0.56
1:B:278:MET:HE2	1:B:1519:ILE:HD11	1.88	0.56
1:A:148:MET:HE1	1:A:989:ALA:HB2	1.87	0.55
1:E:923:THR:HA	1:E:926:LEU:HD23	1.89	0.55
1:E:1913:ILE:HD12	1:E:1913:ILE:O	2.06	0.55
1:C:1913:ILE:HD12	1:C:1913:ILE:O	2.05	0.55
1:D:1331:MET:SD	1:D:1333:TYR:CE2	2.99	0.55
1:A:897:LEU:C	1:A:897:LEU:HD23	2.31	0.55
1:B:897:LEU:C	1:B:897:LEU:HD23	2.31	0.55
1:B:464:VAL:HB	1:B:477:LYS:HD2	1.89	0.55
1:E:897:LEU:HD23	1:E:897:LEU:C	2.33	0.54
1:E:761:GLN:O	1:E:765:VAL:HG23	2.07	0.54
1:C:674:VAL:HG11	1:C:692:MET:HE1	1.90	0.54
1:E:2107:ILE:HG21	1:E:2115:MET:HE1	1.89	0.54
1:A:921:VAL:HG23	1:A:922:LEU:HD12	1.89	0.54
1:E:1193:ASP:OD1	1:E:1193:ASP:O	2.26	0.54
1:C:923:THR:HA	1:C:926:LEU:CD2	2.37	0.54
1:A:476:GLY:O	1:A:480:LEU:HD23	2.07	0.54
1:A:2061:ALA:O	1:A:2064:ILE:HG22	2.08	0.54
1:D:148:MET:HE1	1:D:989:ALA:HB2	1.89	0.54
1:D:179:LEU:CD2	1:D:188:MET:HE1	2.37	0.54
1:D:2195:GLN:OE1	1:D:2195:GLN:N	2.42	0.53
1:E:977:VAL:CG2	1:E:981:ILE:HD12	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:ALA:O	1:C:922:LEU:HD13	2.08	0.53
1:E:291:GLU:OE1	1:E:291:GLU:N	2.41	0.53
1:A:851:ILE:O	1:A:855:ASN:OD1	2.25	0.53
1:C:1331:MET:HE1	1:C:1333:TYR:CE1	2.43	0.53
1:A:2072:ASP:O	1:A:2076:GLU:OE1	2.26	0.53
1:E:654:MET:CE	1:E:764:MET:SD	2.96	0.53
1:E:2168:SER:O	1:E:2172:MET:HG3	2.09	0.53
1:B:148:MET:HE1	1:B:989:ALA:HB2	1.90	0.53
1:B:2491:MET:HB3	1:B:2492:PRO:HD3	1.90	0.53
1:D:761:GLN:O	1:D:765:VAL:HG23	2.09	0.53
1:E:481:THR:HG22	1:E:485:MET:HE3	1.90	0.53
1:B:977:VAL:CG2	1:B:981:ILE:HD12	2.39	0.53
1:D:654:MET:HE1	1:D:764:MET:SD	2.49	0.52
1:D:977:VAL:CG2	1:D:981:ILE:HD12	2.39	0.52
1:A:481:THR:HG22	1:A:485:MET:CE	2.39	0.52
1:B:2328:ALA:HB2	1:B:2516:LYS:HE2	1.91	0.52
1:A:923:THR:HA	1:A:926:LEU:HD23	1.91	0.52
1:B:1381:LEU:HD11	1:B:1492:ALA:HA	1.91	0.52
1:D:476:GLY:O	1:D:480:LEU:HD23	2.10	0.52
1:C:1358:ARG:HG3	1:C:1358:ARG:HH11	1.74	0.52
1:A:2422:LEU:HD13	1:A:2422:LEU:C	2.35	0.52
1:C:977:VAL:CG2	1:C:981:ILE:HD12	2.39	0.52
1:A:977:VAL:CG2	1:A:981:ILE:HD12	2.39	0.52
1:C:381:THR:HG23	1:C:391:TYR:CZ	2.45	0.52
1:B:923:THR:HA	1:B:926:LEU:HD23	1.92	0.52
1:A:187:GLU:HB3	1:A:912:TYR:HB2	1.91	0.52
1:C:654:MET:SD	1:C:765:VAL:HG22	2.49	0.52
1:E:148:MET:HE1	1:E:989:ALA:HB2	1.91	0.51
1:E:918:ALA:C	1:E:922:LEU:HD12	2.35	0.51
1:C:895:SER:HA	1:C:898:VAL:HG22	1.91	0.51
1:C:231:MET:SD	1:C:898:VAL:HA	2.51	0.51
1:D:2328:ALA:HB2	1:D:2516:LYS:HG3	1.91	0.51
1:D:678:LEU:HD11	1:D:692:MET:HE2	1.93	0.51
1:B:179:LEU:CD2	1:B:188:MET:HE1	2.40	0.51
1:B:1176:GLU:C	1:B:1177:ILE:HD12	2.35	0.51
1:E:1177:ILE:HD12	1:E:1195:ARG:NH1	2.26	0.51
1:A:769:THR:HG22	1:A:769:THR:O	2.11	0.51
1:C:1331:MET:CE	1:C:1333:TYR:CZ	2.94	0.51
1:B:839:MET:HE3	1:B:839:MET:N	2.26	0.51
1:B:895:SER:HA	1:B:898:VAL:HG22	1.93	0.51
1:D:921:VAL:HG23	1:D:922:LEU:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2095:ARG:HA	1:D:2095:ARG:NE	2.26	0.50
1:D:769:THR:HG22	1:D:769:THR:O	2.12	0.50
1:D:2172:MET:HE1	1:E:2120:SER:HB2	1.92	0.50
1:E:769:THR:O	1:E:769:THR:HG22	2.12	0.50
1:E:1324:TRP:CD1	1:E:1331:MET:HG3	2.47	0.50
1:C:2195:GLN:OE1	1:C:2195:GLN:N	2.45	0.50
1:C:112:MET:HE1	1:C:1039:TYR:CE1	2.47	0.50
1:E:476:GLY:O	1:E:480:LEU:HD23	2.11	0.50
1:D:2454:MET:HE2	1:D:2454:MET:HA	1.93	0.50
1:E:481:THR:O	1:E:485:MET:HG3	2.12	0.49
1:D:910:PRO:CB	1:D:914:GLN:OE1	2.61	0.49
1:E:187:GLU:HB3	1:E:912:TYR:HB2	1.94	0.49
1:B:2029:MET:HG3	1:B:2272:ARG:HD2	1.95	0.49
1:C:769:THR:HG22	1:C:769:THR:O	2.11	0.49
1:A:481:THR:HG22	1:A:485:MET:HE2	1.94	0.49
1:B:1193:ASP:OD1	1:B:1193:ASP:O	2.30	0.49
1:E:654:MET:CE	1:E:765:VAL:HG22	2.43	0.49
1:E:2107:ILE:CG2	1:E:2115:MET:HE1	2.43	0.49
1:C:2111:GLU:O	1:C:2115:MET:SD	2.71	0.49
1:B:1358:ARG:HG3	1:B:1358:ARG:HH11	1.77	0.49
1:D:699:THR:HG22	1:D:700:LEU:N	2.28	0.49
1:E:654:MET:SD	1:E:765:VAL:HG22	2.53	0.49
1:C:654:MET:HE2	1:C:764:MET:HE3	1.95	0.49
1:C:2061:ALA:O	1:C:2064:ILE:HG22	2.12	0.49
1:B:678:LEU:CD1	1:B:692:MET:HE2	2.42	0.48
1:D:1884:MET:HE1	1:D:1967:VAL:HG21	1.95	0.48
1:B:769:THR:O	1:B:769:THR:HG22	2.12	0.48
1:C:112:MET:HE3	1:C:113:PHE:CZ	2.48	0.48
1:A:700:LEU:HG	1:A:701:GLN:H	1.77	0.48
1:B:910:PRO:CB	1:B:914:GLN:OE1	2.61	0.48
1:E:2111:GLU:O	1:E:2115:MET:SD	2.71	0.48
1:A:699:THR:HG22	1:A:700:LEU:N	2.28	0.48
1:D:895:SER:O	1:D:898:VAL:HG22	2.13	0.48
1:D:2216:ARG:HH11	1:D:2216:ARG:HG3	1.77	0.48
1:E:203:ALA:O	1:E:207:VAL:HG13	2.13	0.48
1:E:1619:THR:HG22	1:E:1619:THR:O	2.13	0.48
1:C:279:PRO:HB3	1:C:293:LEU:HD21	1.95	0.48
1:A:918:ALA:O	1:A:922:LEU:HD13	2.13	0.48
1:B:2095:ARG:HA	1:B:2095:ARG:NE	2.29	0.48
1:D:2029:MET:HG3	1:D:2272:ARG:HD2	1.95	0.48
1:E:341:MET:HE2	1:E:422:ALA:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:MET:SD	1:A:765:VAL:HG22	2.53	0.48
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.79	0.48
1:C:699:THR:HG22	1:C:700:LEU:N	2.29	0.48
1:A:1049:MET:O	1:A:1049:MET:HG2	2.14	0.48
1:B:2085:LEU:HD23	1:B:2210:LEU:CD1	2.44	0.48
1:B:699:THR:HG22	1:B:700:LEU:N	2.29	0.48
1:D:923:THR:HA	1:D:926:LEU:CD2	2.43	0.47
1:A:1381:LEU:HB2	1:A:1525:PHE:HE1	1.79	0.47
1:B:1331:MET:SD	1:B:1333:TYR:CZ	3.06	0.47
1:E:341:MET:SD	1:E:357:TYR:CE2	3.08	0.47
1:A:159:LEU:HD21	1:A:985:ARG:HG3	1.95	0.47
1:E:204:TYR:O	1:E:207:VAL:HG22	2.15	0.47
1:E:2328:ALA:HB2	1:E:2516:LYS:HG3	1.97	0.47
1:C:204:TYR:O	1:C:207:VAL:HG22	2.14	0.47
1:A:761:GLN:O	1:A:765:VAL:HG23	2.15	0.47
1:E:699:THR:HG22	1:E:700:LEU:N	2.29	0.47
1:C:921:VAL:HG13	1:C:922:LEU:CD1	2.45	0.47
1:C:2085:LEU:HD23	1:C:2210:LEU:CD1	2.45	0.47
1:A:1358:ARG:NE	1:A:1527:GLU:OE2	2.48	0.47
1:D:918:ALA:O	1:D:922:LEU:HD13	2.15	0.47
1:D:2061:ALA:O	1:D:2064:ILE:HG22	2.14	0.47
1:E:159:LEU:HD21	1:E:985:ARG:HG3	1.96	0.47
1:E:1720:TRP:HZ2	1:E:1738:LYS:HD2	1.80	0.47
1:A:2085:LEU:HD23	1:A:2210:LEU:CD1	2.45	0.47
1:B:159:LEU:HD21	1:B:985:ARG:HG3	1.96	0.47
1:D:2172:MET:HE3	1:E:2121:ALA:HB2	1.97	0.47
1:E:2229:THR:HG23	1:A:2062:GLU:OE1	2.15	0.47
1:C:1501:ILE:CD1	1:C:1510:THR:HG23	2.45	0.47
1:A:2102:LEU:HD23	1:A:2192:TRP:CD1	2.50	0.47
1:D:341:MET:HE1	1:D:343:VAL:HB	1.96	0.46
1:C:446:LEU:HD12	1:C:457:LEU:HD21	1.96	0.46
1:B:911:THR:HG22	1:B:914:GLN:HG3	1.97	0.46
1:D:204:TYR:O	1:D:207:VAL:HG22	2.15	0.46
1:D:538:LEU:HD22	1:D:562:LEU:HD11	1.97	0.46
1:D:2128:VAL:HG13	1:C:2161:THR:HG22	1.97	0.46
1:B:231:MET:SD	1:B:898:VAL:HA	2.55	0.46
1:E:278:MET:HE2	1:E:1519:ILE:HD11	1.97	0.46
1:E:700:LEU:HG	1:E:701:GLN:H	1.80	0.46
1:E:895:SER:O	1:E:898:VAL:HG22	2.16	0.46
1:C:203:ALA:O	1:C:207:VAL:HG13	2.15	0.46
1:A:1501:ILE:CD1	1:A:1510:THR:HG23	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD22	1:D:164:LEU:HD21	1.98	0.46
1:D:2272:ARG:HG3	1:D:2272:ARG:HH11	1.81	0.46
1:C:159:LEU:HD22	1:C:164:LEU:HD21	1.98	0.46
1:A:2161:THR:HA	1:A:2165:MET:HE1	1.97	0.46
1:B:838:ALA:C	1:B:839:MET:HE3	2.41	0.46
1:D:578:ILE:HG23	1:D:580:ASN:N	2.30	0.46
1:B:654:MET:SD	1:B:764:MET:SD	3.14	0.46
1:E:287:ASN:O	1:E:287:ASN:CG	2.59	0.46
1:E:926:LEU:N	1:E:926:LEU:HD22	2.31	0.46
1:C:2107:ILE:HG21	1:C:2115:MET:HE1	1.98	0.46
1:A:895:SER:HA	1:A:898:VAL:HG22	1.97	0.46
1:A:1193:ASP:O	1:A:1193:ASP:OD2	2.33	0.46
1:C:2029:MET:HG3	1:C:2272:ARG:HD2	1.97	0.45
1:E:2085:LEU:HD23	1:E:2210:LEU:CD1	2.45	0.45
1:C:460:ILE:CG2	1:C:477:LYS:HD3	2.46	0.45
1:A:921:VAL:HG23	1:A:922:LEU:CD1	2.46	0.45
1:B:481:THR:HG22	1:B:485:MET:SD	2.56	0.45
1:B:678:LEU:HD11	1:B:692:MET:HG2	1.98	0.45
1:C:477:LYS:HD2	1:C:478:VAL:N	2.32	0.45
1:A:2095:ARG:HA	1:A:2095:ARG:NE	2.32	0.45
1:B:2061:ALA:O	1:B:2064:ILE:HG22	2.17	0.45
1:D:176:GLU:OE2	1:D:176:GLU:C	2.60	0.45
1:E:176:GLU:C	1:E:176:GLU:OE2	2.60	0.45
1:A:2272:ARG:HG3	1:A:2272:ARG:HH11	1.81	0.45
1:E:2216:ARG:HG3	1:E:2216:ARG:HH11	1.80	0.45
1:C:2085:LEU:HD23	1:C:2210:LEU:HD13	1.99	0.45
1:A:2454:MET:HE2	1:A:2454:MET:HA	1.99	0.45
1:B:1619:THR:O	1:B:1619:THR:HG22	2.16	0.45
1:D:280:GLU:CD	1:D:281:TYR:N	2.75	0.45
1:E:674:VAL:HG11	1:E:692:MET:HE1	1.99	0.45
1:B:473:ASP:OD2	1:B:473:ASP:C	2.60	0.45
1:D:184:LYS:O	1:D:188:MET:HE2	2.17	0.45
1:D:700:LEU:HG	1:D:701:GLN:H	1.81	0.45
1:E:725:MET:HE1	1:E:755:TYR:CD1	2.52	0.45
1:E:2272:ARG:HG3	1:E:2272:ARG:HH11	1.82	0.45
1:C:1050:ARG:NH2	1:C:1057:MET:HE2	2.31	0.45
1:B:700:LEU:HG	1:B:701:GLN:H	1.81	0.45
1:D:1060:LEU:HG	1:D:1077:ALA:HB1	1.98	0.45
1:D:1331:MET:CE	1:D:1332:VAL:O	2.65	0.45
