



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 04:37 pm BST

PDB ID : 9T7J / pdb\_00009t7j  
EMDB ID : EMD-55637  
Title : cryo-EM structure of AKT phosphorylated mTOR complex 2, overall refinement  
Authors : Hay, I.M.; Anandapadamanaban, M.; Williams, R.L.  
Deposited on : 2025-11-10  
Resolution : 3.00 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](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:

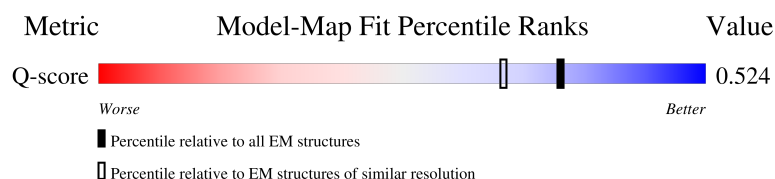
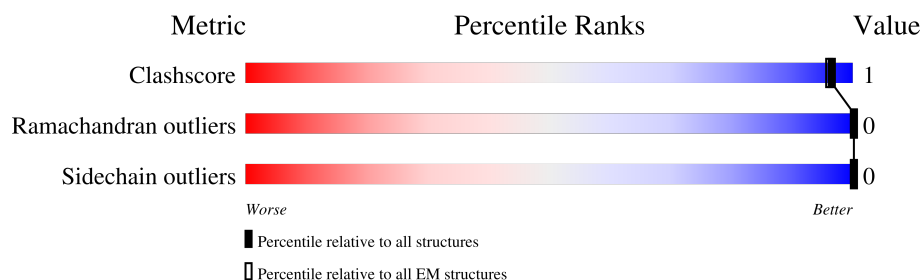
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 3.00 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	14081 ( 2.50 - 3.50 )

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

Mol	Chain	Length	Quality of chain
1	A	2590	
1	B	2590	
2	C	326	
2	D	326	

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Mol	Chain	Length	Quality of chain
3	E	1734	<div><div><div></div><div></div><div></div></div><div>64%35%</div></div>
3	F	1734	<div><div><div></div><div></div><div></div></div><div>5%64%35%</div></div>
4	G	522	<div><div><div></div><div></div><div></div></div><div>9%16%82%</div></div>
4	H	522	<div><div><div></div><div></div><div></div></div><div>9%17%82%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 52802 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	1749	Total	C	N	O	S	0	0
			14145	9037	2478	2532	98		
1	B	1747	Total	C	N	O	S	0	0
			14131	9029	2476	2529	97		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP P42345
A	-39	ALA	-	expression tag	UNP P42345
A	-38	SER	-	expression tag	UNP P42345
A	-37	TRP	-	expression tag	UNP P42345
A	-36	SER	-	expression tag	UNP P42345
A	-35	HIS	-	expression tag	UNP P42345
A	-34	PRO	-	expression tag	UNP P42345
A	-33	GLN	-	expression tag	UNP P42345
A	-32	PHE	-	expression tag	UNP P42345
A	-31	GLU	-	expression tag	UNP P42345
A	-30	LYS	-	expression tag	UNP P42345
A	-29	GLY	-	expression tag	UNP P42345
A	-28	GLY	-	expression tag	UNP P42345
A	-27	GLY	-	expression tag	UNP P42345
A	-26	ALA	-	expression tag	UNP P42345
A	-25	ARG	-	expression tag	UNP P42345
A	-24	GLY	-	expression tag	UNP P42345
A	-23	GLY	-	expression tag	UNP P42345
A	-22	SER	-	expression tag	UNP P42345
A	-21	GLY	-	expression tag	UNP P42345
A	-20	GLY	-	expression tag	UNP P42345
A	-19	GLY	-	expression tag	UNP P42345
A	-18	SER	-	expression tag	UNP P42345
A	-17	TRP	-	expression tag	UNP P42345
A	-16	SER	-	expression tag	UNP P42345
A	-15	HIS	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PRO	-	expression tag	UNP P42345
A	-13	GLN	-	expression tag	UNP P42345
A	-12	PHE	-	expression tag	UNP P42345
A	-11	GLU	-	expression tag	UNP P42345
A	-10	LYS	-	expression tag	UNP P42345
A	-9	GLY	-	expression tag	UNP P42345
A	-8	GLU	-	expression tag	UNP P42345
A	-7	ASN	-	expression tag	UNP P42345
A	-6	LEU	-	expression tag	UNP P42345
A	-5	TYR	-	expression tag	UNP P42345
A	-4	PHE	-	expression tag	UNP P42345
A	-3	GLN	-	expression tag	UNP P42345
A	-2	GLY	-	expression tag	UNP P42345
A	-1	GLY	-	expression tag	UNP P42345
A	0	THR	-	expression tag	UNP P42345
B	-40	MET	-	initiating methionine	UNP P42345
B	-39	ALA	-	expression tag	UNP P42345
B	-38	SER	-	expression tag	UNP P42345
B	-37	TRP	-	expression tag	UNP P42345
B	-36	SER	-	expression tag	UNP P42345
B	-35	HIS	-	expression tag	UNP P42345
B	-34	PRO	-	expression tag	UNP P42345
B	-33	GLN	-	expression tag	UNP P42345
B	-32	PHE	-	expression tag	UNP P42345
B	-31	GLU	-	expression tag	UNP P42345
B	-30	LYS	-	expression tag	UNP P42345
B	-29	GLY	-	expression tag	UNP P42345
B	-28	GLY	-	expression tag	UNP P42345
B	-27	GLY	-	expression tag	UNP P42345
B	-26	ALA	-	expression tag	UNP P42345
B	-25	ARG	-	expression tag	UNP P42345
B	-24	GLY	-	expression tag	UNP P42345
B	-23	GLY	-	expression tag	UNP P42345
B	-22	SER	-	expression tag	UNP P42345
B	-21	GLY	-	expression tag	UNP P42345
B	-20	GLY	-	expression tag	UNP P42345
B	-19	GLY	-	expression tag	UNP P42345
B	-18	SER	-	expression tag	UNP P42345
B	-17	TRP	-	expression tag	UNP P42345
B	-16	SER	-	expression tag	UNP P42345
B	-15	HIS	-	expression tag	UNP P42345
B	-14	PRO	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLN	-	expression tag	UNP P42345
B	-12	PHE	-	expression tag	UNP P42345
B	-11	GLU	-	expression tag	UNP P42345
B	-10	LYS	-	expression tag	UNP P42345
B	-9	GLY	-	expression tag	UNP P42345
B	-8	GLU	-	expression tag	UNP P42345
B	-7	ASN	-	expression tag	UNP P42345
B	-6	LEU	-	expression tag	UNP P42345
B	-5	TYR	-	expression tag	UNP P42345
B	-4	PHE	-	expression tag	UNP P42345
B	-3	GLN	-	expression tag	UNP P42345
B	-2	GLY	-	expression tag	UNP P42345
B	-1	GLY	-	expression tag	UNP P42345
B	0	THR	-	expression tag	UNP P42345

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		
2	D	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		
3	F	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP Q6R327
E	-24	ALA	-	expression tag	UNP Q6R327
E	-23	ASP	-	expression tag	UNP Q6R327
E	-22	TYR	-	expression tag	UNP Q6R327
E	-21	LYS	-	expression tag	UNP Q6R327
E	-20	ASP	-	expression tag	UNP Q6R327
E	-19	HIS	-	expression tag	UNP Q6R327
E	-18	ASP	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	GLY	-	expression tag	UNP Q6R327
E	-16	ASP	-	expression tag	UNP Q6R327
E	-15	TYR	-	expression tag	UNP Q6R327
E	-14	LYS	-	expression tag	UNP Q6R327
E	-13	ASP	-	expression tag	UNP Q6R327
E	-12	HIS	-	expression tag	UNP Q6R327
E	-11	ASP	-	expression tag	UNP Q6R327
E	-10	ILE	-	expression tag	UNP Q6R327
E	-9	ASP	-	expression tag	UNP Q6R327
E	-8	TYR	-	expression tag	UNP Q6R327
E	-7	LYS	-	expression tag	UNP Q6R327
E	-6	ASP	-	expression tag	UNP Q6R327
E	-5	ASP	-	expression tag	UNP Q6R327
E	-4	ASP	-	expression tag	UNP Q6R327
E	-3	ASP	-	expression tag	UNP Q6R327
E	-2	LYS	-	expression tag	UNP Q6R327
E	-1	GLY	-	expression tag	UNP Q6R327
E	0	THR	-	expression tag	UNP Q6R327
F	-25	MET	-	initiating methionine	UNP Q6R327
F	-24	ALA	-	expression tag	UNP Q6R327
F	-23	ASP	-	expression tag	UNP Q6R327
F	-22	TYR	-	expression tag	UNP Q6R327
F	-21	LYS	-	expression tag	UNP Q6R327
F	-20	ASP	-	expression tag	UNP Q6R327
F	-19	HIS	-	expression tag	UNP Q6R327
F	-18	ASP	-	expression tag	UNP Q6R327
F	-17	GLY	-	expression tag	UNP Q6R327
F	-16	ASP	-	expression tag	UNP Q6R327
F	-15	TYR	-	expression tag	UNP Q6R327
F	-14	LYS	-	expression tag	UNP Q6R327
F	-13	ASP	-	expression tag	UNP Q6R327
F	-12	HIS	-	expression tag	UNP Q6R327
F	-11	ASP	-	expression tag	UNP Q6R327
F	-10	ILE	-	expression tag	UNP Q6R327
F	-9	ASP	-	expression tag	UNP Q6R327
F	-8	TYR	-	expression tag	UNP Q6R327
F	-7	LYS	-	expression tag	UNP Q6R327
F	-6	ASP	-	expression tag	UNP Q6R327
F	-5	ASP	-	expression tag	UNP Q6R327
F	-4	ASP	-	expression tag	UNP Q6R327
F	-3	ASP	-	expression tag	UNP Q6R327
F	-2	LYS	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q6R327
F	0	THR	-	expression tag	UNP Q6R327

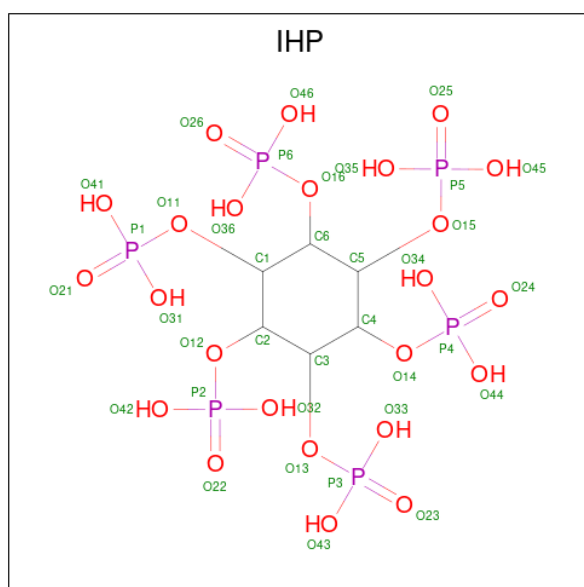
- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	93	Total	C	N	O	P	S	0	0
			735	456	126	148	1	4		
4	H	93	Total	C	N	O	P	S	0	0
			735	456	126	148	1	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ACE	-	acetylation	UNP Q9BPZ7
H	1	ACE	-	acetylation	UNP Q9BPZ7

- 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	
5	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ )



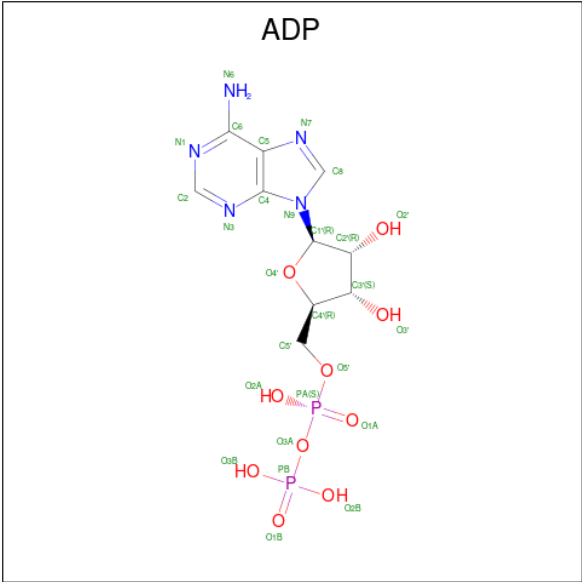
The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at N6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a chain of three phosphate groups (O=P(O)(OH)-O-P(O)(OH)-O-P(O)(OH)-OH) via a triphosphate tail. The structure is labeled with atom names (N1, N3, N7, C2, C4, C5, C6, C8, C9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O8

Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 31	C 10	N 5	O 13	P 3	0
6	B	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Zn 1 1	0
7	F	1	Total Zn 1 1	0

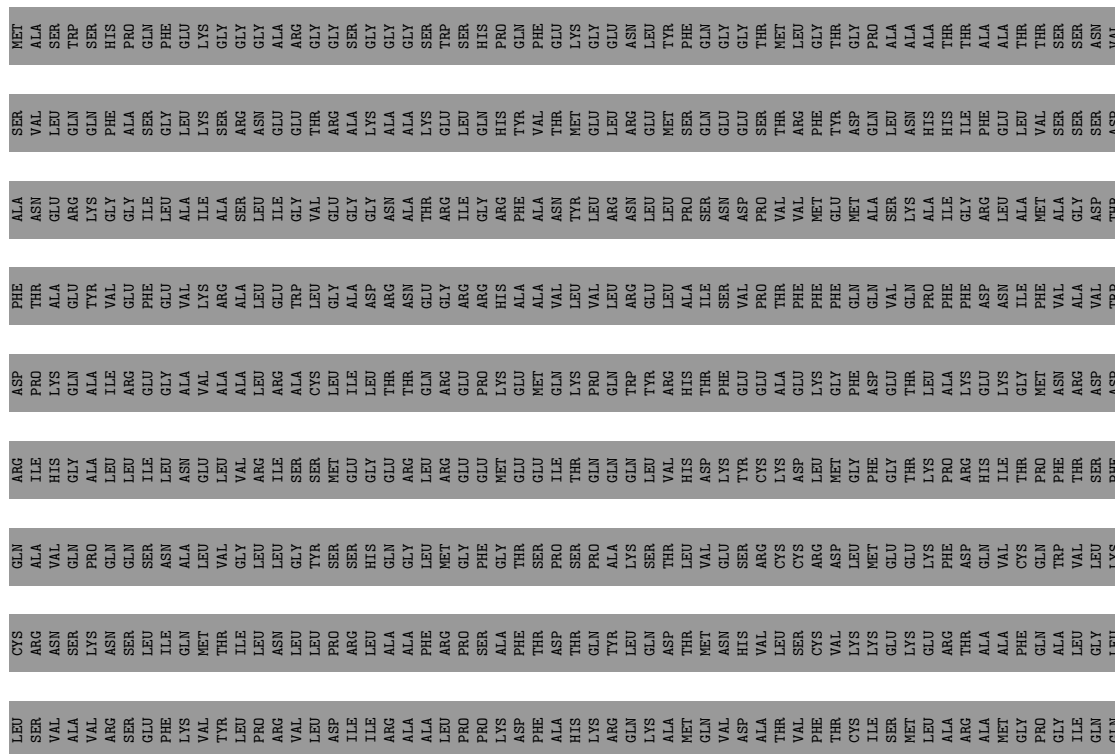
- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

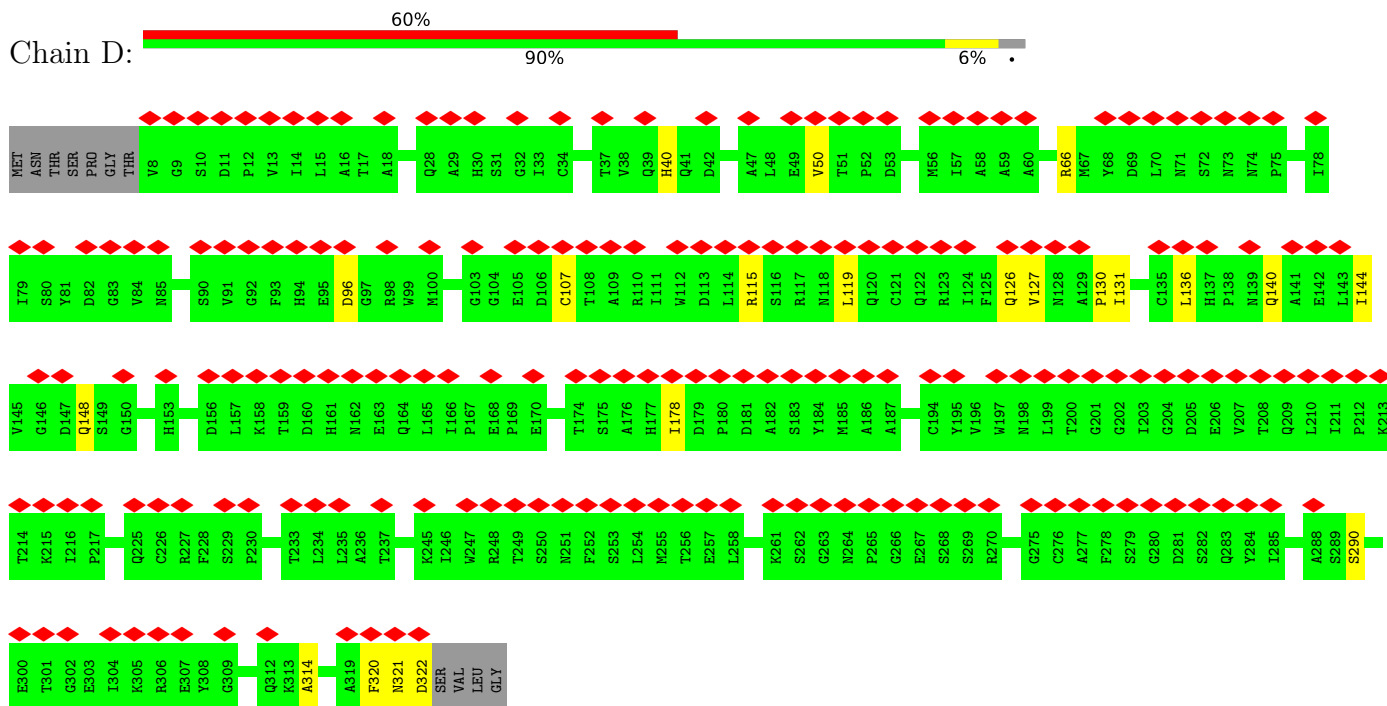


- Molecule 1: Serine/threonine-protein kinase mTOR

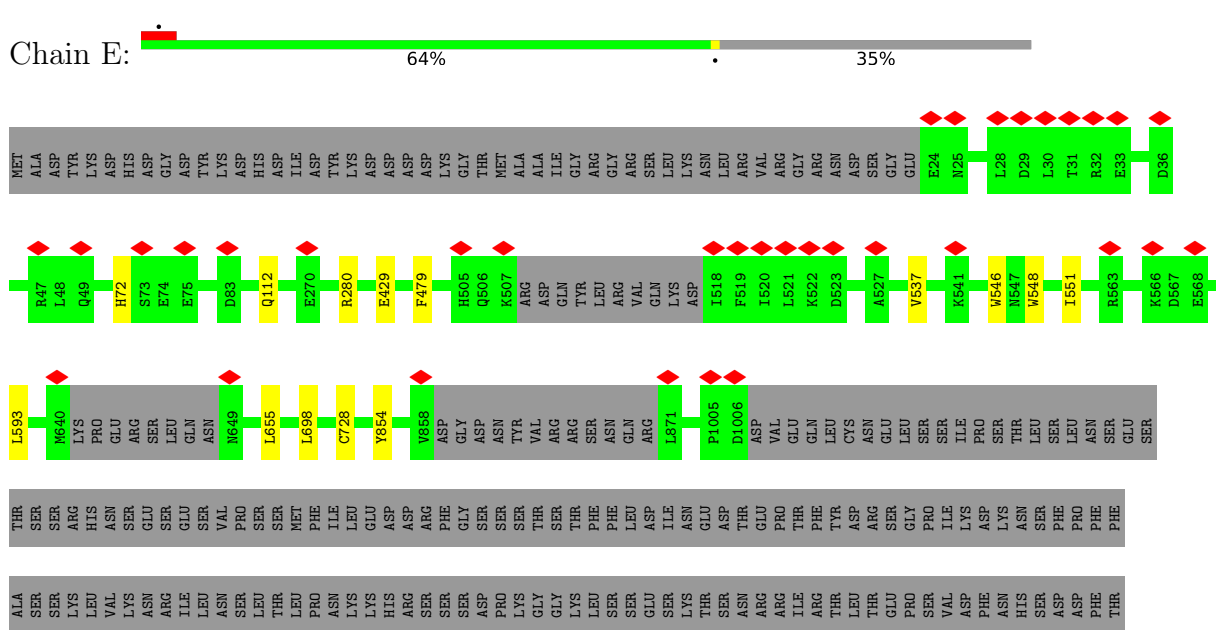




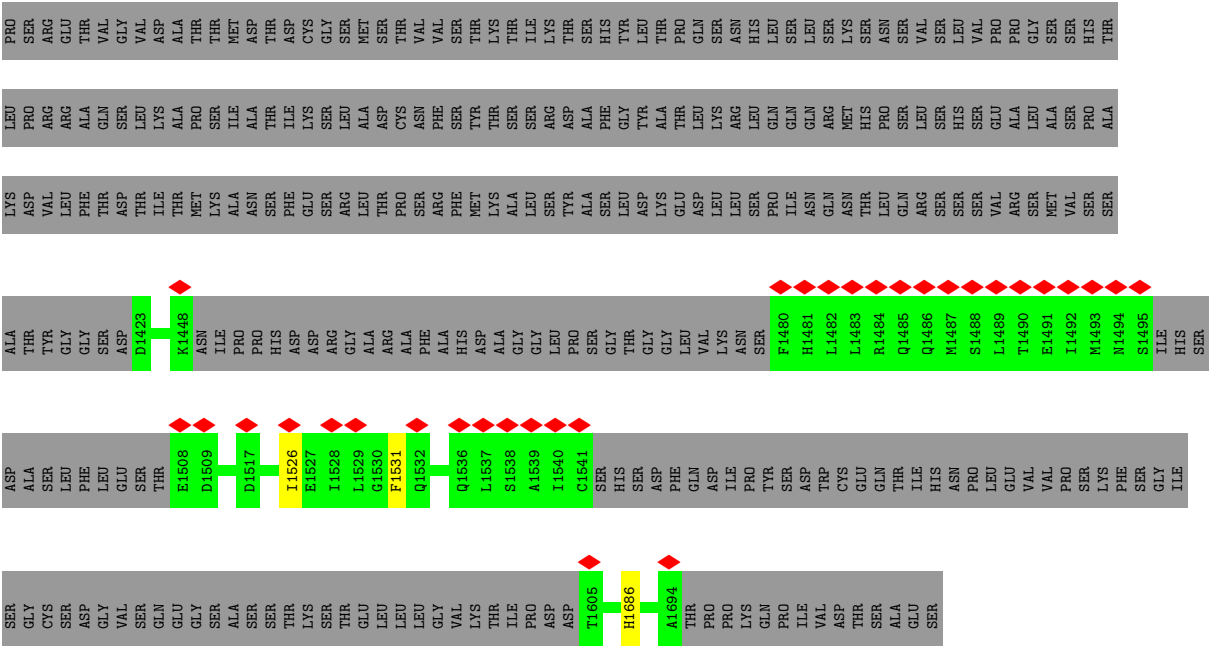
- Molecule 2: Target of rapamycin complex subunit LST8



