wwPDB EM Validation Summary Report

Jul 20, 2023 – 10:36 am BST

PDB ID	:	6TGC
EMDB ID	:	EMD-10498
Title	:	CryoEM structure of the ternary DOCK2-ELMO1-RAC1 complex.
Authors	:	Chang, L.; Yang, J.; Chang, J.H.; Zhang, Z.; Boland, A.; McLaughlin, S.H.; Abu-Thuraia, A.; Killoran, R.C.; Smith, M.J.; Cote, J.F.; Barford, D.
Deposited on	:	2019-11-15
Resolution	:	4.10 Å(reported)

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

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

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

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

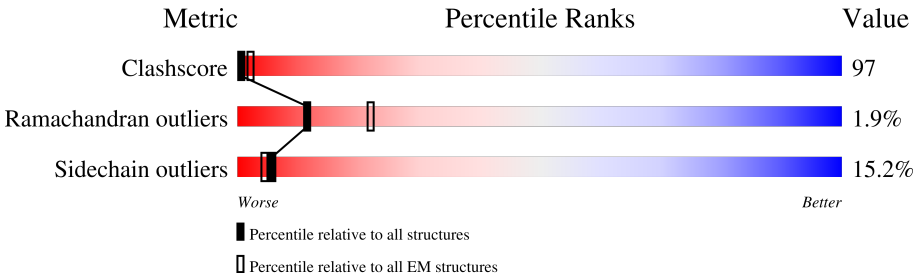
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1830	62% 20% 46% 12% • 21%
1	D	1830	16% 20% 46% 12% • 21%
2	B	727	94% 57% 36% 6%
2	E	727	78% 42% 46% 5% 6%
3	C	192	45% 8% 69% 14% • 8%
3	F	192	45% 8% 67% 15% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33282 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dedicator of cytokinesis protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1450	Total	C	N	O	S	0	0
			10203	6463	1792	1894	54		
1	D	1450	Total	C	N	O	S	0	0
			10203	6463	1792	1894	54		

