



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:28 AM UTC

PDB ID : 6U62 / pdb_00006u62
EMDB ID : EMD-20660
Title : Raptor-Rag-Ragulator complex
Authors : Rogala, K.B.; Sabatini, D.M.
Deposited on : 2019-08-29
Resolution : 3.18 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

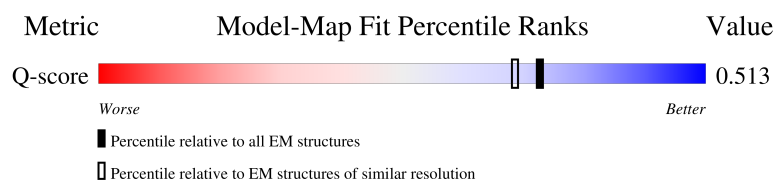
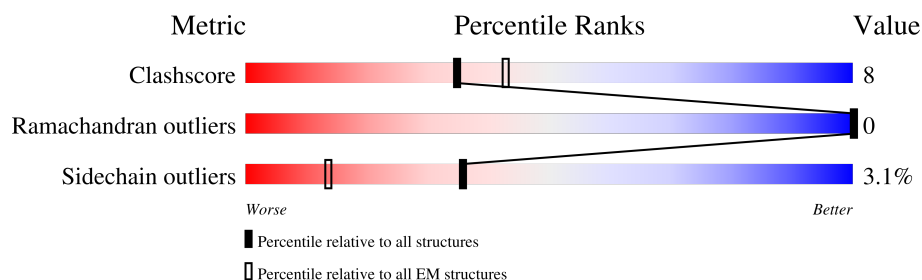
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1392	
2	B	313	
3	C	400	
4	D	158	

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Mol	Chain	Length	Quality of chain
5	E	125	75% 22% ••
6	F	162	56% 18% 26%
7	G	100	74% 10% 16%
8	H	91	71% 26% •

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17036 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 Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1110	Total	C	N	O	S	1	0
			8739	5583	1524	1574	58		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1336	GLY	-	expression tag	UNP Q8N122
A	1337	GLY	-	expression tag	UNP Q8N122
A	1338	GLY	-	expression tag	UNP Q8N122
A	1339	SER	-	expression tag	UNP Q8N122
A	1340	LEU	-	expression tag	UNP Q8N122
A	1341	GLU	-	expression tag	UNP Q8N122
A	1342	VAL	-	expression tag	UNP Q8N122
A	1343	LEU	-	expression tag	UNP Q8N122
A	1344	PHE	-	expression tag	UNP Q8N122
A	1345	GLN	-	expression tag	UNP Q8N122
A	1346	GLY	-	expression tag	UNP Q8N122
A	1347	PRO	-	expression tag	UNP Q8N122
A	1348	GLY	-	expression tag	UNP Q8N122
A	1349	SER	-	expression tag	UNP Q8N122
A	1350	GLY	-	expression tag	UNP Q8N122
A	1351	GLY	-	expression tag	UNP Q8N122
A	1352	GLY	-	expression tag	UNP Q8N122
A	1353	SER	-	expression tag	UNP Q8N122
A	1354	ASP	-	expression tag	UNP Q8N122
A	1355	TYR	-	expression tag	UNP Q8N122
A	1356	LYS	-	expression tag	UNP Q8N122
A	1357	ASP	-	expression tag	UNP Q8N122
A	1358	ASP	-	expression tag	UNP Q8N122
A	1359	ASP	-	expression tag	UNP Q8N122
A	1360	ASP	-	expression tag	UNP Q8N122
A	1361	LYS	-	expression tag	UNP Q8N122
A	1362	SER	-	expression tag	UNP Q8N122
A	1363	SER	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	GLY	-	expression tag	UNP Q8N122
A	1365	TRP	-	expression tag	UNP Q8N122
A	1366	SER	-	expression tag	UNP Q8N122
A	1367	HIS	-	expression tag	UNP Q8N122
A	1368	PRO	-	expression tag	UNP Q8N122
A	1369	GLN	-	expression tag	UNP Q8N122
A	1370	PHE	-	expression tag	UNP Q8N122
A	1371	GLU	-	expression tag	UNP Q8N122
A	1372	LYS	-	expression tag	UNP Q8N122
A	1373	GLY	-	expression tag	UNP Q8N122
A	1374	GLY	-	expression tag	UNP Q8N122
A	1375	GLY	-	expression tag	UNP Q8N122
A	1376	ALA	-	expression tag	UNP Q8N122
A	1377	ARG	-	expression tag	UNP Q8N122
A	1378	GLY	-	expression tag	UNP Q8N122
A	1379	GLY	-	expression tag	UNP Q8N122
A	1380	SER	-	expression tag	UNP Q8N122
A	1381	GLY	-	expression tag	UNP Q8N122
A	1382	GLY	-	expression tag	UNP Q8N122
A	1383	GLY	-	expression tag	UNP Q8N122
A	1384	SER	-	expression tag	UNP Q8N122
A	1385	TRP	-	expression tag	UNP Q8N122
A	1386	SER	-	expression tag	UNP Q8N122
A	1387	HIS	-	expression tag	UNP Q8N122
A	1388	PRO	-	expression tag	UNP Q8N122
A	1389	GLN	-	expression tag	UNP Q8N122
A	1390	PHE	-	expression tag	UNP Q8N122
A	1391	GLU	-	expression tag	UNP Q8N122
A	1392	LYS	-	expression tag	UNP Q8N122

- Molecule 2 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2439	1548	424	450	17		

- Molecule 3 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	281	Total	C	N	O	S	1	0
			2252	1451	368	421	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q9HB90
C	1	PRO	-	expression tag	UNP Q9HB90
C	75	ASN	SER	engineered mutation	UNP Q9HB90
C	90	ASN	THR	engineered mutation	UNP Q9HB90

- Molecule 4 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	108	Total	C	N	O	0	0
			710	449	121	140		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4	GLY	-	expression tag	UNP Q6IAA8
D	5	PRO	-	expression tag	UNP Q6IAA8

- Molecule 5 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	124	Total	C	N	O	S	0	0
			911	575	158	171	7		

- Molecule 6 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	120	Total	C	N	O	S	0	0
			883	572	149	161	1		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	GLU	-	expression tag	UNP Q9UHA4
F	126	ASN	-	expression tag	UNP Q9UHA4
F	127	LEU	-	expression tag	UNP Q9UHA4
F	128	TYR	-	expression tag	UNP Q9UHA4
F	129	PHE	-	expression tag	UNP Q9UHA4
F	130	GLN	-	expression tag	UNP Q9UHA4
F	131	GLY	-	expression tag	UNP Q9UHA4
F	132	SER	-	expression tag	UNP Q9UHA4
F	133	SER	-	expression tag	UNP Q9UHA4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	134	GLY	-	expression tag	UNP Q9UHA4
F	135	TRP	-	expression tag	UNP Q9UHA4
F	136	SER	-	expression tag	UNP Q9UHA4
F	137	HIS	-	expression tag	UNP Q9UHA4
F	138	PRO	-	expression tag	UNP Q9UHA4
F	139	GLN	-	expression tag	UNP Q9UHA4
F	140	PHE	-	expression tag	UNP Q9UHA4
F	141	GLU	-	expression tag	UNP Q9UHA4
F	142	LYS	-	expression tag	UNP Q9UHA4
F	143	GLY	-	expression tag	UNP Q9UHA4
F	144	GLY	-	expression tag	UNP Q9UHA4
F	145	GLY	-	expression tag	UNP Q9UHA4
F	146	SER	-	expression tag	UNP Q9UHA4
F	147	GLY	-	expression tag	UNP Q9UHA4
F	148	GLY	-	expression tag	UNP Q9UHA4
F	149	GLY	-	expression tag	UNP Q9UHA4
F	150	SER	-	expression tag	UNP Q9UHA4
F	151	GLY	-	expression tag	UNP Q9UHA4
F	152	GLY	-	expression tag	UNP Q9UHA4
F	153	GLY	-	expression tag	UNP Q9UHA4
F	154	SER	-	expression tag	UNP Q9UHA4
F	155	TRP	-	expression tag	UNP Q9UHA4
F	156	SER	-	expression tag	UNP Q9UHA4
F	157	HIS	-	expression tag	UNP Q9UHA4
F	158	PRO	-	expression tag	UNP Q9UHA4
F	159	GLN	-	expression tag	UNP Q9UHA4
F	160	PHE	-	expression tag	UNP Q9UHA4
F	161	GLU	-	expression tag	UNP Q9UHA4
F	162	LYS	-	expression tag	UNP Q9UHA4

- Molecule 7 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	84	Total	C	N	O	0	0
			447	270	89	88		

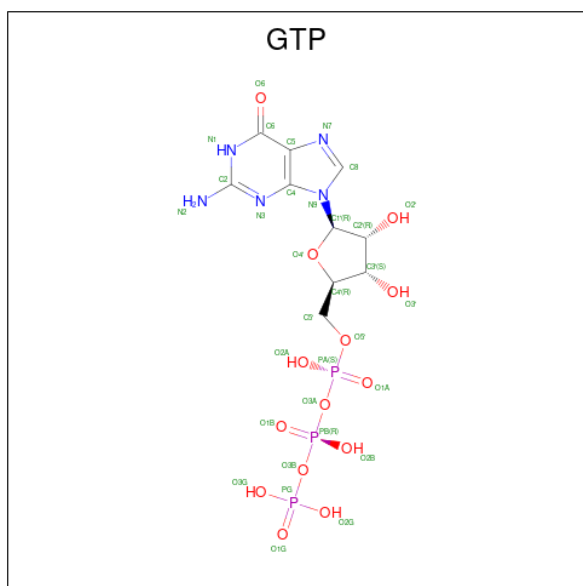
There are 2 discrepancies between the modelled and reference sequences:

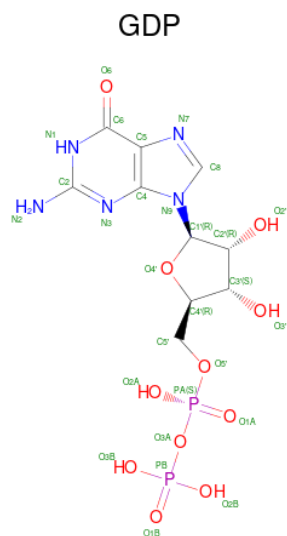
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP Q0VGL1
G	1	PRO	-	expression tag	UNP Q0VGL1

- Molecule 8 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	89	Total	C	N	O	S	0	0
			594	368	106	114	6		

