



## wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:41 pm GMT

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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.3

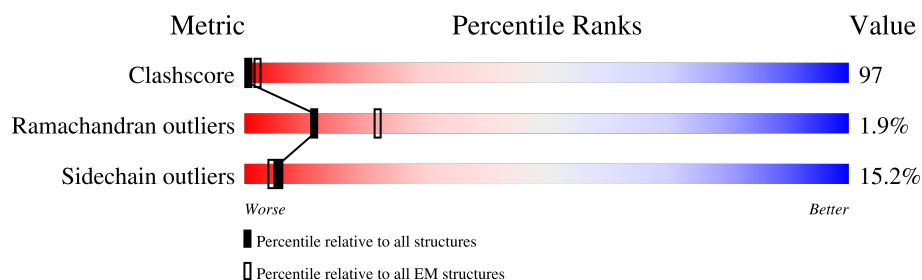
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1830	
1	D	1830	
2	B	727	
2	E	727	
3	C	192	
3	F	192	

## 2 Entry composition

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		

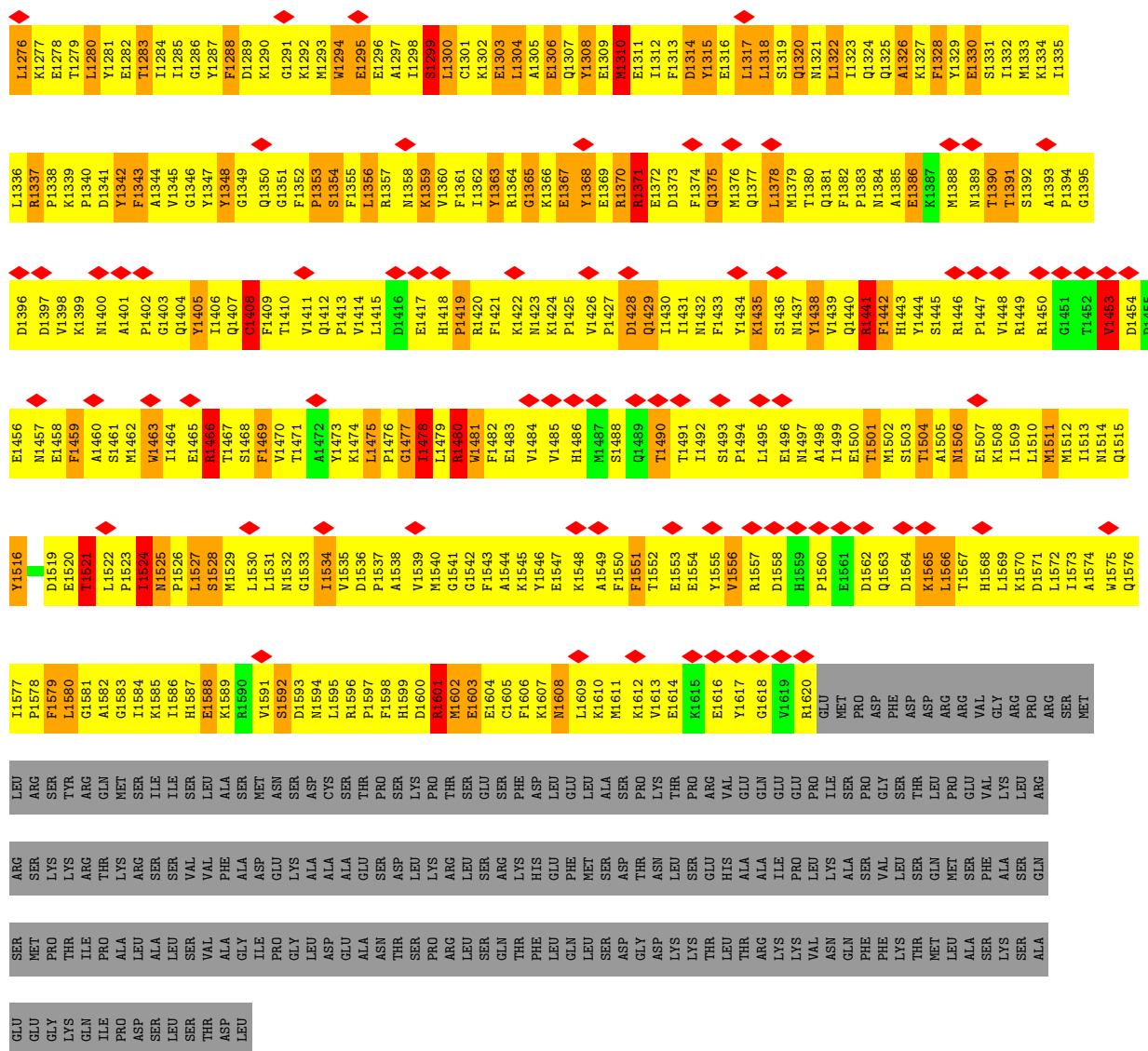




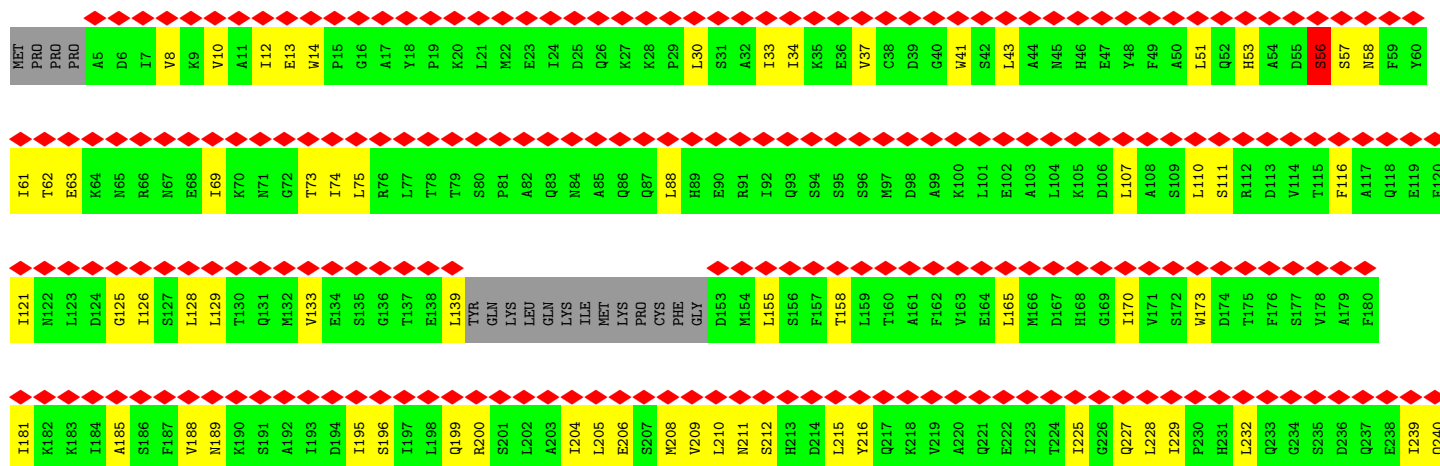
GLN	M1201	E1141	K1081	F1021	X960	X887	X827	X766	X701	M650	S601	T541
VAL	S1202	G1142	I1082	E1022	S962	X888	X828	X767	X702	E651	I602	L542
MET	C1203	G1143	C1083	F1023	S963	X889	X829	X768	X703	H652	T603	H543
THR	T1204	R1144	F1084	Q1024	E964	X890	X830	X769	X704	S653	T604	D544
GLY	V1205	G1145	I1085	L1025	L965	X891	X831	X770	X705	Q654	L605	G545
GLN	N1206	D1146	P1086	V1026	V966	X892	X832	X771	X706	S655	V606	F546
GLN	L1207	E1147	G1087	N1027	D967	X896	X833	X772	X707	D656	C607	H547
HIS	L1208	Q1148	M1088	N1028	F968	X897	X834	X773	X708	E657	S608	D548
PRO	N1209	Q1271	N1209	N1209	F968	X897	X834	X774	X709	Y658	T609	L549
Q1271	N1209	Q1271	N1209	N1209	F968	X897	X834	X774	X709	Y658	T609	L549
F1210	F1210	M1150	G1090	F1030	H970	X899	X836	X775	X710	UNK	UNK	V550
Y1211	Y1211	M1150	G1090	F1030	H970	X899	X836	X775	X710	UNK	UNK	V550
K1274	K1274	Q1275	P1091	H1031	E971	X900	X837	X776	X711	I660	UNK	V551
L1276	L1276	L1152	I1092	L1032	T972	X901	X838	X777	X712	L661	UNK	L552
K1277	K1277	L1153	L1093	L1033	F973	X902	X839	X778	X713	V662	UNK	K553
N1214	N1214	E1154	E1094	V1034	I974	X903	X840	X779	X714	F663	UNK	G554
N1215	N1215	S1155	M1095	A1035	N975	X904	X841	X780	X715	D664	UNK	D555
R1216	R1216	I1156	M1095	F1036	F976	X905	X842	X781	X716	A665	UNK	S556
