



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:29 PM UTC

PDB ID : 6BCX / pdb_00006bcx
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 ⓘ symbol.

The types of validation reports are described at

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

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

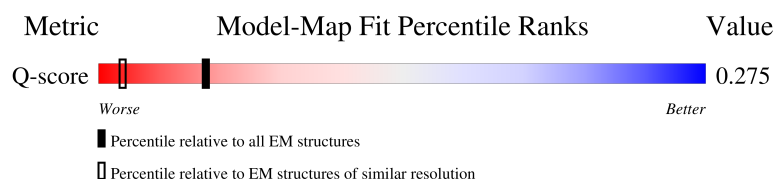
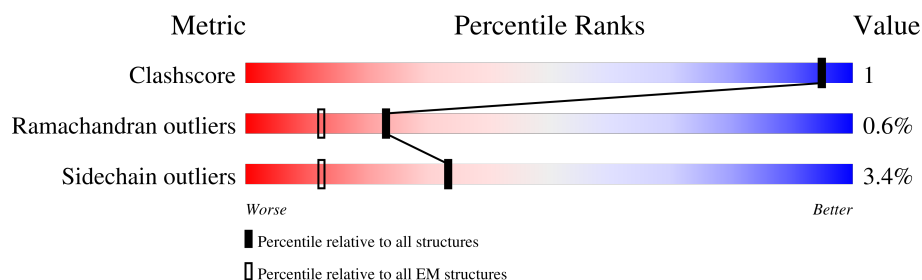
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 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	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	14612 (2.73 - 3.73)

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	20% 80% 5% 15%
1	B	2549	20% 80% 5% 15%
2	D	326	42% 90% 6% ...
2	E	326	39% 90% 7% ...

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Mol	Chain	Length	Quality of chain
3	W	1343	39%73%5%22%
3	Y	1343	39%73%•22%
4	X	122	7%93%
4	Z	122	7%93%

2 Entry composition

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	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		
1	B	2178	Total	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		

- 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
			4809	1526	2353	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		

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

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

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	C	H	N	O	S	0	0
			126	42	58	9	16	1		
4	Z	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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	

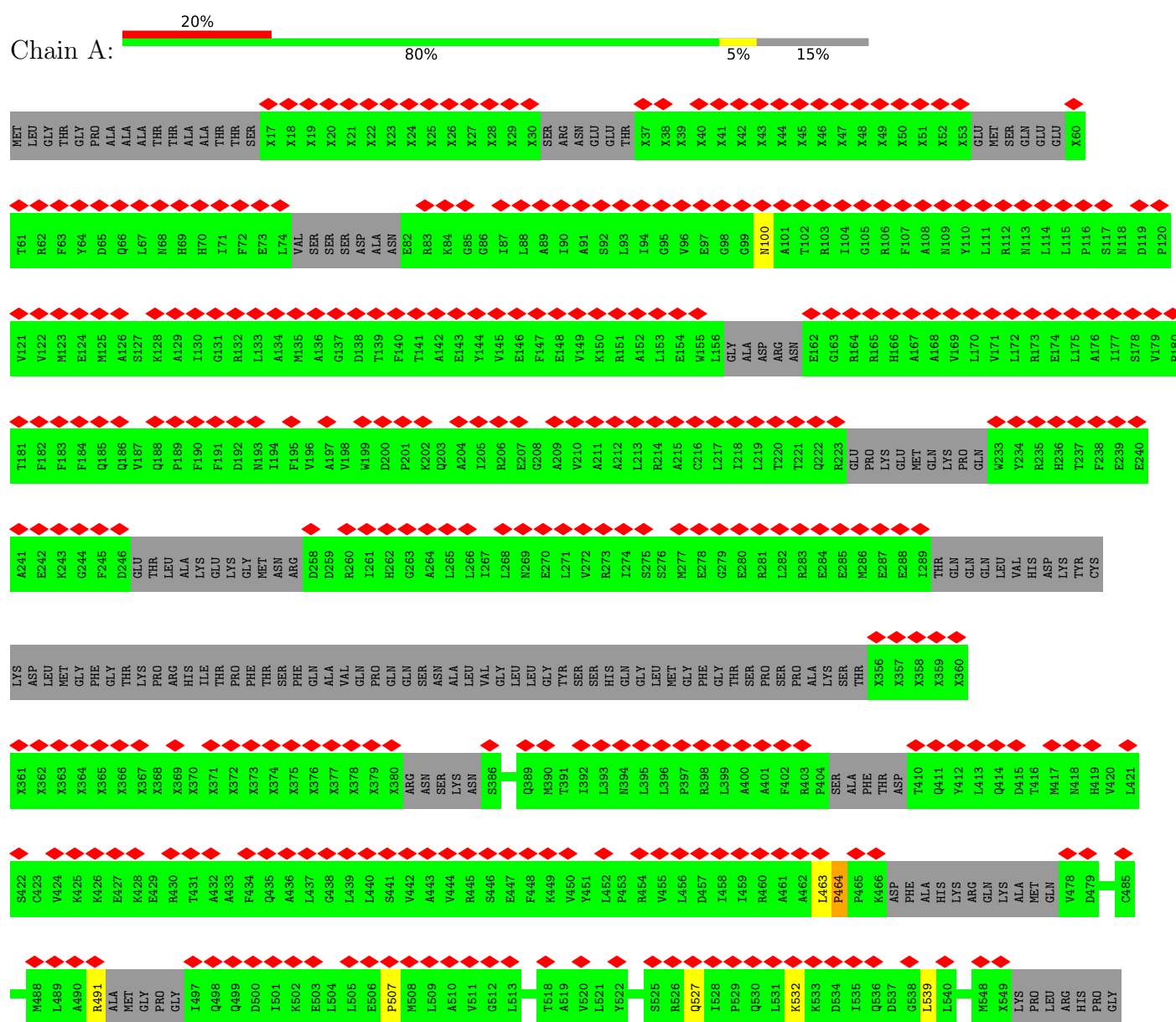
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



