



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:02 AM UTC

PDB ID : 7PEC / pdb_00007pec
EMDB ID : EMD-13352
Title : cryo-EM structure of DEPTOR bound to human mTOR complex 1, DEPT-bound subset local refinement
Authors : Waelchli, M.; Maier, T.
Deposited on : 2021-08-09
Resolution : 4.24 Å(reported)
Based on initial model : 6BCX

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:

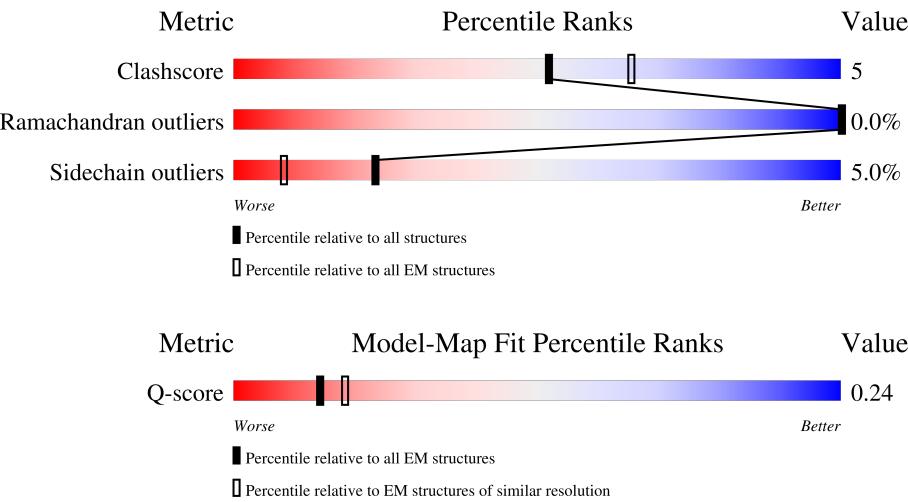
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.24 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	4688 (3.74 - 4.74)

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	2549	13% 73% 13% • 14%
2	C	326	• 79% 17% ••
3	E	1396	8% 62% 12% • 25%
4	I	409	5% 55% 20% • 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30911 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2192	Total	C	N	O	S	0	0
			17454	11152	3058	3133	111		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1052	Total	C	N	O	S	0	0
			8385	5361	1450	1518	56		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-60	MET	-	initiating methionine	UNP Q8N122
E	-59	ALA	-	expression tag	UNP Q8N122
E	-58	HIS	-	expression tag	UNP Q8N122
E	-57	HIS	-	expression tag	UNP Q8N122
E	-56	HIS	-	expression tag	UNP Q8N122
E	-55	HIS	-	expression tag	UNP Q8N122
E	-54	HIS	-	expression tag	UNP Q8N122
E	-53	HIS	-	expression tag	UNP Q8N122
E	-52	HIS	-	expression tag	UNP Q8N122
E	-51	HIS	-	expression tag	UNP Q8N122
E	-50	HIS	-	expression tag	UNP Q8N122
E	-49	HIS	-	expression tag	UNP Q8N122
E	-48	GLY	-	expression tag	UNP Q8N122
E	-47	SER	-	expression tag	UNP Q8N122
E	-46	THR	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-45	SER	-	expression tag	UNP Q8N122
E	-44	GLY	-	expression tag	UNP Q8N122
E	-43	SER	-	expression tag	UNP Q8N122
E	-42	GLY	-	expression tag	UNP Q8N122
E	-41	GLU	-	expression tag	UNP Q8N122
E	-40	GLN	-	expression tag	UNP Q8N122
E	-39	LYS	-	expression tag	UNP Q8N122
E	-38	LEU	-	expression tag	UNP Q8N122
E	-37	ILE	-	expression tag	UNP Q8N122
E	-36	SER	-	expression tag	UNP Q8N122
E	-35	GLU	-	expression tag	UNP Q8N122
E	-34	GLU	-	expression tag	UNP Q8N122
E	-33	ASP	-	expression tag	UNP Q8N122
E	-32	LEU	-	expression tag	UNP Q8N122
E	-31	GLY	-	expression tag	UNP Q8N122
E	-30	SER	-	expression tag	UNP Q8N122
E	-29	THR	-	expression tag	UNP Q8N122
E	-28	SER	-	expression tag	UNP Q8N122
E	-27	GLY	-	expression tag	UNP Q8N122
E	-26	SER	-	expression tag	UNP Q8N122
E	-25	GLY	-	expression tag	UNP Q8N122
E	-24	ASP	-	expression tag	UNP Q8N122
E	-23	TYR	-	expression tag	UNP Q8N122
E	-22	LYS	-	expression tag	UNP Q8N122
E	-21	ASP	-	expression tag	UNP Q8N122
E	-20	ASP	-	expression tag	UNP Q8N122
E	-19	ASP	-	expression tag	UNP Q8N122
E	-18	ASP	-	expression tag	UNP Q8N122
E	-17	LYS	-	expression tag	UNP Q8N122
E	-16	LEU	-	expression tag	UNP Q8N122
E	-15	THR	-	expression tag	UNP Q8N122
E	-14	SER	-	expression tag	UNP Q8N122
E	-13	LEU	-	expression tag	UNP Q8N122
E	-12	TYR	-	expression tag	UNP Q8N122
E	-11	LYS	-	expression tag	UNP Q8N122
E	-10	LYS	-	expression tag	UNP Q8N122
E	-9	ALA	-	expression tag	UNP Q8N122
E	-8	GLY	-	expression tag	UNP Q8N122
E	-7	LEU	-	expression tag	UNP Q8N122
E	-6	GLU	-	expression tag	UNP Q8N122
E	-5	ASN	-	expression tag	UNP Q8N122
E	-4	LEU	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	TYR	-	expression tag	UNP Q8N122
E	-2	PHE	-	expression tag	UNP Q8N122
E	-1	GLN	-	expression tag	UNP Q8N122
E	0	GLY	-	expression tag	UNP Q8N122

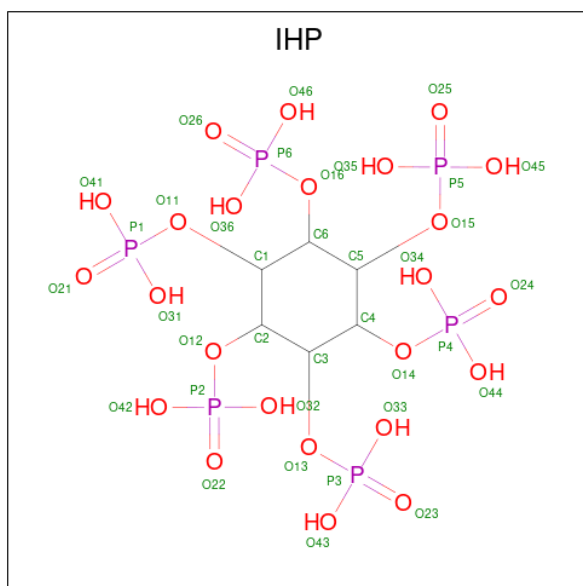
- Molecule 4 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	317	Total	C	N	O	S	0	0
			2580	1627	470	465	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	204	SER	ASN	variant	UNP Q8TB45
I	389	ASN	SER	variant	UNP Q8TB45

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

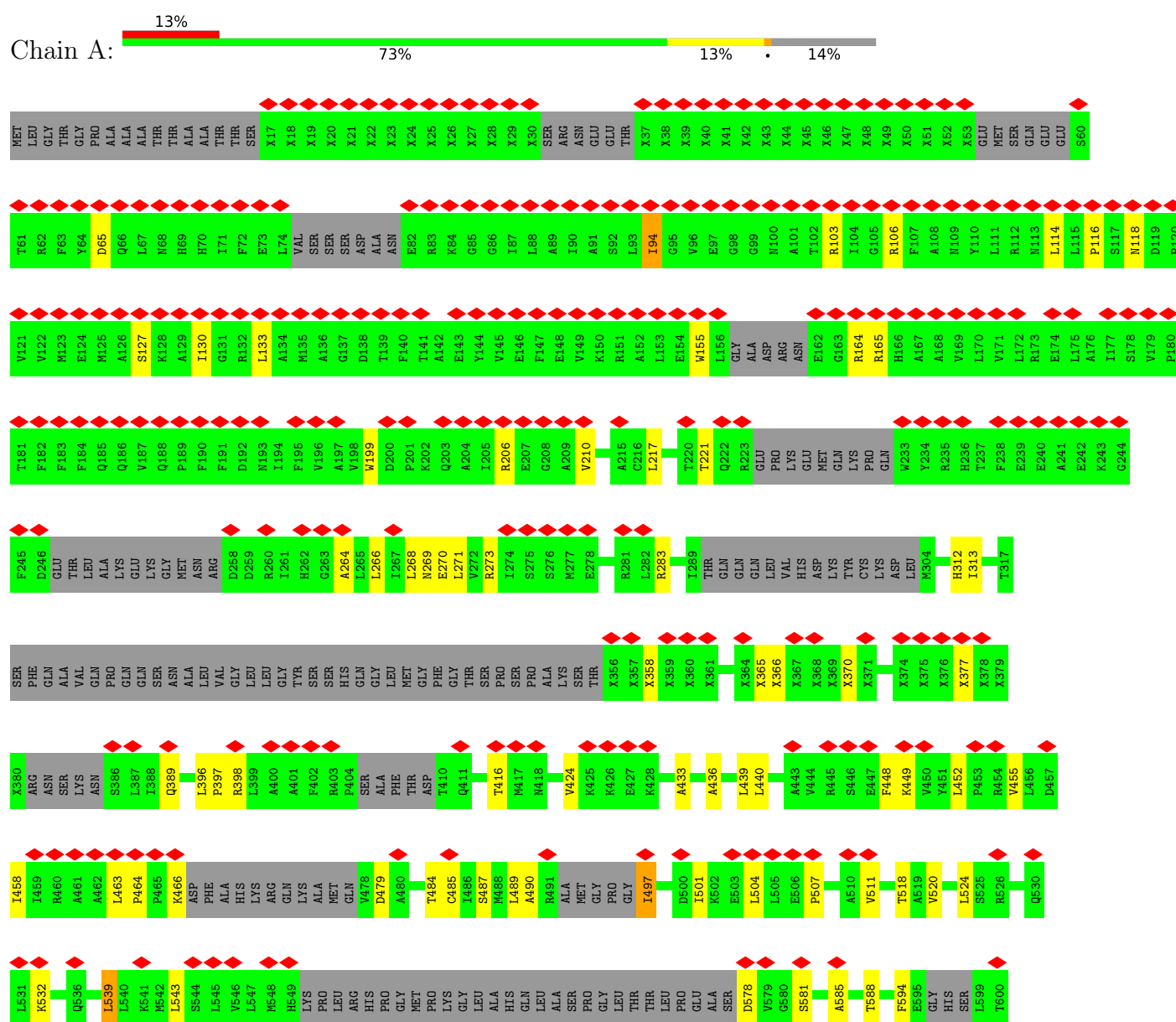


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			36	6	24	6	

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.