E1217	E1217	L1157	L1097	I1037	X977	X906	X843	X782	X717	L666	UNK	K557
E1218	E1218	M1158	I1098	T1038	D976	X907	X844	X783	X718	I667	UNK	K558
M1219	M1219	E1159	P1099	T1039	L979	X908	X845	X784	X719	I667	UNK	K558
Y1220	Y1220	C1160	E1100	D1040	L980	X909	X846	X785	X720	I669	UNK	M559
I1285	I1285	A1161	A1101	S1041	G981	X910	X847	X786	X721	I670	UNK	E560
G1286	G1286	A1162	F1102	L1042	X982	X911	X848	X787	X722	G671	UNK	D561
Y1287	Y1287	E1163	L1103	Q1043	X983	X912	X849	X788	X723	L672	UNK	A562
F1288	F1288	H1164	R1104	L1044	V984	X913	X850	X789	X724	I673	UNK	S563
K1290	K1290	P1165	K1105	E1045	Y985	X914	X851	X790	X725	A674	UNK	A564
G1291	G1291	T1166	A1106	Q1046	P986	X915	X852	X791	X726	A674	UNK	Y565
K1292	K1292	I1167	T1107	Q1047	G987	X916	X853	X792	X727	D675	UNK	L566
M1293	M1293	I1167	T1107	F1047	D988	X917	X854	X793	X728	R676	UNK	T567
W1294	W1294	A1168	I1108	S1048	D988	X918	X855	X794	X729	K677	UNK	L568
E1295	E1295	K1169	P1109	H1049	X989	X919	X856	X795	X730	F678	UNK	P569
A1296	A1296	S1170	I1110	A1050	N990	X919	X856	X795	X730	Q679	UNK	S570
H1231	H1231	V1171	F1111	K1051	A991	X920	X857	X796	X731	UNK	UNK	Y571
D1232	D1232	E1172	F1112	Y1052	N992	X921	X858	X797	X732	UNK	UNK	R572
C1234	C1234	M1173	D1113	M1053	S993	X922	X859	X798	X733	UNK	UNK	H573
E1235	E1235	F1174	M1114	K1054	N994	X923	X860	X799	X734	UNK	UNK	H574
T1238	T1238	V1175	M1115	I1055	V995	X934	X861	X801	X735	UNK	UNK	
E1239	E1239	L1116	L1116	L1056	Q996	X935	X862	X802	X735	UNK	X626	V575
A1241	A1241	L1177	C1117	M1057	N997	X936	X863	X803	X736	UNK	X627	E576
Y1242	Y1242	GLU	GLU	M1057	N997	X936	X863	X803	X736	UNK	X628	N577
Q1307	Q1307	TVR	TVR	K1058	R998	X937	X864	X804	X743	UNK	X629	LYS
T1243	T1243	GLN	GLN	Y1059	V999	X937	X864	X804	X744	UNK	X630	GLY
L1244	L1244	ARG	ARG	G1060	F1000	X938	X865	X805	X744	UNK	X631	ALA