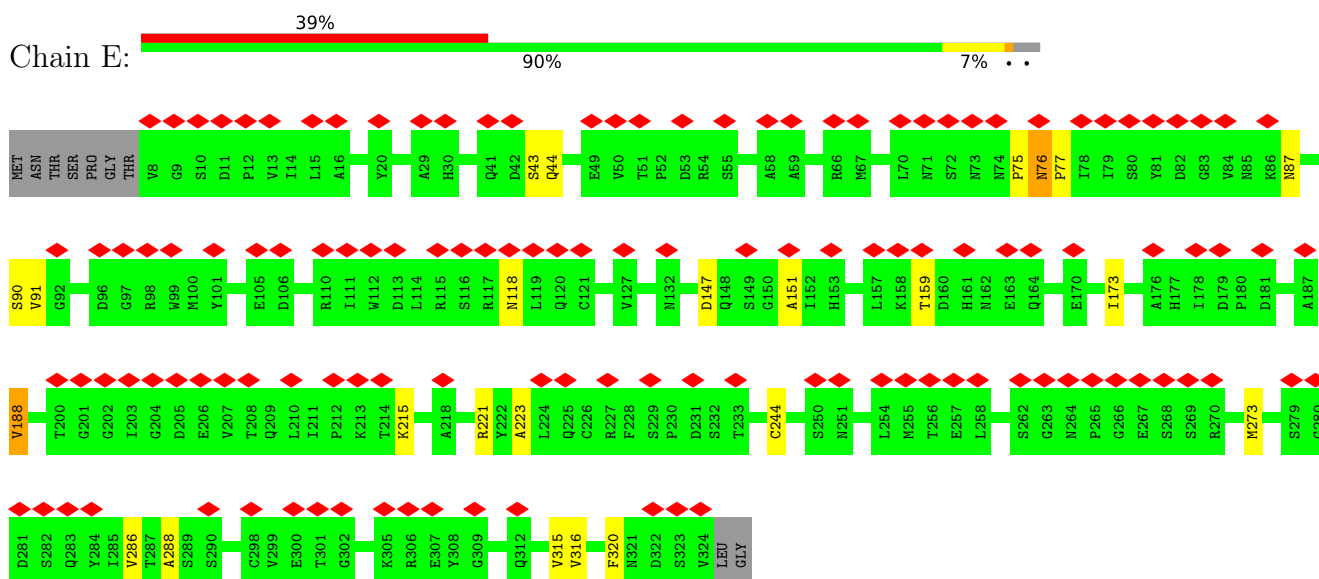


H1084	P896	T665	T484	S422	X361	LYS	A241	T181	V121	T61	MET
D1085	H899	C485	C486	C423	X362	ASP	E242	F182	V122	R62	LEU
M1086	I903	L489	L490	V424	X363	NET	G243	F183	M123	F63	GLY
S1087	I903	L490	R491	K425	X364	GLN	G244	F184	E124	V64	THR
I1091	GLY	A491	A492	K426	X367	PHE	F245	Q186	M125	D65	PRO
L1097	MET	A493	A494	E427	X368	GLY	D246	Q187	A126	Q66	ALA
L1102	ASP	A495	A496	K428	X369	THR	GLU	V187	S127	L67	ALA
L1121	ASP	A497	A498	E429	X370	PRO	THR	Q188	A128	L67	ALA
F1122	ASP	A499	A500	R430	X371	GLY	ALA	Q189	A129	H68	THR
D1123	ASP	A501	A502	T431	X372	ILE	ALA	F189	I130	H70	ALA
E1126	ASP	A503	A504	A432	X373	THR	GLY	F190	GLU	I71	ALA
I1155	ASP	A505	A506	A433	X374	THR	GLY	F191	G131	I71	THR
I1159	ASP	A507	A508	F434	X375	THR	GLY	D192	F72	F72	THR
V1160	ASP	A509	A510	Q435	X376	THR	GLY	M193	E73	E73	SER
R1161	ASP	A511	A512	Q436	X377	THR	GLY	M194	L74	L74	SER
D1164	ASP	A513	A514	A437	X378	THR	GLY	F195	VAL	VAL	SER
E1168	ASP	A515	A516	L437	X379	THR	GLY	V196	SER	SER	SER
S1178	ASP	A517	A518	L438	X380	THR	GLY	A197	SER	SER	SER
S1179	ASP	A519	A520	L439	X381	THR	GLY	V198	ASP	ASP	ASP
Q1183	ASP	A521	A522	L440	X382	THR	GLY	W199	ALA	ALA	ALA
I1192	ASP	A523	A524	L441	X383	THR	GLY	D200	ASN	ASN	ASN
V1198	ASP	A525	A526	V442	X384	THR	GLY	P201	F140	F140	ASN
I1213	ASP	A527	A528	A443	X385	THR	GLY	T141	R83	R83	ASN
T1221	ASP	A529	A530	A444	X386	THR	GLY	A142	K84	K84	ASN
L1222	ASP	A531	A532	V445	X387	THR	GLY	E143	G85	G85	ASN
ALA	ASP	A533	A534	S446	X388	THR	GLY	Y144	G86	G86	ASN
ASP	ASP	A535	A536	E447	X389	THR	GLY	I205	I87	I87	ASN
GLU	ASP	A537	A538	F448	X390	THR	GLY	R206	L88	L88	ASN
GLU	ASP	A539	A540	K449	X391	THR	GLY	E207	A89	A89	ASN
