



## wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 12:55 AM UTC

PDB ID : 9ZE0 / pdb\_00009ze0  
EMDB ID : EMD-74082  
Title : Cryo-EM structure of the endogenous U2/branchpoint spliceosomal complex (Proximal DHX15 state)  
Authors : Liu, S.; Su, T.; Zhou, Z.H.  
Deposited on : 2025-11-26  
Resolution : 3.43 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:

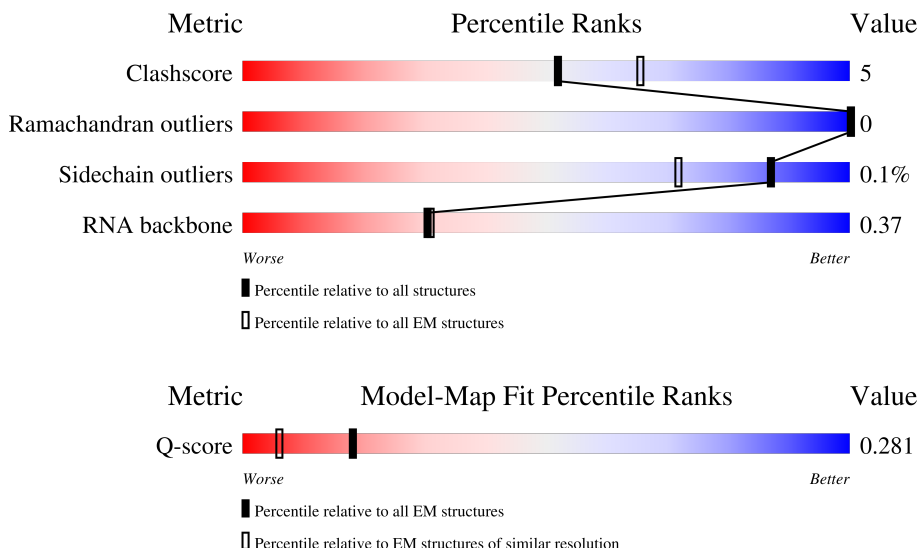
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.43 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13927 ( 2.93 - 3.93 )

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	2	37	<div> <div>5%</div> <div>38%</div> <div>43%</div> <div>11%</div> <div>8%</div> </div>
2	B	795	<div> <div>84%</div> <div>74%</div> <div>10%</div> <div>16%</div> </div>
3	H	110	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	42	
5	C	1029	
6	A	824	
7	B1	1304	
8	B2	895	
9	B3	1217	
10	B4	424	
11	B5	86	
12	B6	125	
13	A1	793	
14	A2	464	
15	A3	501	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 38256 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	37	Total	C	N	O	P	0	0
			781	352	127	265	37		

- Molecule 2 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	665	Total	C	N	O	S	0	0
			5345	3393	924	993	35		

- Molecule 3 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	103	Total	C	N	O	S	0	0
			794	490	142	148	14		

- Molecule 4 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	42	Total	C	N	O	P	0	0
			842	379	89	332	42		

- Molecule 5 is a protein called U2 snRNP-associated SURP motif-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	180	Total	C	N	O	S	0	0
			1451	933	243	269	6		