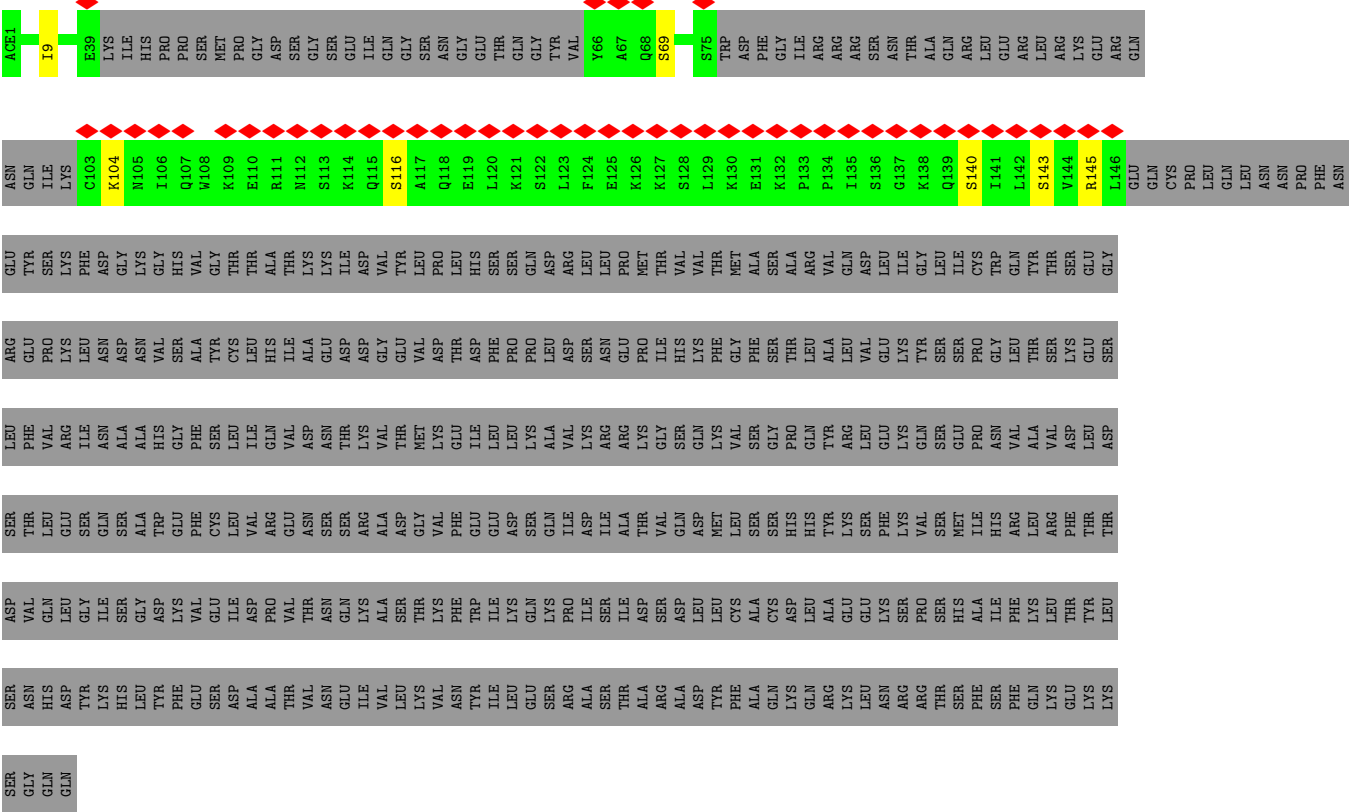
- Molecule 3: Rapamycin-insensitive companion of mTOR







● Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



● Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1





ASN	GLN	ILE	LYS	C103	K104	M105	I106	Q107	M108	K109	E110	R111	M112	S113	K114	Q115	S116	A117	Q118	E119	L120	K121	S122	L123	F124	E125	K126	K127	S128	L129	K130	E131	K132	P133	P134	I135	S136	G137	K138	Q139	S140	I141	L142	S143	V144	R145	L146	GLU	GLN	CYS	PRO	LEU	GLN	LEU	ASN	ASN	PRO	PHE	ASN
GLU	TYR	SER	LYS	PHE	ASP	GLY	GLY	VAL	VAL	GLY	THR	ALA	THR	LYS	LYS	ILE	ASP	THR	LEU	PRO	HIS	SER	GLN	ASP	ARG	LEU	ASN	PRO	MET	THR	VAL	THR	ALA	SER	ARG	VAL	ASP	LEU	ILE	GLY	THR	CYS	GLY	TRP	GLN	TYR	THR	SER	GLY	GLU	SER								
ARG	GLU	PRO	LYS	LEU	ASN	ASP	ASN	SER	ALA	TYR	CYS	HIS	ILE	ASP	GLU	ASP	GLY	VAL	VAL	ASP	THR	PHE	PRO	LYS	LEU	VAL	LYS	ASN	GLY	ILE	THR	PHE	SER	THR	ALA	VAL	VAL	VAL	GLU	LYS	TYR	SER	PRO	GLY	GLY	LEU	ASP	SER											
LEU	PHE	VAL	ARG	ILE	ASN	ALA	HIS	GLY	PHE	SER	ILE	GLN	VAL	ASN	THR	LYS	VAL	MET	LYS	GLU	ILE	LEU	LYS	ALA	VAL	LYS	ARG	GLY	THR	SER	GLY	PRO	THR	GLN	TYR	ARG	LEU	GLU	GLN	SER	GLU	PRO	ASN	VAL	VAL	VAL	ASP												
SER	THR	LEU	GLU	SER	GLN	SER	TRP	PHE	CYS	THR	ARG	GLU	THR	ASN	SER	ARG	THR	GLY	VAL	PHE	GLU	GLY	GLN	ILE	PRO	LYS	ILE	THR	VAL	ASP	LEU	SER	HIS	SER	TYR	ALA	GLU	ARG	LEU	VAL	GLN	VAL	GLU	ILE	HIS	ARG	THR	THR	THR										
ASP	VAL	GLN	GLY	ILE	ILE	SER	ASP	VAL	VAL	GLU	ASP	VAL	THR	ASN	ASN	GLN	THR	LYS	PHE	THR	ILE	LYS	GLN	LYS	PRO	ASP	ILE	SER	ILE	ASP	ALA	ALA	CYS	ASP	GLY	LEU	GLU	GLY	GLU	GLU	GLY	ALA	ILE	ILE	PHE	THR	THR	LEU											
SER	ASN	HIS	TYR	LYS	LYS	HIS	TYR	PHE	GLU	SER	ASP	ALA	VAL	ASN	ASN	VAL	LEU	LYS	VAL	ASN	TYR	LEU	GLU	SER	ARG	ARG	ALA	ALA	ARG	ALA	ALA	GLN	LYS	GLN	ARG	GLY	ASN	ARG	THR	THR	PHE	SER	SER	GLN	LYS	GLY	LYS												
SER	GLY	GLN	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY												

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210421	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)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	488.96, 488.96, 488.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	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: SEP, IHP, ZN, ADP, ACE, ATP

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	0.16	0/14448	0.41	0/19562
1	B	0.15	0/14434	0.40	0/19544
2	C	0.13	0/2501	0.43	0/3408
2	D	0.12	0/2501	0.41	0/3408
3	E	0.15	0/9154	0.39	0/12384
3	F	0.13	0/9154	0.38	0/12384
4	G	0.13	0/730	0.41	0/978
4	H	0.11	0/730	0.35	0/978
All	All	0.15	0/53652	0.40	0/72646

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	14145	0	14307	21	0
1	B	14131	0	14293	23	0
2	C	2443	0	2327	11	0
2	D	2443	0	2327	12	0
3	E	8990	0	9187	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8990	0	9187	9	0
4	G	735	0	738	5	0
4	H	735	0	739	2	0
5	A	36	0	6	0	0
5	B	36	0	6	0	0
6	A	31	0	12	0	0
6	B	31	0	12	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	E	27	0	12	0	0
8	F	27	0	12	0	0
All	All	52802	0	53165	86	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 1.

All (86) 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:C:27:TRP:HH2	2:C:310:GLY:H	1.49	0.59
1:B:2154:GLN:HE21	1:B:2177:SER:HA	1.67	0.57
2:C:79:ILE:HG23	4:G:104:LYS:HB3	1.86	0.57
1:A:1274:ARG:HD3	1:A:1279:ASP:HB3	1.87	0.57
1:A:1119:VAL:HA	1:A:1122:PHE:CE2	2.40	0.56
2:C:30:HIS:CD2	4:G:145:ARG:H	2.24	0.56
1:A:772:MET:SD	1:A:809:SER:HB2	2.47	0.55
2:C:9:GLY:HA3	2:C:70:LEU:HB3	1.87	0.55
2:D:50:VAL:HG21	2:D:321:ASN:HB2	1.88	0.54
3:F:68:CYS:HG	4:H:66:TYR:N	2.05	0.54
3:E:548:TRP:HA	3:E:551:ILE:HD12	1.91	0.53
2:D:127:VAL:HG21	2:D:131:ILE:HD11	1.91	0.53
1:A:2249:LEU:HB3	1:A:2302:LEU:HD21	1.92	0.52
2:D:40:HIS:CE1	2:D:66:ARG:HH21	2.27	0.52
1:B:757:LEU:HD21	1:B:775:ILE:HG23	1.93	0.51
1:B:1119:VAL:HA	1:B:1122:PHE:CE2	2.46	0.51
1:B:965:SER:HA	1:B:968:HIS:CD2	2.47	0.50
1:B:2387:MET:HE1	1:B:2392:LEU:HA	1.94	0.50
2:D:107:CYS:HA	2:D:130:PRO:HA	1.93	0.50
3:F:1526:ILE:HA	3:F:1531:PHE:HB2	1.94	0.50
3:E:1481:HIS:CD2	3:E:1618:ARG:HG3	2.47	0.50
3:F:548:TRP:HA	3:F:551:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2340:HIS:CE1	1:A:2342:SER:HB2	2.47	0.49
2:C:120:GLN:HB3	4:G:116:SER:HB2	1.95	0.48
1:A:1335:ASP:HB3	1:A:1339:ARG:NH1	2.29	0.48
1:B:1101:GLN:HB3	1:B:1141:ARG:HD3	1.96	0.48
1:B:1274:ARG:HD3	1:B:1279:ASP:HB3	1.96	0.47
1:A:2154:GLN:HE21	1:A:2177:SER:HA	1.79	0.47
2:C:278:PHE:HE1	2:C:299:VAL:HG11	1.80	0.47
3:E:593:LEU:HD23	3:E:655:LEU:HD23	1.95	0.47
1:B:1069:LEU:HD23	3:F:467:LEU:HD12	1.96	0.47
2:C:144:ILE:HD12	2:C:178:ILE:HD11	1.96	0.47
1:A:1277:LYS:HE3	1:A:1350:ILE:HG23	1.97	0.47
2:C:138:PRO:HG3	2:C:180:PRO:HA	1.97	0.47
3:F:593:LEU:HD23	3:F:655:LEU:HD23	1.97	0.47
3:E:429:GLU:HG2	3:E:479:PHE:CZ	2.50	0.47
1:A:1808:ASN:ND2	1:A:1873:LEU:HD13	2.31	0.46
3:F:831:TRP:HA	3:F:835:TYR:HB2	1.97	0.46
2:C:230:PRO:HD3	2:C:278:PHE:HB2	1.97	0.46
1:B:604:ARG:NH2	1:B:651:VAL:HG22	2.31	0.45
3:E:698:LEU:HD12	3:E:728:CYS:SG	2.55	0.45
1:B:2340:HIS:CE1	1:B:2342:SER:HB2	2.52	0.45
2:C:129:ALA:HB3	2:C:147:ASP:HB3	1.98	0.45
1:A:791:ASN:O	1:A:794:VAL:HG22	2.17	0.45
1:B:1122:PHE:HB3	1:B:1135:ALA:HB3	1.98	0.45
1:A:761:VAL:HG22	1:A:768:ILE:HG21	1.99	0.44
1:B:630:LEU:HD21	1:B:655:VAL:HB	1.98	0.44
1:A:2194:GLN:HG3	1:A:2421:PHE:HZ	1.82	0.44
1:B:1581:GLU:OE2	1:B:1585:ARG:HD3	2.16	0.44
1:A:2340:HIS:HE1	1:A:2342:SER:HB2	1.83	0.44
1:B:1274:ARG:HG3	1:B:1280:TRP:CE3	2.53	0.43
2:D:119:LEU:HD21	4:H:123:LEU:HD11	2.01	0.43
1:B:872:LEU:HB3	1:B:1576:THR:HG22	2.01	0.43
2:D:96:ASP:HB3	2:D:115:ARG:HH12	1.82	0.43
3:E:854:TYR:CE2	4:G:9:ILE:HD11	2.54	0.43
1:A:2154:GLN:HG3	1:A:2177:SER:HA	2.00	0.43
3:E:537:VAL:HA	3:E:546:TRP:CD1	2.53	0.43
3:F:623:LEU:HD23	3:F:675:MET:HE3	2.01	0.43
2:D:136:LEU:HD11	2:D:140:GLN:HA	2.01	0.42
3:E:280:ARG:HA	3:E:280:ARG:HD3	1.91	0.42
3:E:429:GLU:HG2	3:E:479:PHE:HZ	1.82	0.42
2:C:258:LEU:HD13	2:C:297:TRP:CG	2.55	0.42
4:G:140:SER:HA	4:G:143:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1393:TYR:CZ	1:B:1422:LYS:HD3	2.54	0.42
2:D:290:SER:HA	2:D:314:ALA:HB1	2.00	0.42
1:A:1946:ILE:HD11	1:A:1994:ILE:HD12	2.01	0.42
1:B:1937:GLN:HG3	1:B:1938:VAL:HG13	2.02	0.41
1:A:1504:VAL:HG21	1:A:1508:THR:HG21	2.03	0.41
1:B:604:ARG:HH22	1:B:651:VAL:HG22	1.85	0.41
1:B:947:TYR:HB2	1:B:948:PRO:HD3	2.02	0.41
1:A:825:MET:HE1	1:A:864:LEU:HD13	2.02	0.41
2:D:144:ILE:HD12	2:D:178:ILE:HD11	2.03	0.41
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	2.02	0.41
1:A:709:GLU:OE2	1:A:755:ARG:HD3	2.21	0.41
1:A:1477:MET:HE2	1:A:1500:LYS:HE2	2.03	0.41
1:A:2421:PHE:C	1:A:2421:PHE:CD1	2.97	0.41
3:F:90:LEU:HD13	3:F:1686:HIS:HA	2.03	0.41
1:B:1400:LYS:HE2	1:B:1415:SER:HB3	2.02	0.40
1:B:2340:HIS:HE1	1:B:2342:SER:HB2	1.86	0.40
1:A:1609:PRO:HA	1:A:1612:ARG:HG3	2.03	0.40
1:B:1220:TYR:CD2	1:B:1221:THR:HG22	2.55	0.40
2:D:107:CYS:HB2	2:D:126:GLN:HE22	1.86	0.40
2:D:130:PRO:HB2	2:D:148:GLN:HG3	2.02	0.40
2:D:320:PHE:CZ	2:D:322:ASP:HB3	2.57	0.40
3:E:72:HIS:CE1	3:E:112:GLN:HG3	2.57	0.40
3:F:808:PHE:N	3:F:808:PHE:CD1	2.89	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	1731/2590 (67%)	1707 (99%)	24 (1%)	0	100	100
1	B	1729/2590 (67%)	1701 (98%)	28 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	313/326 (96%)	298 (95%)	15 (5%)	0	100	100
2	D	313/326 (96%)	299 (96%)	14 (4%)	0	100	100
3	E	1103/1734 (64%)	1070 (97%)	33 (3%)	0	100	100
3	F	1103/1734 (64%)	1073 (97%)	30 (3%)	0	100	100
4	G	86/522 (16%)	79 (92%)	7 (8%)	0	100	100
4	H	86/522 (16%)	79 (92%)	7 (8%)	0	100	100
All	All	6464/10344 (62%)	6306 (98%)	158 (2%)	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	1549/2248 (69%)	1549 (100%)	0	100	100
1	B	1547/2248 (69%)	1547 (100%)	0	100	100
2	C	267/276 (97%)	267 (100%)	0	100	100
2	D	267/276 (97%)	267 (100%)	0	100	100
3	E	1005/1562 (64%)	1005 (100%)	0	100	100
3	F	1005/1562 (64%)	1005 (100%)	0	100	100
4	G	85/469 (18%)	85 (100%)	0	100	100
4	H	85/469 (18%)	85 (100%)	0	100	100
All	All	5810/9110 (64%)	5810 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	HIS