GLU	ASP	A541	A542	V450	X392	THR	GLY	G208	I90	I90	ASN
GLU	ASP	A543	A544	Y451	X393	THR	GLY	E148	A91	A91	ASN
GLU	ASP	A545	A546	L452	X394	THR	GLY	V210	S92	S92	ASN
GLU	ASP	A547	A548	L453	X395	THR	GLY	A211	R151	R151	ASN
GLU	ASP	A549	A550	L454	X396	THR	GLY	A152	I94	I94	ASN
GLU	ASP	A551	A552	L455	X397	THR	GLY	L153	G95	G95	ASN
GLU	ASP	A553	A554	L456	X398	THR	GLY	E154	V96	V96	ASN
GLU	ASP	A555	A556	L457	X399	THR	GLY	W155	E97	E97	ASN
GLU	ASP	A557	A558	L458	X400	THR	GLY	C216	G98	G98	ASN
GLU	ASP	A559	A560	L459	X401	THR	GLY	L217	G99	G99	ASN
GLU	ASP	A561	A562	L460	X402	THR	GLY	L218	M100	M100	ASN
GLU	ASP	A563	A564	L461	X403	THR	GLY	L219	A101	A101	ASN
GLU	ASP	A565	A566	L462	X404	THR	GLY	T220	T102	T102	ASN
GLU	ASP	A567	A568	L463	X405	THR	GLY	T221	G163	G163	ASN
GLU	ASP	A569	A570	L464	X406	THR	GLY	Q222	R164	R164	ASN
GLU	ASP	A571	A572	L465	X407	THR	GLY	E162	G165	G165	ASN
GLU	ASP	A573	A574	L466	X408	THR	GLY	R166	R166	R166	ASN
GLU	ASP	A575	A576	L467	X409	THR	GLY	H167	F107	F107	ASN
GLU	ASP	A577	A578	L468	X410	THR	GLY	A168	A108	A108	ASN
GLU	ASP	A579	A580	L469	X411	THR	GLY	V169	M109	M109	ASN
GLU	ASP	A581	A582	L470	X412	THR	GLY	L170	Y110	Y110	ASN
GLU	ASP	A583	A584	L471	X413	THR	GLY	V171	L111	L111	ASN
GLU	ASP	A585	A586	L472	X414	THR	GLY	L172	R112	R112	ASN
GLU	ASP	A587	A588	L473	X415	THR	GLY	M173	M113	M113	ASN
GLU	ASP	A589	A590	L474	X416	THR	GLY	E174	L114	L114	ASN
GLU	ASP	A591	A592	L475	X417	THR	GLY	L175	P116	P116	ASN
GLU	ASP	A593	A594	L476	X418	THR	GLY	T237	I177	I177	ASN
GLU	ASP	A595	A596	L477	X419	THR	GLY	F238	N118	N118	ASN
GLU	ASP	A597	A598	L478	X420	THR	GLY	E239	V179	V179	ASN
GLU	ASP	A599	A600	L479	X421	THR	GLY	E240	P180	P180	ASN