There are 1001 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ALA	-	expression tag	UNP O15042
C	30	HIS	-	expression tag	UNP O15042
C	31	MET	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ASP	-	expression tag	UNP O15042
C	33	ALA	-	expression tag	UNP O15042
C	34	SER	-	expression tag	UNP O15042
C	35	GLY	-	expression tag	UNP O15042
C	36	PRO	-	expression tag	UNP O15042
C	37	SER	-	expression tag	UNP O15042
C	38	ASP	-	expression tag	UNP O15042
C	39	SER	-	expression tag	UNP O15042
C	40	ASP	-	expression tag	UNP O15042
C	41	MET	-	expression tag	UNP O15042
C	42	PRO	-	expression tag	UNP O15042
C	43	SER	-	expression tag	UNP O15042
C	44	ARG	-	expression tag	UNP O15042
C	45	THR	-	expression tag	UNP O15042
C	46	ARG	-	expression tag	UNP O15042
C	47	PRO	-	expression tag	UNP O15042
C	48	LYS	-	expression tag	UNP O15042
C	49	SER	-	expression tag	UNP O15042
C	50	PRO	-	expression tag	UNP O15042
C	51	ARG	-	expression tag	UNP O15042
C	52	LYS	-	expression tag	UNP O15042
C	53	HIS	-	expression tag	UNP O15042
C	54	ASN	-	expression tag	UNP O15042
C	55	TYR	-	expression tag	UNP O15042
C	56	ARG	-	expression tag	UNP O15042
C	57	ASN	-	expression tag	UNP O15042
C	58	GLU	-	expression tag	UNP O15042
C	59	SER	-	expression tag	UNP O15042
C	60	ALA	-	expression tag	UNP O15042
C	61	ARG	-	expression tag	UNP O15042
C	62	GLU	-	expression tag	UNP O15042
C	63	SER	-	expression tag	UNP O15042
C	64	LEU	-	expression tag	UNP O15042
C	65	CYS	-	expression tag	UNP O15042
C	66	ASP	-	expression tag	UNP O15042
C	67	SER	-	expression tag	UNP O15042
C	68	PRO	-	expression tag	UNP O15042
C	69	HIS	-	expression tag	UNP O15042
C	70	GLN	-	expression tag	UNP O15042
C	71	ASN	-	expression tag	UNP O15042
C	72	LEU	-	expression tag	UNP O15042
C	73	SER	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	74	ARG	-	expression tag	UNP O15042
C	75	PRO	-	expression tag	UNP O15042
C	76	LEU	-	expression tag	UNP O15042
C	77	LEU	-	expression tag	UNP O15042
C	78	GLU	-	expression tag	UNP O15042
C	79	ASN	-	expression tag	UNP O15042
C	80	LYS	-	expression tag	UNP O15042
C	81	LEU	-	expression tag	UNP O15042
C	82	LYS	-	expression tag	UNP O15042
C	83	ALA	-	expression tag	UNP O15042
C	84	PHE	-	expression tag	UNP O15042
C	85	SER	-	expression tag	UNP O15042
C	86	ILE	-	expression tag	UNP O15042
C	87	GLY	-	expression tag	UNP O15042
C	88	LYS	-	expression tag	UNP O15042
C	89	MET	-	expression tag	UNP O15042
C	90	SER	-	expression tag	UNP O15042
C	91	THR	-	expression tag	UNP O15042
C	92	ALA	-	expression tag	UNP O15042
C	93	LYS	-	expression tag	UNP O15042
C	94	ARG	-	expression tag	UNP O15042
C	95	THR	-	expression tag	UNP O15042
C	96	LEU	-	expression tag	UNP O15042
C	97	SER	-	expression tag	UNP O15042
C	98	LYS	-	expression tag	UNP O15042
C	99	LYS	-	expression tag	UNP O15042
C	100	GLU	-	expression tag	UNP O15042
C	101	GLN	-	expression tag	UNP O15042
C	102	GLU	-	expression tag	UNP O15042
C	103	GLU	-	expression tag	UNP O15042
C	104	LEU	-	expression tag	UNP O15042
C	105	LYS	-	expression tag	UNP O15042
C	106	LYS	-	expression tag	UNP O15042
C	107	LYS	-	expression tag	UNP O15042
C	108	GLU	-	expression tag	UNP O15042
C	109	ASP	-	expression tag	UNP O15042
C	110	GLU	-	expression tag	UNP O15042
C	111	LYS	-	expression tag	UNP O15042
C	112	ALA	-	expression tag	UNP O15042
C	113	ALA	-	expression tag	UNP O15042
C	114	ALA	-	expression tag	UNP O15042
C	115	GLU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	116	ILE	-	expression tag	UNP O15042
C	117	TYR	-	expression tag	UNP O15042
C	118	GLU	-	expression tag	UNP O15042
C	119	GLU	-	expression tag	UNP O15042
C	120	PHE	-	expression tag	UNP O15042
C	121	LEU	-	expression tag	UNP O15042
C	122	ALA	-	expression tag	UNP O15042
C	123	ALA	-	expression tag	UNP O15042
C	124	PHE	-	expression tag	UNP O15042
C	125	GLU	-	expression tag	UNP O15042
C	126	GLY	-	expression tag	UNP O15042
C	127	SER	-	expression tag	UNP O15042
C	128	ASP	-	expression tag	UNP O15042
C	129	GLY	-	expression tag	UNP O15042
C	130	ASN	-	expression tag	UNP O15042
C	131	LYS	-	expression tag	UNP O15042
C	132	VAL	-	expression tag	UNP O15042
C	133	LYS	-	expression tag	UNP O15042
C	134	THR	-	expression tag	UNP O15042
C	135	PHE	-	expression tag	UNP O15042
C	136	VAL	-	expression tag	UNP O15042
C	137	ARG	-	expression tag	UNP O15042
C	138	GLY	-	expression tag	UNP O15042
C	139	GLY	-	expression tag	UNP O15042
C	140	VAL	-	expression tag	UNP O15042
C	141	VAL	-	expression tag	UNP O15042
C	142	ASN	-	expression tag	UNP O15042
C	143	ALA	-	expression tag	UNP O15042
C	144	ALA	-	expression tag	UNP O15042
C	145	LYS	-	expression tag	UNP O15042
C	146	GLU	-	expression tag	UNP O15042
C	147	GLU	-	expression tag	UNP O15042
C	148	HIS	-	expression tag	UNP O15042
C	149	GLU	-	expression tag	UNP O15042
C	150	THR	-	expression tag	UNP O15042
C	151	ASP	-	expression tag	UNP O15042
C	152	GLU	-	expression tag	UNP O15042
C	153	LYS	-	expression tag	UNP O15042
C	154	ARG	-	expression tag	UNP O15042
C	155	GLY	-	expression tag	UNP O15042
C	156	LYS	-	expression tag	UNP O15042
C	157	ILE	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	158	TYR	-	expression tag	UNP O15042
C	159	LYS	-	expression tag	UNP O15042
C	160	PRO	-	expression tag	UNP O15042
C	161	SER	-	expression tag	UNP O15042
C	162	SER	-	expression tag	UNP O15042
C	163	ARG	-	expression tag	UNP O15042
C	164	PHE	-	expression tag	UNP O15042
C	165	ALA	-	expression tag	UNP O15042
C	166	ASP	-	expression tag	UNP O15042
C	167	GLN	-	expression tag	UNP O15042
C	168	LYS	-	expression tag	UNP O15042
C	169	ASN	-	expression tag	UNP O15042
C	170	PRO	-	expression tag	UNP O15042
C	171	PRO	-	expression tag	UNP O15042
C	172	ASN	-	expression tag	UNP O15042
C	173	GLN	-	expression tag	UNP O15042
C	174	SER	-	expression tag	UNP O15042
C	175	SER	-	expression tag	UNP O15042
C	176	ASN	-	expression tag	UNP O15042
C	177	GLU	-	expression tag	UNP O15042
C	178	ARG	-	expression tag	UNP O15042
C	179	PRO	-	expression tag	UNP O15042
C	180	PRO	-	expression tag	UNP O15042
C	181	SER	-	expression tag	UNP O15042
C	182	LEU	-	expression tag	UNP O15042
C	183	LEU	-	expression tag	UNP O15042
C	184	VAL	-	expression tag	UNP O15042
C	185	ILE	-	expression tag	UNP O15042
C	186	GLU	-	expression tag	UNP O15042
C	187	THR	-	expression tag	UNP O15042
C	188	LYS	-	expression tag	UNP O15042
C	189	LYS	-	expression tag	UNP O15042
C	190	PRO	-	expression tag	UNP O15042
C	191	PRO	-	expression tag	UNP O15042
C	192	LEU	-	expression tag	UNP O15042
C	193	LYS	-	expression tag	UNP O15042
C	194	LYS	-	expression tag	UNP O15042
C	195	GLY	-	expression tag	UNP O15042
C	196	GLU	-	expression tag	UNP O15042
C	197	LYS	-	expression tag	UNP O15042
C	198	GLU	-	expression tag	UNP O15042
C	199	LYS	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	200	LYS	-	expression tag	UNP O15042
C	201	LYS	-	expression tag	UNP O15042
C	202	SER	-	expression tag	UNP O15042
C	203	ASN	-	expression tag	UNP O15042
C	204	LEU	-	expression tag	UNP O15042
C	205	GLU	-	expression tag	UNP O15042
C	206	LEU	-	expression tag	UNP O15042
C	207	PHE	-	expression tag	UNP O15042
C	208	LYS	-	expression tag	UNP O15042
C	209	GLU	-	expression tag	UNP O15042
C	210	GLU	-	expression tag	UNP O15042
C	211	LEU	-	expression tag	UNP O15042
C	212	LYS	-	expression tag	UNP O15042
C	213	GLN	-	expression tag	UNP O15042
C	214	ILE	-	expression tag	UNP O15042
C	215	GLN	-	expression tag	UNP O15042
C	216	GLU	-	expression tag	UNP O15042
C	217	GLU	-	expression tag	UNP O15042
C	218	ARG	-	expression tag	UNP O15042
C	219	ASP	-	expression tag	UNP O15042
C	220	GLU	-	expression tag	UNP O15042
C	221	ARG	-	expression tag	UNP O15042
C	222	HIS	-	expression tag	UNP O15042
C	223	LYS	-	expression tag	UNP O15042
C	224	THR	-	expression tag	UNP O15042
C	225	LYS	-	expression tag	UNP O15042
C	226	GLY	-	expression tag	UNP O15042
C	227	ARG	-	expression tag	UNP O15042
C	228	LEU	-	expression tag	UNP O15042
C	229	SER	-	expression tag	UNP O15042
C	230	ARG	-	expression tag	UNP O15042
C	231	PHE	-	expression tag	UNP O15042
C	232	GLU	-	expression tag	UNP O15042
C	233	PRO	-	expression tag	UNP O15042
C	234	PRO	-	expression tag	UNP O15042
C	235	GLN	-	expression tag	UNP O15042
C	236	SER	-	expression tag	UNP O15042
C	237	ASP	-	expression tag	UNP O15042
C	238	SER	-	expression tag	UNP O15042
C	239	ASP	-	expression tag	UNP O15042
C	240	GLY	-	expression tag	UNP O15042
C	241	GLN	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	242	ARG	-	expression tag	UNP O15042
C	243	ARG	-	expression tag	UNP O15042
C	244	SER	-	expression tag	UNP O15042
C	245	MET	-	expression tag	UNP O15042
C	246	ASP	-	expression tag	UNP O15042
C	247	ALA	-	expression tag	UNP O15042
C	248	PRO	-	expression tag	UNP O15042
C	249	SER	-	expression tag	UNP O15042
C	250	ARG	-	expression tag	UNP O15042
C	251	ARG	-	expression tag	UNP O15042
C	252	ASN	-	expression tag	UNP O15042
C	253	ARG	-	expression tag	UNP O15042
C	254	SER	-	expression tag	UNP O15042
C	255	SER	-	expression tag	UNP O15042
C	256	GLY	-	expression tag	UNP O15042
C	257	VAL	-	expression tag	UNP O15042
C	258	LEU	-	expression tag	UNP O15042
C	259	ASP	-	expression tag	UNP O15042
C	260	ASP	-	expression tag	UNP O15042
C	261	TYR	-	expression tag	UNP O15042
C	262	ALA	-	expression tag	UNP O15042
C	263	PRO	-	expression tag	UNP O15042
C	264	GLY	-	expression tag	UNP O15042
C	265	SER	-	expression tag	UNP O15042
C	266	HIS	-	expression tag	UNP O15042
C	267	ASP	-	expression tag	UNP O15042
C	268	VAL	-	expression tag	UNP O15042
C	269	GLY	-	expression tag	UNP O15042
C	270	ASP	-	expression tag	UNP O15042
C	271	PRO	-	expression tag	UNP O15042
C	272	SER	-	expression tag	UNP O15042
C	273	THR	-	expression tag	UNP O15042
C	274	THR	-	expression tag	UNP O15042
C	275	ASN	-	expression tag	UNP O15042
C	276	LEU	-	expression tag	UNP O15042
C	277	TYR	-	expression tag	UNP O15042
C	278	LEU	-	expression tag	UNP O15042
C	279	GLY	-	expression tag	UNP O15042
C	280	ASN	-	expression tag	UNP O15042
C	281	ILE	-	expression tag	UNP O15042
C	282	ASN	-	expression tag	UNP O15042
C	283	PRO	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	284	GLN	-	expression tag	UNP O15042
C	285	MET	-	expression tag	UNP O15042
C	286	ASN	-	expression tag	UNP O15042
C	287	GLU	-	expression tag	UNP O15042
C	288	GLU	-	expression tag	UNP O15042
C	289	MET	-	expression tag	UNP O15042
C	290	LEU	-	expression tag	UNP O15042
C	291	CYS	-	expression tag	UNP O15042
C	292	GLN	-	expression tag	UNP O15042
C	293	GLU	-	expression tag	UNP O15042
C	294	PHE	-	expression tag	UNP O15042
C	295	GLY	-	expression tag	UNP O15042
C	296	ARG	-	expression tag	UNP O15042
C	297	PHE	-	expression tag	UNP O15042
C	298	GLY	-	expression tag	UNP O15042
C	299	PRO	-	expression tag	UNP O15042
C	300	LEU	-	expression tag	UNP O15042
C	301	ALA	-	expression tag	UNP O15042
C	302	SER	-	expression tag	UNP O15042
C	303	VAL	-	expression tag	UNP O15042
C	304	LYS	-	expression tag	UNP O15042
C	305	ILE	-	expression tag	UNP O15042
C	306	MET	-	expression tag	UNP O15042
C	307	TRP	-	expression tag	UNP O15042
C	308	PRO	-	expression tag	UNP O15042
C	309	ARG	-	expression tag	UNP O15042
C	310	THR	-	expression tag	UNP O15042
C	311	ASP	-	expression tag	UNP O15042
C	312	GLU	-	expression tag	UNP O15042
C	313	GLU	-	expression tag	UNP O15042
C	314	ARG	-	expression tag	UNP O15042
C	315	ALA	-	expression tag	UNP O15042
C	316	ARG	-	expression tag	UNP O15042
C	317	GLU	-	expression tag	UNP O15042
C	318	ARG	-	expression tag	UNP O15042
C	319	ASN	-	expression tag	UNP O15042
C	320	CYS	-	expression tag	UNP O15042
C	321	GLY	-	expression tag	UNP O15042
C	322	PHE	-	expression tag	UNP O15042
C	323	VAL	-	expression tag	UNP O15042
C	324	ALA	-	expression tag	UNP O15042
C	325	PHE	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	326	MET	-	expression tag	UNP O15042
C	327	ASN	-	expression tag	UNP O15042
C	328	ARG	-	expression tag	UNP O15042
C	329	ARG	-	expression tag	UNP O15042
C	330	ASP	-	expression tag	UNP O15042
C	331	ALA	-	expression tag	UNP O15042
C	332	GLU	-	expression tag	UNP O15042
C	333	ARG	-	expression tag	UNP O15042
C	334	ALA	-	expression tag	UNP O15042
C	335	LEU	-	expression tag	UNP O15042
C	336	LYS	-	expression tag	UNP O15042
C	337	ASN	-	expression tag	UNP O15042
C	338	LEU	-	expression tag	UNP O15042
C	339	ASN	-	expression tag	UNP O15042
C	340	GLY	-	expression tag	UNP O15042
C	341	LYS	-	expression tag	UNP O15042
C	342	MET	-	expression tag	UNP O15042
C	343	ILE	-	expression tag	UNP O15042
C	344	MET	-	expression tag	UNP O15042
C	345	SER	-	expression tag	UNP O15042
C	346	PHE	-	expression tag	UNP O15042
C	347	GLU	-	expression tag	UNP O15042
C	348	MET	-	expression tag	UNP O15042
C	349	LYS	-	expression tag	UNP O15042
C	350	LEU	-	expression tag	UNP O15042
C	351	GLY	-	expression tag	UNP O15042
C	352	TRP	-	expression tag	UNP O15042
C	353	GLY	-	expression tag	UNP O15042
C	354	LYS	-	expression tag	UNP O15042
C	355	ALA	-	expression tag	UNP O15042
C	356	VAL	-	expression tag	UNP O15042
C	357	PRO	-	expression tag	UNP O15042
C	358	ILE	-	expression tag	UNP O15042
C	359	PRO	-	expression tag	UNP O15042
C	360	PRO	-	expression tag	UNP O15042
C	361	HIS	-	expression tag	UNP O15042
C	362	PRO	-	expression tag	UNP O15042
C	363	ILE	-	expression tag	UNP O15042
C	364	TYR	-	expression tag	UNP O15042
C	365	ILE	-	expression tag	UNP O15042
C	366	PRO	-	expression tag	UNP O15042
C	367	PRO	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	368	SER	-	expression tag	UNP O15042
C	369	MET	-	expression tag	UNP O15042
C	370	MET	-	expression tag	UNP O15042
C	371	GLU	-	expression tag	UNP O15042
C	372	HIS	-	expression tag	UNP O15042
C	373	THR	-	expression tag	UNP O15042
C	374	LEU	-	expression tag	UNP O15042
C	375	PRO	-	expression tag	UNP O15042
C	376	PRO	-	expression tag	UNP O15042
C	377	PRO	-	expression tag	UNP O15042
C	378	PRO	-	expression tag	UNP O15042
C	379	SER	-	expression tag	UNP O15042
C	380	GLY	-	expression tag	UNP O15042
C	381	LEU	-	expression tag	UNP O15042
C	382	PRO	-	expression tag	UNP O15042
C	383	PHE	-	expression tag	UNP O15042
C	384	ASN	-	expression tag	UNP O15042
C	385	ALA	-	expression tag	UNP O15042
C	386	GLN	-	expression tag	UNP O15042
C	387	PRO	-	expression tag	UNP O15042
C	388	ARG	-	expression tag	UNP O15042
C	389	GLU	-	expression tag	UNP O15042
C	390	ARG	-	expression tag	UNP O15042
C	391	LEU	-	expression tag	UNP O15042
C	392	LYS	-	expression tag	UNP O15042
C	393	ASN	-	expression tag	UNP O15042
C	394	PRO	-	expression tag	UNP O15042
C	395	ASN	-	expression tag	UNP O15042
C	396	ALA	-	expression tag	UNP O15042
C	397	PRO	-	expression tag	UNP O15042
C	398	MET	-	expression tag	UNP O15042
C	399	LEU	-	expression tag	UNP O15042
C	400	PRO	-	expression tag	UNP O15042
C	401	PRO	-	expression tag	UNP O15042
C	402	PRO	-	expression tag	UNP O15042
C	403	LYS	-	expression tag	UNP O15042
C	404	ASN	-	expression tag	UNP O15042
C	405	LYS	-	expression tag	UNP O15042
C	406	GLU	-	expression tag	UNP O15042
C	407	ASP	-	expression tag	UNP O15042
C	408	PHE	-	expression tag	UNP O15042
C	409	GLU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	410	LYS	-	expression tag	UNP O15042
C	411	THR	-	expression tag	UNP O15042
C	412	LEU	-	expression tag	UNP O15042
C	413	SER	-	expression tag	UNP O15042
C	414	GLN	-	expression tag	UNP O15042
C	415	ALA	-	expression tag	UNP O15042
C	416	ILE	-	expression tag	UNP O15042
C	417	VAL	-	expression tag	UNP O15042
C	418	LYS	-	expression tag	UNP O15042
C	419	VAL	-	expression tag	UNP O15042
C	420	VAL	-	expression tag	UNP O15042
C	421	ILE	-	expression tag	UNP O15042
C	422	PRO	-	expression tag	UNP O15042
C	423	THR	-	expression tag	UNP O15042
C	424	GLU	-	expression tag	UNP O15042
C	425	ARG	-	expression tag	UNP O15042
C	426	ASN	-	expression tag	UNP O15042
C	427	LEU	-	expression tag	UNP O15042
C	428	LEU	-	expression tag	UNP O15042
C	429	ALA	-	expression tag	UNP O15042
C	430	LEU	-	expression tag	UNP O15042
C	431	ILE	-	expression tag	UNP O15042
C	432	HIS	-	expression tag	UNP O15042
C	433	ARG	-	expression tag	UNP O15042
C	434	MET	-	expression tag	UNP O15042
C	435	ILE	-	expression tag	UNP O15042
C	436	GLU	-	expression tag	UNP O15042
C	437	PHE	-	expression tag	UNP O15042
C	438	VAL	-	expression tag	UNP O15042
C	439	VAL	-	expression tag	UNP O15042
C	440	ARG	-	expression tag	UNP O15042
C	441	GLU	-	expression tag	UNP O15042
C	442	GLY	-	expression tag	UNP O15042
C	443	PRO	-	expression tag	UNP O15042
C	444	MET	-	expression tag	UNP O15042
C	445	PHE	-	expression tag	UNP O15042
C	446	GLU	-	expression tag	UNP O15042
C	447	ALA	-	expression tag	UNP O15042
C	448	MET	-	expression tag	UNP O15042
C	449	ILE	-	expression tag	UNP O15042
C	450	MET	-	expression tag	UNP O15042
C	451	ASN	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ARG	-	expression tag	UNP O15042
C	453	GLU	-	expression tag	UNP O15042
C	454	ILE	-	expression tag	UNP O15042
C	455	ASN	-	expression tag	UNP O15042
C	456	ASN	-	expression tag	UNP O15042
C	457	PRO	-	expression tag	UNP O15042
C	458	MET	-	expression tag	UNP O15042
C	459	PHE	-	expression tag	UNP O15042
C	460	ARG	-	expression tag	UNP O15042
C	461	PHE	-	expression tag	UNP O15042
C	462	LEU	-	expression tag	UNP O15042
C	463	PHE	-	expression tag	UNP O15042
C	464	GLU	-	expression tag	UNP O15042
C	465	ASN	-	expression tag	UNP O15042
C	466	GLN	-	expression tag	UNP O15042
C	467	THR	-	expression tag	UNP O15042
C	468	PRO	-	expression tag	UNP O15042
C	469	ALA	-	expression tag	UNP O15042
C	470	HIS	-	expression tag	UNP O15042
C	471	VAL	-	expression tag	UNP O15042
C	472	TYR	-	expression tag	UNP O15042
C	473	TYR	-	expression tag	UNP O15042
C	474	ARG	-	expression tag	UNP O15042
C	475	TRP	-	expression tag	UNP O15042
C	476	LYS	-	expression tag	UNP O15042
C	477	LEU	-	expression tag	UNP O15042
C	478	TYR	-	expression tag	UNP O15042
C	479	SER	-	expression tag	UNP O15042
C	480	ILE	-	expression tag	UNP O15042
C	481	LEU	-	expression tag	UNP O15042
C	482	GLN	-	expression tag	UNP O15042
C	483	GLY	-	expression tag	UNP O15042
C	484	ASP	-	expression tag	UNP O15042
C	485	SER	-	expression tag	UNP O15042
C	486	PRO	-	expression tag	UNP O15042
C	487	THR	-	expression tag	UNP O15042
C	488	LYS	-	expression tag	UNP O15042
C	489	TRP	-	expression tag	UNP O15042
C	490	ARG	-	expression tag	UNP O15042
C	491	THR	-	expression tag	UNP O15042
C	492	GLU	-	expression tag	UNP O15042
C	493	ASP	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	PHE	-	expression tag	UNP O15042
C	495	ARG	-	expression tag	UNP O15042
C	496	MET	-	expression tag	UNP O15042
C	497	PHE	-	expression tag	UNP O15042
C	498	LYS	-	expression tag	UNP O15042
C	499	ASN	-	expression tag	UNP O15042
C	500	GLY	-	expression tag	UNP O15042
C	501	SER	-	expression tag	UNP O15042
C	502	PHE	-	expression tag	UNP O15042
C	503	TRP	-	expression tag	UNP O15042
C	504	ARG	-	expression tag	UNP O15042
C	505	PRO	-	expression tag	UNP O15042
C	506	PRO	-	expression tag	UNP O15042
C	507	PRO	-	expression tag	UNP O15042
C	508	LEU	-	expression tag	UNP O15042
C	509	ASN	-	expression tag	UNP O15042
C	510	PRO	-	expression tag	UNP O15042
C	511	TYR	-	expression tag	UNP O15042
C	512	LEU	-	expression tag	UNP O15042
C	513	HIS	-	expression tag	UNP O15042
C	514	GLY	-	expression tag	UNP O15042
C	515	MET	-	expression tag	UNP O15042
C	516	SER	-	expression tag	UNP O15042
C	517	GLU	-	expression tag	UNP O15042
C	518	GLU	-	expression tag	UNP O15042
C	519	GLN	-	expression tag	UNP O15042
C	520	GLU	-	expression tag	UNP O15042
C	521	THR	-	expression tag	UNP O15042
C	522	GLU	-	expression tag	UNP O15042
C	523	ALA	-	expression tag	UNP O15042
C	524	PHE	-	expression tag	UNP O15042
C	525	VAL	-	expression tag	UNP O15042
C	526	GLU	-	expression tag	UNP O15042
C	527	GLU	-	expression tag	UNP O15042
C	528	PRO	-	expression tag	UNP O15042
C	529	SER	-	expression tag	UNP O15042
C	530	LYS	-	expression tag	UNP O15042
C	531	LYS	-	expression tag	UNP O15042
C	532	GLY	-	expression tag	UNP O15042
C	533	ALA	-	expression tag	UNP O15042
C	534	LEU	-	expression tag	UNP O15042
C	535	LYS	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	536	GLU	-	expression tag	UNP O15042
C	537	GLU	-	expression tag	UNP O15042
C	538	GLN	-	expression tag	UNP O15042
C	539	ARG	-	expression tag	UNP O15042
C	540	ASP	-	expression tag	UNP O15042
C	541	LYS	-	expression tag	UNP O15042
C	542	LEU	-	expression tag	UNP O15042
C	543	GLU	-	expression tag	UNP O15042
C	544	GLU	-	expression tag	UNP O15042
C	545	ILE	-	expression tag	UNP O15042
C	546	LEU	-	expression tag	UNP O15042
C	547	ARG	-	expression tag	UNP O15042
C	548	GLY	-	expression tag	UNP O15042
C	549	LEU	-	expression tag	UNP O15042
C	550	THR	-	expression tag	UNP O15042
C	551	PRO	-	expression tag	UNP O15042
C	552	ARG	-	expression tag	UNP O15042
C	553	LYS	-	expression tag	UNP O15042
C	554	ASN	-	expression tag	UNP O15042
C	555	ASP	-	expression tag	UNP O15042
C	556	ILE	-	expression tag	UNP O15042
C	557	GLY	-	expression tag	UNP O15042
C	558	ASP	-	expression tag	UNP O15042
C	559	ALA	-	expression tag	UNP O15042
C	560	MET	-	expression tag	UNP O15042
C	561	VAL	-	expression tag	UNP O15042
C	562	PHE	-	expression tag	UNP O15042
C	563	CYS	-	expression tag	UNP O15042
C	564	LEU	-	expression tag	UNP O15042
C	565	ASN	-	expression tag	UNP O15042
C	566	ASN	-	expression tag	UNP O15042
C	567	ALA	-	expression tag	UNP O15042
C	568	GLU	-	expression tag	UNP O15042
C	569	ALA	-	expression tag	UNP O15042
C	570	ALA	-	expression tag	UNP O15042
C	571	GLU	-	expression tag	UNP O15042
C	572	GLU	-	expression tag	UNP O15042
C	573	ILE	-	expression tag	UNP O15042
C	574	VAL	-	expression tag	UNP O15042
C	575	ASP	-	expression tag	UNP O15042
C	576	CYS	-	expression tag	UNP O15042
C	577	ILE	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	578	THR	-	expression tag	UNP O15042
C	579	GLU	-	expression tag	UNP O15042
C	580	SER	-	expression tag	UNP O15042
C	581	LEU	-	expression tag	UNP O15042
C	582	SER	-	expression tag	UNP O15042
C	583	ILE	-	expression tag	UNP O15042
C	584	LEU	-	expression tag	UNP O15042
C	585	LYS	-	expression tag	UNP O15042
C	586	THR	-	expression tag	UNP O15042
C	587	PRO	-	expression tag	UNP O15042
C	588	LEU	-	expression tag	UNP O15042
C	589	PRO	-	expression tag	UNP O15042
C	590	LYS	-	expression tag	UNP O15042
C	591	LYS	-	expression tag	UNP O15042
C	592	ILE	-	expression tag	UNP O15042
C	593	ALA	-	expression tag	UNP O15042
C	594	ARG	-	expression tag	UNP O15042
C	595	LEU	-	expression tag	UNP O15042
C	596	TYR	-	expression tag	UNP O15042
C	597	LEU	-	expression tag	UNP O15042
C	598	VAL	-	expression tag	UNP O15042
C	599	SER	-	expression tag	UNP O15042
C	600	ASP	-	expression tag	UNP O15042
C	601	VAL	-	expression tag	UNP O15042
C	602	LEU	-	expression tag	UNP O15042
C	603	TYR	-	expression tag	UNP O15042
C	604	ASN	-	expression tag	UNP O15042
C	605	SER	-	expression tag	UNP O15042
C	606	SER	-	expression tag	UNP O15042
C	607	ALA	-	expression tag	UNP O15042
C	608	LYS	-	expression tag	UNP O15042
C	609	VAL	-	expression tag	UNP O15042
C	610	ALA	-	expression tag	UNP O15042
C	611	ASN	-	expression tag	UNP O15042
C	612	ALA	-	expression tag	UNP O15042
C	613	SER	-	expression tag	UNP O15042
C	614	TYR	-	expression tag	UNP O15042
C	615	TYR	-	expression tag	UNP O15042
C	616	ARG	-	expression tag	UNP O15042
C	617	LYS	-	expression tag	UNP O15042
C	618	PHE	-	expression tag	UNP O15042
C	619	PHE	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	620	GLU	-	expression tag	UNP O15042
C	621	THR	-	expression tag	UNP O15042
C	622	LYS	-	expression tag	UNP O15042
C	623	LEU	-	expression tag	UNP O15042
C	624	CYS	-	expression tag	UNP O15042
C	625	GLN	-	expression tag	UNP O15042
C	626	ILE	-	expression tag	UNP O15042
C	627	PHE	-	expression tag	UNP O15042
C	628	SER	-	expression tag	UNP O15042
C	629	ASP	-	expression tag	UNP O15042
C	630	LEU	-	expression tag	UNP O15042
C	631	ASN	-	expression tag	UNP O15042
C	632	ALA	-	expression tag	UNP O15042
C	633	THR	-	expression tag	UNP O15042
C	634	TYR	-	expression tag	UNP O15042
C	635	ARG	-	expression tag	UNP O15042
C	636	THR	-	expression tag	UNP O15042
C	637	ILE	-	expression tag	UNP O15042
C	638	GLN	-	expression tag	UNP O15042
C	639	GLY	-	expression tag	UNP O15042
C	640	HIS	-	expression tag	UNP O15042
C	641	LEU	-	expression tag	UNP O15042
C	642	GLN	-	expression tag	UNP O15042
C	643	SER	-	expression tag	UNP O15042
C	644	GLU	-	expression tag	UNP O15042
C	645	ASN	-	expression tag	UNP O15042
C	646	PHE	-	expression tag	UNP O15042
C	647	LYS	-	expression tag	UNP O15042
C	648	GLN	-	expression tag	UNP O15042
C	649	ARG	-	expression tag	UNP O15042
C	650	VAL	-	expression tag	UNP O15042
C	651	MET	-	expression tag	UNP O15042
C	652	THR	-	expression tag	UNP O15042
C	653	CYS	-	expression tag	UNP O15042
C	654	PHE	-	expression tag	UNP O15042
C	655	ARG	-	expression tag	UNP O15042
C	656	ALA	-	expression tag	UNP O15042
C	657	TRP	-	expression tag	UNP O15042
C	658	GLU	-	expression tag	UNP O15042
C	659	ASP	-	expression tag	UNP O15042
C	660	TRP	-	expression tag	UNP O15042
C	661	ALA	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	662	ILE	-	expression tag	UNP O15042
C	663	TYR	-	expression tag	UNP O15042
C	664	PRO	-	expression tag	UNP O15042
C	665	GLU	-	expression tag	UNP O15042
C	666	PRO	-	expression tag	UNP O15042
C	667	PHE	-	expression tag	UNP O15042
C	668	LEU	-	expression tag	UNP O15042
C	669	ILE	-	expression tag	UNP O15042
C	670	LYS	-	expression tag	UNP O15042
C	671	LEU	-	expression tag	UNP O15042
C	672	GLN	-	expression tag	UNP O15042
C	673	ASN	-	expression tag	UNP O15042
C	674	ILE	-	expression tag	UNP O15042
C	675	PHE	-	expression tag	UNP O15042
C	676	LEU	-	expression tag	UNP O15042
C	677	GLY	-	expression tag	UNP O15042
C	678	LEU	-	expression tag	UNP O15042
C	679	VAL	-	expression tag	UNP O15042
C	680	ASN	-	expression tag	UNP O15042
C	681	ILE	-	expression tag	UNP O15042
C	682	ILE	-	expression tag	UNP O15042
C	683	GLU	-	expression tag	UNP O15042
C	684	GLU	-	expression tag	UNP O15042
C	685	LYS	-	expression tag	UNP O15042
C	686	GLU	-	expression tag	UNP O15042
C	687	THR	-	expression tag	UNP O15042
C	688	GLU	-	expression tag	UNP O15042
C	689	ASP	-	expression tag	UNP O15042
C	690	VAL	-	expression tag	UNP O15042
C	691	PRO	-	expression tag	UNP O15042
C	692	ASP	-	expression tag	UNP O15042
C	693	ASP	-	expression tag	UNP O15042
C	694	LEU	-	expression tag	UNP O15042
C	695	ASP	-	expression tag	UNP O15042
C	696	GLY	-	expression tag	UNP O15042
C	697	ALA	-	expression tag	UNP O15042
C	698	PRO	-	expression tag	UNP O15042
C	699	ILE	-	expression tag	UNP O15042
C	700	GLU	-	expression tag	UNP O15042
C	701	GLU	-	expression tag	UNP O15042
C	702	GLU	-	expression tag	UNP O15042
C	703	LEU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	704	ASP	-	expression tag	UNP O15042
C	705	GLY	-	expression tag	UNP O15042
C	706	ALA	-	expression tag	UNP O15042
C	707	PRO	-	expression tag	UNP O15042
C	708	LEU	-	expression tag	UNP O15042
C	709	GLU	-	expression tag	UNP O15042
C	710	ASP	-	expression tag	UNP O15042
C	711	VAL	-	expression tag	UNP O15042
C	712	ASP	-	expression tag	UNP O15042
C	713	GLY	-	expression tag	UNP O15042
C	714	ILE	-	expression tag	UNP O15042
C	715	PRO	-	expression tag	UNP O15042
C	716	ILE	-	expression tag	UNP O15042
C	717	ASP	-	expression tag	UNP O15042
C	718	ALA	-	expression tag	UNP O15042
C	719	THR	-	expression tag	UNP O15042
C	720	PRO	-	expression tag	UNP O15042
C	721	ILE	-	expression tag	UNP O15042
C	722	ASP	-	expression tag	UNP O15042
C	723	ASP	-	expression tag	UNP O15042
C	724	LEU	-	expression tag	UNP O15042
C	725	ASP	-	expression tag	UNP O15042
C	726	GLY	-	expression tag	UNP O15042
C	727	VAL	-	expression tag	UNP O15042
C	728	PRO	-	expression tag	UNP O15042
C	729	ILE	-	expression tag	UNP O15042
C	730	LYS	-	expression tag	UNP O15042
C	731	SER	-	expression tag	UNP O15042
C	732	LEU	-	expression tag	UNP O15042
C	733	ASP	-	expression tag	UNP O15042
C	734	ASP	-	expression tag	UNP O15042
C	735	ASP	-	expression tag	UNP O15042
C	736	LEU	-	expression tag	UNP O15042
C	737	ASP	-	expression tag	UNP O15042
C	738	GLY	-	expression tag	UNP O15042
C	739	VAL	-	expression tag	UNP O15042
C	740	PRO	-	expression tag	UNP O15042
C	741	LEU	-	expression tag	UNP O15042
C	742	ASP	-	expression tag	UNP O15042
C	743	ALA	-	expression tag	UNP O15042
C	744	THR	-	expression tag	UNP O15042
C	745	GLU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	746	ASP	-	expression tag	UNP O15042
C	747	SER	-	expression tag	UNP O15042
C	748	LYS	-	expression tag	UNP O15042
C	749	LYS	-	expression tag	UNP O15042
C	750	ASN	-	expression tag	UNP O15042
C	751	GLU	-	expression tag	UNP O15042
C	752	PRO	-	expression tag	UNP O15042
C	753	ILE	-	expression tag	UNP O15042
C	754	PHE	-	expression tag	UNP O15042
C	755	LYS	-	expression tag	UNP O15042
C	756	VAL	-	expression tag	UNP O15042
C	757	ALA	-	expression tag	UNP O15042
C	758	PRO	-	expression tag	UNP O15042
C	759	SER	-	expression tag	UNP O15042
C	760	LYS	-	expression tag	UNP O15042
C	761	TRP	-	expression tag	UNP O15042
C	762	GLU	-	expression tag	UNP O15042
C	763	ALA	-	expression tag	UNP O15042
C	764	VAL	-	expression tag	UNP O15042
C	765	ASP	-	expression tag	UNP O15042
C	766	GLU	-	expression tag	UNP O15042
C	767	SER	-	expression tag	UNP O15042
C	768	GLU	-	expression tag	UNP O15042
C	769	LEU	-	expression tag	UNP O15042
C	770	GLU	-	expression tag	UNP O15042
C	771	ALA	-	expression tag	UNP O15042
C	772	GLN	-	expression tag	UNP O15042
C	773	ALA	-	expression tag	UNP O15042
C	774	VAL	-	expression tag	UNP O15042
C	775	THR	-	expression tag	UNP O15042
C	776	THR	-	expression tag	UNP O15042
C	777	SER	-	expression tag	UNP O15042
C	778	LYS	-	expression tag	UNP O15042
C	779	TRP	-	expression tag	UNP O15042
C	780	GLU	-	expression tag	UNP O15042
C	781	LEU	-	expression tag	UNP O15042
C	782	PHE	-	expression tag	UNP O15042
C	783	ASP	-	expression tag	UNP O15042
C	784	GLN	-	expression tag	UNP O15042
C	785	HIS	-	expression tag	UNP O15042
C	786	GLU	-	expression tag	UNP O15042
C	787	GLU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	788	SER	-	expression tag	UNP O15042
C	789	GLU	-	expression tag	UNP O15042
C	790	GLU	-	expression tag	UNP O15042
C	791	GLU	-	expression tag	UNP O15042
C	792	GLU	-	expression tag	UNP O15042
C	793	ASN	-	expression tag	UNP O15042
C	794	GLN	-	expression tag	UNP O15042
C	795	ASN	-	expression tag	UNP O15042
C	796	GLN	-	expression tag	UNP O15042
C	797	GLU	-	expression tag	UNP O15042
C	798	GLU	-	expression tag	UNP O15042
C	799	GLU	-	expression tag	UNP O15042
C	800	SER	-	expression tag	UNP O15042
C	801	GLU	-	expression tag	UNP O15042
C	802	ASP	-	expression tag	UNP O15042
C	803	GLU	-	expression tag	UNP O15042
C	804	GLU	-	expression tag	UNP O15042
C	805	ASP	-	expression tag	UNP O15042
C	806	THR	-	expression tag	UNP O15042
C	807	GLN	-	expression tag	UNP O15042
C	808	SER	-	expression tag	UNP O15042
C	809	SER	-	expression tag	UNP O15042
C	810	LYS	-	expression tag	UNP O15042
C	811	SER	-	expression tag	UNP O15042
C	812	GLU	-	expression tag	UNP O15042
C	813	GLU	-	expression tag	UNP O15042
C	814	HIS	-	expression tag	UNP O15042
C	815	HIS	-	expression tag	UNP O15042
C	816	LEU	-	expression tag	UNP O15042
C	817	TYR	-	expression tag	UNP O15042
C	818	SER	-	expression tag	UNP O15042
C	819	ASN	-	expression tag	UNP O15042
C	820	PRO	-	expression tag	UNP O15042
C	821	ILE	-	expression tag	UNP O15042
C	822	LYS	-	expression tag	UNP O15042
C	823	GLU	-	expression tag	UNP O15042
C	824	GLU	-	expression tag	UNP O15042
C	825	MET	-	expression tag	UNP O15042
C	826	THR	-	expression tag	UNP O15042
C	827	GLU	-	expression tag	UNP O15042
C	828	SER	-	expression tag	UNP O15042
C	829	LYS	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	830	PHE	-	expression tag	UNP O15042
C	831	SER	-	expression tag	UNP O15042
C	832	LYS	-	expression tag	UNP O15042
C	833	TYR	-	expression tag	UNP O15042
C	834	SER	-	expression tag	UNP O15042
C	835	GLU	-	expression tag	UNP O15042
C	836	MET	-	expression tag	UNP O15042
C	837	SER	-	expression tag	UNP O15042
C	838	GLU	-	expression tag	UNP O15042
C	839	GLU	-	expression tag	UNP O15042
C	840	LYS	-	expression tag	UNP O15042
C	841	ARG	-	expression tag	UNP O15042
C	842	ALA	-	expression tag	UNP O15042
C	843	LYS	-	expression tag	UNP O15042
C	844	LEU	-	expression tag	UNP O15042
C	845	ARG	-	expression tag	UNP O15042
C	846	GLU	-	expression tag	UNP O15042
C	847	ILE	-	expression tag	UNP O15042
C	848	GLU	-	expression tag	UNP O15042
C	849	LEU	-	expression tag	UNP O15042
C	850	LYS	-	expression tag	UNP O15042
C	851	VAL	-	expression tag	UNP O15042
C	852	MET	-	expression tag	UNP O15042
C	853	LYS	-	expression tag	UNP O15042
C	854	PHE	-	expression tag	UNP O15042
C	855	GLN	-	expression tag	UNP O15042
C	856	ASP	-	expression tag	UNP O15042
C	857	GLU	-	expression tag	UNP O15042
C	858	LEU	-	expression tag	UNP O15042
C	859	GLU	-	expression tag	UNP O15042
C	860	SER	-	expression tag	UNP O15042
C	861	GLY	-	expression tag	UNP O15042
C	862	LYS	-	expression tag	UNP O15042
C	863	ARG	-	expression tag	UNP O15042
C	864	PRO	-	expression tag	UNP O15042
C	865	LYS	-	expression tag	UNP O15042
C	866	LYS	-	expression tag	UNP O15042
C	867	PRO	-	expression tag	UNP O15042
C	868	GLY	-	expression tag	UNP O15042
C	869	GLN	-	expression tag	UNP O15042
C	870	SER	-	expression tag	UNP O15042
C	871	PHE	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	872	GLN	-	expression tag	UNP O15042
C	873	GLU	-	expression tag	UNP O15042
C	874	GLN	-	expression tag	UNP O15042
C	875	VAL	-	expression tag	UNP O15042
C	876	GLU	-	expression tag	UNP O15042
C	877	HIS	-	expression tag	UNP O15042
C	878	TYR	-	expression tag	UNP O15042
C	879	ARG	-	expression tag	UNP O15042
C	880	ASP	-	expression tag	UNP O15042
C	881	LYS	-	expression tag	UNP O15042
C	882	LEU	-	expression tag	UNP O15042
C	883	LEU	-	expression tag	UNP O15042
C	884	GLN	-	expression tag	UNP O15042
C	885	ARG	-	expression tag	UNP O15042
C	886	GLU	-	expression tag	UNP O15042
C	887	LYS	-	expression tag	UNP O15042
C	888	GLU	-	expression tag	UNP O15042
C	889	LYS	-	expression tag	UNP O15042
C	890	GLU	-	expression tag	UNP O15042
C	891	LEU	-	expression tag	UNP O15042
C	892	GLU	-	expression tag	UNP O15042
C	893	ARG	-	expression tag	UNP O15042
C	894	GLU	-	expression tag	UNP O15042
C	895	ARG	-	expression tag	UNP O15042
C	896	GLU	-	expression tag	UNP O15042
C	897	ARG	-	expression tag	UNP O15042
C	898	ASP	-	expression tag	UNP O15042
C	899	LYS	-	expression tag	UNP O15042
C	900	LYS	-	expression tag	UNP O15042
C	901	ASP	-	expression tag	UNP O15042
C	902	LYS	-	expression tag	UNP O15042
C	903	GLU	-	expression tag	UNP O15042
C	904	LYS	-	expression tag	UNP O15042
C	905	LEU	-	expression tag	UNP O15042
C	906	GLU	-	expression tag	UNP O15042
C	907	SER	-	expression tag	UNP O15042
C	908	ARG	-	expression tag	UNP O15042
C	909	SER	-	expression tag	UNP O15042
C	910	LYS	-	expression tag	UNP O15042
C	911	ASP	-	expression tag	UNP O15042
C	912	LYS	-	expression tag	UNP O15042
C	913	LYS	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	914	GLU	-	expression tag	UNP O15042
C	915	LYS	-	expression tag	UNP O15042
C	916	ASP	-	expression tag	UNP O15042
C	917	GLU	-	expression tag	UNP O15042
C	918	CYS	-	expression tag	UNP O15042
C	919	THR	-	expression tag	UNP O15042
C	920	PRO	-	expression tag	UNP O15042
C	921	THR	-	expression tag	UNP O15042
C	922	ARG	-	expression tag	UNP O15042
C	923	LYS	-	expression tag	UNP O15042
C	924	GLU	-	expression tag	UNP O15042
C	925	ARG	-	expression tag	UNP O15042
C	926	LYS	-	expression tag	UNP O15042
C	927	ARG	-	expression tag	UNP O15042
C	928	ARG	-	expression tag	UNP O15042
C	929	HIS	-	expression tag	UNP O15042
C	930	SER	-	expression tag	UNP O15042
C	931	THR	-	expression tag	UNP O15042
C	932	SER	-	expression tag	UNP O15042
C	933	PRO	-	expression tag	UNP O15042
C	934	SER	-	expression tag	UNP O15042
C	935	PRO	-	expression tag	UNP O15042
C	936	SER	-	expression tag	UNP O15042
C	937	ARG	-	expression tag	UNP O15042
C	938	SER	-	expression tag	UNP O15042
C	939	SER	-	expression tag	UNP O15042
C	940	SER	-	expression tag	UNP O15042
C	941	GLY	-	expression tag	UNP O15042
C	942	ARG	-	expression tag	UNP O15042
C	943	ARG	-	expression tag	UNP O15042
C	944	VAL	-	expression tag	UNP O15042
C	945	LYS	-	expression tag	UNP O15042
C	946	SER	-	expression tag	UNP O15042
C	947	PRO	-	expression tag	UNP O15042
C	948	SER	-	expression tag	UNP O15042
C	949	PRO	-	expression tag	UNP O15042
C	950	LYS	-	expression tag	UNP O15042
C	951	SER	-	expression tag	UNP O15042
C	952	GLU	-	expression tag	UNP O15042
C	953	ARG	-	expression tag	UNP O15042
C	954	SER	-	expression tag	UNP O15042
C	955	GLU	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	956	ARG	-	expression tag	UNP O15042
C	957	SER	-	expression tag	UNP O15042
C	958	GLU	-	expression tag	UNP O15042
C	959	ARG	-	expression tag	UNP O15042
C	960	SER	-	expression tag	UNP O15042
C	961	HIS	-	expression tag	UNP O15042
C	962	LYS	-	expression tag	UNP O15042
C	963	GLU	-	expression tag	UNP O15042
C	964	SER	-	expression tag	UNP O15042
C	965	SER	-	expression tag	UNP O15042
C	966	ARG	-	expression tag	UNP O15042
C	967	SER	-	expression tag	UNP O15042
C	968	ARG	-	expression tag	UNP O15042
C	969	SER	-	expression tag	UNP O15042
C	970	SER	-	expression tag	UNP O15042
C	971	HIS	-	expression tag	UNP O15042
C	972	LYS	-	expression tag	UNP O15042
C	973	ASP	-	expression tag	UNP O15042
C	974	SER	-	expression tag	UNP O15042
C	975	PRO	-	expression tag	UNP O15042
C	976	ARG	-	expression tag	UNP O15042
C	977	ASP	-	expression tag	UNP O15042
C	978	VAL	-	expression tag	UNP O15042
C	979	SER	-	expression tag	UNP O15042
C	980	LYS	-	expression tag	UNP O15042
C	981	LYS	-	expression tag	UNP O15042
C	982	ALA	-	expression tag	UNP O15042
C	983	LYS	-	expression tag	UNP O15042
C	984	ARG	-	expression tag	UNP O15042
C	985	SER	-	expression tag	UNP O15042
C	986	PRO	-	expression tag	UNP O15042
C	987	SER	-	expression tag	UNP O15042
C	988	GLY	-	expression tag	UNP O15042
C	989	SER	-	expression tag	UNP O15042
C	990	ARG	-	expression tag	UNP O15042
C	991	THR	-	expression tag	UNP O15042
C	992	PRO	-	expression tag	UNP O15042
C	993	LYS	-	expression tag	UNP O15042
C	994	ARG	-	expression tag	UNP O15042
C	995	SER	-	expression tag	UNP O15042
C	996	ARG	-	expression tag	UNP O15042
C	997	ARG	-	expression tag	UNP O15042

