WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 08:25 AM EST

PDB ID	:	6BCX
EMDB ID	:	EMD-7087
Title	:	mTORC1 structure refined to 3.0 angstroms
Authors	:	Pavletich, N.P.; Yang, H.
Deposited on	:	2017-10-20
Resolution	:	3.23 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 (i) 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 (i)) were used in the production of this report:

|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.23 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	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		0.6%
Sidechain outliers		3.2%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
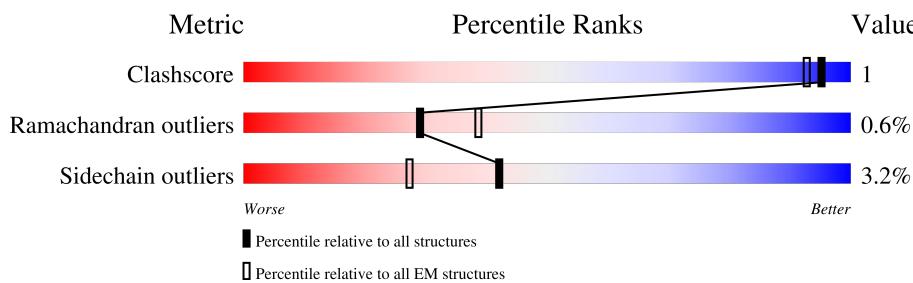
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	20% / 81% / 5% / 15%
1	B	2549	20% / 81% / 5% / 15%
2	D	326	42% / 90% / 7% / •
2	E	326	39% / 90% / 7% / •
3	W	1343	39% / 73% / 5% / 22%
3	Y	1343	39% / 74% / • / 22%
4	X	122	• / 6% / • / 93%
4	Z	122	• / 6% / • / 93%
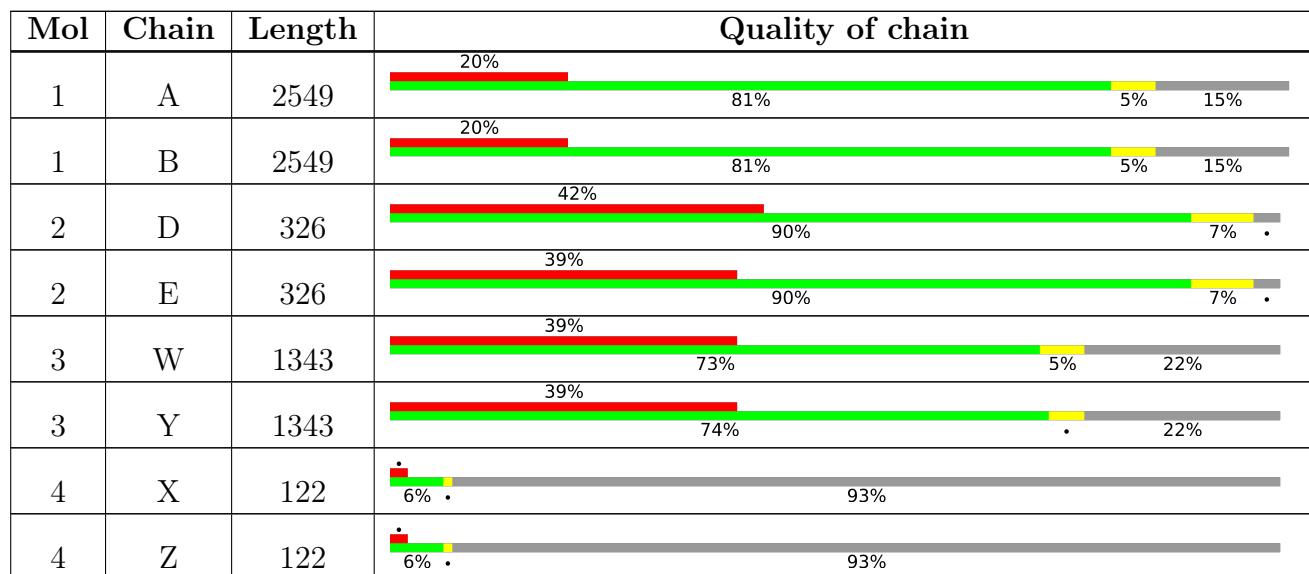
2   Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 113610 atoms, of which 57030 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	2178	Total 35034	C 11082	H 17686	N 3038	O 3117	S 111	0	0
1	B	2178	Total 35034	C 11082	H 17686	N 3038	O 3117	S 111	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total 4809	C 1526	H 2353	N 436	O 476	S 18	0	0
2	E	317	Total 4809	C 1526	H 2353	N 436	O 476	S 18	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	1052	Total 16791	C 5361	H 8406	N 1450	O 1518	S 56	0	0
3	Y	1052	Total 16791	C 5361	H 8406	N 1450	O 1518	S 56	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-7	MET	-	initiating methionine	UNP Q8N122
W	-6	ASP	-	expression tag	UNP Q8N122
W	-5	TYR	-	expression tag	UNP Q8N122
W	-4	LYS	-	expression tag	UNP Q8N122
W	-3	ASP	-	expression tag	UNP Q8N122
W	-2	ASP	-	expression tag	UNP Q8N122
W	-1	ASP	-	expression tag	UNP Q8N122
W	0	ASP	-	expression tag	UNP Q8N122
W	1	LYS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-7	MET	-	initiating methionine	UNP Q8N122
Y	-6	ASP	-	expression tag	UNP Q8N122
Y	-5	TYR	-	expression tag	UNP Q8N122
Y	-4	LYS	-	expression tag	UNP Q8N122
Y	-3	ASP	-	expression tag	UNP Q8N122
Y	-2	ASP	-	expression tag	UNP Q8N122
Y	-1	ASP	-	expression tag	UNP Q8N122
Y	0	ASP	-	expression tag	UNP Q8N122
Y	1	LYS	-	expression tag	UNP Q8N122

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	8	Total 126	C 42	H 58	N 9	O 16	S 1	0	0
4	Z	8	Total 126	C 42	H 58	N 9	O 16	S 1	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	GLY	-	expression tag	UNP Q13541
X	-2	SER	-	expression tag	UNP Q13541
X	-1	GLY	-	expression tag	UNP Q13541
X	0	ARG	-	expression tag	UNP Q13541
Z	-3	GLY	-	expression tag	UNP Q13541
Z	-2	SER	-	expression tag	UNP Q13541
Z	-1	GLY	-	expression tag	UNP Q13541
Z	0	ARG	-	expression tag	UNP Q13541

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP
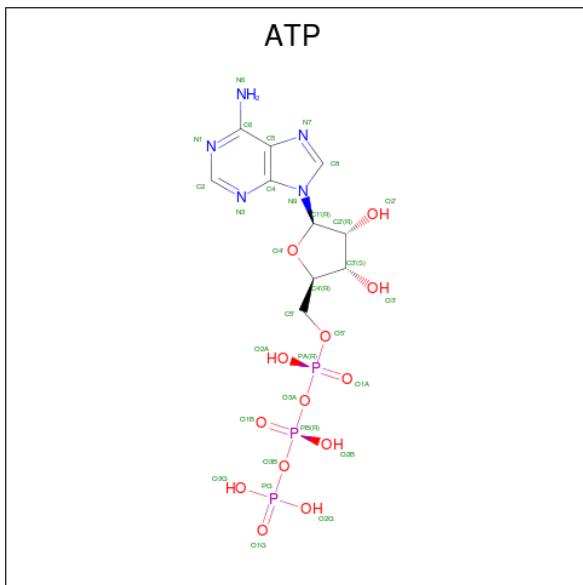
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3   Residue-property plots (i)

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

• Molecule 1: Serine/threonine-protein kinase mTOR
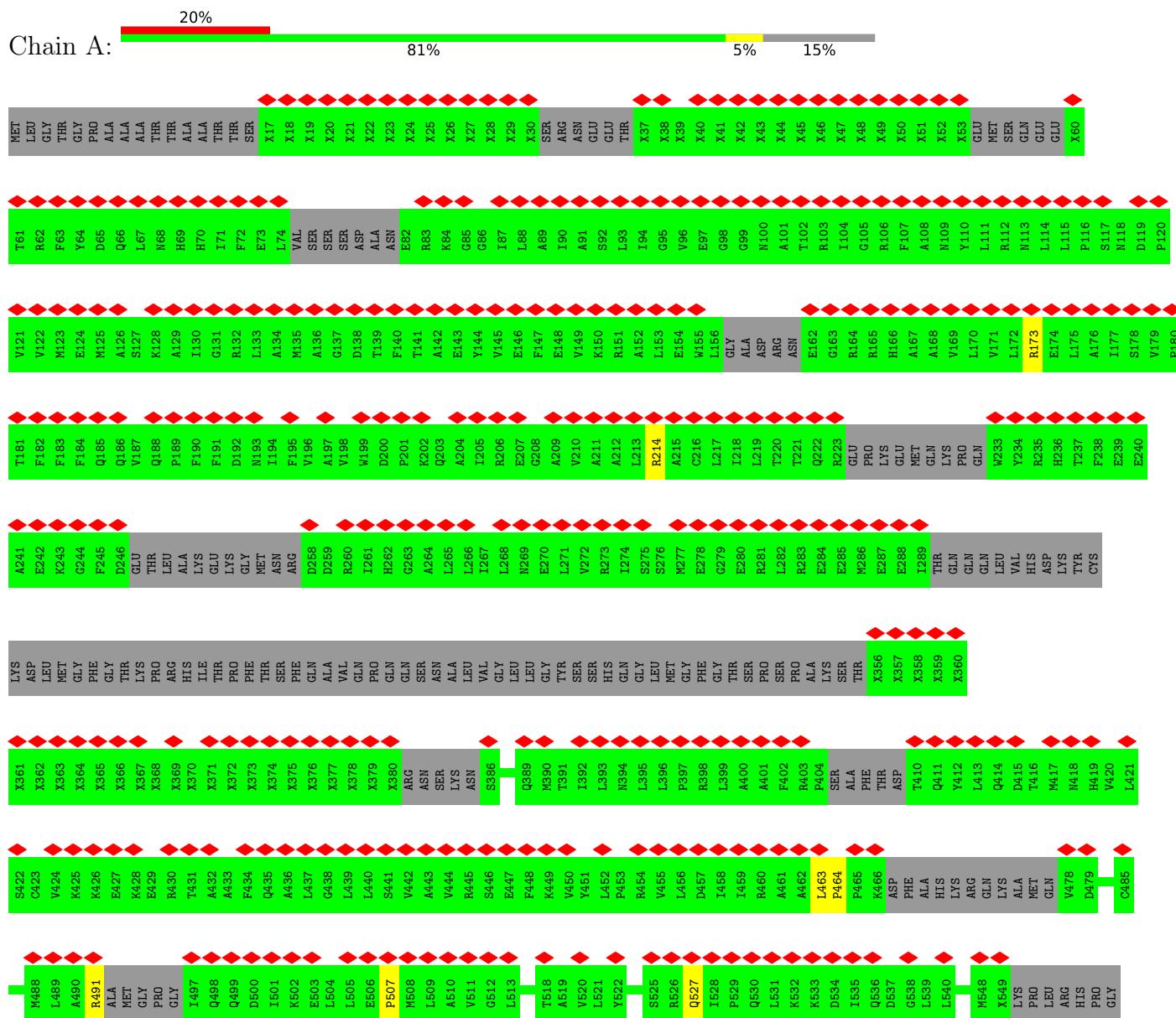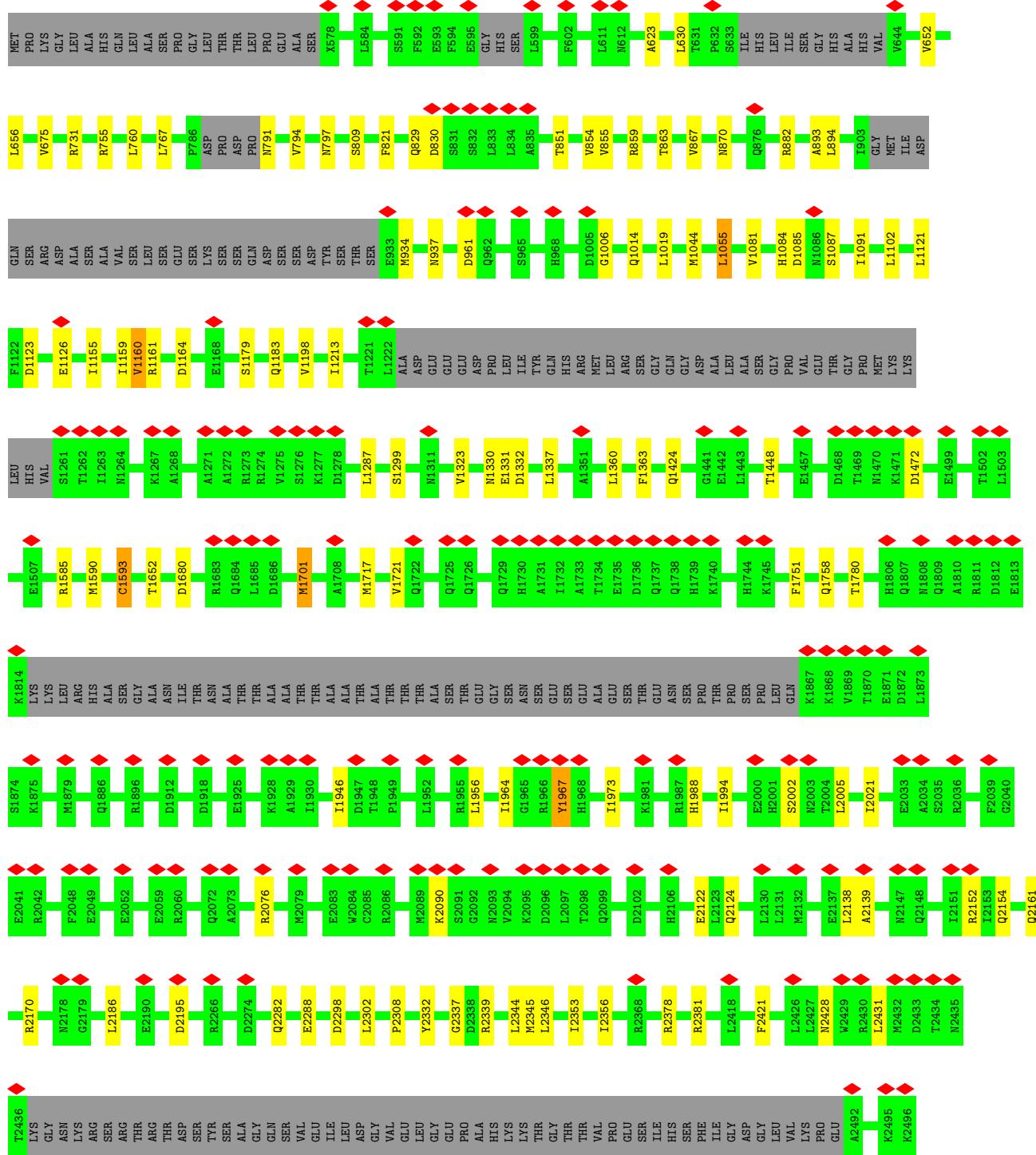
• Molecule 1: Serine/threonine-protein kinase mTOR