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Mol	Chain	Res	Type
1	A	615	HIS
1	A	743	HIS
1	A	1015	GLN
1	A	1106	ASN
1	A	1311	ASN
1	A	1330	ASN
1	A	1398	HIS
1	A	1420	ASN
1	A	1509	GLN
1	A	1782	HIS
1	A	1791	HIS
1	A	1808	ASN
1	A	1937	GLN
1	A	1992	ASN
1	A	2003	ASN
1	A	2007	GLN
1	A	2154	GLN
1	A	2167	GLN
1	A	2180	HIS
1	A	2395	ASN
1	A	2428	ASN
1	A	2515	HIS
1	B	605	HIS
1	B	609	HIS
1	B	694	GLN
1	B	736	GLN
1	B	743	HIS
1	B	759	HIS
1	B	962	GLN
1	B	968	HIS
1	B	1015	GLN
1	B	1106	ASN
1	B	1207	GLN
1	B	1233	GLN
1	B	1308	GLN
1	B	1330	ASN
1	B	1420	ASN
1	B	1439	HIS
1	B	1716	HIS
1	B	1791	HIS
1	B	1898	ASN
1	B	1937	GLN

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Mol	Chain	Res	Type
1	B	1992	ASN
1	B	2003	ASN
1	B	2007	GLN
1	B	2028	HIS
1	B	2117	GLN
1	B	2154	GLN
1	B	2180	HIS
1	B	2540	GLN
2	C	30	HIS
2	C	64	HIS
2	C	71	ASN
2	C	73	ASN
2	C	198	ASN
2	C	242	GLN
2	C	251	ASN
2	D	39	GLN
2	D	126	GLN
2	D	161	HIS
2	D	283	GLN
3	E	37	ASN
3	E	209	ASN
3	E	233	HIS
3	E	435	ASN
3	E	440	HIS
3	E	480	HIS
3	E	600	GLN
3	E	894	HIS
3	E	944	GLN
3	E	1485	GLN
3	E	1494	ASN
3	F	242	GLN
3	F	261	HIS
3	F	432	HIS
3	F	440	HIS
3	F	480	HIS
3	F	600	GLN
3	F	694	GLN
3	F	872	GLN
3	F	885	GLN
3	F	932	ASN
3	F	988	HIS
3	F	999	HIS

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Mol	Chain	Res	Type
3	F	1485	GLN
3	F	1494	ASN
3	F	1535	ASN
3	F	1632	HIS
3	F	1662	HIS
4	G	115	GLN
4	H	13	HIS
4	H	105	ASN
4	H	107	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
4	SEP	H	69	4	8,9,10	1.51	1 (12%)	8,12,14	1.45	2 (25%)
4	SEP	G	69	4	8,9,10	1.49	1 (12%)	8,12,14	1.34	2 (25%)

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
4	SEP	H	69	4	-	1/5/8/10	-
4	SEP	G	69	4	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	69	SEP	P-O1P	3.32	1.61	1.50
4	G	69	SEP	P-O1P	3.26	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	69	SEP	P-OG-CB	-2.94	110.19	118.30
4	G	69	SEP	P-OG-CB	-2.48	111.47	118.30
4	H	69	SEP	OG-CB-CA	2.14	110.23	108.14
4	G	69	SEP	OG-CB-CA	2.11	110.19	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	69	SEP	N-CA-CB-OG
4	H	69	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
6	ATP	B	2601	-	29,33,33	0.31	0	44,52,52	0.49	1 (2%)
6	ATP	A	2602	-	29,33,33	0.31	0	44,52,52	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	IHP	A	2601	-	36,36,36	1.85	6 (16%)	54,60,60	0.92	2 (3%)
8	ADP	F	1801	-	27,29,29	1.36	4 (14%)	42,45,45	2.00	8 (19%)
8	ADP	E	1802	-	27,29,29	1.36	4 (14%)	42,45,45	1.87	9 (21%)
5	IHP	B	2602	-	36,36,36	1.86	6 (16%)	54,60,60	0.92	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
6	ATP	B	2601	-	-	0/22/38/38	0/3/3/3
6	ATP	A	2602	-	-	3/22/38/38	0/3/3/3
5	IHP	A	2601	-	-	6/30/54/54	0/1/1/1
8	ADP	F	1801	-	-	11/16/32/32	0/3/3/3
8	ADP	E	1802	-	-	6/16/32/32	0/3/3/3
5	IHP	B	2602	-	-	9/30/54/54	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1801	ADP	C5-C4	4.65	1.47	1.39
5	B	2602	IHP	P2-O12	4.61	1.68	1.59
5	A	2601	IHP	P2-O12	4.57	1.67	1.59
8	E	1802	ADP	C5-C4	4.54	1.47	1.39
5	B	2602	IHP	P5-O15	4.26	1.67	1.59
5	A	2601	IHP	P5-O15	4.24	1.67	1.59
5	A	2601	IHP	P4-O14	4.23	1.67	1.59
5	B	2602	IHP	P4-O14	4.21	1.67	1.59
5	A	2601	IHP	P6-O16	4.14	1.67	1.59
5	B	2602	IHP	P6-O16	4.07	1.67	1.59
5	B	2602	IHP	P3-O13	4.03	1.66	1.59
5	B	2602	IHP	P1-O11	3.98	1.66	1.59
5	A	2601	IHP	P1-O11	3.96	1.66	1.59
5	A	2601	IHP	P3-O13	3.89	1.66	1.59
8	F	1801	ADP	C5-C6	2.70	1.48	1.41
8	E	1802	ADP	C5-C6	2.66	1.48	1.41
8	E	1802	ADP	C8-N7	2.34	1.36	1.31
8	F	1801	ADP	C8-N7	2.27	1.35	1.31
8	F	1801	ADP	C5-N7	-2.25	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1802	ADP	C5-N7	-2.22	1.34	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1801	ADP	C5-C4-N3	-6.91	117.73	126.75
8	E	1802	ADP	C5-C4-N3	-6.28	118.56	126.75
8	F	1801	ADP	N3-C4-N9	5.49	136.13	127.08
8	E	1802	ADP	N3-C4-N9	4.89	135.14	127.08
8	F	1801	ADP	C2-N3-C4	4.16	121.59	111.75
8	E	1802	ADP	C2-N3-C4	3.87	120.90	111.75
8	E	1802	ADP	C4-C5-N7	-3.25	106.66	110.62
8	F	1801	ADP	N3-C2-N1	-3.22	123.56	128.60
8	E	1802	ADP	N3-C2-N1	-3.17	123.64	128.60
8	F	1801	ADP	C4-C5-N7	-3.11	106.83	110.62
8	F	1801	ADP	PA-O3A-PB	-3.11	122.16	132.83
5	B	2602	IHP	C5-C4-C3	-2.90	104.06	110.41
5	A	2601	IHP	C5-C4-C3	-2.81	104.26	110.41
8	E	1802	ADP	C5-N7-C8	2.71	107.36	103.51
8	F	1801	ADP	C5-N7-C8	2.67	107.30	103.51
8	E	1802	ADP	C4-N9-C8	2.42	108.35	105.73
5	A	2601	IHP	C6-C1-C2	2.42	115.71	110.41
8	E	1802	ADP	PA-O3A-PB	-2.26	125.08	132.83
8	F	1801	ADP	C4-N9-C8	2.12	108.03	105.73
8	E	1802	ADP	C6-C5-N7	2.12	135.97	132.02
6	B	2601	ATP	PB-O3B-PG	2.10	140.01	132.83

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2602	IHP	C2-C1-O11-P1
5	B	2602	IHP	C3-O13-P3-O23
8	E	1802	ADP	C5'-O5'-PA-O1A
8	E	1802	ADP	C5'-O5'-PA-O3A
8	F	1801	ADP	PA-O3A-PB-O2B
8	F	1801	ADP	C5'-O5'-PA-O2A
8	F	1801	ADP	C3'-C4'-C5'-O5'
6	A	2602	ATP	O4'-C4'-C5'-O5'
8	F	1801	ADP	O4'-C4'-C5'-O5'
6	A	2602	ATP	C3'-C4'-C5'-O5'
5	B	2602	IHP	C6-C1-O11-P1