There are 1048 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207A	UNK	ASP	conflict	UNP Q92608
A	207B	UNK	TYR	conflict	UNP Q92608
A	207C	UNK	ALA	conflict	UNP Q92608
A	207D	UNK	MET	conflict	UNP Q92608
A	207E	UNK	TYR	conflict	UNP Q92608
A	207F	UNK	SER	conflict	UNP Q92608
A	207G	UNK	ARG	conflict	UNP Q92608
A	207H	UNK	ILE	conflict	UNP Q92608
A	207I	UNK	SER	conflict	UNP Q92608
A	207J	UNK	SER	conflict	UNP Q92608
A	207K	UNK	SER	conflict	UNP Q92608
A	207L	UNK	PRO	conflict	UNP Q92608
A	207M	UNK	THR	conflict	UNP Q92608
A	207N	UNK	HIS	conflict	UNP Q92608
A	207O	UNK	SER	conflict	UNP Q92608
A	207P	UNK	LEU	conflict	UNP Q92608
A	207Q	UNK	TYR	conflict	UNP Q92608
A	207R	UNK	VAL	conflict	UNP Q92608
A	207S	UNK	PHE	conflict	UNP Q92608
A	207T	UNK	VAL	conflict	UNP Q92608
A	207U	UNK	ARG	conflict	UNP Q92608
A	207V	UNK	ASN	conflict	UNP Q92608
A	207W	UNK	PHE	conflict	UNP Q92608
A	207X	UNK	VAL	conflict	UNP Q92608
A	207Y	UNK	CYS	conflict	UNP Q92608
A	207Z	UNK	ARG	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	208A	UNK	ILE	conflict	UNP Q92608
A	208B	UNK	GLY	conflict	UNP Q92608
A	208C	UNK	GLU	conflict	UNP Q92608
A	208D	UNK	ASP	conflict	UNP Q92608
A	208E	UNK	ALA	conflict	UNP Q92608
A	208F	UNK	GLU	conflict	UNP Q92608
A	208G	UNK	LEU	conflict	UNP Q92608
A	208H	UNK	PHE	conflict	UNP Q92608
A	208I	UNK	MET	conflict	UNP Q92608
A	208J	UNK	SER	conflict	UNP Q92608
A	208K	UNK	LEU	conflict	UNP Q92608
A	208L	UNK	TYR	conflict	UNP Q92608
A	208M	UNK	ASP	conflict	UNP Q92608
A	208N	UNK	PRO	conflict	UNP Q92608
A	208O	UNK	ASN	conflict	UNP Q92608
A	208P	UNK	LYS	conflict	UNP Q92608
A	208Q	UNK	GLN	conflict	UNP Q92608
A	208R	UNK	THR	conflict	UNP Q92608
A	208S	UNK	VAL	conflict	UNP Q92608
A	208T	UNK	ILE	conflict	UNP Q92608
A	208U	UNK	SER	conflict	UNP Q92608
A	208V	UNK	GLU	conflict	UNP Q92608
A	208W	UNK	ASN	conflict	UNP Q92608
A	208X	UNK	TYR	conflict	UNP Q92608
A	208Y	UNK	LEU	conflict	UNP Q92608
A	208Z	UNK	VAL	conflict	UNP Q92608
A	209A	UNK	ARG	conflict	UNP Q92608
A	209B	UNK	TRP	conflict	UNP Q92608
A	209C	UNK	GLY	conflict	UNP Q92608
A	209D	UNK	SER	conflict	UNP Q92608
A	209E	UNK	ARG	conflict	UNP Q92608
A	209F	UNK	GLY	conflict	UNP Q92608
A	209G	UNK	PHE	conflict	UNP Q92608
A	209H	UNK	PRO	conflict	UNP Q92608
A	209I	UNK	LYS	conflict	UNP Q92608
A	209J	UNK	GLU	conflict	UNP Q92608
A	209K	UNK	ILE	conflict	UNP Q92608
A	209L	UNK	GLU	conflict	UNP Q92608
A	209M	UNK	MET	conflict	UNP Q92608
A	209N	UNK	LEU	conflict	UNP Q92608
A	209O	UNK	ASN	conflict	UNP Q92608
A	209P	UNK	ASN	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	209Q	UNK	LEU	conflict	UNP Q92608
A	209R	UNK	LYS	conflict	UNP Q92608
A	209S	UNK	VAL	conflict	UNP Q92608
A	219	UNK	VAL	conflict	UNP Q92608
A	220	UNK	PHE	conflict	UNP Q92608
A	221	UNK	THR	conflict	UNP Q92608
A	222	UNK	ASP	conflict	UNP Q92608
A	223	UNK	LEU	conflict	UNP Q92608
A	224	UNK	GLY	conflict	UNP Q92608
A	225	UNK	ASN	conflict	UNP Q92608
A	226	UNK	LYS	conflict	UNP Q92608
A	227	UNK	ASP	conflict	UNP Q92608
A	228	UNK	LEU	conflict	UNP Q92608
A	229	UNK	ASN	conflict	UNP Q92608
A	230	UNK	ARG	conflict	UNP Q92608
A	231	UNK	ASP	conflict	UNP Q92608
A	232	UNK	LYS	conflict	UNP Q92608
A	233	UNK	ILE	conflict	UNP Q92608
A	234	UNK	TYR	conflict	UNP Q92608
A	235	UNK	LEU	conflict	UNP Q92608
A	236	UNK	ILE	conflict	UNP Q92608
A	237	UNK	CYS	conflict	UNP Q92608
A	238	UNK	GLN	conflict	UNP Q92608
A	239	UNK	ILE	conflict	UNP Q92608
A	240	UNK	VAL	conflict	UNP Q92608
A	241	UNK	ARG	conflict	UNP Q92608
A	242	UNK	VAL	conflict	UNP Q92608
A	243	UNK	GLY	conflict	UNP Q92608
A	244	UNK	LYS	conflict	UNP Q92608
A	245	UNK	MET	conflict	UNP Q92608
A	246	UNK	ASP	conflict	UNP Q92608
A	247	UNK	LEU	conflict	UNP Q92608
A	248	UNK	LYS	conflict	UNP Q92608
A	249	UNK	ASP	conflict	UNP Q92608
A	250	UNK	THR	conflict	UNP Q92608
A	251	UNK	GLY	conflict	UNP Q92608
A	252	UNK	ALA	conflict	UNP Q92608
A	253	UNK	LYS	conflict	UNP Q92608
A	254	UNK	LYS	conflict	UNP Q92608
A	255	UNK	CYS	conflict	UNP Q92608
A	256	UNK	THR	conflict	UNP Q92608
A	257	UNK	GLN	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	258	UNK	GLY	conflict	UNP Q92608
A	259	UNK	LEU	conflict	UNP Q92608
A	260	UNK	ARG	conflict	UNP Q92608
A	261	UNK	ARG	conflict	UNP Q92608
A	262	UNK	PRO	conflict	UNP Q92608
A	263	UNK	PHE	conflict	UNP Q92608
A	264	UNK	GLY	conflict	UNP Q92608
A	265	UNK	VAL	conflict	UNP Q92608
A	266	UNK	ALA	conflict	UNP Q92608
A	267	UNK	VAL	conflict	UNP Q92608
A	268	UNK	MET	conflict	UNP Q92608
A	269	UNK	ASP	conflict	UNP Q92608
A	270	UNK	ILE	conflict	UNP Q92608
A	271	UNK	THR	conflict	UNP Q92608
A	272	UNK	ASP	conflict	UNP Q92608
A	273	UNK	ILE	conflict	UNP Q92608
A	274	UNK	ILE	conflict	UNP Q92608
A	275	UNK	LYS	conflict	UNP Q92608
A	276	UNK	GLY	conflict	UNP Q92608
A	277	UNK	LYS	conflict	UNP Q92608
A	278	UNK	ALA	conflict	UNP Q92608
A	279	UNK	GLU	conflict	UNP Q92608
A	280	UNK	SER	conflict	UNP Q92608
A	281	UNK	ASP	conflict	UNP Q92608
A	282	UNK	GLU	conflict	UNP Q92608
A	283	UNK	GLU	conflict	UNP Q92608
A	284	UNK	LYS	conflict	UNP Q92608
A	285	UNK	GLN	conflict	UNP Q92608
A	286	UNK	HIS	conflict	UNP Q92608
A	287	UNK	PHE	conflict	UNP Q92608
A	288	UNK	ILE	conflict	UNP Q92608
A	289	UNK	PRO	conflict	UNP Q92608
A	290	UNK	PHE	conflict	UNP Q92608
A	291	UNK	HIS	conflict	UNP Q92608
A	292	UNK	PRO	conflict	UNP Q92608
A	293	UNK	VAL	conflict	UNP Q92608
A	294	UNK	THR	conflict	UNP Q92608
A	295	UNK	ALA	conflict	UNP Q92608
A	296	UNK	GLU	conflict	UNP Q92608
A	297	UNK	ASN	conflict	UNP Q92608
A	298	UNK	ASP	conflict	UNP Q92608
A	299	UNK	PHE	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	300	UNK	LEU	conflict	UNP Q92608
A	301	UNK	HIS	conflict	UNP Q92608
A	302	UNK	SER	conflict	UNP Q92608
A	303	UNK	LEU	conflict	UNP Q92608
A	304	UNK	LEU	conflict	UNP Q92608
A	318	UNK	GLY	conflict	UNP Q92608
A	319	UNK	LYS	conflict	UNP Q92608
A	320	UNK	VAL	conflict	UNP Q92608
A	321	UNK	ILE	conflict	UNP Q92608
A	322	UNK	ALA	conflict	UNP Q92608
A	323	UNK	SER	conflict	UNP Q92608
A	324	UNK	LYS	conflict	UNP Q92608
A	325	UNK	GLY	conflict	UNP Q92608
A	326	UNK	ASP	conflict	UNP Q92608
A	327	UNK	SER	conflict	UNP Q92608
A	328	UNK	GLY	conflict	UNP Q92608
A	329	UNK	GLY	conflict	UNP Q92608
A	330	UNK	GLN	conflict	UNP Q92608
A	331	UNK	GLY	conflict	UNP Q92608
A	332	UNK	LEU	conflict	UNP Q92608
A	333	UNK	TRP	conflict	UNP Q92608
A	334	UNK	VAL	conflict	UNP Q92608
A	335	UNK	THR	conflict	UNP Q92608
A	336	UNK	MET	conflict	UNP Q92608
A	337	UNK	LYS	conflict	UNP Q92608
A	338	UNK	MET	conflict	UNP Q92608
A	339	UNK	LEU	conflict	UNP Q92608
A	340	UNK	VAL	conflict	UNP Q92608
A	341	UNK	GLY	conflict	UNP Q92608
A	342	UNK	ASP	conflict	UNP Q92608
A	343	UNK	ILE	conflict	UNP Q92608
A	344	UNK	ILE	conflict	UNP Q92608
A	345	UNK	GLN	conflict	UNP Q92608
A	346	UNK	ILE	conflict	UNP Q92608
A	347	UNK	ARG	conflict	UNP Q92608
A	348	UNK	LYS	conflict	UNP Q92608
A	349	UNK	ASP	conflict	UNP Q92608
A	350	UNK	TYR	conflict	UNP Q92608
A	351	UNK	PRO	conflict	UNP Q92608
A	377	UNK	HIS	conflict	UNP Q92608
A	378	UNK	LEU	conflict	UNP Q92608
A	379	UNK	VAL	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	380	UNK	ASP	conflict	UNP Q92608
A	381	UNK	ARG	conflict	UNP Q92608
A	382	UNK	THR	conflict	UNP Q92608
A	383	UNK	THR	conflict	UNP Q92608
A	384	UNK	VAL	conflict	UNP Q92608
A	385	UNK	VAL	conflict	UNP Q92608
A	386	UNK	ALA	conflict	UNP Q92608
A	387	UNK	ARG	conflict	UNP Q92608
A	388	UNK	LYS	conflict	UNP Q92608
A	389	UNK	LEU	conflict	UNP Q92608
A	609A	UNK	LYS	conflict	UNP Q92608
A	609B	UNK	LEU	conflict	UNP Q92608
A	609C	UNK	THR	conflict	UNP Q92608
A	609D	UNK	GLN	conflict	UNP Q92608
A	609E	UNK	ASN	conflict	UNP Q92608
A	609F	UNK	VAL	conflict	UNP Q92608
A	609G	UNK	GLY	conflict	UNP Q92608
A	609H	UNK	LEU	conflict	UNP Q92608
A	609I	UNK	LEU	conflict	UNP Q92608
A	609J	UNK	GLY	conflict	UNP Q92608
A	609K	UNK	LEU	conflict	UNP Q92608
A	609L	UNK	LEU	conflict	UNP Q92608
A	609M	UNK	LYS	conflict	UNP Q92608
A	609N	UNK	TRP	conflict	UNP Q92608
A	609O	UNK	ARG	conflict	UNP Q92608
A	609P	UNK	MET	conflict	UNP Q92608
A	609Q	UNK	LYS	conflict	UNP Q92608
A	609R	UNK	PRO	conflict	UNP Q92608
A	609S	UNK	GLN	conflict	UNP Q92608
A	609T	UNK	LEU	conflict	UNP Q92608
A	609U	UNK	LEU	conflict	UNP Q92608
A	609V	UNK	GLN	conflict	UNP Q92608
A	609W	UNK	GLU	conflict	UNP Q92608
A	609X	UNK	ASN	conflict	UNP Q92608
A	609Y	UNK	LEU	conflict	UNP Q92608
A	609Z	UNK	GLU	conflict	UNP Q92608
A	610A	UNK	LYS	conflict	UNP Q92608
A	610B	UNK	LEU	conflict	UNP Q92608
A	610C	UNK	LYS	conflict	UNP Q92608
A	610D	UNK	ILE	conflict	UNP Q92608
A	610E	UNK	VAL	conflict	UNP Q92608
A	610F	UNK	ASP	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	626	UNK	GLY	conflict	UNP Q92608
A	627	UNK	GLU	conflict	UNP Q92608
A	628	UNK	GLU	conflict	UNP Q92608
A	629	UNK	VAL	conflict	UNP Q92608
A	630	UNK	VAL	conflict	UNP Q92608
A	631	UNK	LYS	conflict	UNP Q92608
A	632	UNK	PHE	conflict	UNP Q92608
A	633	UNK	LEU	conflict	UNP Q92608
A	634	UNK	GLN	conflict	UNP Q92608
A	635	UNK	ASP	conflict	UNP Q92608
A	636	UNK	THR	conflict	UNP Q92608
A	637	UNK	LEU	conflict	UNP Q92608
A	638	UNK	ASP	conflict	UNP Q92608
A	639	UNK	ALA	conflict	UNP Q92608
A	640	UNK	LEU	conflict	UNP Q92608
A	641	UNK	PHE	conflict	UNP Q92608
A	642	UNK	ASN	conflict	UNP Q92608
A	679A	UNK	HIS	conflict	UNP Q92608
A	679B	UNK	PHE	conflict	UNP Q92608
A	679C	UNK	ASN	conflict	UNP Q92608
A	679D	UNK	THR	conflict	UNP Q92608
A	679E	UNK	VAL	conflict	UNP Q92608
A	679F	UNK	LEU	conflict	UNP Q92608
A	679G	UNK	GLU	conflict	UNP Q92608
A	679H	UNK	ALA	conflict	UNP Q92608
A	679I	UNK	TYR	conflict	UNP Q92608
A	679J	UNK	ILE	conflict	UNP Q92608
A	679K	UNK	GLN	conflict	UNP Q92608
A	679L	UNK	GLN	conflict	UNP Q92608
A	679M	UNK	HIS	conflict	UNP Q92608
A	679N	UNK	PHE	conflict	UNP Q92608
A	679O	UNK	SER	conflict	UNP Q92608
A	679P	UNK	ALA	conflict	UNP Q92608
A	679Q	UNK	THR	conflict	UNP Q92608
A	688	UNK	LEU	conflict	UNP Q92608
A	689	UNK	ALA	conflict	UNP Q92608
A	690	UNK	TYR	conflict	UNP Q92608
A	691	UNK	LYS	conflict	UNP Q92608
A	692	UNK	LYS	conflict	UNP Q92608
A	693	UNK	LEU	conflict	UNP Q92608
A	694	UNK	MET	conflict	UNP Q92608
A	695	UNK	THR	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	696	UNK	VAL	conflict	UNP Q92608
A	697	UNK	LEU	conflict	UNP Q92608
A	698	UNK	LYS	conflict	UNP Q92608
A	699	UNK	THR	conflict	UNP Q92608
A	700	UNK	TYR	conflict	UNP Q92608
A	701	UNK	LEU	conflict	UNP Q92608
A	702	UNK	ASP	conflict	UNP Q92608
A	703	UNK	THR	conflict	UNP Q92608
A	704	UNK	SER	conflict	UNP Q92608
A	705	UNK	SER	conflict	UNP Q92608
A	706	UNK	ARG	conflict	UNP Q92608
A	707	UNK	GLY	conflict	UNP Q92608
A	708	UNK	GLU	conflict	UNP Q92608
A	709	UNK	GLN	conflict	UNP Q92608
A	710	UNK	CYS	conflict	UNP Q92608
A	711	UNK	GLU	conflict	UNP Q92608
A	712	UNK	PRO	conflict	UNP Q92608
A	713	UNK	ILE	conflict	UNP Q92608
A	714	UNK	LEU	conflict	UNP Q92608
A	715	UNK	ARG	conflict	UNP Q92608
A	716	UNK	THR	conflict	UNP Q92608
A	717	UNK	LEU	conflict	UNP Q92608
A	718	UNK	LYS	conflict	UNP Q92608
A	719	UNK	ALA	conflict	UNP Q92608
A	720	UNK	LEU	conflict	UNP Q92608
A	721	UNK	GLU	conflict	UNP Q92608
A	722	UNK	TYR	conflict	UNP Q92608
A	723	UNK	VAL	conflict	UNP Q92608
A	724	UNK	PHE	conflict	UNP Q92608
A	725	UNK	LYS	conflict	UNP Q92608
A	726	UNK	PHE	conflict	UNP Q92608
A	727	UNK	ILE	conflict	UNP Q92608
A	728	UNK	VAL	conflict	UNP Q92608
A	729	UNK	ARG	conflict	UNP Q92608
A	730	UNK	SER	conflict	UNP Q92608
A	731	UNK	ARG	conflict	UNP Q92608
A	732	UNK	THR	conflict	UNP Q92608
A	733	UNK	LEU	conflict	UNP Q92608
A	734	UNK	PHE	conflict	UNP Q92608
A	735	UNK	SER	conflict	UNP Q92608
A	736	UNK	GLN	conflict	UNP Q92608
A	742	UNK	LEU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	743	UNK	TYR	conflict	UNP Q92608
A	744	UNK	GLU	conflict	UNP Q92608
A	745	UNK	GLY	conflict	UNP Q92608
A	746	UNK	LYS	conflict	UNP Q92608
A	747	UNK	GLU	conflict	UNP Q92608
A	748	UNK	GLN	conflict	UNP Q92608
A	749	UNK	MET	conflict	UNP Q92608
A	750	UNK	GLU	conflict	UNP Q92608
A	751	UNK	PHE	conflict	UNP Q92608
A	752	UNK	GLU	conflict	UNP Q92608
A	753	UNK	GLU	conflict	UNP Q92608
A	754	UNK	SER	conflict	UNP Q92608
A	755	UNK	MET	conflict	UNP Q92608
A	756	UNK	ARG	conflict	UNP Q92608
A	757	UNK	ARG	conflict	UNP Q92608
A	758	UNK	LEU	conflict	UNP Q92608
A	759	UNK	PHE	conflict	UNP Q92608
A	760	UNK	GLU	conflict	UNP Q92608
A	761	UNK	SER	conflict	UNP Q92608
A	762	UNK	ILE	conflict	UNP Q92608
A	763	UNK	ASN	conflict	UNP Q92608
A	764	UNK	ASN	conflict	UNP Q92608
A	765	UNK	LEU	conflict	UNP Q92608
A	766	UNK	MET	conflict	UNP Q92608
A	767	UNK	LYS	conflict	UNP Q92608
A	768	UNK	SER	conflict	UNP Q92608
A	769	UNK	GLN	conflict	UNP Q92608
A	770	UNK	TYR	conflict	UNP Q92608
A	771	UNK	LYS	conflict	UNP Q92608
A	772	UNK	THR	conflict	UNP Q92608
A	773	UNK	THR	conflict	UNP Q92608
A	774	UNK	ILE	conflict	UNP Q92608
A	775	UNK	LEU	conflict	UNP Q92608
A	776	UNK	LEU	conflict	UNP Q92608
A	777	UNK	GLN	conflict	UNP Q92608
A	778	UNK	VAL	conflict	UNP Q92608
A	779	UNK	ALA	conflict	UNP Q92608
A	780	UNK	ALA	conflict	UNP Q92608
A	781	UNK	LEU	conflict	UNP Q92608
A	782	UNK	LYS	conflict	UNP Q92608
A	783	UNK	TYR	conflict	UNP Q92608
A	784	UNK	ILE	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	785	UNK	PRO	conflict	UNP Q92608
A	786	UNK	SER	conflict	UNP Q92608
A	787	UNK	VAL	conflict	UNP Q92608
A	788	UNK	LEU	conflict	UNP Q92608
A	789	UNK	HIS	conflict	UNP Q92608
A	790	UNK	ASP	conflict	UNP Q92608
A	791	UNK	VAL	conflict	UNP Q92608
A	792	UNK	GLU	conflict	UNP Q92608
A	793	UNK	MET	conflict	UNP Q92608
A	794	UNK	VAL	conflict	UNP Q92608
A	795	UNK	PHE	conflict	UNP Q92608
A	796	UNK	ASP	conflict	UNP Q92608
A	797	UNK	ALA	conflict	UNP Q92608
A	798	UNK	LYS	conflict	UNP Q92608
A	799	UNK	LEU	conflict	UNP Q92608
A	801	UNK	LEU	conflict	UNP Q92608
A	802	UNK	SER	conflict	UNP Q92608
A	803	UNK	GLN	conflict	UNP Q92608
A	804	UNK	LEU	conflict	UNP Q92608
A	805	UNK	LEU	conflict	UNP Q92608
A	806	UNK	TYR	conflict	UNP Q92608
A	807	UNK	GLU	conflict	UNP Q92608
A	808	UNK	PHE	conflict	UNP Q92608
A	809	UNK	TYR	conflict	UNP Q92608
A	810	UNK	THR	conflict	UNP Q92608
A	811	UNK	CYS	conflict	UNP Q92608
A	812	UNK	ILE	conflict	UNP Q92608
A	813	UNK	PRO	conflict	UNP Q92608
A	814	UNK	PRO	conflict	UNP Q92608
A	815	UNK	VAL	conflict	UNP Q92608
A	816	UNK	LYS	conflict	UNP Q92608
A	817	UNK	LEU	conflict	UNP Q92608
A	818	UNK	GLN	conflict	UNP Q92608
A	819	UNK	LYS	conflict	UNP Q92608
A	820	UNK	GLN	conflict	UNP Q92608
A	821	UNK	LYS	conflict	UNP Q92608
A	822	UNK	VAL	conflict	UNP Q92608
A	823	UNK	GLN	conflict	UNP Q92608
A	824	UNK	SER	conflict	UNP Q92608
A	825	UNK	MET	conflict	UNP Q92608
A	826	UNK	ASN	conflict	UNP Q92608
A	827	UNK	GLU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	828	UNK	ILE	conflict	UNP Q92608
A	829	UNK	VAL	conflict	UNP Q92608
A	830	UNK	GLN	conflict	UNP Q92608
A	831	UNK	SER	conflict	UNP Q92608
A	832	UNK	ASN	conflict	UNP Q92608
A	833	UNK	LEU	conflict	UNP Q92608
A	834	UNK	PHE	conflict	UNP Q92608
A	835	UNK	LYS	conflict	UNP Q92608
A	836	UNK	LYS	conflict	UNP Q92608
A	837	UNK	GLN	conflict	UNP Q92608
A	838	UNK	GLU	conflict	UNP Q92608
A	839	UNK	CYS	conflict	UNP Q92608
A	840	UNK	ARG	conflict	UNP Q92608
A	841	UNK	ASP	conflict	UNP Q92608
A	842	UNK	ILE	conflict	UNP Q92608
A	843	UNK	LEU	conflict	UNP Q92608
A	844	UNK	LEU	conflict	UNP Q92608
A	845	UNK	PRO	conflict	UNP Q92608
A	846	UNK	VAL	conflict	UNP Q92608
A	847	UNK	ILE	conflict	UNP Q92608
A	848	UNK	THR	conflict	UNP Q92608
A	849	UNK	LYS	conflict	UNP Q92608
A	850	UNK	GLU	conflict	UNP Q92608
A	851	UNK	LEU	conflict	UNP Q92608
A	852	UNK	LYS	conflict	UNP Q92608
A	853	UNK	GLU	conflict	UNP Q92608
A	854	UNK	LEU	conflict	UNP Q92608
A	855	UNK	LEU	conflict	UNP Q92608
A	856	UNK	GLU	conflict	UNP Q92608
A	857	UNK	GLN	conflict	UNP Q92608
A	858	UNK	LYS	conflict	UNP Q92608
A	859	UNK	ASP	conflict	UNP Q92608
A	860	UNK	ASP	conflict	UNP Q92608
A	861	UNK	MET	conflict	UNP Q92608
A	862	UNK	GLN	conflict	UNP Q92608
A	863	UNK	HIS	conflict	UNP Q92608
A	864	UNK	GLN	conflict	UNP Q92608
A	865	UNK	VAL	conflict	UNP Q92608
A	866	UNK	LEU	conflict	UNP Q92608
A	867	UNK	GLU	conflict	UNP Q92608
A	868	UNK	ARG	conflict	UNP Q92608
A	869	UNK	LYS	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	870	UNK	TYR	conflict	UNP Q92608
A	871	UNK	CYS	conflict	UNP Q92608
A	872	UNK	VAL	conflict	UNP Q92608
A	873	UNK	GLU	conflict	UNP Q92608
A	874	UNK	LEU	conflict	UNP Q92608
A	875	UNK	LEU	conflict	UNP Q92608
A	876	UNK	ASN	conflict	UNP Q92608
A	877	UNK	SER	conflict	UNP Q92608
A	878	UNK	ILE	conflict	UNP Q92608
A	879	UNK	LEU	conflict	UNP Q92608
A	880	UNK	GLU	conflict	UNP Q92608
A	881	UNK	VAL	conflict	UNP Q92608
A	882	UNK	LEU	conflict	UNP Q92608
A	883	UNK	SER	conflict	UNP Q92608
A	884	UNK	TYR	conflict	UNP Q92608
A	885	UNK	GLN	conflict	UNP Q92608
A	886	UNK	ASP	conflict	UNP Q92608
A	887	UNK	ALA	conflict	UNP Q92608
A	888	UNK	ALA	conflict	UNP Q92608
A	889	UNK	PHE	conflict	UNP Q92608
A	890	UNK	THR	conflict	UNP Q92608
A	891	UNK	TYR	conflict	UNP Q92608
A	892	UNK	HIS	conflict	UNP Q92608
A	896	UNK	HIS	conflict	UNP Q92608
A	897	UNK	ILE	conflict	UNP Q92608
A	898	UNK	GLN	conflict	UNP Q92608
A	899	UNK	GLU	conflict	UNP Q92608
A	900	UNK	ILE	conflict	UNP Q92608
A	901	UNK	MET	conflict	UNP Q92608
A	902	UNK	VAL	conflict	UNP Q92608
A	903	UNK	GLN	conflict	UNP Q92608
A	904	UNK	LEU	conflict	UNP Q92608
A	905	UNK	LEU	conflict	UNP Q92608
A	906	UNK	ARG	conflict	UNP Q92608
A	907	UNK	THR	conflict	UNP Q92608
A	908	UNK	VAL	conflict	UNP Q92608
A	909	UNK	ASN	conflict	UNP Q92608
A	910	UNK	ARG	conflict	UNP Q92608
A	911	UNK	THR	conflict	UNP Q92608
A	912	UNK	VAL	conflict	UNP Q92608
A	913	UNK	ILE	conflict	UNP Q92608
A	914	UNK	THR	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
A	915	UNK	MET	conflict	UNP Q92608
A	916	UNK	GLY	conflict	UNP Q92608
A	917	UNK	ARG	conflict	UNP Q92608
A	918	UNK	ASP	conflict	UNP Q92608
A	919	UNK	HIS	conflict	UNP Q92608
A	920	UNK	ILE	conflict	UNP Q92608
A	921	UNK	LEU	conflict	UNP Q92608
A	922	UNK	ILE	conflict	UNP Q92608
A	923	UNK	SER	conflict	UNP Q92608
A	934	UNK	HIS	conflict	UNP Q92608
A	935	UNK	PHE	conflict	UNP Q92608
A	936	UNK	VAL	conflict	UNP Q92608
A	937	UNK	ALA	conflict	UNP Q92608
A	938	UNK	CYS	conflict	UNP Q92608
A	939	UNK	MET	conflict	UNP Q92608
A	940	UNK	THR	conflict	UNP Q92608
A	941	UNK	ALA	conflict	UNP Q92608
A	942	UNK	ILE	conflict	UNP Q92608
A	943	UNK	LEU	conflict	UNP Q92608
A	944	UNK	ASN	conflict	UNP Q92608
A	945	UNK	GLN	conflict	UNP Q92608
A	946	UNK	MET	conflict	UNP Q92608
A	947	UNK	GLY	conflict	UNP Q92608
A	948	UNK	ASP	conflict	UNP Q92608
A	949	UNK	GLN	conflict	UNP Q92608
A	950	UNK	HIS	conflict	UNP Q92608
A	951	UNK	TYR	conflict	UNP Q92608
A	952	UNK	SER	conflict	UNP Q92608