E1309	E1309	L1181	SER	D1061	L1001	X940	X866	X806	X745	UNK	X632	THR
M1310	M1310	L1245	GLY	M1062	R1002	X941	X867	X807	X746	UNK	X633	LEU
E1311	E1311	L1246	L1246	R1062	R1002	X941	X868	X808	X747	UNK	X634	ARG
I1312	I1312	L1182	L1182	R1063	A1003	X942	X869	X809	X748	UNK	X635	SER
F1313	F1313	K1184	F1125	R1064	A1003	X943	X870	X810	X749	UNK	X636	ARG
D1314	D1314	K1184	F1125	R1064	A1003	X943	X870	X810	X749	UNK	X636	SER
Y1315	Y1315	L1185	K1126	L1065	N1005	X944	X871	X811	X750	X688	X638	SER
E1316	E1316	L1186	K1127	I1066	N1005	X945	X872	X812	X751	X689	X638	SER
L1317	L1317	L1186	F1128	I1066	K1006	X945	X873	X813	X752	X690	X638	SER
K1252	K1252	D1187	F1128	G1067	F1007	X946	X874	X814	X753	X691	X639	VAL
W1253	W1253	D1187	E1129	F1068	F1007	X946	X874	X814	X753	X692	X640	G590
S1254	S1254	Y1188	N1130	S1069	A1008	X947	X875	X815	X754	X693	X641	G591
D1255	D1255	R1189	E1131	I1070	E1009	X948	X876	X816	X755	X694	X642	S593
E1256	E1256	G1190	L1132	I1071	T1010	X949	X877	X817	X756	X695	I648	V594
		V1191	T1132	R1071	M1011	X950	X878	X818	X757	X696	S595	S595
GLN	GLN	M1192	L1133	D1072	N1012	X951	X878	X818	X757	X697	M649	S596
CYS	CYS	M1192	L1133	D1072	N1012	X951	X878	X818	X757	X697	M649	S596
ALA	ALA	T1193	L1134	M1073	Q1013	X952	X879	X819	X758	X698		R597
SER	SER	K1135	L1135	M1073	Q1013	X952	X879	X819	X758	X698		R597
		L1194	K1136	Y1074	F1014	X953	X880	X820	X759	X699		D598
		E1195	D1137	Y1075	F1015	X954	X881	X821	X760	X700		V599
		S1196	D1137	K1076	L1016	X955	X882	X822	X761			F600
		K1197	H1138	L1077	E1017	X956	X883	X823	X762			
		N1198	E1139	G1076	H1018	X957	X884	X824	X763			
		N1199	E1139	G1076	H1018	X957	X884	X824	X763			
			V1140	Q1079	T1019	X958	X885	X825	X764			
			N1080	N1080	N1020	X959	X886	X826	X765			