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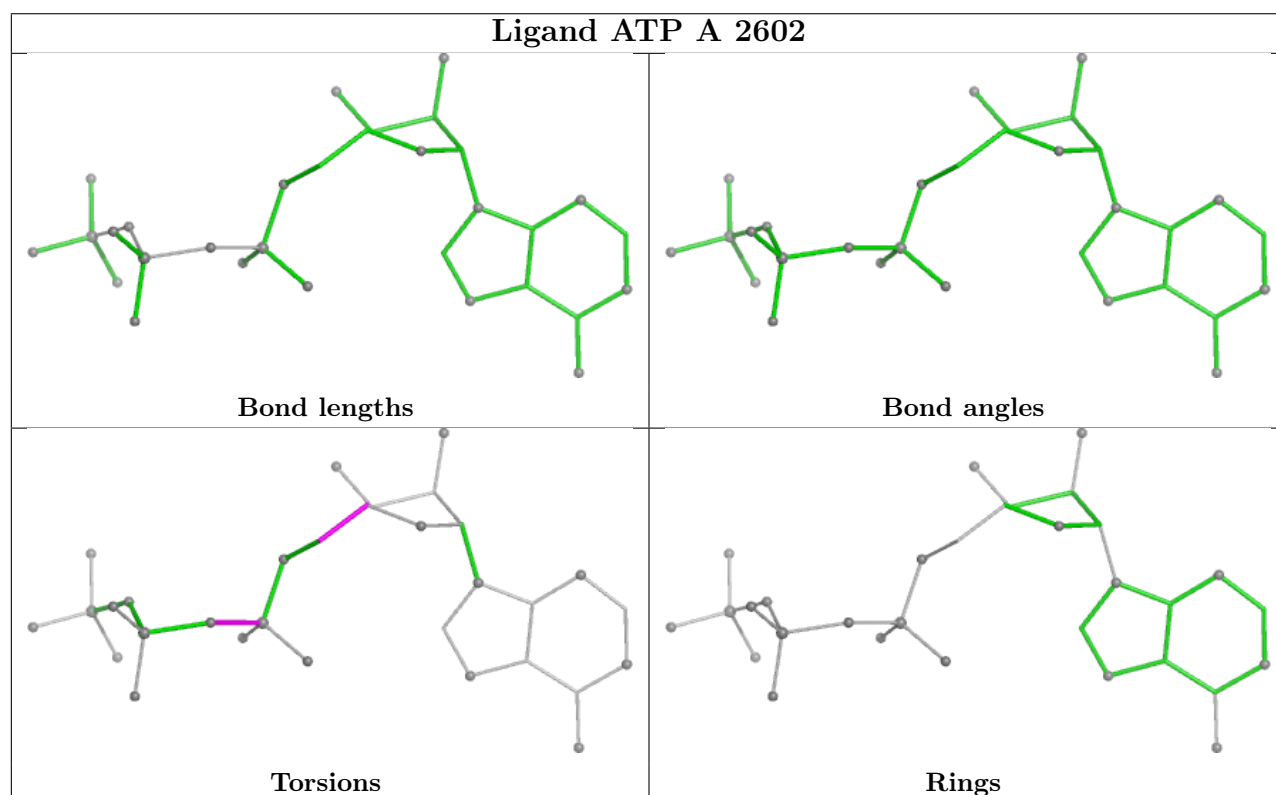
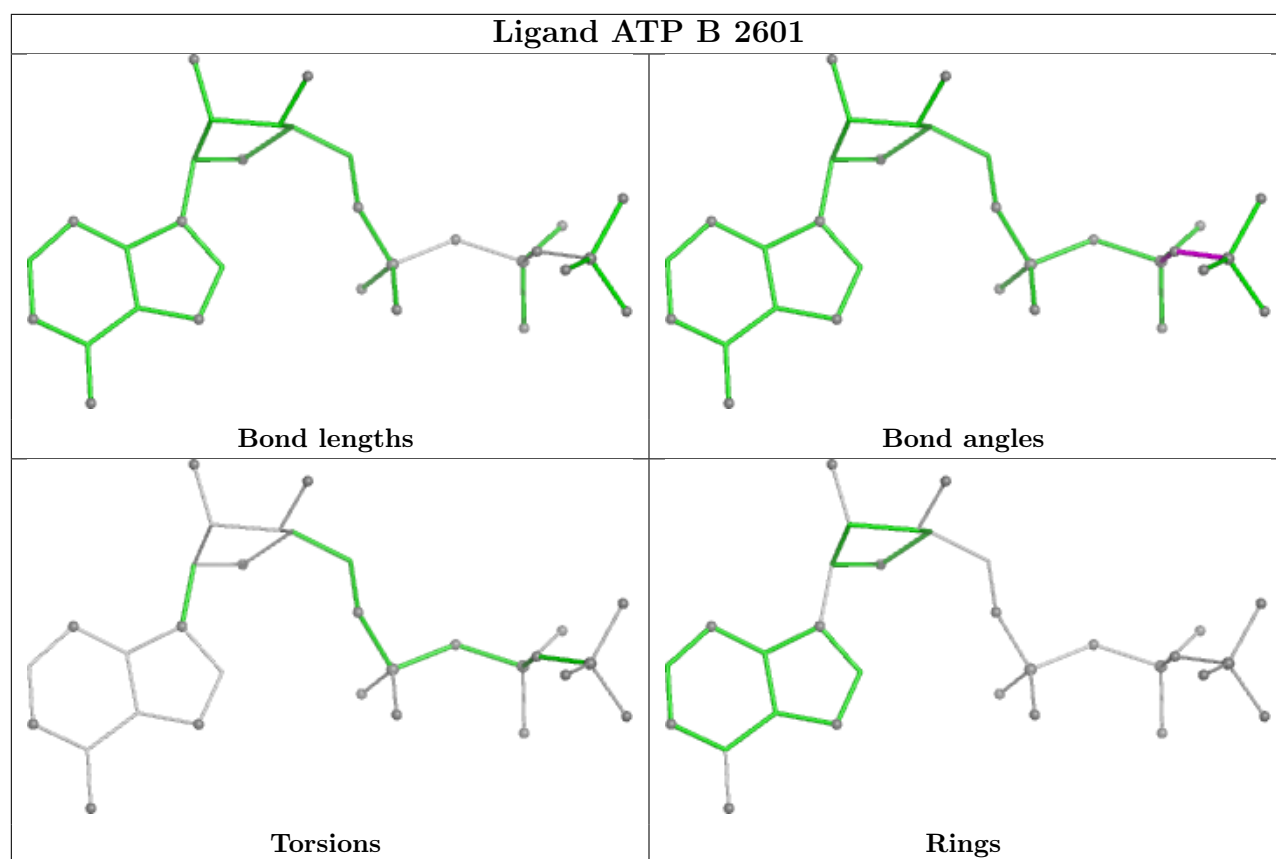
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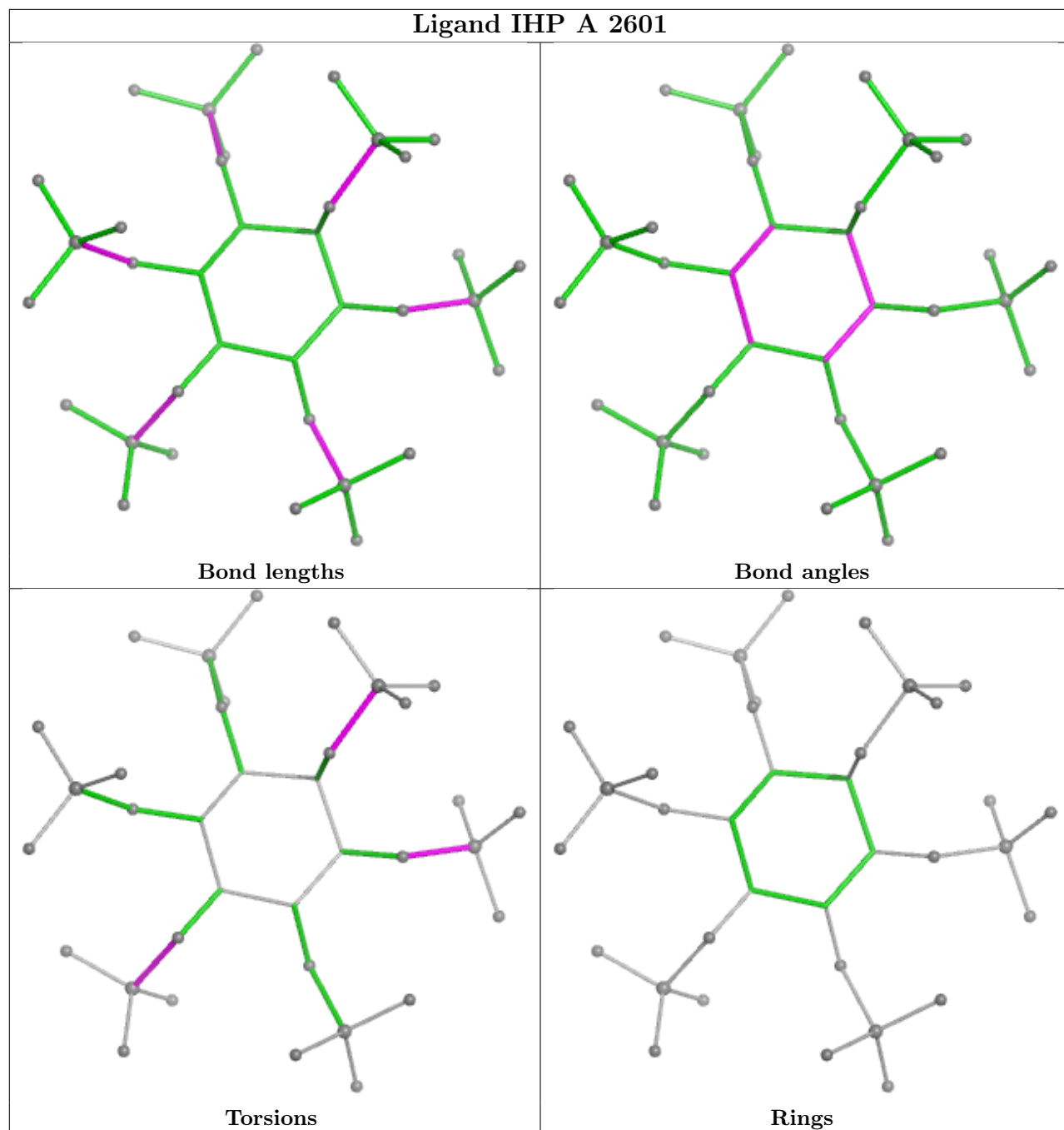
Mol	Chain	Res	Type	Atoms
8	E	1802	ADP	PB-O3A-PA-O1A
8	F	1801	ADP	C4'-C5'-O5'-PA
8	F	1801	ADP	C5'-O5'-PA-O3A
6	A	2602	ATP	PB-O3A-PA-O1A
8	F	1801	ADP	C2'-C1'-N9-C4
8	E	1802	ADP	C5'-O5'-PA-O2A
8	F	1801	ADP	C5'-O5'-PA-O1A
8	E	1802	ADP	PB-O3A-PA-O2A
8	F	1801	ADP	C2'-C1'-N9-C8
5	A	2601	IHP	C1-O11-P1-O21
5	A	2601	IHP	C2-O12-P2-O22
5	B	2602	IHP	C2-O12-P2-O22
5	B	2602	IHP	C4-O14-P4-O24
8	F	1801	ADP	PA-O3A-PB-O3B
5	A	2601	IHP	C1-O11-P1-O31
5	A	2601	IHP	C1-O11-P1-O41
5	A	2601	IHP	C2-O12-P2-O32
5	A	2601	IHP	C5-O15-P5-O35
5	B	2602	IHP	C2-O12-P2-O42
5	B	2602	IHP	C3-O13-P3-O43
5	B	2602	IHP	C4-O14-P4-O44
5	B	2602	IHP	C6-O16-P6-O46
8	F	1801	ADP	O4'-C1'-N9-C8
8	E	1802	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