1:B:204:TYR:O	1:B:207:VAL:HG22	2.17	0.45
1:B:2161:THR:O	1:B:2165:MET:SD	2.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD21	1:D:985:ARG:HG3	1.98	0.45
1:E:2061:ALA:O	1:E:2064:ILE:HG22	2.17	0.45
1:C:863:THR:OG1	1:C:864:PRO:HD2	2.17	0.45
1:B:481:THR:O	1:B:485:MET:SD	2.75	0.45
1:D:1682:THR:HG22	1:D:1683:ASP:N	2.32	0.44
1:C:1195:ARG:HG3	1:C:1218:ASN:HD21	1.82	0.44
1:D:654:MET:SD	1:D:764:MET:SD	3.15	0.44
1:C:2128:VAL:HG13	1:B:2161:THR:HG22	1.98	0.44
1:C:2478:ASP:OD2	1:C:2478:ASP:C	2.60	0.44
1:A:926:LEU:HD22	1:A:926:LEU:N	2.32	0.44
1:D:473:ASP:O	1:D:477:LYS:HG2	2.17	0.44
1:B:863:THR:OG1	1:B:864:PRO:HD2	2.18	0.44
1:B:1050:ARG:NH2	1:B:1057:MET:HE2	2.33	0.44
1:D:911:THR:HG22	1:D:914:GLN:HG3	1.99	0.44
1:D:2062:GLU:OE2	1:C:2229:THR:HG23	2.18	0.44
1:C:184:LYS:HB3	1:C:188:MET:HG2	1.99	0.44
1:B:1060:LEU:HG	1:B:1077:ALA:HB1	1.98	0.44
1:E:341:MET:HG3	1:E:422:ALA:HB1	2.00	0.44
1:E:1170:LEU:HG	1:E:1198:LEU:HD11	1.98	0.44
1:A:1110:PHE:O	1:A:1123:TRP:HA	2.18	0.44
1:B:2191:GLU:OE1	1:B:2192:TRP:CD1	2.71	0.44
1:D:187:GLU:HB3	1:D:912:TYR:HB2	1.99	0.44
1:C:176:GLU:C	1:C:176:GLU:OE2	2.60	0.44
1:C:981:ILE:HG12	1:B:1973:ASN:HB2	2.00	0.44
1:C:1110:PHE:O	1:C:1123:TRP:HA	2.18	0.44
1:A:1060:LEU:HG	1:A:1077:ALA:HB1	1.98	0.44
1:A:1973:ASN:HB2	1:B:981:ILE:HG12	2.00	0.44
1:B:1110:PHE:O	1:B:1123:TRP:HA	2.18	0.44
1:D:1973:ASN:HB2	1:E:981:ILE:HG12	2.00	0.44
1:E:279:PRO:HB3	1:E:293:LEU:HD21	1.99	0.44
1:E:863:THR:OG1	1:E:864:PRO:HD2	2.18	0.44
1:E:2095:ARG:HA	1:E:2095:ARG:NE	2.32	0.44
1:E:1973:ASN:HB2	1:A:981:ILE:HG12	2.00	0.44
1:C:159:LEU:HD21	1:C:985:ARG:HG3	1.98	0.44
1:C:654:MET:HE2	1:C:764:MET:CE	2.47	0.44
1:A:2029:MET:HG3	1:A:2272:ARG:HD2	2.00	0.44
1:D:921:VAL:HG23	1:D:922:LEU:HD13	1.98	0.44
1:D:1110:PHE:O	1:D:1123:TRP:HA	2.18	0.44
1:C:1060:LEU:HG	1:C:1077:ALA:HB1	2.00	0.44
1:B:176:GLU:OE2	1:B:176:GLU:C	2.61	0.44
1:D:1151:ILE:CG2	1:D:1153:PRO:HD3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:C	1:A:176:GLU:OE2	2.61	0.43
1:A:1655:HIS:HA	1:A:1711:PHE:CE2	2.53	0.43
1:C:477:LYS:HD2	1:C:477:LYS:C	2.42	0.43
1:C:1682:THR:HG22	1:C:1683:ASP:N	2.32	0.43
1:D:981:ILE:HG12	1:C:1973:ASN:HB2	2.00	0.43
1:E:1110:PHE:O	1:E:1123:TRP:HA	2.18	0.43
1:E:1151:ILE:CG2	1:E:1153:PRO:HD3	2.48	0.43
1:E:1501:ILE:CD1	1:E:1510:THR:HG23	2.48	0.43
1:E:1560:GLU:N	1:E:1560:GLU:OE1	2.52	0.43
1:A:1682:THR:HG22	1:A:1683:ASP:N	2.33	0.43
1:B:1682:THR:HG22	1:B:1683:ASP:N	2.32	0.43
1:C:237:LEU:HD13	1:C:479:PHE:HB3	2.00	0.43
1:B:906:MET:HE2	1:B:908:GLU:HB2	2.01	0.43
1:C:674:VAL:HG11	1:C:692:MET:CE	2.48	0.43
1:C:755:TYR:O	1:C:759:LEU:HG	2.19	0.43
1:A:188:MET:SD	1:A:188:MET:N	2.92	0.43
1:A:1177:ILE:O	1:A:1193:ASP:OD2	2.37	0.43
1:A:863:THR:OG1	1:A:864:PRO:HD2	2.18	0.43
1:D:1720:TRP:HZ2	1:D:1738:LYS:HD2	1.84	0.43
1:A:838:ALA:C	1:A:839:MET:HE3	2.42	0.43
1:B:926:LEU:N	1:B:926:LEU:HD22	2.33	0.43
1:D:269:GLY:O	1:D:270:ASN:CG	2.61	0.43
1:E:1655:HIS:HA	1:E:1711:PHE:CE2	2.52	0.43
1:C:2272:ARG:HG3	1:C:2272:ARG:HH11	1.84	0.43
1:B:184:LYS:O	1:B:188:MET:HE2	2.18	0.43
1:B:761:GLN:O	1:B:765:VAL:HG23	2.19	0.43
1:B:2272:ARG:HG3	1:B:2272:ARG:HH11	1.84	0.43
1:D:646:TRP:CH2	1:D:654:MET:HE2	2.54	0.43
1:C:280:GLU:CD	1:C:281:TYR:N	2.76	0.43
1:D:381:THR:HG23	1:D:391:TYR:CE1	2.54	0.43
1:E:911:THR:O	1:E:914:GLN:HG2	2.19	0.43
1:E:1060:LEU:HG	1:E:1077:ALA:HB1	2.00	0.43
1:A:1376:ASN:HA	1:A:1525:PHE:CD2	2.53	0.43
1:B:287:ASN:CG	1:B:287:ASN:O	2.61	0.43
1:B:456:ILE:N	1:B:456:ILE:HD12	2.33	0.43
1:B:906:MET:CE	1:B:908:GLU:HB2	2.48	0.43
1:E:327:VAL:HG11	1:E:435:SER:H	1.84	0.42
1:E:2029:MET:HE1	1:A:2315:ALA:HB1	2.00	0.42
1:C:761:GLN:O	1:C:765:VAL:HG23	2.18	0.42
1:C:897:LEU:C	1:C:897:LEU:HD13	2.44	0.42
1:C:2454:MET:HE2	1:C:2454:MET:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:THR:HA	1:B:926:LEU:CD2	2.48	0.42
1:D:693:ALA:HB3	1:D:694:PRO:HD3	2.01	0.42
1:C:1151:ILE:CG2	1:C:1153:PRO:HD3	2.48	0.42
1:C:446:LEU:HD12	1:C:457:LEU:CD2	2.49	0.42
1:A:188:MET:HE1	1:A:912:TYR:CZ	2.55	0.42
1:A:269:GLY:O	1:A:270:ASN:CG	2.63	0.42
1:B:755:TYR:O	1:B:759:LEU:HG	2.20	0.42
1:D:381:THR:HG23	1:D:391:TYR:CZ	2.53	0.42
1:D:458:GLU:HA	1:D:461:VAL:HG12	2.01	0.42
1:B:919:ALA:O	1:B:923:THR:HG23	2.20	0.42
1:A:1151:ILE:CG2	1:A:1153:PRO:HD3	2.48	0.42
1:D:2117:LEU:HD22	1:C:2172:MET:SD	2.59	0.42
1:E:269:GLY:O	1:E:270:ASN:CG	2.62	0.42
1:E:693:ALA:HB3	1:E:694:PRO:HD3	2.02	0.42
1:E:1177:ILE:O	1:E:1193:ASP:OD1	2.37	0.42
1:A:204:TYR:O	1:A:207:VAL:HG22	2.19	0.42
1:B:269:GLY:O	1:B:270:ASN:CG	2.63	0.42
1:B:1501:ILE:CD1	1:B:1510:THR:HG23	2.49	0.42
1:E:674:VAL:CG1	1:E:692:MET:HE1	2.49	0.42
1:E:1757:PRO:O	1:E:1758:MET:C	2.63	0.42
1:E:2229:THR:CG2	1:A:2062:GLU:OE1	2.68	0.42
1:C:464:VAL:HG21	1:C:477:LYS:HE2	2.01	0.42
1:C:474:VAL:O	1:C:477:LYS:HE3	2.20	0.42
1:A:1331:MET:CG	1:A:1333:TYR:CE2	3.03	0.42
1:D:2191:GLU:OE1	1:D:2192:TRP:CD1	2.73	0.42
1:E:1177:ILE:HD12	1:E:1195:ARG:HH11	1.83	0.42
1:E:1682:THR:HG22	1:E:1683:ASP:N	2.35	0.42
1:C:700:LEU:HG	1:C:701:GLN:H	1.84	0.42
1:A:2478:ASP:OD2	1:A:2478:ASP:C	2.63	0.42
1:D:863:THR:OG1	1:D:864:PRO:HD2	2.19	0.41
1:E:895:SER:HA	1:E:898:VAL:HG22	2.02	0.41
1:A:485:MET:SD	1:A:492:ALA:HB2	2.60	0.41
1:A:1078:PHE:CZ	1:A:1775:THR:HG21	2.55	0.41
1:C:240:ASN:OD1	1:C:240:ASN:C	2.64	0.41
1:B:690:HIS:O	1:B:694:PRO:HD3	2.19	0.41
1:C:654:MET:HE1	1:C:764:MET:HB3	2.01	0.41
1:C:1757:PRO:O	1:C:1758:MET:C	2.64	0.41
1:B:1151:ILE:CG2	1:B:1153:PRO:HD3	2.48	0.41
1:B:2030:VAL:O	1:B:2034:THR:HG23	2.20	0.41
1:D:477:LYS:NZ	1:D:499:CYS:O	2.53	0.41
1:D:897:LEU:HD13	1:D:897:LEU:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1836:ASP:OD2	1:D:1836:ASP:O	2.38	0.41
1:E:192:PHE:O	1:E:192:PHE:CD1	2.74	0.41
1:C:919:ALA:O	1:C:923:THR:HG23	2.20	0.41
1:A:674:VAL:HG11	1:A:692:MET:CE	2.48	0.41
1:D:475:LEU:O	1:D:479:PHE:CD2	2.74	0.41
1:D:919:ALA:O	1:D:923:THR:HG23	2.21	0.41
1:C:269:GLY:O	1:C:270:ASN:CG	2.63	0.41
1:E:2454:MET:HA	1:E:2454:MET:HE2	2.03	0.41
1:C:711:VAL:HG21	1:C:763:GLU:HG3	2.01	0.41
1:C:1501:ILE:HD13	1:C:1510:THR:HG23	2.03	0.41
1:B:814:LEU:HD21	1:B:839:MET:HE1	2.02	0.41
1:C:906:MET:CE	1:C:908:GLU:HB2	2.49	0.41
1:A:690:HIS:O	1:A:694:PRO:CD	2.69	0.41
1:A:1333:TYR:O	1:A:1358:ARG:HB2	2.20	0.41
1:B:692:MET:HE1	1:B:730:PHE:HD2	1.85	0.41
1:B:1078:PHE:CZ	1:B:1775:THR:HG21	2.56	0.41
1:A:551:LEU:C	1:A:551:LEU:HD23	2.46	0.41
1:D:192:PHE:O	1:D:192:PHE:CD2	2.73	0.41
1:D:240:ASN:OD1	1:D:240:ASN:C	2.64	0.41
1:D:291:GLU:O	1:D:291:GLU:CD	2.64	0.41
1:D:755:TYR:O	1:D:759:LEU:HG	2.21	0.41
1:D:2161:THR:HG22	1:E:2128:VAL:HG13	2.03	0.41
1:E:1331:MET:SD	1:E:1333:TYR:CZ	3.14	0.41
1:E:1836:ASP:OD2	1:E:1839:ALA:HB3	2.21	0.41
1:C:188:MET:HG3	1:C:189:LEU:N	2.36	0.41
1:A:209:GLU:O	1:A:213:LEU:CD2	2.69	0.41
1:A:237:LEU:HA	1:A:240:ASN:ND2	2.36	0.41
1:A:919:ALA:O	1:A:923:THR:HG23	2.21	0.41
1:A:923:THR:HA	1:A:926:LEU:CD2	2.50	0.41
1:E:458:GLU:HA	1:E:461:VAL:HG12	2.03	0.41
1:B:278:MET:CE	1:B:1519:ILE:HD11	2.49	0.41
1:D:481:THR:O	1:D:485:MET:HG3	2.21	0.40
1:D:803:MET:HE1	1:D:871:TRP:CD1	2.56	0.40
1:D:1836:ASP:OD2	1:D:1839:ALA:HB3	2.21	0.40
1:C:112:MET:HE1	1:C:1039:TYR:CZ	2.56	0.40
1:A:159:LEU:HD13	1:A:164:LEU:HG	2.03	0.40
1:E:578:ILE:HG23	1:E:580:ASN:N	2.34	0.40
1:C:1655:HIS:HA	1:C:1711:PHE:CE2	2.56	0.40
1:A:755:TYR:O	1:A:759:LEU:HG	2.20	0.40
1:A:2476:ALA:C	1:A:2478:ASP:H	2.29	0.40
1:E:1048:THR:HG22	1:E:1778:LEU:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:HIS:O	1:B:694:PRO:CD	2.69	0.40
1:D:2085:LEU:HD23	1:D:2210:LEU:CD1	2.52	0.40
1:C:458:GLU:HA	1:C:461:VAL:HG12	2.02	0.40
1:C:2030:VAL:O	1:C:2034:THR:HG23	2.22	0.40
1:D:2030:VAL:O	1:D:2034:THR:HG23	2.21	0.40
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.30	0.40
1:A:2281:ARG:HD2	1:A:2287:ASP:HA	2.04	0.40
1:B:693:ALA:HB3	1:B:694:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2286/2535 (90%)	2219 (97%)	66 (3%)	1 (0%)	100	100
1	B	2286/2535 (90%)	2219 (97%)	66 (3%)	1 (0%)	100	100
1	C	2286/2535 (90%)	2217 (97%)	68 (3%)	1 (0%)	100	100
1	D	2286/2535 (90%)	2214 (97%)	71 (3%)	1 (0%)	100	100
1	E	2286/2535 (90%)	2215 (97%)	70 (3%)	1 (0%)	100	100
All	All	11430/12675 (90%)	11084 (97%)	341 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1668	VAL
1	E	1668	VAL
1	C	1668	VAL
1	A	1668	VAL
1	B	1668	VAL