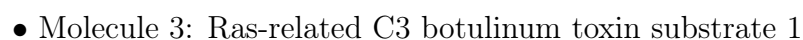


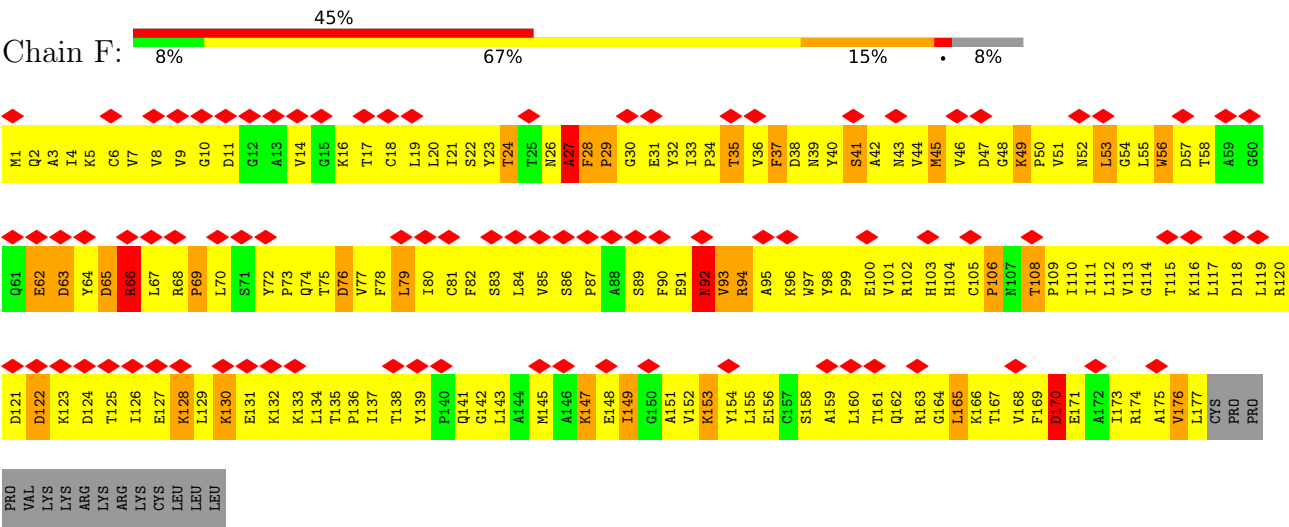


● Molecule 2: Engulfment and cell motility protein 1











## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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(°)	Ideal(°)
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 ⓘ

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 ⓘ

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

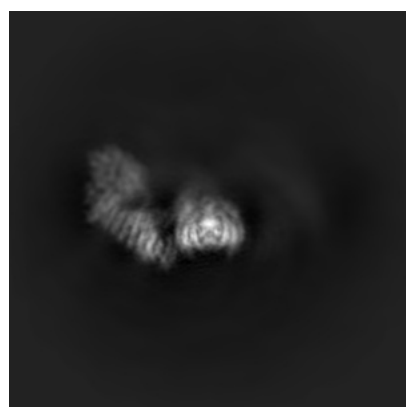
## 6 Map visualisation [i](#)

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.

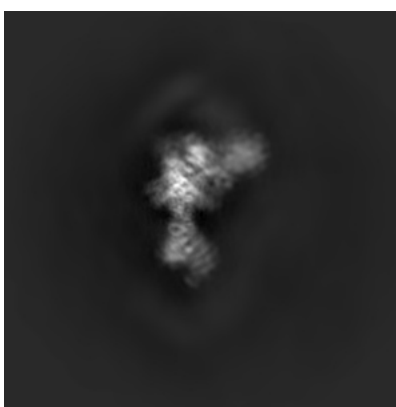
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

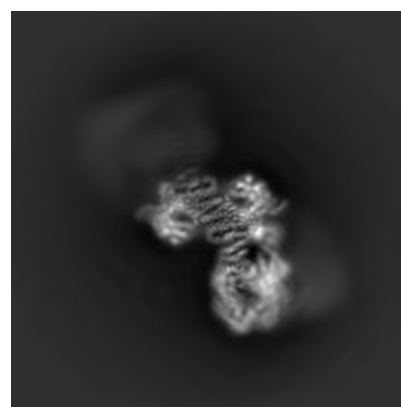
#### 6.1.1 Primary map



X



Y

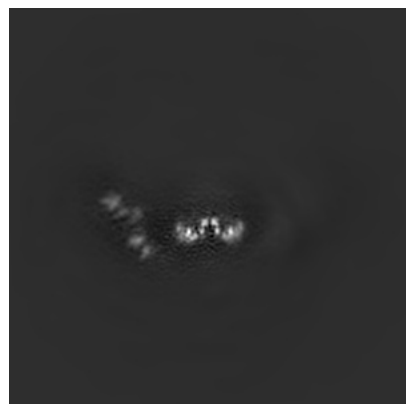


Z

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

### 6.2 Central slices [i](#)

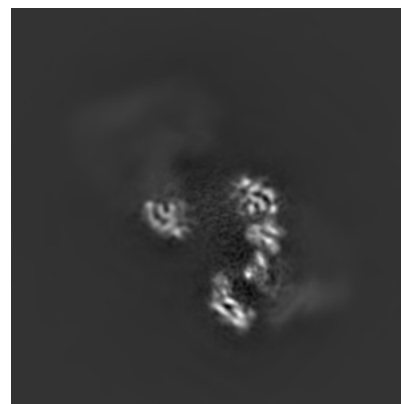
#### 6.2.1 Primary map



X Index: 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](#)

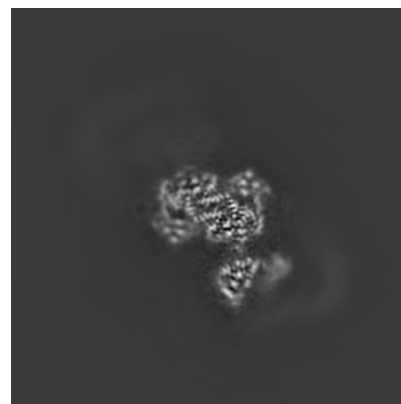
### 6.3.1 Primary map



X Index: 156



Y Index: 124

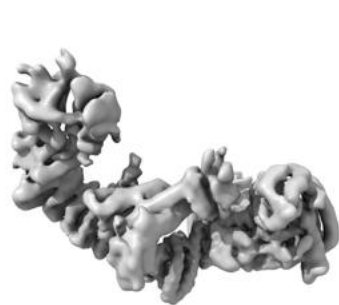


Z Index: 124

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 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.