A	953	UNK	PHE	conflict	UNP Q92608
A	954	UNK	TYR	conflict	UNP Q92608
A	955	UNK	ILE	conflict	UNP Q92608
A	956	UNK	GLU	conflict	UNP Q92608
A	957	UNK	THR	conflict	UNP Q92608
A	958	UNK	PHE	conflict	UNP Q92608
A	959	UNK	GLN	conflict	UNP Q92608
A	960	UNK	THR	conflict	UNP Q92608
D	207A	UNK	ASP	conflict	UNP Q92608
D	207B	UNK	TYR	conflict	UNP Q92608
D	207C	UNK	ALA	conflict	UNP Q92608
D	207D	UNK	MET	conflict	UNP Q92608
D	207E	UNK	TYR	conflict	UNP Q92608
D	207F	UNK	SER	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	207G	UNK	ARG	conflict	UNP Q92608
D	207H	UNK	ILE	conflict	UNP Q92608
D	207I	UNK	SER	conflict	UNP Q92608
D	207J	UNK	SER	conflict	UNP Q92608
D	207K	UNK	SER	conflict	UNP Q92608
D	207L	UNK	PRO	conflict	UNP Q92608
D	207M	UNK	THR	conflict	UNP Q92608
D	207N	UNK	HIS	conflict	UNP Q92608
D	207O	UNK	SER	conflict	UNP Q92608
D	207P	UNK	LEU	conflict	UNP Q92608
D	207Q	UNK	TYR	conflict	UNP Q92608
D	207R	UNK	VAL	conflict	UNP Q92608
D	207S	UNK	PHE	conflict	UNP Q92608
D	207T	UNK	VAL	conflict	UNP Q92608
D	207U	UNK	ARG	conflict	UNP Q92608
D	207V	UNK	ASN	conflict	UNP Q92608
D	207W	UNK	PHE	conflict	UNP Q92608
D	207X	UNK	VAL	conflict	UNP Q92608
D	207Y	UNK	CYS	conflict	UNP Q92608
D	207Z	UNK	ARG	conflict	UNP Q92608
D	208A	UNK	ILE	conflict	UNP Q92608
D	208B	UNK	GLY	conflict	UNP Q92608
D	208C	UNK	GLU	conflict	UNP Q92608
D	208D	UNK	ASP	conflict	UNP Q92608
D	208E	UNK	ALA	conflict	UNP Q92608
D	208F	UNK	GLU	conflict	UNP Q92608
D	208G	UNK	LEU	conflict	UNP Q92608
D	208H	UNK	PHE	conflict	UNP Q92608
D	208I	UNK	MET	conflict	UNP Q92608
D	208J	UNK	SER	conflict	UNP Q92608
D	208K	UNK	LEU	conflict	UNP Q92608
D	208L	UNK	TYR	conflict	UNP Q92608
D	208M	UNK	ASP	conflict	UNP Q92608
D	208N	UNK	PRO	conflict	UNP Q92608
D	208O	UNK	ASN	conflict	UNP Q92608
D	208P	UNK	LYS	conflict	UNP Q92608
D	208Q	UNK	GLN	conflict	UNP Q92608
D	208R	UNK	THR	conflict	UNP Q92608
D	208S	UNK	VAL	conflict	UNP Q92608
D	208T	UNK	ILE	conflict	UNP Q92608
D	208U	UNK	SER	conflict	UNP Q92608
D	208V	UNK	GLU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	208W	UNK	ASN	conflict	UNP Q92608
D	208X	UNK	TYR	conflict	UNP Q92608
D	208Y	UNK	LEU	conflict	UNP Q92608
D	208Z	UNK	VAL	conflict	UNP Q92608
D	209A	UNK	ARG	conflict	UNP Q92608
D	209B	UNK	TRP	conflict	UNP Q92608
D	209C	UNK	GLY	conflict	UNP Q92608
D	209D	UNK	SER	conflict	UNP Q92608
D	209E	UNK	ARG	conflict	UNP Q92608
D	209F	UNK	GLY	conflict	UNP Q92608
D	209G	UNK	PHE	conflict	UNP Q92608
D	209H	UNK	PRO	conflict	UNP Q92608
D	209I	UNK	LYS	conflict	UNP Q92608
D	209J	UNK	GLU	conflict	UNP Q92608
D	209K	UNK	ILE	conflict	UNP Q92608
D	209L	UNK	GLU	conflict	UNP Q92608
D	209M	UNK	MET	conflict	UNP Q92608
D	209N	UNK	LEU	conflict	UNP Q92608
D	209O	UNK	ASN	conflict	UNP Q92608
D	209P	UNK	ASN	conflict	UNP Q92608
D	209Q	UNK	LEU	conflict	UNP Q92608
D	209R	UNK	LYS	conflict	UNP Q92608
D	209S	UNK	VAL	conflict	UNP Q92608
D	219	UNK	VAL	conflict	UNP Q92608
D	220	UNK	PHE	conflict	UNP Q92608
D	221	UNK	THR	conflict	UNP Q92608
D	222	UNK	ASP	conflict	UNP Q92608
D	223	UNK	LEU	conflict	UNP Q92608
D	224	UNK	GLY	conflict	UNP Q92608
D	225	UNK	ASN	conflict	UNP Q92608
D	226	UNK	LYS	conflict	UNP Q92608
D	227	UNK	ASP	conflict	UNP Q92608
D	228	UNK	LEU	conflict	UNP Q92608
D	229	UNK	ASN	conflict	UNP Q92608
D	230	UNK	ARG	conflict	UNP Q92608
D	231	UNK	ASP	conflict	UNP Q92608
D	232	UNK	LYS	conflict	UNP Q92608
D	233	UNK	ILE	conflict	UNP Q92608
D	234	UNK	TYR	conflict	UNP Q92608
D	235	UNK	LEU	conflict	UNP Q92608
D	236	UNK	ILE	conflict	UNP Q92608
D	237	UNK	CYS	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	238	UNK	GLN	conflict	UNP Q92608
D	239	UNK	ILE	conflict	UNP Q92608
D	240	UNK	VAL	conflict	UNP Q92608
D	241	UNK	ARG	conflict	UNP Q92608
D	242	UNK	VAL	conflict	UNP Q92608
D	243	UNK	GLY	conflict	UNP Q92608
D	244	UNK	LYS	conflict	UNP Q92608
D	245	UNK	MET	conflict	UNP Q92608
D	246	UNK	ASP	conflict	UNP Q92608
D	247	UNK	LEU	conflict	UNP Q92608
D	248	UNK	LYS	conflict	UNP Q92608
D	249	UNK	ASP	conflict	UNP Q92608
D	250	UNK	THR	conflict	UNP Q92608
D	251	UNK	GLY	conflict	UNP Q92608
D	252	UNK	ALA	conflict	UNP Q92608
D	253	UNK	LYS	conflict	UNP Q92608
D	254	UNK	LYS	conflict	UNP Q92608
D	255	UNK	CYS	conflict	UNP Q92608
D	256	UNK	THR	conflict	UNP Q92608
D	257	UNK	GLN	conflict	UNP Q92608
D	258	UNK	GLY	conflict	UNP Q92608
D	259	UNK	LEU	conflict	UNP Q92608
D	260	UNK	ARG	conflict	UNP Q92608
D	261	UNK	ARG	conflict	UNP Q92608
D	262	UNK	PRO	conflict	UNP Q92608
D	263	UNK	PHE	conflict	UNP Q92608
D	264	UNK	GLY	conflict	UNP Q92608
D	265	UNK	VAL	conflict	UNP Q92608
D	266	UNK	ALA	conflict	UNP Q92608
D	267	UNK	VAL	conflict	UNP Q92608
D	268	UNK	MET	conflict	UNP Q92608
D	269	UNK	ASP	conflict	UNP Q92608
D	270	UNK	ILE	conflict	UNP Q92608
D	271	UNK	THR	conflict	UNP Q92608
D	272	UNK	ASP	conflict	UNP Q92608
D	273	UNK	ILE	conflict	UNP Q92608
D	274	UNK	ILE	conflict	UNP Q92608
D	275	UNK	LYS	conflict	UNP Q92608
D	276	UNK	GLY	conflict	UNP Q92608
D	277	UNK	LYS	conflict	UNP Q92608
D	278	UNK	ALA	conflict	UNP Q92608
D	279	UNK	GLU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	280	UNK	SER	conflict	UNP Q92608
D	281	UNK	ASP	conflict	UNP Q92608
D	282	UNK	GLU	conflict	UNP Q92608
D	283	UNK	GLU	conflict	UNP Q92608
D	284	UNK	LYS	conflict	UNP Q92608
D	285	UNK	GLN	conflict	UNP Q92608
D	286	UNK	HIS	conflict	UNP Q92608
D	287	UNK	PHE	conflict	UNP Q92608
D	288	UNK	ILE	conflict	UNP Q92608
D	289	UNK	PRO	conflict	UNP Q92608
D	290	UNK	PHE	conflict	UNP Q92608
D	291	UNK	HIS	conflict	UNP Q92608
D	292	UNK	PRO	conflict	UNP Q92608
D	293	UNK	VAL	conflict	UNP Q92608
D	294	UNK	THR	conflict	UNP Q92608
D	295	UNK	ALA	conflict	UNP Q92608
D	296	UNK	GLU	conflict	UNP Q92608
D	297	UNK	ASN	conflict	UNP Q92608
D	298	UNK	ASP	conflict	UNP Q92608
D	299	UNK	PHE	conflict	UNP Q92608
D	300	UNK	LEU	conflict	UNP Q92608
D	301	UNK	HIS	conflict	UNP Q92608
D	302	UNK	SER	conflict	UNP Q92608
D	303	UNK	LEU	conflict	UNP Q92608
D	304	UNK	LEU	conflict	UNP Q92608
D	318	UNK	GLY	conflict	UNP Q92608
D	319	UNK	LYS	conflict	UNP Q92608
D	320	UNK	VAL	conflict	UNP Q92608
D	321	UNK	ILE	conflict	UNP Q92608
D	322	UNK	ALA	conflict	UNP Q92608
D	323	UNK	SER	conflict	UNP Q92608
D	324	UNK	LYS	conflict	UNP Q92608
D	325	UNK	GLY	conflict	UNP Q92608
D	326	UNK	ASP	conflict	UNP Q92608
D	327	UNK	SER	conflict	UNP Q92608
D	328	UNK	GLY	conflict	UNP Q92608
D	329	UNK	GLY	conflict	UNP Q92608
D	330	UNK	GLN	conflict	UNP Q92608
D	331	UNK	GLY	conflict	UNP Q92608
D	332	UNK	LEU	conflict	UNP Q92608
D	333	UNK	TRP	conflict	UNP Q92608
D	334	UNK	VAL	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	335	UNK	THR	conflict	UNP Q92608
D	336	UNK	MET	conflict	UNP Q92608
D	337	UNK	LYS	conflict	UNP Q92608
D	338	UNK	MET	conflict	UNP Q92608
D	339	UNK	LEU	conflict	UNP Q92608
D	340	UNK	VAL	conflict	UNP Q92608
D	341	UNK	GLY	conflict	UNP Q92608
D	342	UNK	ASP	conflict	UNP Q92608
D	343	UNK	ILE	conflict	UNP Q92608
D	344	UNK	ILE	conflict	UNP Q92608
D	345	UNK	GLN	conflict	UNP Q92608
D	346	UNK	ILE	conflict	UNP Q92608
D	347	UNK	ARG	conflict	UNP Q92608
D	348	UNK	LYS	conflict	UNP Q92608
D	349	UNK	ASP	conflict	UNP Q92608
D	350	UNK	TYR	conflict	UNP Q92608
D	351	UNK	PRO	conflict	UNP Q92608
D	377	UNK	HIS	conflict	UNP Q92608
D	378	UNK	LEU	conflict	UNP Q92608
D	379	UNK	VAL	conflict	UNP Q92608
D	380	UNK	ASP	conflict	UNP Q92608
D	381	UNK	ARG	conflict	UNP Q92608
D	382	UNK	THR	conflict	UNP Q92608
D	383	UNK	THR	conflict	UNP Q92608
D	384	UNK	VAL	conflict	UNP Q92608
D	385	UNK	VAL	conflict	UNP Q92608
D	386	UNK	ALA	conflict	UNP Q92608
D	387	UNK	ARG	conflict	UNP Q92608
D	388	UNK	LYS	conflict	UNP Q92608
D	389	UNK	LEU	conflict	UNP Q92608
D	609A	UNK	LYS	conflict	UNP Q92608
D	609B	UNK	LEU	conflict	UNP Q92608
D	609C	UNK	THR	conflict	UNP Q92608
D	609D	UNK	GLN	conflict	UNP Q92608
D	609E	UNK	ASN	conflict	UNP Q92608
D	609F	UNK	VAL	conflict	UNP Q92608
D	609G	UNK	GLY	conflict	UNP Q92608
D	609H	UNK	LEU	conflict	UNP Q92608
D	609I	UNK	LEU	conflict	UNP Q92608
D	609J	UNK	GLY	conflict	UNP Q92608
D	609K	UNK	LEU	conflict	UNP Q92608
D	609L	UNK	LEU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	609M	UNK	LYS	conflict	UNP Q92608
D	609N	UNK	TRP	conflict	UNP Q92608
D	609O	UNK	ARG	conflict	UNP Q92608
D	609P	UNK	MET	conflict	UNP Q92608
D	609Q	UNK	LYS	conflict	UNP Q92608
D	609R	UNK	PRO	conflict	UNP Q92608
D	609S	UNK	GLN	conflict	UNP Q92608
D	609T	UNK	LEU	conflict	UNP Q92608
D	609U	UNK	LEU	conflict	UNP Q92608
D	609V	UNK	GLN	conflict	UNP Q92608
D	609W	UNK	GLU	conflict	UNP Q92608
D	609X	UNK	ASN	conflict	UNP Q92608
D	609Y	UNK	LEU	conflict	UNP Q92608
D	609Z	UNK	GLU	conflict	UNP Q92608
D	610A	UNK	LYS	conflict	UNP Q92608
D	610B	UNK	LEU	conflict	UNP Q92608
D	610C	UNK	LYS	conflict	UNP Q92608
D	610D	UNK	ILE	conflict	UNP Q92608
D	610E	UNK	VAL	conflict	UNP Q92608
D	610F	UNK	ASP	conflict	UNP Q92608
D	626	UNK	GLY	conflict	UNP Q92608
D	627	UNK	GLU	conflict	UNP Q92608
D	628	UNK	GLU	conflict	UNP Q92608
D	629	UNK	VAL	conflict	UNP Q92608
D	630	UNK	VAL	conflict	UNP Q92608
D	631	UNK	LYS	conflict	UNP Q92608
D	632	UNK	PHE	conflict	UNP Q92608
D	633	UNK	LEU	conflict	UNP Q92608
D	634	UNK	GLN	conflict	UNP Q92608
D	635	UNK	ASP	conflict	UNP Q92608
D	636	UNK	THR	conflict	UNP Q92608
D	637	UNK	LEU	conflict	UNP Q92608
D	638	UNK	ASP	conflict	UNP Q92608
D	639	UNK	ALA	conflict	UNP Q92608
D	640	UNK	LEU	conflict	UNP Q92608
D	641	UNK	PHE	conflict	UNP Q92608
D	642	UNK	ASN	conflict	UNP Q92608
D	679A	UNK	HIS	conflict	UNP Q92608
D	679B	UNK	PHE	conflict	UNP Q92608
D	679C	UNK	ASN	conflict	UNP Q92608
D	679D	UNK	THR	conflict	UNP Q92608
D	679E	UNK	VAL	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	679F	UNK	LEU	conflict	UNP Q92608
D	679G	UNK	GLU	conflict	UNP Q92608
D	679H	UNK	ALA	conflict	UNP Q92608
D	679I	UNK	TYR	conflict	UNP Q92608
D	679J	UNK	ILE	conflict	UNP Q92608
D	679K	UNK	GLN	conflict	UNP Q92608
D	679L	UNK	GLN	conflict	UNP Q92608
D	679M	UNK	HIS	conflict	UNP Q92608
D	679N	UNK	PHE	conflict	UNP Q92608
D	679O	UNK	SER	conflict	UNP Q92608
D	679P	UNK	ALA	conflict	UNP Q92608
D	679Q	UNK	THR	conflict	UNP Q92608
D	688	UNK	LEU	conflict	UNP Q92608
D	689	UNK	ALA	conflict	UNP Q92608
D	690	UNK	TYR	conflict	UNP Q92608
D	691	UNK	LYS	conflict	UNP Q92608
D	692	UNK	LYS	conflict	UNP Q92608
D	693	UNK	LEU	conflict	UNP Q92608
D	694	UNK	MET	conflict	UNP Q92608
D	695	UNK	THR	conflict	UNP Q92608
D	696	UNK	VAL	conflict	UNP Q92608
D	697	UNK	LEU	conflict	UNP Q92608
D	698	UNK	LYS	conflict	UNP Q92608
D	699	UNK	THR	conflict	UNP Q92608
D	700	UNK	TYR	conflict	UNP Q92608
D	701	UNK	LEU	conflict	UNP Q92608
D	702	UNK	ASP	conflict	UNP Q92608
D	703	UNK	THR	conflict	UNP Q92608
D	704	UNK	SER	conflict	UNP Q92608
D	705	UNK	SER	conflict	UNP Q92608
D	706	UNK	ARG	conflict	UNP Q92608
D	707	UNK	GLY	conflict	UNP Q92608
D	708	UNK	GLU	conflict	UNP Q92608
D	709	UNK	GLN	conflict	UNP Q92608
D	710	UNK	CYS	conflict	UNP Q92608
D	711	UNK	GLU	conflict	UNP Q92608
D	712	UNK	PRO	conflict	UNP Q92608
D	713	UNK	ILE	conflict	UNP Q92608
D	714	UNK	LEU	conflict	UNP Q92608
D	715	UNK	ARG	conflict	UNP Q92608
D	716	UNK	THR	conflict	UNP Q92608
D	717	UNK	LEU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	718	UNK	LYS	conflict	UNP Q92608
D	719	UNK	ALA	conflict	UNP Q92608
D	720	UNK	LEU	conflict	UNP Q92608
D	721	UNK	GLU	conflict	UNP Q92608
D	722	UNK	TYR	conflict	UNP Q92608
D	723	UNK	VAL	conflict	UNP Q92608
D	724	UNK	PHE	conflict	UNP Q92608
D	725	UNK	LYS	conflict	UNP Q92608
D	726	UNK	PHE	conflict	UNP Q92608
D	727	UNK	ILE	conflict	UNP Q92608
D	728	UNK	VAL	conflict	UNP Q92608
D	729	UNK	ARG	conflict	UNP Q92608
D	730	UNK	SER	conflict	UNP Q92608
D	731	UNK	ARG	conflict	UNP Q92608
D	732	UNK	THR	conflict	UNP Q92608
D	733	UNK	LEU	conflict	UNP Q92608
D	734	UNK	PHE	conflict	UNP Q92608
D	735	UNK	SER	conflict	UNP Q92608
D	736	UNK	GLN	conflict	UNP Q92608
D	742	UNK	LEU	conflict	UNP Q92608
D	743	UNK	TYR	conflict	UNP Q92608
D	744	UNK	GLU	conflict	UNP Q92608
D	745	UNK	GLY	conflict	UNP Q92608
D	746	UNK	LYS	conflict	UNP Q92608
D	747	UNK	GLU	conflict	UNP Q92608
D	748	UNK	GLN	conflict	UNP Q92608
D	749	UNK	MET	conflict	UNP Q92608
D	750	UNK	GLU	conflict	UNP Q92608
D	751	UNK	PHE	conflict	UNP Q92608
D	752	UNK	GLU	conflict	UNP Q92608
D	753	UNK	GLU	conflict	UNP Q92608
D	754	UNK	SER	conflict	UNP Q92608
D	755	UNK	MET	conflict	UNP Q92608
D	756	UNK	ARG	conflict	UNP Q92608
D	757	UNK	ARG	conflict	UNP Q92608
D	758	UNK	LEU	conflict	UNP Q92608
D	759	UNK	PHE	conflict	UNP Q92608
D	760	UNK	GLU	conflict	UNP Q92608
D	761	UNK	SER	conflict	UNP Q92608
D	762	UNK	ILE	conflict	UNP Q92608
D	763	UNK	ASN	conflict	UNP Q92608
D	764	UNK	ASN	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	765	UNK	LEU	conflict	UNP Q92608
D	766	UNK	MET	conflict	UNP Q92608
D	767	UNK	LYS	conflict	UNP Q92608
D	768	UNK	SER	conflict	UNP Q92608
D	769	UNK	GLN	conflict	UNP Q92608
D	770	UNK	TYR	conflict	UNP Q92608
D	771	UNK	LYS	conflict	UNP Q92608
D	772	UNK	THR	conflict	UNP Q92608
D	773	UNK	THR	conflict	UNP Q92608
D	774	UNK	ILE	conflict	UNP Q92608
D	775	UNK	LEU	conflict	UNP Q92608
D	776	UNK	LEU	conflict	UNP Q92608
D	777	UNK	GLN	conflict	UNP Q92608
D	778	UNK	VAL	conflict	UNP Q92608
D	779	UNK	ALA	conflict	UNP Q92608
D	780	UNK	ALA	conflict	UNP Q92608
D	781	UNK	LEU	conflict	UNP Q92608
D	782	UNK	LYS	conflict	UNP Q92608
D	783	UNK	TYR	conflict	UNP Q92608
D	784	UNK	ILE	conflict	UNP Q92608
D	785	UNK	PRO	conflict	UNP Q92608
D	786	UNK	SER	conflict	UNP Q92608
D	787	UNK	VAL	conflict	UNP Q92608
D	788	UNK	LEU	conflict	UNP Q92608
D	789	UNK	HIS	conflict	UNP Q92608
D	790	UNK	ASP	conflict	UNP Q92608
D	791	UNK	VAL	conflict	UNP Q92608
D	792	UNK	GLU	conflict	UNP Q92608
D	793	UNK	MET	conflict	UNP Q92608
D	794	UNK	VAL	conflict	UNP Q92608
D	795	UNK	PHE	conflict	UNP Q92608
D	796	UNK	ASP	conflict	UNP Q92608
D	797	UNK	ALA	conflict	UNP Q92608
D	798	UNK	LYS	conflict	UNP Q92608
D	799	UNK	LEU	conflict	UNP Q92608
D	801	UNK	LEU	conflict	UNP Q92608
D	802	UNK	SER	conflict	UNP Q92608
D	803	UNK	GLN	conflict	UNP Q92608
D	804	UNK	LEU	conflict	UNP Q92608
D	805	UNK	LEU	conflict	UNP Q92608
D	806	UNK	TYR	conflict	UNP Q92608
D	807	UNK	GLU	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	808	UNK	PHE	conflict	UNP Q92608
D	809	UNK	TYR	conflict	UNP Q92608
D	810	UNK	THR	conflict	UNP Q92608
D	811	UNK	CYS	conflict	UNP Q92608
D	812	UNK	ILE	conflict	UNP Q92608
D	813	UNK	PRO	conflict	UNP Q92608
D	814	UNK	PRO	conflict	UNP Q92608
D	815	UNK	VAL	conflict	UNP Q92608
D	816	UNK	LYS	conflict	UNP Q92608
D	817	UNK	LEU	conflict	UNP Q92608
D	818	UNK	GLN	conflict	UNP Q92608
D	819	UNK	LYS	conflict	UNP Q92608
D	820	UNK	GLN	conflict	UNP Q92608
D	821	UNK	LYS	conflict	UNP Q92608
D	822	UNK	VAL	conflict	UNP Q92608
D	823	UNK	GLN	conflict	UNP Q92608
D	824	UNK	SER	conflict	UNP Q92608
D	825	UNK	MET	conflict	UNP Q92608
D	826	UNK	ASN	conflict	UNP Q92608
D	827	UNK	GLU	conflict	UNP Q92608
D	828	UNK	ILE	conflict	UNP Q92608
D	829	UNK	VAL	conflict	UNP Q92608
D	830	UNK	GLN	conflict	UNP Q92608
D	831	UNK	SER	conflict	UNP Q92608
D	832	UNK	ASN	conflict	UNP Q92608
D	833	UNK	LEU	conflict	UNP Q92608
D	834	UNK	PHE	conflict	UNP Q92608
D	835	UNK	LYS	conflict	UNP Q92608
D	836	UNK	LYS	conflict	UNP Q92608
D	837	UNK	GLN	conflict	UNP Q92608
D	838	UNK	GLU	conflict	UNP Q92608
D	839	UNK	CYS	conflict	UNP Q92608
D	840	UNK	ARG	conflict	UNP Q92608
D	841	UNK	ASP	conflict	UNP Q92608
D	842	UNK	ILE	conflict	UNP Q92608
D	843	UNK	LEU	conflict	UNP Q92608
D	844	UNK	LEU	conflict	UNP Q92608
D	845	UNK	PRO	conflict	UNP Q92608
D	846	UNK	VAL	conflict	UNP Q92608
D	847	UNK	ILE	conflict	UNP Q92608
D	848	UNK	THR	conflict	UNP Q92608
D	849	UNK	LYS	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	850	UNK	GLU	conflict	UNP Q92608
D	851	UNK	LEU	conflict	UNP Q92608
D	852	UNK	LYS	conflict	UNP Q92608
D	853	UNK	GLU	conflict	UNP Q92608
D	854	UNK	LEU	conflict	UNP Q92608
D	855	UNK	LEU	conflict	UNP Q92608
D	856	UNK	GLU	conflict	UNP Q92608
D	857	UNK	GLN	conflict	UNP Q92608
D	858	UNK	LYS	conflict	UNP Q92608
D	859	UNK	ASP	conflict	UNP Q92608
D	860	UNK	ASP	conflict	UNP Q92608
D	861	UNK	MET	conflict	UNP Q92608
D	862	UNK	GLN	conflict	UNP Q92608
D	863	UNK	HIS	conflict	UNP Q92608
D	864	UNK	GLN	conflict	UNP Q92608
D	865	UNK	VAL	conflict	UNP Q92608
D	866	UNK	LEU	conflict	UNP Q92608
D	867	UNK	GLU	conflict	UNP Q92608
D	868	UNK	ARG	conflict	UNP Q92608
D	869	UNK	LYS	conflict	UNP Q92608
D	870	UNK	TYR	conflict	UNP Q92608
D	871	UNK	CYS	conflict	UNP Q92608
D	872	UNK	VAL	conflict	UNP Q92608
D	873	UNK	GLU	conflict	UNP Q92608
D	874	UNK	LEU	conflict	UNP Q92608
D	875	UNK	LEU	conflict	UNP Q92608
D	876	UNK	ASN	conflict	UNP Q92608
D	877	UNK	SER	conflict	UNP Q92608
D	878	UNK	ILE	conflict	UNP Q92608
D	879	UNK	LEU	conflict	UNP Q92608
D	880	UNK	GLU	conflict	UNP Q92608
D	881	UNK	VAL	conflict	UNP Q92608
D	882	UNK	LEU	conflict	UNP Q92608
D	883	UNK	SER	conflict	UNP Q92608
D	884	UNK	TYR	conflict	UNP Q92608
D	885	UNK	GLN	conflict	UNP Q92608
D	886	UNK	ASP	conflict	UNP Q92608
D	887	UNK	ALA	conflict	UNP Q92608
D	888	UNK	ALA	conflict	UNP Q92608
D	889	UNK	PHE	conflict	UNP Q92608
D	890	UNK	THR	conflict	UNP Q92608
D	891	UNK	TYR	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	892	UNK	HIS	conflict	UNP Q92608
D	896	UNK	HIS	conflict	UNP Q92608
D	897	UNK	ILE	conflict	UNP Q92608
D	898	UNK	GLN	conflict	UNP Q92608
D	899	UNK	GLU	conflict	UNP Q92608
D	900	UNK	ILE	conflict	UNP Q92608
D	901	UNK	MET	conflict	UNP Q92608
D	902	UNK	VAL	conflict	UNP Q92608
D	903	UNK	GLN	conflict	UNP Q92608
D	904	UNK	LEU	conflict	UNP Q92608
D	905	UNK	LEU	conflict	UNP Q92608
D	906	UNK	ARG	conflict	UNP Q92608
D	907	UNK	THR	conflict	UNP Q92608
D	908	UNK	VAL	conflict	UNP Q92608
D	909	UNK	ASN	conflict	UNP Q92608
D	910	UNK	ARG	conflict	UNP Q92608
D	911	UNK	THR	conflict	UNP Q92608
D	912	UNK	VAL	conflict	UNP Q92608
D	913	UNK	ILE	conflict	UNP Q92608
D	914	UNK	THR	conflict	UNP Q92608
D	915	UNK	MET	conflict	UNP Q92608
D	916	UNK	GLY	conflict	UNP Q92608
D	917	UNK	ARG	conflict	UNP Q92608
D	918	UNK	ASP	conflict	UNP Q92608
D	919	UNK	HIS	conflict	UNP Q92608
D	920	UNK	ILE	conflict	UNP Q92608
D	921	UNK	LEU	conflict	UNP Q92608
D	922	UNK	ILE	conflict	UNP Q92608
D	923	UNK	SER	conflict	UNP Q92608
D	934	UNK	HIS	conflict	UNP Q92608
D	935	UNK	PHE	conflict	UNP Q92608
D	936	UNK	VAL	conflict	UNP Q92608
D	937	UNK	ALA	conflict	UNP Q92608
D	938	UNK	CYS	conflict	UNP Q92608
D	939	UNK	MET	conflict	UNP Q92608
D	940	UNK	THR	conflict	UNP Q92608
D	941	UNK	ALA	conflict	UNP Q92608
D	942	UNK	ILE	conflict	UNP Q92608
D	943	UNK	LEU	conflict	UNP Q92608
D	944	UNK	ASN	conflict	UNP Q92608
D	945	UNK	GLN	conflict	UNP Q92608
D	946	UNK	MET	conflict	UNP Q92608