Chain B:

• Molecule 2: Target of rapamycin complex subunit LST8


Chain D:

• Molecule 2: Target of rapamycin complex subunit LST8

Chain E:

• Molecule 3: Regulatory-associated protein of mTOR

Chain W:

• Molecule 3: Regulatory-associated protein of mTOR
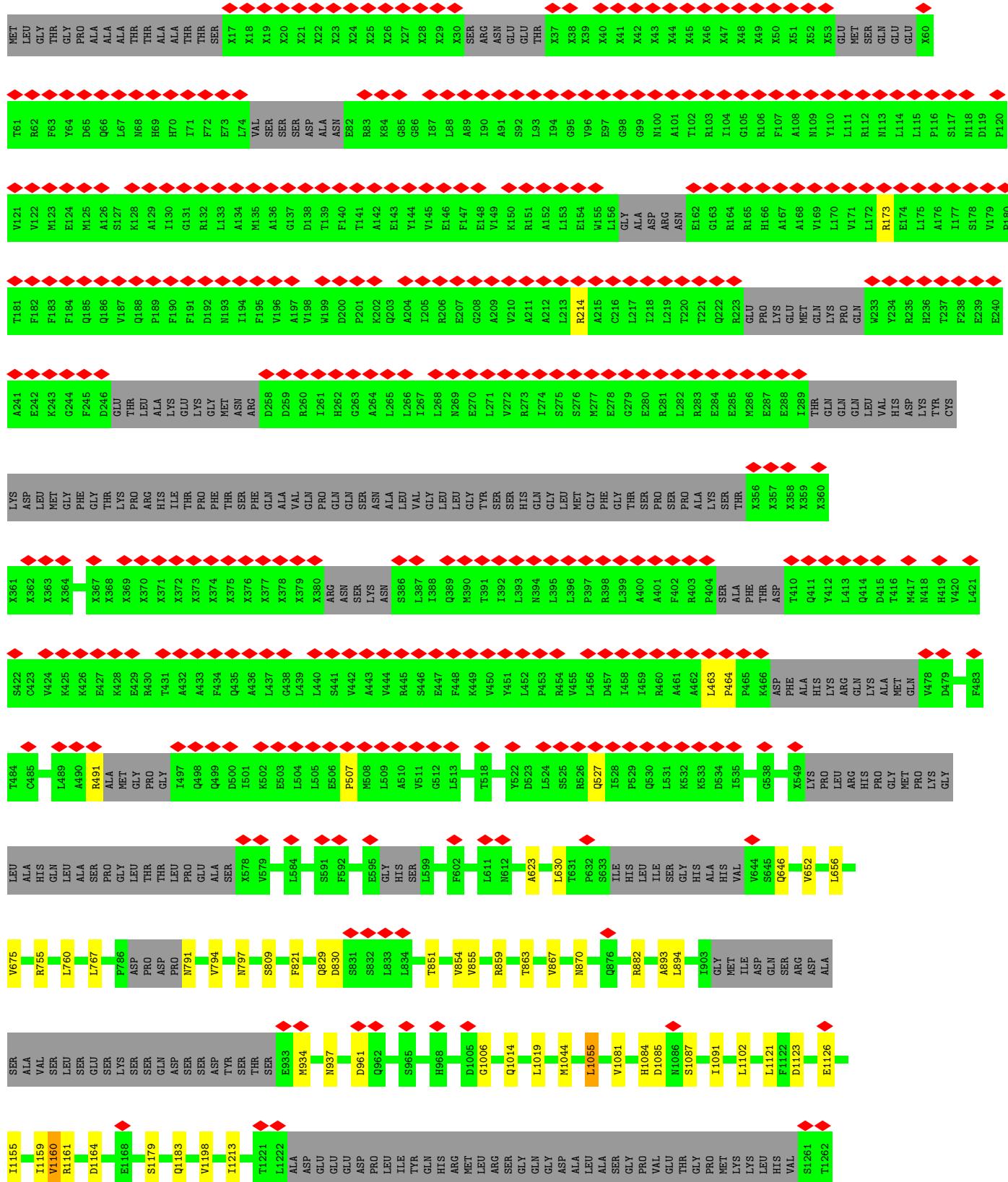