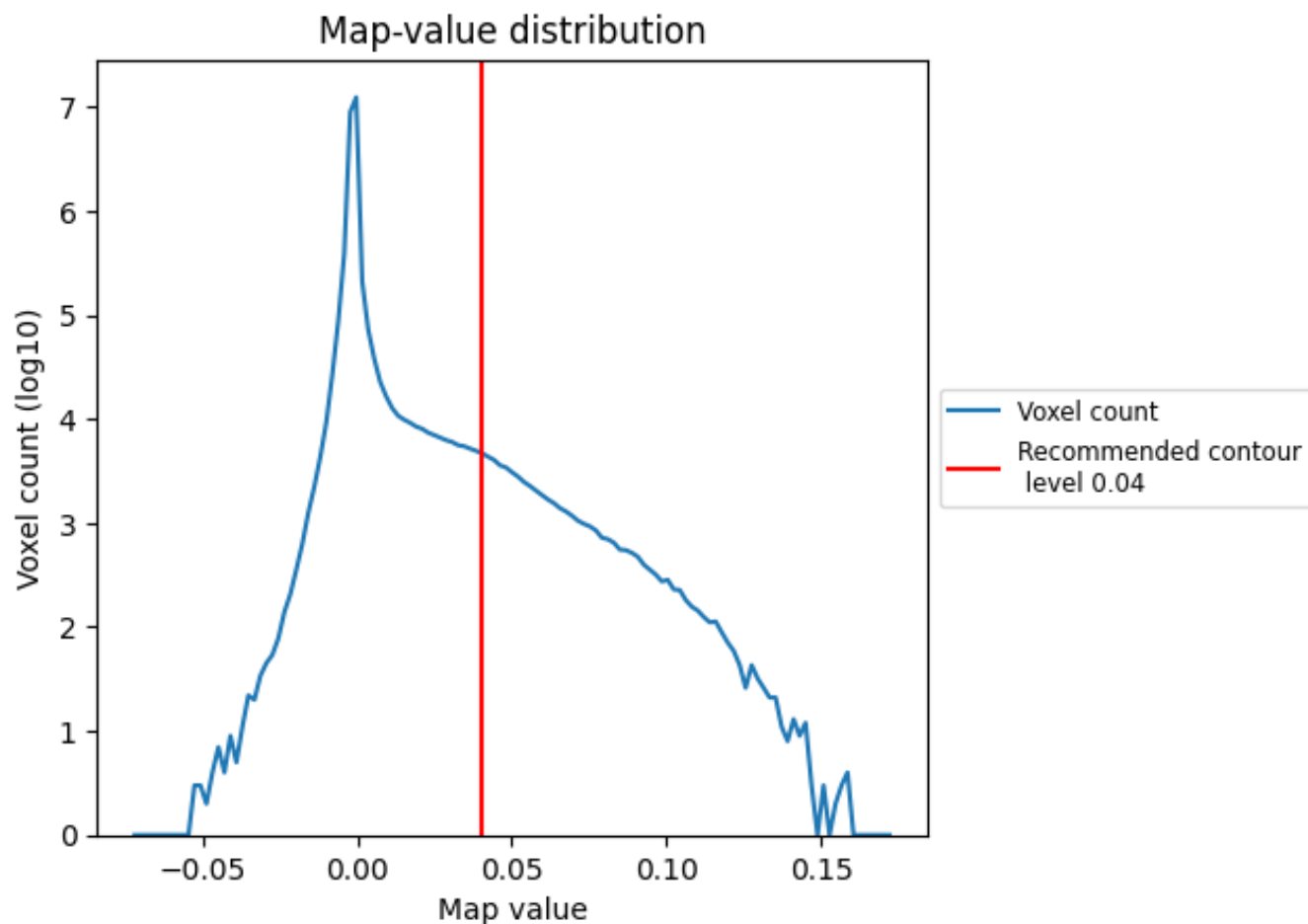
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