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Chain	Residue	Modelled	Actual	Comment	Reference
D	947	UNK	GLY	conflict	UNP Q92608
D	948	UNK	ASP	conflict	UNP Q92608
D	949	UNK	GLN	conflict	UNP Q92608
D	950	UNK	HIS	conflict	UNP Q92608
D	951	UNK	TYR	conflict	UNP Q92608
D	952	UNK	SER	conflict	UNP Q92608
D	953	UNK	PHE	conflict	UNP Q92608
D	954	UNK	TYR	conflict	UNP Q92608
D	955	UNK	ILE	conflict	UNP Q92608
D	956	UNK	GLU	conflict	UNP Q92608
D	957	UNK	THR	conflict	UNP Q92608
D	958	UNK	PHE	conflict	UNP Q92608
D	959	UNK	GLN	conflict	UNP Q92608
D	960	UNK	THR	conflict	UNP Q92608

- Molecule 2 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	680	Total	C	N	O	S	0	0
			5054	3269	841	917	27		
2	E	680	Total	C	N	O	S	0	0
			5056	3270	840	917	29		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	LEU	ARG	conflict	UNP Q92556
E	139	LEU	ARG	conflict	UNP Q92556

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

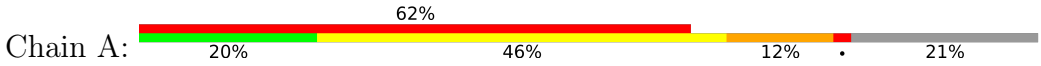
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1383	889	228	258	8		
3	F	177	Total	C	N	O	S	0	0
			1383	889	228	258	8		