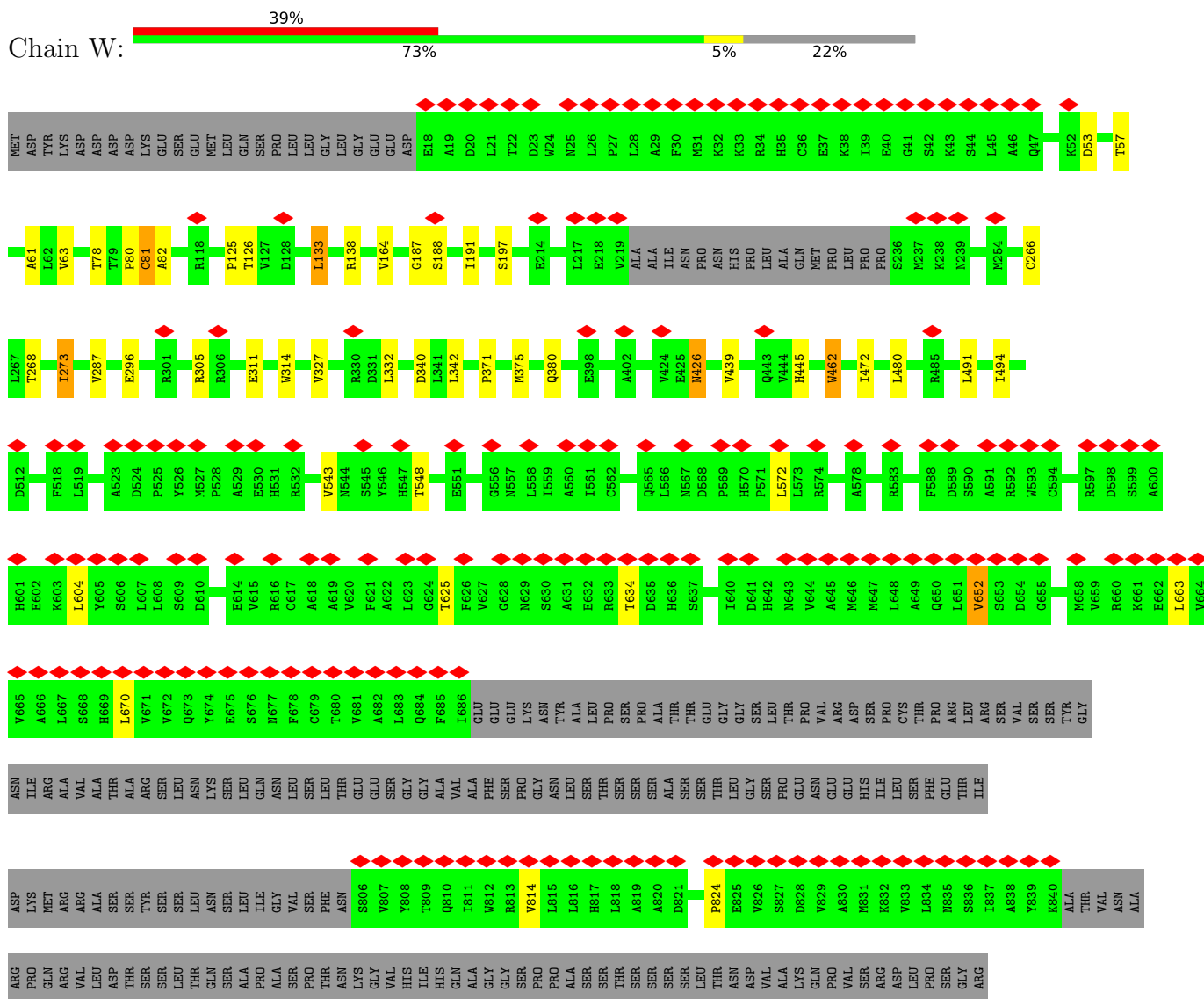


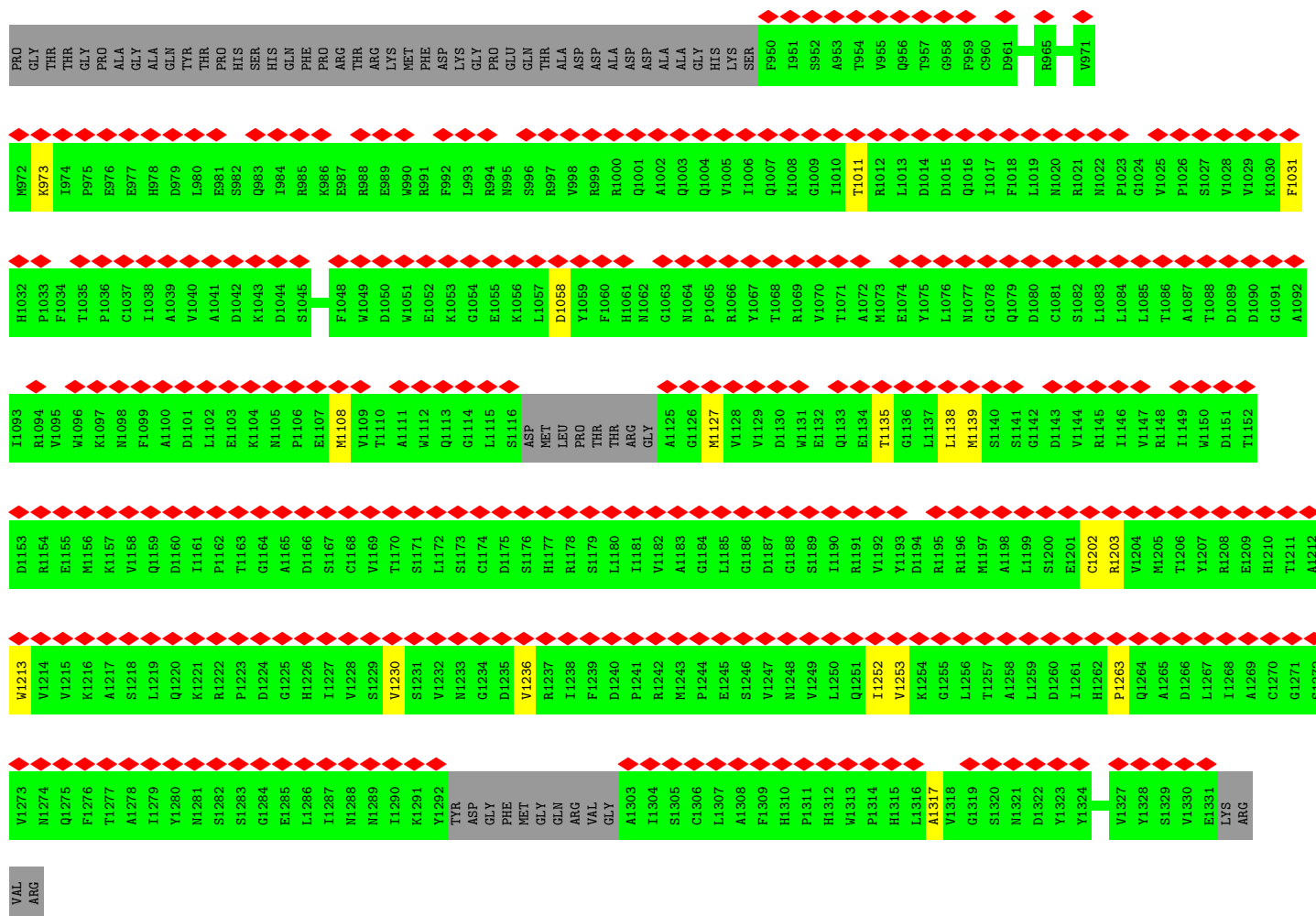
S268	S269	S270	M273	F278	S279	G280	D281	S282	Q283	Y284	I285	V286	T287	A288	S289	S290	L293	C298	V299	E300	T301	G302	K305	R306	E307	V308	G309	G310	H311	Q312	V315	V316	F320	M321	D322	S323	V324	LEU	GLY											
I178	D179	D181	A187	V188	T200	G201	G202	T203	G204	D205	E206	V207	T208	Q209	L210	K213	T214	K215	A218	R221	A223	E225	L224	Q226	C226	R227	F228	S229	P230	D231	S232	T233	A236	C244	K245	T246	S250	N251	M255	T256	E257	L258	S262	Q263	M264	P265	Q266	E267		
N85	K86	N87	S90	V91	G92	F93	D96	G97	R98	E105	D106	R110	I111	W112	D113	L114	R115	S116	R117	N118	L119	Q120	C121	F125	Q126	V127	I131	M132	N139	A151	I152	H153	L157	I158	T159	D160	H161	N162	E163	Q164	P167	E168	P169	E170	I173	A176	H177			
MET	ASN	THR	SER	PRO	GLY	THR	V8	G9	S10	D11	P12	V13	I14	L15	A16	Y20	A29	R20	I33	T37	Q41	D42	S43	Q44	E49	V50	T51	P52	D53	R54	S55	A58	A59	R66	M67	L70	N71	S72	N73	N74	P75	N76	P77	I78	I79	S80	Y81	D82	G83	V84