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



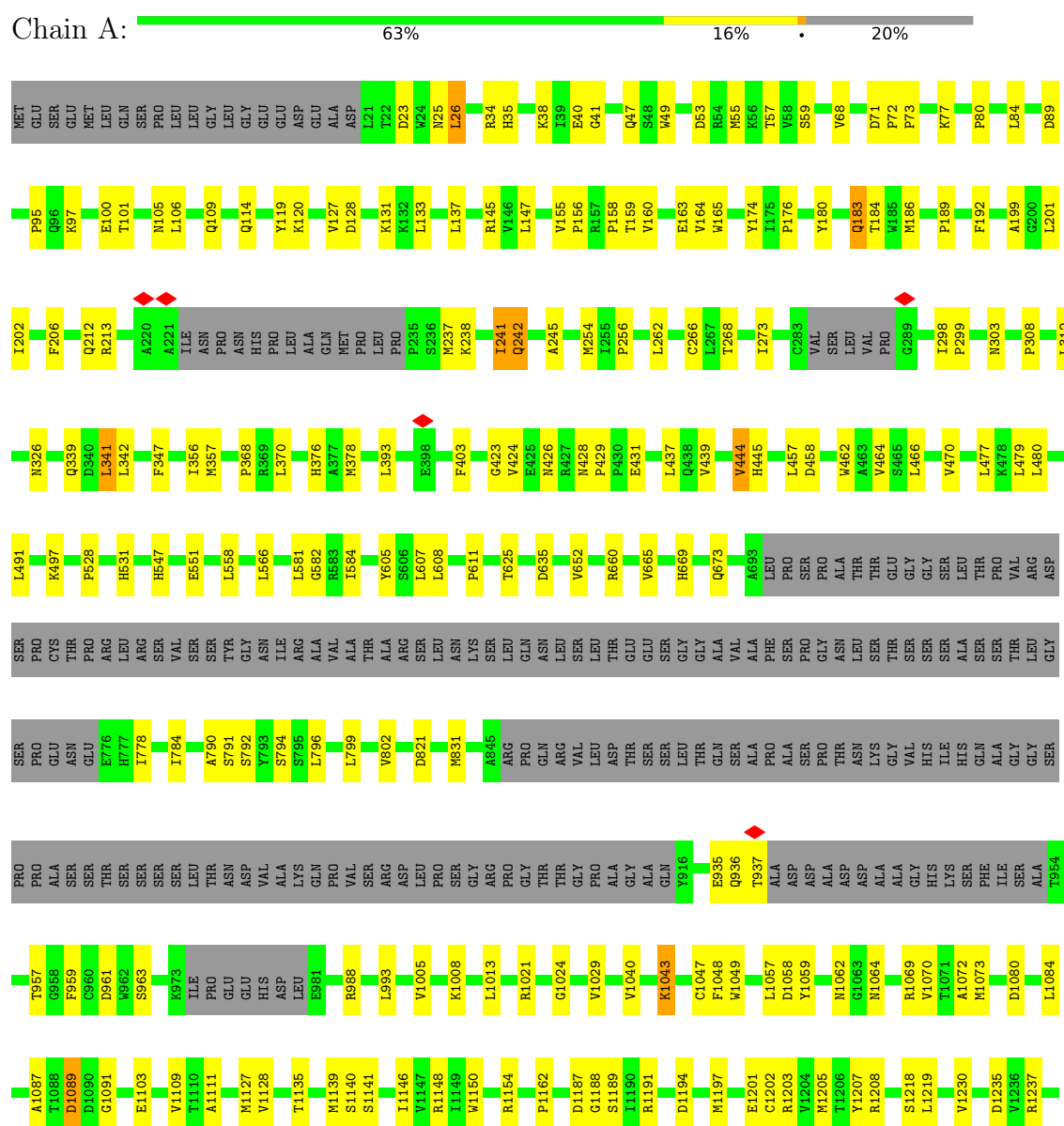


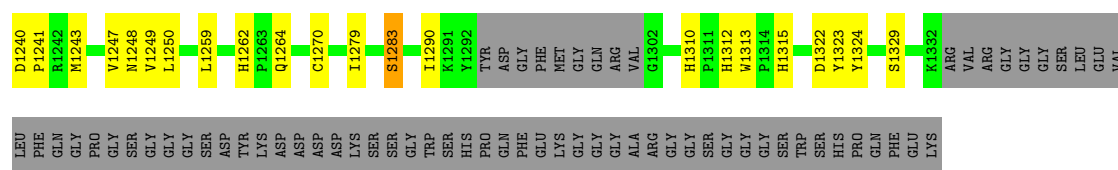
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

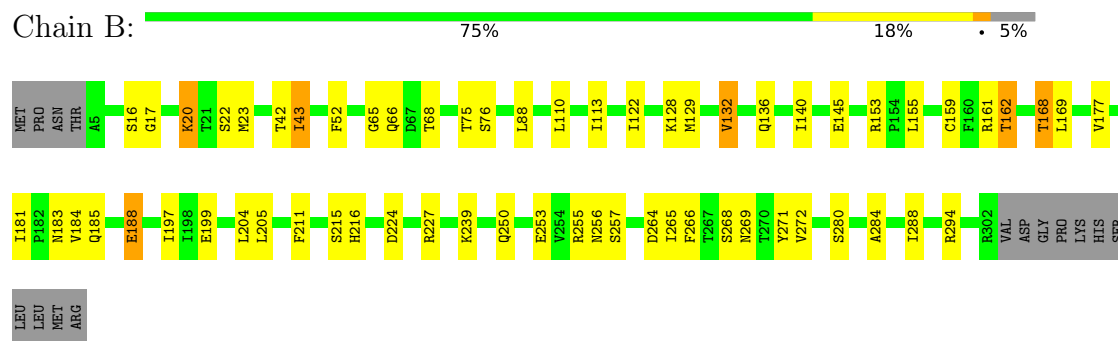
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

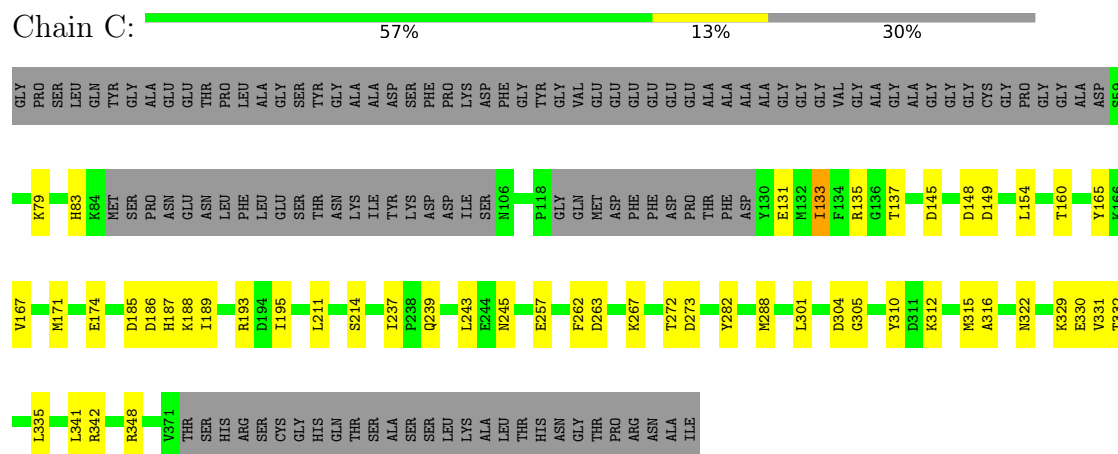




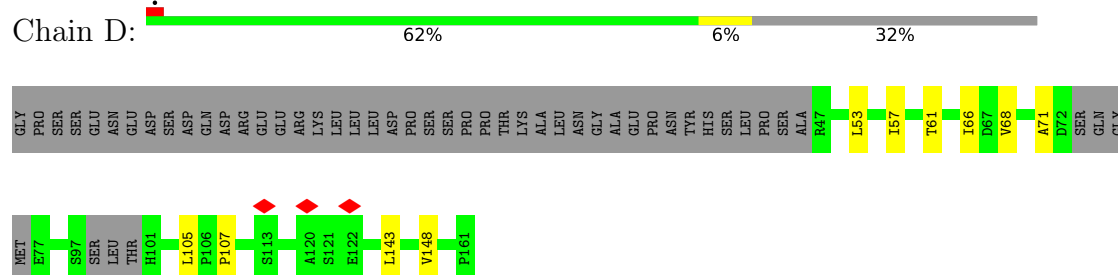
• Molecule 2: Ras-related GTP-binding protein A



• Molecule 3: Ras-related GTP-binding protein C

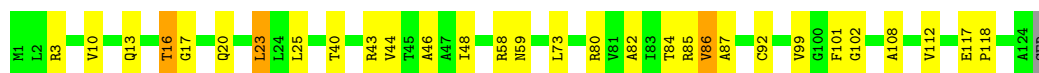


• Molecule 4: Regulator complex protein LAMTOR1

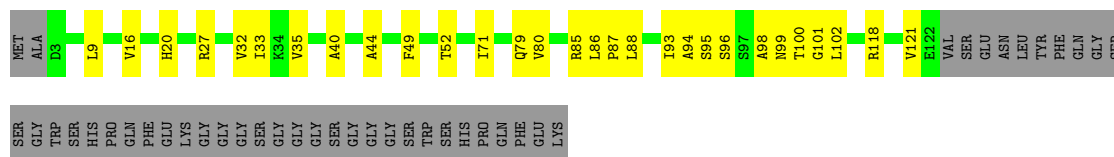


• Molecule 5: Regulator complex protein LAMTOR2

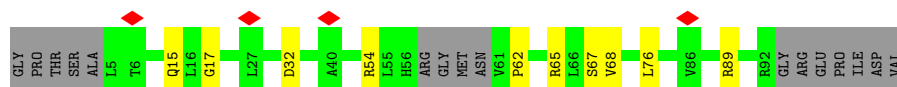




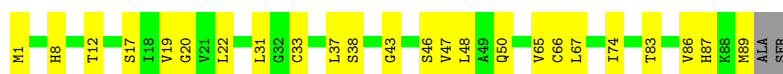
• Molecule 6: Regulator complex protein LAMTOR3



• Molecule 7: Regulator complex protein LAMTOR4



• Molecule 8: Regulator complex protein LAMTOR5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	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	0.064	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG

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	0.17	0/8951	0.39	0/12178
2	B	0.28	0/2484	0.45	0/3346
3	C	0.19	0/2298	0.36	0/3101
4	D	0.13	0/720	0.32	0/991
5	E	0.16	0/921	0.32	0/1249
6	F	0.15	0/899	0.42	0/1224
7	G	0.12	0/448	0.34	0/619
8	H	0.12	0/600	0.31	0/821
All	All	0.19	0/17321	0.39	0/23529

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 [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	8739	0	8626	140	0
2	B	2439	0	2421	43	0
3	C	2252	0	2235	31	0
4	D	710	0	593	6	0
5	E	911	0	919	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	883	0	878	20	0
7	G	447	0	268	6	0
8	H	594	0	560	18	0
9	B	32	0	12	7	0
10	B	1	0	0	0	0
11	C	28	0	12	0	0
All	All	17036	0	16524	268	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 8.