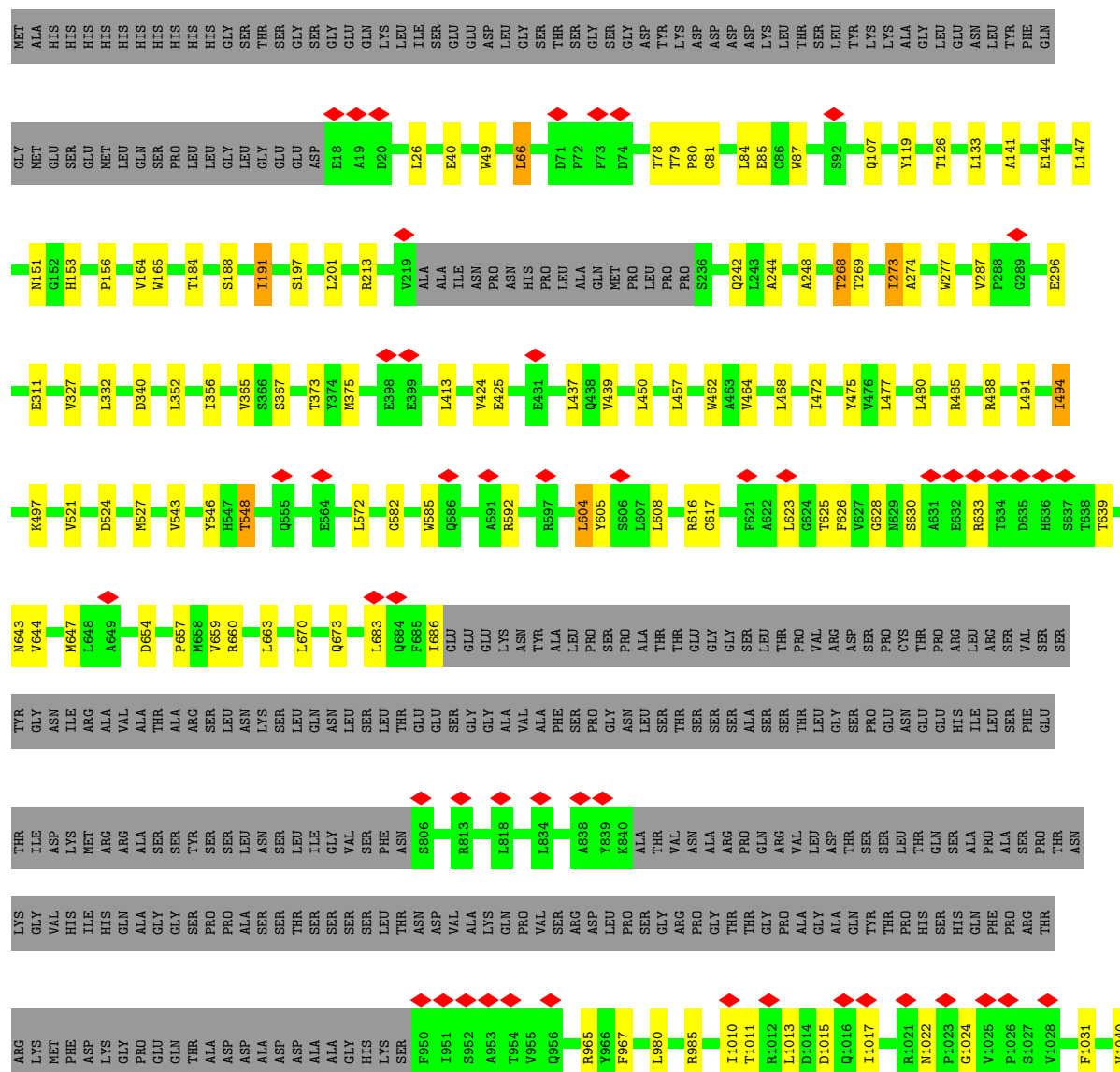
- Molecule 1: Serine/threonine-protein kinase mTOR

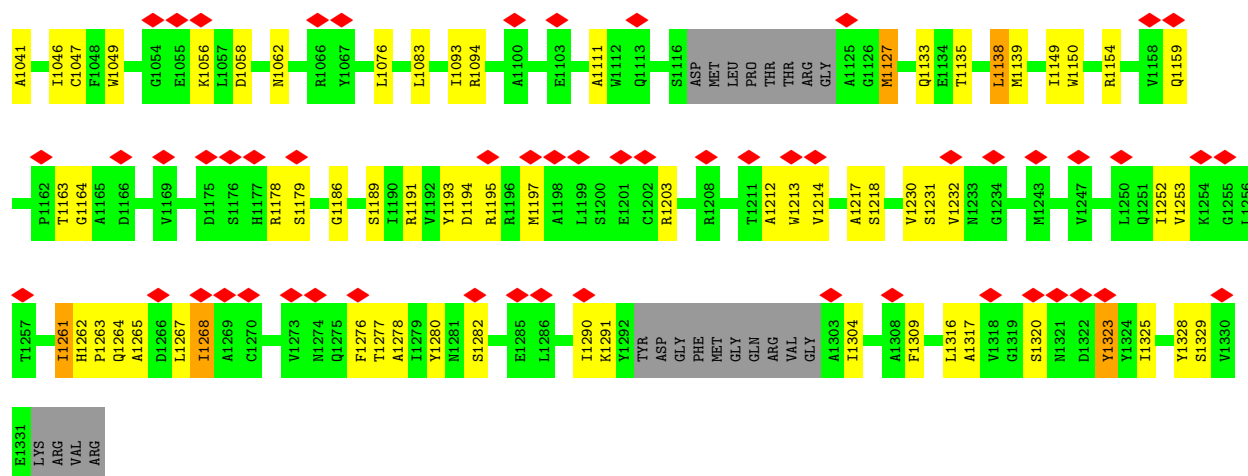




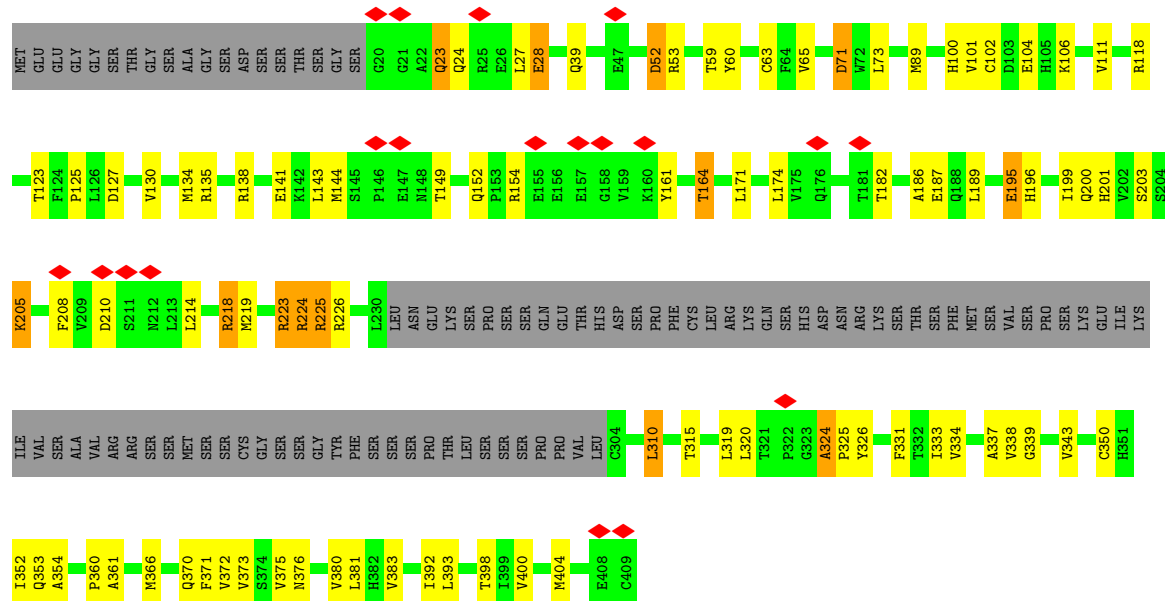
[illegible]

Chain E:





- Molecule 4: DEP domain-containing mTOR-interacting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.658	Depositor
Minimum map value	-0.219	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0944	Depositor
Map size (Å)	533.76, 533.76, 533.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.112, 1.112, 1.112	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: IHP

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	0.09	0/17523	0.27	0/23716
2	C	0.09	0/2514	0.28	0/3426
3	E	0.08	0/8585	0.25	0/11680
4	I	0.10	0/2631	0.32	0/3539
All	All	0.09	0/31253	0.27	0/42361

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	17454	0	17472	173	0
2	C	2456	0	2341	28	0
3	E	8385	0	8375	88	0
4	I	2580	0	2592	50	0
5	A	36	0	6	1	0
All	All	30911	0	30786	333	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.