- Molecule 2: Target of rapamycin complex subunit LST8



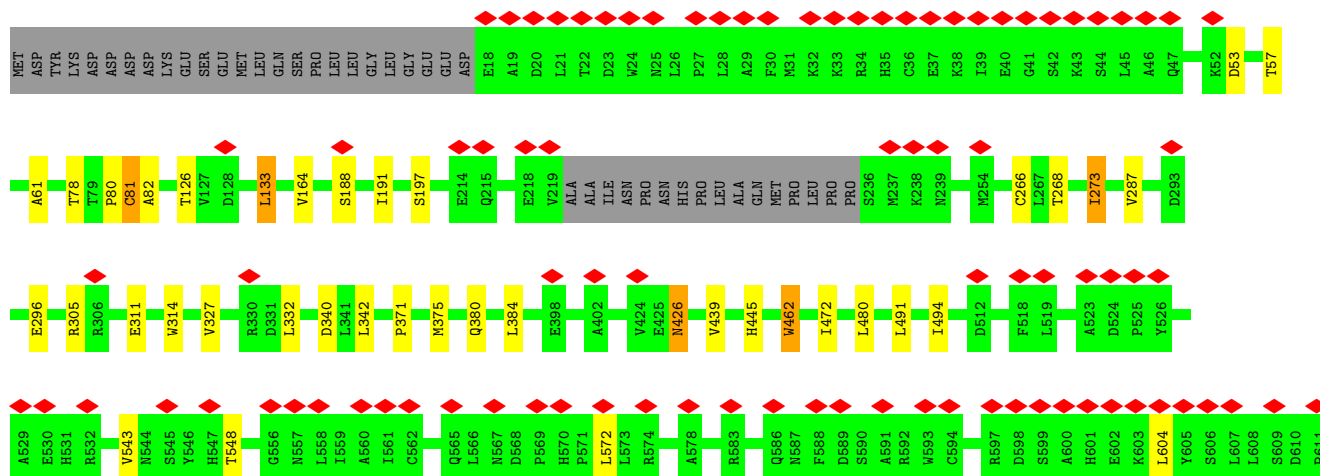
- Molecule 3: Regulatory-associated protein of mTOR

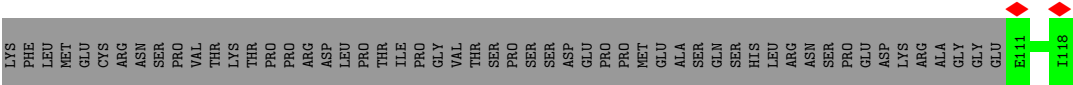




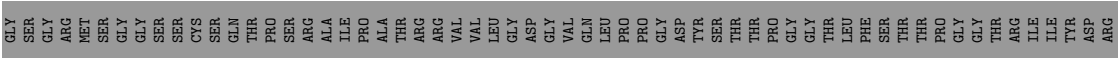
• Molecule 3: Regulatory-associated protein of mTOR

Chain Y:





● 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, 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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.61	1/17398 (0.0%)	0.90	8/23547 (0.0%)
1	B	0.61	1/17398 (0.0%)	0.90	7/23547 (0.0%)
2	D	0.57	0/2514	0.75	0/3426
2	E	0.57	0/2514	0.75	0/3426
3	W	0.58	0/8585	0.84	1/11680 (0.0%)
3	Y	0.58	0/8585	0.83	1/11680 (0.0%)
4	X	0.53	0/68	0.65	0/89
4	Z	0.52	0/68	0.65	0/89
All	All	0.60	2/57130 (0.0%)	0.87	17/77484 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ASN	CA-C	6.00	1.55	1.52
1	B	100	ASN	CA-C	5.96	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	PRO	N-CA-C	7.63	120.01	110.70
1	B	464	PRO	N-CA-C	7.63	120.00	110.70
1	B	1973	ILE	N-CA-CB	6.05	118.77	110.54
1	A	1973	ILE	N-CA-CB	6.02	118.73	110.54
1	B	895	ASP	CA-C-N	5.77	127.05	119.84
1	B	895	ASP	C-N-CA	5.77	127.05	119.84
1	A	895	ASP	CA-C-N	5.73	127.01	119.84
1	A	895	ASP	C-N-CA	5.73	127.01	119.84
1	B	1192	ILE	CA-C-N	5.58	125.04	119.24
1	B	1192	ILE	C-N-CA	5.58	125.04	119.24
1	A	899	HIS	N-CA-C	5.42	119.06	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1192	ILE	CA-C-N	5.41	124.86	119.24
1	A	1192	ILE	C-N-CA	5.41	124.86	119.24
1	B	899	HIS	N-CA-C	5.37	119.00	112.23
3	W	652	VAL	N-CA-C	-5.16	106.04	110.74
1	A	1116	PRO	N-CA-C	5.09	116.91	110.70
3	Y	652	VAL	N-CA-C	-5.04	106.15	110.74

There are no chirality outliers.