All (268) 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)
2:B:250:GLN:HB2	2:B:265:ILE:HD11	1.59	0.85
2:B:162:THR:HA	2:B:168:THR:HG23	1.60	0.84
1:A:192:PHE:HB2	1:A:242:GLN:HB3	1.64	0.79
2:B:162:THR:HA	2:B:168:THR:CG2	2.13	0.78
2:B:22:SER:HB3	9:B:401:GTP:O1A	1.85	0.77
1:A:1310:HIS:HD2	1:A:1312:HIS:H	1.34	0.74
7:G:17:GLY:HA3	7:G:32:ASP:H	1.52	0.73
1:A:660:ARG:NH2	1:A:821:ASP:OD2	2.21	0.73
2:B:17:GLY:CA	9:B:401:GTP:O1B	2.36	0.73
1:A:165:TRP:HB3	1:A:174:TYR:HB2	1.71	0.73
1:A:428:ASN:ND2	1:A:429:PRO:O	2.22	0.72
2:B:17:GLY:HA2	9:B:401:GTP:O1B	1.89	0.72
2:B:42:THR:N	9:B:401:GTP:O3G	2.20	0.72
1:A:1043:LYS:HB2	1:A:1069:ARG:HB2	1.74	0.69
1:A:1062:ASN:HD22	1:A:1064:ASN:HD22	1.40	0.69
6:F:86:LEU:HB2	6:F:87:PRO:HD3	1.75	0.69
3:C:331:VAL:HG12	3:C:332:THR:HG23	1.75	0.68
1:A:158:PRO:HB2	1:A:201:LEU:HD11	1.76	0.67
2:B:224:ASP:HB3	2:B:227:ARG:HB3	1.77	0.66
2:B:162:THR:HG22	2:B:169:LEU:HA	1.79	0.65
1:A:558:LEU:HD23	1:A:584:ILE:HD12	1.77	0.65
1:A:53:ASP:OD2	1:A:339:GLN:NE2	2.30	0.64
2:B:145:GLU:HG3	2:B:159:CYS:HB2	1.79	0.64
1:A:59:SER:HB2	1:A:137:LEU:HD22	1.80	0.63
2:B:199:GLU:OE2	5:E:3:ARG:NH1	2.31	0.63
2:B:181:ILE:HB	2:B:184:VAL:HG22	1.81	0.62
1:A:988:ARG:NH1	1:A:1080:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:ALA:HB1	6:F:98:ALA:HB3	1.81	0.62
1:A:660:ARG:NH1	1:A:1111:ALA:O	2.32	0.62
1:A:1103:GLU:N	1:A:1103:GLU:OE1	2.33	0.61
5:E:59:ASN:ND2	6:F:52:THR:OG1	2.33	0.60
1:A:423:GLY:O	1:A:426:ASN:ND2	2.35	0.59
3:C:148:ASP:OD1	3:C:149:ASP:N	2.33	0.59
6:F:99:ASN:HD22	6:F:102:LEU:H	1.49	0.59
1:A:38:LYS:NZ	1:A:40:GLU:OE1	2.35	0.58
1:A:1047:CYS:SG	1:A:1049:TRP:NE1	2.76	0.58
3:C:165:TYR:HB2	3:C:211:LEU:HD21	1.84	0.58
2:B:17:GLY:N	9:B:401:GTP:O1B	2.37	0.58
1:A:1247:VAL:HG12	1:A:1248:ASN:HD22	1.68	0.57
1:A:158:PRO:HG2	1:A:202:ILE:HD11	1.86	0.57
1:A:1313:TRP:HB3	1:A:1315:HIS:HD2	1.69	0.56
4:D:71:ALA:HB1	5:E:58:ARG:HH22	1.70	0.56
6:F:102:LEU:HD22	8:H:47:VAL:HG21	1.87	0.56
2:B:197:ILE:O	5:E:3:ARG:NH2	2.38	0.56
2:B:204:LEU:HD23	2:B:216:HIS:HB2	1.88	0.56
2:B:280:SER:O	5:E:43:ARG:NH1	2.33	0.56
6:F:9:LEU:HD23	6:F:35:VAL:HG23	1.88	0.56
5:E:20:GLN:NE2	5:E:40:THR:OG1	2.39	0.55
1:A:665:VAL:HG21	1:A:957:THR:HG23	1.88	0.55
2:B:110:LEU:HD11	2:B:122:ILE:HD13	1.89	0.55
6:F:79:GLN:NE2	6:F:100:THR:OG1	2.39	0.55
1:A:1062:ASN:HD22	1:A:1064:ASN:ND2	2.05	0.55
1:A:1043:LYS:HA	1:A:1070:VAL:H	1.71	0.55
2:B:266:PHE:O	2:B:294:ARG:HG3	2.07	0.55
1:A:71:ASP:O	1:A:73:PRO:HD3	2.07	0.55
6:F:16:VAL:HG22	6:F:102:LEU:HD23	1.89	0.54
1:A:1218:SER:OG	1:A:1219:LEU:N	2.41	0.54
8:H:20:GLY:O	8:H:87:HIS:N	2.41	0.54
1:A:1191:ARG:HB3	1:A:1203:ARG:HD2	1.90	0.54
6:F:44:ALA:HB1	6:F:93:ILE:HG12	1.88	0.54
1:A:1207:TYR:OH	1:A:1240:ASP:O	2.23	0.54
3:C:185:ASP:HA	3:C:188:LYS:HE3	1.91	0.53
6:F:32:VAL:HG12	6:F:33:ILE:HG23	1.89	0.53
7:G:15:GLN:HA	7:G:89:ARG:HA	1.90	0.53
1:A:1259:LEU:HD12	1:A:1270:CYS:HB3	1.90	0.53
8:H:74:ILE:HB	8:H:87:HIS:ND1	2.24	0.53
1:A:156:PRO:HG2	1:A:165:TRP:CD1	2.44	0.53
5:E:16:THR:OG1	5:E:17:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:CYS:HA	1:A:273:ILE:HG21	1.91	0.52
1:A:298:ILE:HD13	1:A:393:LEU:HD11	1.91	0.52
1:A:163:GLU:HB2	1:A:176:PRO:HB3	1.92	0.51
1:A:41:GLY:HA3	1:A:961:ASP:HB3	1.93	0.51
5:E:86:VAL:HG12	5:E:87:ALA:H	1.76	0.51
1:A:47:GLN:HG3	1:A:49:TRP:CD1	2.46	0.51
1:A:1091:GLY:HA2	1:A:1127:MET:SD	2.50	0.51
2:B:255:ARG:HB3	3:C:315:MET:HG3	1.91	0.51
8:H:46:SER:HA	8:H:83:THR:HG21	1.92	0.51
1:A:1047:CYS:HB2	1:A:1059:TYR:HD1	1.76	0.51
3:C:135:ARG:NH1	3:C:167:VAL:O	2.44	0.51
4:D:57:ILE:O	4:D:61:THR:HG22	2.11	0.51
3:C:348:ARG:HD3	4:D:68:VAL:HB	1.92	0.51
1:A:444:VAL:HG13	1:A:445:HIS:ND1	2.26	0.50
1:A:57:THR:HG22	1:A:145:ARG:HB2	1.91	0.50
3:C:310:TYR:OH	3:C:335:LEU:O	2.30	0.50
2:B:23:MET:HB2	2:B:169:LEU:HD11	1.93	0.50
3:C:154:LEU:HD21	3:C:195:ILE:HG23	1.93	0.50
5:E:80:ARG:NH1	5:E:99:VAL:O	2.44	0.50
1:A:105:ASN:O	1:A:109:GLN:N	2.42	0.50
1:A:611:PRO:HB3	1:A:1154:ARG:HD2	1.92	0.50
1:A:1262:HIS:HD2	1:A:1264:GLN:H	1.60	0.50
3:C:322:ASN:OD1	3:C:322:ASN:N	2.45	0.50
6:F:85:ARG:O	6:F:88:LEU:N	2.45	0.50
1:A:184:THR:HG22	1:A:213:ARG:NH1	2.26	0.50
1:A:1237:ARG:HD3	1:A:1249:VAL:HG13	1.94	0.50
3:C:79:LYS:HA	3:C:83:HIS:HB2	1.93	0.50
3:C:237:ILE:HG13	3:C:237:ILE:O	2.12	0.49
1:A:241:ILE:HG22	1:A:368:PRO:HD3	1.94	0.49
2:B:211:PHE:HE2	2:B:239:LYS:HD2	1.76	0.49
1:A:1230:VAL:HG11	1:A:1259:LEU:HD13	1.95	0.49
1:A:35:HIS:HB3	1:A:1109:VAL:HG13	1.95	0.49
1:A:114:GLN:O	1:A:119:TYR:OH	2.31	0.49
1:A:1310:HIS:CD2	1:A:1313:TRP:H	2.31	0.49
5:E:84:THR:HG22	5:E:85:ARG:H	1.76	0.49
1:A:652:VAL:HG11	1:A:796:LEU:HD13	1.95	0.48
3:C:239:GLN:O	3:C:243:LEU:HG	2.14	0.48
2:B:52:PHE:CZ	2:B:177:VAL:HG11	2.49	0.48
1:A:1058:ASP:OD1	1:A:1059:TYR:N	2.47	0.48
1:A:1013:LEU:HD23	1:A:1279:ILE:HD13	1.95	0.48
1:A:1047:CYS:HG	1:A:1049:TRP:CD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:TYR:HD1	1:A:608:LEU:HD12	1.79	0.48
1:A:1024:GLY:HA2	1:A:1323:TYR:CD2	2.49	0.48
8:H:66:CYS:SG	8:H:67:LEU:N	2.87	0.47
1:A:1315:HIS:ND1	1:A:1329:SER:HB3	2.29	0.47
2:B:185:GLN:CD	2:B:185:GLN:H	2.22	0.47
1:A:155:VAL:HB	1:A:165:TRP:HB2	1.96	0.47
1:A:71:ASP:C	1:A:73:PRO:HD3	2.40	0.47
1:A:120:LYS:HB3	1:A:133:LEU:HD11	1.96	0.47
1:A:347:PHE:HD2	1:A:370:LEU:HD11	1.78	0.47
2:B:255:ARG:HG3	2:B:255:ARG:O	2.15	0.47
8:H:8:HIS:O	8:H:12:THR:OG1	2.22	0.47
1:A:1029:VAL:HG22	1:A:1040:VAL:HG22	1.96	0.47
5:E:73:LEU:HB3	5:E:101:PHE:CE1	2.50	0.47
1:A:1250:LEU:HG	1:A:1283:SER:O	2.14	0.47
4:D:66:ILE:HD12	5:E:48:ILE:HD12	1.97	0.47
5:E:16:THR:HG21	8:H:1:MET:HB2	1.97	0.47
1:A:1146:ILE:HD13	1:A:1162:PRO:HA	1.98	0.46
1:A:1310:HIS:CD2	1:A:1312:HIS:H	2.25	0.46
3:C:137:THR:OG1	3:C:171:MET:SD	2.73	0.46
1:A:186:MET:HE3	1:A:186:MET:HB2	1.79	0.46
3:C:186:ASP:OD1	3:C:187:HIS:N	2.48	0.46
7:G:67:SER:HB3	8:H:66:CYS:HB3	1.97	0.46
1:A:147:LEU:HD22	1:A:342:LEU:HD21	1.97	0.46
1:A:1187:ASP:OD1	1:A:1188:GLY:N	2.48	0.46
7:G:68:VAL:HG22	8:H:65:VAL:HG13	1.97	0.46
1:A:180:TYR:HE2	1:A:212:GLN:HE22	1.64	0.46
8:H:17:SER:O	8:H:89:MET:N	2.44	0.46
1:A:528:PRO:HG2	1:A:531:HIS:HD2	1.80	0.46
2:B:205:LEU:HD12	2:B:205:LEU:HA	1.80	0.46
8:H:22:LEU:HD22	8:H:37:LEU:HD13	1.97	0.46
1:A:109:GLN:OE1	1:A:268:THR:OG1	2.34	0.46
1:A:458:ASP:HA	1:A:497:LYS:HE2	1.98	0.46
1:A:376:HIS:HD2	1:A:378:MET:H	1.63	0.45
6:F:101:GLY:C	8:H:43:GLY:HA3	2.42	0.45
8:H:74:ILE:HB	8:H:87:HIS:CE1	2.52	0.45
1:A:326:ASN:HD21	1:A:431:GLU:HB2	1.80	0.45
