



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:18 AM UTC

PDB ID : 8RCH / pdb_00008rch
EMDB ID : EMD-19052
Title : CryoEM structure of mTORC1 with a paediatric kidney cancer-associated 1455-EWED-1458 duplication in mTOR, overall refinement
Authors : Anandapadamanaban, M.; Hay, I.M.; Perisic, O.; Williams, R.L.
Deposited on : 2023-12-06
Resolution : 4.00 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

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:

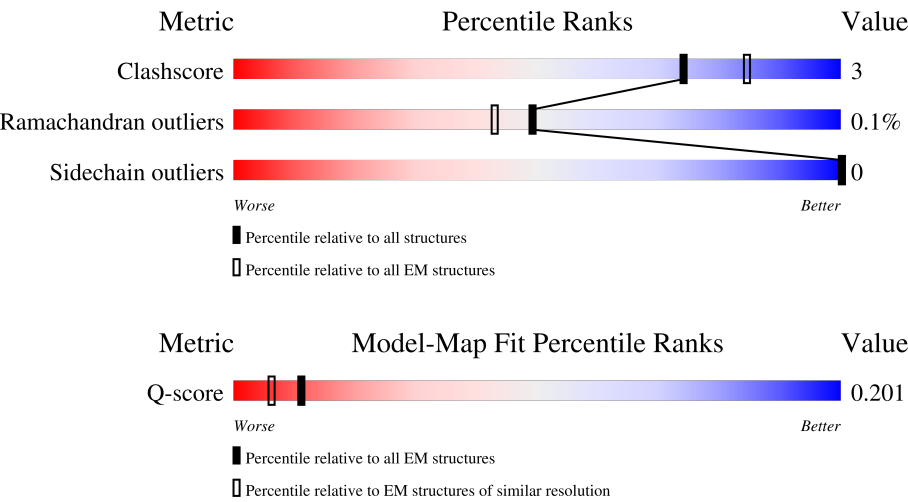
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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	7587 (3.50 - 4.50)

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 ≥ 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	
1	B	2549	
2	D	326	
2	E	326	

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Mol	Chain	Length	Quality of chain
3	W	1335	8%29%68%
3	Y	1335	12%71%7%22%
4	X	118	7%93%
4	Z	118	5%7%93%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 99566 atoms, of which 49958 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	2036	Total	C	H	N	O	S	0	0
			33036	10476	16667	2863	2926	104		
1	B	2036	Total	C	H	N	O	S	0	0
			33036	10476	16667	2863	2926	104		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total	C	H	N	O	S	0	0
			4798	1526	2342	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4798	1526	2342	436	476	18		

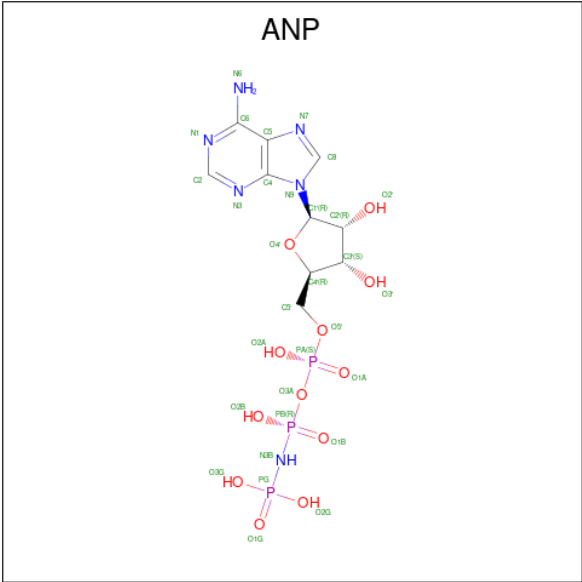
- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	428	Total	C	H	N	O	S	0	0
			6933	2225	3504	581	602	21		
3	Y	1044	Total	C	H	N	O	S	0	0
			16645	5322	8320	1441	1506	56		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Z	8	Total	C	H	N	O	S	0	0
			127	42	58	9	17	1		
4	X	8	Total	C	H	N	O	S	0	0
			127	42	58	9	17	1		

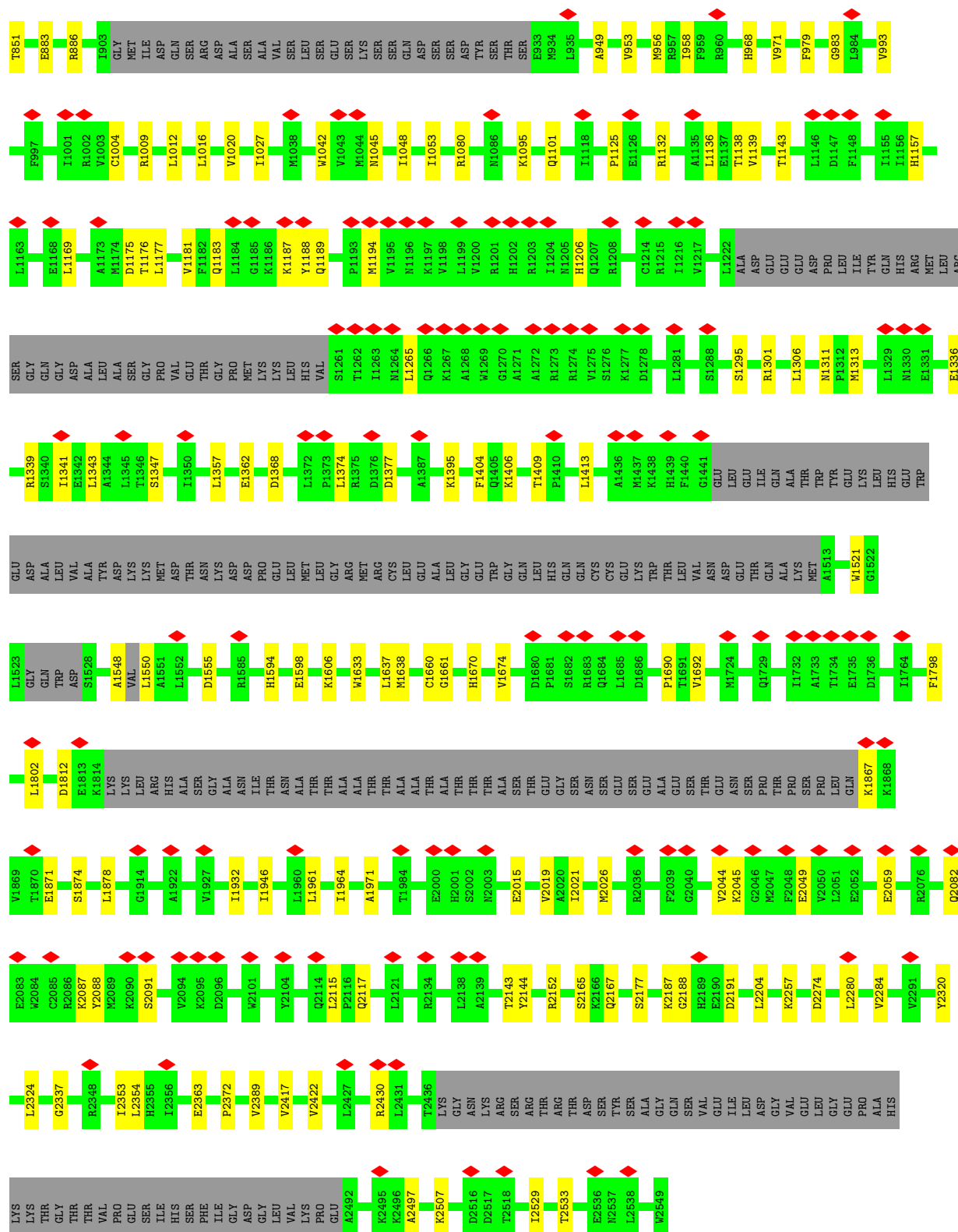
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



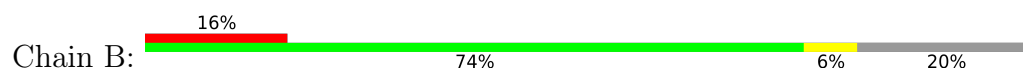
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

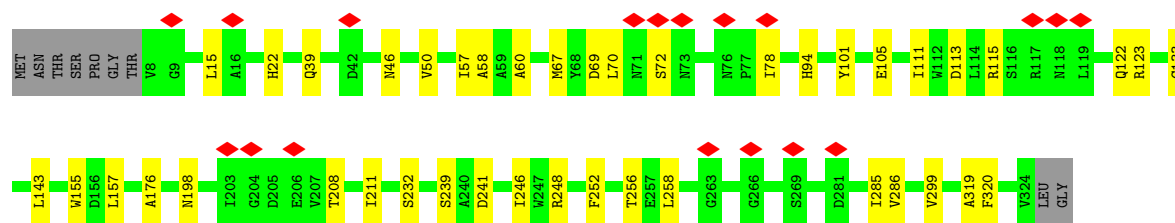
Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Mg	0
			2	2	
6	B	2	Total	Mg	0
			2	2	



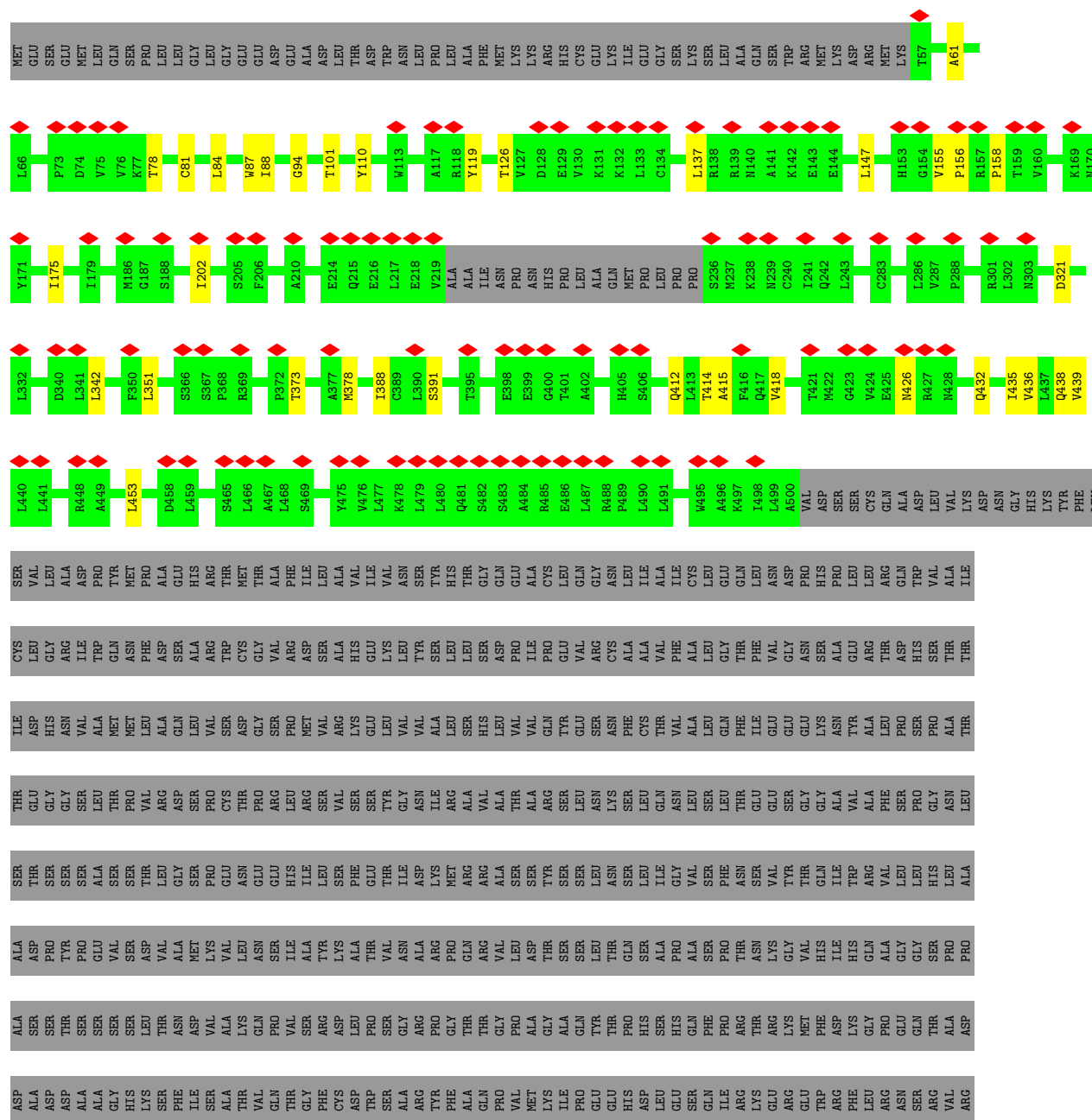
• Molecule 1: Serine/threonine-protein kinase mTOR