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	1960/2173 (90%)	1944 (99%)	16 (1%)	73 85
1	B	1960/2173 (90%)	1946 (99%)	14 (1%)	76 87
1	C	1960/2173 (90%)	1948 (99%)	12 (1%)	78 89
1	D	1960/2173 (90%)	1945 (99%)	15 (1%)	73 85
1	E	1960/2173 (90%)	1945 (99%)	15 (1%)	73 85
All	All	9800/10865 (90%)	9728 (99%)	72 (1%)	73 87

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	159	LEU
1	D	176	GLU
1	D	192	PHE
1	D	211	ILE
1	D	341	MET
1	D	480	LEU
1	D	654	MET
1	D	922	LEU
1	D	968	TYR
1	D	1195	ARG
1	D	1328	TYR
1	D	1720	TRP
1	D	2195	GLN
1	D	2454	MET
1	D	2478	ASP
1	E	159	LEU
1	E	176	GLU
1	E	211	ILE
1	E	291	GLU
1	E	341	MET
1	E	448	ARG
1	E	480	LEU
1	E	725	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	846	LEU
1	E	897	LEU
1	E	968	TYR
1	E	1328	TYR
1	E	2454	MET
1	E	2478	ASP
1	E	2516	LYS
1	C	159	LEU
1	C	176	GLU
1	C	477	LYS
1	C	764	MET
1	C	922	LEU
1	C	929	GLN
1	C	968	TYR
1	C	1195	ARG
1	C	1720	TRP
1	C	1913	ILE
1	C	2195	GLN
1	C	2454	MET
1	A	159	LEU
1	A	176	GLU
1	A	211	ILE
1	A	240	ASN
1	A	480	LEU
1	A	839	MET
1	A	897	LEU
1	A	914	GLN
1	A	922	LEU
1	A	968	TYR
1	A	1328	TYR
1	A	1720	TRP
1	A	2029	MET
1	A	2076	GLU
1	A	2216	ARG
1	A	2454	MET
1	B	159	LEU
1	B	176	GLU
1	B	211	ILE
1	B	480	LEU
1	B	485	MET
1	B	839	MET
1	B	897	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	968	TYR
1	B	1177	ILE
1	B	1328	TYR
1	B	2206	ILE
1	B	2216	ARG
1	B	2408	LYS
1	B	2454	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	394	ASN
1	D	556	ASN
1	D	709	HIS
1	D	735	ASN
1	D	1292	GLN
1	D	1303	ASN
1	D	1361	HIS
1	D	1582	ASN
1	D	1671	ASN
1	D	1680	GLN
1	D	1870	GLN
1	D	2057	GLN
1	D	2237	GLN
1	D	2248	GLN
1	E	240	ASN
1	E	267	ASN
1	E	352	ASN
1	E	709	HIS
1	E	767	HIS
1	E	812	ASN
1	E	1102	ASN
1	E	1303	ASN
1	E	1376	ASN
1	E	1499	GLN
1	E	1633	GLN
1	E	1671	ASN
1	E	1680	GLN
1	E	1870	GLN
1	E	2057	GLN
1	E	2237	GLN
1	E	2248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	352	ASN
1	C	394	ASN
1	C	527	GLN
1	C	676	HIS
1	C	709	HIS
1	C	929	GLN
1	C	1303	ASN
1	C	1499	GLN
1	C	1533	ASN
1	C	1631	ASN
1	C	1633	GLN
1	C	1671	ASN
1	C	1870	GLN
1	C	1961	GLN
1	C	2032	GLN
1	C	2057	GLN
1	C	2237	GLN
1	C	2248	GLN
1	C	2348	ASN
1	C	2452	HIS
1	C	2461	GLN
1	C	2510	HIS
1	A	312	GLN
1	A	352	ASN
1	A	709	HIS
1	A	1303	ASN
1	A	1341	ASN
1	A	1499	GLN
1	A	1655	HIS
1	A	1671	ASN
1	A	1680	GLN
1	A	1810	GLN
1	A	1870	GLN
1	A	2237	GLN
1	A	2248	GLN
1	A	2461	GLN
1	A	2510	HIS
1	B	644	GLN
1	B	735	ASN
1	B	1303	ASN
1	B	1376	ASN
1	B	1533	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1631	ASN
1	B	1633	GLN
1	B	1671	ASN
1	B	1680	GLN
1	B	1810	GLN
1	B	1870	GLN
1	B	2057	GLN
1	B	2248	GLN
1	B	2414	GLN
1	B	2497	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.