1:A:778:ILE:HD12	1:A:778:ILE:H	1.80	0.45
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.88	0.45
2:B:136:GLN:O	2:B:140:ILE:HG13	2.16	0.45
3:C:273:ASP:OD1	3:C:273:ASP:N	2.47	0.45
1:A:1139:MET:H	1:A:1139:MET:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLU:HG2	1:A:936:GLN:N	2.32	0.45
7:G:54:ARG:H	7:G:62:PRO:HB2	1.81	0.45
1:A:457:LEU:HG	1:A:464:VAL:HG22	1.98	0.45
1:A:791:SER:OG	1:A:792:SER:N	2.49	0.45
1:A:1048:PHE:HZ	1:A:1084:LEU:HD22	1.82	0.45
1:A:1208:ARG:HA	1:A:1208:ARG:HD3	1.77	0.45
1:A:1072:ALA:HB3	1:A:1087:ALA:HB3	1.99	0.45
1:A:582:GLY:O	1:A:625:THR:HG21	2.17	0.45
1:A:784:ILE:HD12	1:A:831:MET:SD	2.57	0.45
3:C:304:ASP:N	3:C:304:ASP:OD1	2.50	0.45
1:A:959:PHE:O	1:A:963:SER:OG	2.31	0.45
5:E:23:LEU:HD22	5:E:46:ALA:HB2	1.98	0.45
1:A:566:LEU:HD22	1:A:607:LEU:HD11	1.99	0.44
4:D:105:LEU:O	4:D:107:PRO:HD3	2.16	0.44
6:F:118:ARG:O	6:F:121:VAL:HG12	2.17	0.44
1:A:1047:CYS:HB2	1:A:1059:TYR:CD1	2.52	0.44
2:B:266:PHE:HB2	2:B:272:VAL:HB	1.98	0.44
5:E:25:LEU:HD11	5:E:46:ALA:HB1	1.99	0.44
1:A:1240:ASP:HB3	1:A:1243:MET:HB2	2.00	0.44
6:F:99:ASN:OD1	8:H:46:SER:OG	2.28	0.44
1:A:55:MET:HE1	1:A:189:PRO:HD2	1.99	0.44
3:C:262:PHE:HE1	3:C:282:TYR:HE1	1.65	0.44
6:F:27:ARG:HB3	6:F:27:ARG:HH11	1.82	0.44
1:A:159:THR:OG1	1:A:163:GLU:OE1	2.26	0.44
1:A:1148:ARG:HD2	1:A:1150:TRP:NE1	2.32	0.44
3:C:174:GLU:OE1	3:C:214:SER:OG	2.35	0.44
1:A:1313:TRP:CB	1:A:1315:HIS:HD2	2.31	0.44
2:B:284:ALA:O	2:B:288:ILE:HG13	2.17	0.44
1:A:72:PRO:HB2	1:A:174:TYR:HE2	1.83	0.44
3:C:131:GLU:HG2	3:C:167:VAL:HG13	2.00	0.44
1:A:57:THR:O	1:A:114:GLN:NE2	2.33	0.44
2:B:122:ILE:HD11	2:B:155:LEU:HD23	2.00	0.44
2:B:256:ASN:CG	2:B:257:SER:H	2.26	0.44
1:A:799:LEU:HB2	1:A:802:VAL:HG12	1.98	0.43
5:E:82:ALA:O	5:E:92:CYS:HA	2.18	0.43
5:E:108:ALA:O	5:E:112:VAL:HG23	2.18	0.43
2:B:132:VAL:HG11	2:B:140:ILE:HD12	2.00	0.43
2:B:253:GLU:O	3:C:316:ALA:HA	2.18	0.43
1:A:184:THR:HG22	1:A:213:ARG:HH12	1.82	0.43
1:A:547:HIS:NE2	1:A:551:GLU:OE2	2.52	0.43
1:A:1128:VAL:HG22	1:A:1141:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ASP:HB3	1:A:1197:MET:HG3	2.01	0.43
1:A:183:GLN:HB2	1:A:237:MET:HG3	1.99	0.43
2:B:128:LYS:HG2	9:B:401:GTP:C6	2.53	0.43
6:F:79:GLN:HB2	6:F:96:SER:HA	2.01	0.43
1:A:97:LYS:O	1:A:101:THR:HG23	2.18	0.43
2:B:188:GLU:HG2	2:B:215:SER:HB2	2.01	0.43
1:A:199:ALA:HB3	1:A:245:ALA:H	1.83	0.43
1:A:1127:MET:HE3	1:A:1140:SER:HB2	2.00	0.43
1:A:262:LEU:HD23	1:A:357:MET:SD	2.59	0.43
1:A:1205:MET:HG3	1:A:1241:PRO:O	2.19	0.43
1:A:1235:ASP:OD1	1:A:1235:ASP:N	2.52	0.43
1:A:1021:ARG:HB2	1:A:1324:TYR:HE1	1.84	0.42
1:A:77:LYS:HA	1:A:254:MET:HE1	2.01	0.42
1:A:299:PRO:HG2	1:A:308:PRO:HG2	2.01	0.42
1:A:1187:ASP:OD1	1:A:1189:SER:OG	2.35	0.42
4:D:148:VAL:HG21	5:E:10:VAL:HG13	2.00	0.42
1:A:23:ASP:HA	1:A:26:LEU:HG	2.01	0.42
1:A:128:ASP:HA	1:A:131:LYS:HD3	2.01	0.42
1:A:790:ALA:O	1:A:794:SER:OG	2.26	0.42
5:E:84:THR:HG22	5:E:85:ARG:N	2.34	0.42
1:A:1008:LYS:HB2	1:A:1008:LYS:HE3	1.85	0.42
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.90	0.42
1:A:105:ASN:OD1	1:A:106:LEU:N	2.51	0.42
1:A:1069:ARG:HG2	1:A:1089:ASP:OD2	2.20	0.42
2:B:129:MET:HG3	2:B:161:ARG:HB2	2.01	0.42
7:G:65:ARG:HH11	7:G:76:LEU:HD13	1.85	0.42
8:H:33:CYS:HB2	8:H:38:SER:HA	2.01	0.42
1:A:439:VAL:CG1	1:A:445:HIS:HB2	2.50	0.42
1:A:479:LEU:HB3	1:A:491:LEU:HD11	2.01	0.42
2:B:264:ASP:O	2:B:271:TYR:HD1	2.02	0.42
3:C:272:THR:OG1	3:C:273:ASP:N	2.52	0.42
1:A:158:PRO:HB3	1:A:164:VAL:HG12	2.02	0.41
2:B:88:LEU:HD22	2:B:113:ILE:HG13	2.02	0.41
1:A:183:GLN:H	1:A:183:GLN:HG2	1.62	0.41
3:C:145:ASP:OD1	3:C:145:ASP:N	2.35	0.41
5:E:102:GLY:HA3	8:H:31:LEU:HD12	2.02	0.41
1:A:155:VAL:HG11	1:A:165:TRP:O	2.20	0.41
1:A:202:ILE:O	1:A:206:PHE:HB2	2.21	0.41
1:A:201:LEU:HD12	1:A:202:ILE:N	2.35	0.41
6:F:88:LEU:HD23	6:F:88:LEU:HA	1.83	0.41
1:A:341:LEU:HD13	1:A:341:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LEU:O	1:A:584:ILE:HG22	2.20	0.41
8:H:47:VAL:HA	8:H:50:GLN:HG2	2.00	0.41
8:H:74:ILE:HA	8:H:86:VAL:O	2.20	0.41
1:A:308:PRO:HG3	1:A:403:PHE:CZ	2.55	0.41
1:A:1043:LYS:O	1:A:1069:ARG:HA	2.21	0.41
1:A:80:PRO:HG2	1:A:256:PRO:HG3	2.01	0.41
3:C:263:ASP:O	3:C:267:LYS:N	2.50	0.41
5:E:117:GLU:HB3	5:E:118:PRO:HD3	2.03	0.41
2:B:75:THR:OG1	2:B:76:SER:N	2.54	0.41
2:B:183:ASN:OD1	2:B:183:ASN:N	2.48	0.41
1:A:424:VAL:HG12	1:A:462:TRP:HZ2	1.86	0.41
1:A:831:MET:HE3	1:A:831:MET:HB3	2.00	0.41
2:B:20:LYS:HE3	9:B:401:GTP:O2B	2.21	0.41
3:C:262:PHE:CE1	3:C:282:TYR:HE1	2.39	0.41
6:F:20:HIS:NE2	6:F:95:SER:HB2	2.35	0.41
1:A:439:VAL:HG13	1:A:445:HIS:HB2	2.02	0.41
1:A:669:HIS:O	1:A:673:GLN:HG2	2.20	0.41
1:A:1322:ASP:O	1:A:1323:TYR:HB2	2.21	0.41
2:B:16:SER:HB2	2:B:65:GLY:C	2.46	0.41
2:B:153:ARG:NE	2:B:153:ARG:HA	2.35	0.41
3:C:133:ILE:O	3:C:137:THR:HG23	2.21	0.41
6:F:86:LEU:HD12	6:F:86:LEU:H	1.85	0.40
1:A:202:ILE:H	1:A:202:ILE:HG13	1.76	0.40
3:C:193:ARG:HE	3:C:193:ARG:HB2	1.71	0.40
3:C:312:LYS:HA	3:C:330:GLU:CD	2.46	0.40
1:A:466:LEU:O	1:A:470:VAL:HG23	2.21	0.40
1:A:1201:GLU:HG2	1:A:1202:CYS:H	1.86	0.40
3:C:329:LYS:HE3	3:C:329:LYS:HB3	1.93	0.40
1:A:238:LYS:HE3	1:A:238:LYS:HB3	1.92	0.40
3:C:257:GLU:OE2	3:C:342:ARG:HG3	2.22	0.40
3:C:301:LEU:HD13	3:C:305:GLY:HA2	2.04	0.40
1:A:68:VAL:HG21	1:A:95:PRO:C	2.47	0.40
1:A:84:LEU:HA	1:A:89:ASP:HA	2.03	0.40
1:A:326:ASN:ND2	1:A:431:GLU:HB2	2.37	0.40
2:B:43:ILE:HD13	2:B:43:ILE:HA	1.82	0.40
6:F:20:HIS:HB3	6:F:40:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1095/1392 (79%)	993 (91%)	102 (9%)	0	100	100
2	B	296/313 (95%)	275 (93%)	21 (7%)	0	100	100
3	C	276/400 (69%)	258 (94%)	18 (6%)	0	100	100
4	D	102/158 (65%)	98 (96%)	4 (4%)	0	100	100
5	E	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
6	F	118/162 (73%)	105 (89%)	13 (11%)	0	100	100
7	G	80/100 (80%)	71 (89%)	9 (11%)	0	100	100
8	H	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
All	All	2176/2741 (79%)	2000 (92%)	176 (8%)	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	
1	A	946/1202 (79%)	919 (97%)	27 (3%)	37	64
2	B	271/287 (94%)	261 (96%)	10 (4%)	30	59
3	C	251/340 (74%)	245 (98%)	6 (2%)	43	67
4	D	55/138 (40%)	53 (96%)	2 (4%)	31	60
5	E	90/98 (92%)	85 (94%)	5 (6%)	19	48
6	F	91/135 (67%)	88 (97%)	3 (3%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	12/83 (14%)	12 (100%)	0	100	100
8	H	58/77 (75%)	56 (97%)	2 (3%)	32	61
All	All	1774/2360 (75%)	1719 (97%)	55 (3%)	36	62