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Chain	Residue	Modelled	Actual	Comment	Reference
C	998	SER	-	expression tag	UNP O15042
C	999	ARG	-	expression tag	UNP O15042
C	1000	SER	-	expression tag	UNP O15042
C	1001	ARG	-	expression tag	UNP O15042
C	1002	SER	-	expression tag	UNP O15042
C	1003	PRO	-	expression tag	UNP O15042
C	1004	LYS	-	expression tag	UNP O15042
C	1005	LYS	-	expression tag	UNP O15042
C	1006	SER	-	expression tag	UNP O15042
C	1007	GLY	-	expression tag	UNP O15042
C	1008	LYS	-	expression tag	UNP O15042
C	1009	LYS	-	expression tag	UNP O15042
C	1010	SER	-	expression tag	UNP O15042
C	1011	ARG	-	expression tag	UNP O15042
C	1012	SER	-	expression tag	UNP O15042
C	1013	GLN	-	expression tag	UNP O15042
C	1014	SER	-	expression tag	UNP O15042
C	1015	ARG	-	expression tag	UNP O15042
C	1016	SER	-	expression tag	UNP O15042
C	1017	PRO	-	expression tag	UNP O15042
C	1018	HIS	-	expression tag	UNP O15042
C	1019	ARG	-	expression tag	UNP O15042
C	1020	SER	-	expression tag	UNP O15042
C	1021	HIS	-	expression tag	UNP O15042
C	1022	LYS	-	expression tag	UNP O15042
C	1023	LYS	-	expression tag	UNP O15042
C	1024	SER	-	expression tag	UNP O15042
C	1025	LYS	-	expression tag	UNP O15042
C	1026	LYS	-	expression tag	UNP O15042
C	1027	ASN	-	expression tag	UNP O15042
C	1028	LYS	-	expression tag	UNP O15042
C	1029	HIS	-	expression tag	UNP O15042