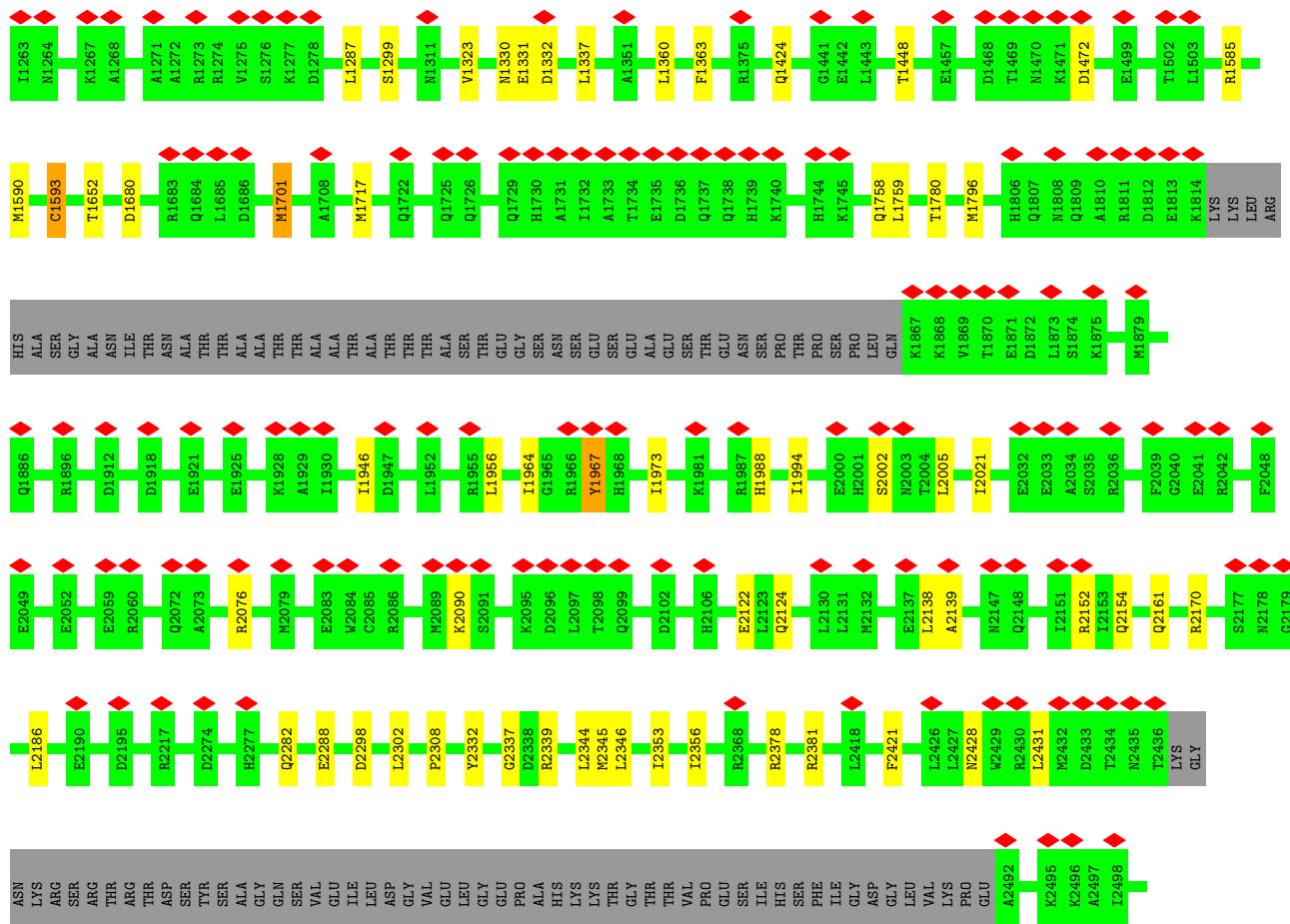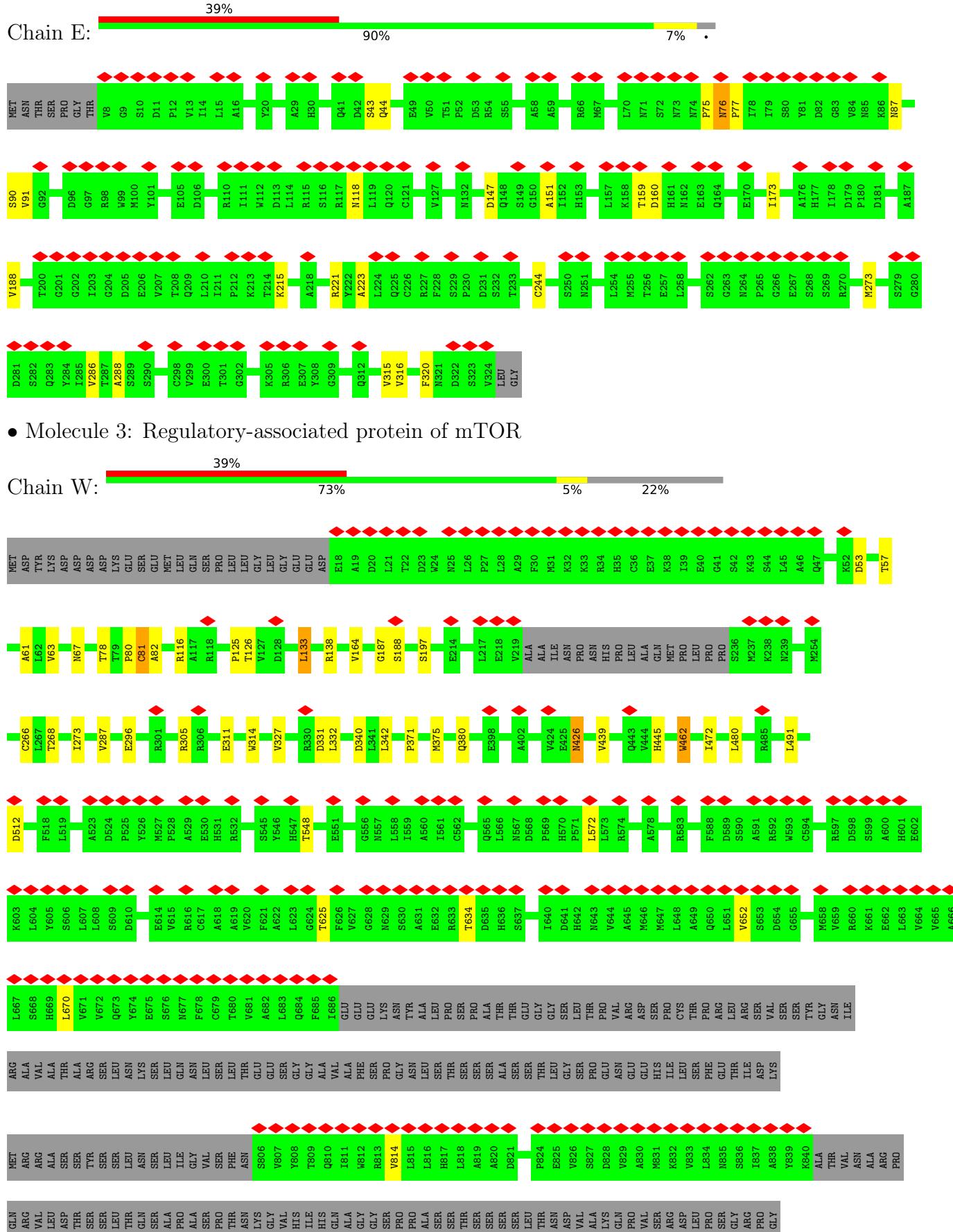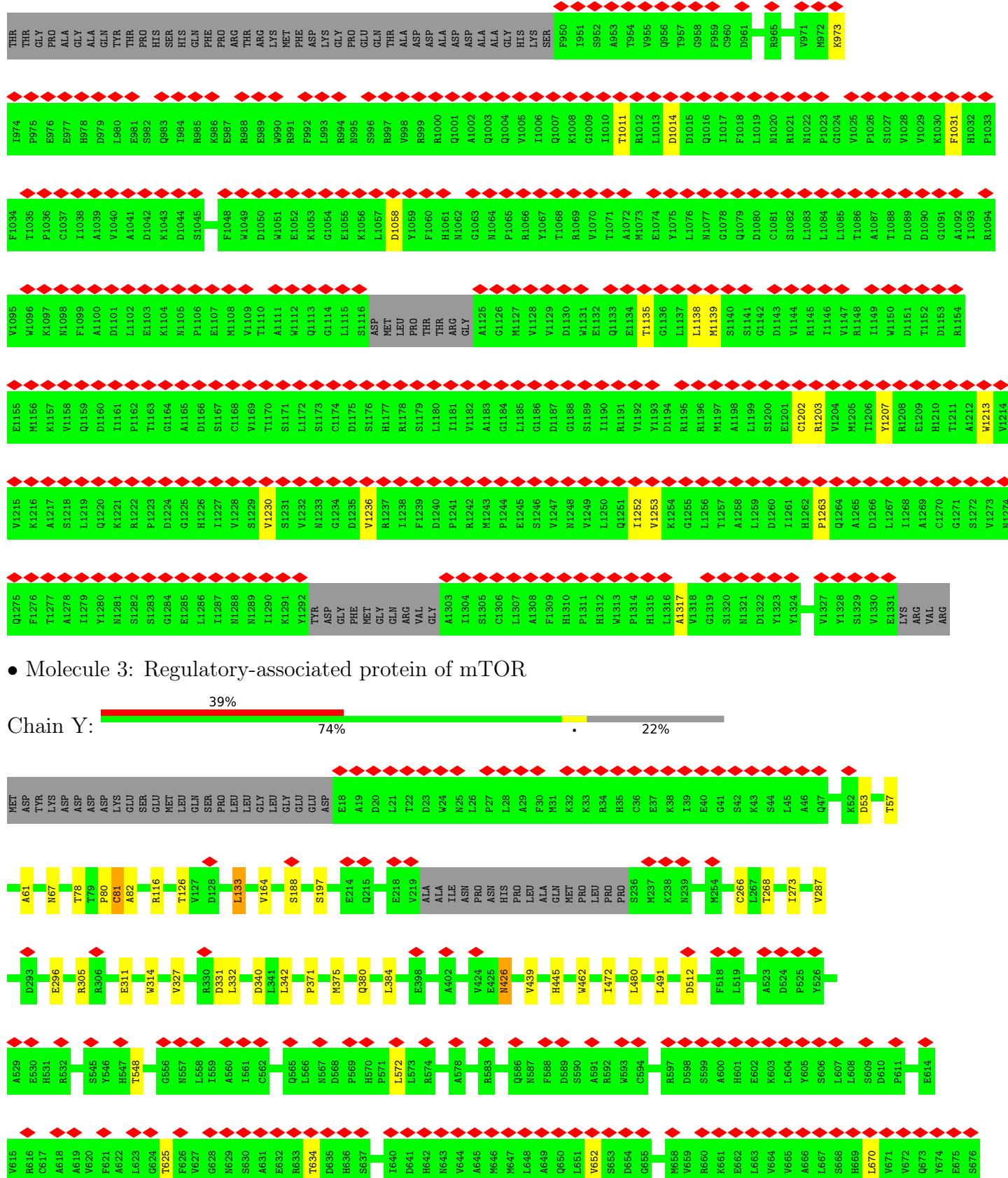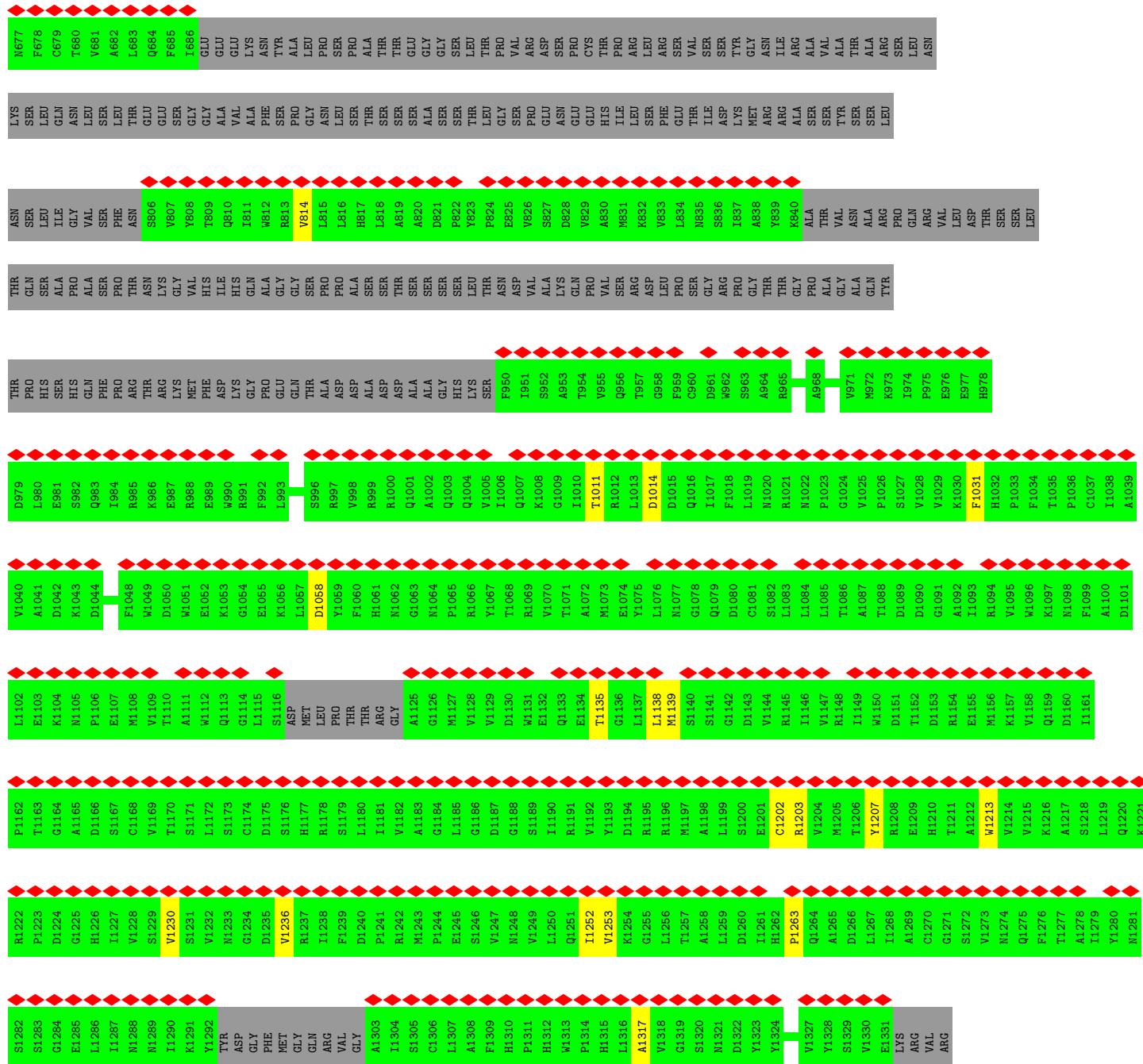
Chain Y:

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

Chain X: 6%   93%

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

Chain Z:

6%

93%

GLY SER GLY ARG MET SER GLY GLY SER SER CYS SER GLN THR PRO SER ARG ALA ILE PRO ALA THR ARG ARG VAL VAL LEU GLY ASP GLY VAL GLN LEU PRO PRO GLY ASP TYR SER THR THR PRO GLY GLY THR LEU PHE SER THR THR PRO GLY GLY THR ARG ILE ILE TYR ASP ARG

LYS PHE LEU MET GLU CYS ARG ASN SER PRO VAL THR LYS THR PRO ARG ASP LEU PRO THR ILE PRO GLY VAL THR SER PRO SER SER ASP GLU PRO PRO MET GLU ALA SER GLN SER HIS LEU ARG ASN SER PRO GLU ASP LYS ARG ALA GLY GLY GLU E111 D117 I118

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	580768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	497.6444, 497.6444, 497.6444	wwPDB
Map dimensions	374, 374, 374	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3306, 1.3306, 1.3306	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: MG, 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	0.42	0/17398	0.63	1/23547 (0.0%)
1	B	0.42	0/17398	0.62	1/23547 (0.0%)
2	D	0.39	0/2514	0.59	0/3426
2	E	0.39	0/2514	0.60	0/3426
3	W	0.41	0/8585	0.63	0/11680
3	Y	0.41	0/8585	0.63	0/11680
4	X	0.50	0/68	0.58	0/89
4	Z	0.51	0/68	0.58	0/89
All	All	0.41	0/57130	0.62	2/77484 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1055	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	1055	LEU	CA-CB-CG	5.43	127.79	115.30

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	17348	17686	17376	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	17348	17686	17376	34	0
2	D	2456	2353	2341	9	0
2	E	2456	2353	2341	9	0
3	W	8385	8406	8375	18	0
3	Y	8385	8406	8375	15	0
4	X	68	58	57	0	0
4	Z	68	58	57	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	56580	57030	56322	113	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 (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.18	0.77
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.18	0.77
3:Y:426:ASN:N	3:Y:426:ASN:HD22	1.96	0.63
3:W:426:ASN:HD22	3:W:426:ASN:N	1.96	0.60
1:B:755:ARG:HB2	1:B:797:ASN:HD22	1.68	0.58
1:A:755:ARG:HB2	1:A:797:ASN:HD22	1.68	0.58
3:W:973:LYS:HD3	1:B:646:GLN:HE22	1.69	0.56
1:B:829:GLN:HE21	1:B:867:VAL:HG21	1.70	0.56
1:A:829:GLN:HE21	1:A:867:VAL:HG21	1.69	0.55
3:W:439:VAL:HG13	3:W:445:HIS:HB2	1.91	0.53
1:B:1701:MET:CE	1:B:1717:MET:HA	2.40	0.52
3:Y:305:ARG:HD2	3:Y:314:TRP:CD2	2.45	0.52
1:A:1701:MET:CE	1:A:1717:MET:HA	2.40	0.52
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.43	0.51
3:Y:439:VAL:HG13	3:Y:445:HIS:HB2	1.92	0.51
1:B:491:ARG:HG3	1:B:527:GLN:HE22	1.76	0.51
1:A:491:ARG:HG3	1:A:527:GLN:HE22	1.76	0.51
3:W:652:VAL:HG22	3:W:814:VAL:HG13	1.93	0.51
2:E:188:VAL:HG13	2:E:223:ALA:HB3	1.94	0.50
3:W:305:ARG:HD2	3:W:314:TRP:CD2	2.45	0.50
1:B:755:ARG:HB2	1:B:797:ASN:ND2	2.28	0.49
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.94	0.49
3:Y:1252:ILE:HG22	3:Y:1253:VAL:HG23	1.95	0.49
3:Y:652:VAL:HG22	3:Y:814:VAL:HG13	1.94	0.48
1:B:2282:GLN:HE21	2:E:316:VAL:HG11	1.77	0.48
1:A:1330:ASN:O	1:A:1332:ASP:N	2.47	0.48
1:B:1330:ASN:O	1:B:1332:ASP:N	2.47	0.48
3:Y:480:LEU:HD23	3:Y:491:LEU:HD13	1.95	0.48
1:B:791:ASN:HD22	1:B:794:VAL:HG23	1.78	0.48
1:A:755:ARG:HB2	1:A:797:ASN:ND2	2.28	0.47
1:A:791:ASN:HD22	1:A:794:VAL:HG23	1.78	0.47
1:A:1323:VAL:HG21	1:A:1363:PHE:HE2	1.79	0.47
3:W:480:LEU:HD23	3:W:491:LEU:HD13	1.95	0.47
1:B:1323:VAL:HG21	1:B:1363:PHE:HE2	1.79	0.47
1:A:2282:GLN:HE21	2:D:316:VAL:HG11	1.79	0.47
3:W:1252:ILE:HG22	3:W:1253:VAL:HG23	1.95	0.47
1:B:1160:VAL:HG13	1:B:1198:VAL:HG21	1.98	0.46
1:B:1123:ASP:OD2	1:B:1161:ARG:NH1	2.45	0.46
1:A:1155:ILE:HG22	1:A:1159:ILE:HD12	1.97	0.46
1:B:1155:ILE:HG22	1:B:1159:ILE:HD12	1.98	0.46
1:B:2288:GLU:OE1	2:E:221:ARG:NH2	2.49	0.46
1:A:731:ARG:HD2	3:Y:384:LEU:HD13	1.97	0.45
1:A:623:ALA:HB1	1:A:675:VAL:HG22	1.99	0.45
1:A:1160:VAL:HG13	1:A:1198:VAL:HG21	1.98	0.45
3:Y:81:CYS:SG	3:Y:82:ALA:N	2.90	0.45
1:A:1087:SER:OG	1:A:1091:ILE:HG13	2.17	0.44
3:W:266:CYS:HA	3:W:273:ILE:HD11	1.99	0.44
1:A:1123:ASP:OD2	1:A:1161:ARG:NH1	2.45	0.44
1:A:1424:GLN:HE22	1:A:1585:ARG:HG2	1.83	0.44
3:Y:266:CYS:HA	3:Y:273:ILE:HD11	1.99	0.44
1:A:1081:VAL:O	1:A:1085:ASP:HB2	2.19	0.43
1:B:623:ALA:HB1	1:B:675:VAL:HG22	1.99	0.43
1:B:1087:SER:OG	1:B:1091:ILE:HG13	2.17	0.43
3:Y:327:VAL:HG12	3:Y:371:PRO:HG2	2.01	0.43
1:B:1424:GLN:HE22	1:B:1585:ARG:HG2	1.83	0.43
1:B:2332:TYR:CZ	1:B:2528:LEU:HD21	2.54	0.43
3:Y:1230:VAL:HG22	3:Y:1236:VAL:HG22	2.01	0.43
3:W:81:CYS:SG	3:W:82:ALA:N	2.91	0.43
1:A:463:LEU:N	1:A:464:PRO:HD2	2.34	0.43
2:D:288:ALA:HB1	2:D:315:VAL:HG12	2.01	0.43
3:W:426:ASN:N	3:W:426:ASN:ND2	2.67	0.43
1:B:1081:VAL:O	1:B:1085:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:ASN:HB3	2:E:77:PRO:CD	2.49	0.43
3:W:1230:VAL:HG22	3:W:1236:VAL:HG22	2.01	0.42
1:B:463:LEU:N	1:B:464:PRO:HD2	2.34	0.42
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	2.00	0.42
1:A:2428:ASN:HD22	1:A:2431:LEU:HD12	1.84	0.42
1:A:1946:ILE:HD11	1:A:1994:ILE:HD12	2.02	0.42
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	2.01	0.42
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.53	0.42
2:E:288:ALA:HB1	2:E:315:VAL:HG12	2.01	0.42
1:A:2332:TYR:CZ	1:A:2528:LEU:HD21	2.53	0.42
3:W:327:VAL:HG12	3:W:371:PRO:HG2	2.01	0.42
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.49	0.41
1:B:2002:SER:HB3	1:B:2005:LEU:HB3	2.02	0.41
3:Y:57:THR:HG21	3:Y:342:LEU:HD23	2.02	0.41
1:B:1946:ILE:HD11	1:B:1994:ILE:HD12	2.01	0.41
1:B:2170:ARG:HB2	1:B:2186:LEU:HB3	2.01	0.41
1:B:2428:ASN:HD22	1:B:2431:LEU:HD12	1.84	0.41
3:Y:1031:PHE:CZ	3:Y:1317:ALA:HB2	2.55	0.41
2:D:286:VAL:HG21	2:D:320:PHE:CD1	2.55	0.41
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.53	0.41
1:A:1590:MET:HA	1:A:1593:CYS:SG	2.61	0.41
3:W:57:THR:HG21	3:W:342:LEU:HD23	2.02	0.41
1:B:854:VAL:HG12	1:B:855:VAL:HG23	2.03	0.41
3:W:462:TRP:CD1	3:W:462:TRP:C	2.94	0.41
2:D:244:CYS:HB2	2:D:273:MET:HG2	2.03	0.41
3:W:63:VAL:HG13	3:W:125:PRO:HG3	2.03	0.41
1:A:854:VAL:HG12	1:A:855:VAL:HG23	2.03	0.41
1:A:2002:SER:HB3	1:A:2005:LEU:HB3	2.02	0.41
1:A:2122:GLU:HG2	1:A:2124:GLN:HE21	1.86	0.41
3:W:61:ALA:HB1	3:W:133:LEU:HD11	2.03	0.41
3:W:1031:PHE:CZ	3:W:1317:ALA:HB2	2.55	0.41
1:B:2139:ALA:HA	1:B:2152:ARG:HA	2.02	0.41
3:Y:61:ALA:HB1	3:Y:133:LEU:HD11	2.03	0.41
2:D:43:SER:OG	2:D:44:GLN:N	2.54	0.41
3:Y:426:ASN:N	3:Y:426:ASN:ND2	2.66	0.41
1:A:2139:ALA:HA	1:A:2152:ARG:HA	2.02	0.40
1:B:2122:GLU:HG2	1:B:2124:GLN:HE21	1.86	0.40
1:A:630:LEU:HD22	1:A:652:VAL:HG22	2.04	0.40
1:A:1721:VAL:HG11	1:A:1751:PHE:CE1	2.56	0.40
2:D:76:ASN:CB	2:D:77:PRO:CD	2.99	0.40
1:B:1590:MET:HA	1:B:1593:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1964:ILE:O	1:B:1967:TYR:O	2.40	0.40
2:E:43:SER:OG	2:E:44:GLN:N	2.55	0.40
2:E:147:ASP:OD1	2:E:151:ALA:N	2.55	0.40
1:A:2288:GLU:OE1	2:D:221:ARG:NH2	2.54	0.40
1:B:630:LEU:HD22	1:B:652:VAL:HG22	2.03	0.40
2:E:286:VAL:HG21	2:E:320:PHE:CD1	2.56	0.40
1:A:1964:ILE:O	1:A:1967:TYR:O	2.39	0.40
3:W:138:ARG:NE	3:W:187:GLY:HA3	2.37	0.40
2:E:244:CYS:HB2	2:E:273:MET:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2088/2549 (82%)	1972 (94%)	107 (5%)	9 (0%)	34	68
1	B	2088/2549 (82%)	1973 (94%)	106 (5%)	9 (0%)	34	68
2	D	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	12	44
2	E	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	12	44
3	W	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	22	58
3	Y	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	22	58
4	X	6/122 (5%)	6 (100%)	0	0	100	100
4	Z	6/122 (5%)	5 (83%)	1 (17%)	0	100	100
All	All	6898/8680 (80%)	6410 (93%)	448 (6%)	40 (1%)	29	61