All (333) 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)
4:I:224:ARG:H	4:I:224:ARG:HE	1.22	0.88
1:A:1280:TRP:HE1	1:A:1348:GLN:HB3	1.51	0.75
1:A:424:VAL:HG22	1:A:433:ALA:HB1	1.70	0.73
3:E:141:ALA:HB1	3:E:144:GLU:HB2	1.69	0.73
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.24	0.71
3:E:1047:CYS:SG	3:E:1056:LYS:NZ	2.65	0.69
1:A:490:ALA:HA	1:A:497:ILE:HG12	1.76	0.68
1:A:199:TRP:HA	1:A:206:ARG:HH21	1.58	0.68
1:A:268:LEU:HD22	1:A:365:UNK:HA	1.75	0.68
1:A:873:LYS:NZ	1:A:1576:THR:O	2.28	0.67
1:A:2018:ARG:NH1	1:A:2067:GLU:OE2	2.27	0.67
1:A:676:LEU:HB3	1:A:710:LEU:HD23	1.76	0.66
1:A:854:VAL:HG12	1:A:855:VAL:HG23	1.78	0.66
4:I:118:ARG:HD2	4:I:125:PRO:HD2	1.76	0.66
4:I:134:MET:HE2	4:I:138:ARG:HH12	1.60	0.66
1:A:1115:LEU:HD21	1:A:1155:ILE:HD11	1.77	0.66
1:A:210:VAL:HG11	1:A:266:LEU:HD13	1.77	0.65
1:A:882:ARG:NH2	1:A:1565:ASP:OD2	2.29	0.65
1:A:1170:ARG:HD3	1:A:1204:ILE:HG12	1.79	0.64
1:A:837:ARG:NH1	1:A:875:GLU:OE2	2.29	0.64
1:A:1514:ARG:HH21	1:A:1540:THR:HG21	1.63	0.63
3:E:1252:ILE:HG22	3:E:1253:VAL:HG23	1.80	0.63
3:E:1277:THR:HB	3:E:1290:ILE:HB	1.79	0.63
4:I:218:ARG:HH12	4:I:219:MET:HB2	1.62	0.63
1:A:463:LEU:HD22	1:A:511:VAL:HG21	1.81	0.63
4:I:224:ARG:H	4:I:224:ARG:NE	1.95	0.63
1:A:1174:MET:HE3	1:A:1204:ILE:HG21	1.80	0.62
3:E:1041:ALA:HA	3:E:1046:ILE:HA	1.82	0.62
1:A:487:SER:HB3	1:A:520:VAL:HG13	1.81	0.62
4:I:376:ASN:HA	4:I:400:VAL:HB	1.82	0.62
2:C:31:SER:O	2:C:306:ARG:NH1	2.33	0.62
3:E:1022:ASN:OD1	3:E:1049:TRP:NE1	2.32	0.61
4:I:123:THR:HG23	4:I:125:PRO:HD3	1.83	0.61
2:C:294:ALA:HB3	2:C:308:TYR:HB2	1.81	0.61
1:A:965:SER:HA	1:A:968:HIS:HD2	1.65	0.61
2:C:285:ILE:HG23	2:C:297:TRP:HB2	1.83	0.61
1:A:1538:ARG:NH2	4:I:339:GLY:O	2.34	0.61
4:I:154:ARG:NH1	4:I:164:THR:O	2.34	0.60
2:C:248:ARG:HD2	2:C:251:ASN:HB2	1.83	0.60
4:I:324:ALA:HB3	4:I:325:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	1.84	0.60
3:E:268:THR:HG23	3:E:269:THR:HG23	1.82	0.60
2:C:91:VAL:HG12	2:C:102:THR:HG22	1.83	0.60
1:A:1042:TRP:HE1	1:A:1049:GLN:HG2	1.67	0.60
3:E:616:ARG:NH2	3:E:1154:ARG:O	2.35	0.59
3:E:1304:ILE:HA	3:E:1320:SER:HA	1.85	0.59
1:A:1350:ILE:HG22	1:A:1353:VAL:H	1.68	0.58
1:A:1123:ASP:OD2	1:A:1161:ARG:NH1	2.36	0.58
3:E:40:GLU:O	3:E:965:ARG:NH2	2.34	0.58
1:A:377:UNK:O	1:A:389:GLN:NE2	2.37	0.58
3:E:1040:VAL:HG21	3:E:1325:ILE:HD13	1.85	0.58
4:I:53:ARG:O	4:I:60:TYR:N	2.37	0.58
2:C:225:GLN:OE1	2:C:227:ARG:NH2	2.37	0.58
1:A:520:VAL:O	1:A:524:LEU:N	2.38	0.57
3:E:521:VAL:HG13	3:E:527:MET:HE3	1.88	0.56
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.86	0.56
3:E:1010:ILE:HG21	3:E:1267:LEU:HD11	1.87	0.56
1:A:155:TRP:HB3	1:A:165:ARG:HD3	1.86	0.56
3:E:1062:ASN:O	3:E:1094:ARG:NH1	2.39	0.56
1:A:1266:GLN:NE2	1:A:1336:GLU:OE1	2.34	0.56
4:I:223:ARG:O	4:I:223:ARG:NE	2.39	0.56
1:A:1911:PHE:O	1:A:1950:ARG:NH1	2.40	0.55
3:E:592:ARG:NH1	3:E:626:PHE:O	2.40	0.55
3:E:683:LEU:HA	3:E:686:ILE:HD12	1.88	0.55
1:A:397:PRO:HG3	1:A:436:ALA:HA	1.89	0.55
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.72	0.55
1:A:1878:LEU:HD11	1:A:1918:ASP:HB2	1.89	0.55
4:I:100:HIS:HB3	4:I:104:GLU:HA	1.88	0.55
4:I:333:ILE:HD11	4:I:360:PRO:HB2	1.88	0.55
4:I:135:ARG:HG2	4:I:138:ARG:HH21	1.72	0.55
4:I:223:ARG:HH22	4:I:225:ARG:HH22	1.54	0.55
1:A:1478:LEU:HD11	1:A:1508:THR:HG23	1.89	0.54
1:A:518:THR:HG21	1:A:588:THR:HG23	1.88	0.54
1:A:1535:MET:HE3	4:I:354:ALA:HB1	1.89	0.54
2:C:40:HIS:ND1	2:C:68:TYR:OH	2.29	0.54
3:E:26:LEU:HD22	3:E:1133:GLN:HG3	1.90	0.54
1:A:676:LEU:HG	1:A:707:ILE:HG23	1.89	0.54
1:A:856:GLU:HA	1:A:859:ARG:HE	1.74	0.53
4:I:152:GLN:O	4:I:164:THR:OG1	2.25	0.53
1:A:607:ALA:HA	1:A:610:PHE:CE2	2.43	0.53
1:A:817:VAL:HG21	1:A:851:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:PRO:HB3	1:A:834:LEU:HB3	1.89	0.53
1:A:1605:TYR:O	1:A:1612:ARG:NE	2.40	0.53
1:A:269:ASN:ND2	1:A:273:ARG:HB2	2.23	0.53
2:C:16:ALA:HB3	2:C:319:ALA:HB3	1.91	0.53
3:E:1212:ALA:HB1	3:E:1232:VAL:HB	1.89	0.53
3:E:1017:ILE:HD11	3:E:1329:SER:HB3	1.90	0.53
1:A:959:PHE:HA	1:A:964:LEU:HG	1.91	0.53
3:E:660:ARG:NH2	3:E:1111:ALA:O	2.34	0.53
1:A:1206:HIS:HB3	1:A:1209:TYR:HB3	1.92	0.52
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.91	0.52
4:I:23:GLN:NE2	4:I:195:GLU:O	2.42	0.52
3:E:437:LEU:HD21	3:E:475:TYR:CE2	2.44	0.52
3:E:485:ARG:HA	3:E:488:ARG:HG3	1.91	0.52
4:I:27:LEU:HD13	4:I:196:HIS:HA	1.91	0.52
1:A:1306:LEU:HD13	1:A:1313:MET:HE3	1.90	0.52
1:A:2418:LEU:HA	1:A:2421:PHE:CE1	2.44	0.52
3:E:1076:LEU:HB2	3:E:1083:LEU:HB2	1.91	0.52
2:C:173:ILE:HA	2:C:189:ASN:HA	1.90	0.52
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.92	0.52
1:A:539:LEU:HD22	1:A:594:PHE:HE1	1.74	0.52
1:A:1598:GLU:OE2	1:A:1622:ARG:NH1	2.43	0.52
1:A:266:LEU:O	1:A:270:GLU:HG2	2.10	0.52
3:E:1138:LEU:O	3:E:1150:TRP:N	2.40	0.52
3:E:1189:SER:OG	3:E:1191:ARG:NH1	2.43	0.52
4:I:71:ASP:OD1	4:I:71:ASP:N	2.40	0.52
2:C:178:ILE:HB	2:C:185:MET:HG3	1.92	0.51
1:A:2268:MET:HE2	1:A:2287:PHE:HA	1.92	0.51
1:A:1556:LEU:HD11	4:I:393:LEU:HD22	1.92	0.51
3:E:1214:VAL:HG11	3:E:1217:ALA:HB2	1.93	0.51
4:I:373:VAL:O	4:I:380:VAL:N	2.37	0.51
3:E:1262:HIS:CE1	3:E:1264:GLN:HB2	2.46	0.51
4:I:224:ARG:HE	4:I:224:ARG:N	2.01	0.51
1:A:283:ARG:HB2	1:A:439:LEU:HD11	1.92	0.51
3:E:1262:HIS:HD2	3:E:1263:PRO:HD2	1.76	0.51
1:A:2296:GLY:O	1:A:2385:ASN:ND2	2.44	0.51
1:A:1973:ILE:HD12	1:A:1974:TYR:H	1.75	0.50
3:E:657:PRO:HA	3:E:660:ARG:HB2	1.93	0.50
4:I:334:VAL:HG23	4:I:398:THR:HG22	1.93	0.50
1:A:366:UNK:O	1:A:370:UNK:N	2.44	0.50
1:A:1277:LYS:HA	1:A:1350:ILE:HG12	1.92	0.50
4:I:63:CYS:SG	4:I:101:VAL:HG21	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:218:ARG:HG2	4:I:218:ARG:HH11	1.77	0.50
1:A:94:ILE:HD13	1:A:133:LEU:HD13	1.92	0.50
1:A:2418:LEU:HA	1:A:2421:PHE:HE1	1.77	0.50
3:E:488:ARG:NH2	3:E:524:ASP:OD2	2.45	0.50
1:A:466:LYS:HD2	1:A:479:ASP:HB2	1.92	0.50
3:E:616:ARG:NH1	3:E:654:ASP:OD2	2.44	0.49
4:I:218:ARG:HH11	4:I:218:ARG:CG	2.25	0.49
3:E:78:THR:O	3:E:81:CYS:HB3	2.12	0.49
1:A:628:ARG:O	1:A:631:THR:OG1	2.29	0.49
3:E:1031:PHE:HZ	3:E:1317:ALA:HB2	1.76	0.49
2:C:100:MET:HE2	2:C:112:TRP:HB2	1.93	0.49
3:E:1276:PHE:HE1	3:E:1291:LYS:HE2	1.77	0.49
1:A:65:ASP:OD2	1:A:106:ARG:NH1	2.46	0.49
3:E:1309:PHE:CE1	3:E:1316:LEU:HB2	2.47	0.49
1:A:312:HIS:CD2	1:A:313:ILE:HG12	2.47	0.49
1:A:1661:GLY:HA2	1:A:1666:LEU:HD23	1.95	0.49
2:C:89:ALA:N	2:C:103:GLY:O	2.46	0.49
4:I:361:ALA:HB1	4:I:366:MET:HG2	1.95	0.49
1:A:271:LEU:HB3	1:A:358:UNK:HA	1.95	0.48
3:E:980:LEU:HA	3:E:985:ARG:HD3	1.95	0.48
3:E:1268:ILE:HD11	3:E:1282:SER:HA	1.95	0.48
1:A:1350:ILE:O	1:A:1354:THR:OG1	2.32	0.48
3:E:79:THR:HB	3:E:80:PRO:HD3	1.95	0.48
3:E:1149:ILE:HD12	3:E:1159:GLN:HB2	1.96	0.48
4:I:60:TYR:HB3	4:I:63:CYS:SG	2.53	0.48
4:I:100:HIS:CE1	4:I:102:CYS:HB2	2.48	0.48
2:C:284:TYR:HB3	2:C:296:LEU:HD11	1.96	0.48
1:A:485:CYS:O	1:A:489:LEU:N	2.42	0.48
2:C:198:ASN:HB2	2:C:211:ILE:HB	1.96	0.48
2:C:255:MET:HE2	2:C:255:MET:HB3	1.82	0.47
2:C:275:GLY:HA3	2:C:288:ALA:H	1.79	0.47
1:A:504:LEU:O	1:A:507:PRO:HD2	2.14	0.47
1:A:934:MET:HE1	1:A:1319:ASN:HB2	1.95	0.47
3:E:1212:ALA:HB3	3:E:1231:SER:HB2	1.95	0.47
4:I:343:VAL:O	4:I:353:GLN:N	2.41	0.47
1:A:879:GLY:HA2	1:A:882:ARG:HD3	1.96	0.47
1:A:396:LEU:HB3	1:A:416:THR:HG23	1.95	0.47
3:E:277:TRP:CD2	3:E:356:ILE:HG12	2.50	0.47
3:E:630:SER:O	3:E:633:ARG:HG2	2.13	0.47
4:I:375:VAL:HG21	4:I:392:ILE:HG22	1.96	0.47
1:A:751:GLU:HB2	1:A:794:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:GLU:OE1	2:C:195:TYR:OH	2.31	0.47
4:I:24:GLN:O	4:I:28:GLU:HB3	2.15	0.47
1:A:65:ASP:OD1	1:A:103:ARG:NH1	2.48	0.47
1:A:1044:MET:SD	1:A:1044:MET:N	2.88	0.47
2:C:93:PHE:HE1	2:C:114:LEU:HD11	1.79	0.47
4:I:174:LEU:HD13	4:I:186:ALA:HB1	1.97	0.47
4:I:226:ARG:HA	4:I:226:ARG:HD2	1.69	0.47
1:A:2169:PRO:HB3	1:A:2187:LYS:HD3	1.97	0.47