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	26	LEU
1	A	34	ARG
1	A	100	GLU
1	A	127	VAL
1	A	160	VAL
1	A	183	GLN
1	A	241	ILE
1	A	242	GLN
1	A	303	ASN
1	A	341	LEU
1	A	356	ILE
1	A	437	LEU
1	A	444	VAL
1	A	477	LEU
1	A	480	LEU
1	A	635	ASP
1	A	937	THR
1	A	993	LEU
1	A	1005	VAL
1	A	1043	LYS
1	A	1057	LEU
1	A	1073	MET
1	A	1089	ASP
1	A	1135	THR
1	A	1283	SER
1	A	1290	ILE
2	B	20	LYS
2	B	43	ILE
2	B	66	GLN
2	B	68	THR
2	B	132	VAL
2	B	162	THR
2	B	168	THR

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Mol	Chain	Res	Type
2	B	188	GLU
2	B	268	SER
2	B	269	ASN
3	C	133	ILE
3	C	160	THR
3	C	189	ILE
3	C	245	ASN
3	C	288	MET
3	C	341	LEU
4	D	53	LEU
4	D	143	LEU
5	E	13	GLN
5	E	16	THR
5	E	23	LEU
5	E	44	VAL
5	E	86	VAL
6	F	49	PHE
6	F	71	ILE
6	F	80	VAL
8	H	19	VAL
8	H	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	339	GLN
1	A	349	ASN
1	A	361	ASN
1	A	376	HIS
1	A	417	GLN
1	A	531	HIS
1	A	557	ASN
1	A	636	HIS
1	A	805	ASN
1	A	817	HIS
1	A	835	ASN
1	A	1016	GLN
1	A	1061	HIS
1	A	1064	ASN
1	A	1098	ASN
1	A	1248	ASN

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Mol	Chain	Res	Type
1	A	1251	GLN
1	A	1262	HIS
1	A	1275	GLN
1	A	1310	HIS
1	A	1315	HIS
2	B	107	GLN
2	B	179	GLN
2	B	193	ASN
3	C	196	HIS
3	C	200	ASN
5	E	20	GLN
5	E	59	ASN
5	E	109	GLN
6	F	79	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
11	GDP	C	401	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
9	GTP	B	401	10	33,34,34	0.58	0	50,54,54	0.54	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
11	GDP	C	401	-	-	3/16/32/32	0/3/3/3
9	GTP	B	401	10	-	6/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	401	GDP	C5-C4	2.87	1.46	1.38
11	C	401	GDP	C6-N1	-2.67	1.33	1.38
11	C	401	GDP	C5-N7	-2.24	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	401	GDP	C5-C4-N3	-6.06	118.75	128.39
11	C	401	GDP	C2-N3-C4	4.95	120.83	112.30
11	C	401	GDP	N9-C4-N3	4.55	135.04	125.95
11	C	401	GDP	C6-C5-N7	3.21	136.13	130.29
11	C	401	GDP	C4-C5-N7	-2.47	106.76	110.67
11	C	401	GDP	O6-C6-C5	-2.26	120.58	126.53
11	C	401	GDP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	401	GTP	PB-O3A-PA-O5'
9	B	401	GTP	C5'-O5'-PA-O3A
9	B	401	GTP	C5'-O5'-PA-O1A
11	C	401	GDP	C5'-O5'-PA-O3A
11	C	401	GDP	C5'-O5'-PA-O1A
11	C	401	GDP	C5'-O5'-PA-O2A

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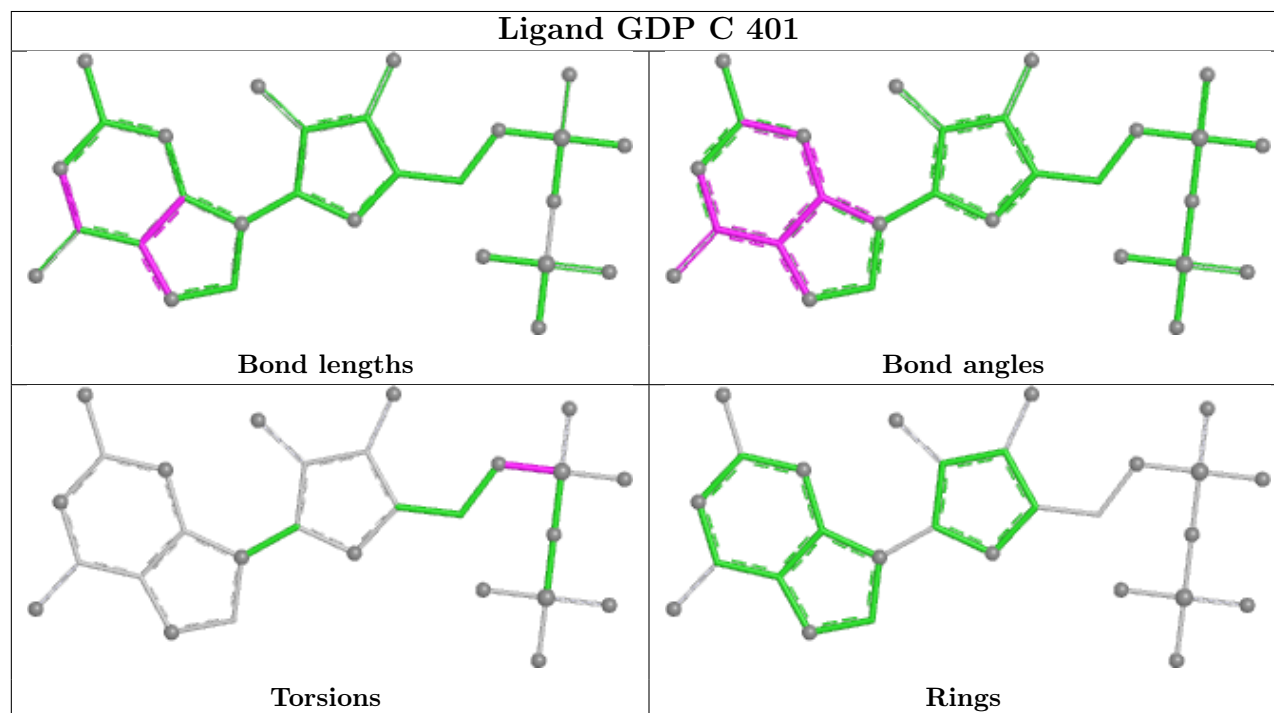
Mol	Chain	Res	Type	Atoms
9	B	401	GTP	C3'-C4'-C5'-O5'
9	B	401	GTP	O4'-C4'-C5'-O5'
9	B	401	GTP	C5'-O5'-PA-O2A