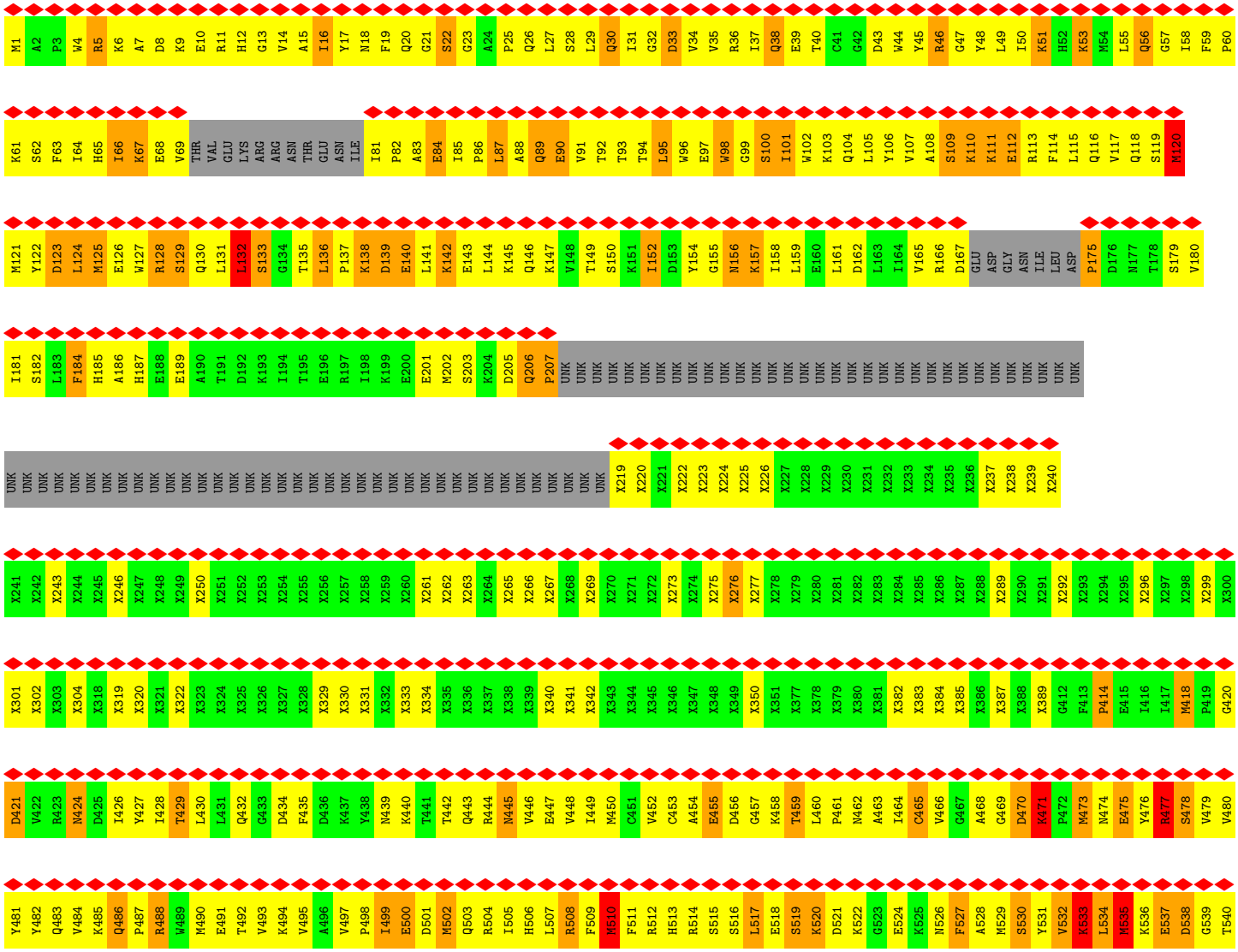
3 Residue-property plots (i)

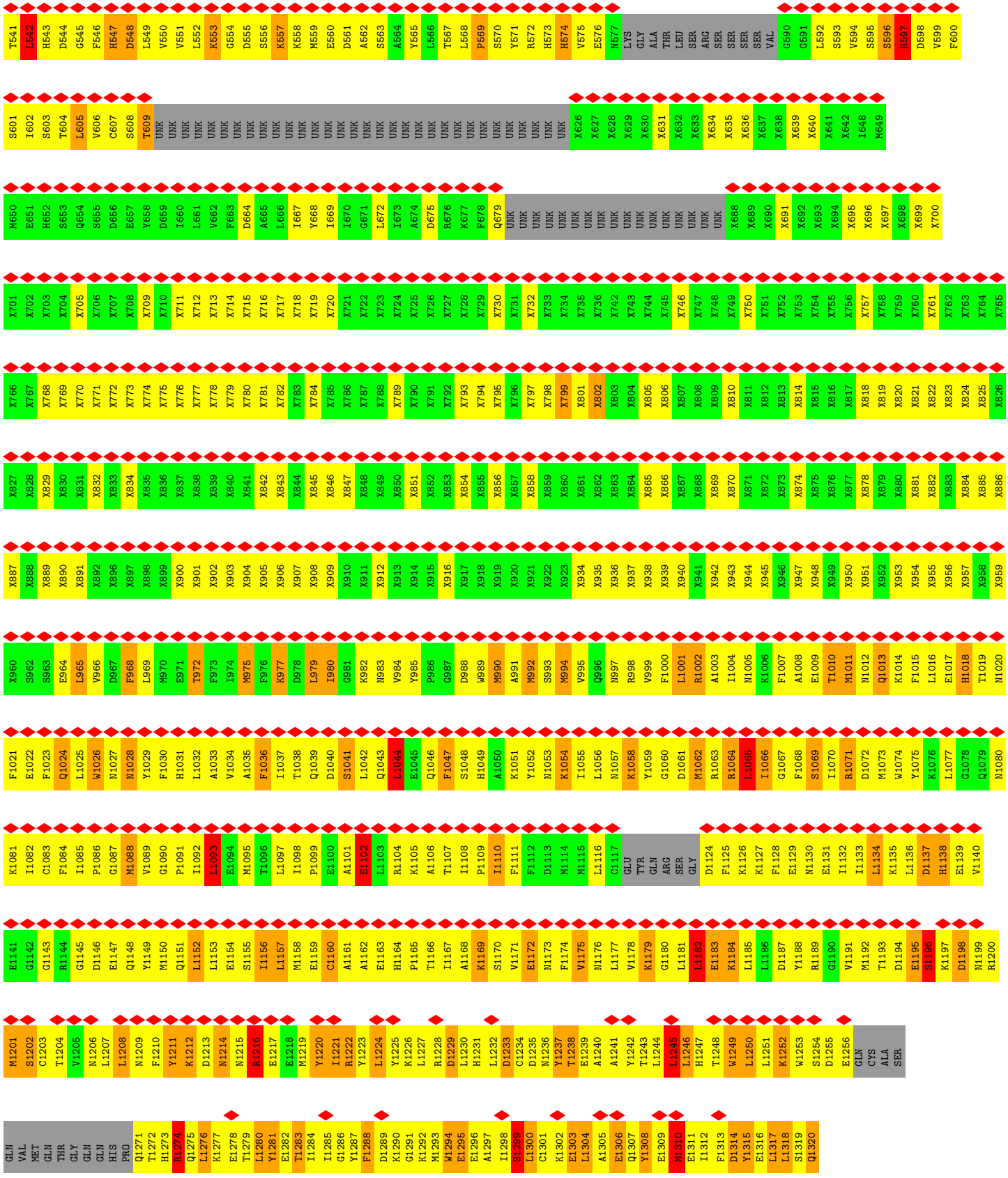
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

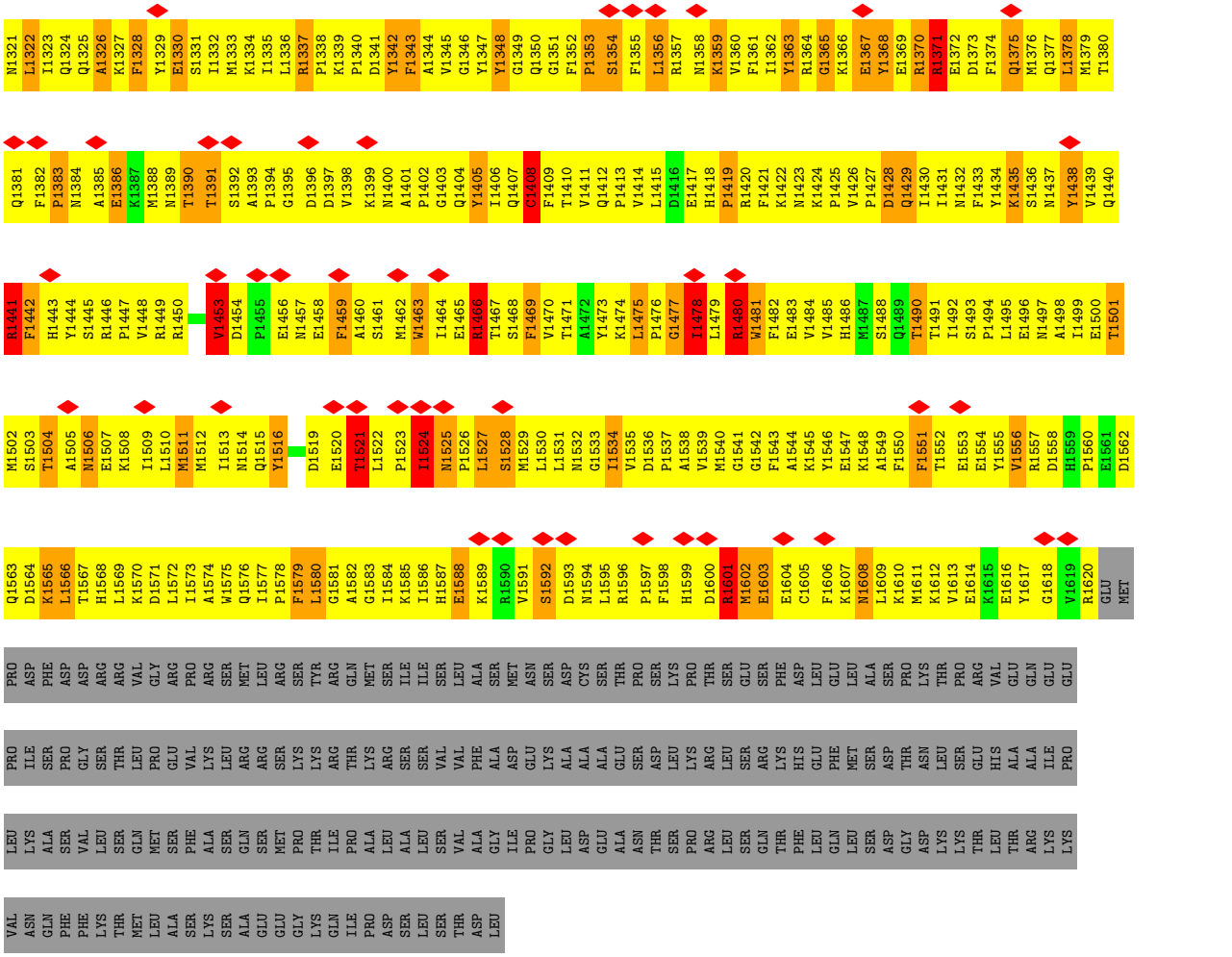
- Molecule 1: Dedicator of cytokinesis protein 2

Chain A:



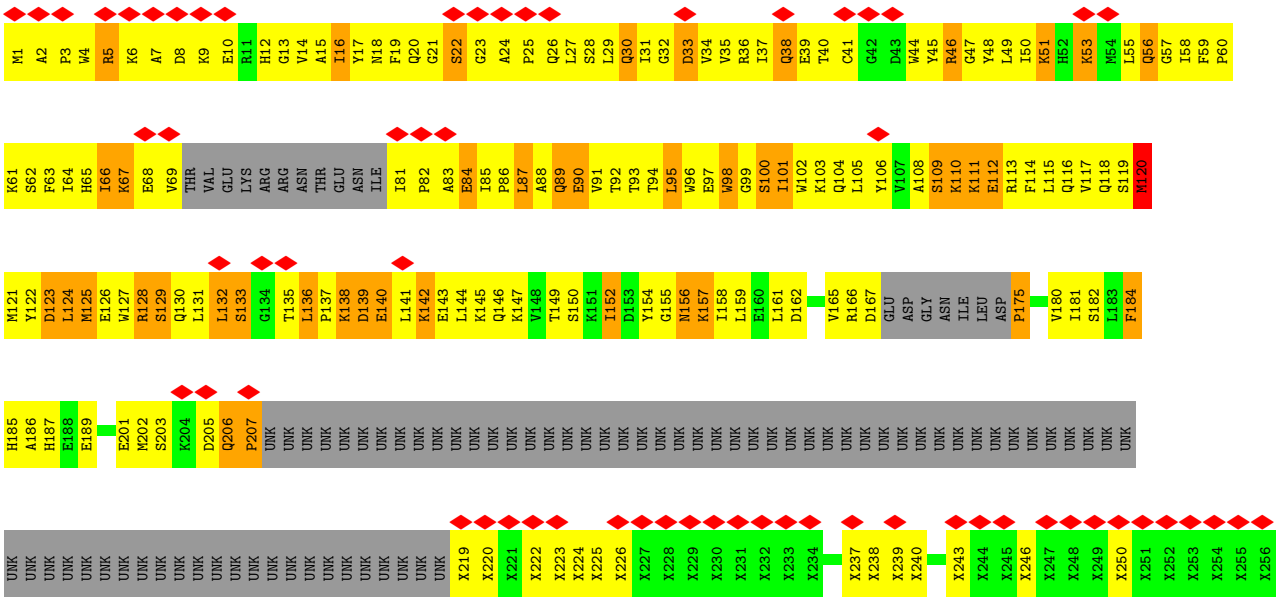


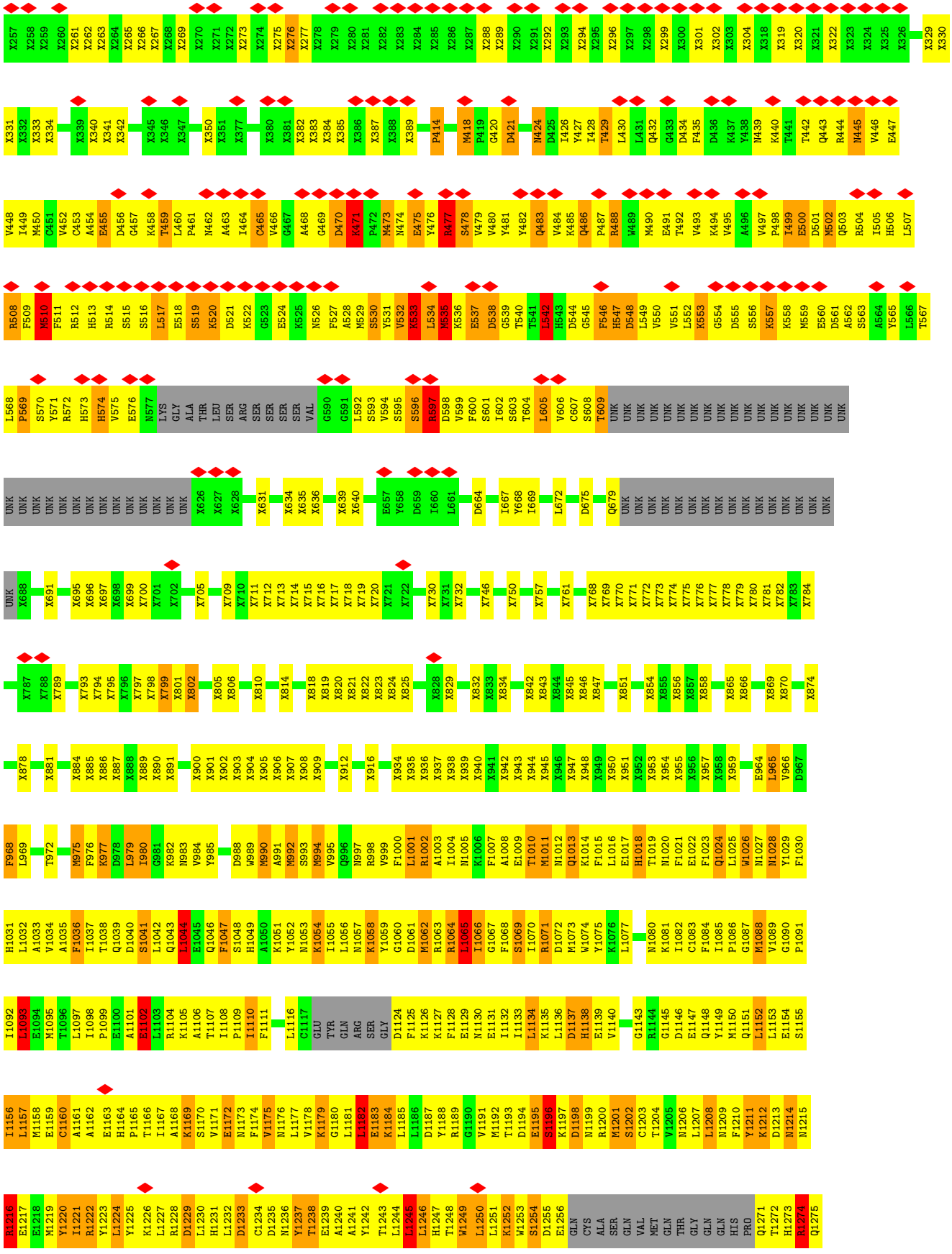

T541 L542 H543 D544 G545 F546 H547 D548 L549 V550 V551 L552 K553 G554 D555 S556 K557 K558 M559 E560 D561 A562 S563 A564 Y565 L566 T567 L568 P569 S570 Y571 R572 H573 H574 V575 E576 N577 LYS GLY ALA THR LEU SER ARG SER SER SER SER VAL G590 G591 L592 S593 V594 S595 S596 R597 D598 V599 F600
S601 I602 S603 T604 L605 V606 C607 S608 T609 UNK UNK UNK