- Molecule 6 is a protein called RNA-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	157	Total	C	N	O	S	0	0
			1262	776	242	233	11		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	MET	-	expression tag	UNP P52756
A	817	ASP	-	expression tag	UNP P52756
A	818	TYR	-	expression tag	UNP P52756
A	819	LYS	-	expression tag	UNP P52756
A	820	ASP	-	expression tag	UNP P52756
A	821	ASP	-	expression tag	UNP P52756
A	822	ASP	-	expression tag	UNP P52756
A	823	ASP	-	expression tag	UNP P52756
A	824	LYS	-	expression tag	UNP P52756

- Molecule 7 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B1	895	Total	C	N	O	S	0	0
			7142	4581	1225	1295	41		

- Molecule 8 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B2	251	Total	C	N	O	S	0	0
			1967	1265	349	346	7		

- Molecule 9 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B3	1198	Total	C	N	O	S	0	0
			9396	5959	1598	1794	45		

- Molecule 10 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B4	205	Total	C	N	O	S	0	0
			1593	1011	270	305	7		

- Molecule 11 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B5	75	Total	C	N	O	S	0	0
			616	390	108	113	5		

- Molecule 12 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B6	98	Total	C	N	O	S	0	0
			805	515	144	142	4		

- Molecule 13 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	159	Total	C	N	O	S	0	0
			1344	864	229	249	2		

- Molecule 14 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	197	Total	C	N	O	S	0	0
			1645	1042	300	295	8		

- Molecule 15 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	388	Total	C	N	O	S	0	0
			3270	2068	570	618	14		

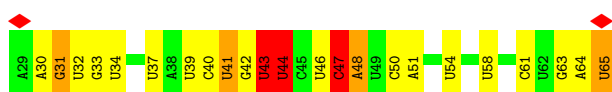
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	H	3	Total	Zn	0
			3	3	

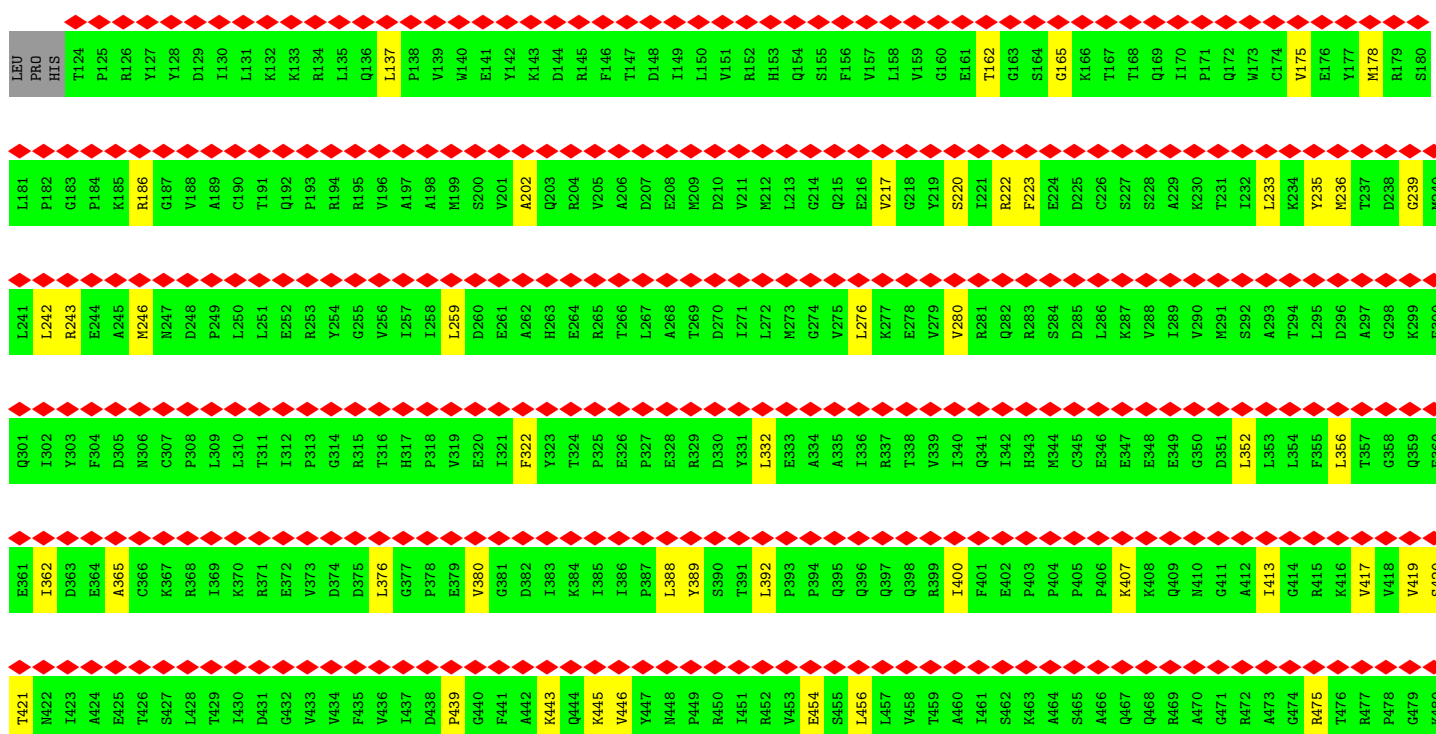
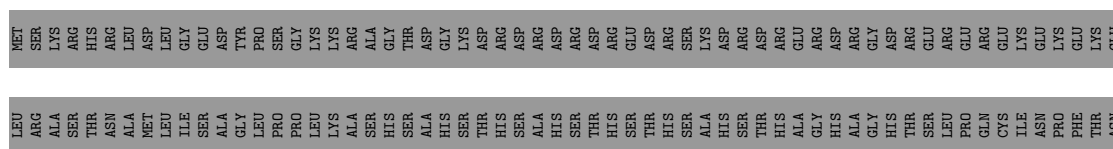
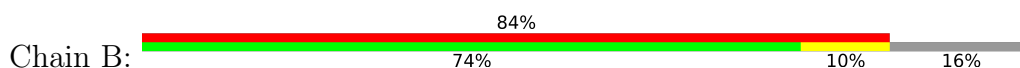
### 3 Residue-property plots