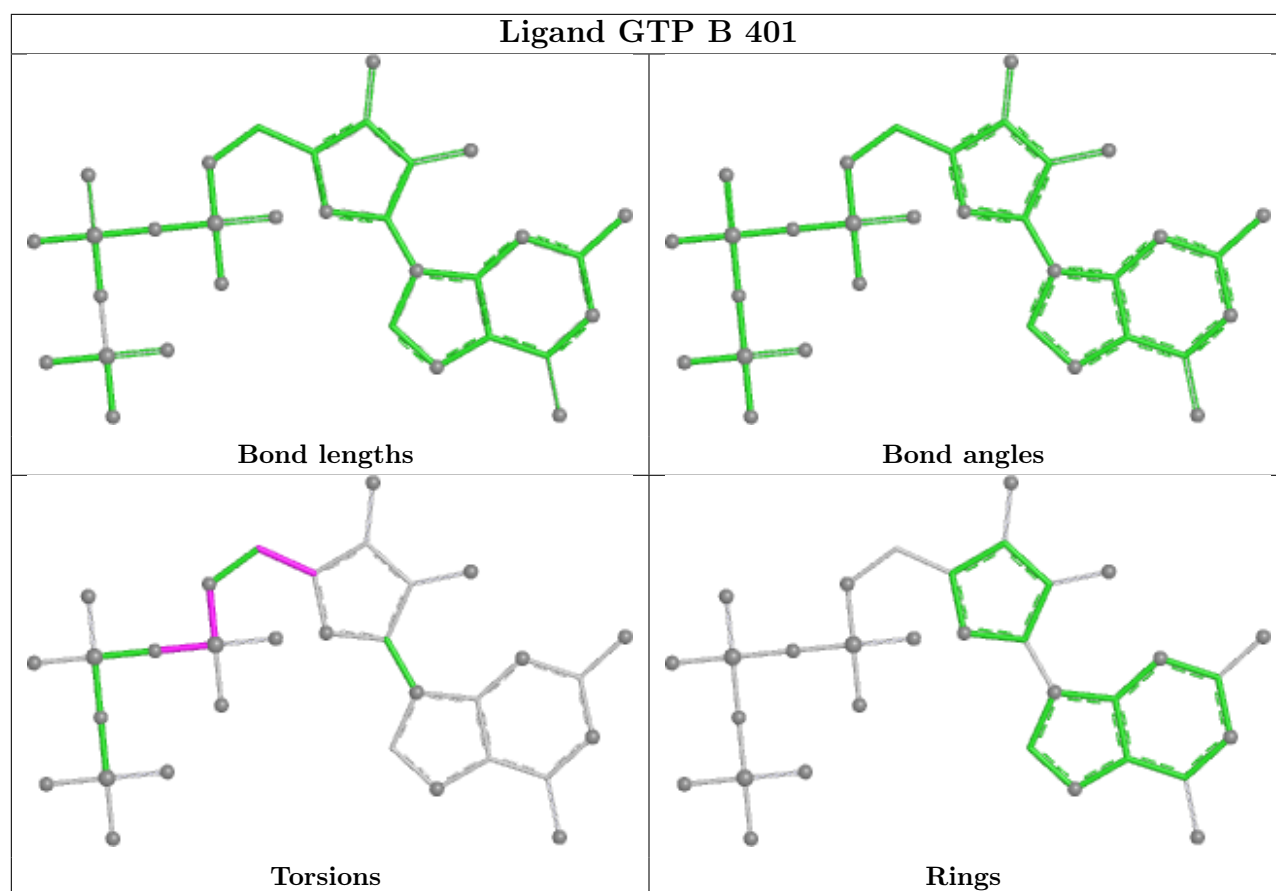
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	401	GTP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

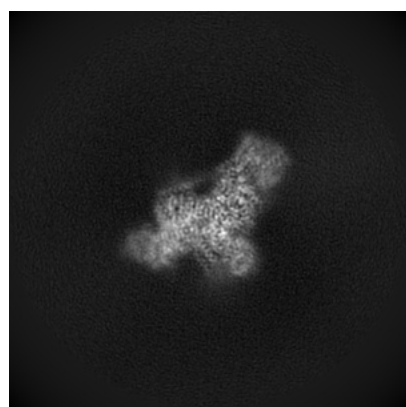
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20660. These allow visual inspection of the internal detail of the map and identification of artifacts.

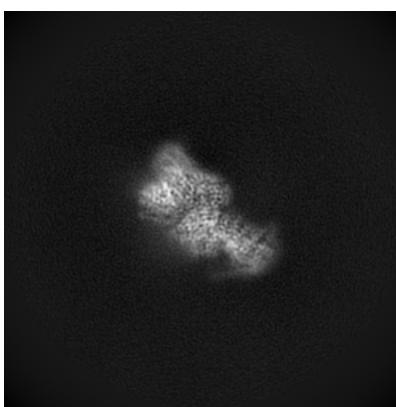
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

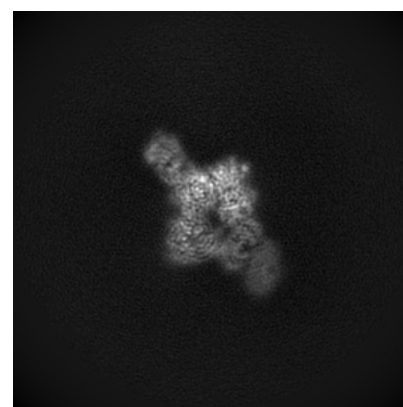
6.1.1 Primary map



X



Y



Z

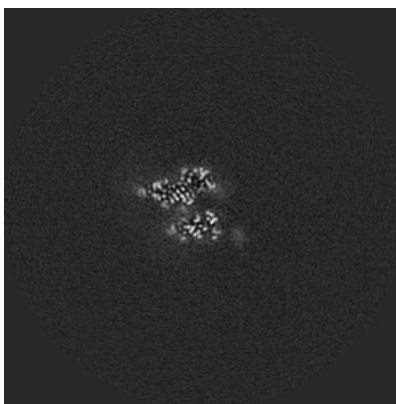
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

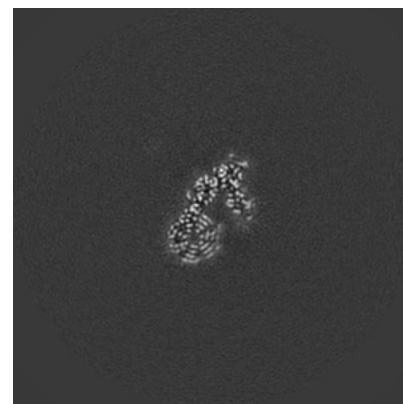
6.2.1 Primary map



X Index: 176



Y Index: 176

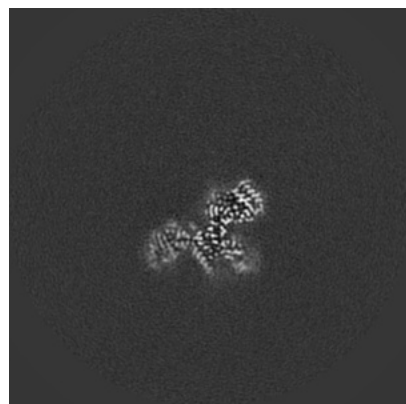


Z Index: 176

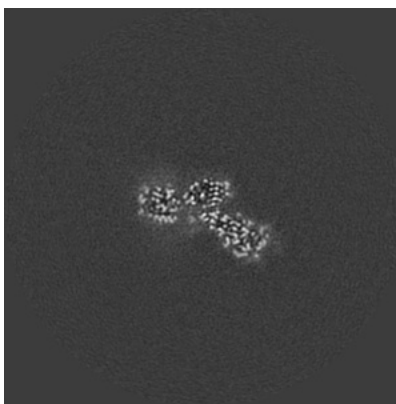
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

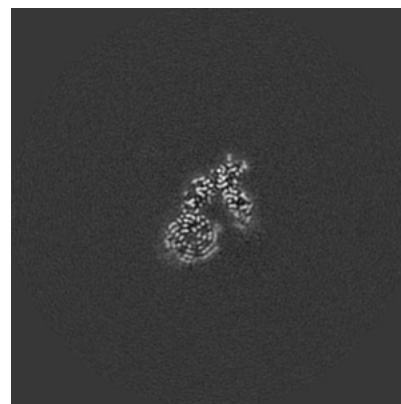
6.3.1 Primary map



X Index: 192



Y Index: 202

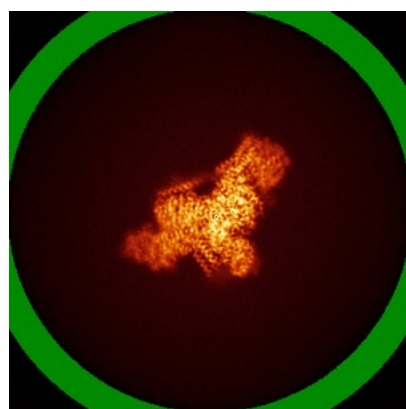


Z Index: 174

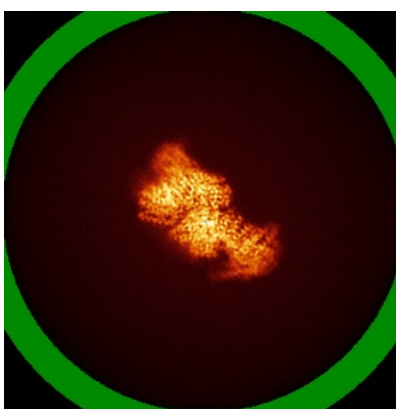
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