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	893	ALA

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Mol	Chain	Res	Type
3	W	53	ASP
1	B	893	ALA
3	Y	53	ASP
1	A	1006	GLY
1	A	1331	GLU
1	A	2308	PRO
2	D	87	ASN
1	B	1006	GLY
1	B	1331	GLU
1	B	2308	PRO
2	E	87	ASN
1	A	1472	ASP
3	W	1203	ARG
3	W	1213	TRP
1	B	1472	ASP
3	Y	1203	ARG
3	Y	1213	TRP
2	D	75	PRO
2	D	118	ASN
3	W	80	PRO
3	W	81	CYS
3	W	1202	CYS
2	E	75	PRO
2	E	118	ASN
3	Y	80	PRO
3	Y	81	CYS
3	Y	1202	CYS
1	A	809	SER
1	A	830	ASP
1	A	961	ASP
3	W	1263	PRO
1	B	809	SER
1	B	830	ASP
1	B	961	ASP
3	Y	1263	PRO
2	D	76	ASN
2	E	76	ASN
1	A	507	PRO
1	B	507	PRO

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	1861/2166 (86%)	1803 (97%)	58 (3%)	40	70
1	B	1861/2166 (86%)	1804 (97%)	57 (3%)	40	70
2	D	269/276 (98%)	263 (98%)	6 (2%)	52	76
2	E	269/276 (98%)	263 (98%)	6 (2%)	52	76
3	W	928/1171 (79%)	895 (96%)	33 (4%)	35	66
3	Y	928/1171 (79%)	895 (96%)	33 (4%)	35	66
4	X	8/104 (8%)	7 (88%)	1 (12%)	4	20
4	Z	8/104 (8%)	7 (88%)	1 (12%)	4	20
All	All	6132/7434 (82%)	5937 (97%)	195 (3%)	42	69

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	214	ARG
1	A	656	LEU
1	A	760	LEU
1	A	767	LEU
1	A	821	PHE
1	A	851	THR
1	A	859	ARG
1	A	863	THR
1	A	870	ASN
1	A	882	ARG
1	A	894	LEU
1	A	934	MET
1	A	937	ASN
1	A	1014	GLN
1	A	1019	LEU
1	A	1044	MET
1	A	1055	LEU
1	A	1084	HIS

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Mol	Chain	Res	Type
1	A	1102	LEU
1	A	1121	LEU
1	A	1126	GLU
1	A	1160	VAL
1	A	1164	ASP
1	A	1179	SER
1	A	1183	GLN
1	A	1213	ILE
1	A	1287	LEU
1	A	1299	SER
1	A	1337	LEU
1	A	1360	LEU
1	A	1448	THR
1	A	1593	CYS
1	A	1652	THR
1	A	1680	ASP
1	A	1701	MET
1	A	1758	GLN
1	A	1780	THR
1	A	1956	LEU
1	A	1967	TYR
1	A	1973	ILE
1	A	1988	HIS
1	A	2021	ILE
1	A	2076	ARG
1	A	2090	LYS
1	A	2138	LEU
1	A	2154	GLN
1	A	2161	GLN
1	A	2195	ASP
1	A	2298	ASP
1	A	2302	LEU
1	A	2344	LEU
1	A	2345	MET
1	A	2346	LEU
1	A	2353	ILE
1	A	2381	ARG
1	A	2421	PHE
1	A	2548	PHE
2	D	90	SER
2	D	91	VAL
2	D	159	THR

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Mol	Chain	Res	Type
2	D	160	ASP
2	D	173	ILE
2	D	215	LYS
3	W	67	ASN
3	W	78	THR
3	W	116	ARG
3	W	126	THR
3	W	133	LEU
3	W	164	VAL
3	W	188	SER
3	W	197	SER
3	W	268	THR
3	W	287	VAL
3	W	296	GLU
3	W	311	GLU
3	W	331	ASP
3	W	332	LEU
3	W	340	ASP
3	W	375	MET
3	W	380	GLN
3	W	426	ASN
3	W	462	TRP
3	W	472	ILE
3	W	512	ASP
3	W	548	THR
3	W	572	LEU
3	W	625	THR
3	W	634	THR
3	W	670	LEU
3	W	1011	THR
3	W	1014	ASP
3	W	1058	ASP
3	W	1135	THR
3	W	1138	LEU
3	W	1139	MET
3	W	1207	TYR
4	X	117	ASP
1	B	173	ARG
1	B	214	ARG
1	B	656	LEU
1	B	760	LEU
1	B	767	LEU

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Mol	Chain	Res	Type
1	B	821	PHE
1	B	851	THR
1	B	859	ARG
1	B	863	THR
1	B	870	ASN
1	B	882	ARG
1	B	894	LEU
1	B	934	MET
1	B	937	ASN
1	B	1014	GLN
1	B	1019	LEU
1	B	1044	MET
1	B	1055	LEU
1	B	1084	HIS
1	B	1102	LEU
1	B	1121	LEU
1	B	1126	GLU
1	B	1160	VAL
1	B	1164	ASP
1	B	1179	SER
1	B	1183	GLN
1	B	1213	ILE
1	B	1287	LEU
1	B	1299	SER
1	B	1337	LEU
1	B	1360	LEU
1	B	1448	THR
1	B	1593	CYS
1	B	1652	THR
1	B	1680	ASP
1	B	1701	MET
1	B	1758	GLN
1	B	1780	THR
1	B	1956	LEU
1	B	1967	TYR
1	B	1973	ILE
1	B	1988	HIS
1	B	2021	ILE
1	B	2076	ARG
1	B	2090	LYS
1	B	2138	LEU
1	B	2154	GLN

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Mol	Chain	Res	Type
1	B	2161	GLN
1	B	2298	ASP
1	B	2302	LEU
1	B	2344	LEU
1	B	2345	MET
1	B	2346	LEU
1	B	2353	ILE
1	B	2381	ARG
1	B	2421	PHE
1	B	2548	PHE
2	E	90	SER
2	E	91	VAL
2	E	159	THR
2	E	160	ASP
2	E	173	ILE
2	E	215	LYS
3	Y	67	ASN
3	Y	78	THR
3	Y	116	ARG
3	Y	126	THR
3	Y	133	LEU
3	Y	164	VAL
3	Y	188	SER
3	Y	197	SER
3	Y	268	THR
3	Y	287	VAL
3	Y	296	GLU
3	Y	311	GLU
3	Y	331	ASP
3	Y	332	LEU
3	Y	340	ASP
3	Y	375	MET
3	Y	380	GLN
3	Y	426	ASN
3	Y	462	TRP
3	Y	472	ILE
3	Y	512	ASP
3	Y	548	THR
3	Y	572	LEU
3	Y	625	THR
3	Y	634	THR
3	Y	670	LEU

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Mol	Chain	Res	Type
3	Y	1011	THR
3	Y	1014	ASP
3	Y	1058	ASP
3	Y	1135	THR
3	Y	1138	LEU
3	Y	1139	MET
3	Y	1207	TYR
4	Z	117	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	527	GLN
1	A	646	GLN
1	A	791	ASN
1	A	829	GLN
1	A	1014	GLN
1	A	1058	GLN
1	A	1496	GLN
1	A	1554	GLN
1	A	2124	GLN
1	A	2154	GLN
1	A	2223	GLN
1	A	2385	ASN
2	D	321	ASN
3	W	67	ASN
3	W	242	GLN
3	W	339	GLN
3	W	426	ASN
3	W	995	ASN
1	B	193	ASN
1	B	527	GLN
1	B	646	GLN
1	B	791	ASN
1	B	829	GLN
1	B	1014	GLN
1	B	1058	GLN
1	B	1496	GLN
1	B	1554	GLN
1	B	2124	GLN
1	B	2154	GLN

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Mol	Chain	Res	Type
1	B	2223	GLN
1	B	2385	ASN
2	E	321	ASN
3	Y	67	ASN
3	Y	242	GLN
3	Y	412	GLN
3	Y	426	ASN
3	Y	995	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	ATP	A	3000	6	26,33,33	1.01	2 (7%)	31,52,52	1.38	5 (16%)
5	ATP	B	3000	6	26,33,33	1.05	1 (3%)	31,52,52	1.46	6 (19%)

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	ATP	A	3000	6	-	2/18/38/38	0/3/3/3
5	ATP	B	3000	6	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3000	ATP	C5-C4	2.68	1.48	1.40
5	A	3000	ATP	C5-C4	2.48	1.47	1.40
5	A	3000	ATP	O4'-C1'	2.01	1.43	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3000	ATP	N3-C2-N1	-3.83	122.70	128.68
5	A	3000	ATP	N3-C2-N1	-3.80	122.73	128.68
5	B	3000	ATP	C4-C5-N7	-2.98	106.29	109.40
5	A	3000	ATP	C4-C5-N7	-2.81	106.47	109.40
5	B	3000	ATP	C3'-C2'-C1'	2.47	104.70	100.98
5	B	3000	ATP	PB-O3B-PG	-2.43	124.48	132.83
5	A	3000	ATP	PB-O3B-PG	-2.38	124.66	132.83
5	B	3000	ATP	C1'-N9-C4	-2.29	122.62	126.64
5	A	3000	ATP	C3'-C2'-C1'	2.19	104.27	100.98
5	B	3000	ATP	C2-N1-C6	2.17	122.46	118.75
5	A	3000	ATP	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3000	ATP	PG-O3B-PB-O1B
5	B	3000	ATP	PA-O3A-PB-O1B
5	A	3000	ATP	PA-O3A-PB-O2B
5	B	3000	ATP	PA-O3A-PB-O2B
5	A	3000	ATP	C4'-C5'-O5'-PA
5	B	3000	ATP	PG-O3B-PB-O2B

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 then 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.