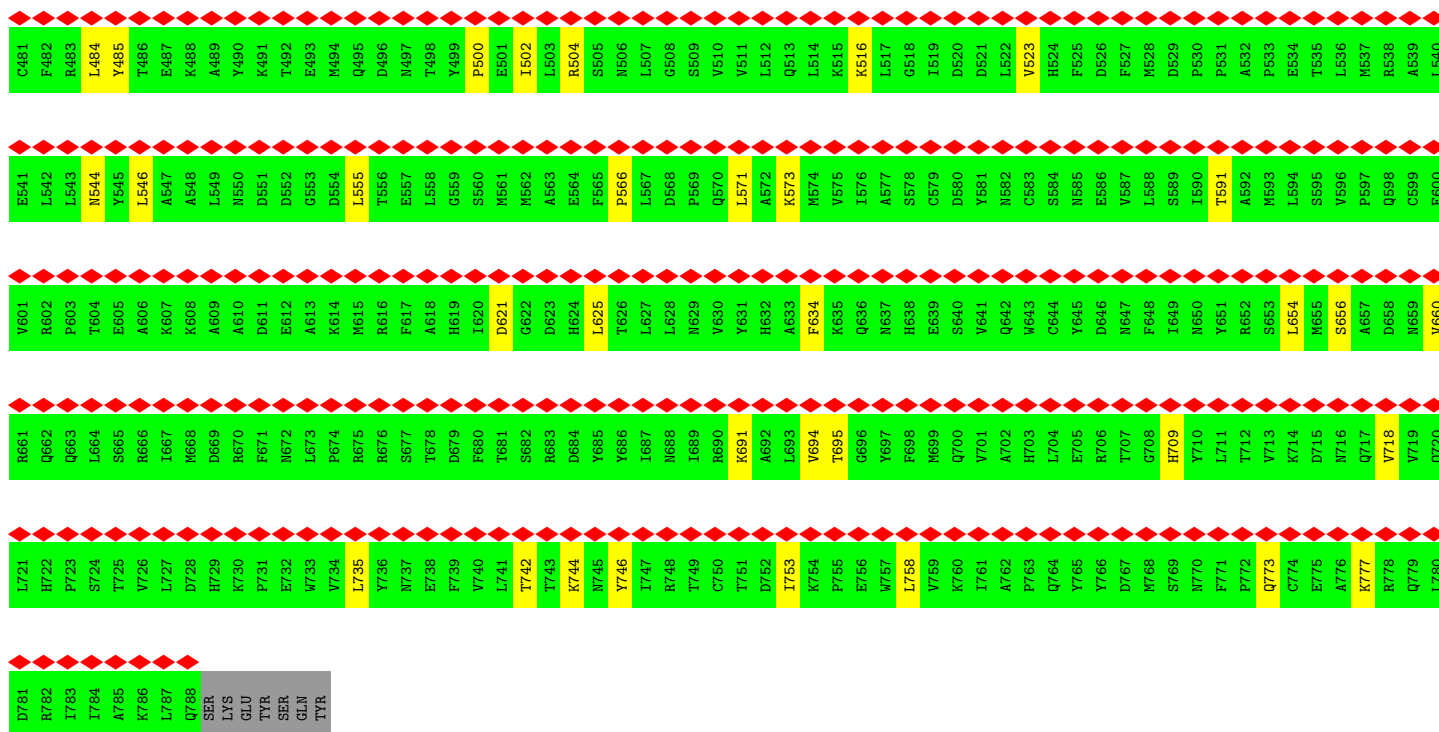
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: U2 snRNA

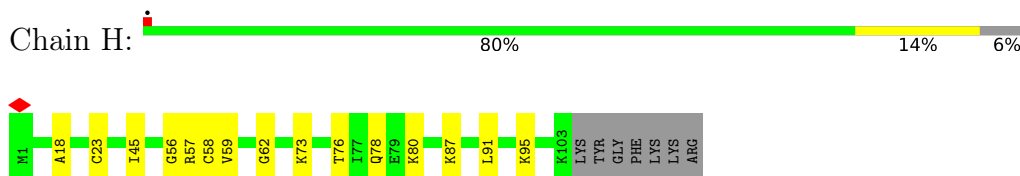


#### • Molecule 2: ATP-dependent RNA helicase DHX15

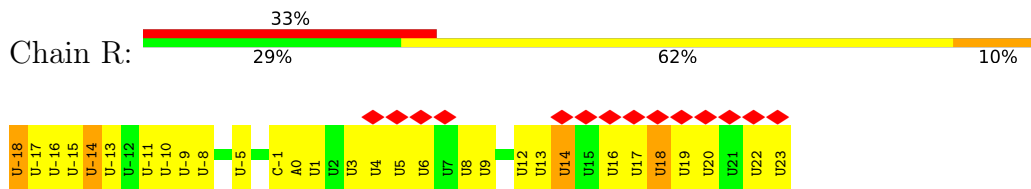




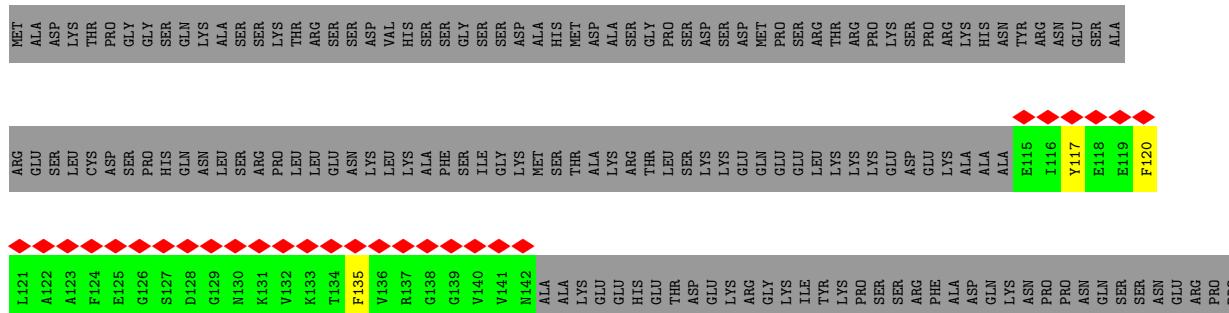
- Molecule 3: PHD finger-like domain-containing protein 5A



- Molecule 4: pre-mRNA



- Molecule 5: U2 snRNP-associated SURP motif-containing protein





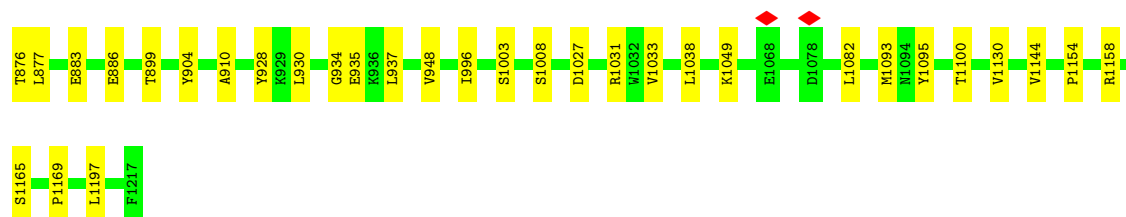
- Molecule 6: RNA-binding protein 5

[illegible]

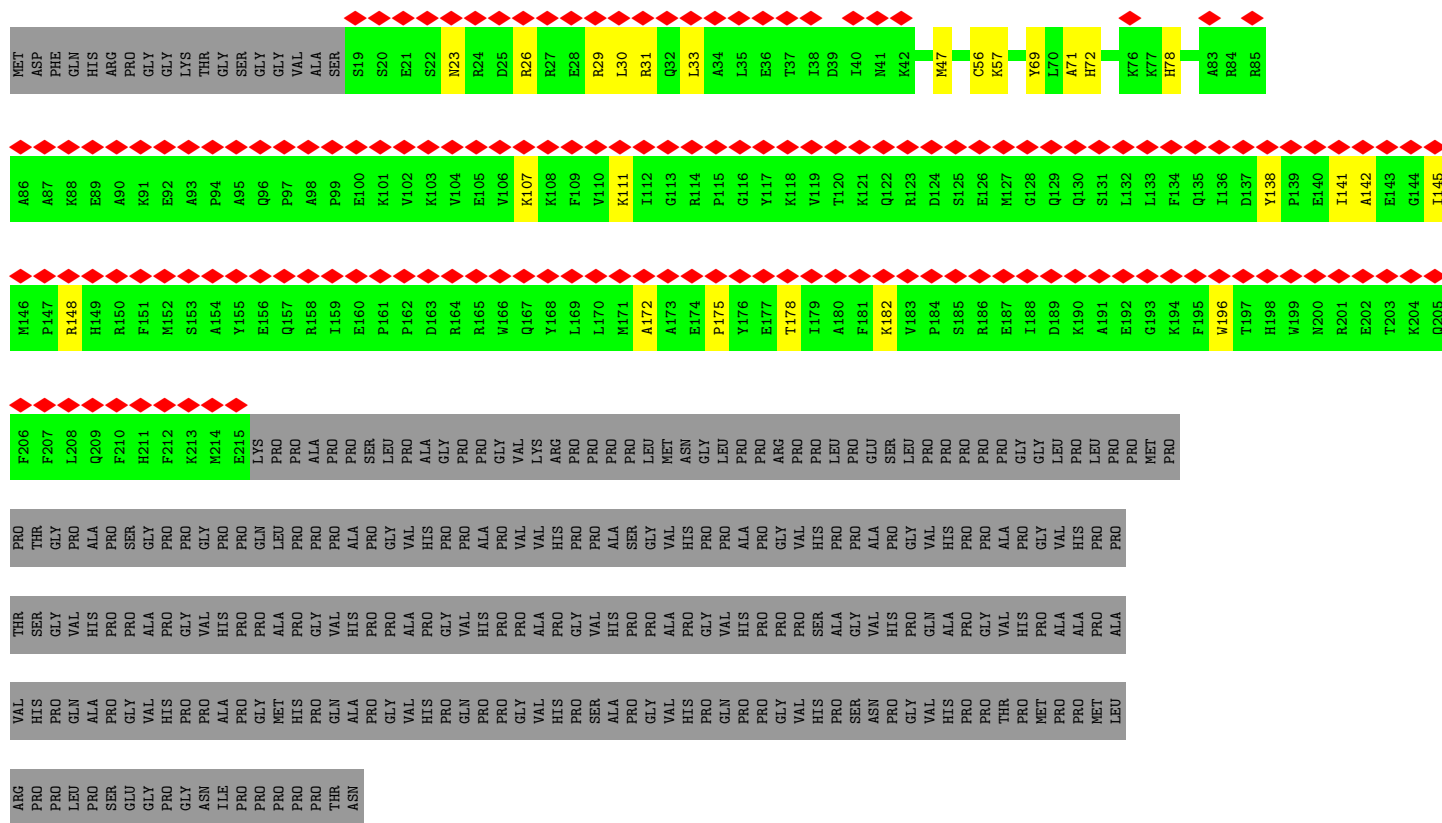






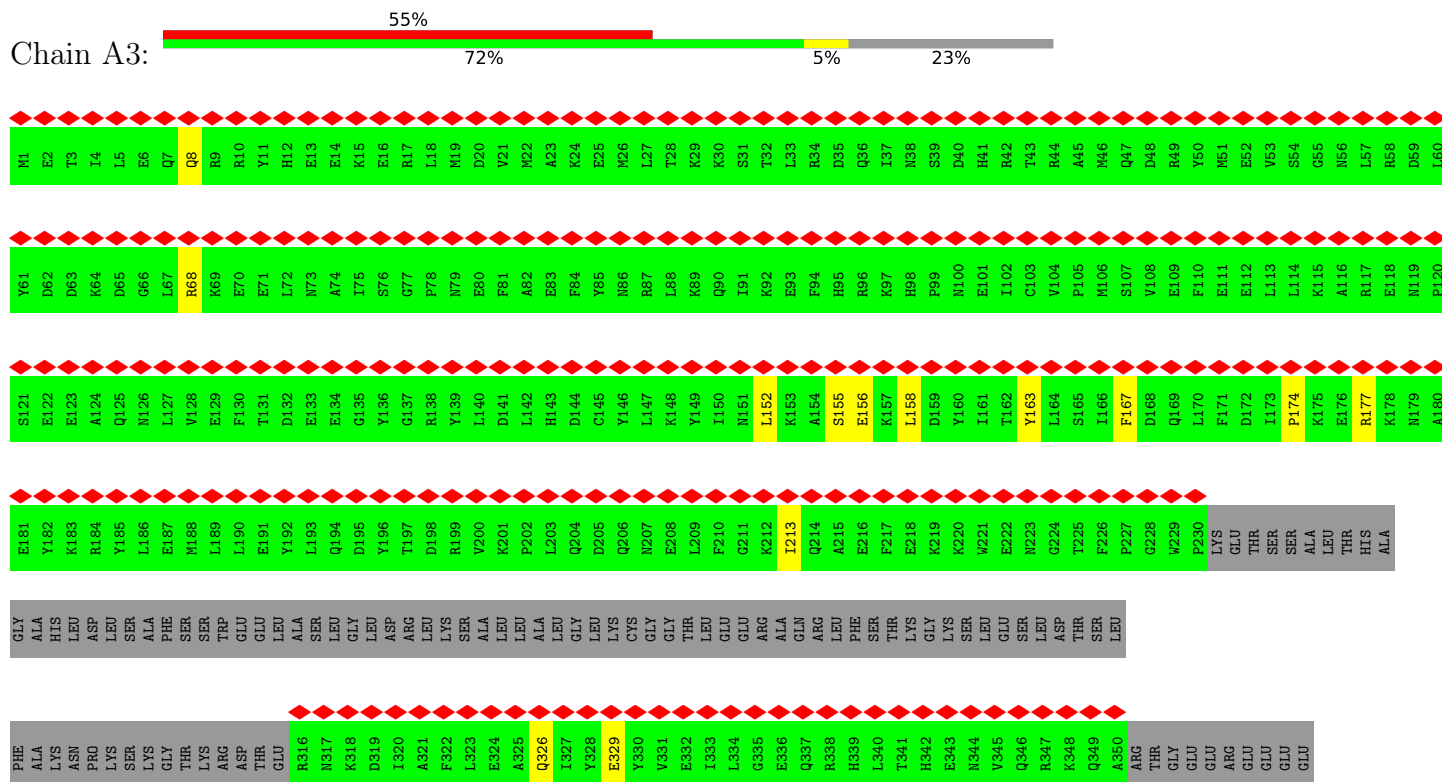




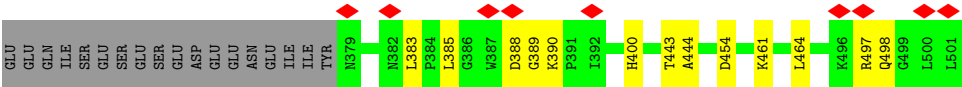


• Molecule 15: Splicing factor 3A subunit 3

Chain A3:







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.317	Depositor
Minimum map value	-2.008	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, OMC

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	2	0.14	0/625	0.27	0/972
2	B	0.06	0/5455	0.19	0/7392
3	H	0.17	0/807	0.36	0/1082
4	R	0.19	0/926	0.37	0/1429
5	C	0.07	0/1477	0.21	0/1990
6	A	0.06	0/1279	0.18	0/1700
7	B1	0.15	0/7284	0.28	0/9868
8	B2	0.20	0/2025	0.38	0/2747
9	B3	0.15	0/9590	0.31	0/13015
10	B4	0.24	0/1627	0.34	0/2200
11	B5	0.16	0/634	0.23	0/857
12	B6	0.09	0/823	0.22	0/1114
13	A1	0.07	0/1377	0.19	0/1857
14	A2	0.09	0/1686	0.22	0/2264
15	A3	0.10	0/3345	0.20	0/4503
All	All	0.14	0/38960	0.27	0/52990

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	781	0	398	17	0
2	B	5345	0	5378	50	0
3	H	794	0	775	10	0
4	R	842	0	424	14	0
5	C	1451	0	1463	17	0
6	A	1262	0	1259	19	0
7	B1	7142	0	7319	94	0
8	B2	1967	0	1918	38	0
9	B3	9396	0	9309	102	0
10	B4	1593	0	1556	25	0
11	B5	616	0	579	10	0
12	B6	805	0	802	12	0
13	A1	1344	0	1309	9	0
14	A2	1645	0	1629	19	0
15	A3	3270	0	3163	16	0
16	H	3	0	0	0	0
All	All	38256	0	37281	405	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 5.