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.97	0.47
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	1.95	0.47
3:E:156:PRO:HG2	3:E:165:TRP:CG	2.50	0.47
1:A:2034:ALA:HB1	1:A:2047:MET:HG2	1.95	0.47
3:E:244:ALA:HB3	3:E:365:VAL:HB	1.97	0.47
1:A:2254:ARG:NH2	1:A:2264:GLU:OE2	2.39	0.46
2:C:63:GLN:HG2	2:C:85:ASN:HA	1.96	0.46
4:I:23:GLN:O	4:I:27:LEU:HD12	2.16	0.46
4:I:164:THR:HB	4:I:214:LEU:HD22	1.98	0.46
1:A:2336:LEU:HG	1:A:2339:ARG:HD2	1.97	0.46
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.48	0.46
1:A:2300:ALA:HB2	1:A:2386:ALA:HA	1.98	0.46
4:I:326:TYR:CD2	4:I:404:MET:HG3	2.51	0.46
1:A:619:ARG:NH2	1:A:668:ASP:OD2	2.49	0.46
1:A:2251:ARG:HG3	1:A:2261:LEU:HD22	1.98	0.46
4:I:352:ILE:HD12	4:I:370:GLN:HB2	1.98	0.46
1:A:990:LEU:HD11	1:A:1023:VAL:HG13	1.97	0.46
1:A:1655:LYS:NZ	5:A:2601:IHP:O43	2.49	0.46
3:E:628:GLY:O	3:E:673:GLN:NE2	2.49	0.46
1:A:1391:ARG:HD3	1:A:1581:GLU:HG3	1.97	0.45
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.97	0.45
3:E:1031:PHE:CZ	3:E:1317:ALA:HB2	2.51	0.45
3:E:1186:GLY:HA2	3:E:1213:TRP:HA	1.97	0.45
1:A:578:ASP:N	1:A:581:SER:HG	2.13	0.45
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.98	0.45
2:C:74:ASN:N	2:C:75:PRO:HD3	2.31	0.45
1:A:608:ASP:OD1	1:A:612:ASN:ND2	2.49	0.45
1:A:581:SER:O	1:A:585:ALA:N	2.44	0.45
1:A:864:LEU:HD23	1:A:864:LEU:HA	1.82	0.45
1:A:1268:ALA:HA	1:A:1286:ARG:HH22	1.82	0.45
1:A:1444:GLU:N	1:A:1444:GLU:OE1	2.50	0.45
1:A:2378:ARG:NH2	1:A:2546:CYS:O	2.49	0.45
3:E:1164:GLY:HA3	3:E:1203:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:413:LEU:HD11	3:E:439:VAL:HG11	1.99	0.45
3:E:477:LEU:HD12	3:E:480:LEU:HD12	1.99	0.45
3:E:1197:MET:H	3:E:1197:MET:HG2	1.58	0.45
1:A:1024:LYS:HG3	1:A:1025:SER:H	1.81	0.45
2:C:40:HIS:CE1	2:C:66:ARG:HD2	2.52	0.45
1:A:273:ARG:HH11	1:A:398:ARG:NH1	2.15	0.45
1:A:755:ARG:HB2	1:A:797:ASN:HD22	1.82	0.45
1:A:1087:SER:OG	1:A:1091:ILE:HG13	2.17	0.45
1:A:1081:VAL:O	1:A:1085:ASP:HB2	2.17	0.44
3:E:1164:GLY:HA3	3:E:1203:ARG:NH2	2.32	0.44
4:I:52:ASP:OD1	4:I:52:ASP:N	2.50	0.44
1:A:217:LEU:O	1:A:221:THR:OG1	2.35	0.44
1:A:796:ASN:HD21	1:A:836:LYS:HG3	1.83	0.44
1:A:1740:LYS:HE3	1:A:1740:LYS:HB3	1.87	0.44
2:C:200:THR:OG1	2:C:209:GLN:HB2	2.18	0.44
3:E:147:LEU:HA	3:E:191:ILE:HG23	1.98	0.44
3:E:1218:SER:HB3	3:E:1261:ILE:HD12	1.99	0.44
1:A:1119:VAL:HA	1:A:1122:PHE:CE2	2.53	0.44
4:I:350:CYS:O	4:I:372:VAL:HG22	2.17	0.44
1:A:424:VAL:HG12	1:A:458:ILE:HG21	1.99	0.44
1:A:463:LEU:N	1:A:464:PRO:HD2	2.33	0.44
3:E:605:TYR:HA	3:E:608:LEU:HG	2.00	0.44
1:A:1053:ILE:HA	1:A:1056:ILE:HD12	1.99	0.44
1:A:1072:PRO:HA	1:A:1075:ILE:HD12	1.99	0.44
1:A:664:ILE:HD11	1:A:699:ALA:HB2	1.99	0.43
1:A:1023:VAL:O	1:A:1024:LYS:HG2	2.18	0.43
3:E:623:LEU:HD22	3:E:644:VAL:HG13	2.00	0.43
4:I:201:HIS:HB3	4:I:205:LYS:HA	1.99	0.43
1:A:1710:LYS:HE2	1:A:1710:LYS:HB3	1.77	0.43
3:E:582:GLY:HA2	3:E:585:TRP:CE2	2.54	0.43
3:E:1179:SER:HB2	3:E:1194:ASP:OD1	2.17	0.43
3:E:1262:HIS:CD2	3:E:1263:PRO:HD2	2.53	0.43
1:A:484:THR:O	1:A:487:SER:OG	2.31	0.43
1:A:1189:GLN:HA	1:A:1192:ILE:HD12	2.01	0.43
1:A:1873:LEU:HG	1:A:1877:LEU:HG	2.01	0.43
1:A:2274:ASP:O	1:A:2278:LEU:HG	2.19	0.43
3:E:184:THR:OG1	3:E:213:ARG:NH2	2.52	0.43
1:A:396:LEU:HD13	1:A:416:THR:HG23	2.01	0.43
1:A:1280:TRP:NE1	1:A:1348:GLN:HB3	2.28	0.43
4:I:310:LEU:HD22	4:I:310:LEU:HA	1.82	0.43
1:A:735:ILE:O	1:A:739:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:GLU:N	1:A:857:PRO:HD2	2.34	0.43
1:A:875:GLU:O	1:A:881:ARG:NH1	2.48	0.43
1:A:1728:ALA:HB2	1:A:1743:LEU:HD23	2.00	0.43
1:A:2230:LEU:HD11	1:A:2236:LEU:HG	2.00	0.43
4:I:320:LEU:HD21	4:I:381:LEU:HD12	2.00	0.43
1:A:1552:LEU:O	1:A:1606:LYS:NZ	2.50	0.43
1:A:1912:ASP:O	1:A:1950:ARG:NH1	2.52	0.43
3:E:107:GLN:HG3	3:E:119:TYR:CG	2.54	0.43
1:A:199:TRP:HH2	1:A:264:ALA:HB2	1.84	0.43
1:A:1055:LEU:HD22	1:A:1055:LEU:O	2.19	0.43
1:A:971:VAL:HG22	1:A:1306:LEU:HD11	2.00	0.42
3:E:457:LEU:HD22	3:E:464:VAL:HG22	2.00	0.42
1:A:1598:GLU:O	1:A:1602:VAL:HG23	2.19	0.42
3:E:201:LEU:HG	3:E:248:ALA:HB1	2.01	0.42
3:E:450:LEU:HD22	3:E:494:ILE:HD13	2.01	0.42
1:A:2246:LEU:HD23	1:A:2341:PRO:HB3	2.00	0.42
3:E:49:TRP:CG	3:E:468:LEU:HB3	2.54	0.42
3:E:87:TRP:HZ2	3:E:273:ILE:HG23	1.83	0.42
3:E:1163:THR:O	3:E:1193:TYR:OH	2.27	0.42
1:A:283:ARG:HB2	1:A:439:LEU:HD21	2.02	0.42
1:A:776:LEU:HD11	1:A:820:LEU:HD11	2.02	0.42
1:A:283:ARG:HG2	1:A:398:ARG:HH21	1.85	0.42
1:A:850:SER:O	1:A:1611:ARG:NH2	2.53	0.42
1:A:1280:TRP:HB3	1:A:1353:VAL:HG21	2.01	0.42
1:A:1689:LEU:HG	1:A:1716:HIS:ND1	2.35	0.42
1:A:2193:ARG:O	1:A:2197:ARG:HG2	2.19	0.42
3:E:633:ARG:HA	3:E:633:ARG:HD3	1.72	0.42
2:C:150:GLY:HA2	2:C:173:ILE:HG23	2.01	0.42
3:E:66:LEU:HD11	3:E:85:GLU:HG2	2.02	0.42
3:E:617:CYS:HB2	3:E:659:VAL:HG22	2.00	0.42
3:E:1015:ASP:O	3:E:1328:TYR:HA	2.20	0.42
1:A:116:PRO:HB3	1:A:164:ARG:HH22	1.85	0.42
3:E:639:THR:O	3:E:643:ASN:ND2	2.44	0.42
1:A:1005:ASP:O	1:A:1008:ILE:HG13	2.18	0.42
1:A:1199:LEU:HA	1:A:1204:ILE:HD12	2.02	0.42
1:A:2192:LEU:HD21	1:A:2237:ILE:HD11	2.02	0.42
1:A:501:ILE:HA	1:A:504:LEU:HB2	2.02	0.42
1:A:2368:ARG:NH1	1:A:2370:LYS:O	2.53	0.42
3:E:274:ALA:HB2	3:E:352:LEU:HD21	2.02	0.42
1:A:127:SER:HA	1:A:130:ILE:HD12	2.02	0.41
1:A:397:PRO:HB3	1:A:440:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:LYS:HG3	1:A:1304:TRP:CD1	2.55	0.41
1:A:114:LEU:HD22	1:A:118:ASN:HD21	1.85	0.41
1:A:894:LEU:HD23	1:A:894:LEU:HA	1.83	0.41
1:A:2003:ASN:O	1:A:2007:GLN:HG2	2.20	0.41
4:I:218:ARG:HG2	4:I:218:ARG:NH1	2.35	0.41
1:A:1326:TRP:O	1:A:1334:GLN:NE2	2.53	0.41
1:A:824:ILE:O	1:A:828:LEU:N	2.51	0.41
3:E:497:LYS:NZ	3:E:967:PHE:O	2.30	0.41
3:E:605:TYR:CZ	3:E:647:MET:HG3	2.55	0.41
1:A:999:ASN:O	1:A:1003:VAL:HG23	2.20	0.41
1:A:1136:LEU:HD22	1:A:1173:ALA:HA	2.02	0.41
1:A:1329:LEU:HB3	1:A:1333:GLN:HB2	2.02	0.41
2:C:279:SER:HA	2:C:320:PHE:CE2	2.56	0.41
1:A:1031:MET:HG2	1:A:1063:LEU:HD11	2.03	0.41
1:A:1372:LEU:HA	1:A:1373:PRO:HD3	1.93	0.41
3:E:604:LEU:HD12	3:E:604:LEU:HA	1.85	0.41
1:A:448:PHE:CZ	1:A:455:VAL:HG21	2.55	0.41
1:A:829:GLN:O	1:A:830:ASP:HB2	2.21	0.41
1:A:1142:LEU:HB3	1:A:1146:LEU:HD12	2.03	0.41
1:A:2368:ARG:HH12	1:A:2371:PHE:HB2	1.84	0.41
3:E:242:GLN:HB2	3:E:367:SER:HB2	2.03	0.41
1:A:968:HIS:CG	1:A:1008:ILE:HG21	2.56	0.41
1:A:1026:HIS:ND1	3:E:78:THR:HG23	2.36	0.41
1:A:1097:LEU:HD13	1:A:1097:LEU:HA	1.92	0.41
3:E:327:VAL:HG11	3:E:373:THR:HG22	2.03	0.41
4:I:73:LEU:HD11	4:I:89:MET:HE3	2.02	0.41
1:A:449:LYS:HA	1:A:452:LEU:HG	2.01	0.41
1:A:539:LEU:HD23	1:A:543:LEU:HD13	2.03	0.41
1:A:963:SER:HA	1:A:966:HIS:CE1	2.56	0.41
1:A:1781:GLU:OE2	1:A:1784:ARG:NH2	2.53	0.41
3:E:151:ASN:OD1	3:E:153:HIS:ND1	2.53	0.41
3:E:1041:ALA:HB2	3:E:1046:ILE:HG23	2.03	0.41
3:E:1278:ALA:HB1	3:E:1280:TYR:CZ	2.56	0.41
1:A:1042:TRP:NE1	1:A:1049:GLN:HG2	2.35	0.40
3:E:1024:GLY:O	3:E:1323:TYR:HB3	2.20	0.40
1:A:1566:LYS:HZ2	4:I:337:ALA:HB3	1.86	0.40
3:E:480:LEU:HD23	3:E:491:LEU:HD13	2.03	0.40
1:A:1024:LYS:HE2	1:A:1024:LYS:HB3	1.87	0.40
1:A:1097:LEU:HD12	1:A:1138:THR:HG21	2.04	0.40
3:E:546:TYR:CZ	3:E:548:THR:HB	2.56	0.40
3:E:1093:ILE:HD11	3:E:1127:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1159:GLN:OE1	3:E:1195:ARG:HB2	2.21	0.40
1:A:1071:LEU:N	1:A:1072:PRO:HD2	2.37	0.40
4:I:334:VAL:HA	4:I:398:THR:HG22	2.03	0.40
1:A:1901:GLN:HG3	1:A:2413:SER:HA	2.04	0.40
3:E:1262:HIS:HB3	3:E:1265:ALA:O	2.22	0.40
4:I:371:PHE:HB2	4:I:404:MET:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2100/2549 (82%)	2033 (97%)	67 (3%)	0	100	100
2	C	315/326 (97%)	291 (92%)	24 (8%)	0	100	100
3	E	1040/1396 (74%)	978 (94%)	62 (6%)	0	100	100
4	I	313/409 (76%)	293 (94%)	19 (6%)	1 (0%)	36	71
All	All	3768/4680 (80%)	3595 (95%)	172 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	324	ALA