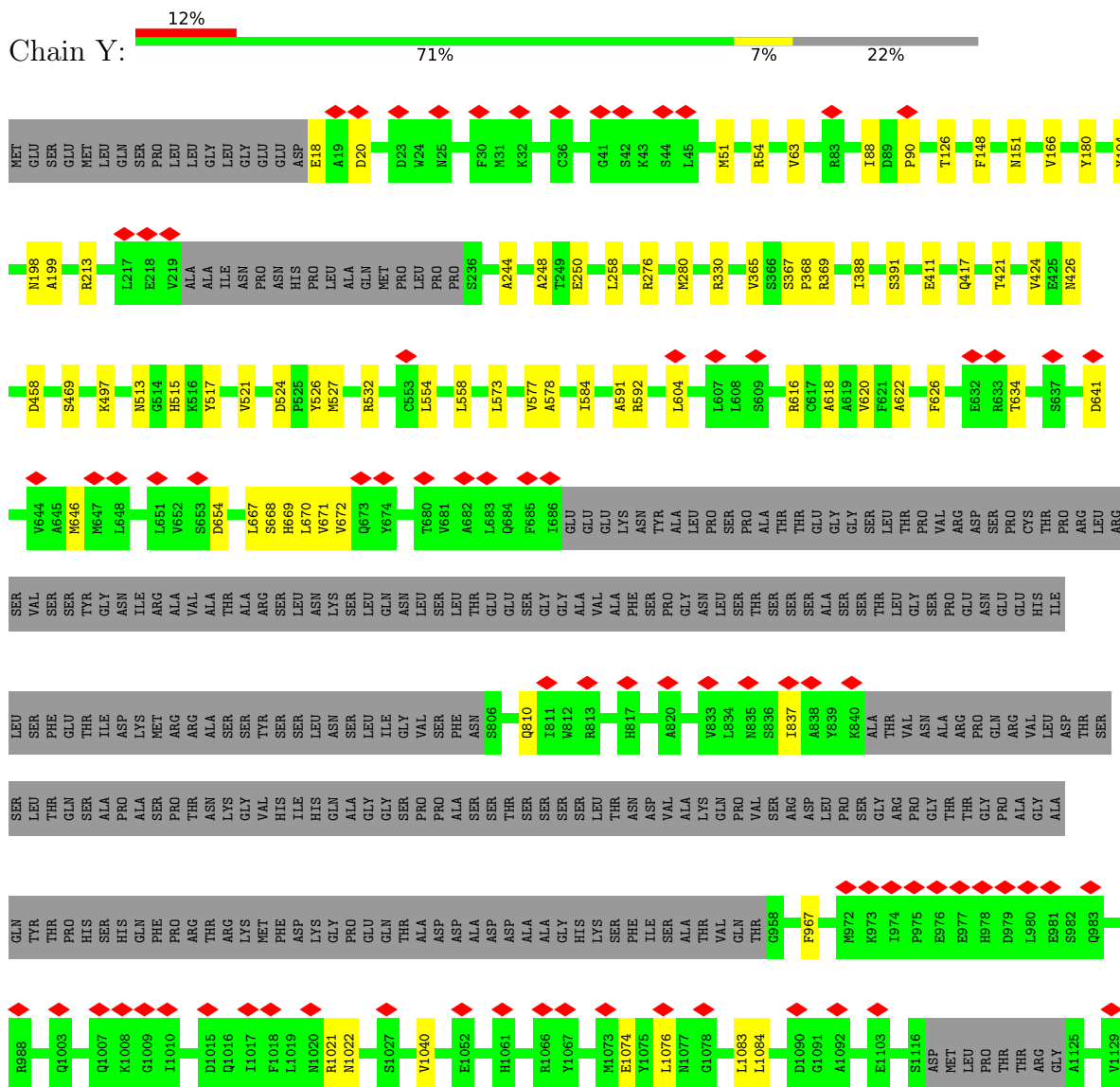


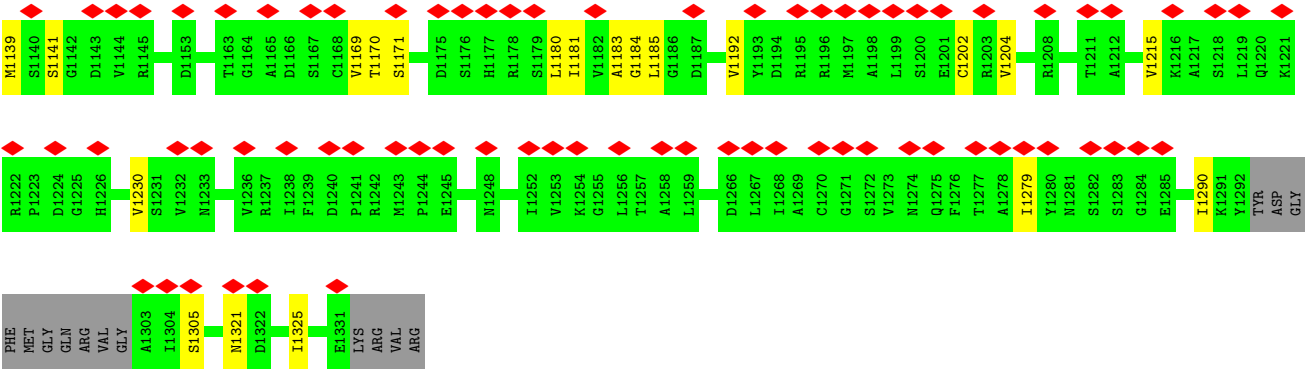


• Molecule 3: Regulatory-associated protein of mTOR

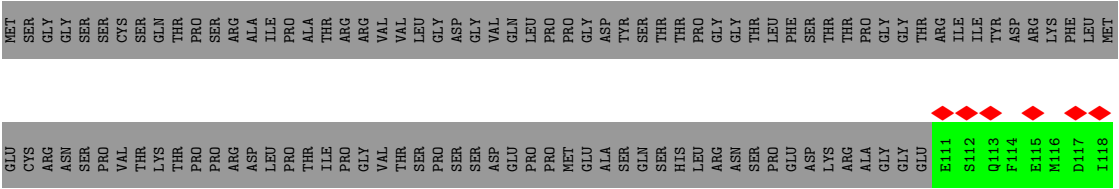


- Molecule 3: Regulatory-associated protein of mTOR

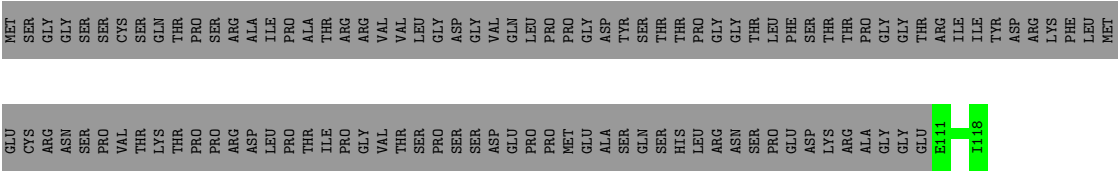




● Molecule 4: Eukaryotic translation initiation factor 4E-binding protein 1



● Molecule 4: Eukaryotic translation initiation factor 4E-binding protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	264890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/16696	0.46	7/22592 (0.0%)
1	B	0.19	0/16696	0.44	4/22592 (0.0%)
2	D	0.22	0/2514	0.64	10/3426 (0.3%)
2	E	0.22	0/2514	0.58	8/3426 (0.2%)
3	W	0.20	0/3516	0.41	0/4797
3	Y	0.21	0/8524	0.48	4/11596 (0.0%)
4	X	0.25	0/69	0.26	0/89
4	Z	0.27	0/69	0.31	0/89
All	All	0.20	0/50598	0.47	33/68607 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
3	W	0	2
3	Y	0	3
All	All	0	8

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TYR	CA-C-N	10.86	141.26	121.70
1	A	234	TYR	C-N-CA	10.86	141.26	121.70
1	A	2372	PRO	CA-C-N	9.07	138.03	121.70
1	A	2372	PRO	C-N-CA	9.07	138.03	121.70
1	B	2372	PRO	CA-C-N	7.95	136.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2372	PRO	C-N-CA	7.95	136.00	121.70
2	D	79	ILE	CA-C-N	7.54	135.27	121.70
2	D	79	ILE	C-N-CA	7.54	135.27	121.70
2	D	81	TYR	CA-C-N	7.37	134.96	121.70
2	D	81	TYR	C-N-CA	7.37	134.96	121.70
2	D	105	GLU	CA-C-N	7.24	134.73	121.70
2	D	105	GLU	C-N-CA	7.24	134.73	121.70
2	E	72	SER	CA-C-N	6.85	134.03	121.70
2	E	72	SER	C-N-CA	6.85	134.03	121.70
1	A	2143	THR	CA-C-N	6.65	133.67	121.70
1	A	2143	THR	C-N-CA	6.65	133.67	121.70
1	B	1309	ALA	CA-C-N	6.51	133.41	121.70
1	B	1309	ALA	C-N-CA	6.51	133.41	121.70
2	E	232	SER	CA-C-N	5.96	132.42	121.70
2	E	232	SER	C-N-CA	5.96	132.42	121.70
3	Y	151	ASN	CA-C-N	5.72	131.99	121.70
3	Y	151	ASN	C-N-CA	5.72	131.99	121.70
2	D	208	THR	CA-C-N	5.43	131.47	121.70
2	D	208	THR	C-N-CA	5.43	131.47	121.70
2	E	105	GLU	CA-C-N	5.36	131.35	121.70
2	E	105	GLU	C-N-CA	5.36	131.35	121.70
2	E	208	THR	CA-C-N	5.34	131.31	121.70
2	E	208	THR	C-N-CA	5.34	131.31	121.70
2	D	200	THR	CA-C-N	5.33	131.29	121.70
2	D	200	THR	C-N-CA	5.33	131.29	121.70
3	Y	1141	SER	CA-C-N	5.28	131.20	121.70
3	Y	1141	SER	C-N-CA	5.28	131.20	121.70
1	A	764	ALA	N-CA-C	5.21	121.33	109.81

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1189	GLN	Peptide
1	A	183	PHE	Peptide
1	A	2115	LEU	Peptide
3	W	155	VAL	Peptide
3	W	426	ASN	Peptide
3	Y	1184	GLY	Peptide
3	Y	367	SER	Peptide
3	Y	458	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16369	16667	16646	103	0
1	B	16369	16667	16646	90	0
2	D	2456	2342	2341	34	0
2	E	2456	2342	2341	21	0
3	W	3429	3504	3502	22	0
3	Y	8325	8320	8314	54	0
4	X	69	58	57	0	0
4	Z	69	58	57	0	0
5	A	31	0	13	1	0
5	B	31	0	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	49608	49958	49929	315	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 3.