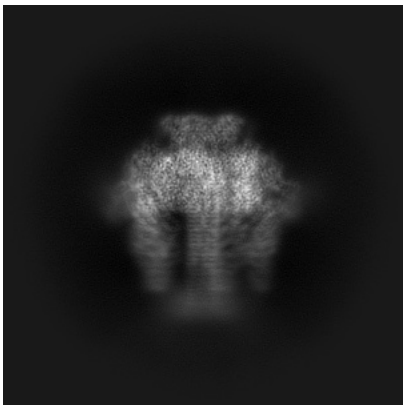
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58628. These allow visual inspection of the internal detail of the map and identification of artifacts.

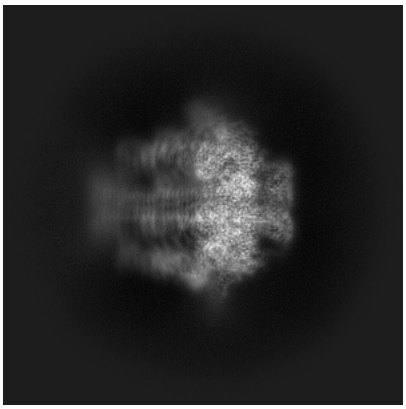
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

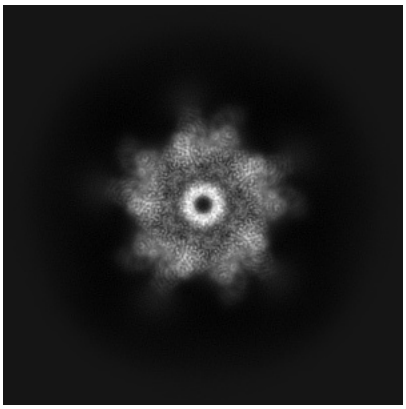
6.1.1 Primary map



X

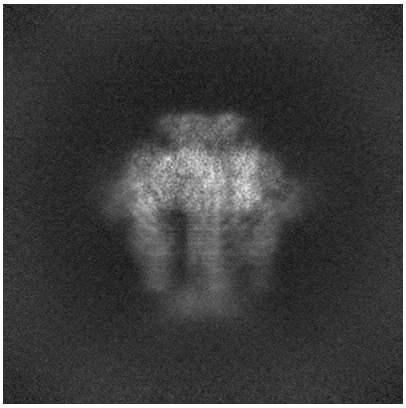


Y

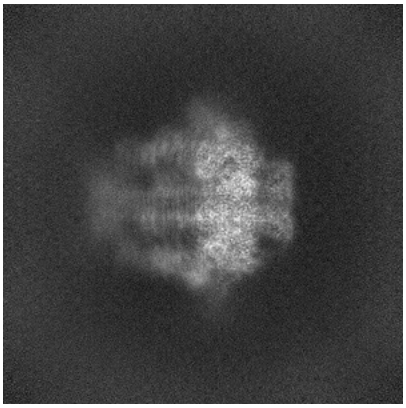


Z

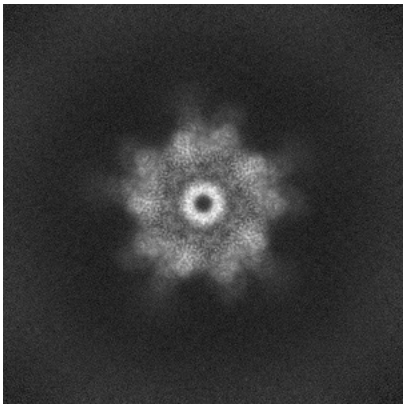
6.1.2 Raw map



X



Y



Z

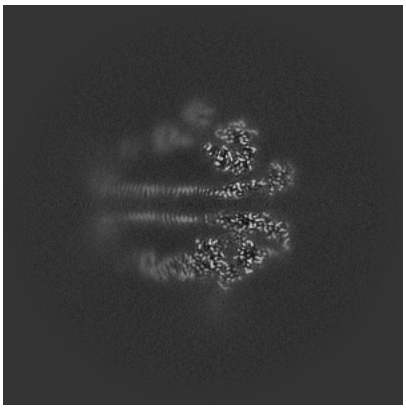
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