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1871/2169 (86%)	1793 (96%)	78 (4%)	26	48
2	C	269/276 (98%)	258 (96%)	11 (4%)	27	49
3	E	928/1214 (76%)	888 (96%)	40 (4%)	26	48
4	I	281/364 (77%)	243 (86%)	38 (14%)	4	16
All	All	3349/4023 (83%)	3182 (95%)	167 (5%)	23	44

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	497	ILE
1	A	532	LYS
1	A	539	LEU
1	A	656	LEU
1	A	665	THR
1	A	760	LEU
1	A	767	LEU
1	A	768	ILE
1	A	811	LEU
1	A	821	PHE
1	A	851	THR
1	A	863	THR
1	A	882	ARG
1	A	894	LEU
1	A	895	ASP
1	A	934	MET
1	A	959	PHE
1	A	964	LEU
1	A	968	HIS
1	A	969	THR
1	A	970	MET
1	A	1003	VAL
1	A	1008	ILE
1	A	1014	GLN
1	A	1019	LEU
1	A	1055	LEU
1	A	1084	HIS
1	A	1097	LEU
1	A	1102	LEU
1	A	1121	LEU

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Mol	Chain	Res	Type
1	A	1160	VAL
1	A	1179	SER
1	A	1183	GLN
1	A	1213	ILE
1	A	1262	THR
1	A	1275	VAL
1	A	1287	LEU
1	A	1299	SER
1	A	1306	LEU
1	A	1337	LEU
1	A	1350	ILE
1	A	1354	THR
1	A	1360	LEU
1	A	1374	LEU
1	A	1380	ILE
1	A	1448	THR
1	A	1515	MET
1	A	1552	LEU
1	A	1558	SER
1	A	1575	LEU
1	A	1593	CYS
1	A	1617	GLN
1	A	1652	THR
1	A	1701	MET
1	A	1752	LEU
1	A	1758	GLN
1	A	1780	THR
1	A	1803	HIS
1	A	1899	ASN
1	A	1956	LEU
1	A	1967	TYR
1	A	1973	ILE
1	A	1988	HIS
1	A	2005	LEU
1	A	2021	ILE
1	A	2138	LEU
1	A	2260	LEU
1	A	2302	LEU
1	A	2311	GLU
1	A	2344	LEU
1	A	2345	MET
1	A	2346	LEU

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Mol	Chain	Res	Type
1	A	2390	THR
1	A	2398	ILE
1	A	2493	LEU
1	A	2501	ILE
1	A	2533	THR
2	C	84	VAL
2	C	91	VAL
2	C	108	THR
2	C	159	THR
2	C	173	ILE
2	C	188	VAL
2	C	215	LYS
2	C	225	GLN
2	C	243	THR
2	C	273	MET
2	C	274	TRP
3	E	66	LEU
3	E	84	LEU
3	E	126	THR
3	E	133	LEU
3	E	164	VAL
3	E	188	SER
3	E	191	ILE
3	E	197	SER
3	E	268	THR
3	E	273	ILE
3	E	287	VAL
3	E	296	GLU
3	E	311	GLU
3	E	332	LEU
3	E	340	ASP
3	E	375	MET
3	E	424	VAL
3	E	425	GLU
3	E	462	TRP
3	E	472	ILE
3	E	494	ILE
3	E	543	VAL
3	E	548	THR
3	E	572	LEU
3	E	604	LEU
3	E	625	THR

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Mol	Chain	Res	Type
3	E	663	LEU
3	E	670	LEU
3	E	1011	THR
3	E	1013	LEU
3	E	1058	ASP
3	E	1127	MET
3	E	1135	THR
3	E	1138	LEU
3	E	1139	MET
3	E	1178	ARG
3	E	1230	VAL
3	E	1261	ILE
3	E	1268	ILE
3	E	1323	TYR
4	I	23	GLN
4	I	28	GLU
4	I	39	GLN
4	I	52	ASP
4	I	59	THR
4	I	65	VAL
4	I	71	ASP
4	I	106	LYS
4	I	111	VAL
4	I	127	ASP
4	I	130	VAL
4	I	141	GLU
4	I	143	LEU
4	I	144	MET
4	I	149	THR
4	I	161	TYR
4	I	164	THR
4	I	171	LEU
4	I	182	THR
4	I	187	GLU
4	I	189	LEU
4	I	195	GLU
4	I	199	ILE
4	I	200	GLN
4	I	203	SER
4	I	205	LYS
4	I	208	PHE
4	I	210	ASP

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Mol	Chain	Res	Type
4	I	218	ARG
4	I	223	ARG
4	I	224	ARG
4	I	225	ARG
4	I	310	LEU
4	I	315	THR
4	I	319	LEU
4	I	331	PHE
4	I	338	VAL
4	I	383	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	609	HIS
1	A	703	GLN
1	A	791	ASN
1	A	846	GLN
1	A	968	HIS
1	A	1015	GLN
1	A	1106	ASN
1	A	1446	GLN
1	A	1553	HIS
1	A	1604	GLN
1	A	1627	GLN
1	A	1693	HIS
1	A	1727	GLN
1	A	1806	HIS
1	A	1992	ASN
1	A	2003	ASN
1	A	2007	GLN
1	A	2028	HIS
1	A	2289	HIS
1	A	2535	HIS
2	C	39	GLN
2	C	122	GLN
2	C	283	GLN
3	E	105	ASN
3	E	550	GLN
3	E	570	HIS
3	E	1105	ASN

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Mol	Chain	Res	Type
3	E	1177	HIS
3	E	1289	ASN
4	I	39	GLN
4	I	99	HIS
4	I	196	HIS
4	I	216	GLN
4	I	220	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
5	IHP	A	2601	-	36,36,36	0.74	2 (5%)	60,60,60	0.57	1 (1%)

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
5	IHP	A	2601	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2601	IHP	P3-O13	2.83	1.64	1.59
5	A	2601	IHP	P1-O11	2.05	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2601	IHP	P2-O12-C2	2.94	131.30	123.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