Ligand ATP A 3000

Bond lengths   Bond angles

Torsions   Rings

Ligand ATP B 3000

Bond lengths

Bond angles

Torsions

Rings
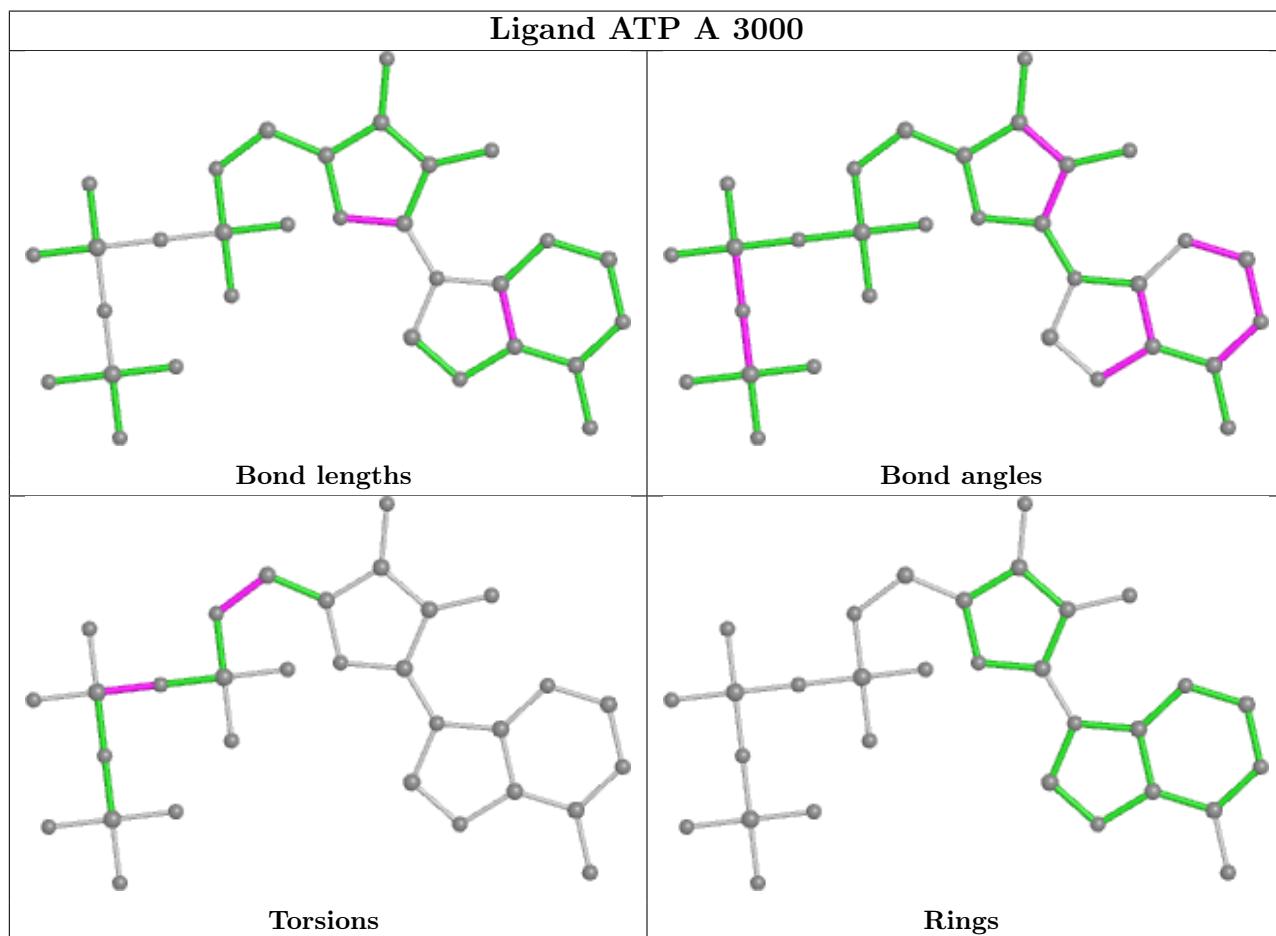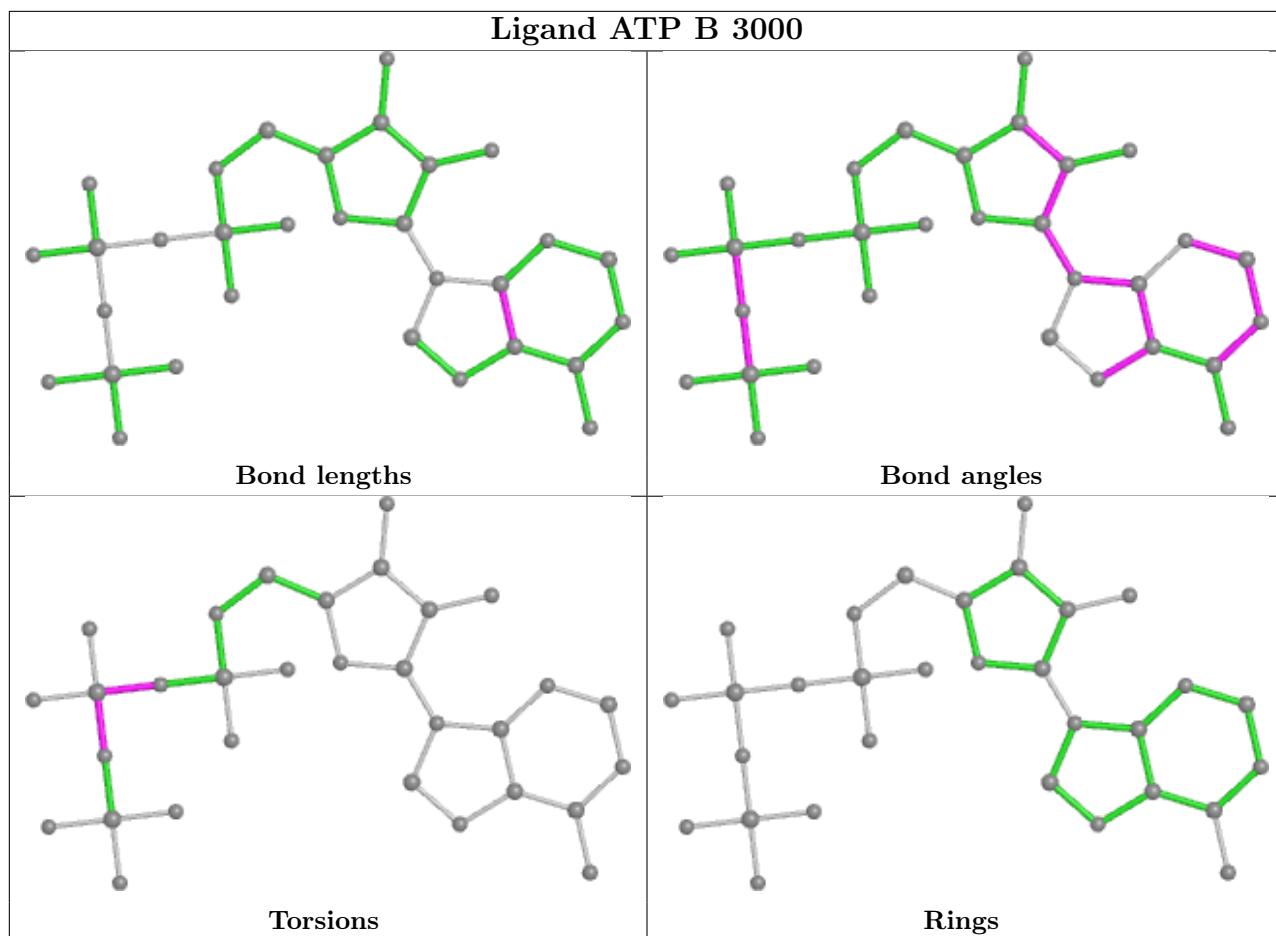
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7087. 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 |
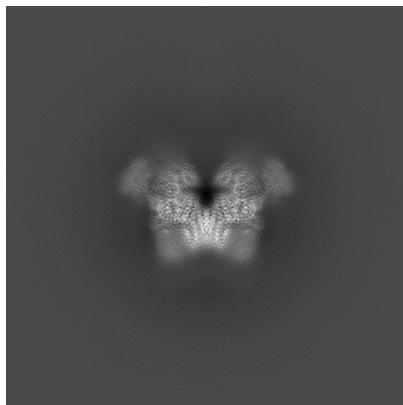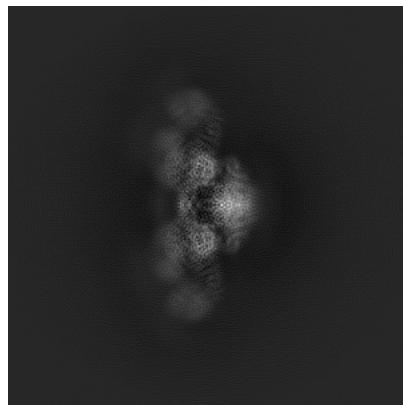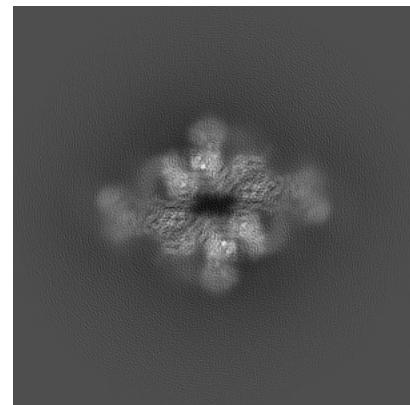
The images above show the map projected in three orthogonal directions.