The worst 5 of 405 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)
1:2:33:G:H1	4:R:1:U:H3	1.19	0.87
8:B2:536:MET:HE1	8:B2:566:ILE:HD12	1.59	0.84
7:B1:1017:LEU:HD21	7:B1:1042:ILE:HG21	1.60	0.84
7:B1:460:PRO:HD3	7:B1:467:LEU:HD11	1.60	0.83
1:2:42:G:H1	4:R:-9:U:H3	1.29	0.79

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	
2	B	663/795 (83%)	658 (99%)	5 (1%)	0	100	100
3	H	101/110 (92%)	91 (90%)	10 (10%)	0	100	100
5	C	176/1029 (17%)	174 (99%)	2 (1%)	0	100	100
6	A	153/824 (19%)	151 (99%)	2 (1%)	0	100	100
7	B1	891/1304 (68%)	866 (97%)	25 (3%)	0	100	100
8	B2	247/895 (28%)	233 (94%)	14 (6%)	0	100	100
9	B3	1192/1217 (98%)	1130 (95%)	62 (5%)	0	100	100
10	B4	201/424 (47%)	195 (97%)	6 (3%)	0	100	100
11	B5	73/86 (85%)	69 (94%)	4 (6%)	0	100	100
12	B6	96/125 (77%)	95 (99%)	1 (1%)	0	100	100
13	A1	157/793 (20%)	154 (98%)	3 (2%)	0	100	100
14	A2	195/464 (42%)	187 (96%)	8 (4%)	0	100	100
15	A3	382/501 (76%)	378 (99%)	4 (1%)	0	100	100
All	All	4527/8567 (53%)	4381 (97%)	146 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	B	592/704 (84%)	592 (100%)	0	100	100
3	H	89/95 (94%)	89 (100%)	0	100	100
5	C	157/934 (17%)	157 (100%)	0	100	100
6	A	128/704 (18%)	128 (100%)	0	100	100
7	B1	775/1104 (70%)	775 (100%)	0	100	100
8	B2	202/776 (26%)	199 (98%)	3 (2%)	57	71
9	B3	1037/1051 (99%)	1037 (100%)	0	100	100
10	B4	167/336 (50%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	B5	66/77 (86%)	66 (100%)	0	100	100
12	B6	84/109 (77%)	84 (100%)	0	100	100
13	A1	144/709 (20%)	144 (100%)	0	100	100
14	A2	174/382 (46%)	174 (100%)	0	100	100
15	A3	350/446 (78%)	350 (100%)	0	100	100
All	All	3965/7427 (53%)	3962 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B2	567	ASP
8	B2	706	THR
8	B2	713	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
7	B1	1277	GLN
9	B3	138	GLN
14	A2	209	GLN
9	B3	9	GLN
9	B3	804	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/37 (97%)	8 (22%)	0
4	R	42/42 (100%)	21 (50%)	3 (7%)
All	All	78/79 (98%)	29 (37%)	3 (3%)

5 of 29 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	30	A
1	2	31	G
1	2	43	PSU
1	2	44	PSU
1	2	46	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	R	-18	U
4	R	-14	U
4	R	8	U

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PSU	2	39	4,1	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
1	PSU	2	41	4,1	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
1	PSU	2	58	1	18,21,22	1.06	1 (5%)	21,30,33	1.79	4 (19%)
1	PSU	2	37	1	18,21,22	1.07	1 (5%)	21,30,33	1.92	4 (19%)
1	PSU	2	54	1	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
1	OMC	2	40	4,1	19,22,23	0.55	0	25,31,34	0.66	0
1	PSU	2	34	4,1	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
1	PSU	2	43	1	18,21,22	1.12	1 (5%)	21,30,33	1.62	4 (19%)
1	PSU	2	44	1	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
1	OMC	2	47	1	19,22,23	0.50	0	25,31,34	0.91	2 (8%)
1	OMC	2	61	1	19,22,23	0.55	0	25,31,34	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	39	4,1	-	0/7/25/26	0/2/2/2
1	PSU	2	41	4,1	-	0/7/25/26	0/2/2/2
1	PSU	2	58	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	37	1	-	0/7/25/26	0/2/2/2
1	PSU	2	54	1	-	0/7/25/26	0/2/2/2
1	OMC	2	40	4,1	-	1/9/27/28	0/2/2/2
1	PSU	2	34	4,1	-	0/7/25/26	0/2/2/2
1	PSU	2	43	1	-	6/7/25/26	0/2/2/2
1	PSU	2	44	1	-	2/7/25/26	0/2/2/2
1	OMC	2	47	1	-	6/9/27/28	0/2/2/2
1	OMC	2	61	1	-	0/9/27/28	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	43	PSU	C6-C5	3.90	1.39	1.35
1	2	44	PSU	C6-C5	3.66	1.39	1.35
1	2	34	PSU	C6-C5	3.61	1.39	1.35
1	2	58	PSU	C6-C5	3.61	1.39	1.35
1	2	39	PSU	C6-C5	3.59	1.39	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	44	PSU	N1-C2-N3	5.05	120.50	115.17
1	2	37	PSU	C4-N3-C2	-5.03	119.45	126.37
1	2	41	PSU	C4-N3-C2	-4.99	119.50	126.37
1	2	41	PSU	N1-C2-N3	4.91	120.34	115.17
1	2	39	PSU	N1-C2-N3	4.89	120.33	115.17

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	40	OMC	C1'-C2'-O2'-CM2
1	2	43	PSU	O4'-C1'-C5-C4
1	2	43	PSU	O4'-C1'-C5-C6
1	2	43	PSU	O4'-C4'-C5'-O5'
1	2	44	PSU	O4'-C1'-C5-C4

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	41	PSU	2	0
1	2	40	OMC	1	0
1	2	43	PSU	2	0
1	2	44	PSU	1	0
1	2	47	OMC	1	0
1	2	61	OMC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

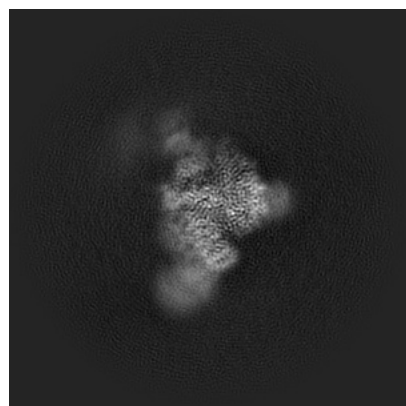
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74082. These allow visual inspection of the internal detail of the map and identification of artifacts.

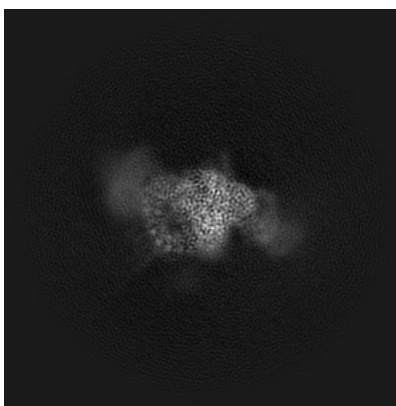
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

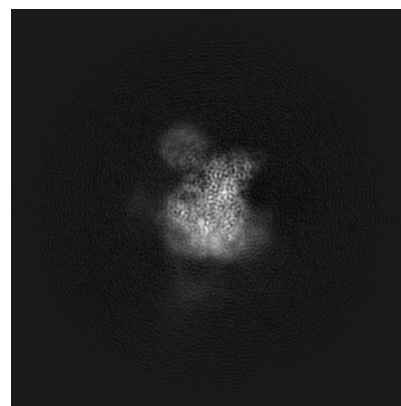
#### 6.1.1 Primary map



X

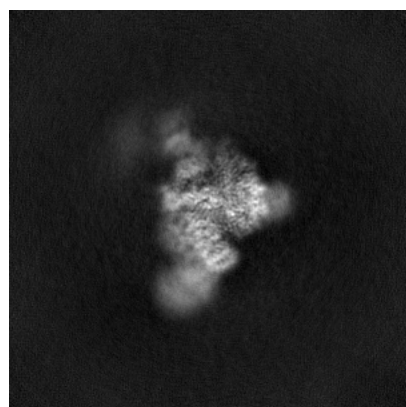


Y

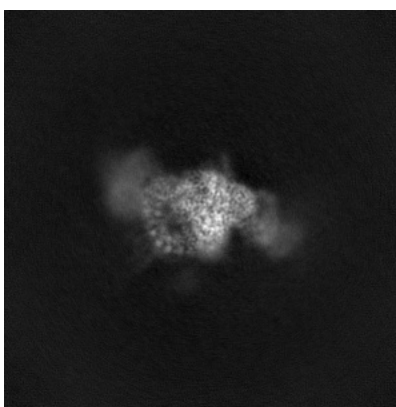


Z

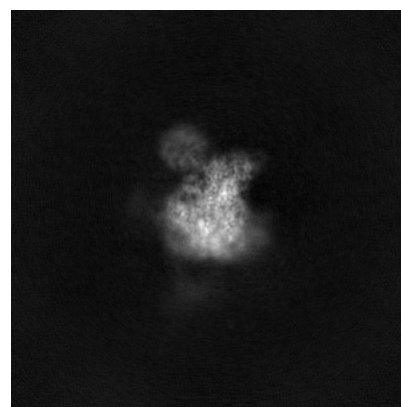
#### 6.1.2 Raw map



X



Y

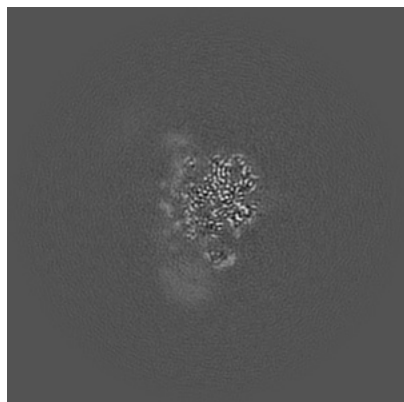


Z

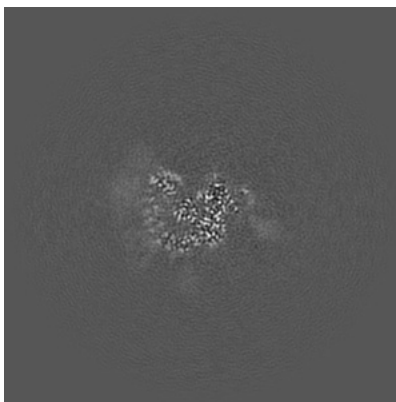
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

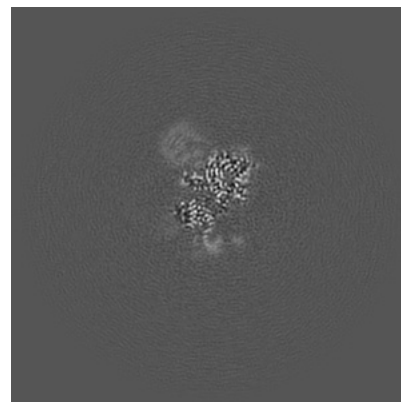
### 6.2.1 Primary map



X Index: 192

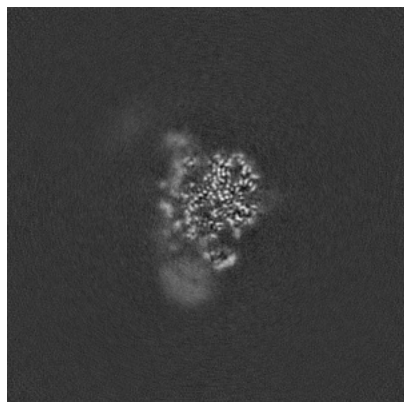


Y Index: 192

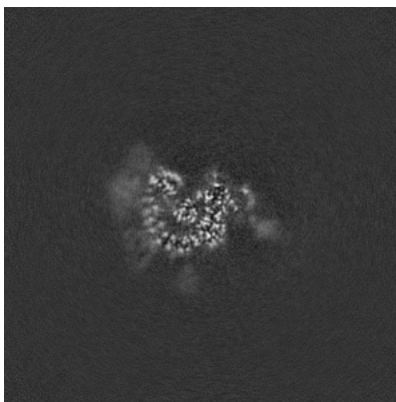


Z Index: 192

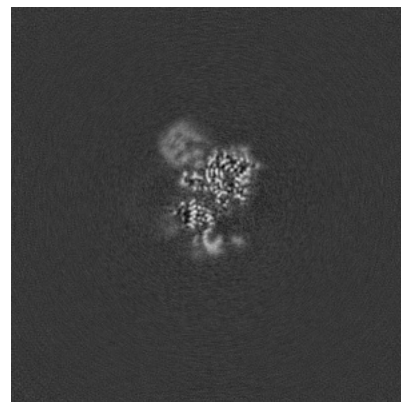
### 6.2.2 Raw map



X Index: 192



Y Index: 192

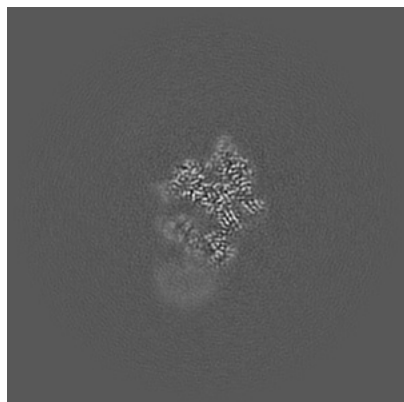


Z Index: 192

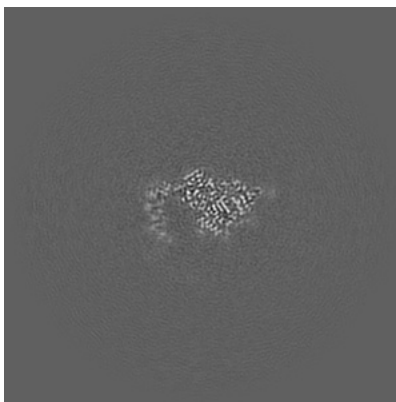
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

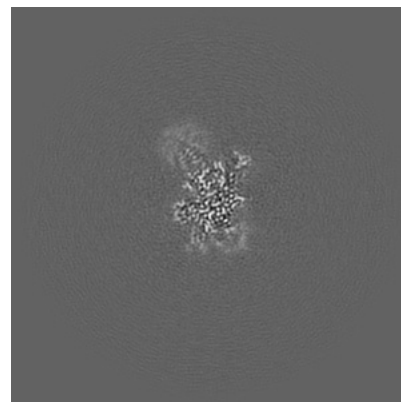
### 6.3.1 Primary map



X Index: 206

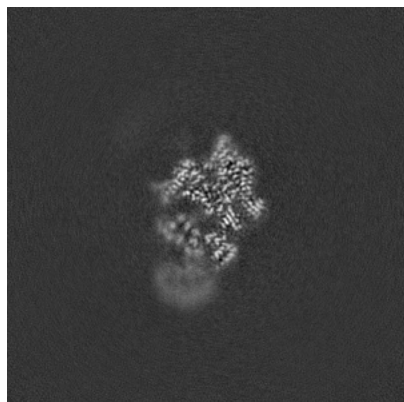


Y Index: 211

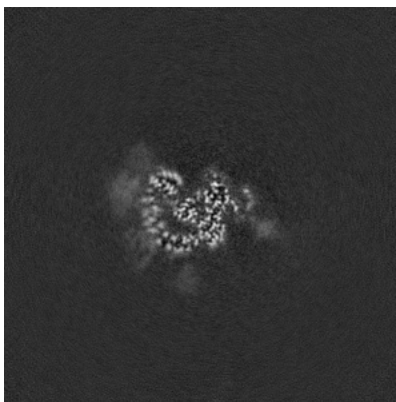


Z Index: 203

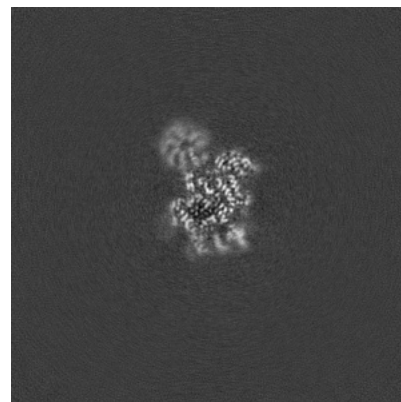
### 6.3.2 Raw map



X Index: 205



Y Index: 193

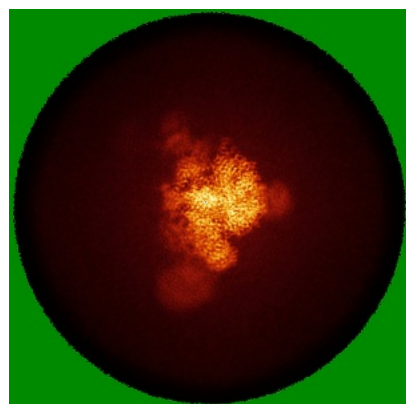


Z Index: 199

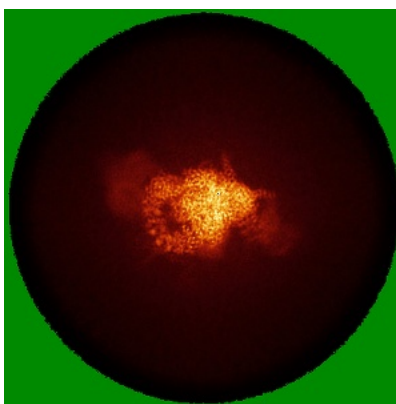
The images above show the largest variance slices of the map in three orthogonal directions.