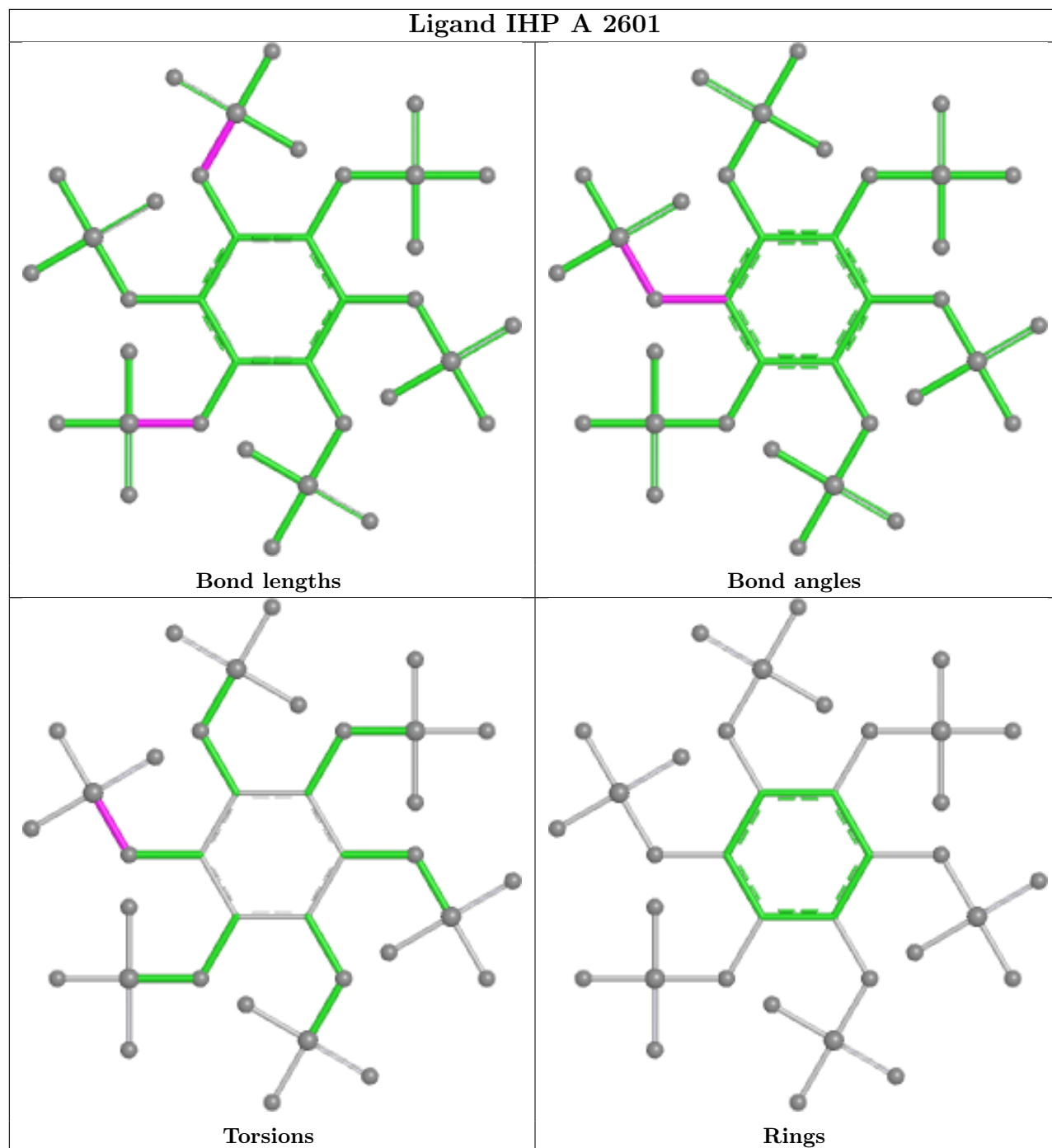
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2601	IHP	1	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.

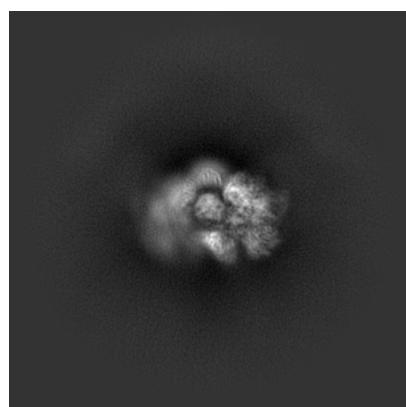
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13352. These allow visual inspection of the internal detail of the map and identification of artifacts.

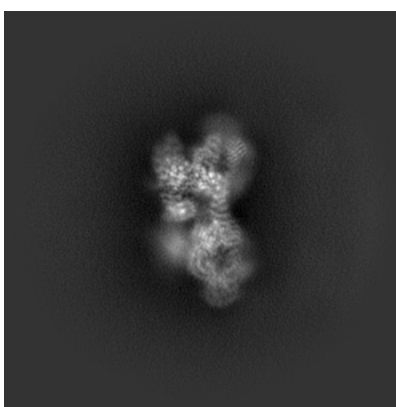
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

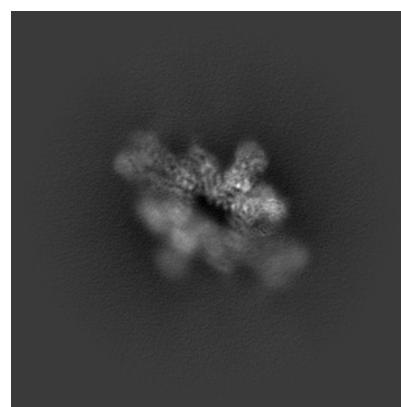
6.1.1 Primary map



X



Y

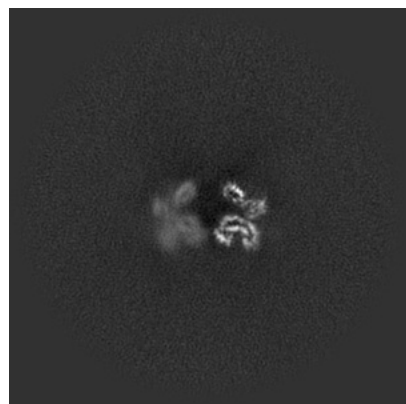


Z

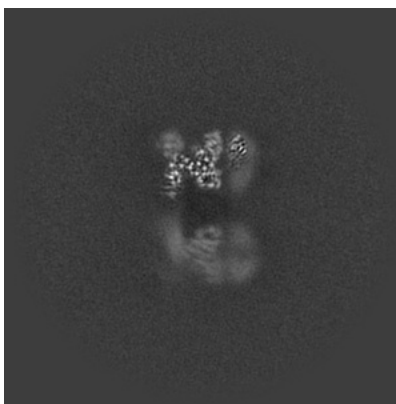
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

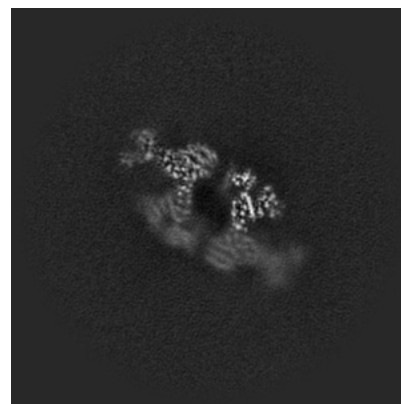
6.2.1 Primary map



X Index: 240



Y Index: 240

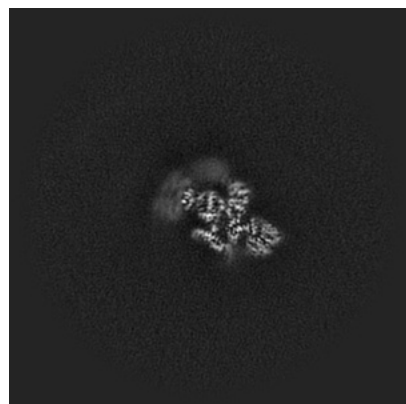


Z Index: 240

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

6.3 Largest variance slices [i](#)

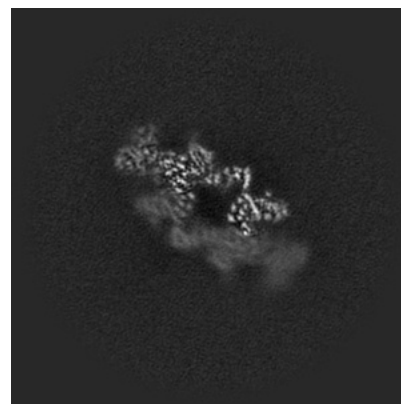
6.3.1 Primary map



X Index: 281



Y Index: 269

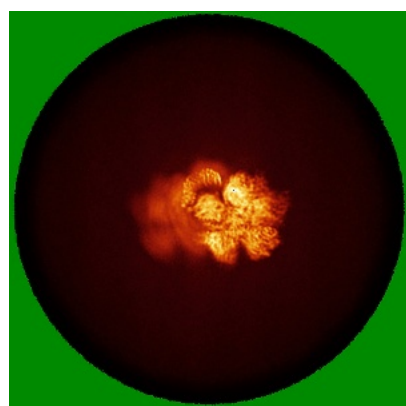


Z Index: 248

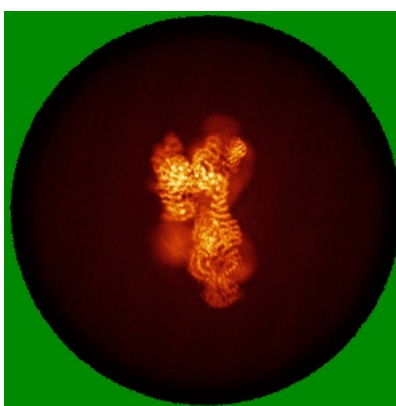
The images above show the largest variance slices of the map in three orthogonal directions.

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

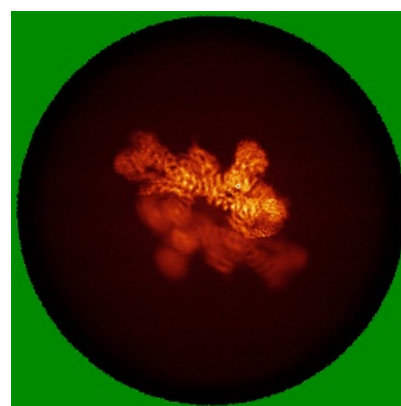
6.4.1 Primary map



X



Y

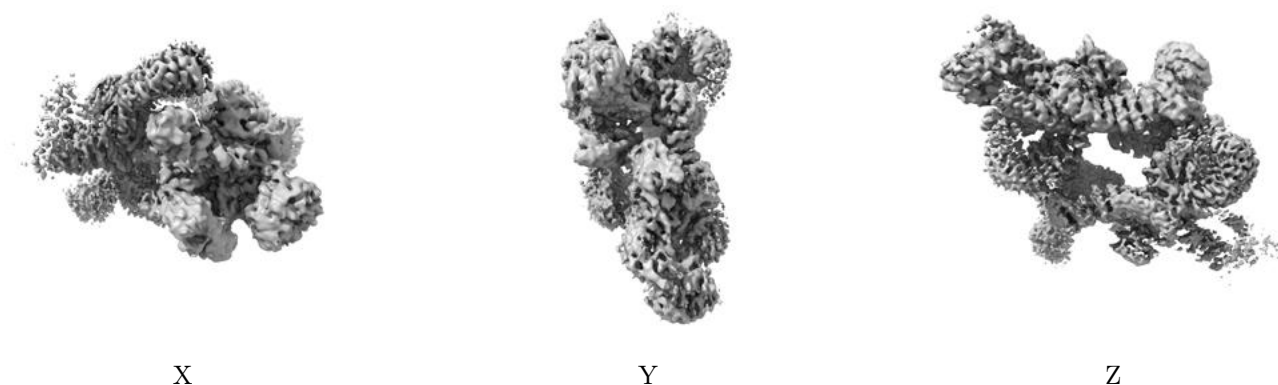


Z

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 0.0944. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

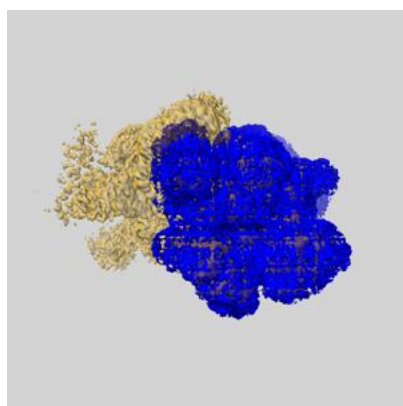
6.6 Mask visualisation [i](#)