All (315) 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:E:94:HIS:NE2	2:E:101:TYR:OH	2.17	0.78
1:A:285:GLU:O	1:A:491:ARG:NH1	2.17	0.77
1:A:2274:ASP:O	2:D:44:GLN:NE2	2.22	0.73
3:W:61:ALA:HB2	3:W:137:LEU:HD11	1.72	0.71
1:B:1362:GLU:OE1	1:B:1395:LYS:NZ	2.24	0.70
1:A:724:ALA:N	3:Y:411:GLU:OE2	2.25	0.70
1:A:502:LYS:NZ	1:A:534:ASP:OD2	2.25	0.69
2:E:46:ASN:N	2:E:60:ALA:O	2.25	0.69
1:B:459:ILE:HG21	1:B:486:ILE:HD11	1.74	0.69
1:B:719:SER:O	1:B:766:ARG:NH1	2.27	0.68
3:Y:1040:VAL:HG21	3:Y:1325:ILE:HD13	1.74	0.68
1:A:1143:THR:O	1:A:1183:GLN:NE2	2.28	0.66
1:B:1598:GLU:OE1	1:B:1619:TRP:NE1	2.29	0.66
1:A:524:LEU:HD11	1:A:528:ILE:HD12	1.78	0.66
1:A:1362:GLU:OE2	1:A:1395:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:1305:SER:N	3:Y:1321:ASN:OD1	2.29	0.65
1:B:1902:ASP:OD1	1:B:1905:ARG:NH1	2.30	0.64
1:B:2189:HIS:N	1:B:2233:ASN:O	2.30	0.64
3:Y:592:ARG:NH2	3:Y:641:ASP:OD1	2.30	0.64
1:B:1555:ASP:OD1	1:B:1606:LYS:NZ	2.28	0.64
1:A:91:ALA:O	1:A:132:ARG:NH1	2.31	0.63
1:A:1521:TRP:NE1	1:A:1638:MET:O	2.31	0.63
1:B:1124:ALA:O	1:B:1132:ARG:NH1	2.32	0.63
5:A:3000:ANP:H8	5:A:3000:ANP:H5'2	1.81	0.63
1:A:114:LEU:O	1:A:118:ASN:N	2.31	0.63
1:A:2204:LEU:HD22	1:A:2417:VAL:HG21	1.81	0.62
1:A:586:LEU:HD13	1:A:622:ALA:HB2	1.81	0.62
3:Y:616:ARG:NH1	3:Y:654:ASP:OD2	2.33	0.62
1:A:883:GLU:OE1	1:A:886:ARG:NH1	2.33	0.61
1:B:1657:ALA:O	1:B:1663:SER:OG	2.15	0.61
1:B:2204:LEU:HD22	1:B:2417:VAL:HG21	1.82	0.61
1:A:1377:ASP:OD1	1:A:1406:LYS:NZ	2.33	0.61
3:W:321:ASP:OD2	3:W:438:GLN:NE2	2.33	0.61
1:B:2209:LEU:O	1:B:2215:SER:OG	2.19	0.61
1:A:74:LEU:O	1:A:83:ARG:NH1	2.34	0.60
2:E:133:CYS:SG	2:E:176:ALA:N	2.74	0.60
1:B:1309:ALA:HB3	1:B:1310:TYR:HA	1.83	0.60
1:A:1368:ASP:OD1	1:A:2257:LYS:NZ	2.33	0.60
1:B:2106:HIS:O	1:B:2110:ARG:NE	2.30	0.60
1:A:764:ALA:HB1	1:A:768:ILE:HG23	1.83	0.60
1:A:1187:LYS:NZ	1:B:694:GLN:OE1	2.34	0.60
1:A:176:ALA:HB3	1:A:215:ALA:HB1	1.84	0.59
1:B:2339:ARG:O	1:B:2545:TRP:NE1	2.35	0.59
1:A:268:LEU:O	1:A:272:VAL:HG22	2.01	0.59
3:Y:1169:VAL:O	3:Y:1185:LEU:N	2.36	0.59
1:A:1139:VAL:O	1:A:1143:THR:OG1	2.19	0.59
1:B:661:VAL:O	1:B:665:THR:HG23	2.03	0.59
2:E:123:ARG:NE	2:E:157:LEU:O	2.36	0.59
3:Y:88:ILE:HG22	3:Y:90:PRO:HD3	1.85	0.59
1:A:1042:TRP:O	1:A:1080:ARG:NH2	2.36	0.58
1:A:2529:ILE:O	1:A:2533:THR:HG23	2.03	0.58
2:E:22:HIS:O	2:E:39:GLN:NE2	2.36	0.58
1:B:1548:ALA:O	1:B:1550:LEU:N	2.36	0.58
3:Y:604:LEU:HD21	3:Y:622:ALA:HB3	1.85	0.58
3:W:78:THR:HG1	3:W:81:CYS:HG	1.47	0.57
3:Y:1074:GLU:O	3:Y:1084:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:SER:HB3	2:D:70:LEU:HD23	1.87	0.56
1:B:433:ALA:HB1	1:B:481:THR:HG21	1.86	0.56
3:Y:1169:VAL:HG11	3:Y:1183:ALA:HB1	1.88	0.56
2:D:168:GLU:OE1	2:D:189:ASN:ND2	2.39	0.56
1:A:1177:LEU:O	1:A:1181:VAL:HG23	2.04	0.56
3:W:158:PRO:CB	3:W:202:ILE:HD11	2.35	0.56
1:B:437:LEU:HD22	1:B:455:VAL:HG21	1.87	0.56
1:B:2020:ALA:O	1:B:2170:ARG:NH1	2.38	0.56
1:B:742:GLU:OE2	1:B:782:LYS:NZ	2.27	0.56
2:E:57:ILE:HG13	2:E:70:LEU:HD11	1.87	0.56
2:D:280:GLY:N	2:D:322:ASP:OD1	2.39	0.55
2:D:103:GLY:O	2:D:110:ARG:NH2	2.40	0.55
1:A:1339:ARG:NH2	1:A:1374:LEU:O	2.40	0.55
3:W:378:MET:HE1	3:W:435:ILE:HD11	1.88	0.55
2:E:239:SER:OG	2:E:241:ASP:OD1	2.24	0.55
1:B:2088:TYR:O	1:B:2092:GLY:N	2.38	0.55
2:D:18:ALA:HB1	2:D:45:VAL:HG21	1.89	0.55
2:D:224:LEU:HD12	2:D:273:MET:O	2.06	0.55
3:Y:517:TYR:O	3:Y:521:VAL:HG23	2.06	0.55
1:A:783:LEU:HD11	1:A:802:ILE:CD1	2.37	0.55
3:Y:1169:VAL:CG1	3:Y:1183:ALA:HB1	2.36	0.54
1:A:533:LYS:NZ	1:A:537:ASP:OD2	2.41	0.54
1:A:810:GLY:O	1:A:851:THR:OG1	2.25	0.54
1:A:1020:VAL:HG22	1:A:1027:ILE:HD11	1.89	0.54
3:Y:1139:MET:SD	3:Y:1181:ILE:HD12	2.48	0.54
3:Y:63:VAL:HG21	3:Y:148:PHE:CZ	2.43	0.54
3:Y:198:ASN:ND2	3:Y:250:GLU:O	2.41	0.54
1:A:1594:HIS:NE2	1:A:1598:GLU:OE2	2.41	0.54
2:E:198:ASN:N	2:E:211:ILE:O	2.41	0.54
1:B:1653:TRP:HE3	1:B:1672:THR:HG23	1.74	0.53
1:B:2063:GLN:N	1:B:2067:GLU:OE1	2.40	0.53
3:W:351:LEU:HD22	3:W:373:THR:OG1	2.08	0.53
1:B:1998:MET:O	1:B:2002:SER:N	2.39	0.53
1:A:979:PHE:O	1:A:983:GLY:N	2.42	0.53
1:A:1343:LEU:O	1:A:1347:SER:OG	2.18	0.53
1:A:1053:ILE:HG21	1:A:1095:LYS:HG2	1.90	0.53
1:B:1551:ALA:O	1:B:1555:ASP:N	2.42	0.53
3:Y:1076:LEU:HD12	3:Y:1083:LEU:HB2	1.91	0.53
1:B:722:ASN:O	1:B:726:VAL:HG12	2.09	0.53
1:B:1377:ASP:OD1	1:B:1406:LYS:NZ	2.42	0.53
2:D:60:ALA:HB2	2:D:91:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HG23	1:B:482:VAL:CG1	2.39	0.53
1:B:727:MET:SD	1:B:767:LEU:HD21	2.49	0.53
1:B:1970:GLN:OE1	1:B:1973:ILE:HD11	2.09	0.53
1:B:2339:ARG:NH2	1:B:2357:ASP:O	2.42	0.53
3:Y:558:LEU:HD23	3:Y:584:ILE:HD11	1.91	0.53
2:E:50:VAL:HG23	2:E:319:ALA:HB1	1.90	0.52
1:B:459:ILE:HG12	1:B:482:VAL:HG13	1.90	0.52
1:B:2035:SER:O	1:B:2039:PHE:N	2.42	0.52
1:A:1016:LEU:O	1:A:1020:VAL:HG23	2.09	0.52
1:A:2152:ARG:O	1:A:2177:SER:N	2.42	0.52
1:A:194:ILE:O	1:A:198:VAL:HG23	2.09	0.52
1:A:217:LEU:HB3	1:A:274:ILE:HD13	1.91	0.51
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.42	0.51
1:A:949:ALA:O	1:A:953:VAL:HG23	2.09	0.51
2:D:18:ALA:CB	2:D:45:VAL:HG21	2.39	0.51
2:D:58:ALA:HB1	2:D:100:MET:HE1	1.93	0.51
3:W:61:ALA:HB2	3:W:137:LEU:CD1	2.39	0.51
1:B:1422:LYS:O	1:B:1424:GLN:NE2	2.44	0.51
1:B:490:ALA:HB2	1:B:501:ILE:HD12	1.92	0.51
3:W:378:MET:CE	3:W:435:ILE:HD11	2.41	0.51
1:A:2320:TYR:CZ	1:A:2324:LEU:HD11	2.45	0.51
1:A:2117:GLN:OE1	3:W:94:GLY:N	2.40	0.51
1:A:971:VAL:HA	1:A:1306:LEU:HD11	1.92	0.50
1:B:1998:MET:O	1:B:2002:SER:OG	2.29	0.50
3:W:388:ILE:O	3:W:391:SER:OG	2.26	0.50
3:Y:554:LEU:HD21	3:Y:591:ALA:HB2	1.92	0.50
1:B:2297:ASP:OD1	1:B:2385:ASN:ND2	2.44	0.50
1:A:191:PHE:CE2	1:A:267:ILE:HD11	2.47	0.50
2:D:174:THR:HG21	2:D:222:TYR:CE1	2.47	0.50
2:E:15:LEU:HD13	2:E:286:VAL:HG21	1.94	0.49
1:A:1194:MET:HB2	1:B:665:THR:HG22	1.94	0.49
1:A:2059:GLU:OE2	1:A:2082:GLN:NE2	2.45	0.49
2:E:113:ASP:OD2	2:E:115:ARG:NH1	2.45	0.49
1:A:2087:LYS:O	1:A:2091:SER:OG	2.09	0.49
2:D:143:LEU:HD22	2:D:155:TRP:CZ2	2.47	0.49
1:A:2187:LYS:NZ	1:A:2188:GLY:O	2.41	0.49
1:A:1548:ALA:O	1:A:1550:LEU:N	2.45	0.49
2:D:143:LEU:HD22	2:D:155:TRP:CE2	2.48	0.49
3:Y:258:LEU:HD23	3:Y:280:MET:HE1	1.94	0.49
3:Y:573:LEU:O	3:Y:577:VAL:HG23	2.13	0.49
1:A:702:ASP:OD1	1:A:703:GLN:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:646:MET:HE1	3:Y:810:GLN:HB3	1.95	0.49
1:A:2422:VAL:HG12	1:A:2497:ALA:HB1	1.94	0.48
1:B:459:ILE:HG21	1:B:486:ILE:CD1	2.43	0.48
3:Y:198:ASN:ND2	3:Y:248:ALA:O	2.46	0.48
1:A:1045:ASN:HB3	1:A:1048:ILE:HG22	1.95	0.48
3:Y:578:ALA:HB3	3:Y:618:ALA:HB1	1.94	0.48
2:E:246:ILE:HD12	2:E:256:THR:HG23	1.95	0.48
1:A:1157:HIS:ND1	1:B:664:ILE:O	2.43	0.48
1:A:2191:ASP:OD2	1:A:2430:ARG:NH1	2.47	0.48
3:W:414:THR:O	3:W:418:VAL:HG23	2.13	0.48
1:A:1971:ALA:N	1:A:2144:TYR:OH	2.46	0.48
2:D:222:TYR:O	2:D:240:ALA:N	2.45	0.48
1:B:1140:ASP:OD1	1:B:1176:THR:OG1	2.21	0.48
2:E:58:ALA:HB2	2:E:67:MET:HE1	1.94	0.48
3:Y:330:ARG:NH2	3:Y:469:SER:O	2.46	0.48
1:B:1537:PRO:O	1:B:1540:THR:HG22	2.14	0.48
2:D:79:ILE:HG21	2:D:81:TYR:CE1	2.49	0.47
3:W:432:GLN:HG3	3:W:435:ILE:HD12	1.96	0.47
1:B:441:SER:OG	1:B:488:MET:O	2.20	0.47
1:A:195:PHE:CZ	1:A:267:ILE:HD12	2.48	0.47
1:B:1552:LEU:HD12	1:B:1599:LEU:HD22	1.96	0.47
3:Y:276:ARG:HG2	3:Y:280:MET:HE2	1.97	0.47
2:E:248:ARG:O	2:E:252:PHE:N	2.45	0.47
3:W:84:LEU:HD13	3:W:87:TRP:HA	1.95	0.47
3:W:126:THR:O	3:W:175:ILE:HD13	2.15	0.47
3:Y:667:LEU:HD23	3:Y:670:LEU:HD12	1.96	0.47
2:D:246:ILE:HD11	2:D:285:ILE:HD13	1.96	0.47
1:A:1020:VAL:HG22	1:A:1027:ILE:CD1	2.44	0.47
2:D:25:ARG:NE	2:D:310:GLY:O	2.48	0.47
1:B:2338:ASP:OD2	1:B:2340:HIS:NE2	2.48	0.47
3:Y:18:GLU:N	3:Y:20:ASP:OD1	2.48	0.47
2:E:258:LEU:HD11	2:E:285:ILE:HG21	1.97	0.47
3:Y:244:ALA:HB3	3:Y:365:VAL:HB	1.97	0.47
2:D:145:VAL:HG21	2:D:155:TRP:CZ3	2.49	0.46
1:B:2422:VAL:O	1:B:2428:ASN:ND2	2.46	0.46
1:B:455:VAL:HG12	1:B:459:ILE:HD12	1.98	0.46
2:D:25:ARG:HG2	2:D:37:THR:HG22	1.98	0.46
1:B:1530:GLU:OE2	1:B:1554:GLN:NE2	2.44	0.46
1:B:2320:TYR:CZ	1:B:2324:LEU:HD11	2.50	0.46
3:Y:671:VAL:HG11	3:Y:837:ILE:HD11	1.97	0.46
1:A:1871:GLU:O	1:A:1874:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:PRO:O	1:A:1132:ARG:NH2	2.48	0.46
1:A:630:LEU:HD11	1:A:655:VAL:HG11	1.97	0.46
1:A:1660:CYS:SG	1:A:1661:GLY:N	2.89	0.46
1:A:2363:GLU:OE1	1:A:2507:LYS:NZ	2.48	0.46
1:B:1143:THR:O	1:B:1183:GLN:NE2	2.49	0.46
1:B:518:THR:HG21	1:B:588:THR:HG21	1.98	0.46
1:B:586:LEU:O	1:B:625:THR:HG21	2.16	0.45
1:B:1004:CYS:O	1:B:1009:ARG:NH2	2.49	0.45
3:Y:616:ARG:O	3:Y:620:VAL:HG23	2.16	0.45
1:B:631:THR:HG23	1:B:644:VAL:HG11	1.98	0.45
1:A:1175:ASP:OD1	1:A:1206:HIS:NE2	2.49	0.45
3:Y:1040:VAL:HG21	3:Y:1325:ILE:CD1	2.45	0.45
1:A:740:GLU:O	1:A:744:SER:OG	2.19	0.45
1:B:2333:ILE:HG13	1:B:2407:LEU:HD13	1.99	0.45
1:B:2347:ASP:OD1	1:B:2348:ARG:N	2.49	0.45
3:Y:669:HIS:O	3:Y:672:VAL:HG12	2.16	0.45
2:D:43:SER:OG	2:D:44:GLN:N	2.49	0.45
2:E:69:ASP:OD1	2:E:70:LEU:N	2.50	0.45
3:Y:592:ARG:NE	3:Y:626:PHE:O	2.43	0.45
1:A:265:LEU:HD12	1:A:395:LEU:HD11	1.98	0.45
2:D:245:LYS:NZ	2:D:257:GLU:OE1	2.49	0.45
3:Y:180:TYR:O	3:Y:213:ARG:NH2	2.50	0.45
3:Y:668:SER:HA	3:Y:671:VAL:HG22	1.99	0.45
3:W:110:TYR:O	3:W:119:TYR:OH	2.34	0.45
1:B:486:ILE:HD13	1:B:489:LEU:HD12	1.98	0.45
1:A:1946:ILE:HD12	1:A:1961:LEU:HD12	1.99	0.45
1:B:1056:ILE:O	1:B:1060:VAL:HG23	2.16	0.45
3:Y:524:ASP:OD1	3:Y:526:TYR:N	2.50	0.45
1:A:1690:PRO:HG2	1:A:1692:VAL:HG12	1.99	0.45
1:B:1159:ILE:HG21	1:B:1177:LEU:HD21	1.99	0.45
2:E:69:ASP:HB2	2:E:78:ILE:HD11	1.98	0.45
3:Y:1170:THR:OG1	3:Y:1171:SER:N	2.49	0.45
1:A:1932:ILE:HD11	1:A:1964:ILE:CG1	2.46	0.44
3:W:415:ALA:HB1	1:B:725:PHE:CZ	2.52	0.44
1:B:719:SER:HA	1:B:726:VAL:HG11	1.97	0.44
3:Y:1215:VAL:N	3:Y:1230:VAL:O	2.50	0.44
1:A:281:ARG:NH1	1:A:285:GLU:OE1	2.49	0.44
3:Y:194:TYR:HB2	3:Y:199:ALA:HB1	1.99	0.44
1:B:217:LEU:HG	1:B:274:ILE:HD13	1.99	0.44
3:W:412:GLN:NE2	1:B:724:ALA:HB1	2.32	0.44
1:B:516:ALA:O	1:B:520:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:LEU:HD13	2:D:210:LEU:CD2	2.48	0.44
3:W:435:ILE:O	3:W:439:VAL:HG23	2.17	0.44
1:B:393:LEU:HD13	1:B:433:ALA:O	2.17	0.44
1:A:2044:VAL:HG11	1:A:2088:TYR:CE2	2.53	0.44
2:D:242:GLN:OE1	2:D:269:SER:N	2.47	0.44
1:A:2045:LYS:NZ	1:A:2049:GLU:OE2	2.50	0.44
1:B:590:GLY:HA2	1:B:629:LEU:HD21	1.99	0.44
1:A:1341:ILE:HG23	1:A:1357:LEU:HD22	2.00	0.43
2:D:103:GLY:HA2	2:D:131:ILE:HD12	2.00	0.43
3:Y:1021:ARG:NE	3:Y:1022:ASN:O	2.45	0.43
1:B:1653:TRP:CB	1:B:1676:LEU:HD11	2.48	0.43
3:Y:51:MET:O	3:Y:54:ARG:NE	2.45	0.43
1:A:2165:SER:OG	1:A:2167:GLN:O	2.30	0.43
1:B:1653:TRP:HB2	1:B:1676:LEU:HD11	1.99	0.43
1:A:1136:LEU:O	1:A:1176:THR:OG1	2.24	0.43
1:A:1295:SER:O	1:A:1301:ARG:NH1	2.44	0.43
1:A:1798:PHE:CE2	1:A:1802:LEU:HD11	2.54	0.43
3:Y:604:LEU:HD21	3:Y:622:ALA:CB	2.48	0.43
1:A:724:ALA:HB2	3:Y:411:GLU:HG3	2.00	0.43
1:A:757:LEU:O	1:A:761:VAL:HG23	2.19	0.43
1:B:452:LEU:HD22	1:B:456:LEU:HG	2.01	0.43
1:B:200:ASP:O	1:B:206:ARG:NE	2.52	0.43
1:B:590:GLY:HA3	1:B:625:THR:HG23	2.01	0.43
1:B:686:HIS:O	1:B:692:ASN:ND2	2.47	0.43
1:B:1940:PRO:O	1:B:1944:ALA:N	2.48	0.43
2:E:111:ILE:O	2:E:122:GLN:N	2.52	0.43
1:A:2280:LEU:O	1:A:2284:VAL:HG23	2.19	0.43
3:W:415:ALA:HB2	1:B:724:ALA:HB3	2.00	0.43
3:Y:527:MET:O	3:Y:532:ARG:NH1	2.51	0.43
1:A:958:ILE:HD12	1:A:1313:MET:HE3	2.01	0.42
1:B:997:PHE:CE2	1:B:1001:ILE:HD11	2.54	0.42
1:A:465:PRO:HA	1:A:466:LYS:HB2	2.01	0.42
1:A:1132:ARG:HB3	1:A:1169:LEU:HD11	2.01	0.42
3:Y:513:ASN:O	3:Y:515:HIS:N	2.52	0.42
1:A:1555:ASP:OD1	1:A:1606:LYS:NZ	2.30	0.42
1:B:163:GLY:O	1:B:166:HIS:NE2	2.51	0.42
1:A:1404:PHE:CE2	1:A:2389:VAL:HG13	2.54	0.42
1:A:1812:ASP:OD1	1:A:1867:LYS:N	2.53	0.42
1:B:1548:ALA:O	1:B:1551:ALA:N	2.52	0.42
3:Y:424:VAL:HG12	3:Y:426:ASN:H	1.84	0.42
1:A:138:ASP:OD1	1:A:139:THR:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:O	1:A:287:GLU:N	2.48	0.42
2:D:50:VAL:HG13	2:D:70:LEU:HD22	2.01	0.42
3:Y:126:THR:HA	3:Y:166:VAL:HG13	2.01	0.42
1:B:1181:VAL:HG13	1:B:1188:TYR:CE2	2.55	0.42
3:Y:365:VAL:HG13	3:Y:369:ARG:NH2	2.35	0.42
2:D:109:ALA:HB2	2:D:131:ILE:HD11	2.02	0.42
1:B:702:ASP:OD1	1:B:703:GLN:N	2.50	0.42
2:D:58:ALA:HB2	2:D:93:PHE:CZ	2.55	0.42
1:B:2411:LYS:HG3	1:B:2508:LEU:HD13	2.01	0.42
3:Y:1202:CYS:O	3:Y:1204:VAL:HG13	2.19	0.42
2:E:143:LEU:HD23	2:E:155:TRP:NE1	2.35	0.41
3:Y:1180:LEU:HD11	3:Y:1192:VAL:HG12	2.02	0.41
1:A:628:ARG:O	1:A:631:THR:HG23	2.21	0.41
1:A:1633:TRP:CH2	1:A:1637:LEU:HD22	2.55	0.41
3:W:147:LEU:HD22	3:W:342:LEU:HD21	2.01	0.41
1:B:511:VAL:HG13	1:B:517:LEU:HD22	2.02	0.41
1:A:1101:GLN:HG3	1:A:1138:THR:HG23	2.02	0.41
3:Y:1279:ILE:HD12	3:Y:1290:ILE:HD13	2.01	0.41
1:B:1923:LEU:O	1:B:1927:VAL:HG23	2.21	0.41
1:B:2369:GLU:OE1	1:B:2369:GLU:N	2.46	0.41
2:D:99:TRP:CE3	2:D:111:ILE:HG21	2.55	0.41
3:W:436:VAL:HG11	3:W:453:LEU:HD21	2.01	0.41
2:E:50:VAL:HG21	2:E:320:PHE:O	2.21	0.41
2:D:58:ALA:HB2	2:D:93:PHE:CE2	2.56	0.41
1:A:195:PHE:CE2	1:A:267:ILE:HD12	2.56	0.41
1:A:1181:VAL:HG22	1:A:1188:TYR:CZ	2.55	0.41
1:A:1265:LEU:HD13	1:A:1336:GLU:OE1	2.21	0.41
1:A:1670:HIS:O	1:A:1674:VAL:HG23	2.21	0.41
1:A:176:ALA:O	1:A:219:LEU:HD11	2.21	0.41
1:A:1874:SER:O	1:A:1878:LEU:HD12	2.21	0.41
1:A:2015:GLU:O	1:A:2019:VAL:HG23	2.21	0.41
2:D:65:ILE:HD11	2:D:88:ILE:CG2	2.51	0.41
1:A:2353:ILE:C	1:A:2354:LEU:HD12	2.45	0.41
2:D:161:HIS:ND1	2:D:204:GLY:O	2.47	0.41
2:D:321:ASN:OD1	2:D:322:ASP:N	2.52	0.41
1:B:821:PHE:CD2	1:B:844:LEU:HD22	2.56	0.40
1:B:2210:ALA:O	1:B:2216:LEU:HD21	2.20	0.40
3:Y:388:ILE:O	3:Y:391:SER:OG	2.33	0.40
3:Y:417:GLN:O	3:Y:421:THR:HG23	2.21	0.40
1:A:2422:VAL:CG1	1:A:2497:ALA:HB1	2.52	0.40
2:D:248:ARG:O	2:D:252:PHE:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1528:SER:OG	1:B:1529:MET:N	2.54	0.40
2:D:30:HIS:O	2:D:306:ARG:NE	2.54	0.40
3:W:88:ILE:HD13	3:W:101:THR:HB	2.03	0.40
1:B:433:ALA:CB	1:B:481:THR:HG21	2.50	0.40
1:A:706:GLU:OE1	1:A:706:GLU:N	2.53	0.40
1:A:956:MET:SD	1:A:993:VAL:HG22	2.61	0.40
1:A:1409:THR:O	1:A:1413:LEU:HD23	2.21	0.40
1:B:1540:THR:HG23	1:B:1543:GLY:H	1.87	0.40
2:E:285:ILE:HG13	2:E:299:VAL:HG22	2.03	0.40
3:Y:497:LYS:NZ	3:Y:967:PHE:O	2.52	0.40
1:A:968:HIS:NE2	1:A:1012:LEU:HD21	2.37	0.40
1:A:2021:ILE:HG22	1:A:2026:MET:HG3	2.04	0.40
1:B:2428:ASN:O	1:B:2432:MET:N	2.49	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	1994/2549 (78%)	1927 (97%)	65 (3%)	2 (0%)	48	81
1	B	1994/2549 (78%)	1940 (97%)	52 (3%)	2 (0%)	48	81
2	D	315/326 (97%)	283 (90%)	32 (10%)	0	100	100
2	E	315/326 (97%)	296 (94%)	19 (6%)	0	100	100
3	W	424/1335 (32%)	403 (95%)	20 (5%)	1 (0%)	43	75
3	Y	1032/1335 (77%)	971 (94%)	59 (6%)	2 (0%)	43	75
4	X	6/118 (5%)	6 (100%)	0	0	100	100
4	Z	6/118 (5%)	6 (100%)	0	0	100	100
All	All	6086/8656 (70%)	5832 (96%)	247 (4%)	7 (0%)	49	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1311	ASN
1	B	1311	ASN
3	Y	634	THR
1	A	2337	GLY
3	W	156	PRO
1	B	116	PRO
3	Y	368	PRO