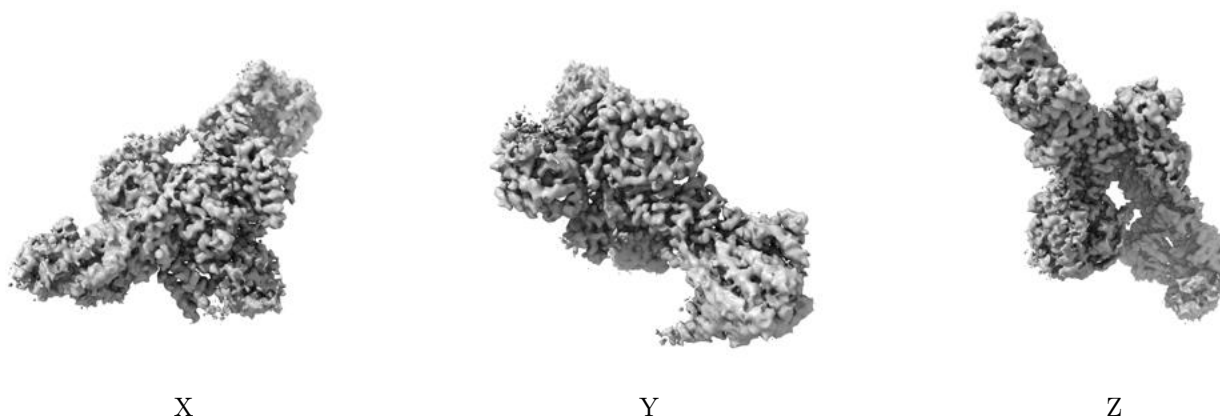


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

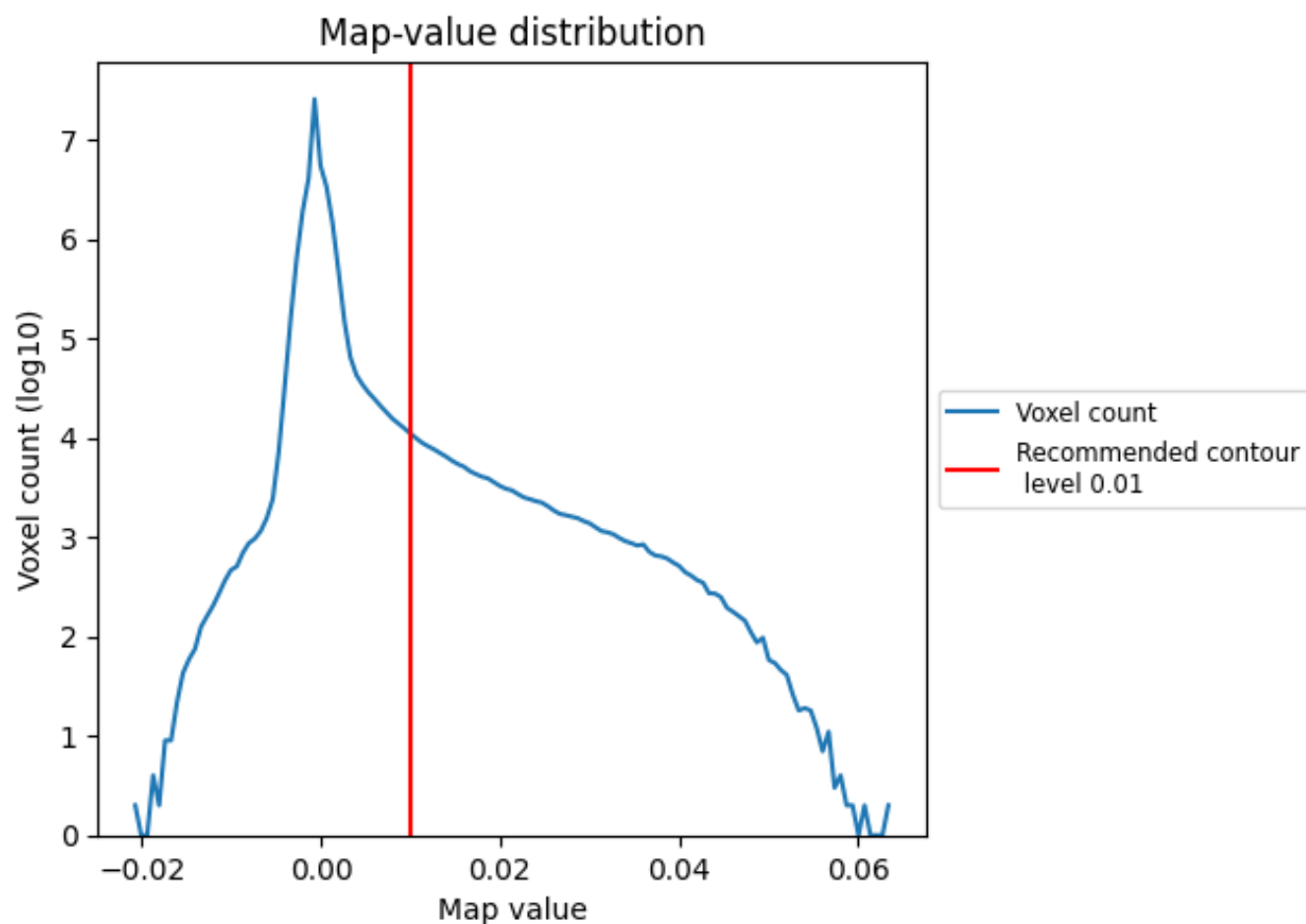
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

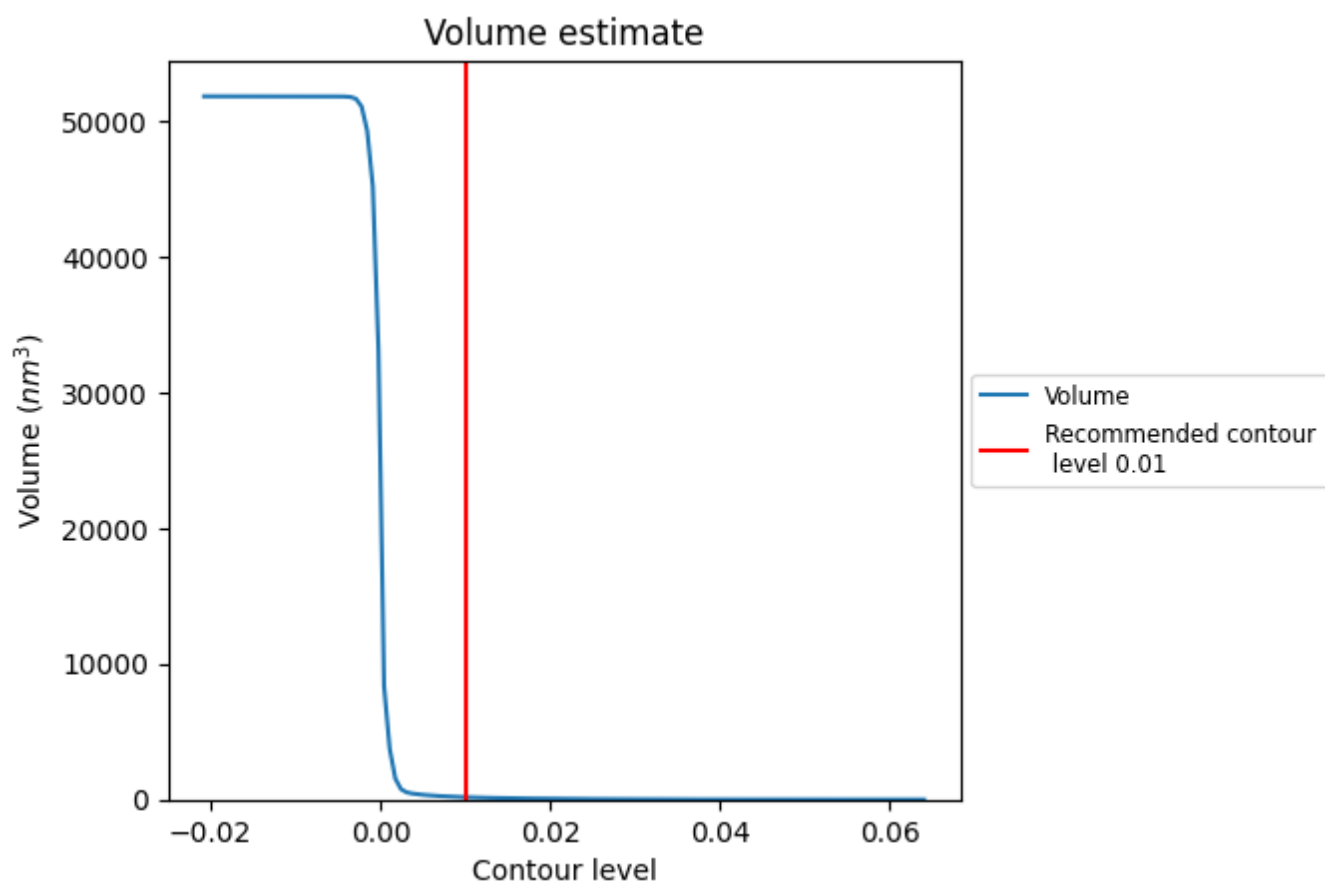
This section contains the results of statistical analysis of the map.

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.

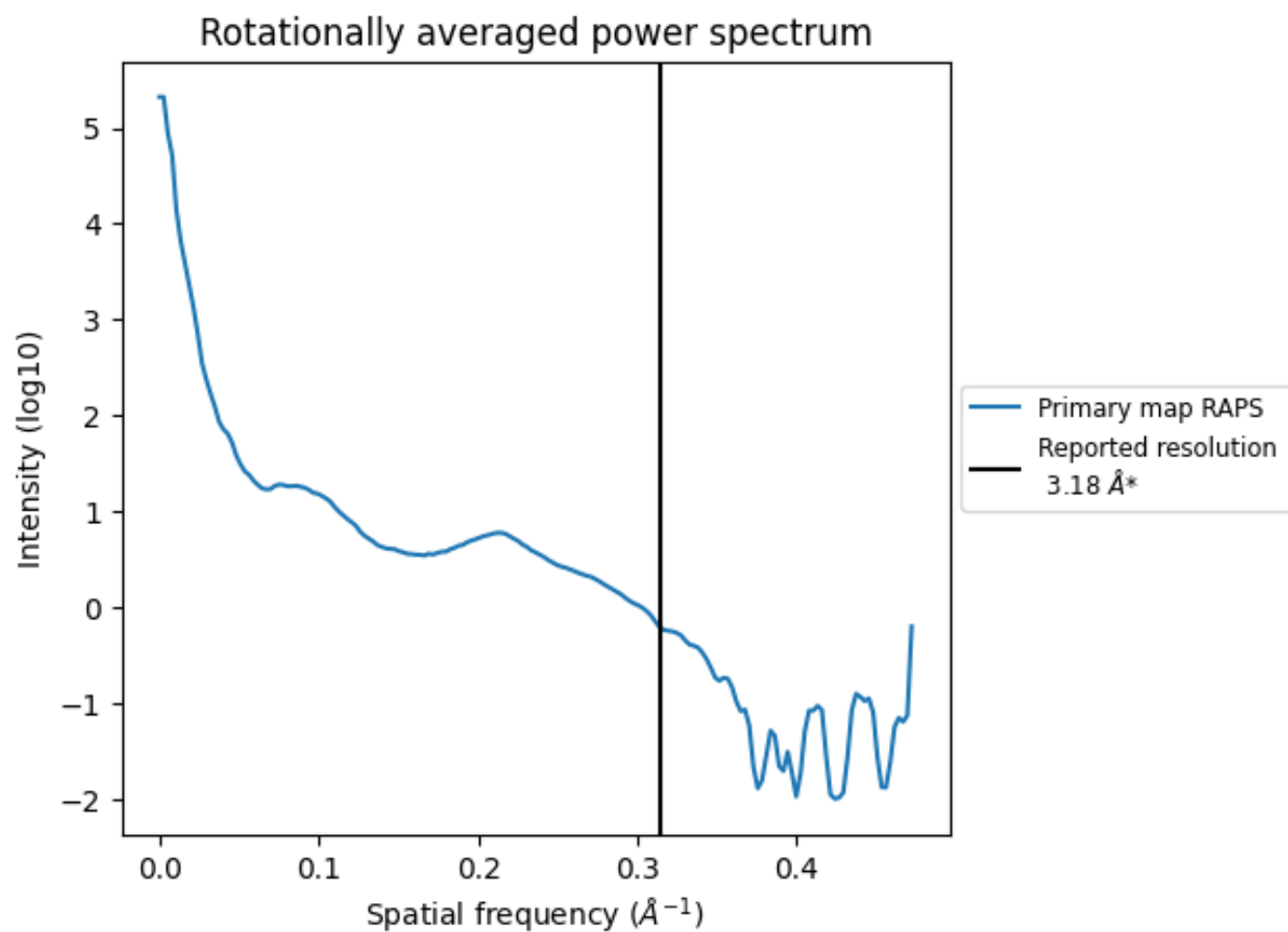
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm^3 ; this corresponds to an approximate mass of 157 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 0.314 Å⁻¹