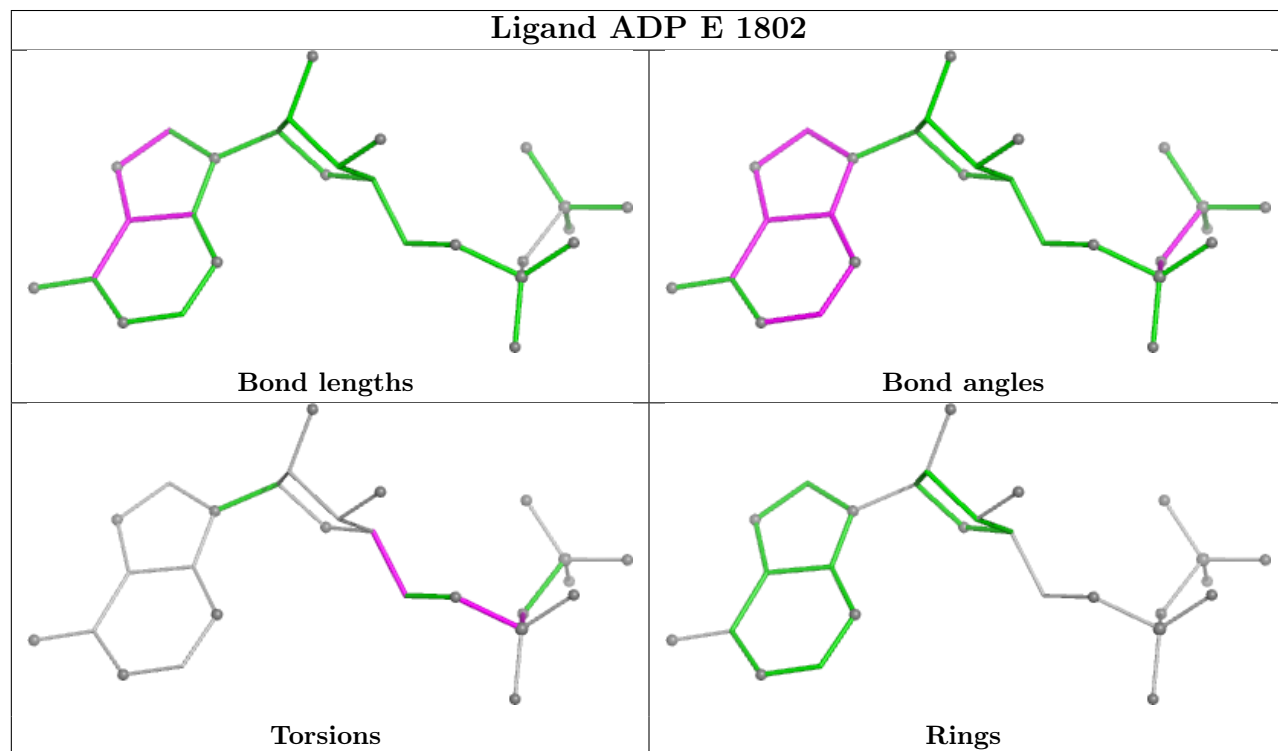
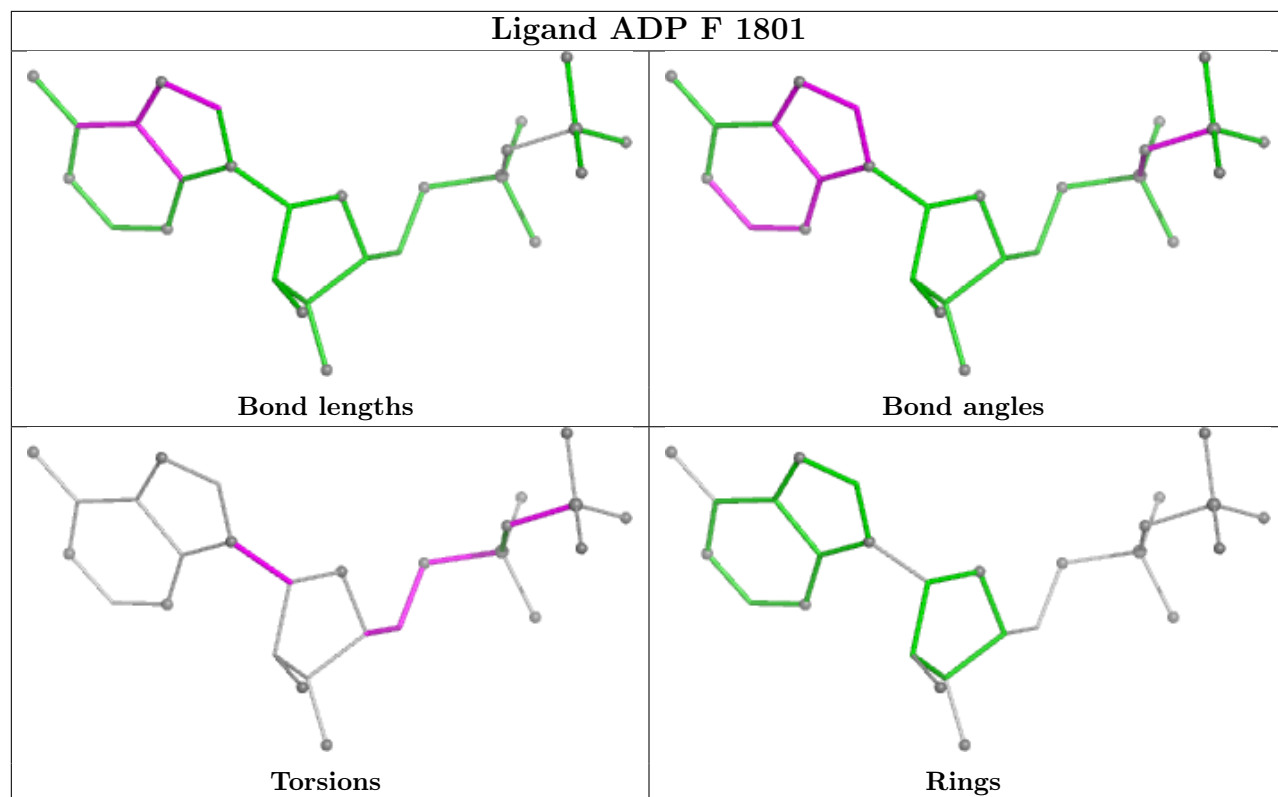
No monomer is involved in short contacts.

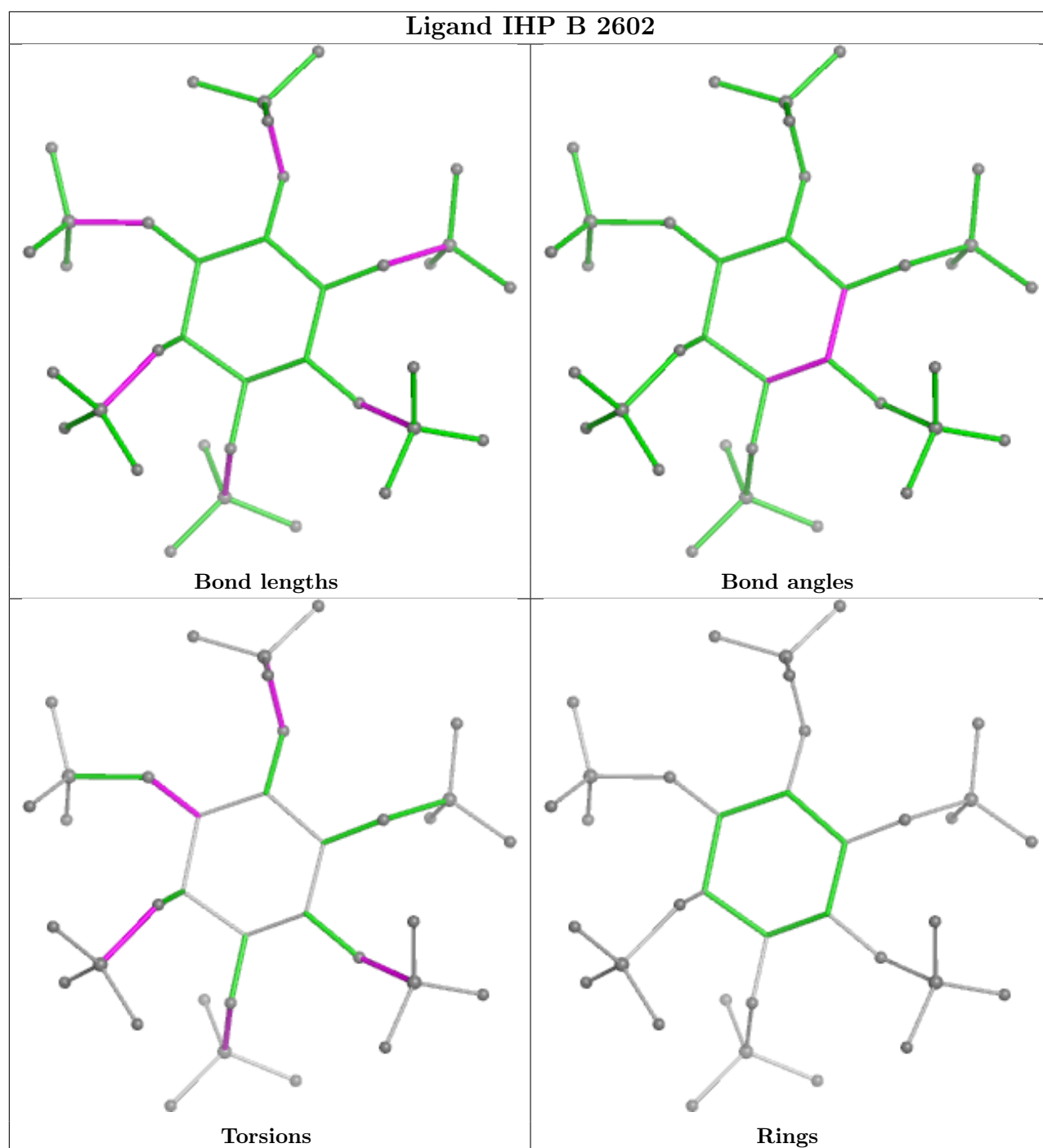
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

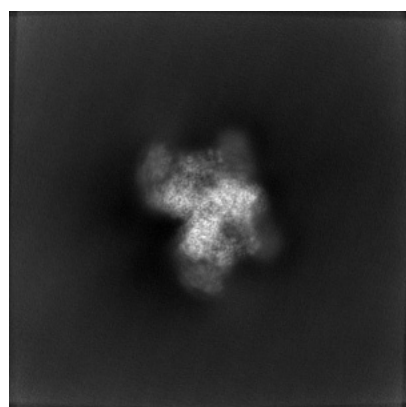
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55637. These allow visual inspection of the internal detail of the map and identification of artifacts.

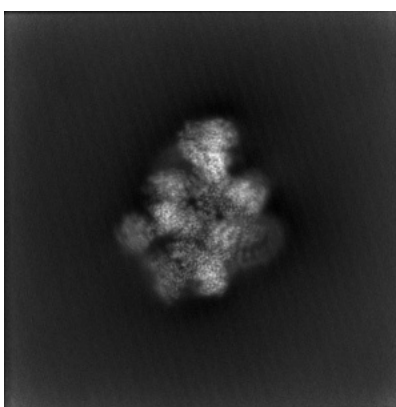
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

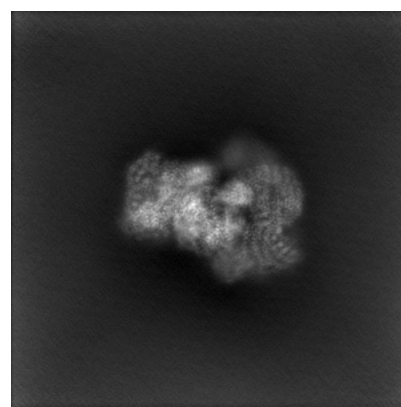
#### 6.1.1 Primary map



X



Y

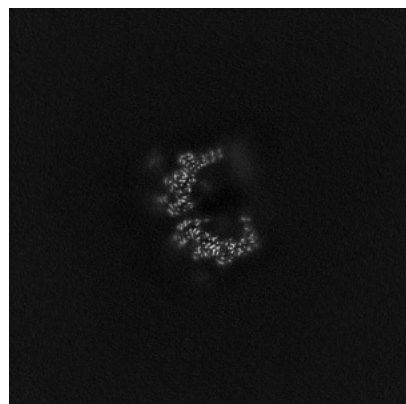


Z

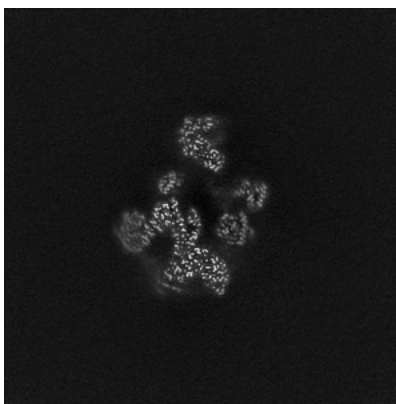
The images above show the map projected in three orthogonal directions.