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	1789/2220 (81%)	1789 (100%)	0	100	100
1	B	1789/2220 (81%)	1789 (100%)	0	100	100
2	D	269/276 (98%)	269 (100%)	0	100	100
2	E	269/276 (98%)	269 (100%)	0	100	100
3	W	383/1163 (33%)	383 (100%)	0	100	100
3	Y	921/1163 (79%)	921 (100%)	0	100	100
4	X	8/102 (8%)	8 (100%)	0	100	100
4	Z	8/102 (8%)	8 (100%)	0	100	100
All	All	5436/7522 (72%)	5436 (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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	262	HIS
1	A	1553	HIS
1	A	1624	GLN
1	A	1627	GLN

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Mol	Chain	Res	Type
1	A	1727	GLN
1	A	2063	GLN
1	A	2540	GLN
3	W	173	GLN
3	W	380	GLN
3	W	412	GLN
1	B	188	GLN
1	B	527	GLN
1	B	530	GLN
1	B	1183	GLN
1	B	1424	GLN
1	B	1541	HIS
1	B	1627	GLN
1	B	1807	GLN
1	B	1808	ASN
1	B	2154	GLN
1	B	2194	GLN
2	E	39	GLN
3	Y	544	ASN
3	Y	565	GLN
3	Y	575	GLN
3	Y	673	GLN
3	Y	1133	GLN

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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ANP	A	3000	6	33,33,33	3.54	17 (51%)	45,52,52	2.62	15 (33%)
5	ANP	B	3000	6	33,33,33	3.53	18 (54%)	45,52,52	2.54	15 (33%)