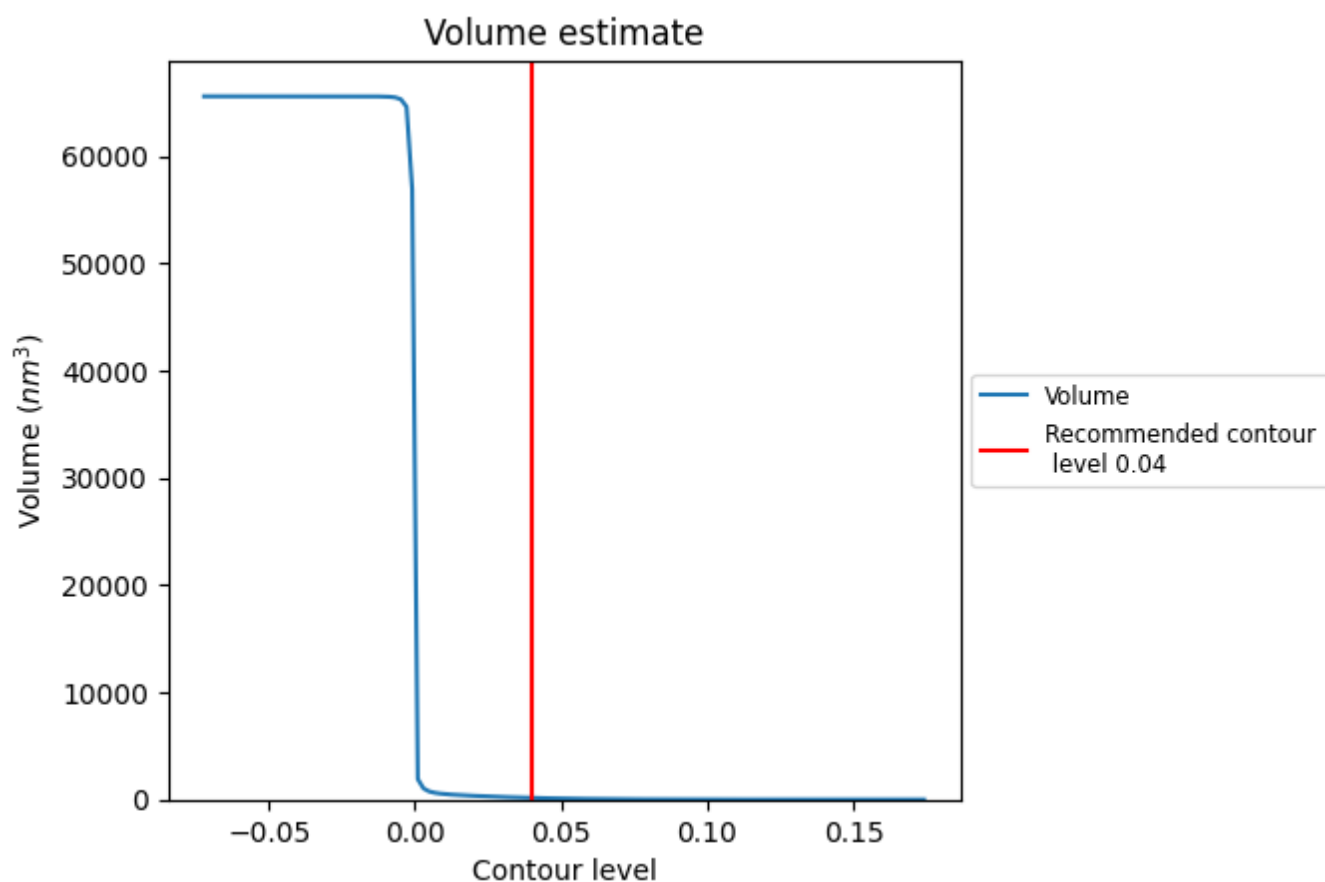
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

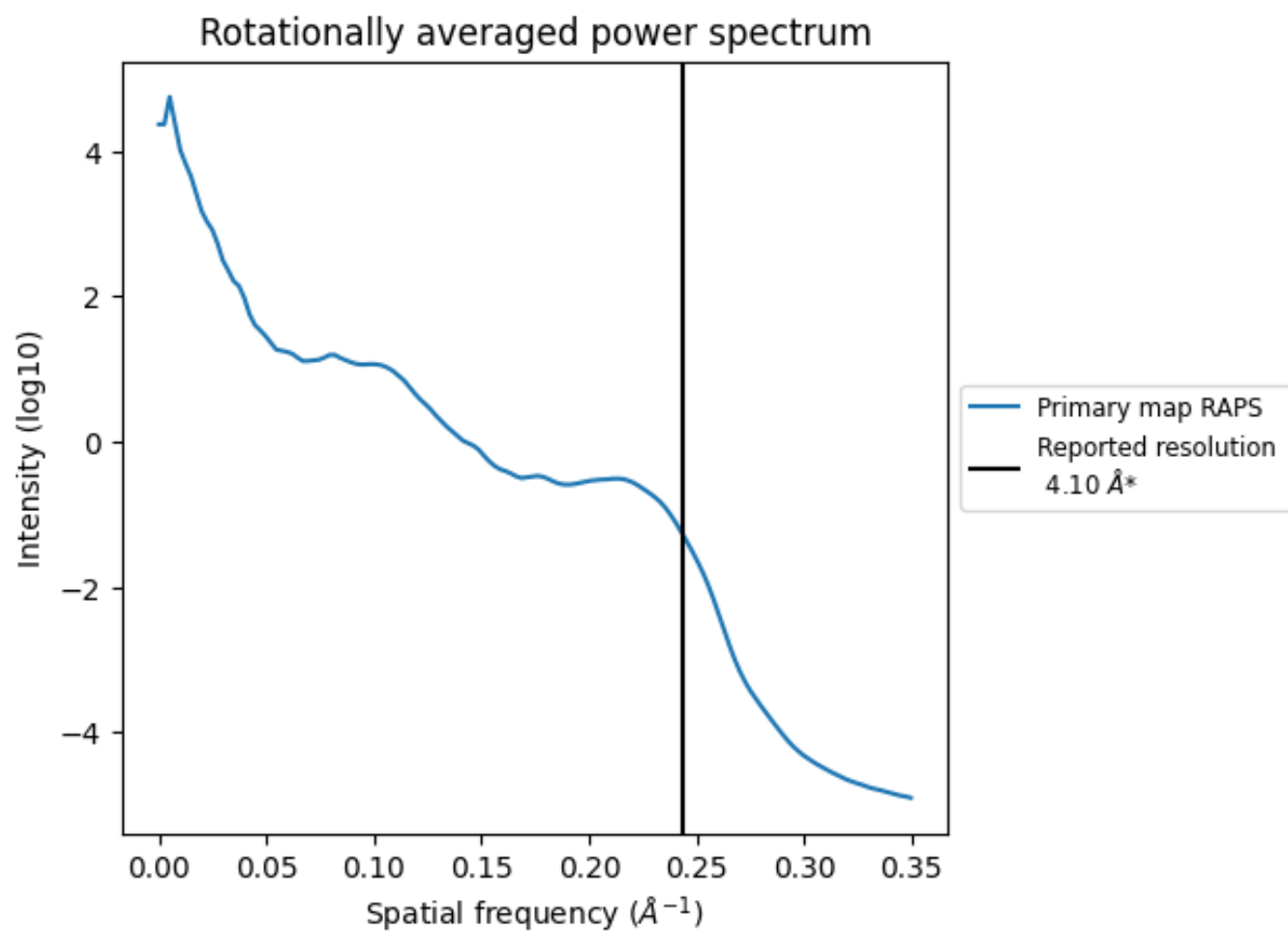
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm<sup>3</sup>; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.244  $\text{\AA}^{-1}$