There are no planarity outliers.

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	17348	17686	17376	38	0
1	B	17348	17686	17376	38	0
2	D	2456	2353	2341	9	0
2	E	2456	2353	2341	9	0
3	W	8385	8406	8375	19	0
3	Y	8385	8406	8375	16	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	123	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 (123) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1759:LEU:HD11	1:A:1796:MET:HE3	1.88	0.56
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	1.87	0.55
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:A:1018:MET:HE2	1:A:1058:GLN:HE22	1.76	0.49
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.44	0.49
1:B:1018:MET:HE2	1:B:1058:GLN:HE22	1.77	0.49
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.94	0.49
3:W:824:PRO:HD3	3:W:1108:MET:HE3	1.95	0.49
3:Y:824:PRO:HD3	3:Y:1108:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:MET:HE1	1:B:1319:ASN:HB2	1.97	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
3:W:462:TRP:CD1	3:W:462:TRP:C	2.94	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
1:B:873:LYS:NZ	1:B:1576:THR:O	2.42	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:934:MET:HE1	1:A:1319:ASN:HB2	2.00	0.43
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
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
3:Y:462:TRP:CD1	3:Y:462:TRP:C	2.95	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: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
1:B:799:LEU:HD11	1:B:827:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:327:VAL:HG12	3:W:371:PRO:HG2	2.01	0.42
1:A:799:LEU:HD11	1:A:827:MET:HE1	2.01	0.41
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
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
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
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%)	30	60
1	B	2088/2549 (82%)	1973 (94%)	106 (5%)	9 (0%)	30	60
2	D	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	9	37
2	E	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	9	37
3	W	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	18	50
3	Y	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	18	50
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%)	23	53

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	893	ALA
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

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Mol	Chain	Res	Type
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%)	1795 (96%)	66 (4%)	32	60
1	B	1861/2166 (86%)	1797 (97%)	64 (3%)	32	61
2	D	269/276 (98%)	263 (98%)	6 (2%)	45	68
2	E	269/276 (98%)	263 (98%)	6 (2%)	45	68
3	W	928/1171 (79%)	894 (96%)	34 (4%)	30	59
3	Y	928/1171 (79%)	894 (96%)	34 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	8/104 (8%)	8 (100%)	0	100	100
4	Z	8/104 (8%)	8 (100%)	0	100	100
All	All	6132/7434 (82%)	5922 (97%)	210 (3%)	33	61

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	LYS
1	A	539	LEU
1	A	656	LEU
1	A	659	LEU
1	A	665	THR
1	A	698	VAL
1	A	760	LEU
1	A	767	LEU
1	A	768	ILE
1	A	821	PHE
1	A	851	THR
1	A	863	THR
1	A	870	ASN
1	A	882	ARG
1	A	894	LEU
1	A	896	PRO
1	A	934	MET
1	A	1014	GLN
1	A	1019	LEU
1	A	1023	VAL
1	A	1055	LEU
1	A	1066	GLU
1	A	1084	HIS
1	A	1097	LEU
1	A	1102	LEU
1	A	1121	LEU
1	A	1160	VAL
1	A	1164	ASP
1	A	1178	SER
1	A	1179	SER
1	A	1183	GLN
1	A	1213	ILE
1	A	1262	THR
1	A	1275	VAL

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Mol	Chain	Res	Type
1	A	1287	LEU
1	A	1299	SER
1	A	1337	LEU
1	A	1360	LEU
1	A	1402	LEU
1	A	1448	THR
1	A	1515	MET
1	A	1552	LEU
1	A	1575	LEU
1	A	1593	CYS
1	A	1617	GLN
1	A	1652	THR
1	A	1701	MET
1	A	1752	LEU
1	A	1758	GLN
1	A	1780	THR
1	A	1956	LEU
1	A	1967	TYR
1	A	1973	ILE
1	A	1988	HIS
1	A	2005	LEU
1	A	2021	ILE
1	A	2138	LEU
1	A	2232	THR
1	A	2260	LEU
1	A	2302	LEU
1	A	2344	LEU
1	A	2345	MET
1	A	2346	LEU
1	A	2353	ILE
1	A	2501	ILE
1	A	2548	PHE
2	D	90	SER
2	D	91	VAL
2	D	159	THR
2	D	173	ILE
2	D	188	VAL
2	D	215	LYS
3	W	78	THR
3	W	126	THR
3	W	133	LEU
3	W	164	VAL