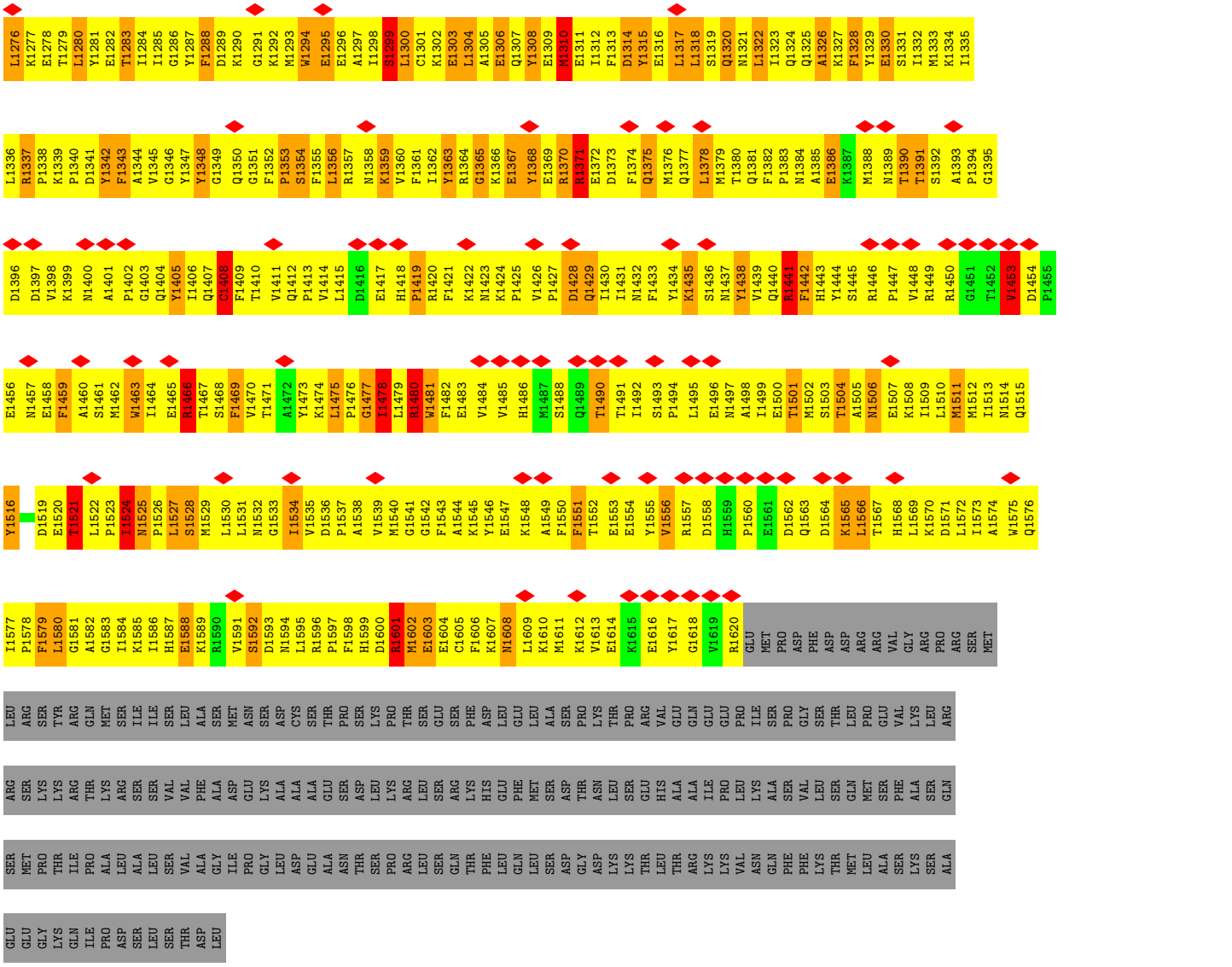


• Molecule 1: Dedicator of cytokinesis protein 2

Chain D:

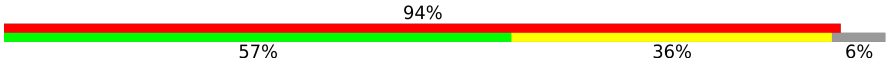


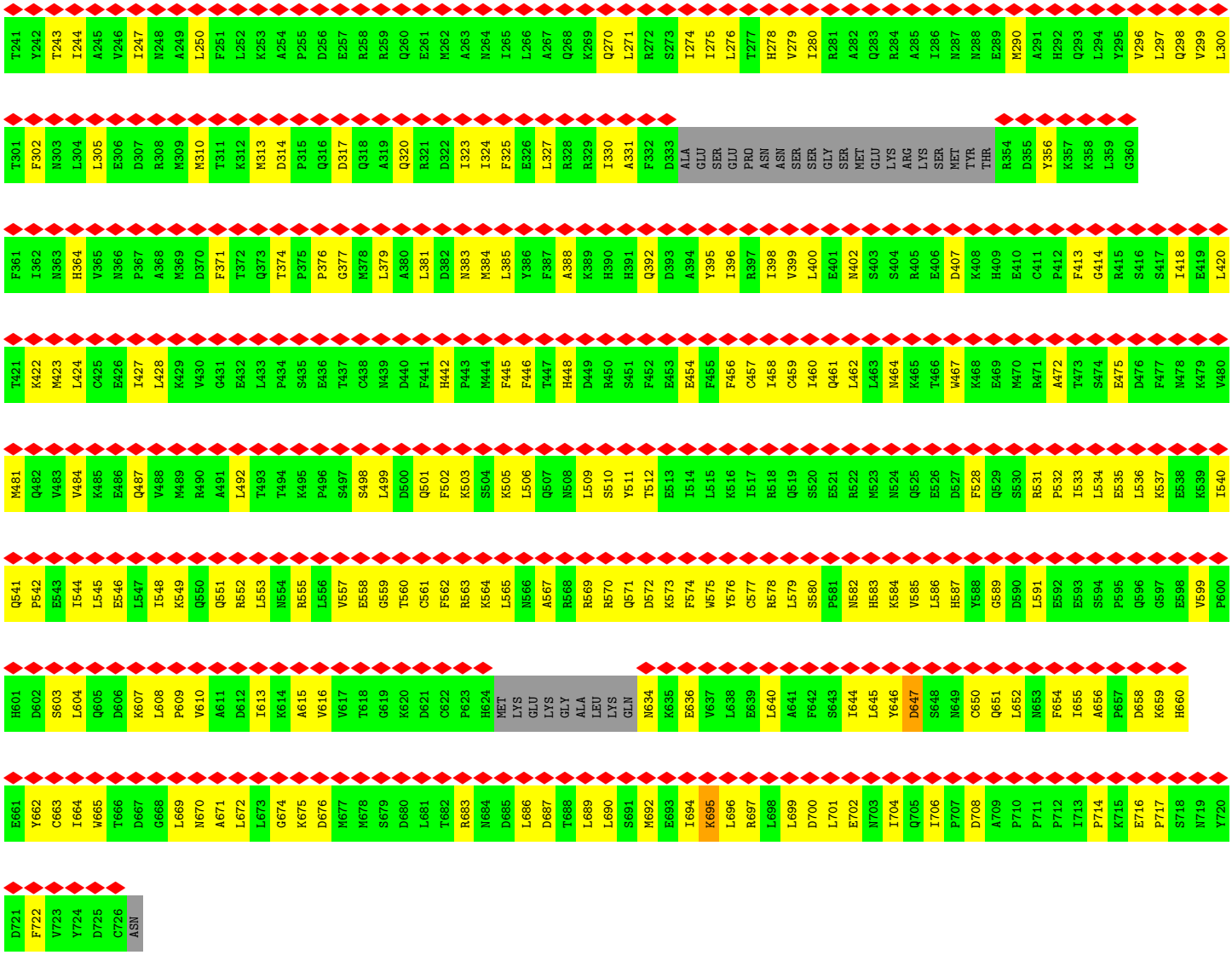




• Molecule 2: Engulfment and cell motility protein 1

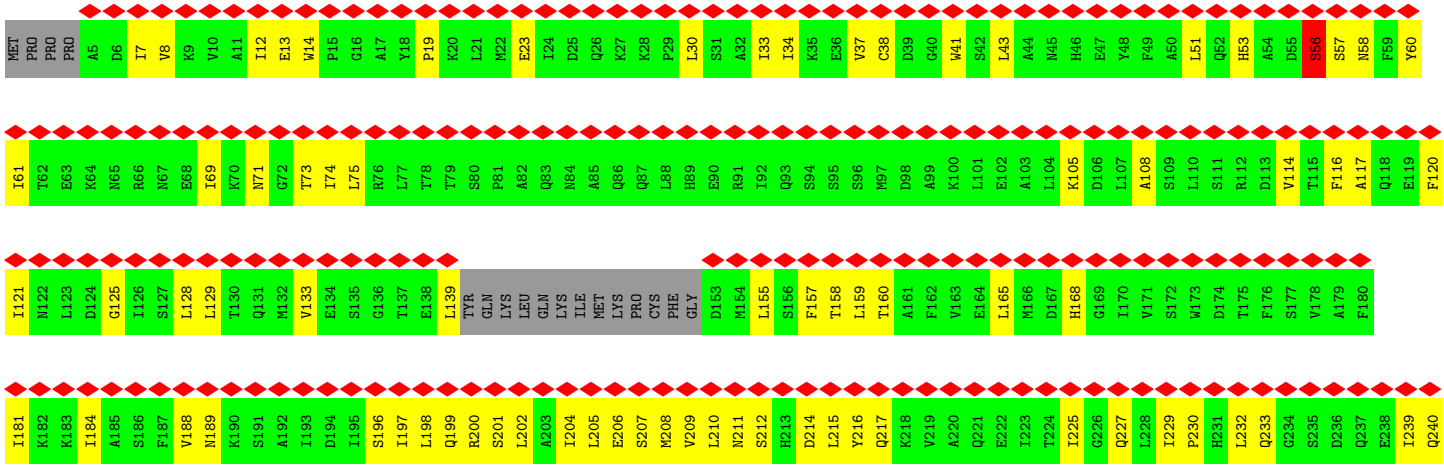
Chain B:

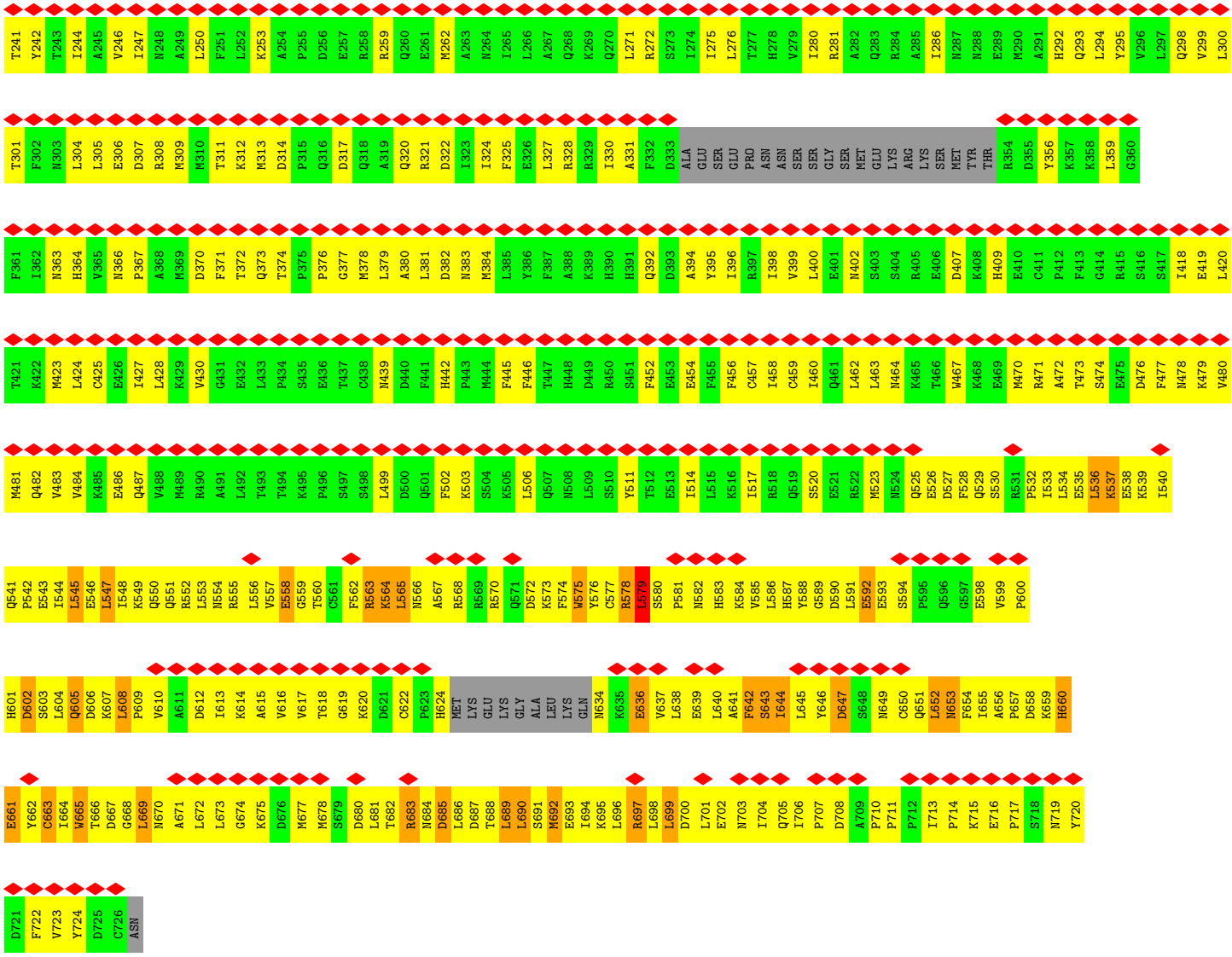




• Molecule 2: Engulfment and cell motility protein 1

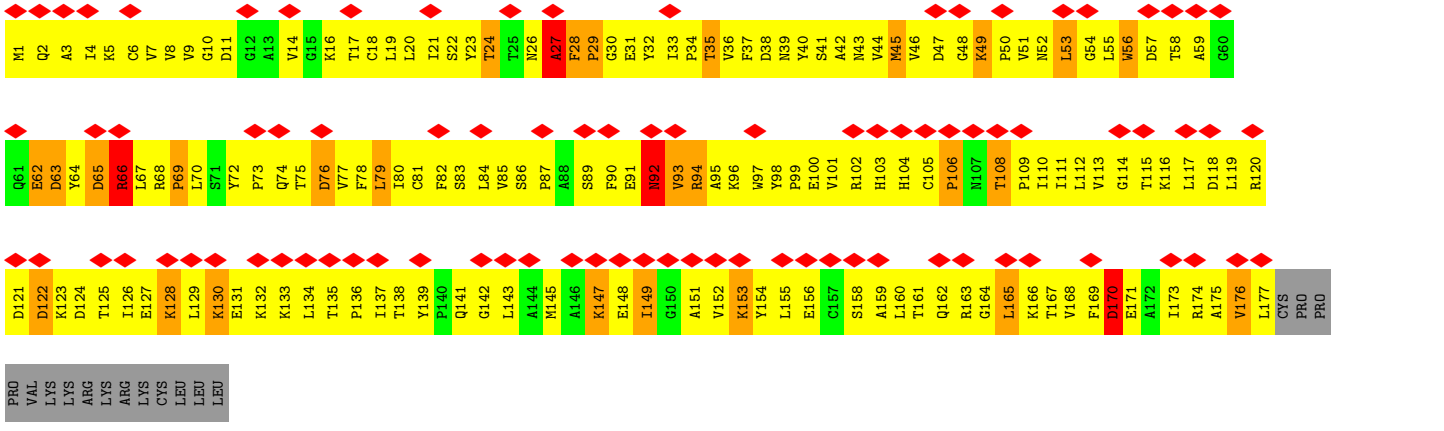
Chain E:





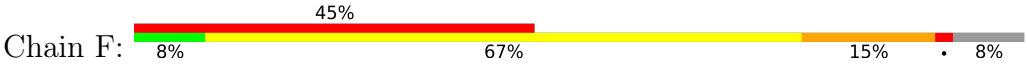
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

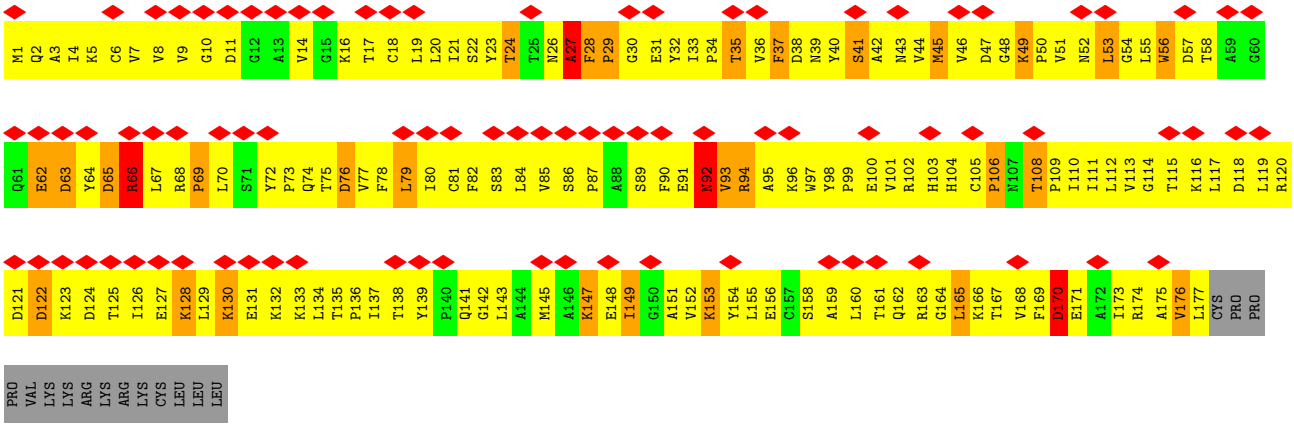
Chain C:



• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F:


45%
8%
67%
15%
8%


M1 Q2 A3 I4 K5 C6 V7 V8 V9 G10 D11 G12 A13 V14 G15 K16 T17 C18 L19 L20 I21 S22 Y23 T24 T25 N26 A27 F28 P29 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 Y40 S41 A42 N43 V44 M45 V46 D47 G48 K49 P50 V51 N52 L53 G54 L55 W56 D57 T58 A59 G60
Q61 E62 D63 Y64 D65 R66 L67 R68 P69 L70 S71 Y72 P73 Q74 T75 D76 V77 F78 L79 I80 C81 F82 S83 L84 V85 S86 P87 A88 S89 F90 E91 N92 V93 R94 A95 K96 W97 Y98 P99 E100 V101 R102 H103 H104 C105 P106 N107 T108 P109 I110 I111 L112 V113 G114 T115 K116 L117 D118 L119 R120
D121 D122 K123 D124 T125 I126 E127 K128 L129 K130 E131 K132 K133 L134 T135 P136 I137 T138 Y139 P140 Q141 G142 L143 A144 M145 A146 K147 E148 I149 G150 A151 V152 K153 Y154 L155 E156 C157 S158 A159 L160 T161 Q162 R163 G164 L165 K166 T167 V168 F169 D170 E171 A172 I173 R174 A175 V176 L177 CYS PRO PRO
PRO VAL LYS LYS ARG LYS ARG LYS CYS LEU LEU LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	245763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	403.25998, 403.25998, 403.25998	wwPDB
Map dimensions	282, 282, 282	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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	0.97	28/8364 (0.3%)	1.08	52/11318 (0.5%)
1	D	0.97	27/8364 (0.3%)	1.08	52/11318 (0.5%)
2	B	0.27	0/5147	0.50	0/6959
2	E	0.56	6/5149 (0.1%)	0.76	15/6961 (0.2%)
3	C	0.80	2/1413 (0.1%)	1.12	9/1922 (0.5%)
3	F	0.80	2/1413 (0.1%)	1.12	9/1922 (0.5%)
All	All	0.81	65/29850 (0.2%)	0.95	137/40400 (0.3%)

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	33
1	D	0	33
2	B	0	2
2	E	0	8
3	C	0	2
3	F	0	3
All	All	0	81

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1363	TYR	CD2-CE2	-10.37	1.23	1.39
1	D	1363	TYR	CD2-CE2	-10.32	1.23	1.39
1	A	1294	TRP	CB-CG	-10.23	1.31	1.50
1	D	1294	TRP	CB-CG	-10.18	1.31	1.50
2	E	661	GLU	CB-CG	-8.07	1.36	1.52

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1300	LEU	CA-CB-CG	-15.88	78.78	115.30
1	D	1300	LEU	CA-CB-CG	-15.88	78.78	115.30
1	D	1521	THR	C-N-CA	12.32	152.51	121.70
1	A	1521	THR	C-N-CA	12.32	152.49	121.70
2	E	699	LEU	CA-CB-CG	-11.82	88.12	115.30

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	LEU	Peptide
1	A	276	UNK	Peptide
1	A	341	UNK	Peptide
1	A	418	MET	Peptide
1	A	66	ILE	Peptide

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	10203	0	8220	2225	0
1	D	10203	0	8220	2247	0
2	B	5054	0	4721	255	0
2	E	5056	0	4724	670	0
3	C	1383	0	1405	443	0
3	F	1383	0	1405	416	0
All	All	33282	0	28695	5998	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 97.

The worst 5 of 5998 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:D:1441:ARG:HA	1:D:1469:PHE:O	1.25	1.31
2:E:641:ALA:HA	2:E:654:PHE:O	1.33	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:ARG:HA	1:A:1469:PHE:O	1.25	1.24
1:D:1585:LYS:O	1:D:1588:GLU:HB3	1.36	1.20
1:D:1346:GLY:O	1:D:1406:ILE:HA	1.39	1.20

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	1029/1830 (56%)	689 (67%)	312 (30%)	28 (3%)	5 33
1	D	1029/1830 (56%)	689 (67%)	312 (30%)	28 (3%)	5 33
2	B	672/727 (92%)	641 (95%)	29 (4%)	2 (0%)	41 75
2	E	672/727 (92%)	593 (88%)	75 (11%)	4 (1%)	25 63
3	C	175/192 (91%)	121 (69%)	49 (28%)	5 (3%)	4 32
3	F	175/192 (91%)	121 (69%)	49 (28%)	5 (3%)	4 32
All	All	3752/5498 (68%)	2854 (76%)	826 (22%)	72 (2%)	11 39

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	A	414	PRO
1	A	1196	SER
1	A	1238	THR
1	A	1428	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	829/1180 (70%)	635 (77%)	194 (23%)	1 5
1	D	829/1180 (70%)	635 (77%)	194 (23%)	1 5
2	B	497/662 (75%)	493 (99%)	4 (1%)	81 88
2	E	498/662 (75%)	486 (98%)	12 (2%)	49 69
3	C	153/168 (91%)	130 (85%)	23 (15%)	3 17
3	F	153/168 (91%)	130 (85%)	23 (15%)	3 17
All	All	2959/4020 (74%)	2509 (85%)	450 (15%)	6 16

5 of 450 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
3	F	122	ASP
1	D	508	ARG
3	F	86	SER
1	D	1466	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1199	ASN
2	E	240	GLN
1	D	1275	GLN
1	D	1568	HIS
2	E	303	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
1	D	7

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	389:UNK	C	412:GLY	N	30.55
1	D	389:UNK	C	412:GLY	N	30.55
1	A	351:UNK	C	377:UNK	N	20.14
1	D	351:UNK	C	377:UNK	N	20.14
1	A	892:UNK	C	896:UNK	N	9.23

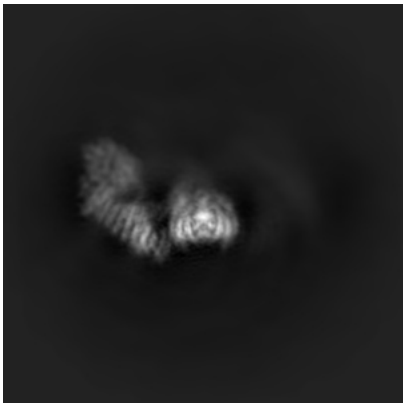
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10498. These allow visual inspection of the internal detail of the map and identification of artifacts.

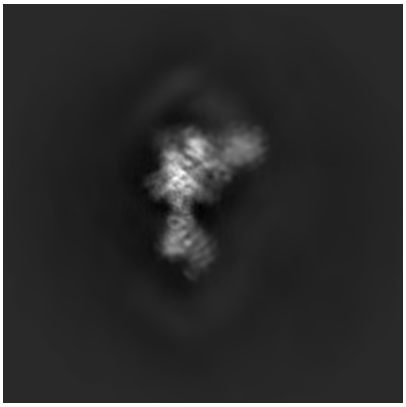
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

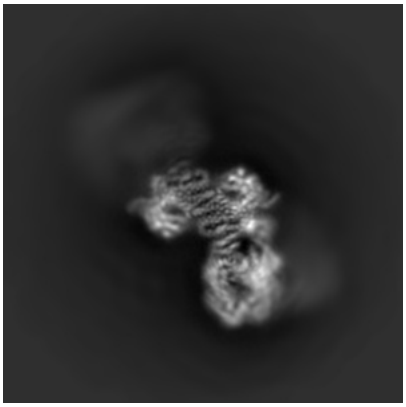
6.1.1 Primary map



X



Y



Z

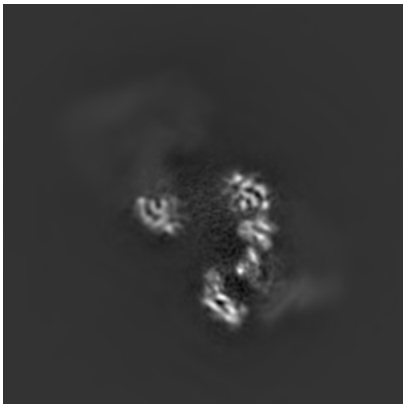
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 141

Y Index: 141

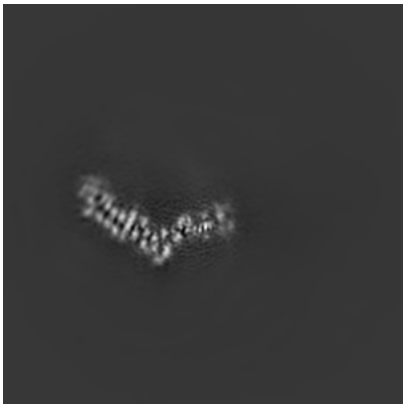


Z Index: 141

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

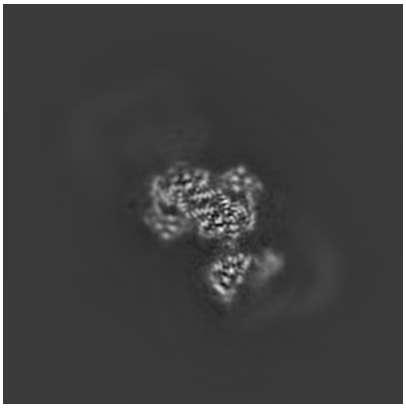
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 156

Y Index: 124



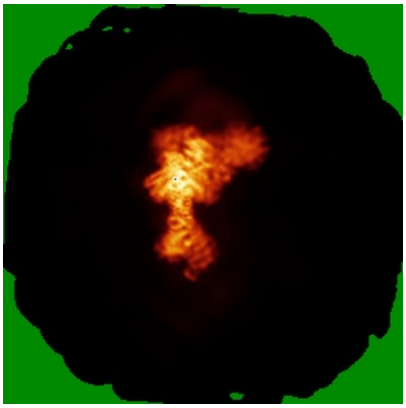
Z Index: 124

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

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

6.4.1 Primary map

X



Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

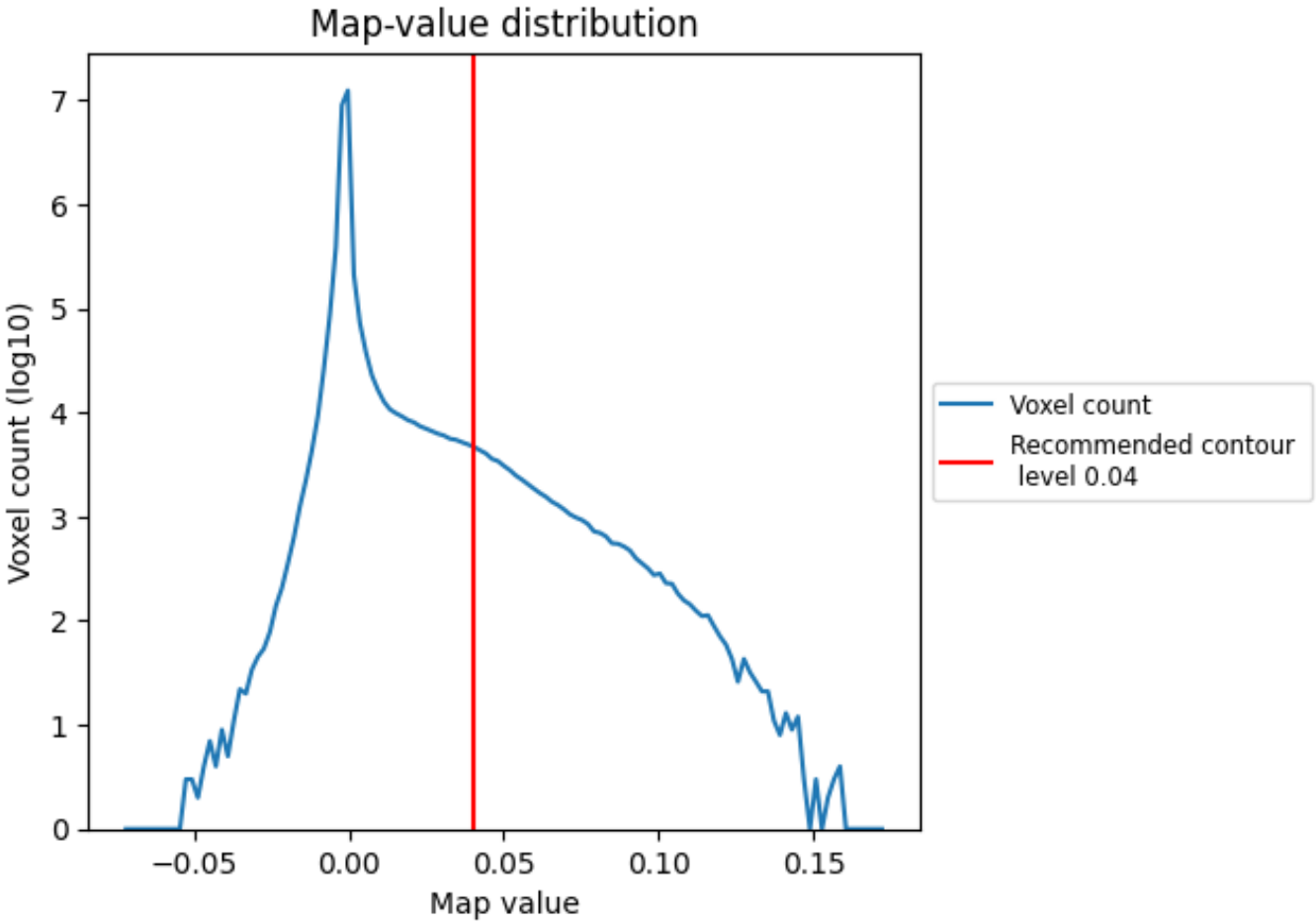
6.6 Mask visualisation (i)