6.2   Central slices (i)

6.2.1   Primary map
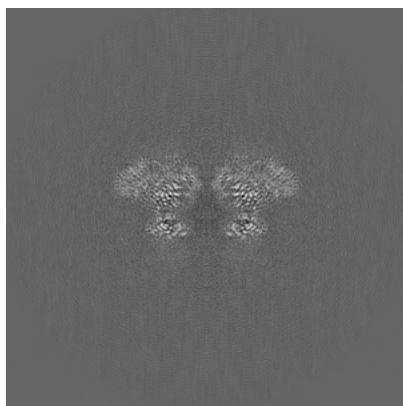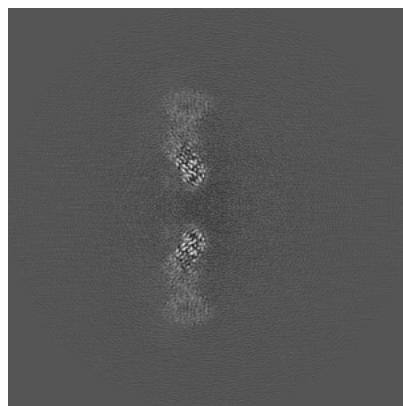
| X Index: 187 | Y Index: 187 | Z Index: 187 |
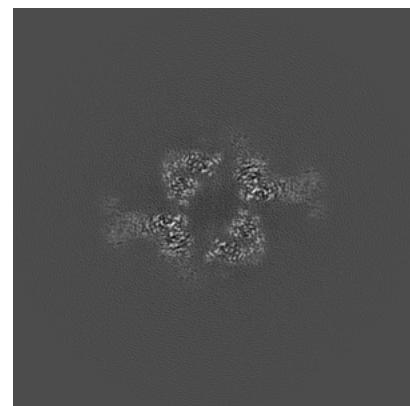
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
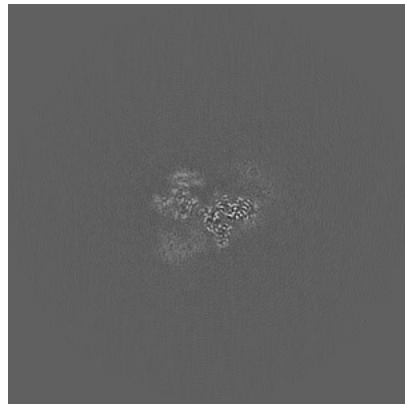
| X Index: 222 | Y Index: 169 | Z Index: 177 |
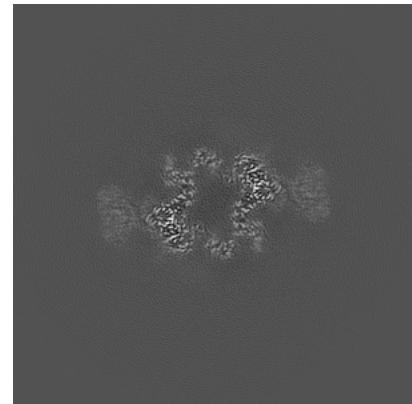
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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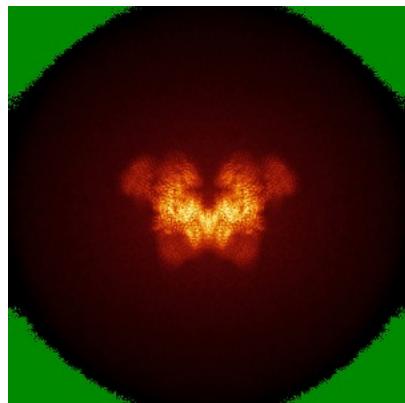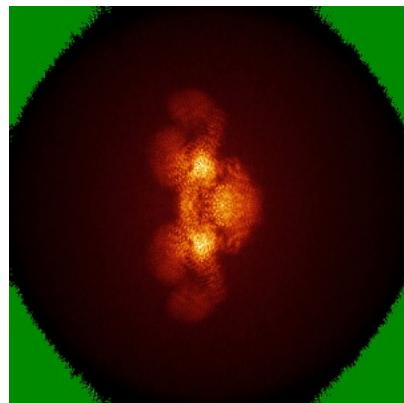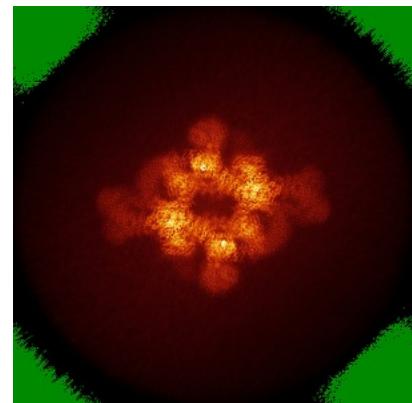
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
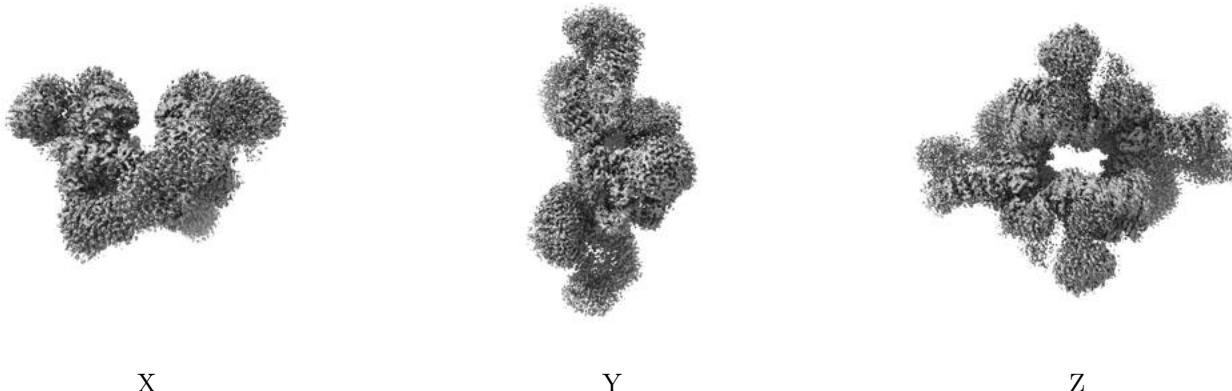
The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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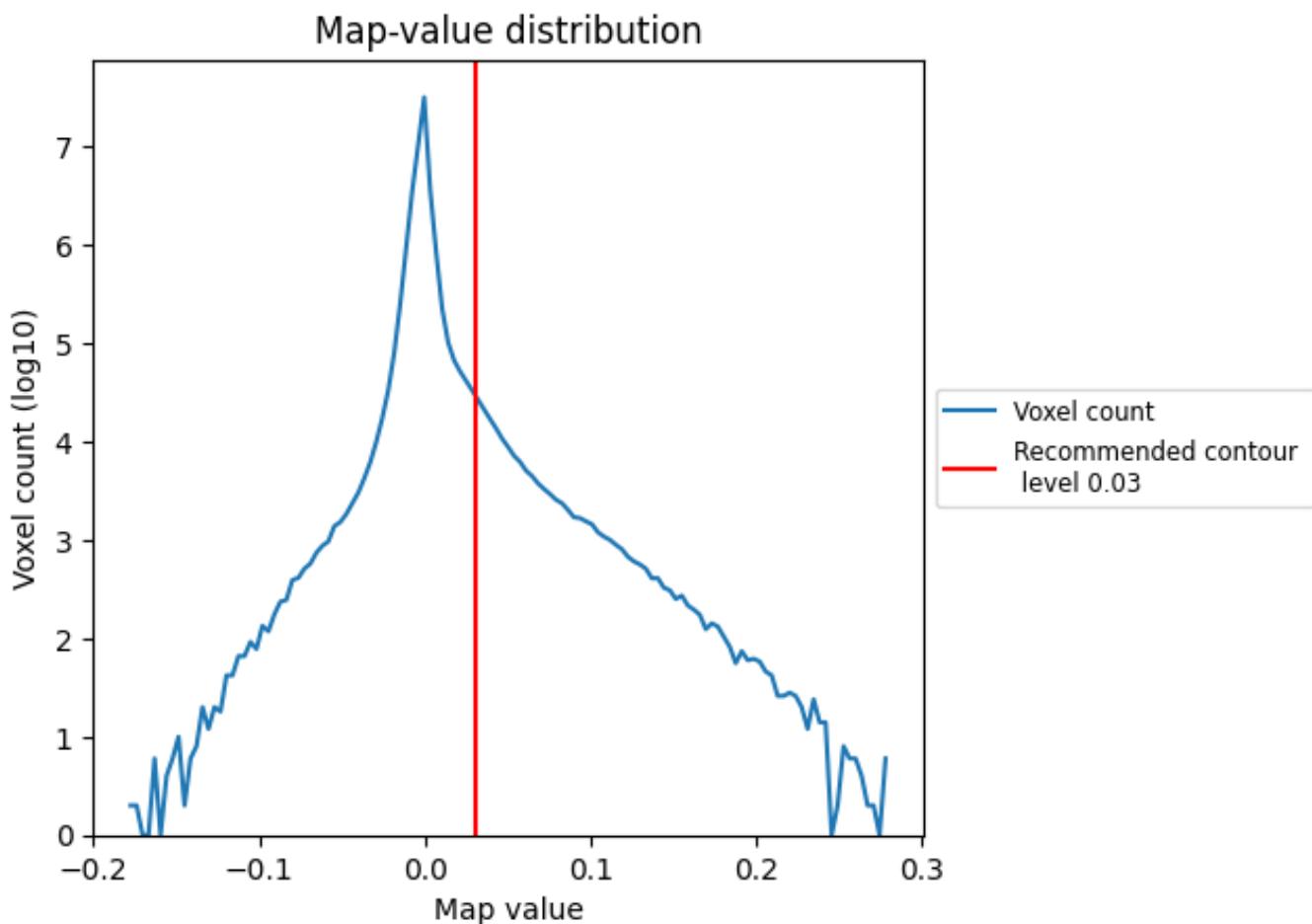
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
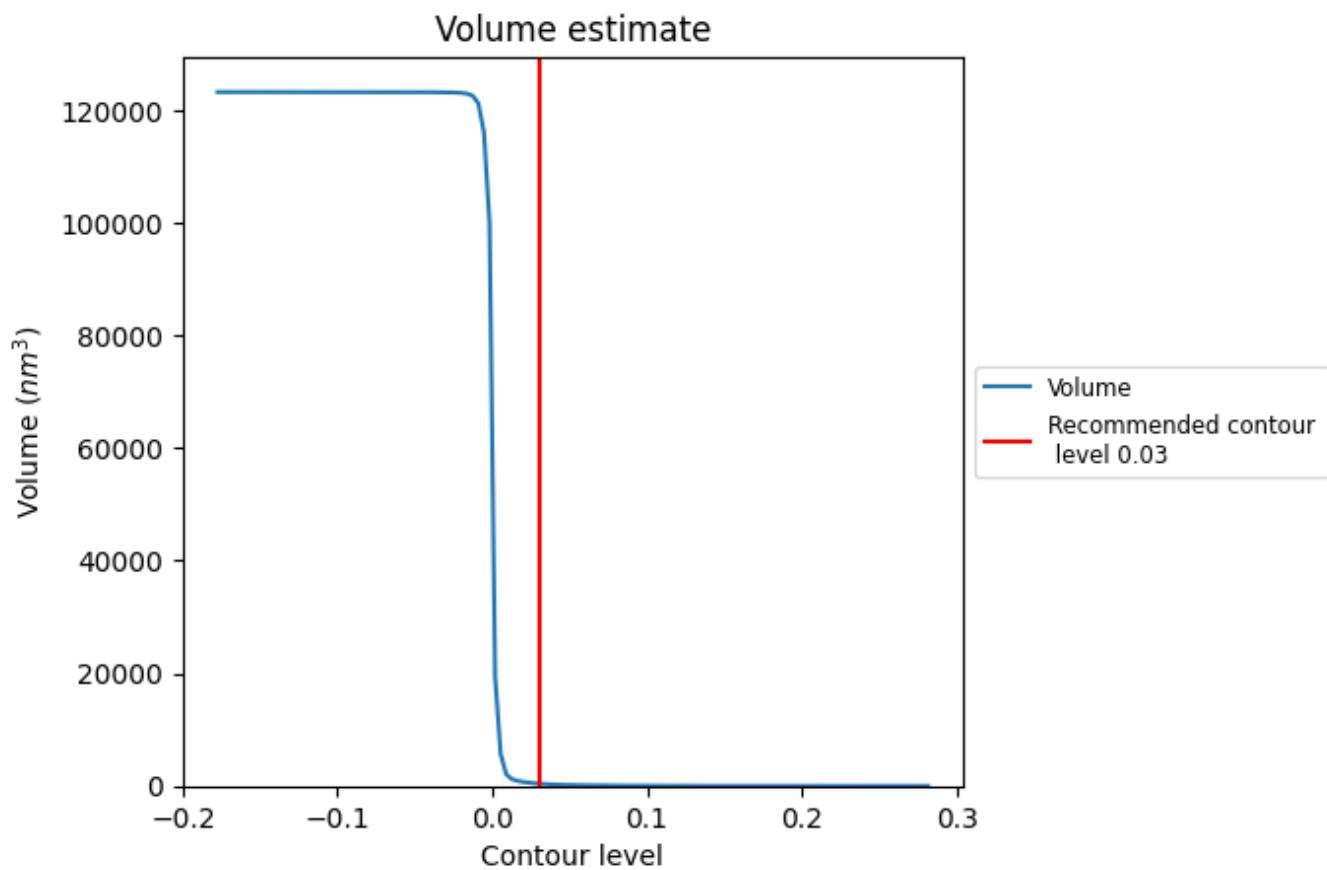
The volume at the recommended contour level is 412 nm^3; this corresponds to an approximate mass of 372 kDa.