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

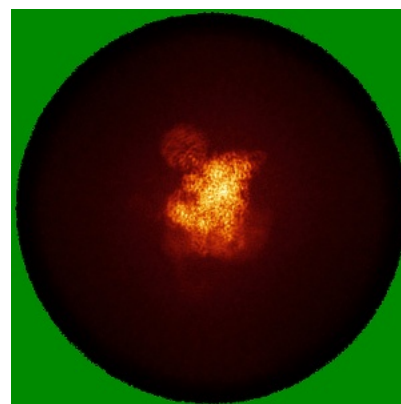
### 6.4.1 Primary map



X

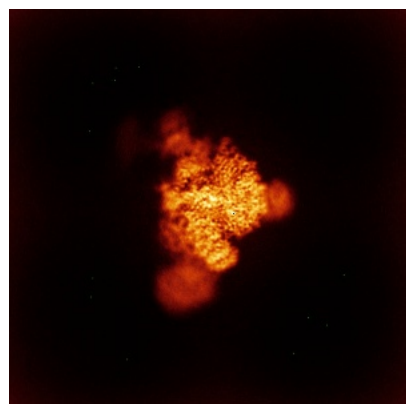


Y

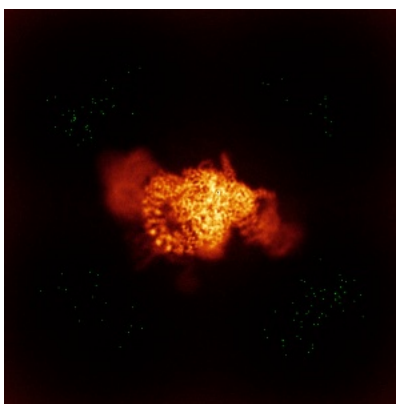


Z

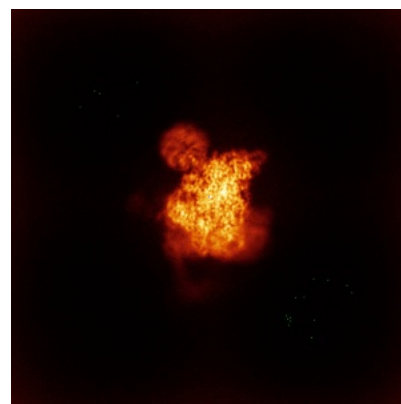
### 6.4.2 Raw map



X



Y



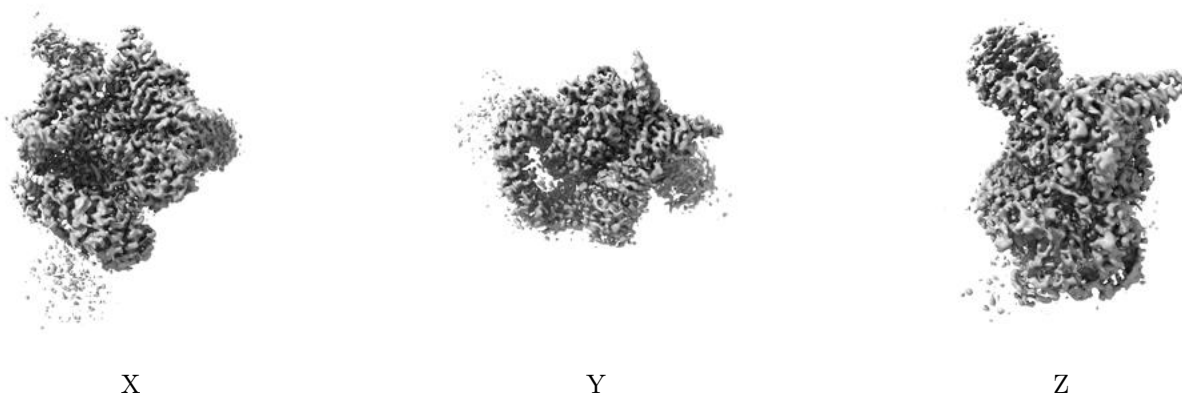
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

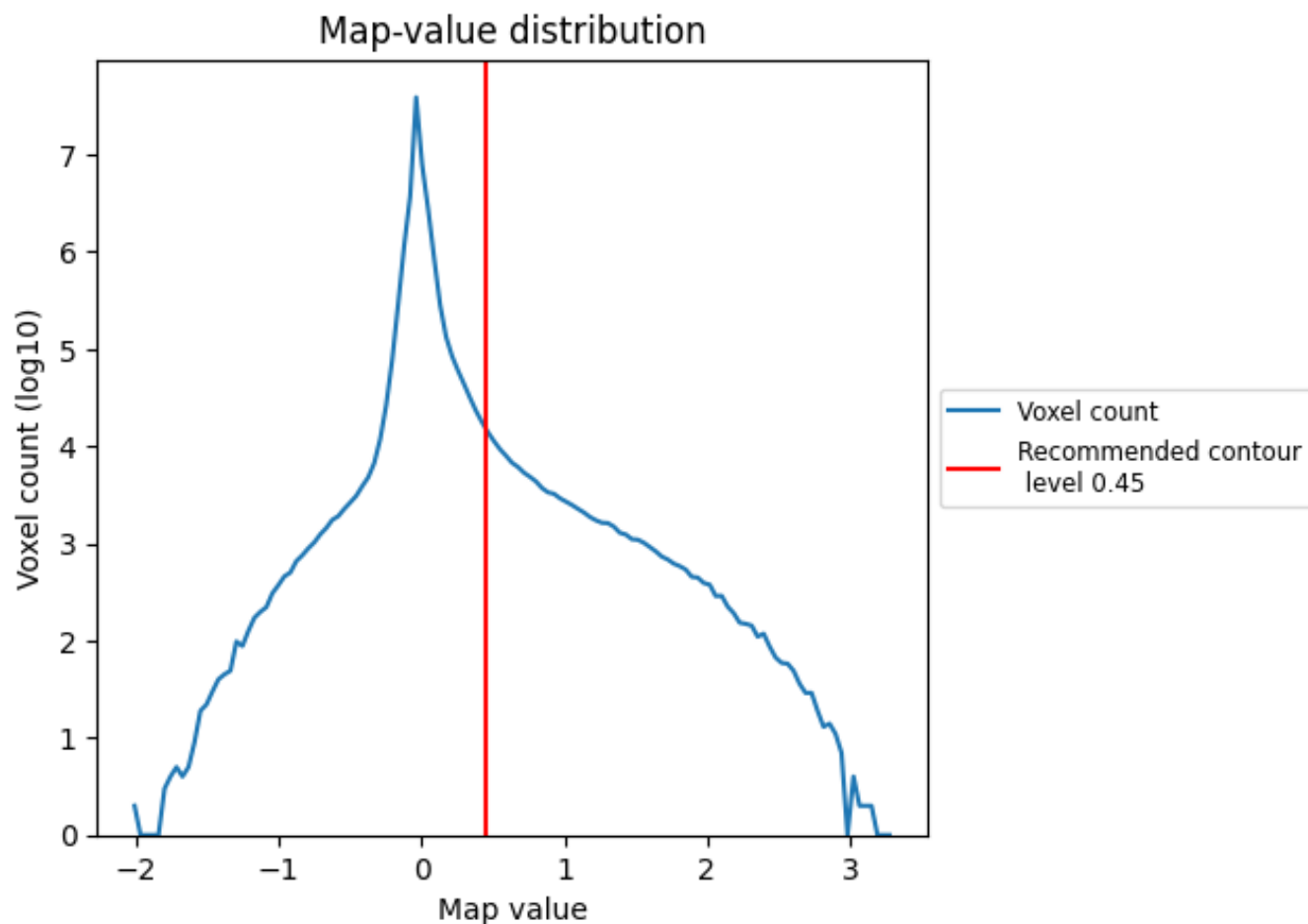
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

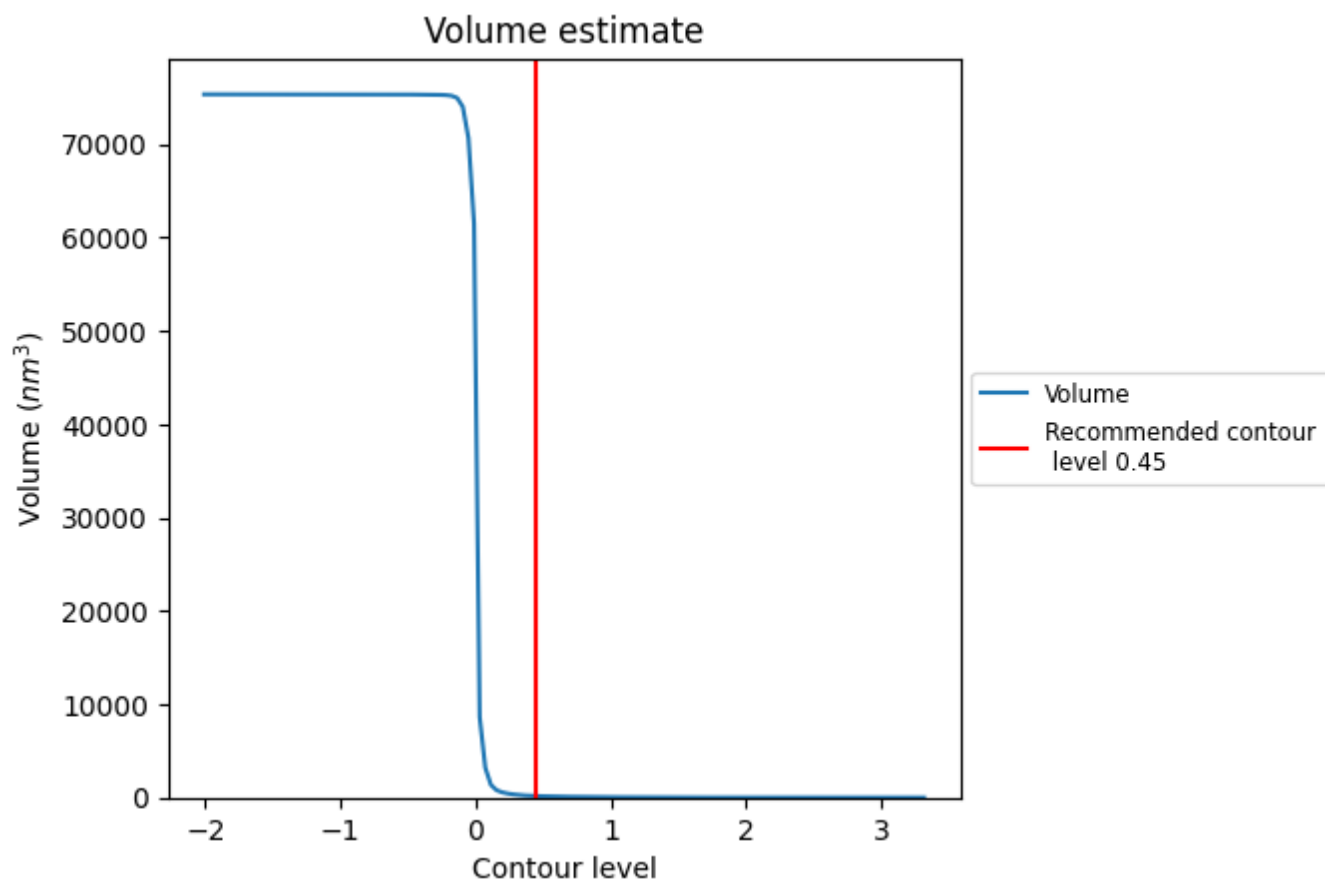
This section contains the results of statistical analysis of the map.