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

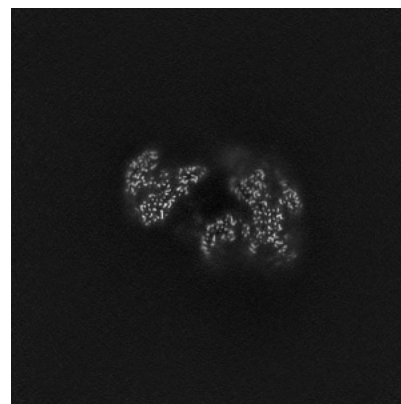
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

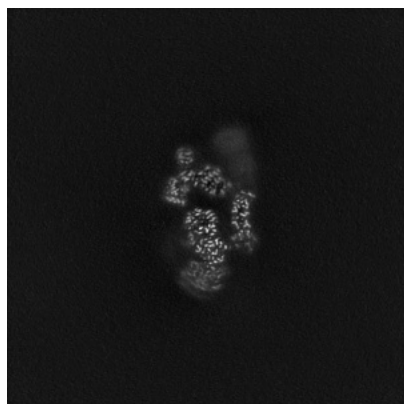


Z Index: 256

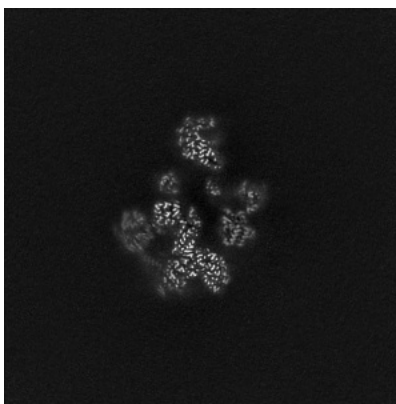
The images above show central slices of the map in three orthogonal directions.

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

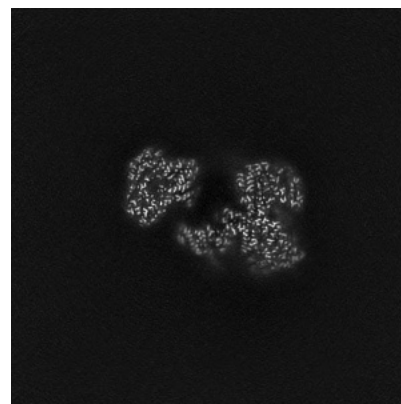
### 6.3.1 Primary map



X Index: 234



Y Index: 252

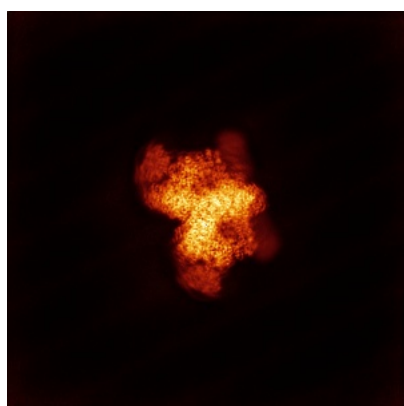


Z Index: 270

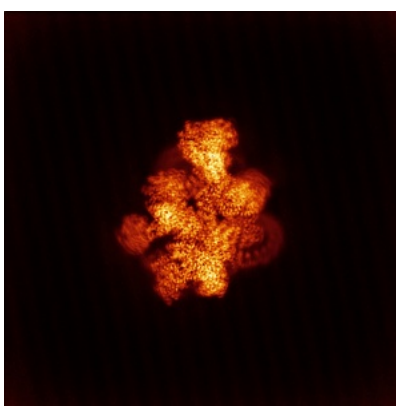
The images above show the largest variance slices of the map in three orthogonal directions.

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

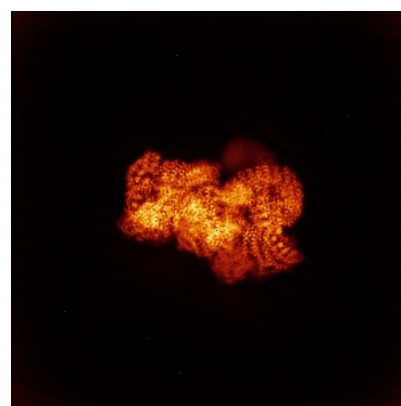
### 6.4.1 Primary map



X



Y



Z

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

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

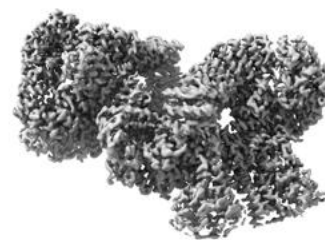
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

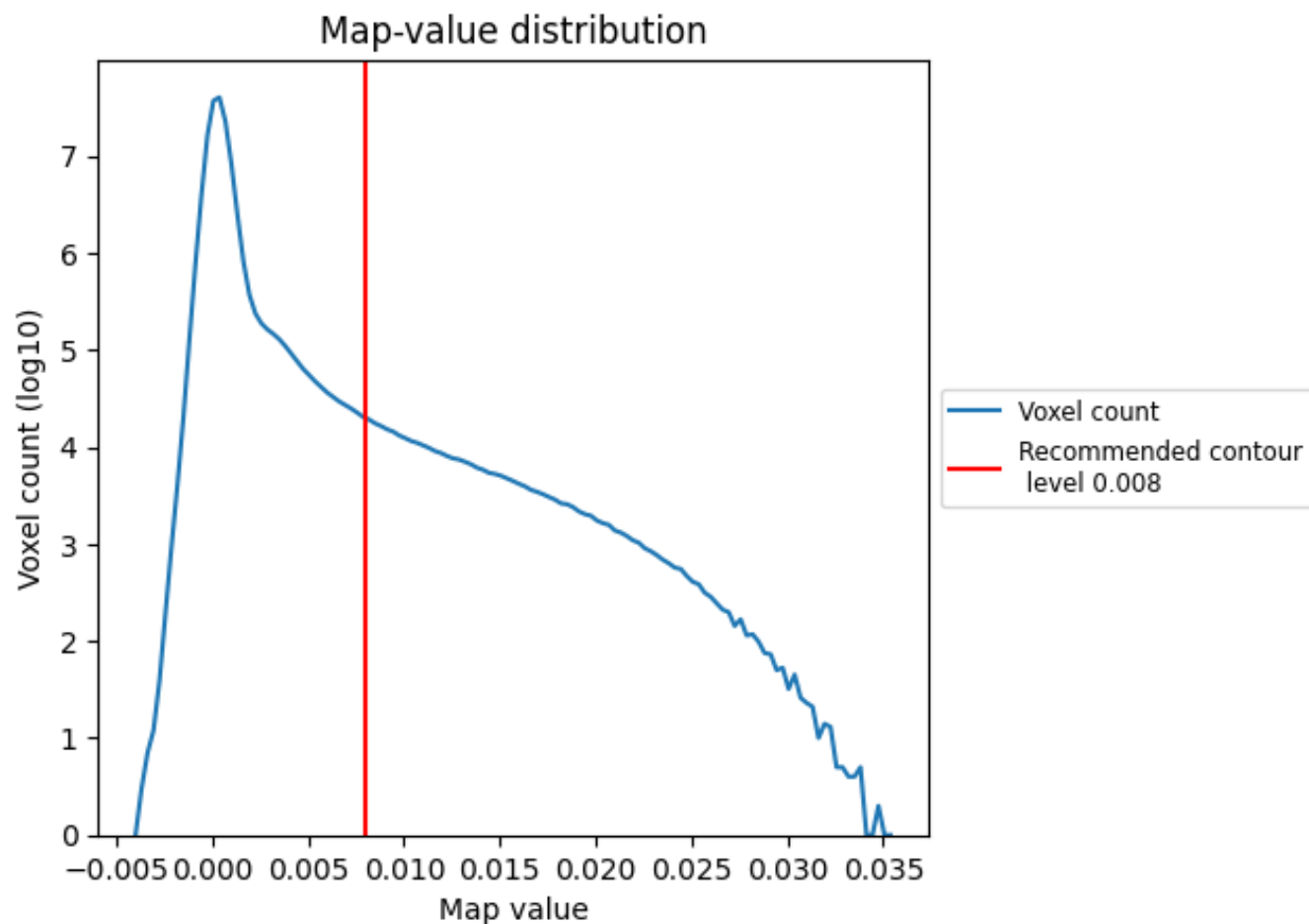
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

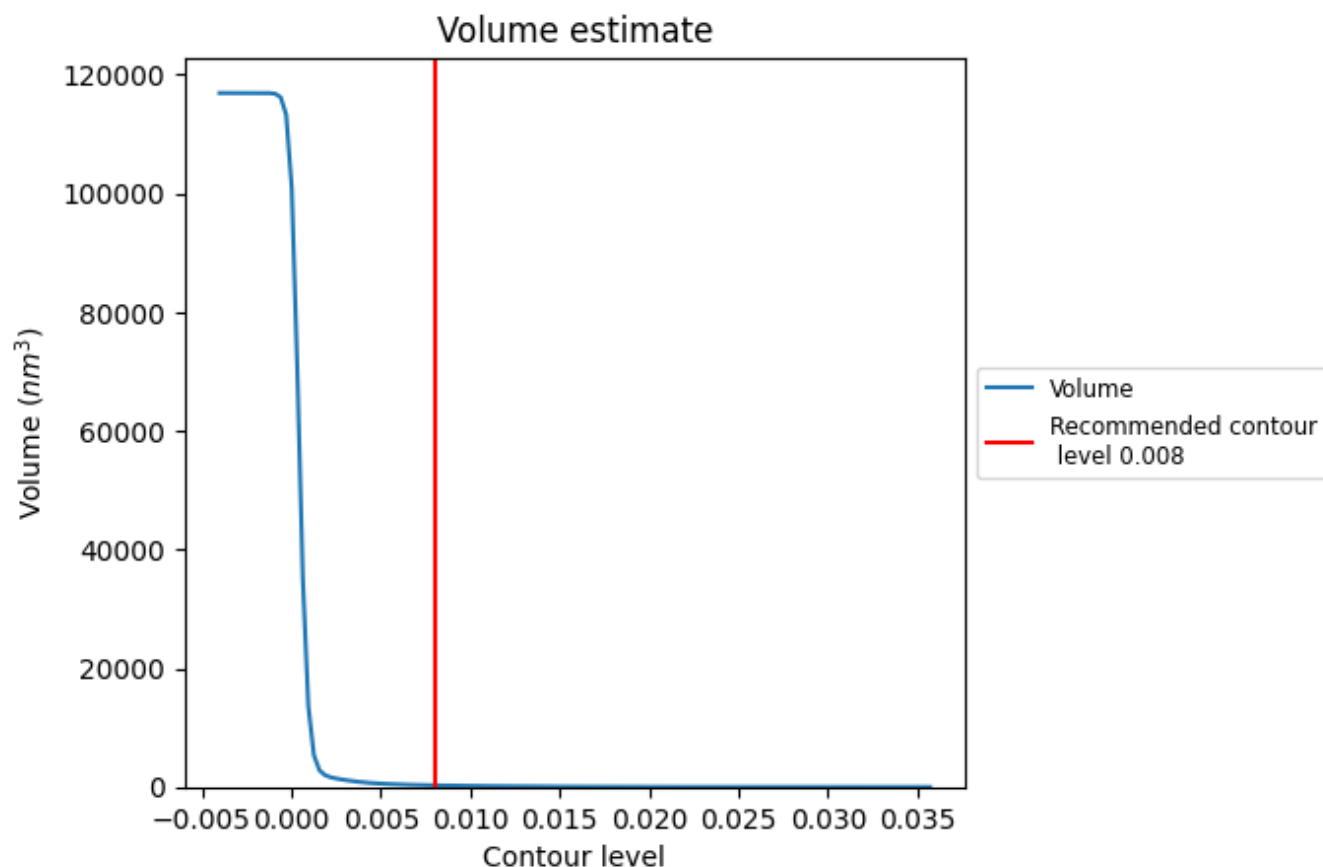
This section contains the results of statistical analysis of the map.