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	ANP	A	3000	6	-	5/18/38/38	0/3/3/3
5	ANP	B	3000	6	-	5/18/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3000	ANP	C3'-C4'	-9.98	1.27	1.53
5	B	3000	ANP	C3'-C4'	-9.85	1.28	1.53
5	B	3000	ANP	C2'-C1'	-8.27	1.27	1.53
5	A	3000	ANP	C2'-C1'	-8.10	1.28	1.53
5	A	3000	ANP	PA-O3A	6.77	1.66	1.59
5	B	3000	ANP	PA-O3A	6.69	1.66	1.59
5	A	3000	ANP	O4'-C1'	5.89	1.55	1.42
5	B	3000	ANP	O4'-C1'	5.76	1.55	1.42
5	B	3000	ANP	O4'-C4'	4.82	1.55	1.45
5	A	3000	ANP	O4'-C4'	4.68	1.55	1.45
5	B	3000	ANP	C2'-C3'	4.65	1.66	1.53
5	A	3000	ANP	C2'-C3'	4.63	1.65	1.53
5	A	3000	ANP	C6-N6	4.29	1.45	1.34
5	B	3000	ANP	C6-N6	4.23	1.45	1.34
5	A	3000	ANP	PG-O1G	4.08	1.52	1.46
5	B	3000	ANP	PG-O1G	4.06	1.52	1.46
5	A	3000	ANP	PB-O3A	3.74	1.63	1.59
5	B	3000	ANP	PB-O3A	3.62	1.63	1.59
5	B	3000	ANP	PB-N3B	3.29	1.72	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3000	ANP	PB-N3B	3.27	1.71	1.63
5	B	3000	ANP	C5-C4	-2.97	1.33	1.39
5	A	3000	ANP	C5-C4	-2.84	1.34	1.39
5	A	3000	ANP	PB-O1B	2.79	1.50	1.46
5	B	3000	ANP	PB-O1B	2.75	1.50	1.46
5	B	3000	ANP	PG-N3B	2.32	1.69	1.63
5	A	3000	ANP	PG-N3B	2.29	1.69	1.63
5	B	3000	ANP	PB-O2B	-2.21	1.50	1.56
5	A	3000	ANP	PB-O2B	-2.16	1.51	1.56
5	B	3000	ANP	PG-O3G	-2.16	1.51	1.56
5	A	3000	ANP	PG-O3G	-2.13	1.51	1.56
5	A	3000	ANP	C5'-C4'	2.13	1.58	1.51
5	B	3000	ANP	C5'-C4'	2.11	1.57	1.51
5	B	3000	ANP	C8-N9	-2.04	1.34	1.37
5	B	3000	ANP	C5-N7	-2.04	1.35	1.39
5	A	3000	ANP	C8-N9	-2.04	1.34	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3000	ANP	N6-C6-N1	-6.64	103.59	118.38
5	B	3000	ANP	N6-C6-N1	-6.35	104.23	118.38
5	A	3000	ANP	C4-N9-C1'	-6.26	111.98	126.63
5	B	3000	ANP	C4-N9-C1'	-6.15	112.25	126.63
5	A	3000	ANP	C1'-N9-C8	5.78	139.93	127.09
5	A	3000	ANP	N3-C2-N1	-5.74	119.89	128.58
5	B	3000	ANP	C1'-N9-C8	5.64	139.61	127.09
5	B	3000	ANP	N3-C2-N1	-5.63	120.07	128.58
5	A	3000	ANP	C5-C6-N6	5.24	136.25	123.29
5	B	3000	ANP	C5-C4-N3	-4.99	119.84	126.72
5	B	3000	ANP	C5-C6-N6	4.89	135.39	123.29
5	A	3000	ANP	C5-C4-N3	-4.86	120.03	126.72
5	A	3000	ANP	N9-C8-N7	-4.22	107.95	113.94
5	B	3000	ANP	N9-C8-N7	-4.20	107.98	113.94
5	A	3000	ANP	C3'-C2'-C1'	3.50	108.08	101.46
5	A	3000	ANP	C2-N3-C4	3.39	120.12	111.83
5	B	3000	ANP	C2-N3-C4	3.39	120.10	111.83
5	B	3000	ANP	N3-C4-N9	3.10	132.44	127.17
5	A	3000	ANP	C5-N7-C8	2.94	108.07	103.45
5	A	3000	ANP	N3-C4-N9	2.84	132.00	127.17
5	B	3000	ANP	C5-N7-C8	2.84	107.91	103.45
5	B	3000	ANP	C2'-C3'-C4'	2.45	107.35	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3000	ANP	C3'-C2'-C1'	2.37	105.94	101.46
5	A	3000	ANP	C4-C5-N7	-2.33	107.92	110.58
5	B	3000	ANP	C4-N9-C8	2.29	108.14	105.74
5	A	3000	ANP	C2'-C3'-C4'	2.28	107.02	102.61
5	A	3000	ANP	C4-N9-C8	2.23	108.08	105.74
5	A	3000	ANP	C4'-O4'-C1'	-2.09	104.86	109.47
5	B	3000	ANP	C4'-O4'-C1'	-2.06	104.92	109.47
5	B	3000	ANP	C4-C5-N7	-2.04	108.25	110.58

There are no chirality outliers.

All (10) torsion outliers are listed below:

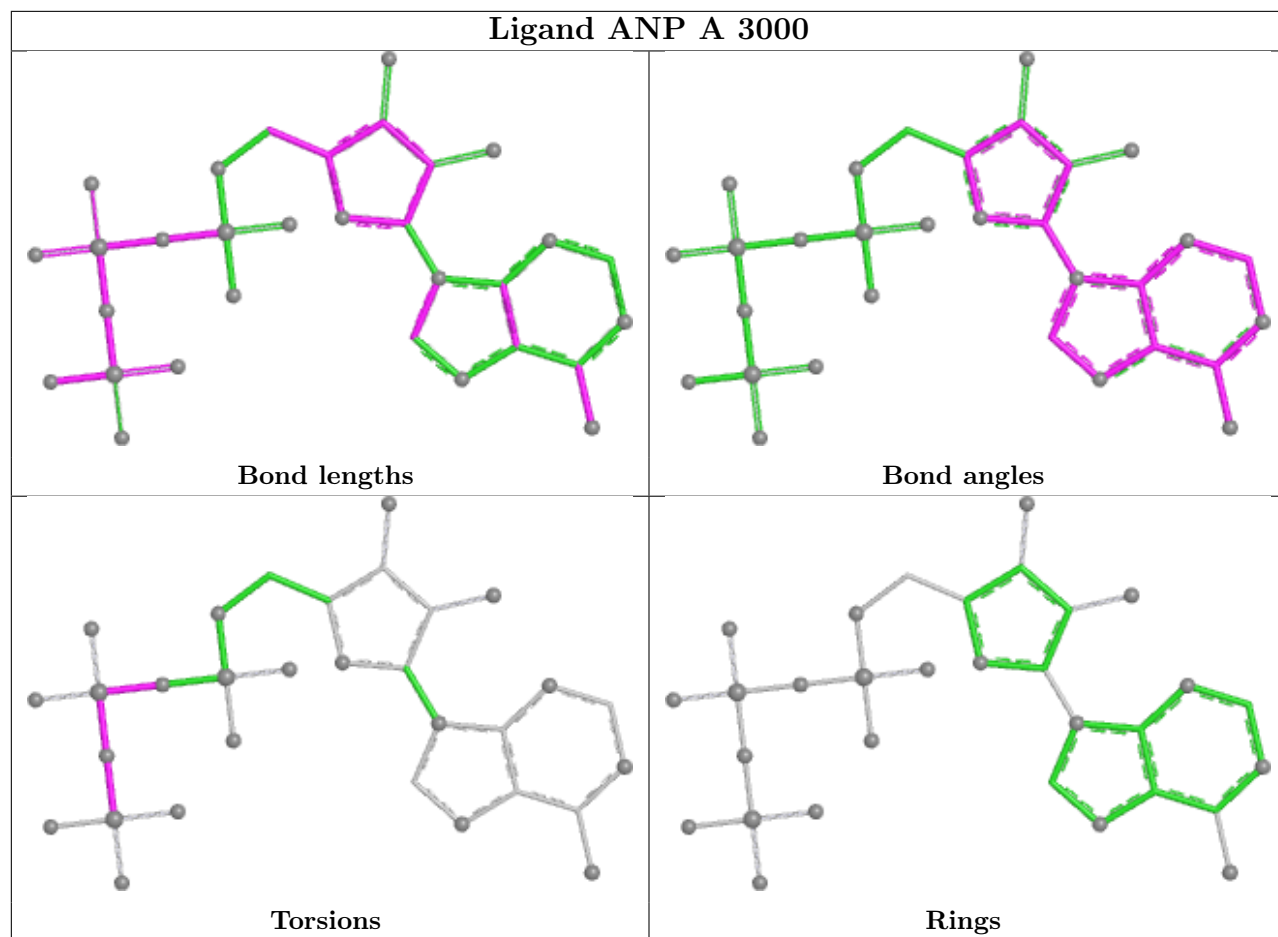
Mol	Chain	Res	Type	Atoms
5	A	3000	ANP	PB-N3B-PG-O1G
5	A	3000	ANP	PG-N3B-PB-O1B
5	A	3000	ANP	PG-N3B-PB-O3A
5	A	3000	ANP	PA-O3A-PB-O2B
5	B	3000	ANP	PB-N3B-PG-O1G
5	B	3000	ANP	PG-N3B-PB-O1B
5	B	3000	ANP	O4'-C4'-C5'-O5'
5	B	3000	ANP	C3'-C4'-C5'-O5'
5	B	3000	ANP	PB-O3A-PA-O5'
5	A	3000	ANP	PA-O3A-PB-O1B

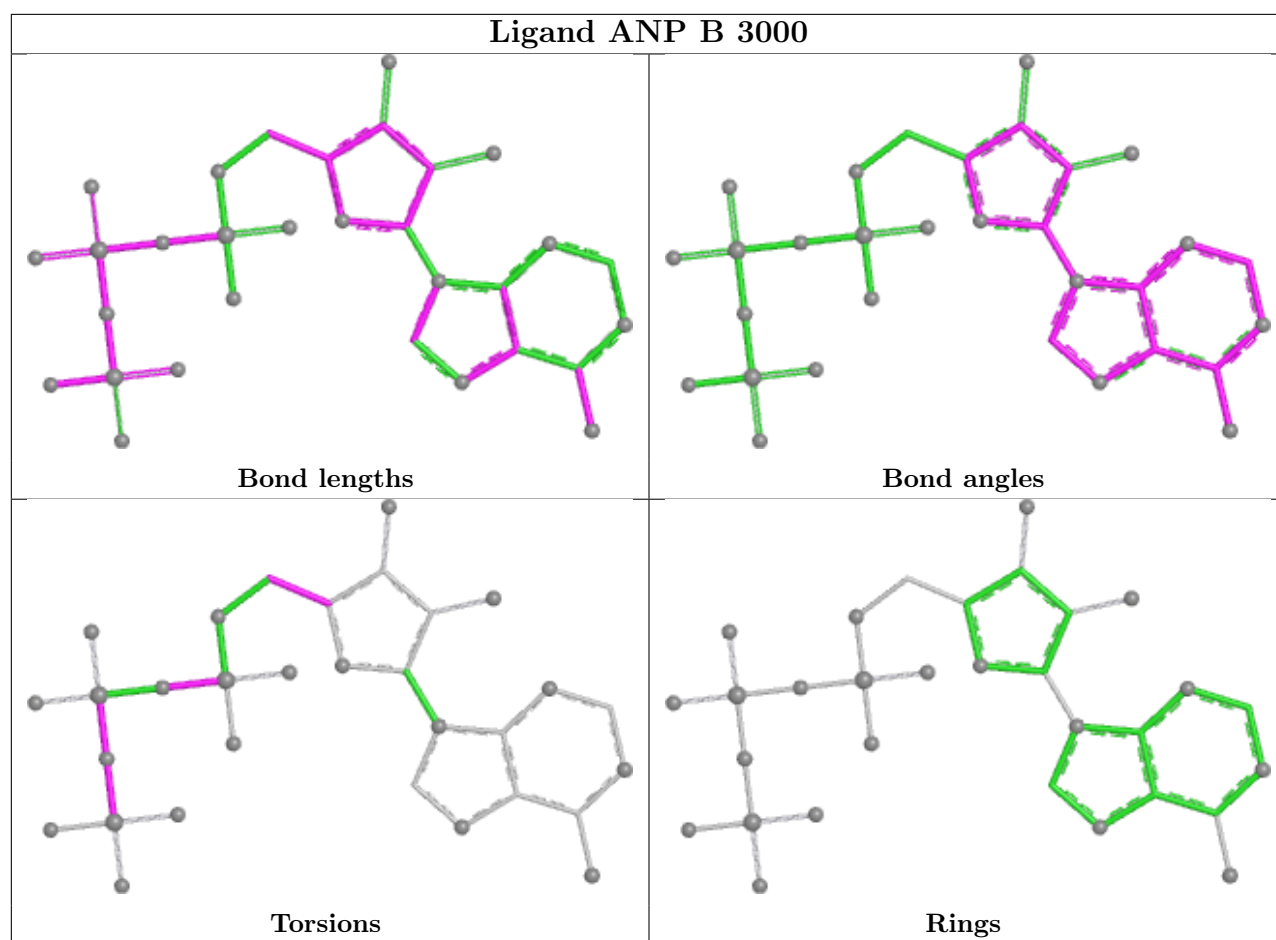
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3000	ANP	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.

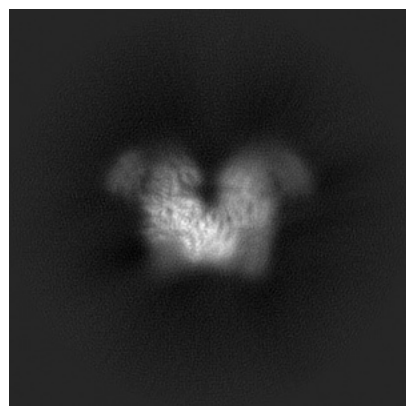
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19052. These allow visual inspection of the internal detail of the map and identification of artifacts.