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



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

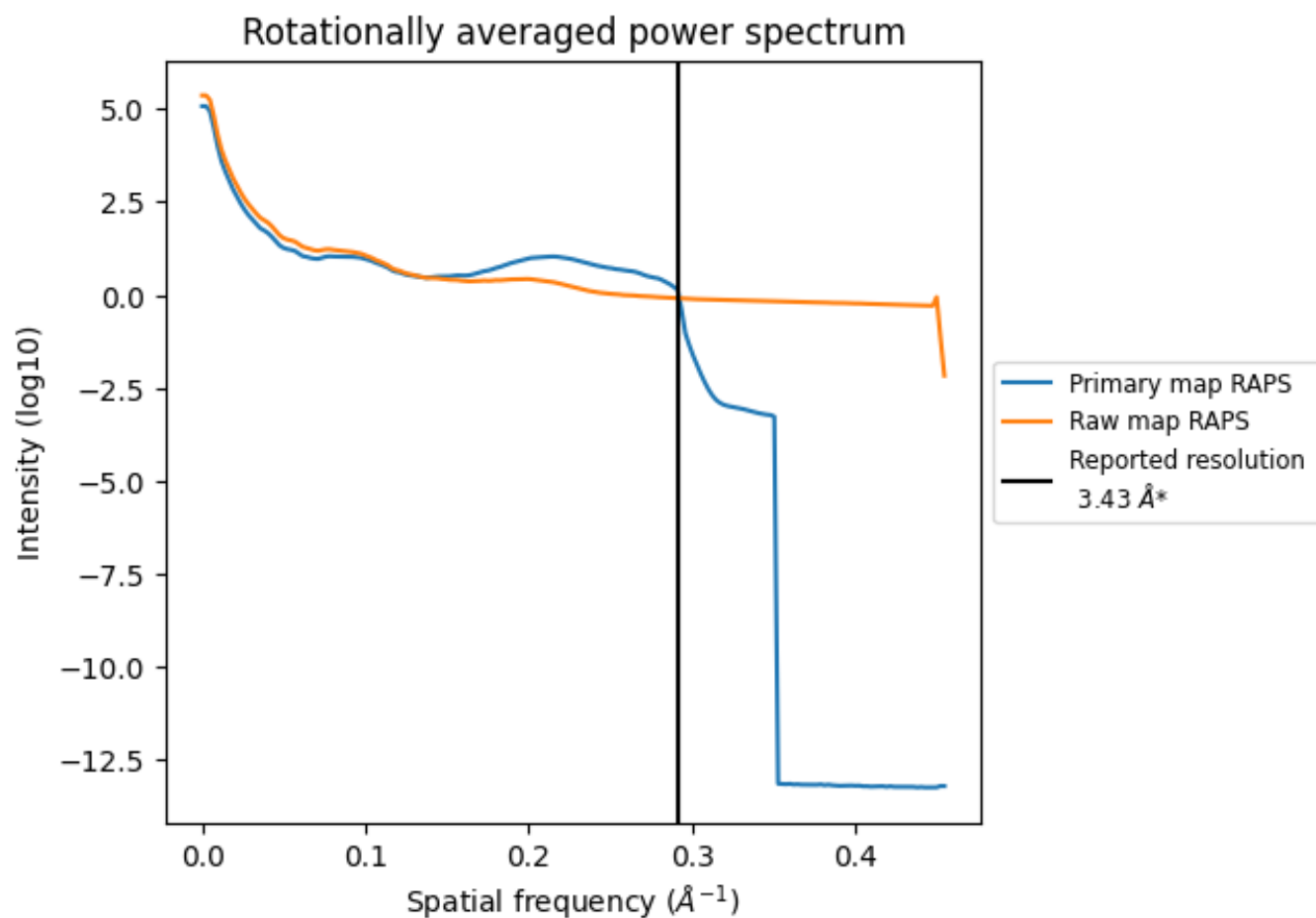
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm<sup>3</sup>; this corresponds to an approximate mass of 147 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 ⓘ

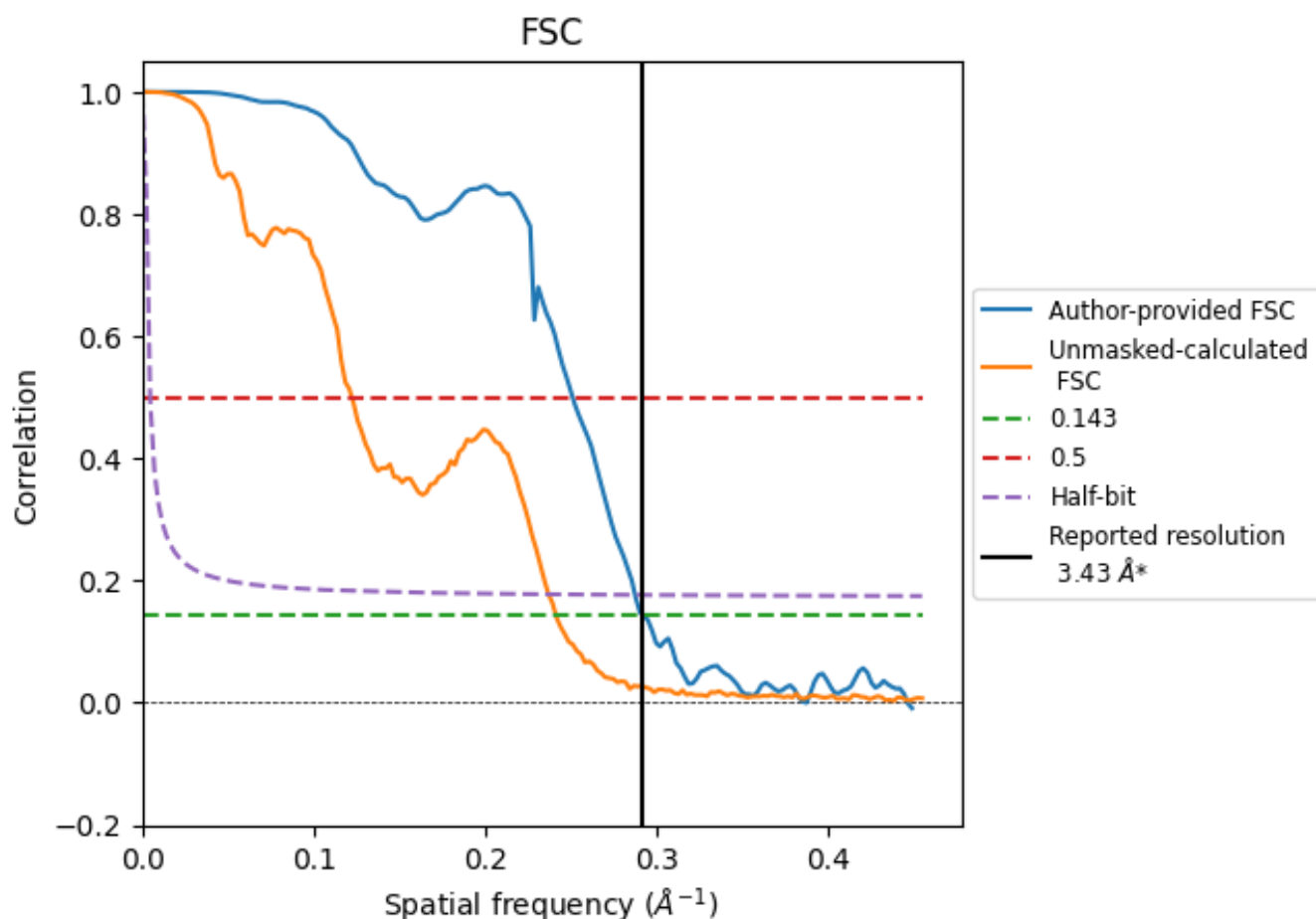


\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

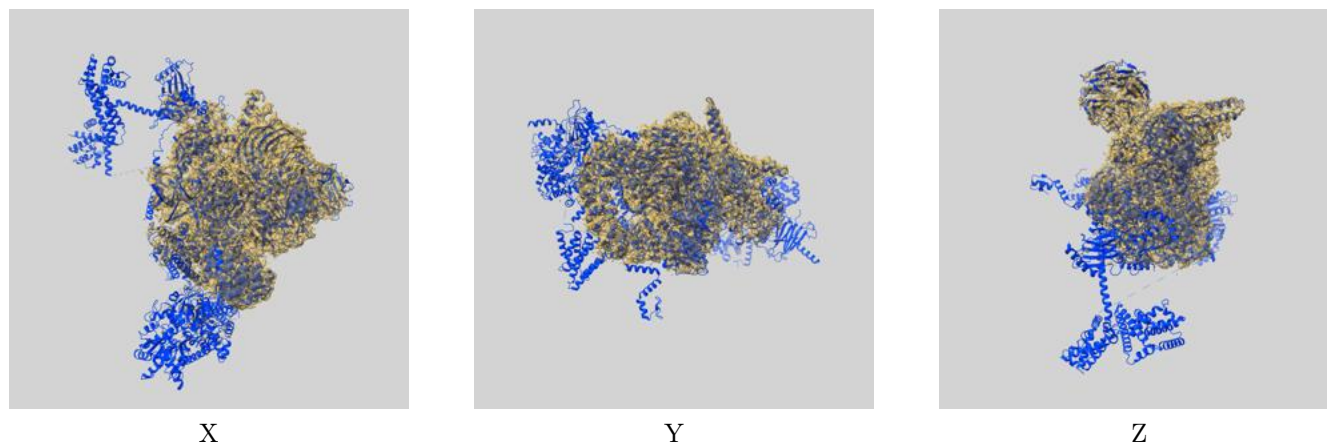
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.43	3.99	3.48
Unmasked-calculated*	4.15	8.18	4.22

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.43 by more than 10 %

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

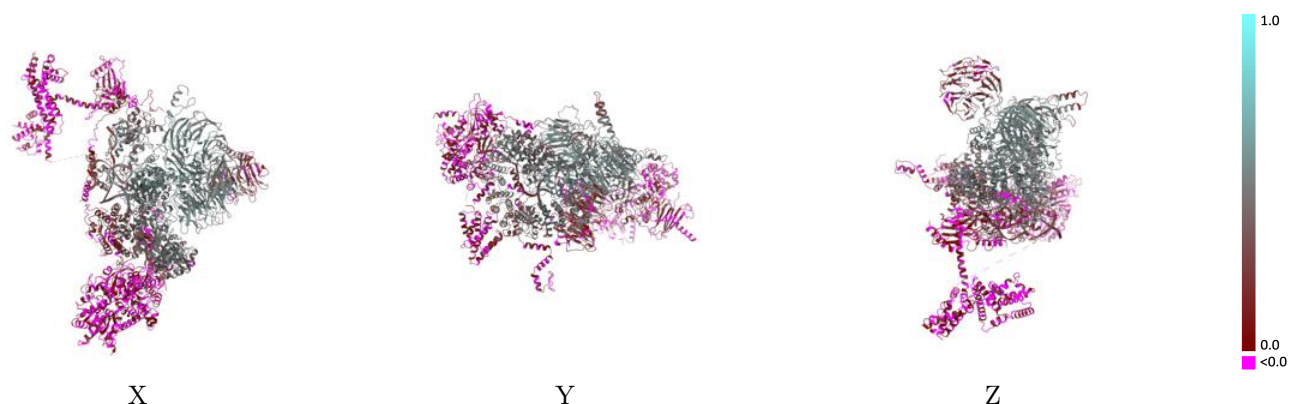
This section contains information regarding the fit between EMDB map EMD-74082 and PDB model 9ZE0. Per-residue inclusion information can be found in section [3](#) on page [31](#).

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



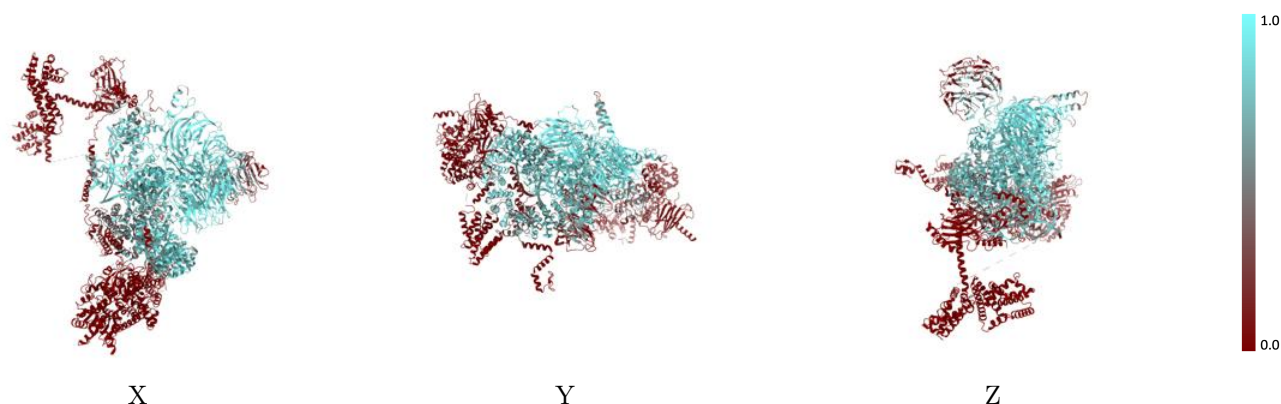
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

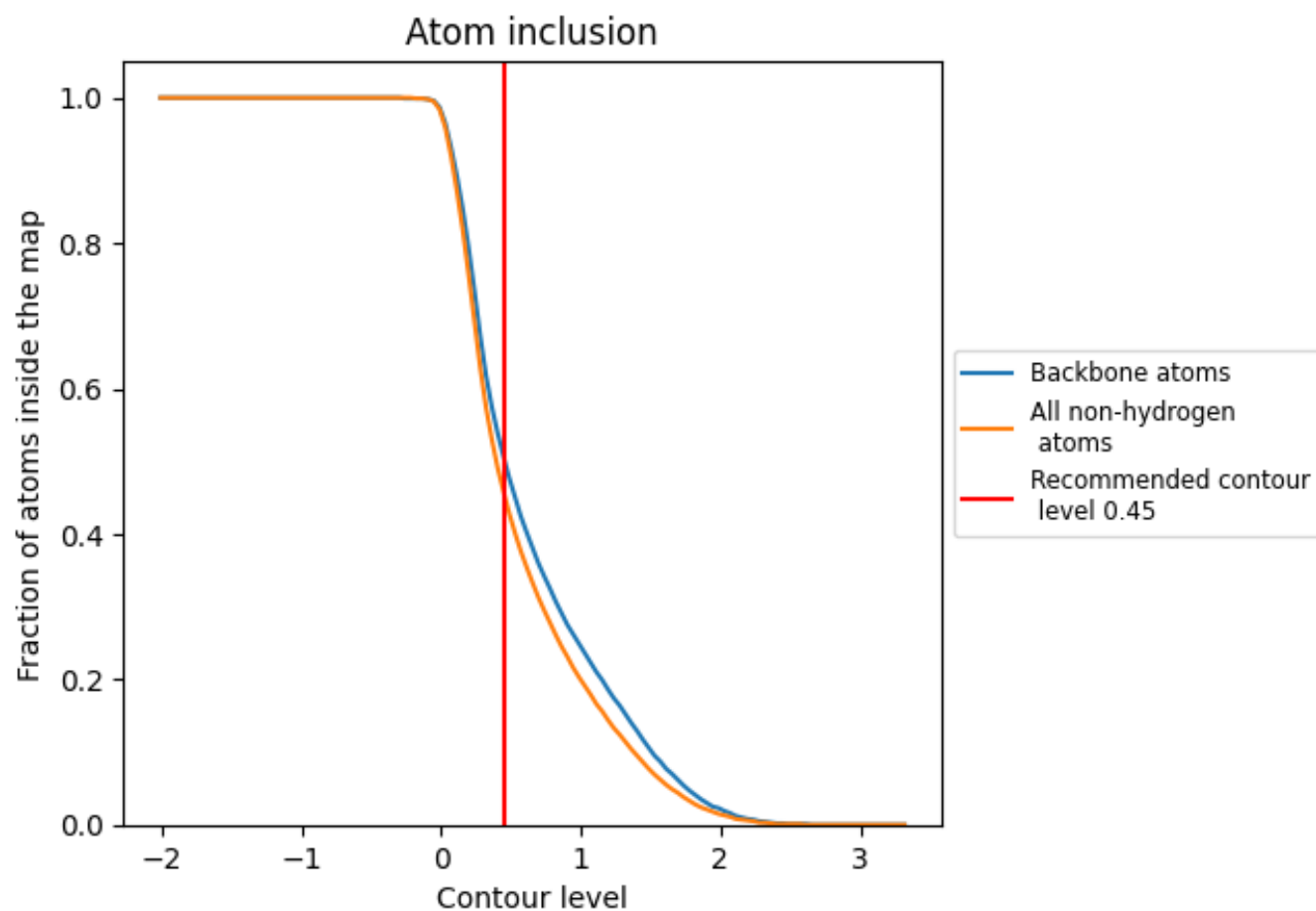
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.45).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 46% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4560	<div></div> 0.2810
2	<div></div> 0.8120	<div></div> 0.3820
A	<div></div> 0.0780	<div></div> 0.0930
A1	<div></div> 0.0020	<div></div> 0.0050
A2	<div></div> 0.1640	<div></div> 0.1480
A3	<div></div> 0.2400	<div></div> 0.1420
B	<div></div> 0.0030	<div></div> 0.0160
B1	<div></div> 0.7170	<div></div> 0.4260
B2	<div></div> 0.6290	<div></div> 0.3880
B3	<div></div> 0.7360	<div></div> 0.4410
B4	<div></div> 0.3390	<div></div> 0.2270
B5	<div></div> 0.8840	<div></div> 0.5320
B6	<div></div> 0.0950	<div></div> 0.2340
C	<div></div> 0.0070	<div></div> 0.0480
H	<div></div> 0.8780	<div></div> 0.5180
R	<div></div> 0.5390	<div></div> 0.2880