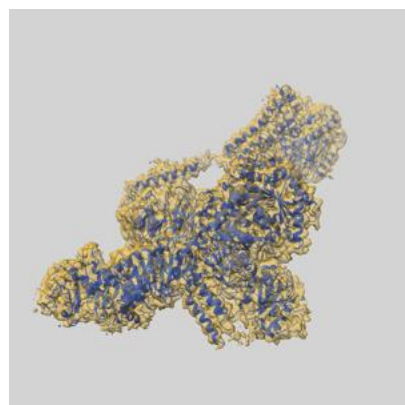
8 Fourier-Shell correlation

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

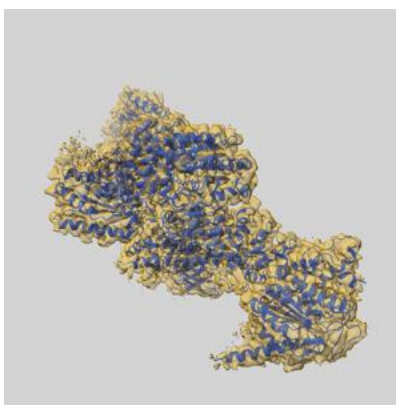
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20660 and PDB model 6U62. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

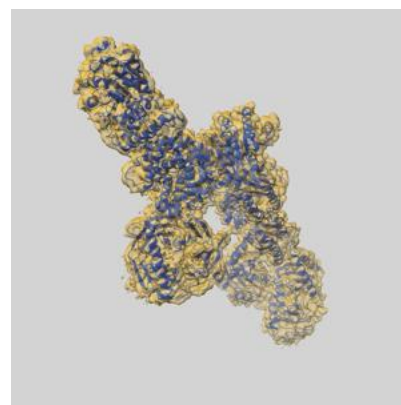
9.1 Map-model overlay [i](#)



X



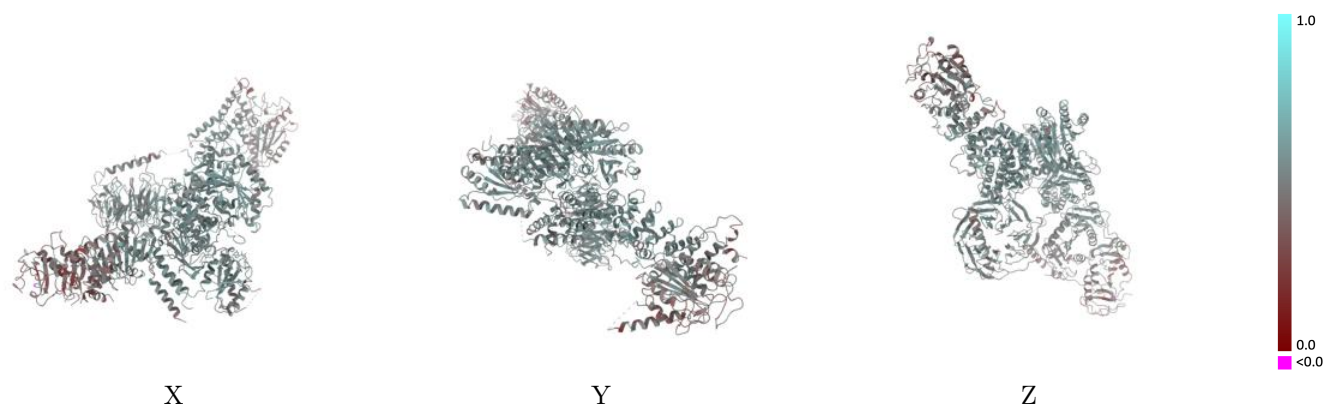
Y



Z

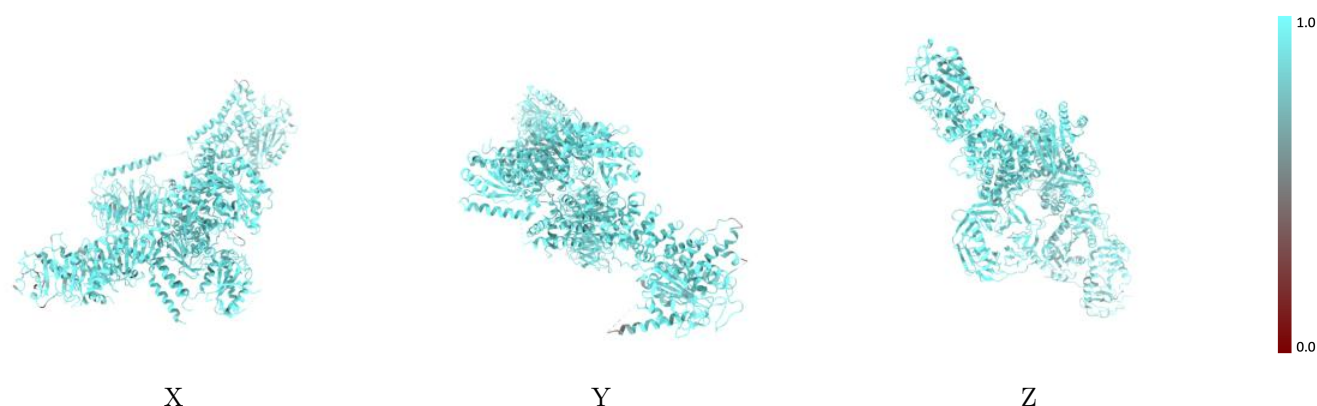
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



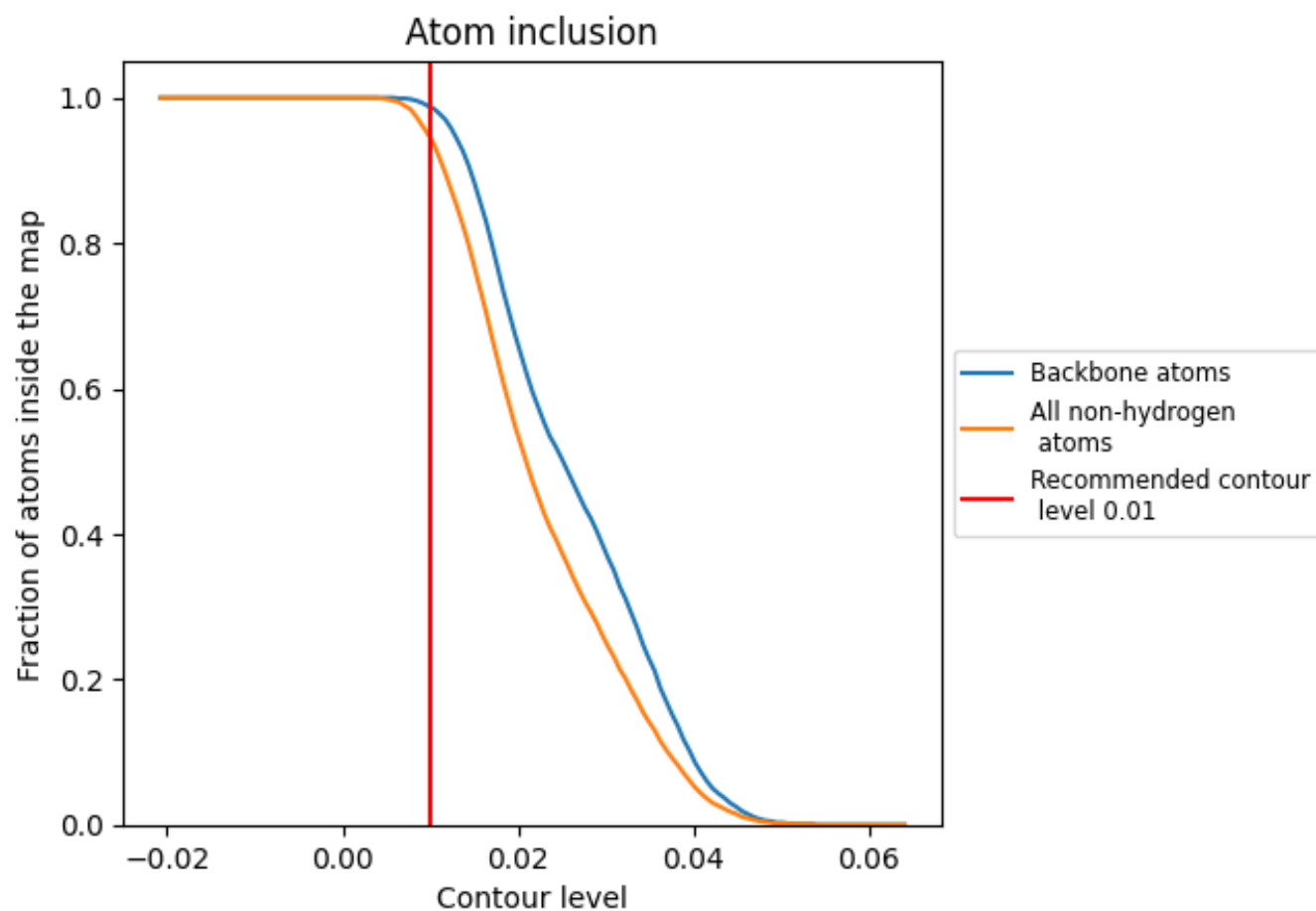
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.5130
A	0.9460	0.5150
B	0.9620	0.5580
C	0.9590	0.5420
D	0.9060	0.4370
E	0.9400	0.5200
F	0.9320	0.4720
G	0.8900	0.3880
H	0.9220	0.4410

1.0

0.0

<0.0