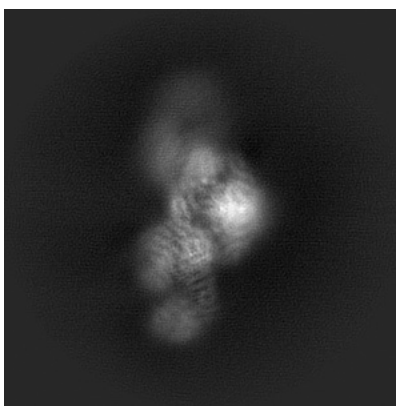
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

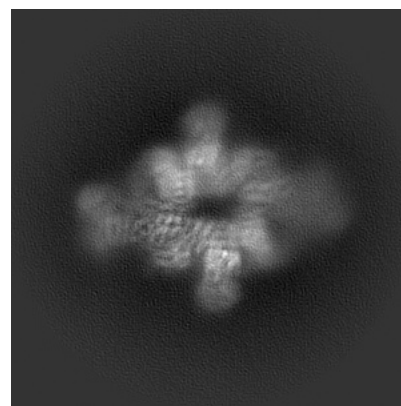
6.1.1 Primary map



X

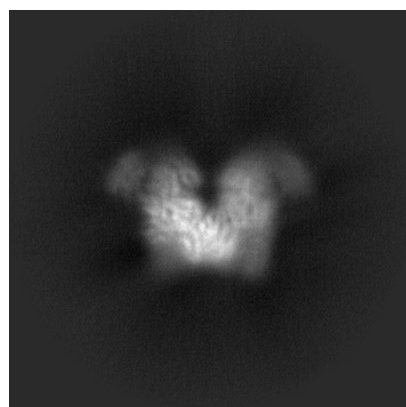


Y

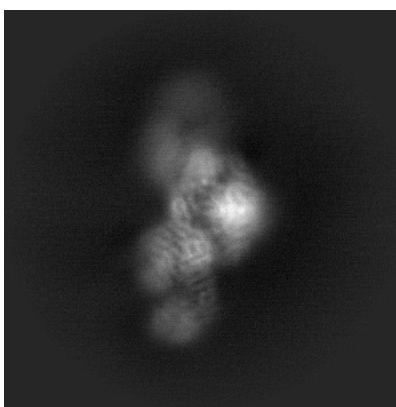


Z

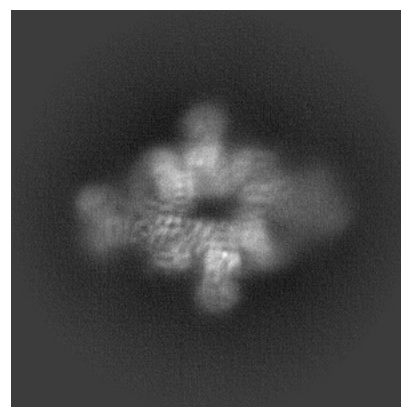
6.1.2 Raw map



X



Y

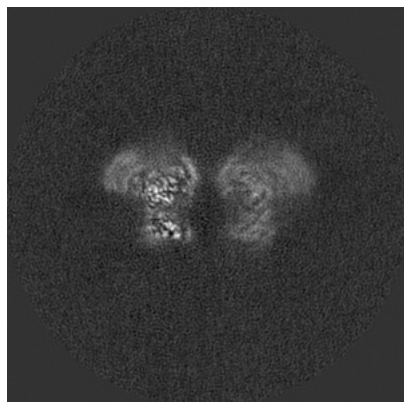


Z

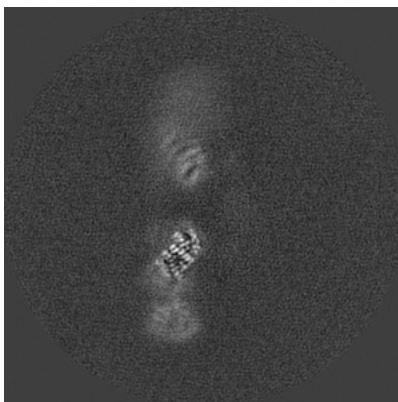
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

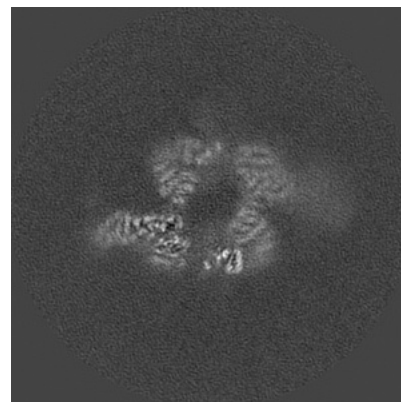
6.2.1 Primary map



X Index: 256



Y Index: 256

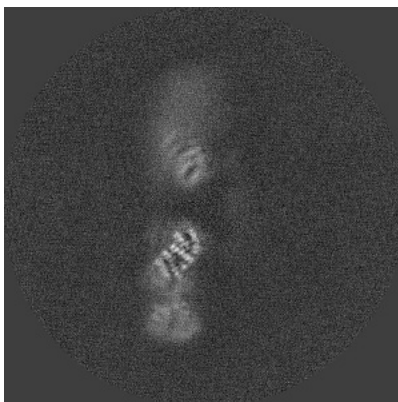


Z Index: 256

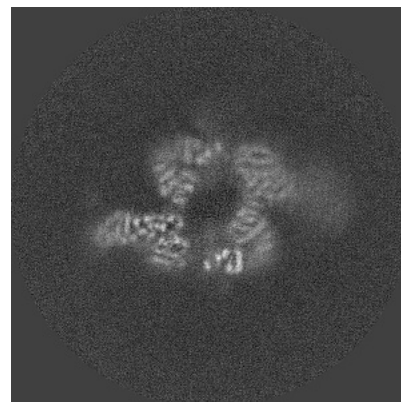
6.2.2 Raw map



X Index: 256



Y Index: 256

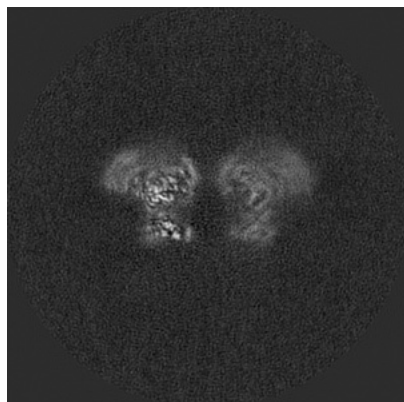


Z Index: 256

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

6.3 Largest variance slices [i](#)

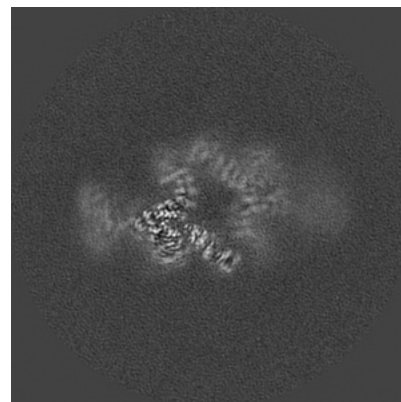
6.3.1 Primary map



X Index: 255

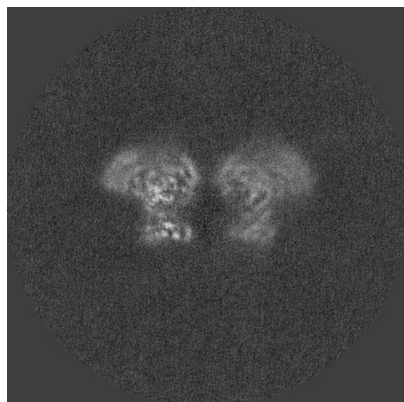


Y Index: 227

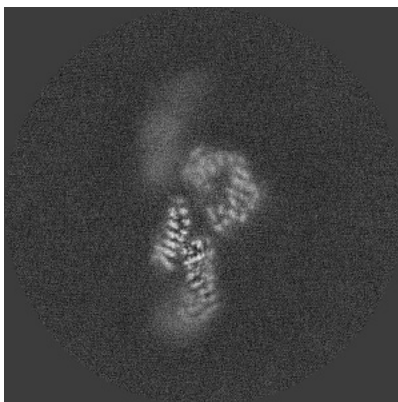


Z Index: 236

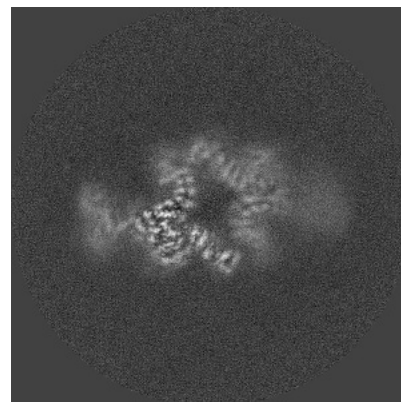
6.3.2 Raw map



X Index: 255



Y Index: 227

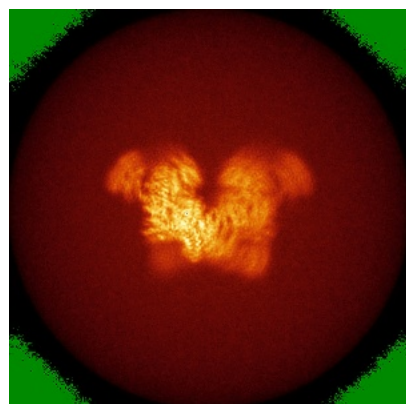


Z Index: 237

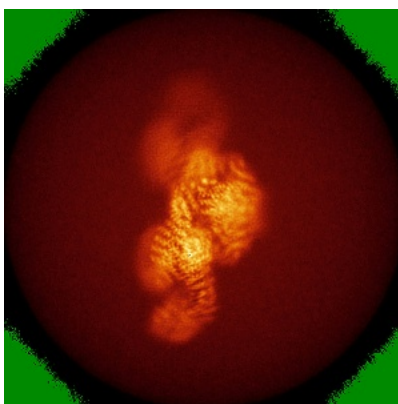
The images above show the largest variance slices of the map in three orthogonal directions.

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

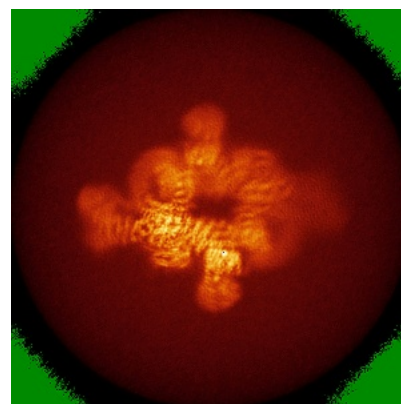
6.4.1 Primary map



X

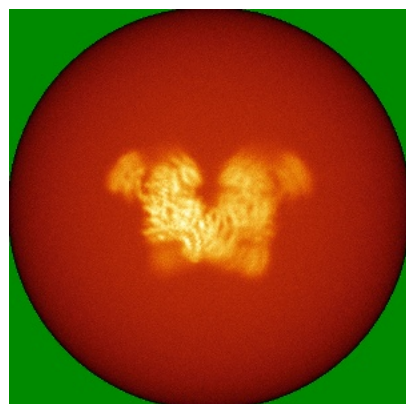


Y

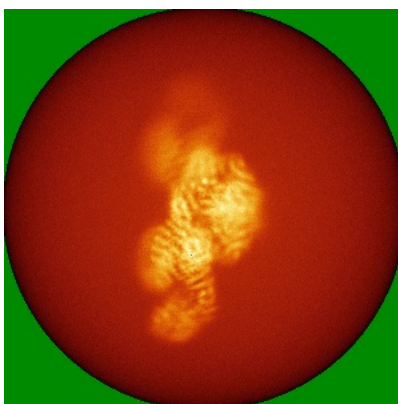


Z

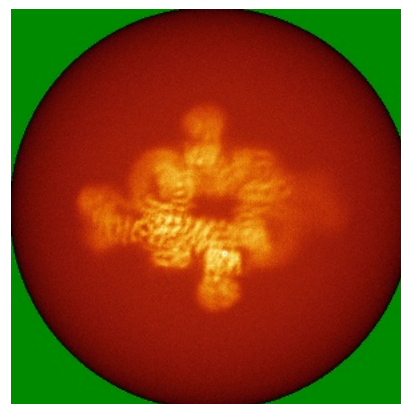
6.4.2 Raw map



X



Y

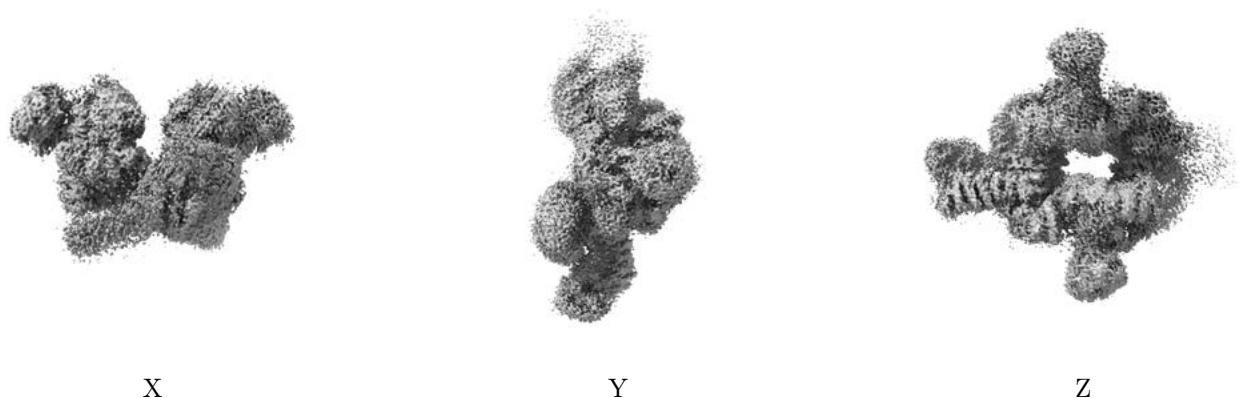


Z

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

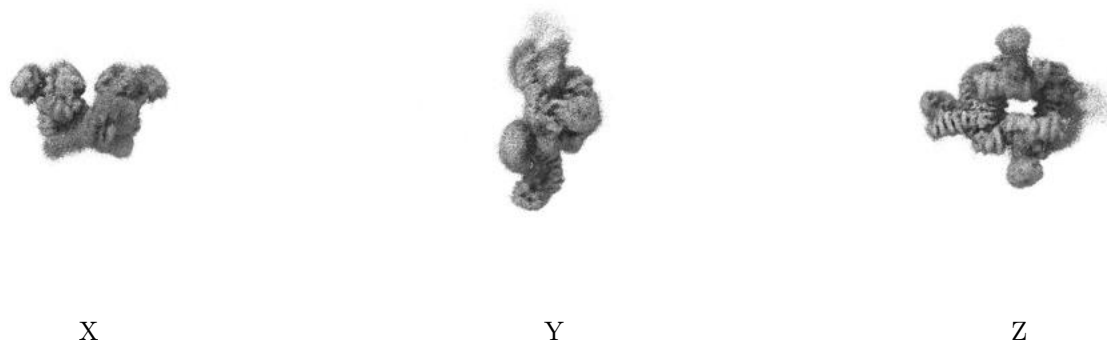
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