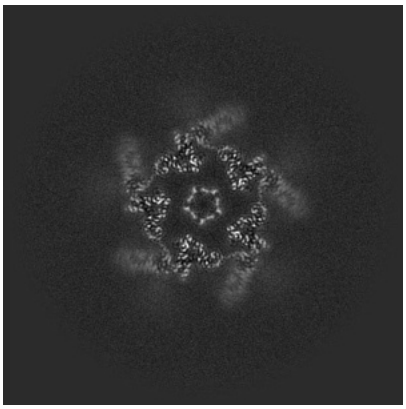
6.2.1 Primary map



X Index: 320



Y Index: 320

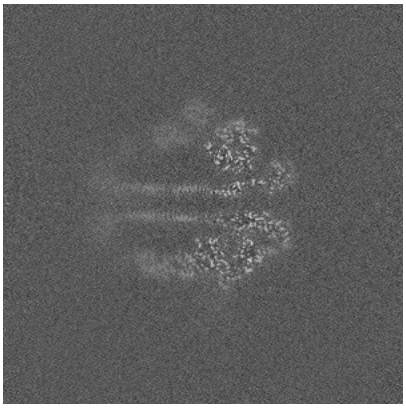


Z Index: 320

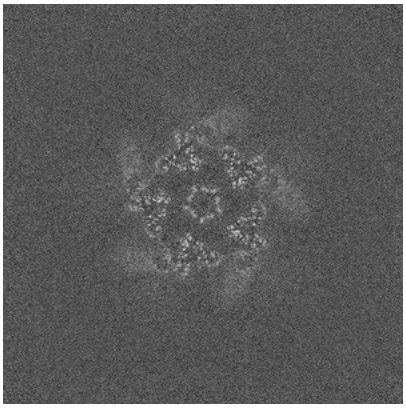
6.2.2 Raw map



X Index: 320



Y Index: 320

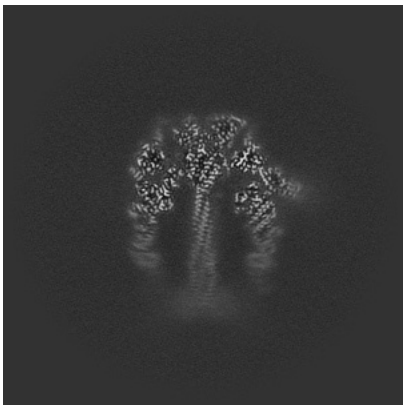


Z Index: 320

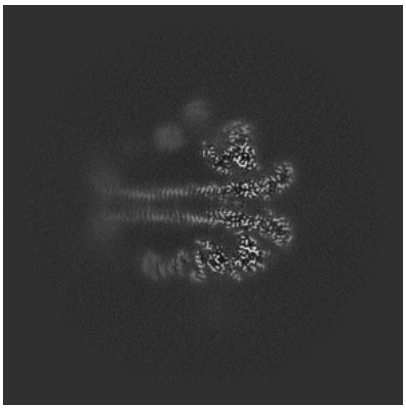
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

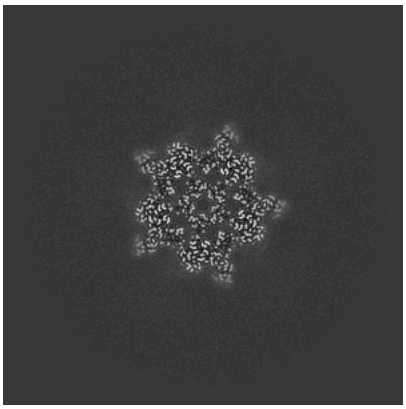
6.3.1 Primary map



X Index: 295

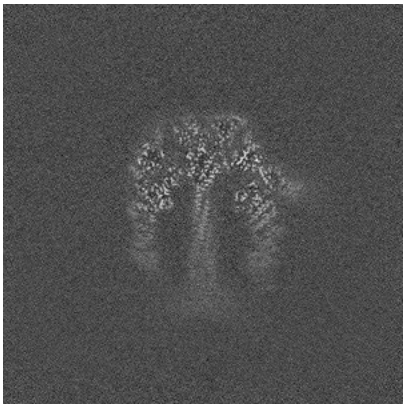


Y Index: 310

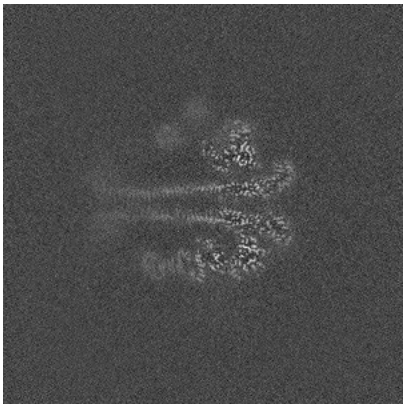


Z Index: 386

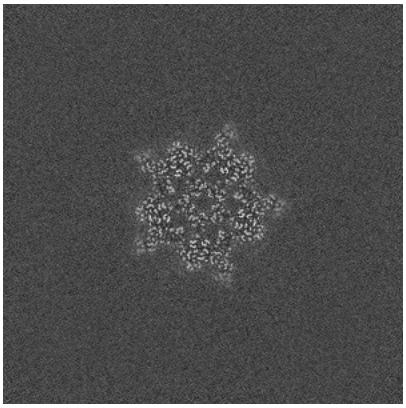
6.3.2 Raw map



X Index: 295



Y Index: 311

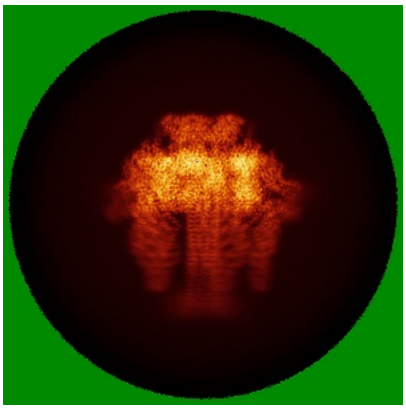


Z Index: 386

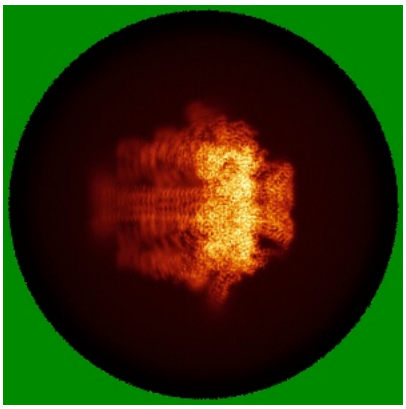
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

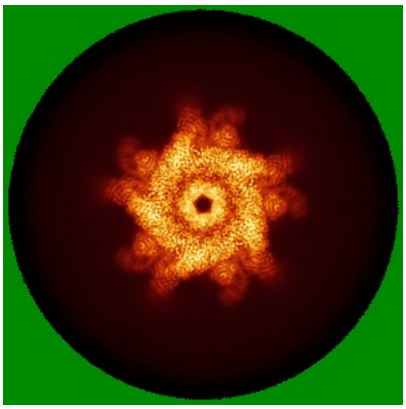
6.4.1 Primary map



X

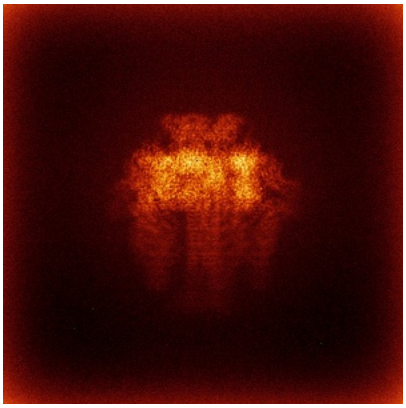


Y

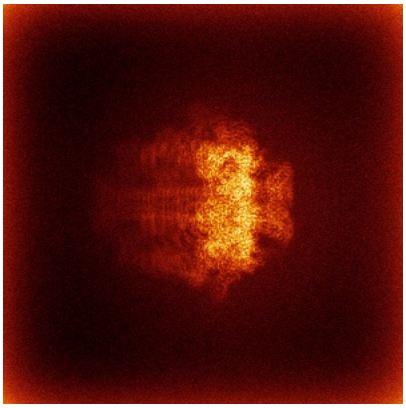


Z

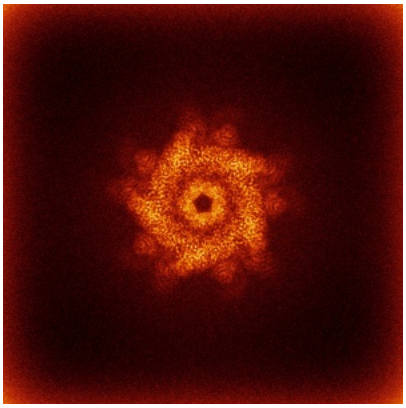
6.4.2 Raw map



X



Y

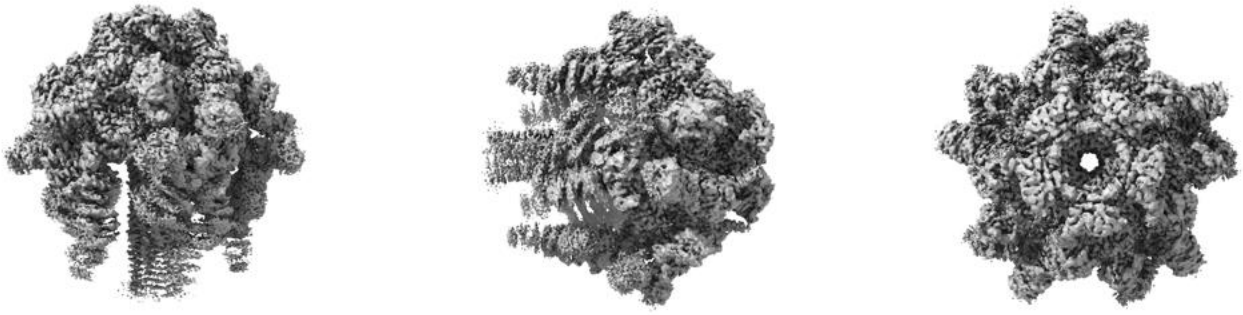


Z

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)