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

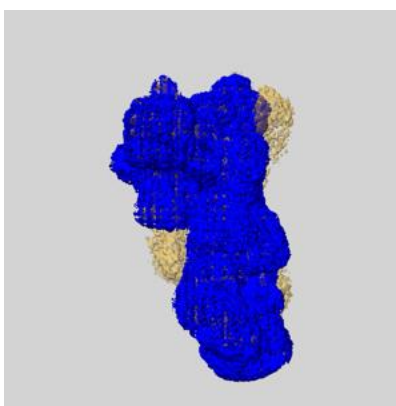
A mask typically either:

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

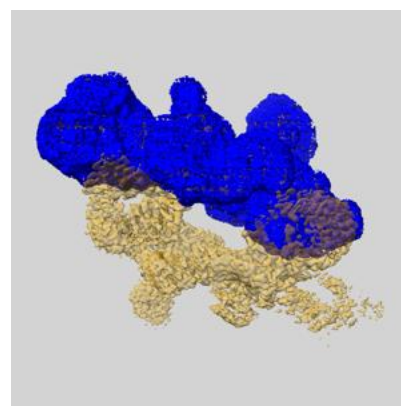
6.6.1 emd_13352_msk_1.map [i](#)



X



Y

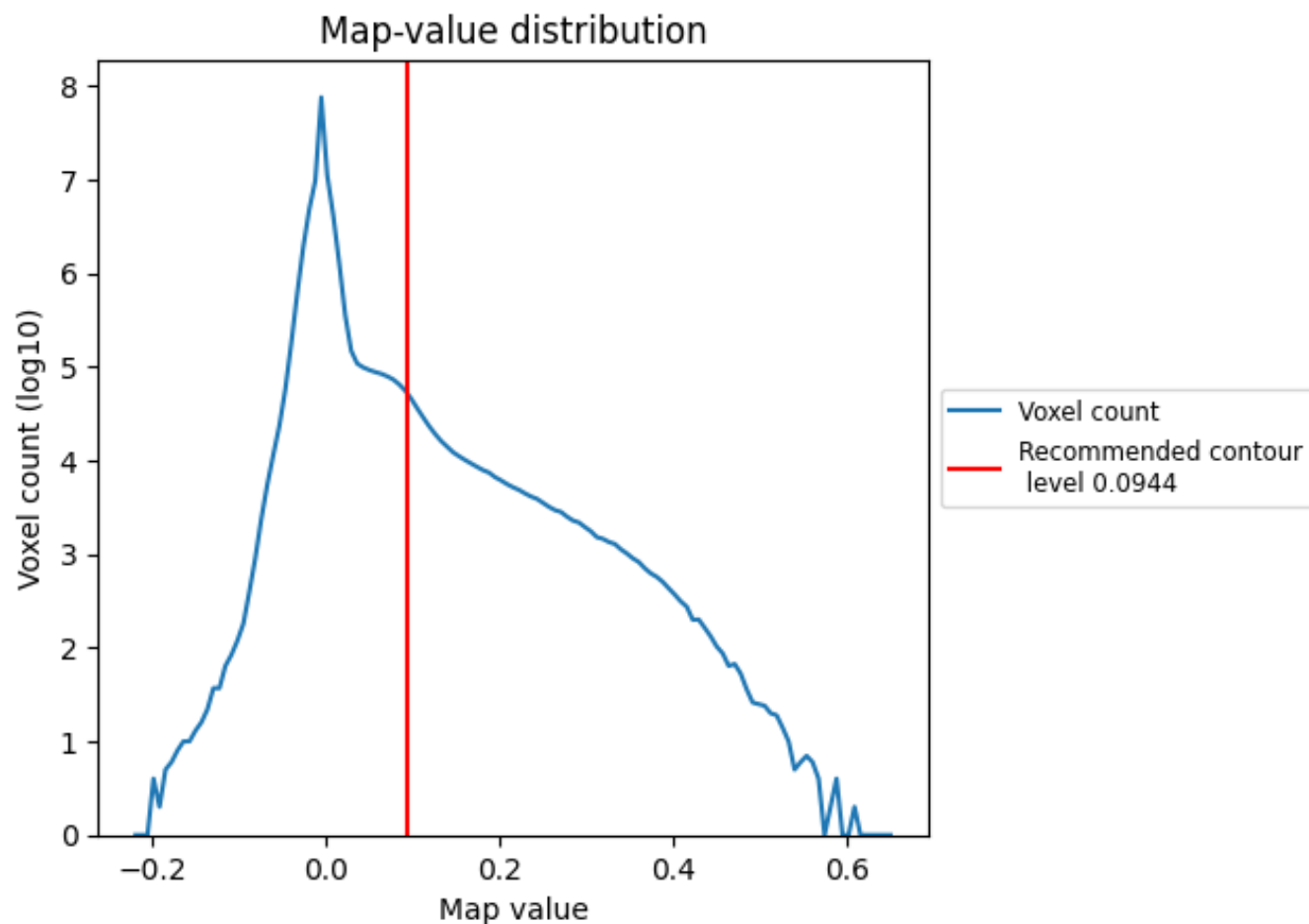


Z

7 Map analysis [i](#)

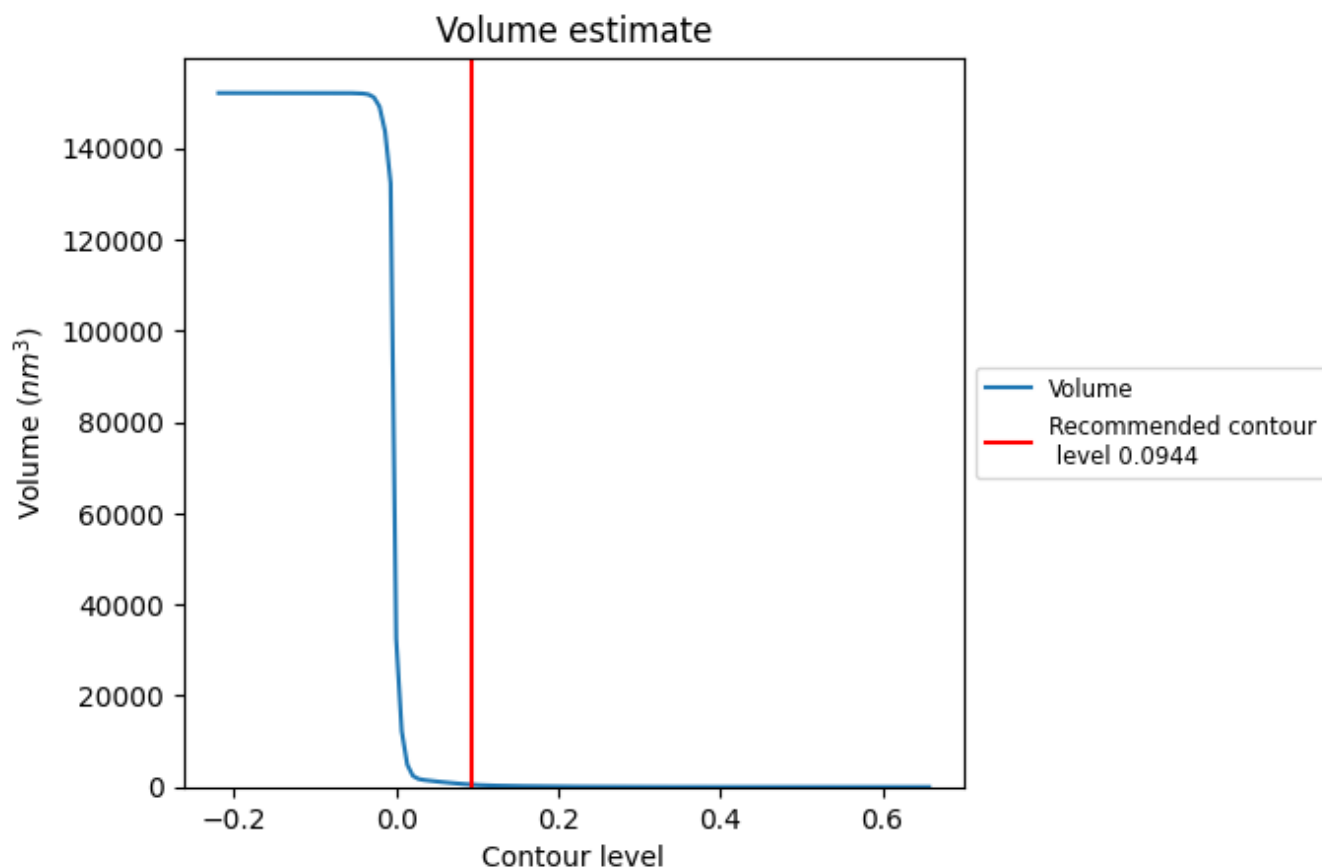
This section contains the results of statistical analysis of the map.

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.

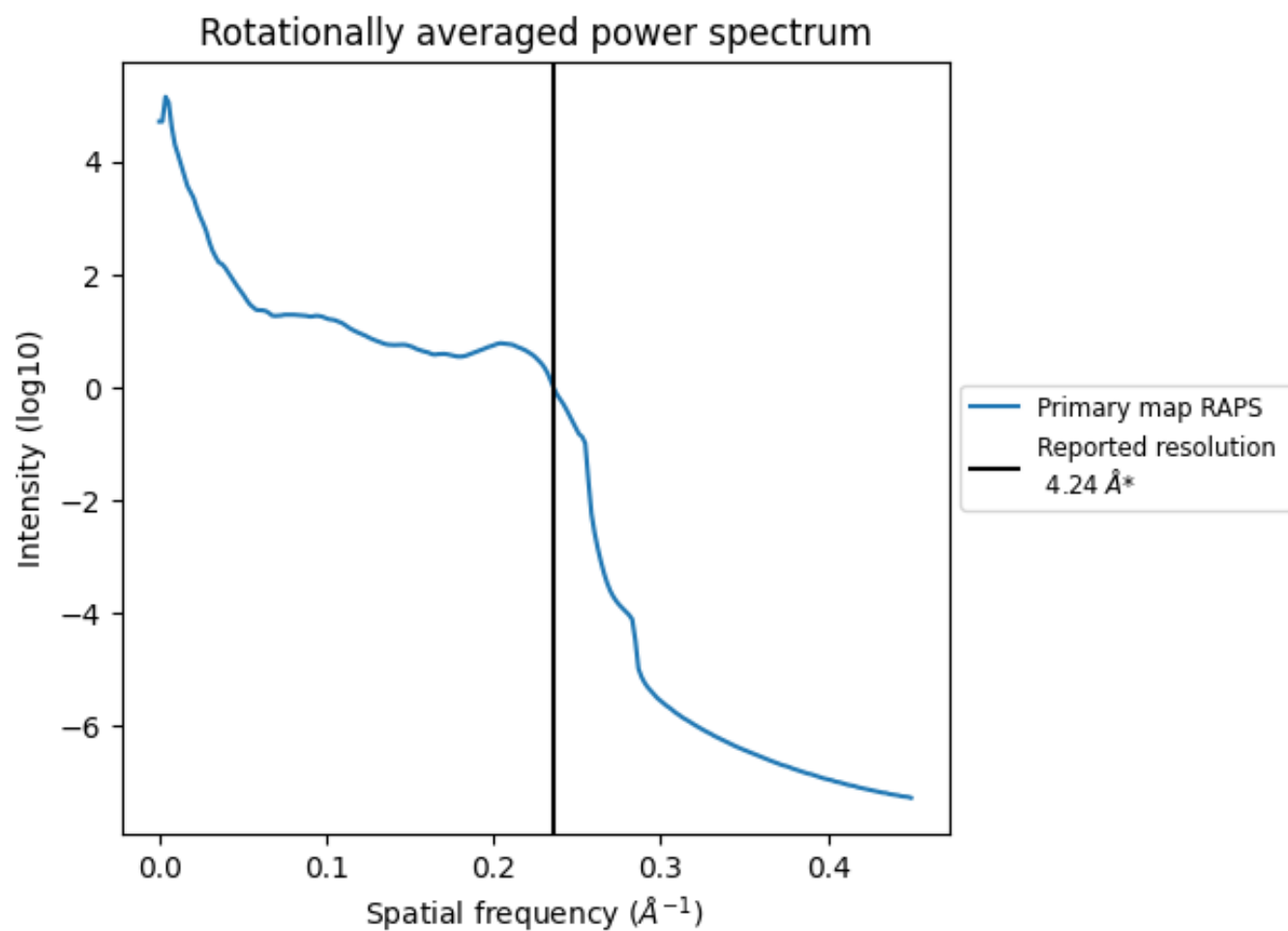
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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 0.236 Å⁻¹