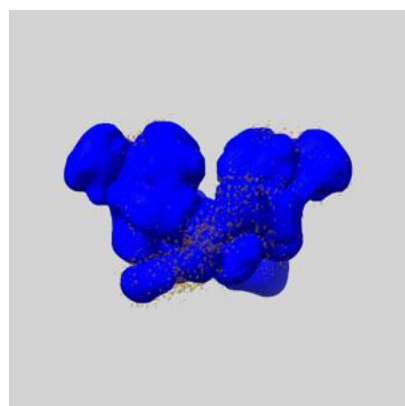
6.6 Mask visualisation [i](#)

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

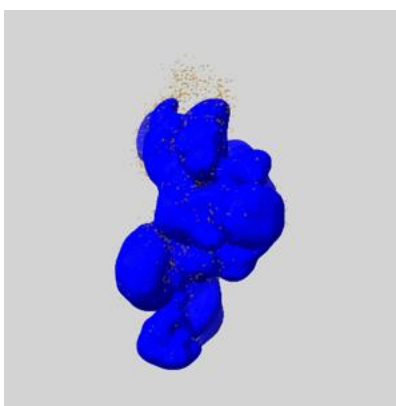
A mask typically either:

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

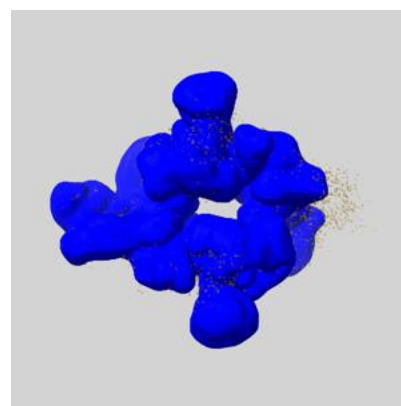
6.6.1 emd_19052_msk_1.map [i](#)



X



Y

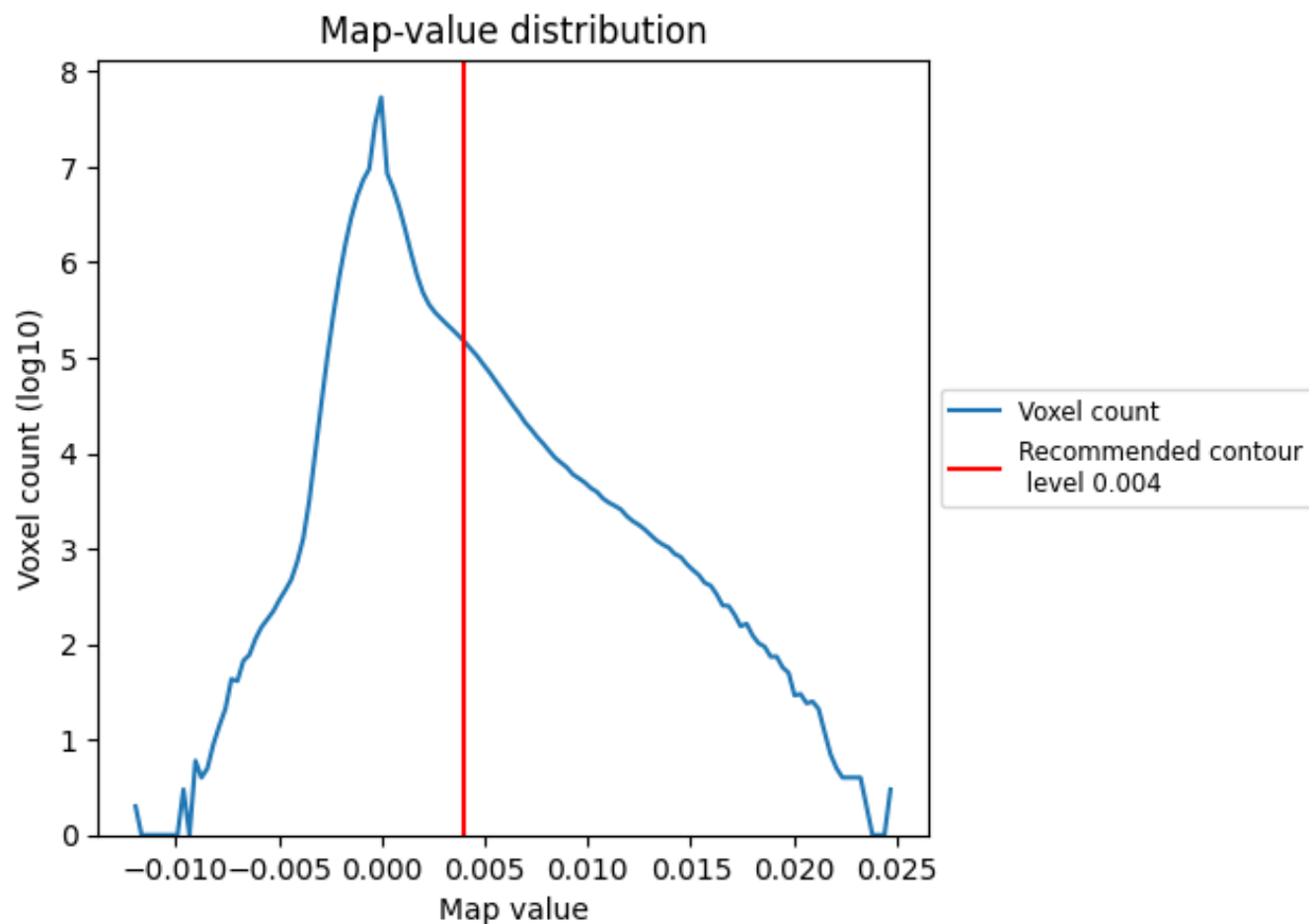


Z

7 Map analysis [i](#)

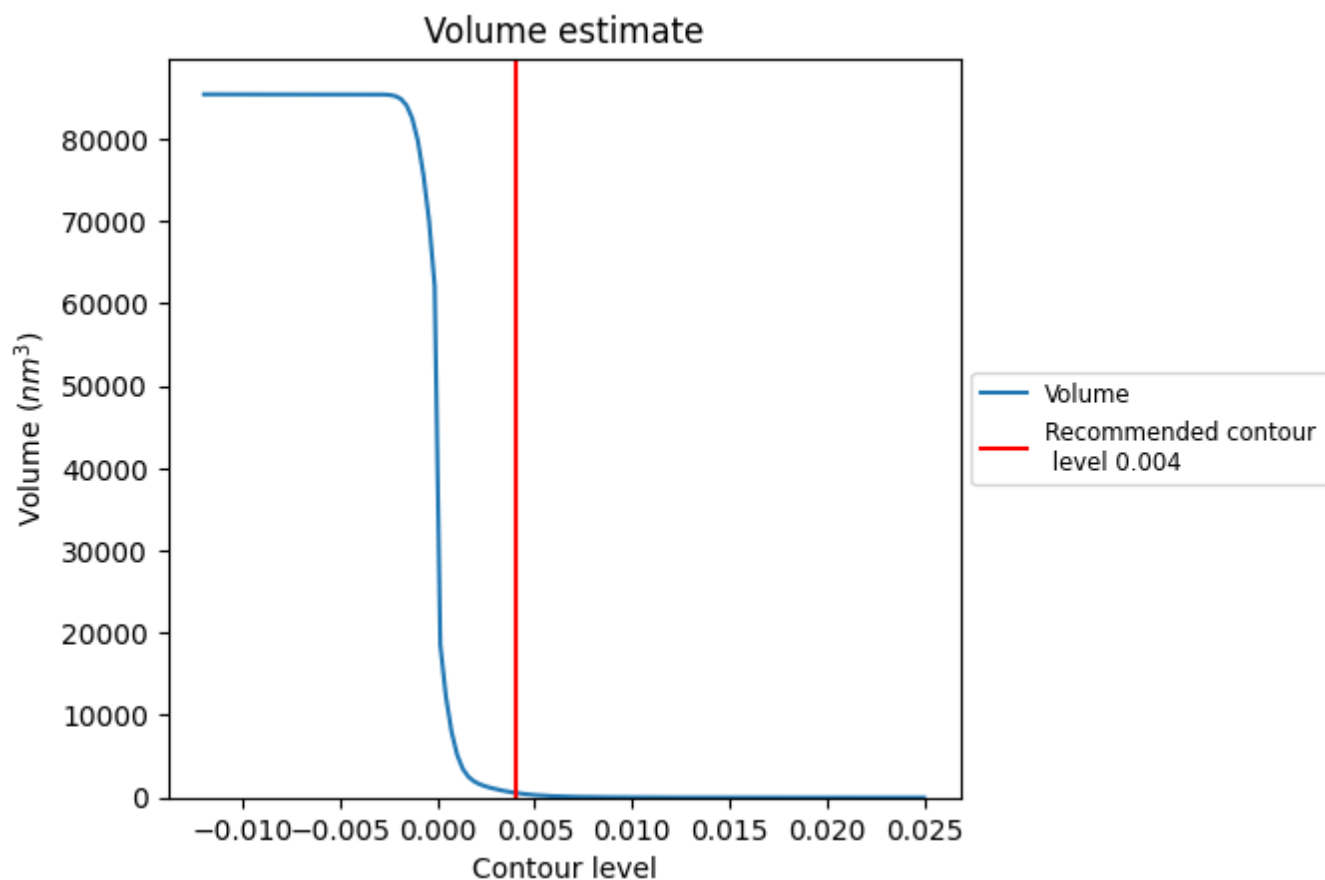
This section contains the results of statistical analysis of the map.

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.

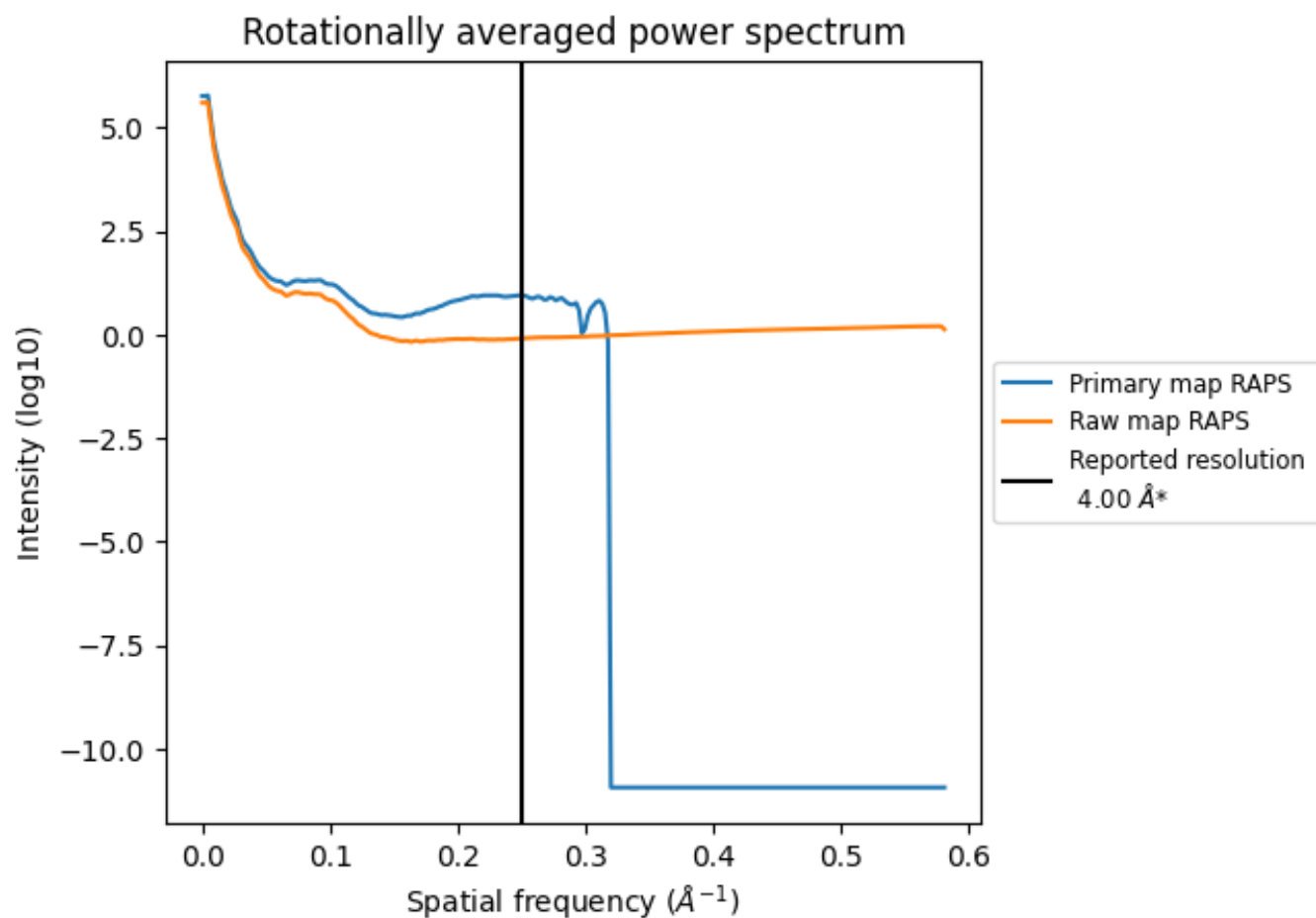
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 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 ⓘ