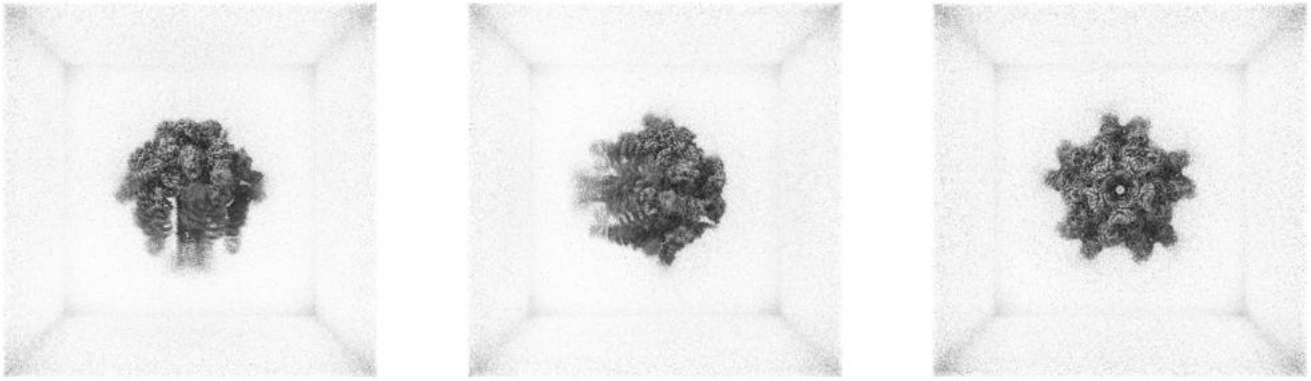
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0262. 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.

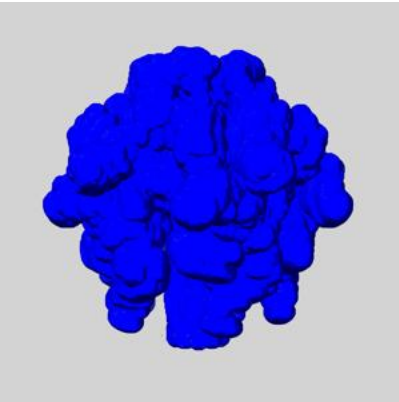
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

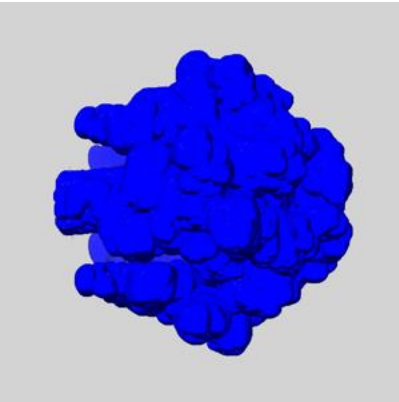
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

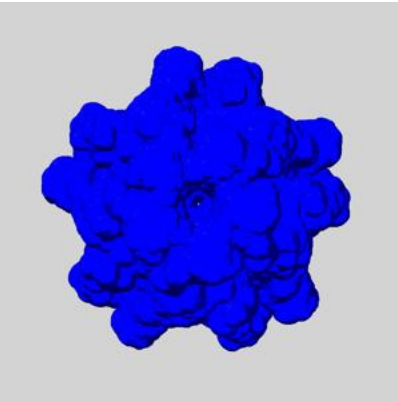
6.6.1 emd_58628_msk_1.map (i)