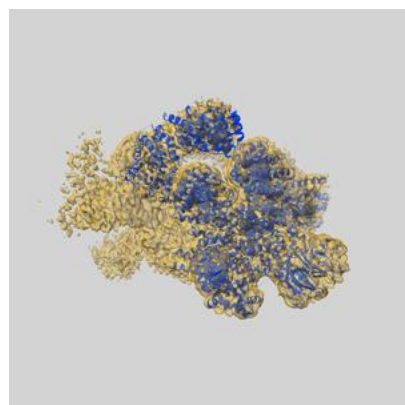
8 Fourier-Shell correlation

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

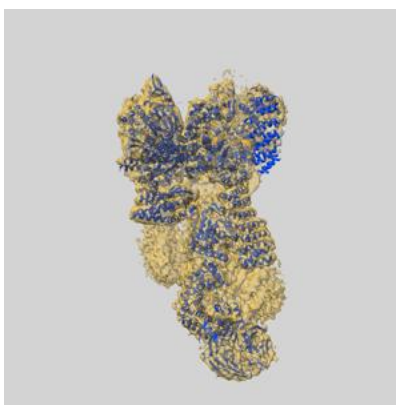
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13352 and PDB model 7PEC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

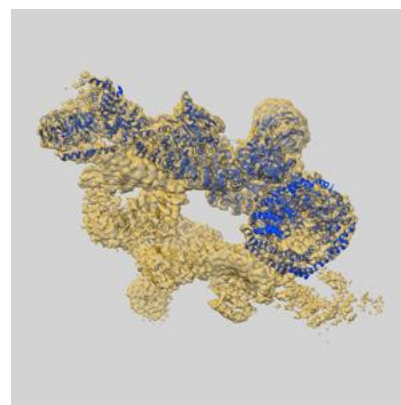
9.1 Map-model overlay [i](#)



X



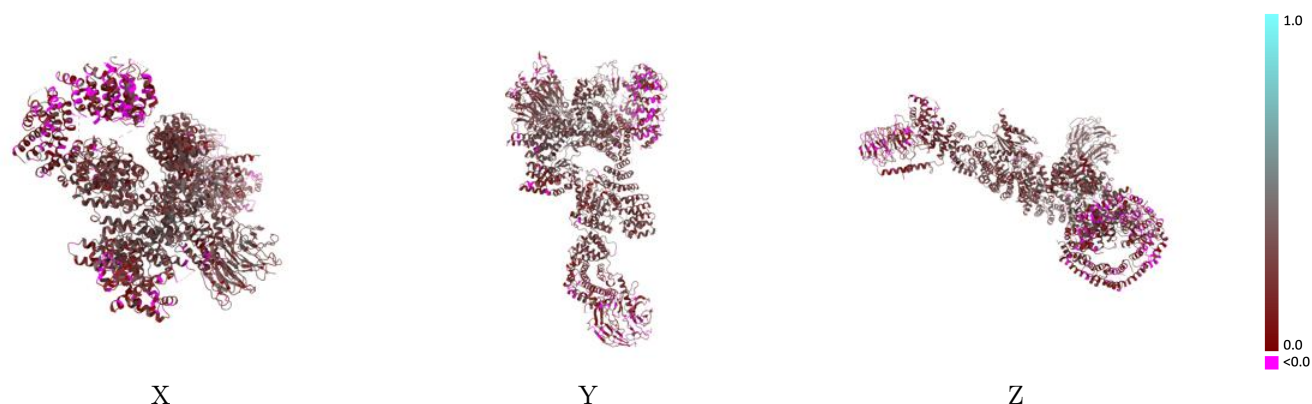
Y



Z

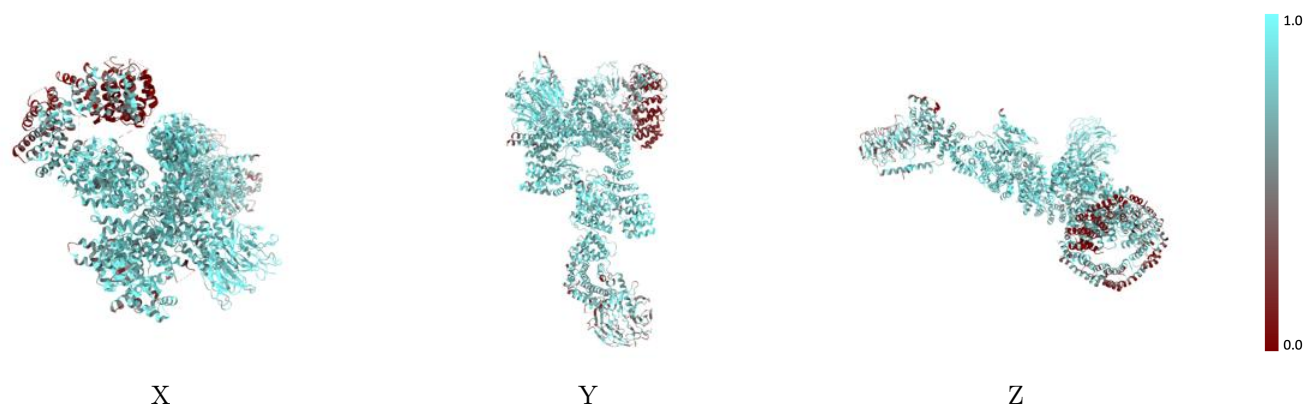
The images above show the 3D surface view of the map at the recommended contour level 0.0944 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



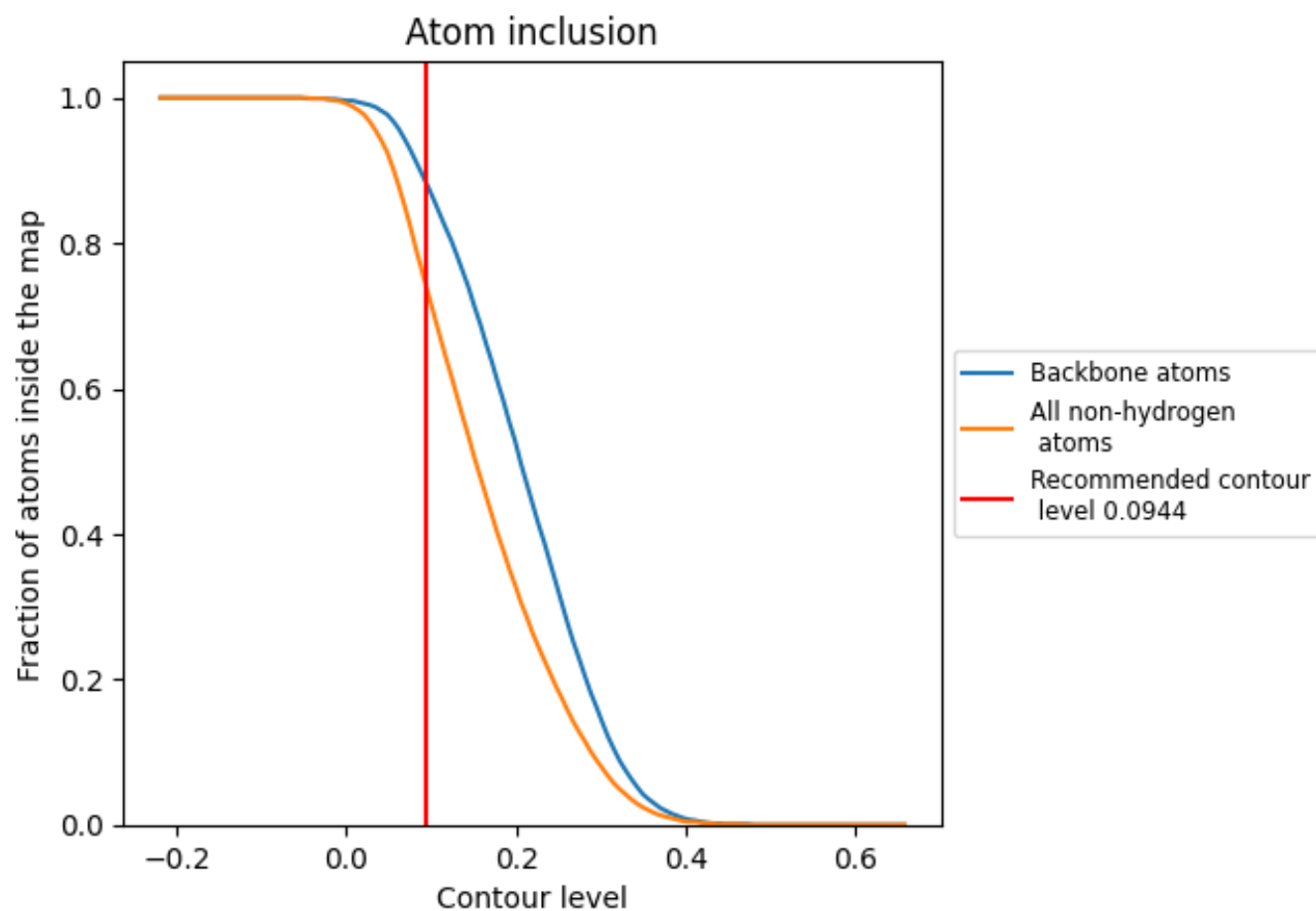
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0944).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0944) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.2400
A	0.7210	0.2450
C	0.8710	0.3070
E	0.7220	0.2270
I	0.7970	0.1860