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 ⓘ
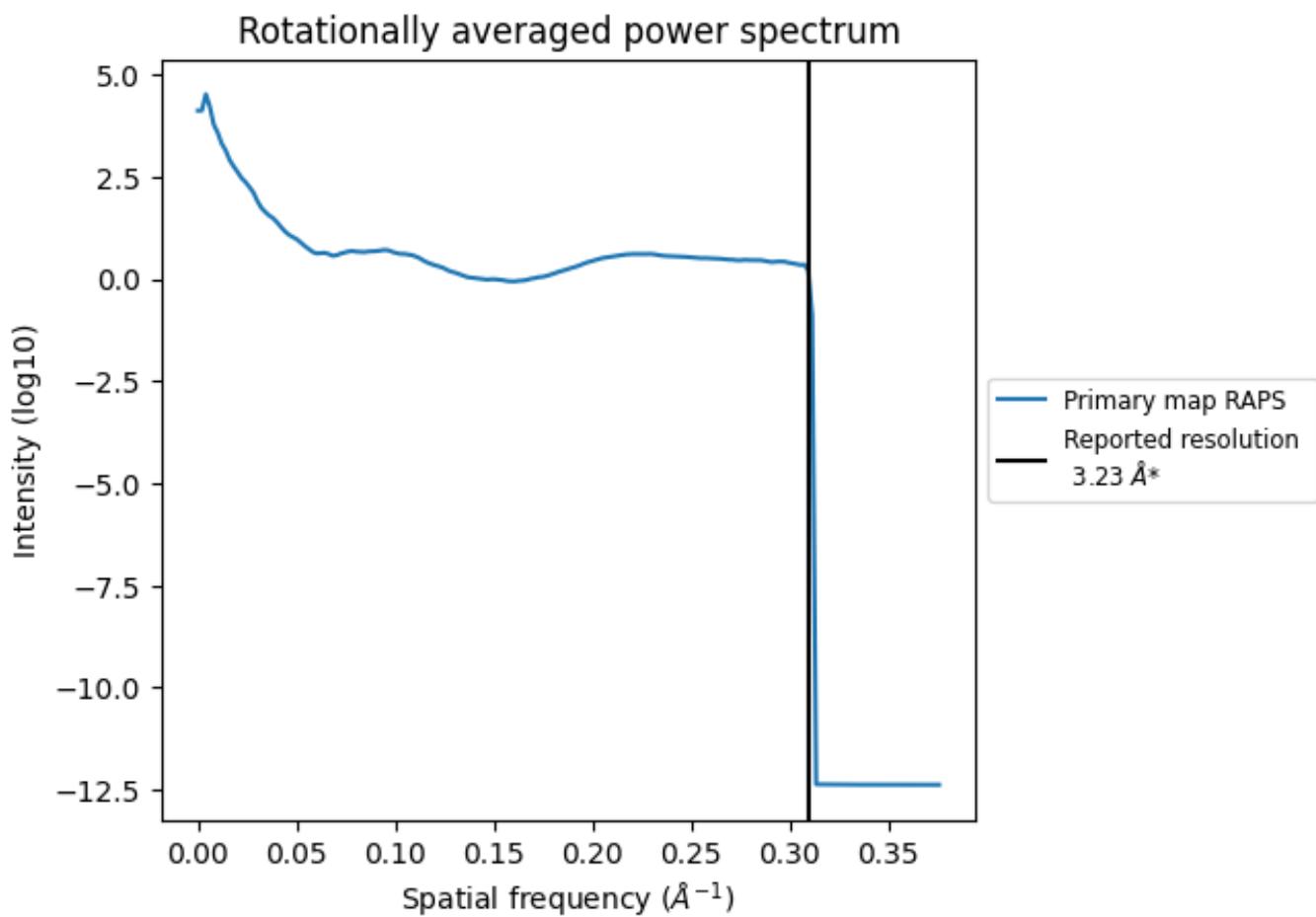
*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-7087 and PDB model 6BCX. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlay ⓘ

X   Y   Z
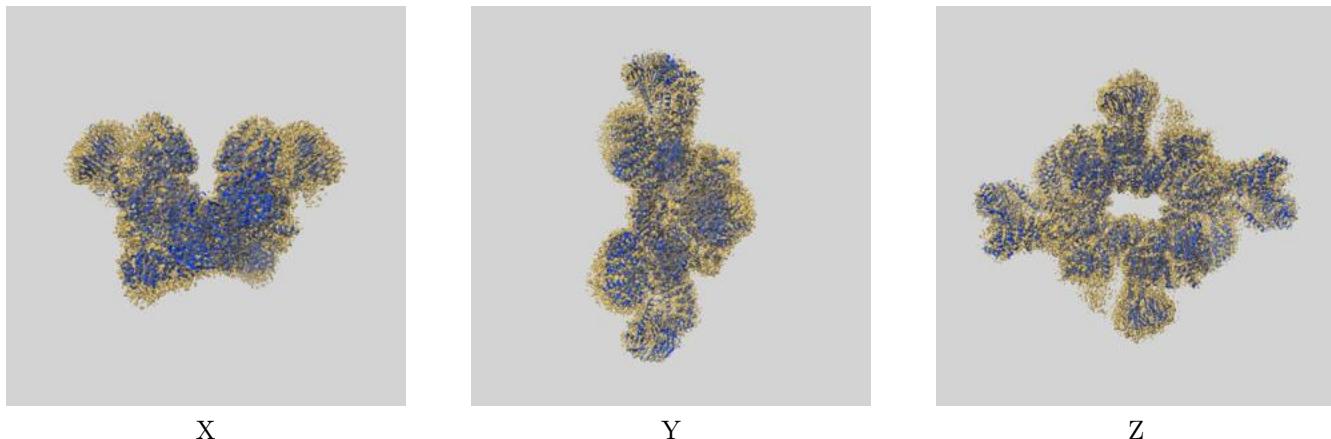
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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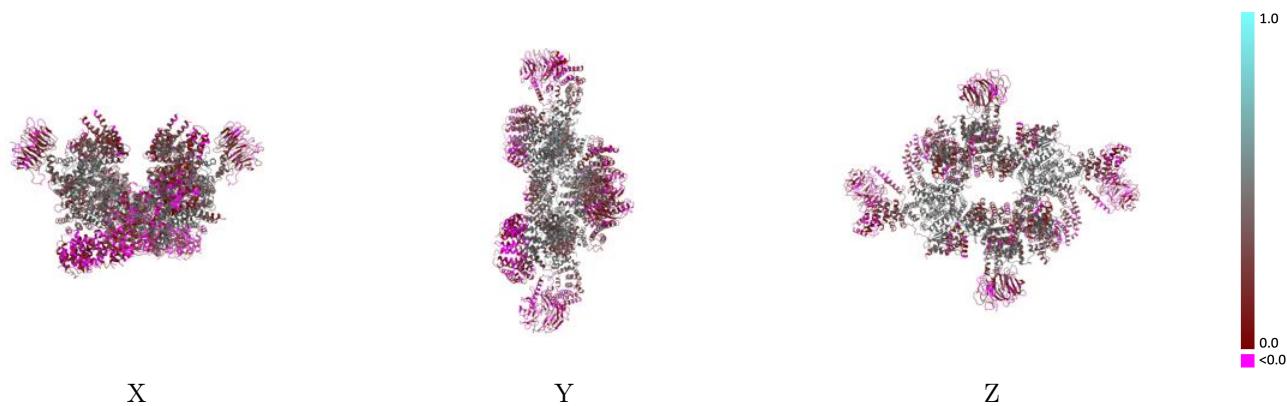
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
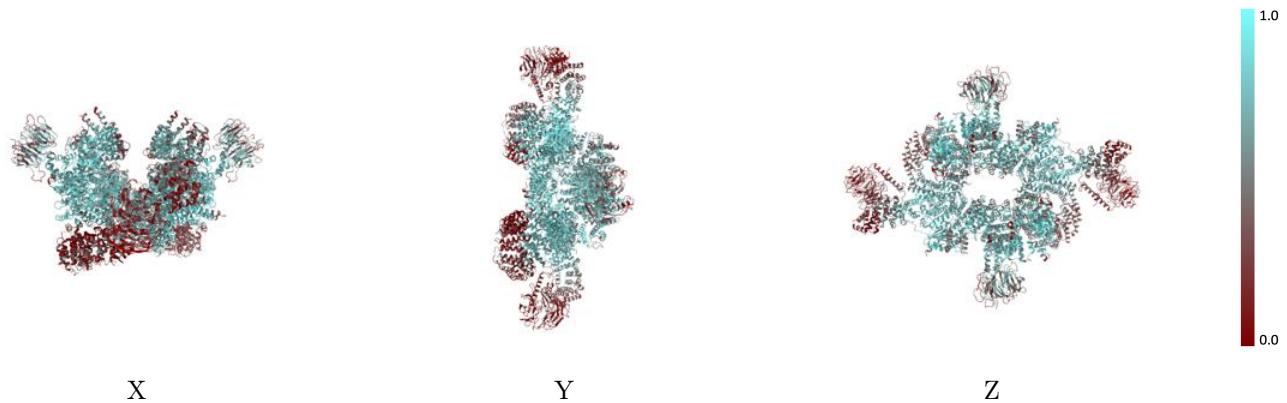
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4   Atom inclusion ⓘ
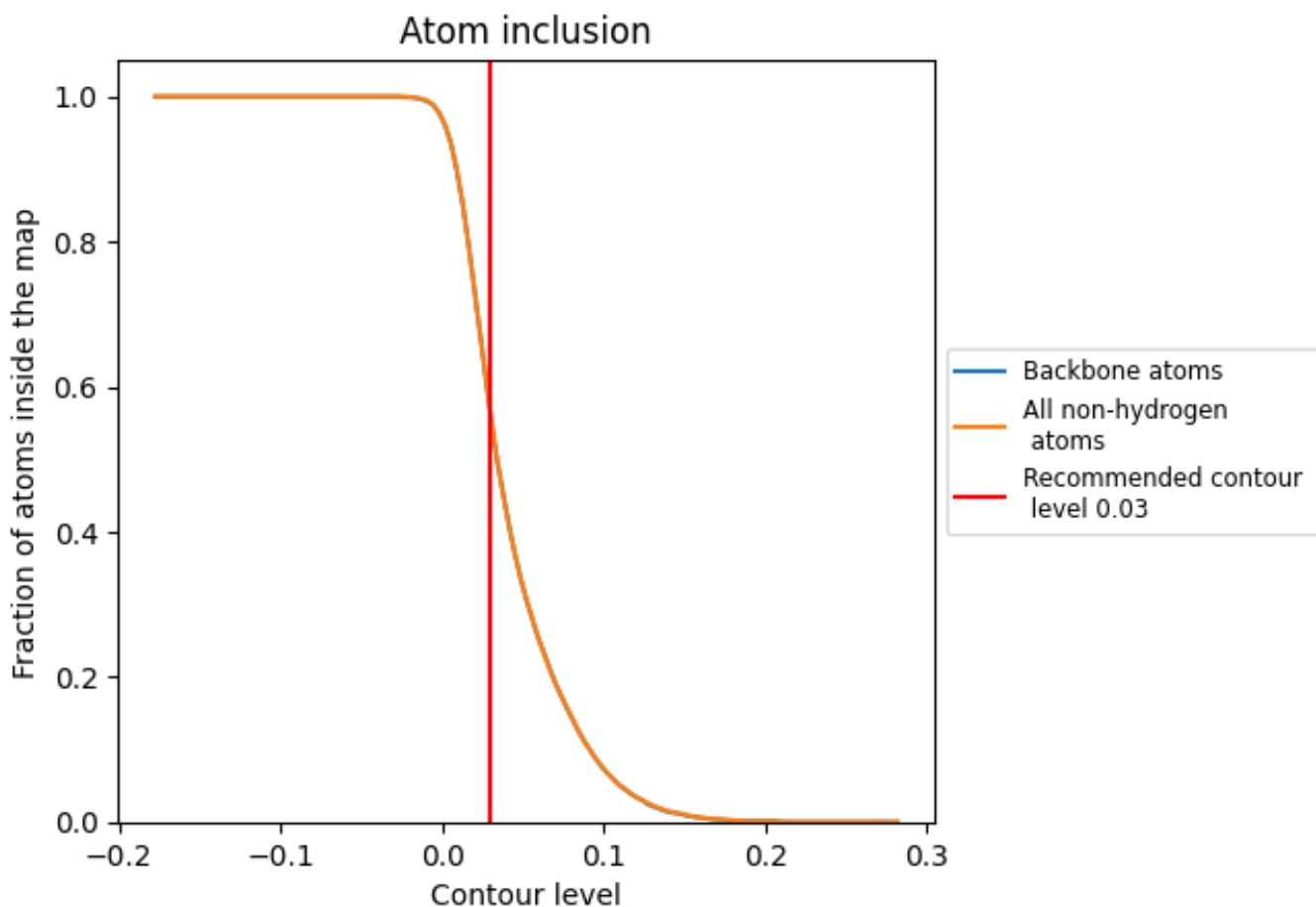
At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.2750
A	0.6340	0.3120
B	0.6310	0.3100
D	0.4590	0.1190
E	0.4640	0.1270
W	0.4600	0.2440
X	0.6180	0.3600
Y	0.4580	0.2470
Z	0.6030	0.3710

1.0

0.0
<0.0