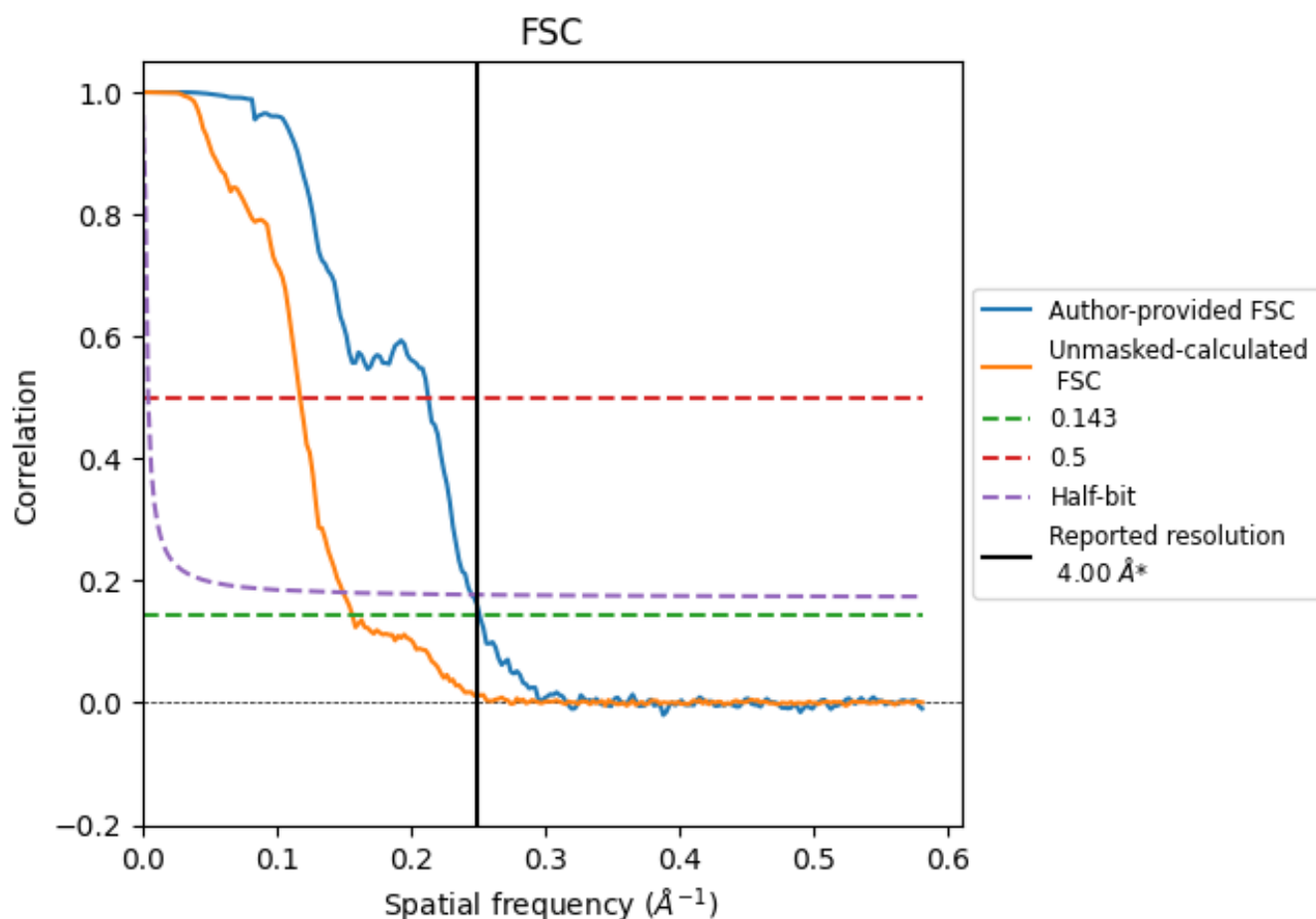


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

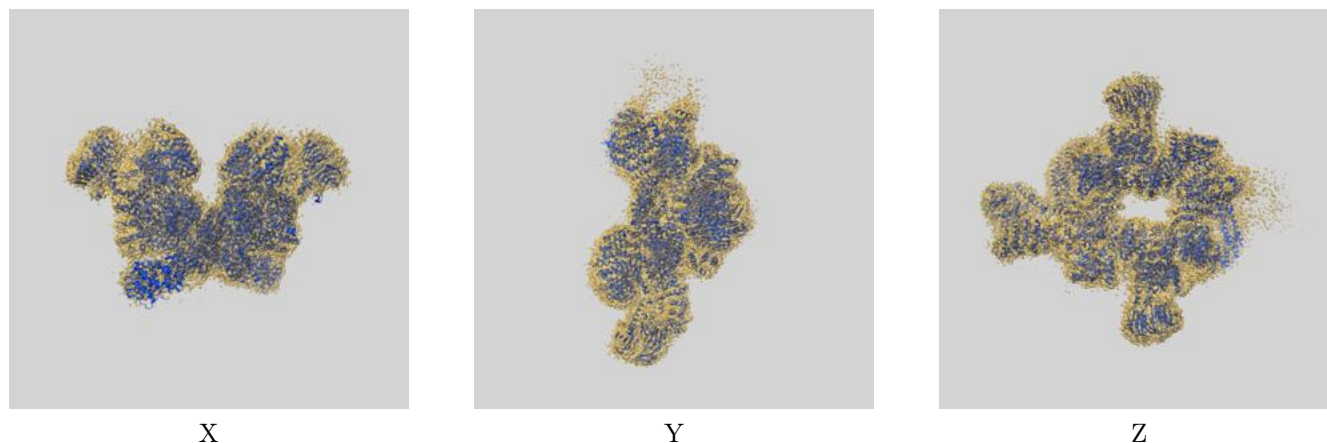
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.69	4.07
Unmasked-calculated*	6.38	8.50	6.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.38 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

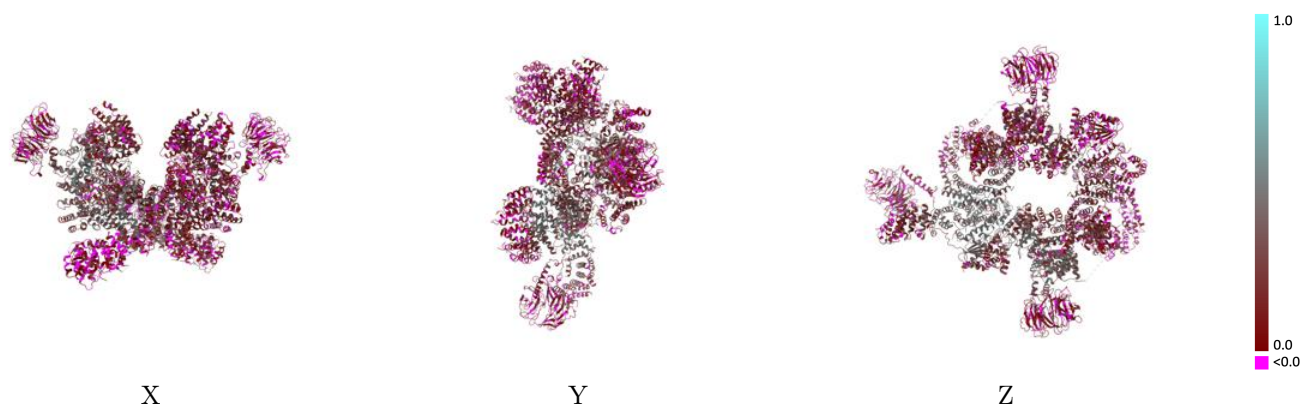
This section contains information regarding the fit between EMDB map EMD-19052 and PDB model 8RCH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



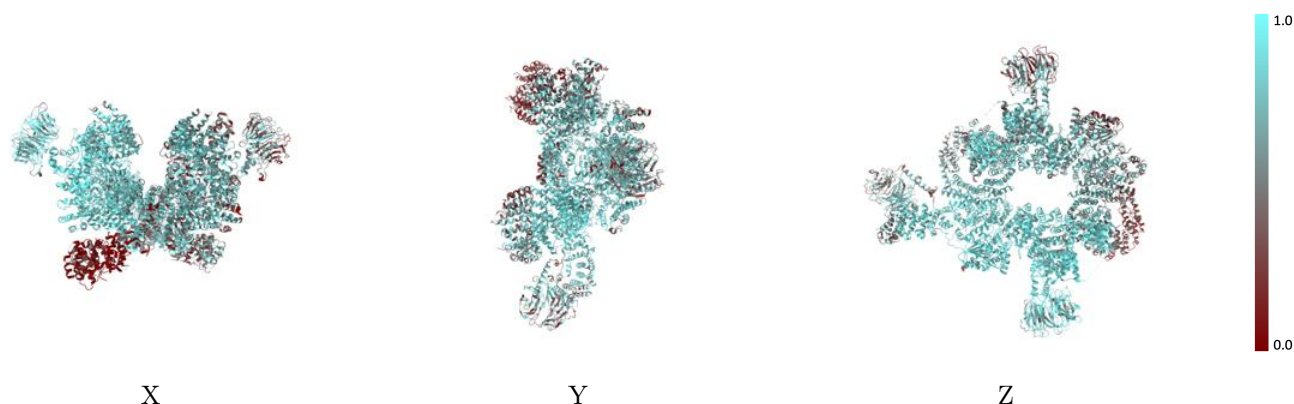
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



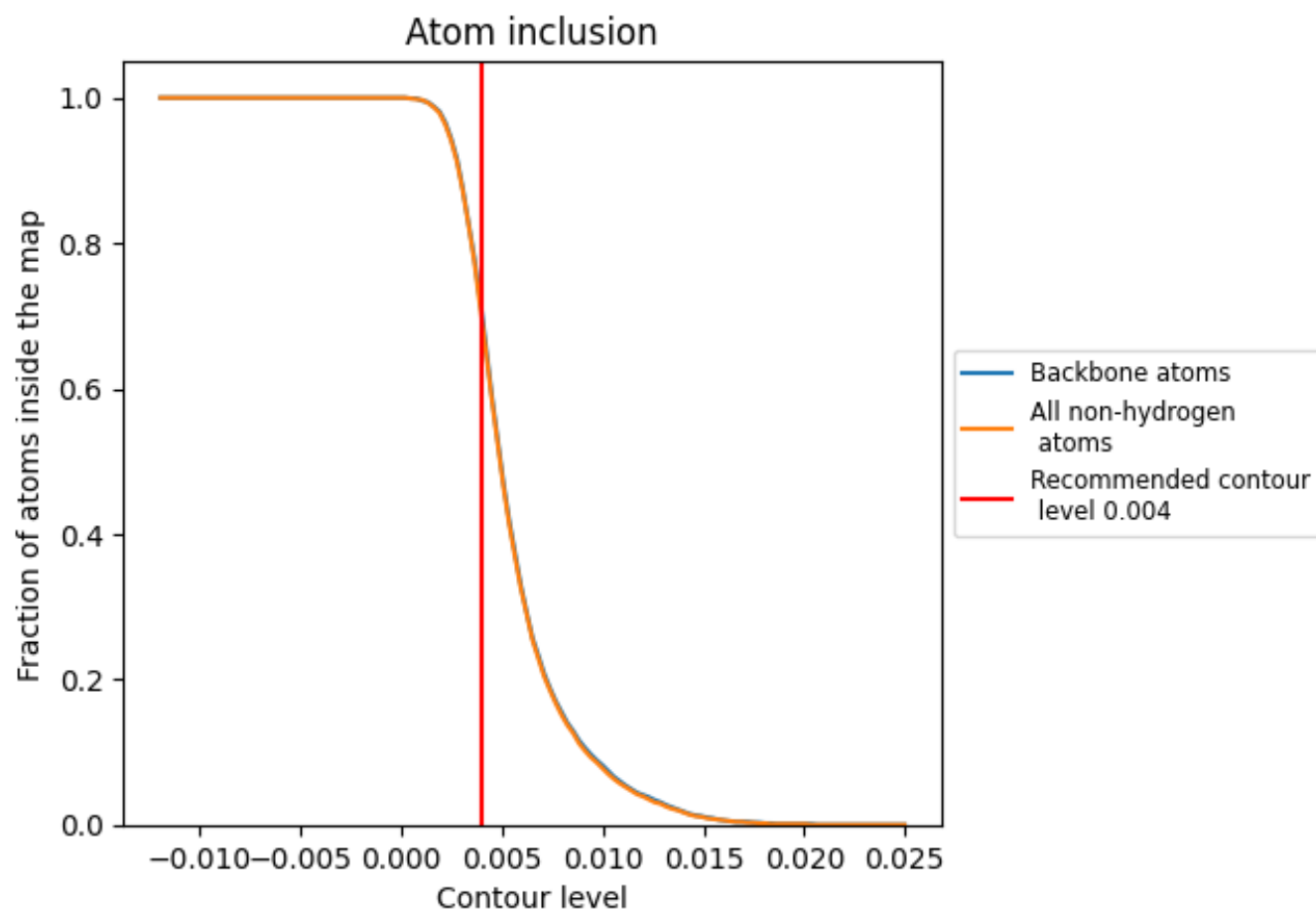
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.2010
A	0.7150	0.1850
B	0.7130	0.2430
D	0.4710	0.0680
E	0.7930	0.1230
W	0.5950	0.1270
X	0.8840	0.4040
Y	0.7380	0.2410
Z	0.3040	0.1530

1.0

0.0

<0.0