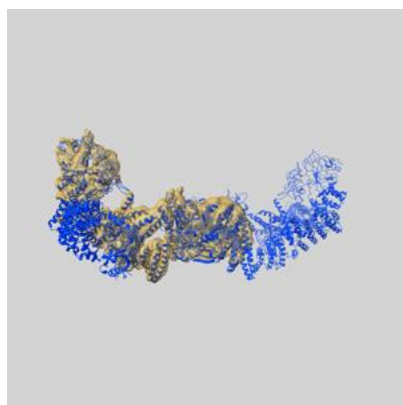
## 8 Fourier-Shell correlation

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

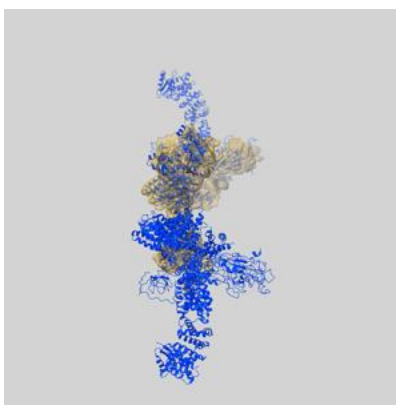
## 9 Map-model fit [i](#)

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](#).

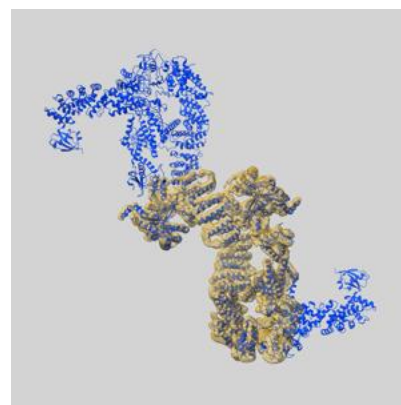
### 9.1 Map-model overlay [i](#)



X



Y

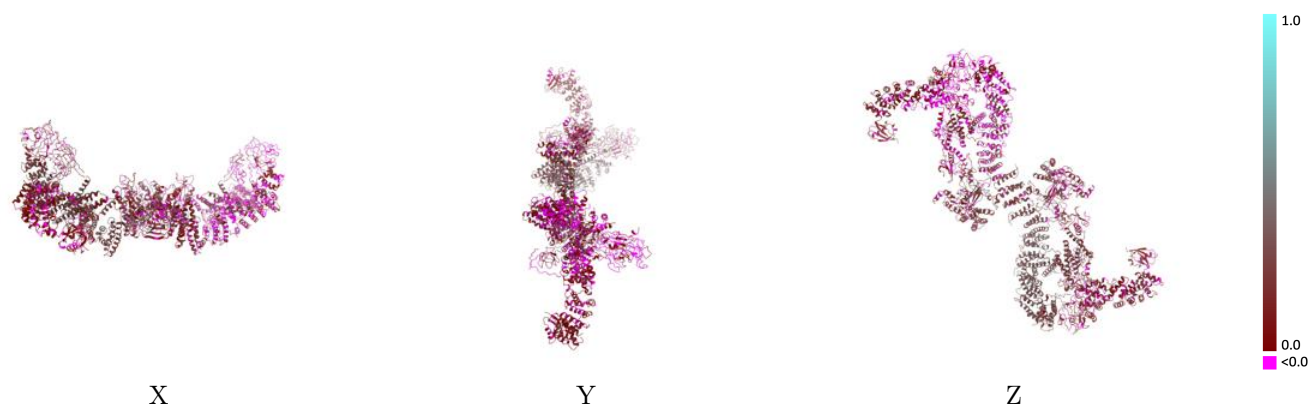


Z

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.