X



Y

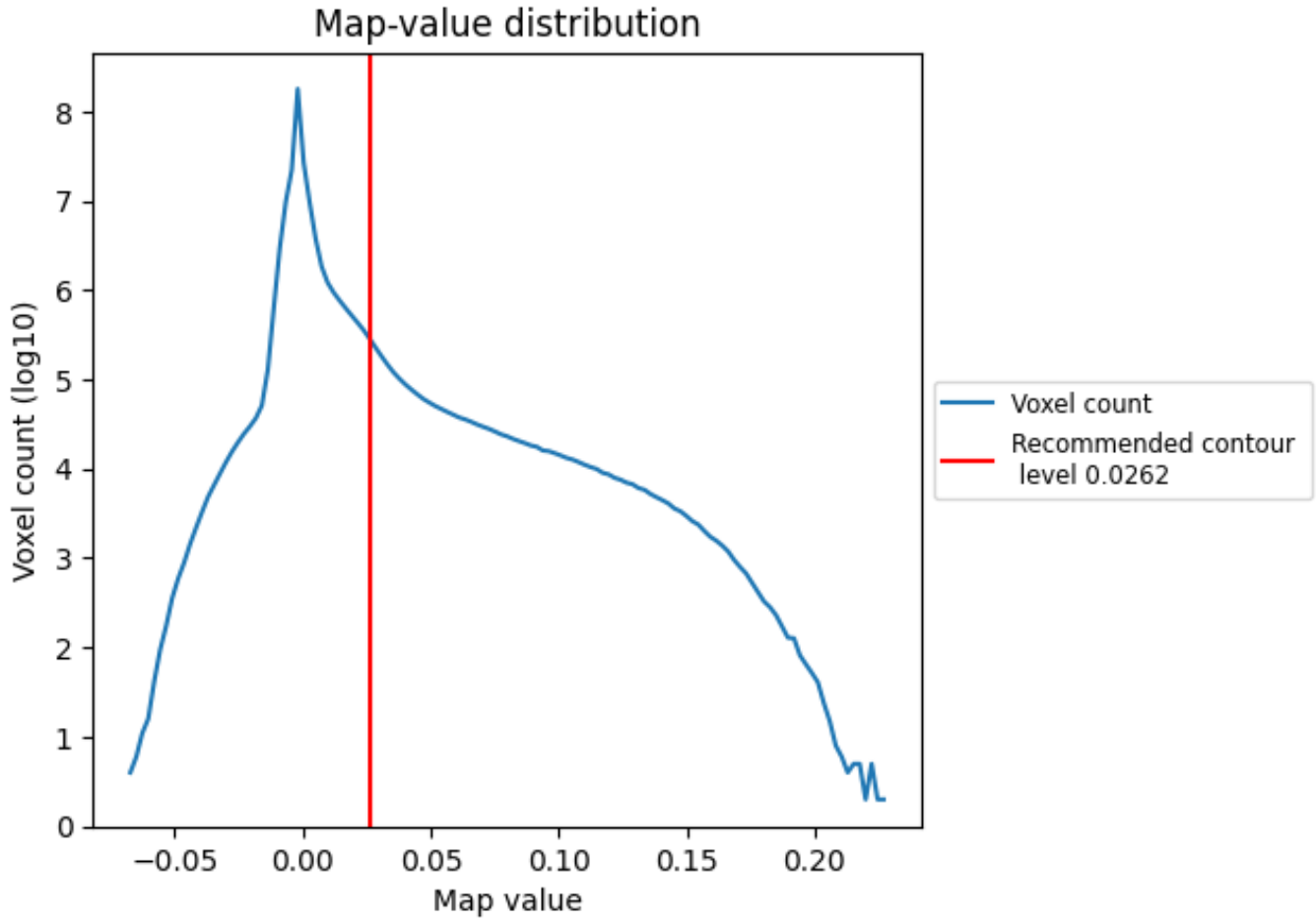


Z

7 Map analysis

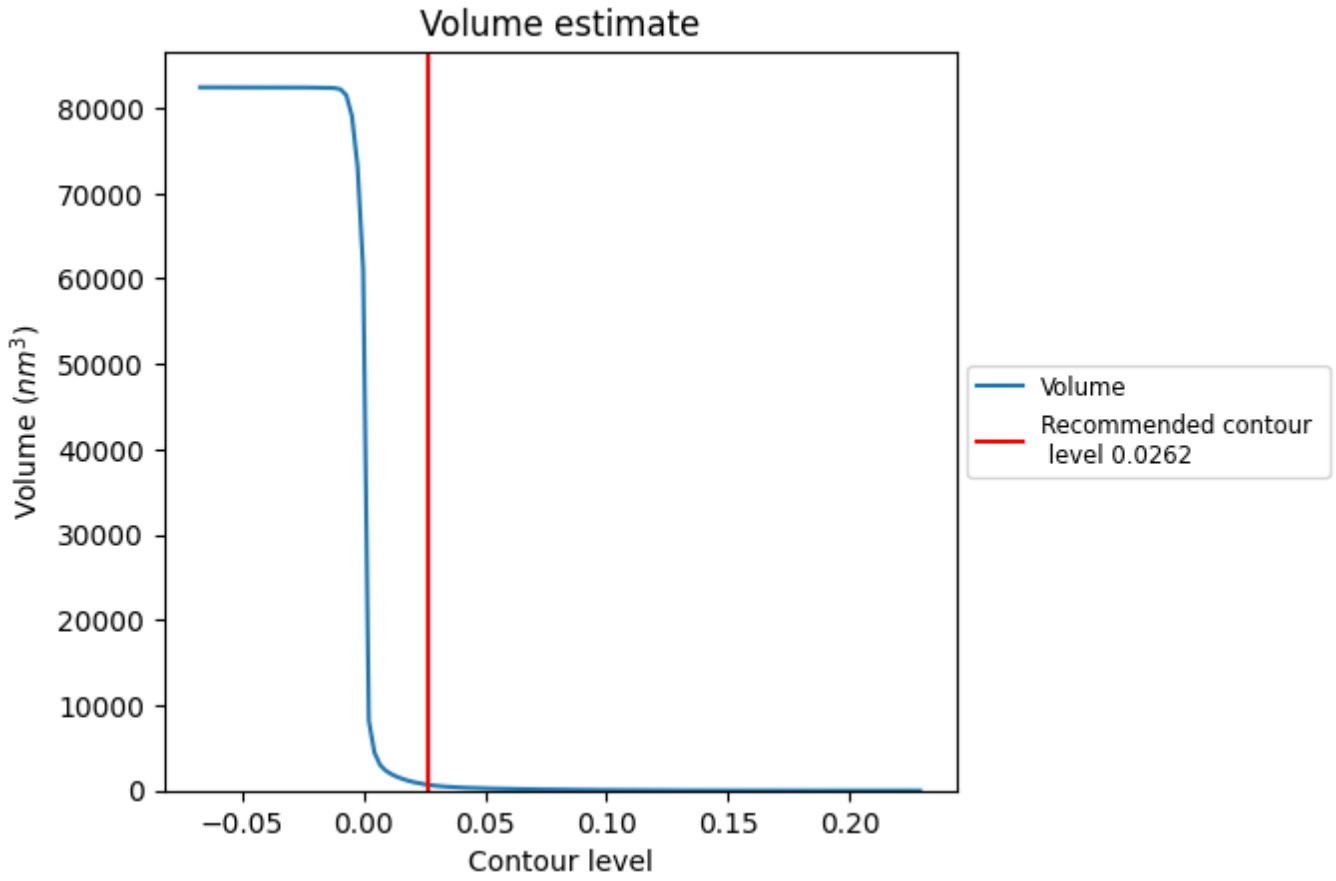
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

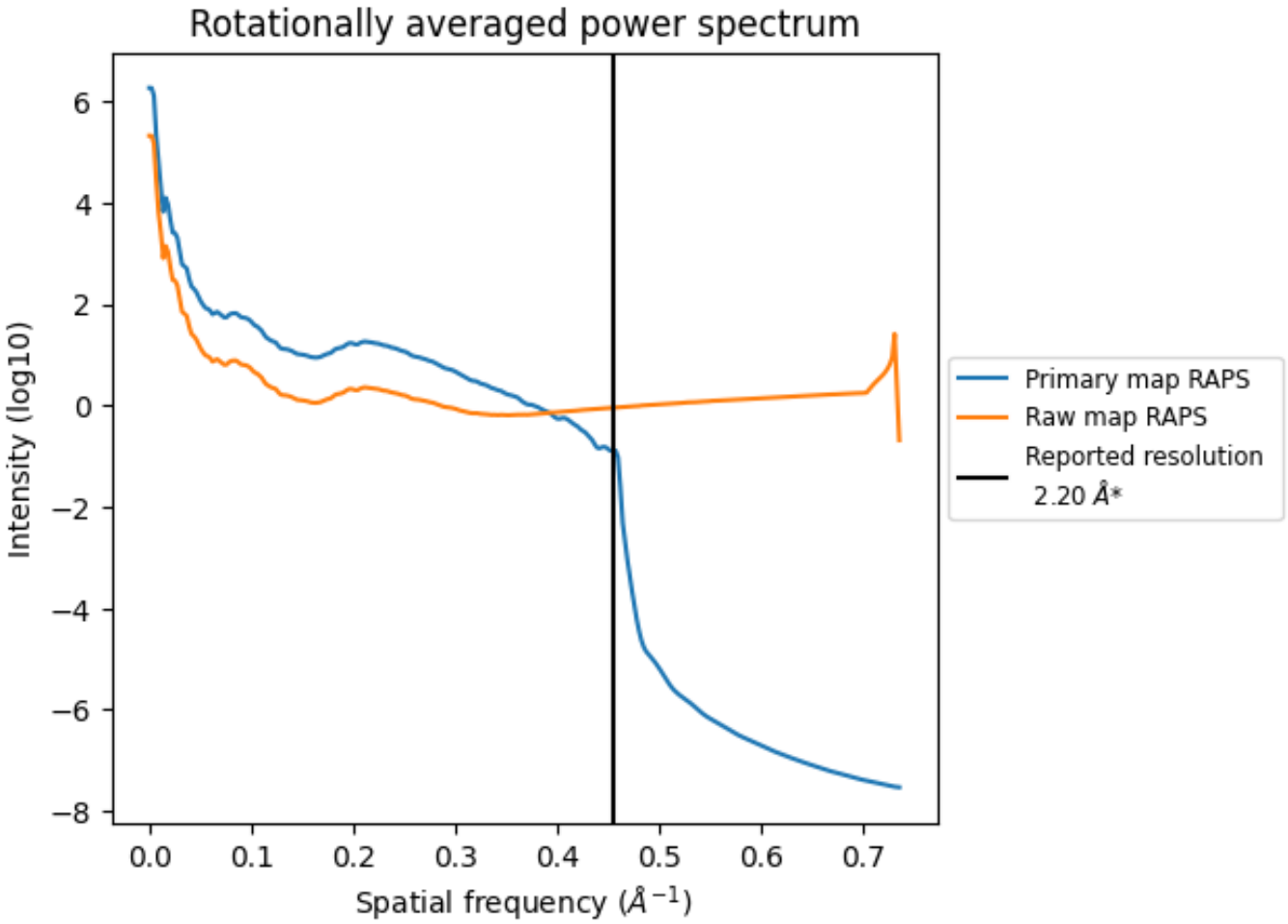
7.2 Volume estimate



The volume at the recommended contour level is 687 nm^3; this corresponds to an approximate mass of 621 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 (i)

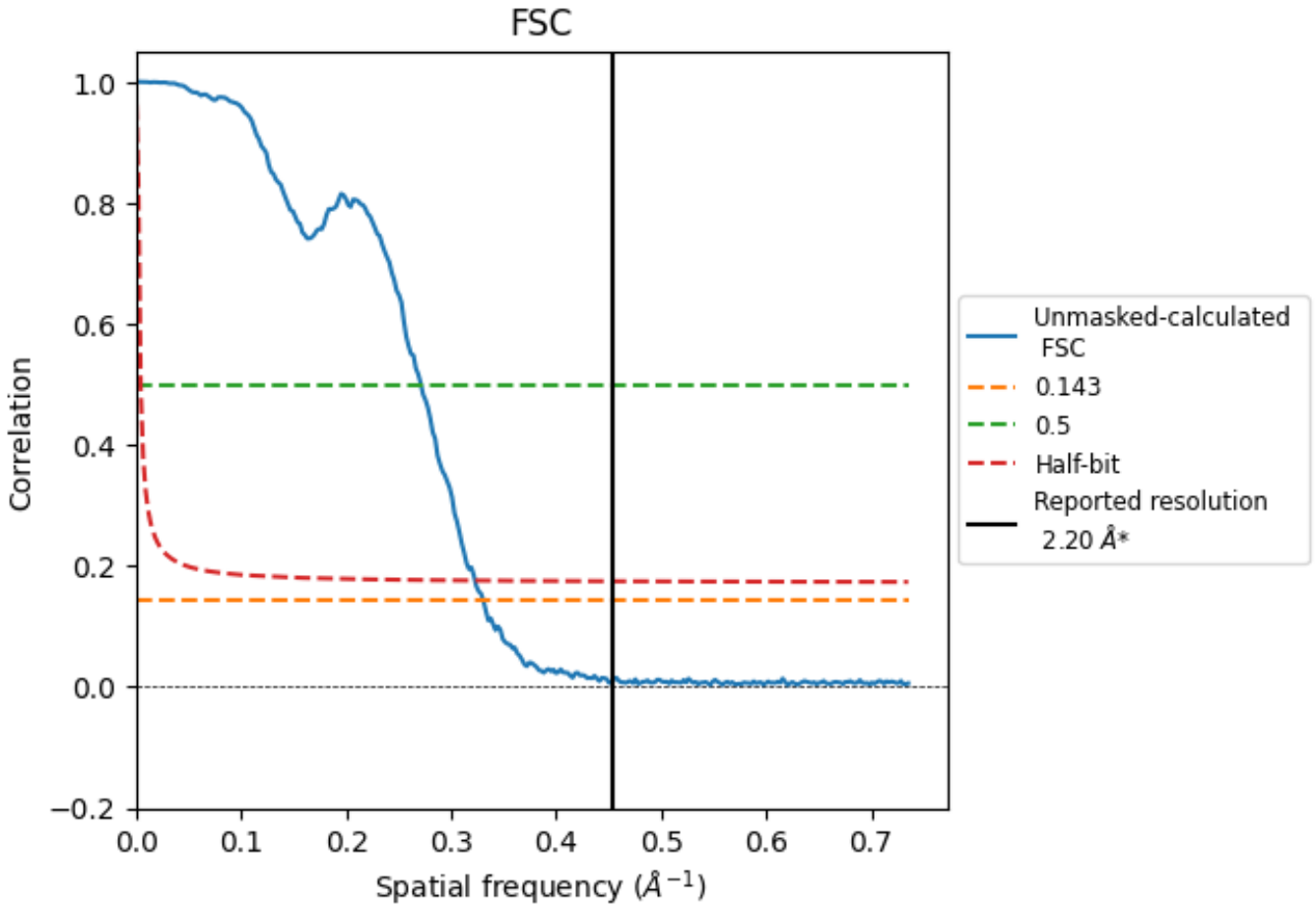


*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8.2 Resolution estimates (i)