### 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.

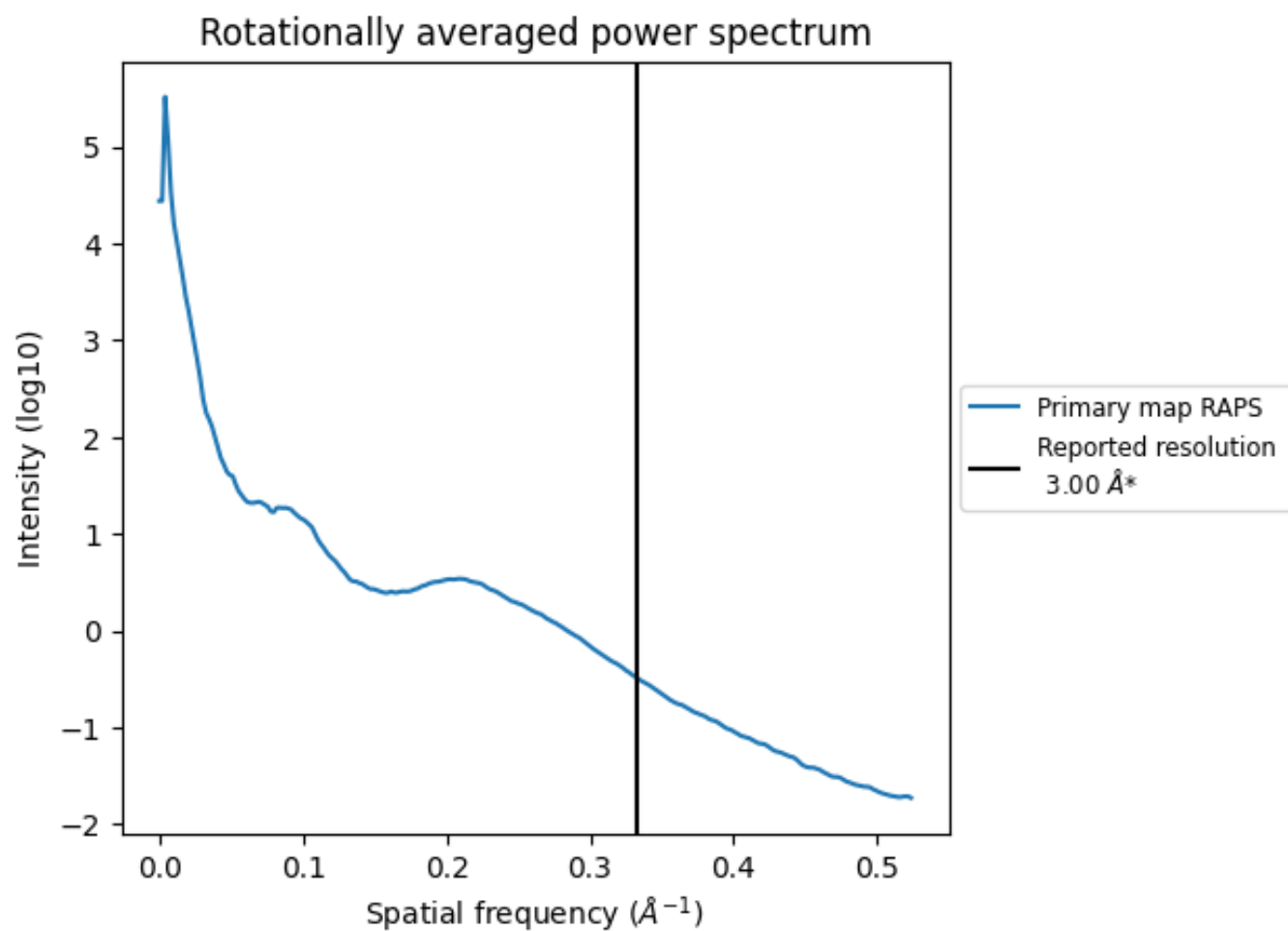
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271  $\text{nm}^3$ ; this corresponds to an approximate mass of 245 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 0.333 Å<sup>-1</sup>



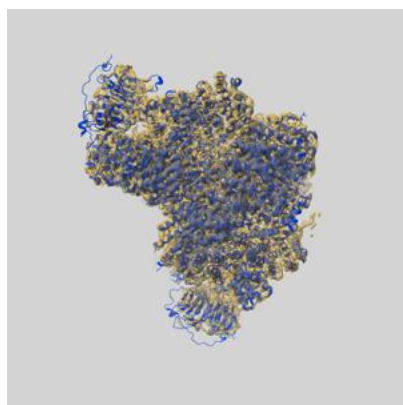
## 8 Fourier-Shell correlation

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

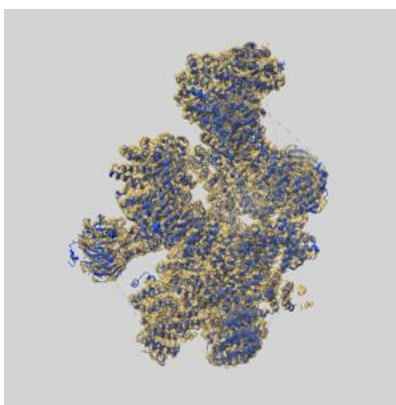
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55637 and PDB model 9T7J. Per-residue inclusion information can be found in section [3](#) on page [11](#).

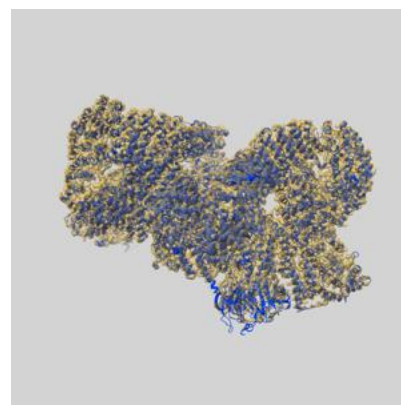
### 9.1 Map-model overlay [i](#)



X



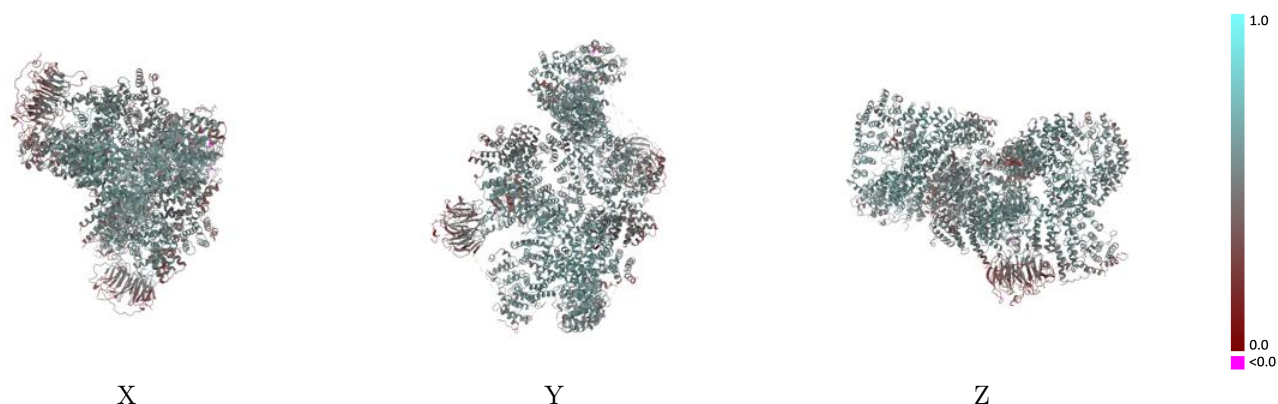
Y



Z

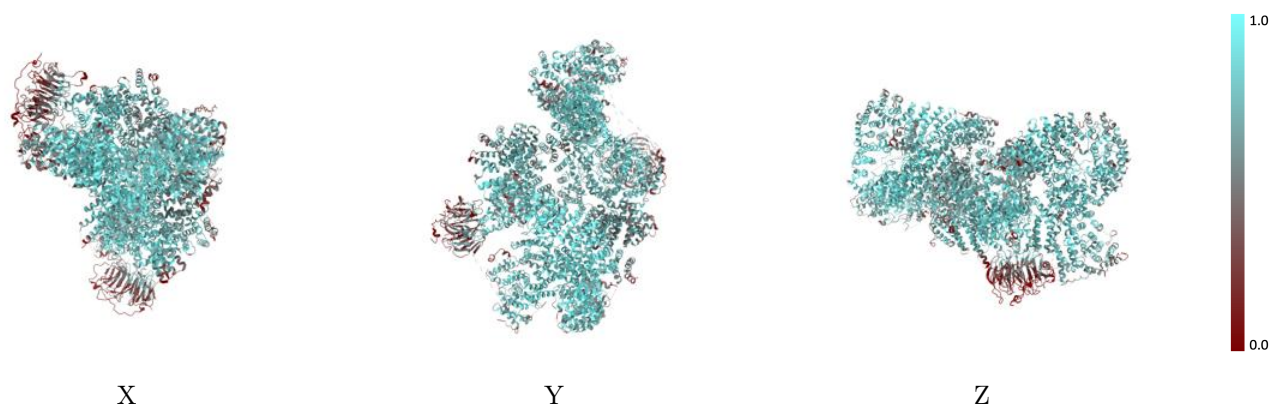
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



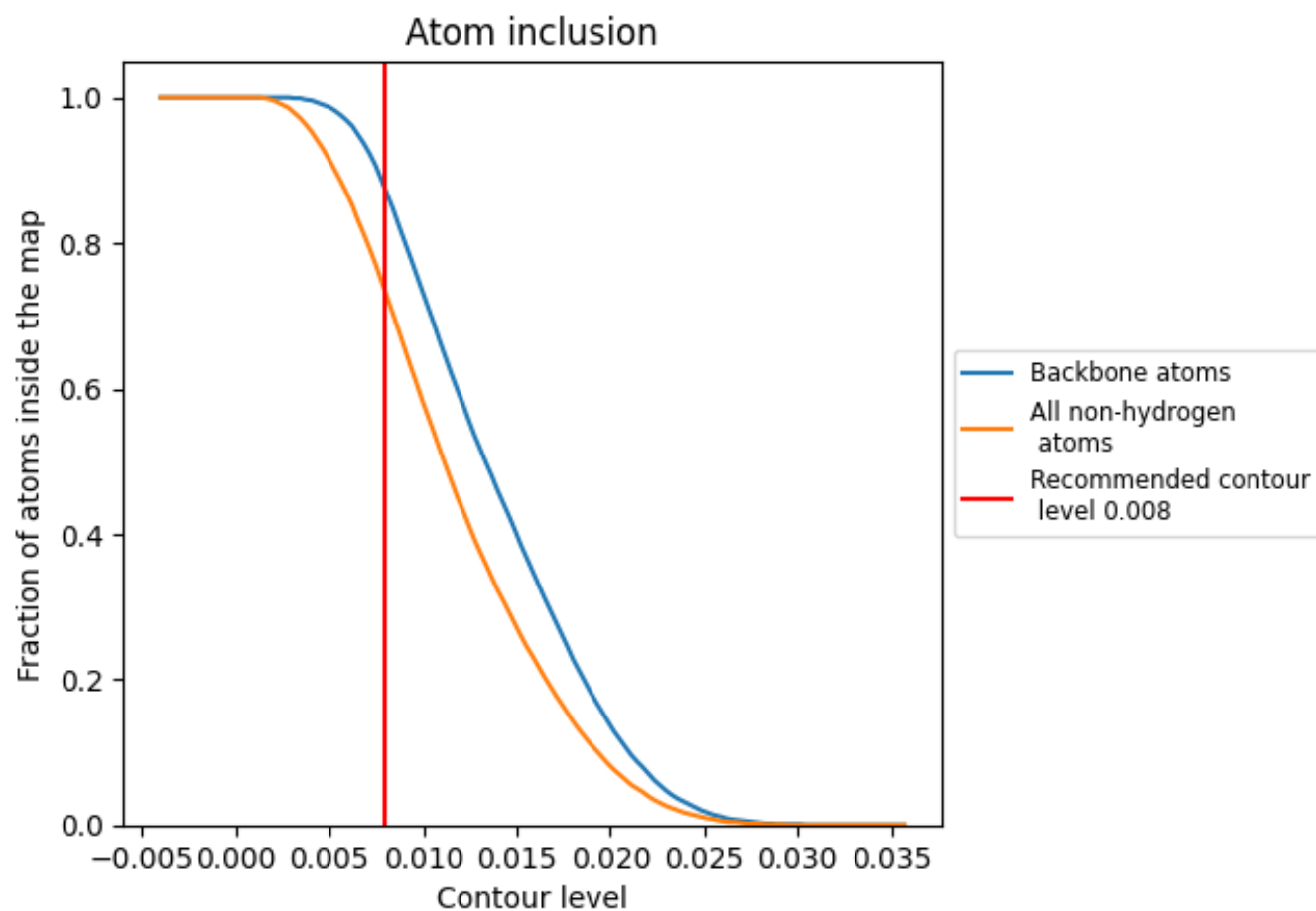
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7320	<div></div> 0.5240
A	<div></div> 0.7920	<div></div> 0.5460
B	<div></div> 0.7680	<div></div> 0.5320
C	<div></div> 0.3570	<div></div> 0.3770
D	<div></div> 0.3400	<div></div> 0.3740
E	<div></div> 0.8120	<div></div> 0.5640
F	<div></div> 0.7620	<div></div> 0.5350
G	<div></div> 0.4350	<div></div> 0.4100
H	<div></div> 0.4020	<div></div> 0.4030

1.0

0.0

<0.0