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

7 Map analysis

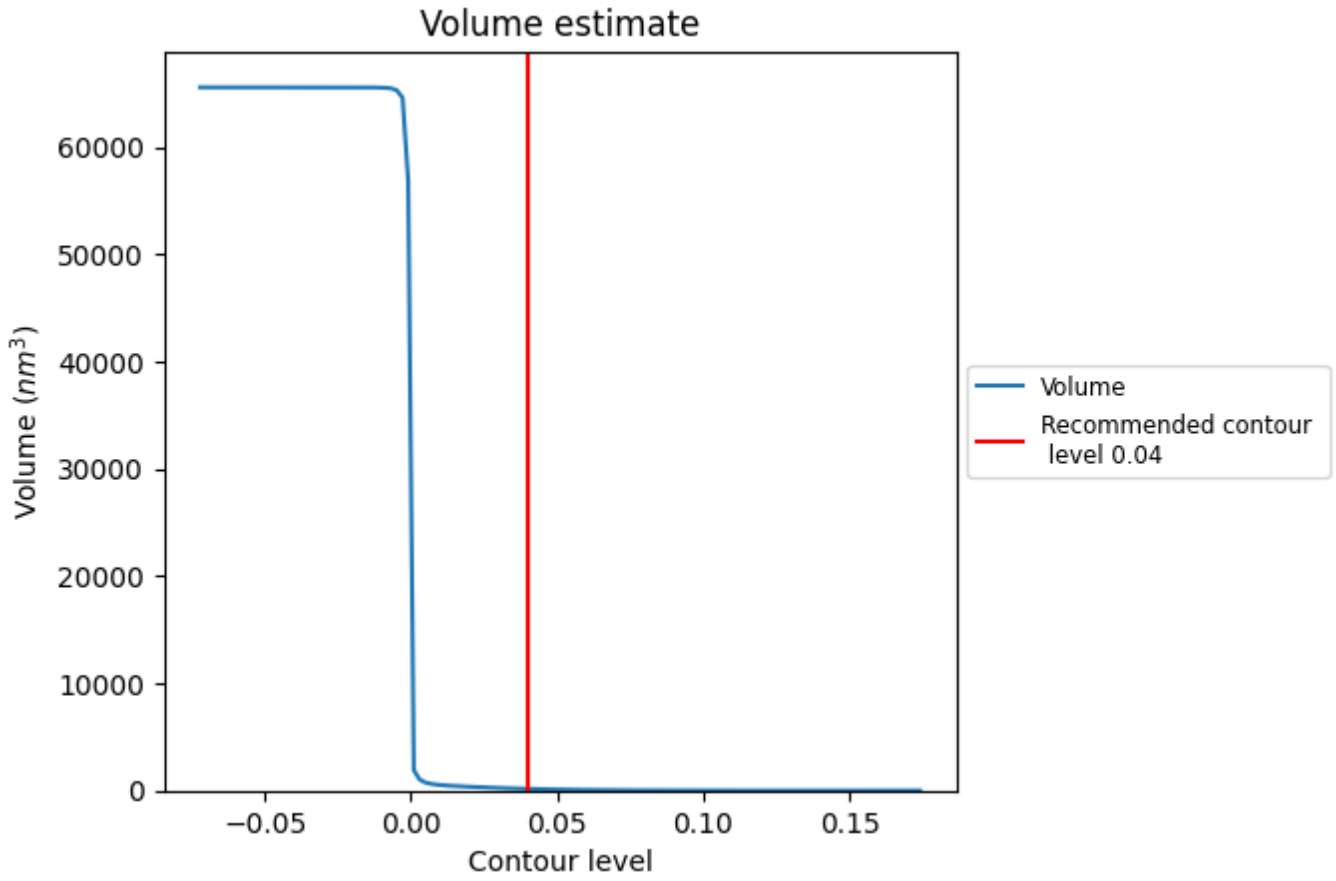
This section contains the results of statistical analysis of the map.

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.

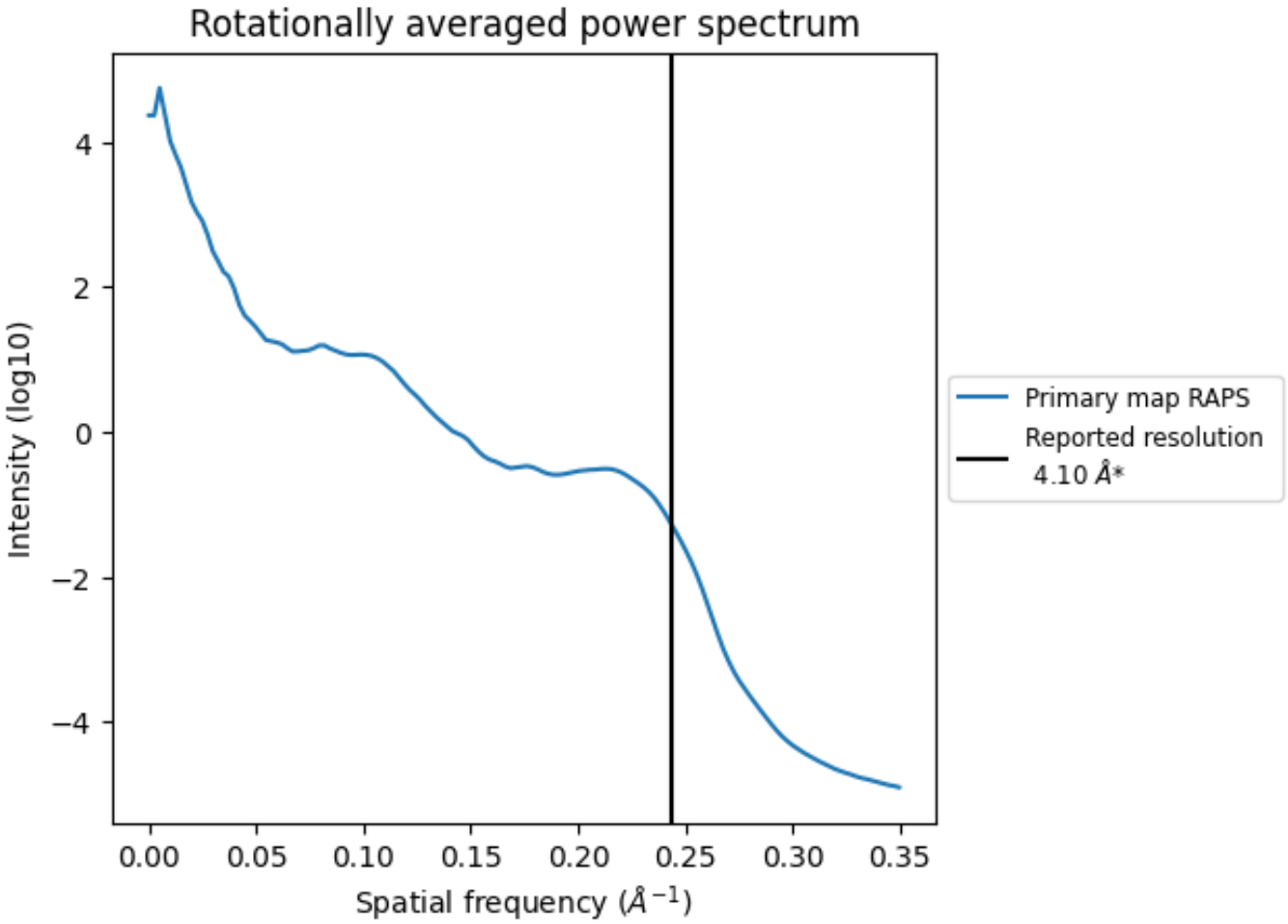
7.2 Volume estimate (i)



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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 0.244 Å^{-1}

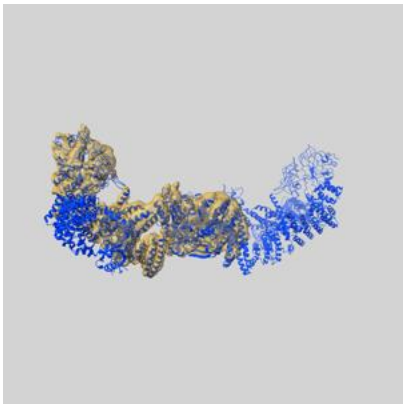
8 Fourier-Shell correlation (i)

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

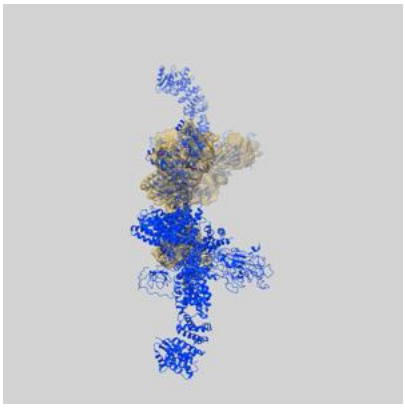
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10498 and PDB model 6TGC. Per-residue inclusion information can be found in section 3 on page 29.

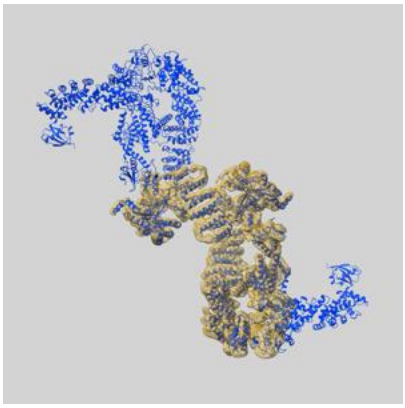
9.1 Map-model overlay



X



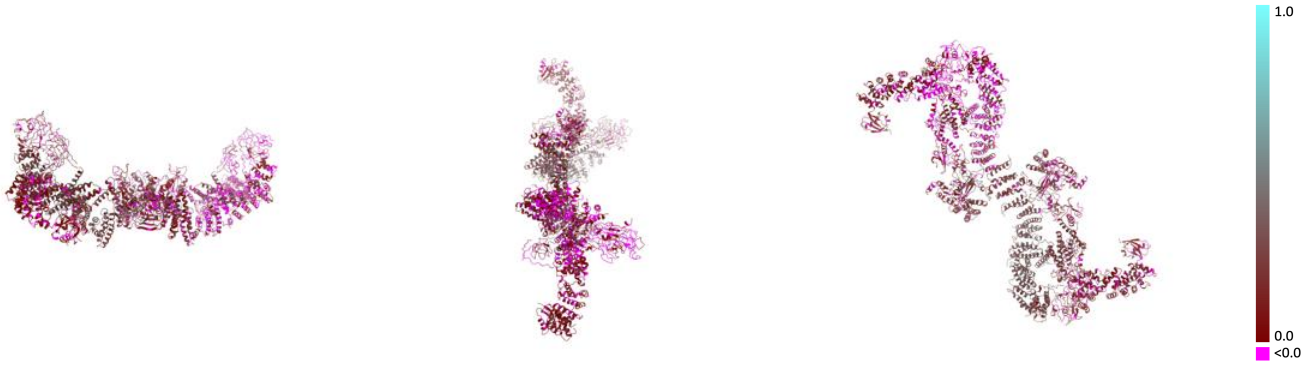
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

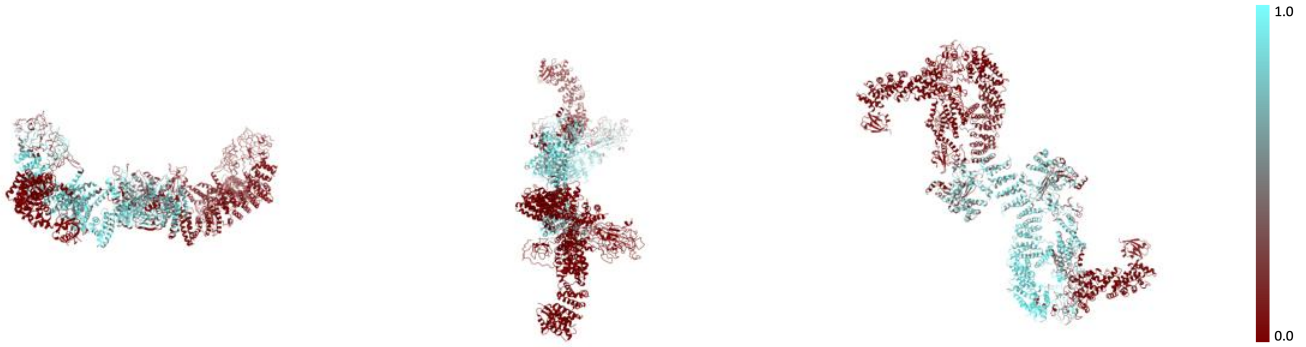
9.2 Q-score mapped to coordinate model (i)



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.

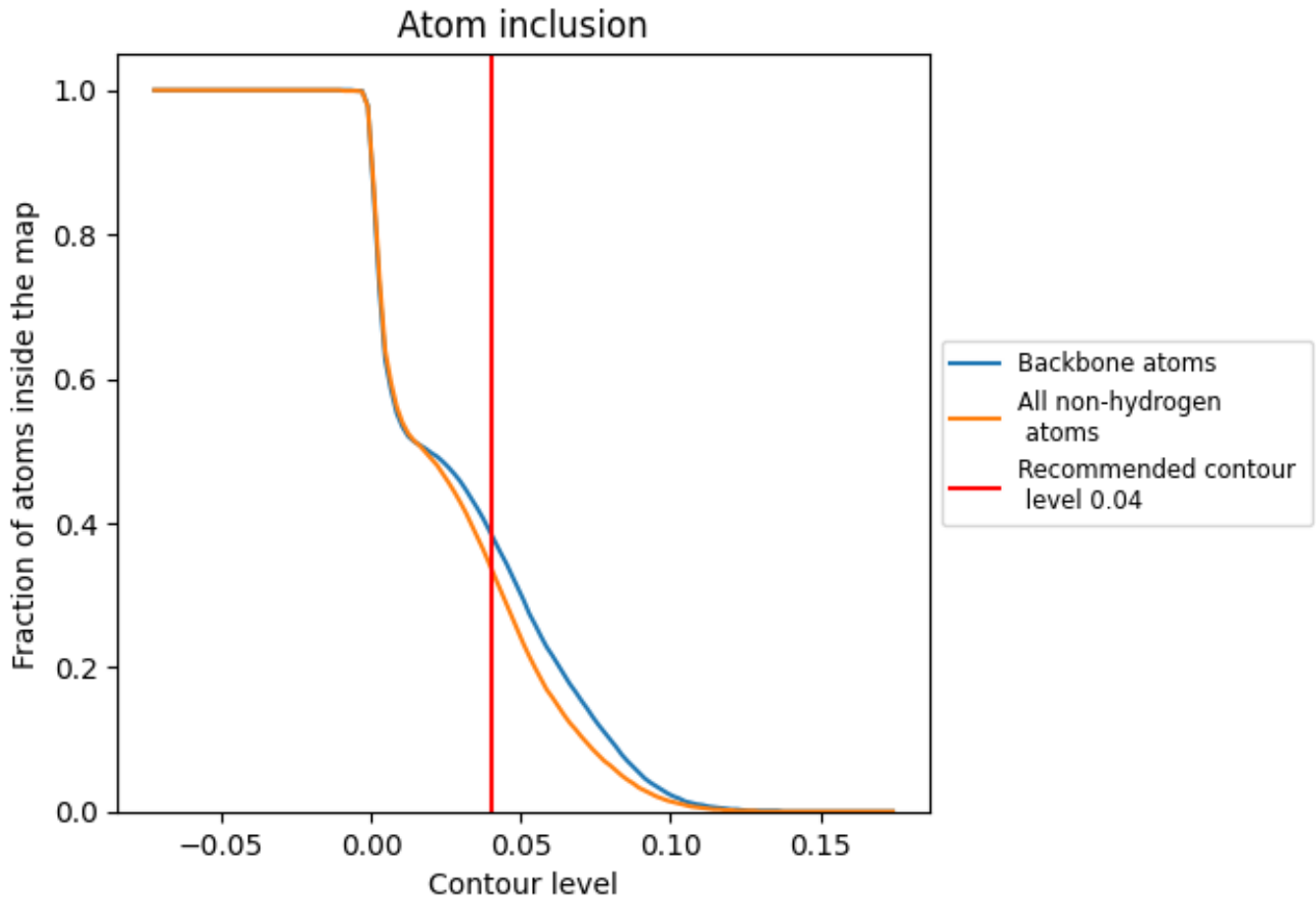
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 39% of all backbone atoms, 34% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3390	0.1290
A	0.2110	0.0740
B	0.0010	0.0570
C	0.4220	0.1730
D	0.6980	0.2220
E	0.1610	0.1160
F	0.4460	0.1180