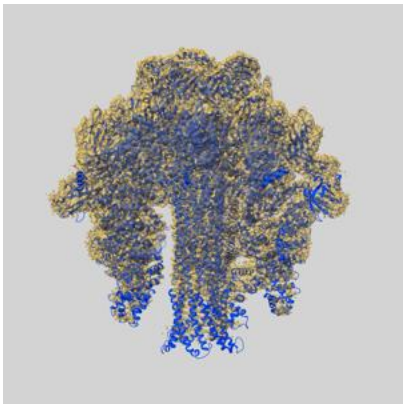
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.68	3.10

*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 3.02 differs from the reported value 2.2 by more than 10 %

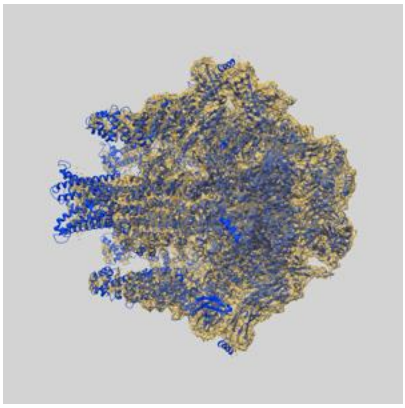
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58628 and PDB model 31QH. Per-residue inclusion information can be found in section 3 on page 29.

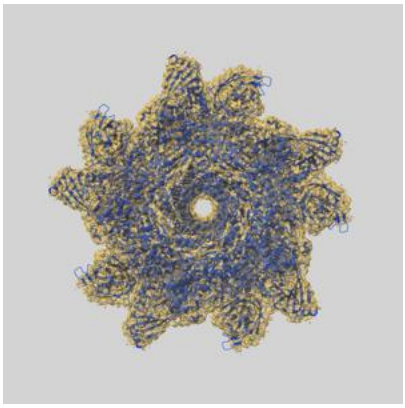
9.1 Map-model overlay



X



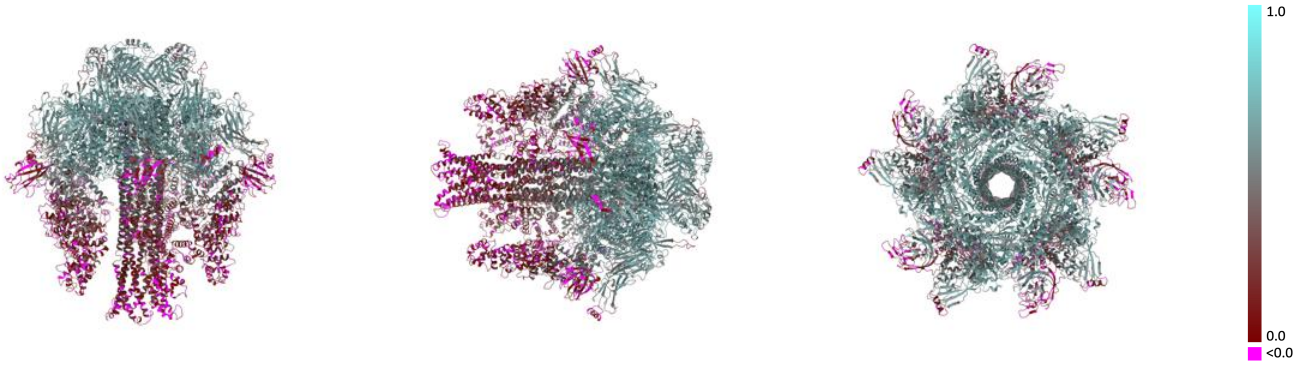
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0262 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.

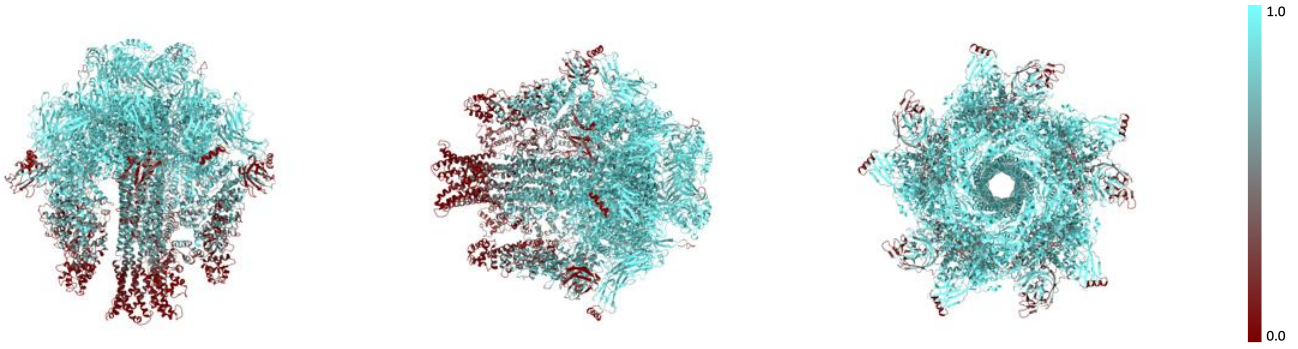
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

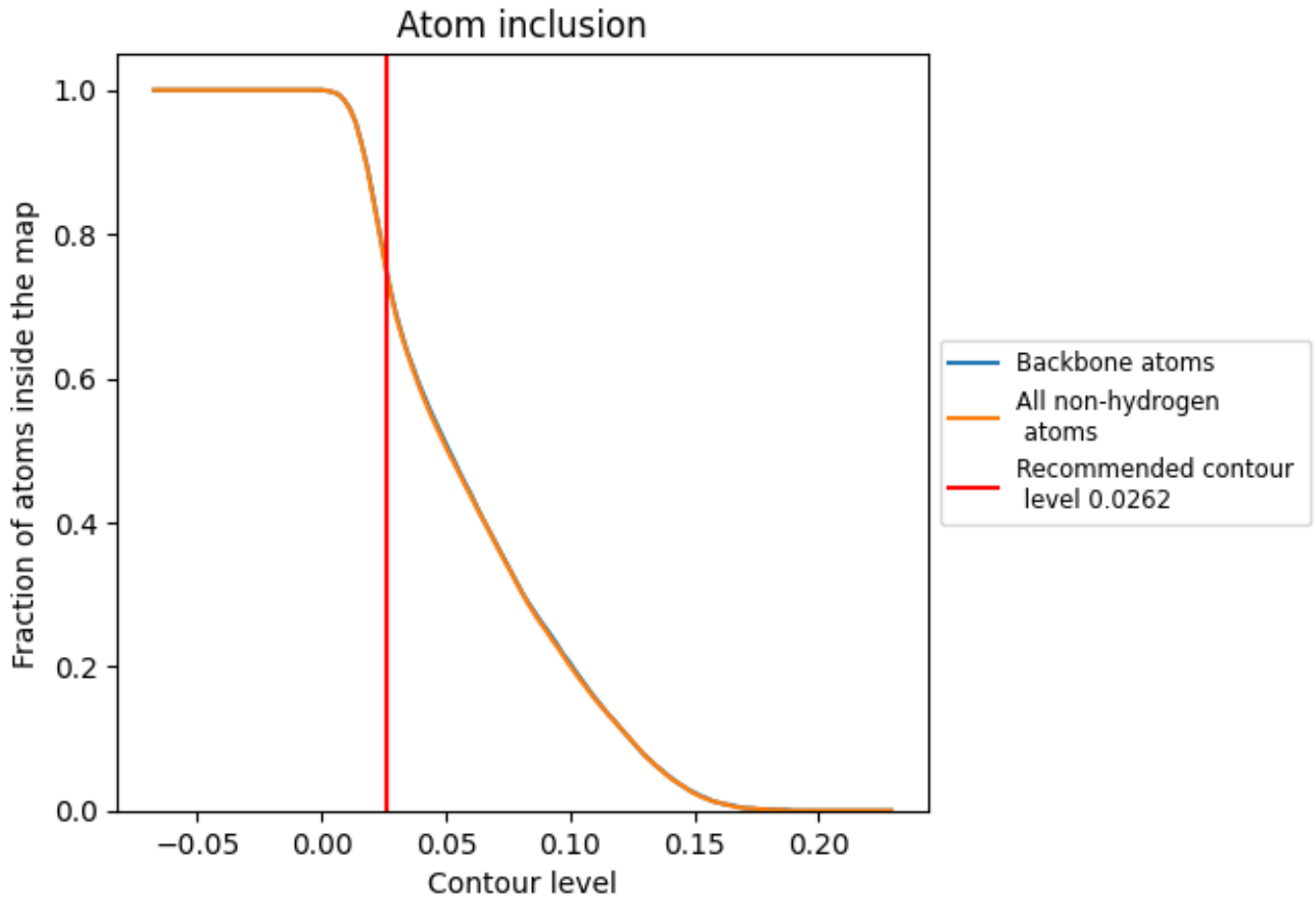
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0262).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.0262) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7450	0.4380
A	0.7480	0.4380
B	0.7510	0.4400
C	0.7460	0.4360
D	0.7440	0.4380
E	0.7500	0.4400