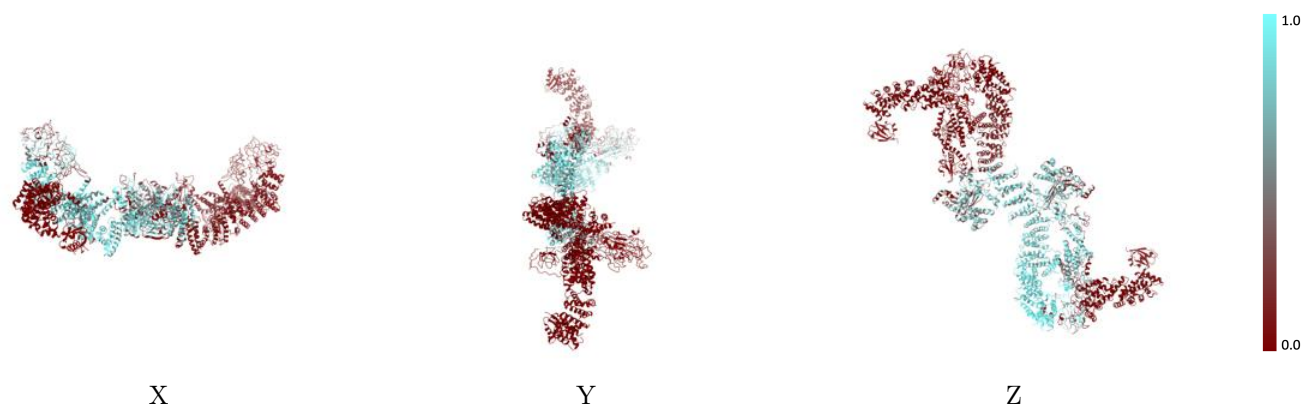


## 9.2 Q-score mapped to coordinate model [i](#)



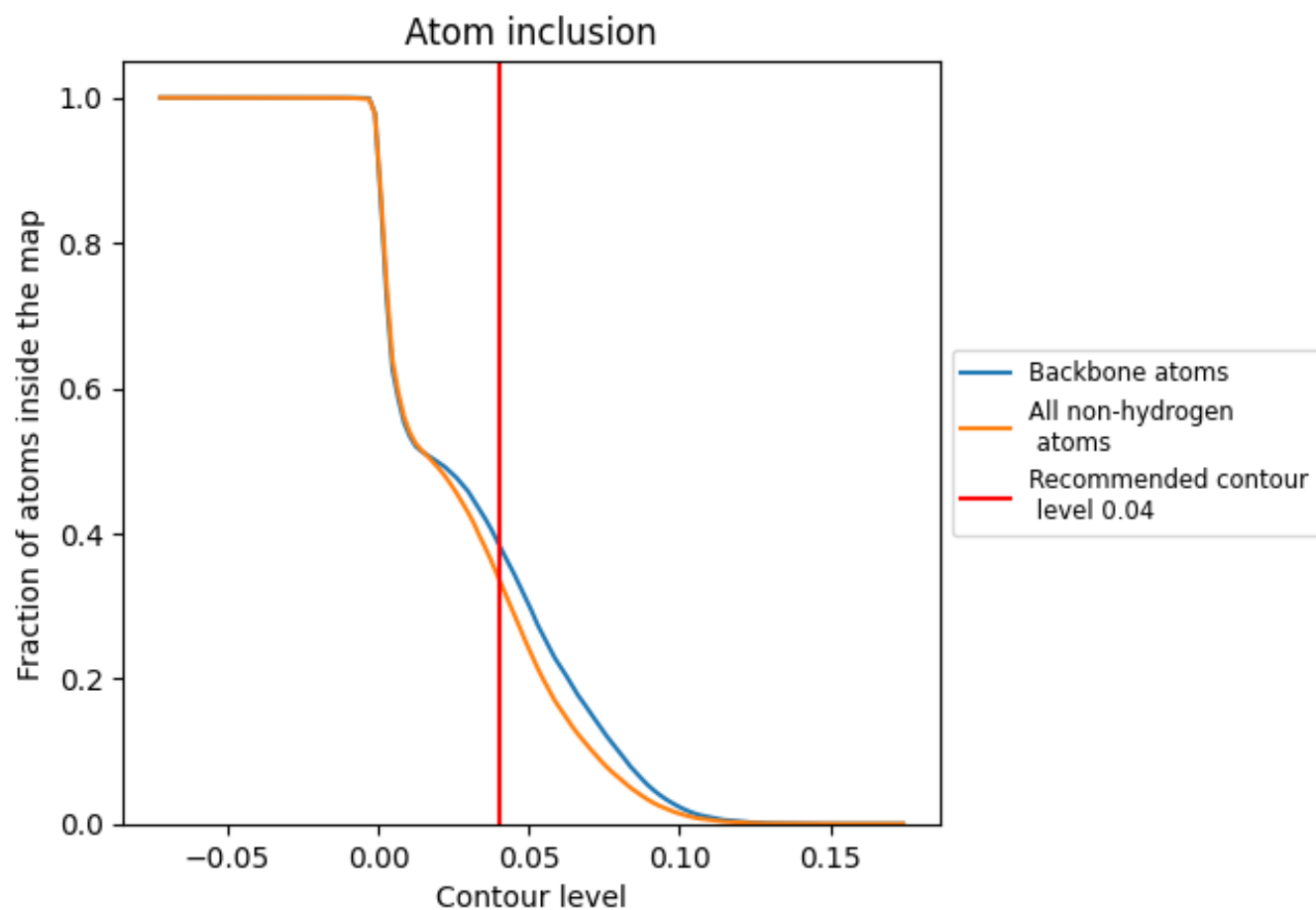
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 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	<div></div> 0.3389	<div></div> 0.1290
A	<div></div> 0.2110	<div></div> 0.0740
B	<div></div> 0.0008	<div></div> 0.0570
C	<div></div> 0.4216	<div></div> 0.1730
D	<div></div> 0.6976	<div></div> 0.2220
E	<div></div> 0.1612	<div></div> 0.1160
F	<div></div> 0.4459	<div></div> 0.1180