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Mol	Chain	Res	Type
3	W	188	SER
3	W	191	ILE
3	W	197	SER
3	W	268	THR
3	W	273	ILE
3	W	287	VAL
3	W	296	GLU
3	W	311	GLU
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	494	ILE
3	W	543	VAL
3	W	548	THR
3	W	572	LEU
3	W	604	LEU
3	W	625	THR
3	W	634	THR
3	W	663	LEU
3	W	670	LEU
3	W	1011	THR
3	W	1058	ASP
3	W	1127	MET
3	W	1135	THR
3	W	1138	LEU
3	W	1139	MET
1	B	532	LYS
1	B	539	LEU
1	B	656	LEU
1	B	665	THR
1	B	698	VAL
1	B	760	LEU
1	B	767	LEU
1	B	768	ILE
1	B	821	PHE
1	B	851	THR
1	B	863	THR
1	B	870	ASN

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Mol	Chain	Res	Type
1	B	882	ARG
1	B	894	LEU
1	B	896	PRO
1	B	934	MET
1	B	1014	GLN
1	B	1019	LEU
1	B	1023	VAL
1	B	1055	LEU
1	B	1084	HIS
1	B	1097	LEU
1	B	1102	LEU
1	B	1121	LEU
1	B	1160	VAL
1	B	1164	ASP
1	B	1178	SER
1	B	1179	SER
1	B	1183	GLN
1	B	1213	ILE
1	B	1262	THR
1	B	1275	VAL
1	B	1287	LEU
1	B	1299	SER
1	B	1337	LEU
1	B	1360	LEU
1	B	1402	LEU
1	B	1448	THR
1	B	1515	MET
1	B	1552	LEU
1	B	1575	LEU
1	B	1593	CYS
1	B	1617	GLN
1	B	1652	THR
1	B	1701	MET
1	B	1752	LEU
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	2005	LEU
1	B	2021	ILE

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Mol	Chain	Res	Type
1	B	2138	LEU
1	B	2232	THR
1	B	2260	LEU
1	B	2302	LEU
1	B	2344	LEU
1	B	2345	MET
1	B	2346	LEU
1	B	2353	ILE
1	B	2501	ILE
1	B	2548	PHE
2	E	90	SER
2	E	91	VAL
2	E	159	THR
2	E	173	ILE
2	E	188	VAL
2	E	215	LYS
3	Y	78	THR
3	Y	126	THR
3	Y	133	LEU
3	Y	164	VAL
3	Y	188	SER
3	Y	191	ILE
3	Y	197	SER
3	Y	268	THR
3	Y	273	ILE
3	Y	287	VAL
3	Y	296	GLU
3	Y	311	GLU
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	494	ILE
3	Y	543	VAL
3	Y	548	THR
3	Y	572	LEU
3	Y	604	LEU
3	Y	625	THR
3	Y	634	THR

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Mol	Chain	Res	Type
3	Y	663	LEU
3	Y	670	LEU
3	Y	1011	THR
3	Y	1058	ASP
3	Y	1127	MET
3	Y	1135	THR
3	Y	1138	LEU
3	Y	1139	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	193	ASN
1	A	389	GLN
1	A	527	GLN
1	A	646	GLN
1	A	722	ASN
1	A	791	ASN
1	A	829	GLN
1	A	1014	GLN
1	A	1015	GLN
1	A	1045	ASN
1	A	1058	GLN
1	A	1334	GLN
1	A	1525	GLN
1	A	1808	ASN
1	A	1959	GLN
1	A	2003	ASN
1	A	2028	HIS
1	A	2071	ASN
1	A	2124	GLN
1	A	2154	GLN
1	A	2223	GLN
1	A	2385	ASN
1	A	2428	ASN
1	A	2540	GLN
2	D	39	GLN
2	D	41	GLN
3	W	67	ASN
3	W	107	GLN
3	W	212	GLN

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Mol	Chain	Res	Type
3	W	339	GLN
3	W	392	GLN
3	W	405	HIS
3	W	426	ASN
3	W	506	GLN
3	W	531	HIS
3	W	669	HIS
3	W	995	ASN
3	W	1105	ASN
3	W	1113	GLN
3	W	1159	GLN
3	W	1226	HIS
3	W	1233	ASN
3	W	1264	GLN
3	W	1289	ASN
1	B	193	ASN
1	B	389	GLN
1	B	498	GLN
1	B	527	GLN
1	B	646	GLN
1	B	791	ASN
1	B	829	GLN
1	B	1014	GLN
1	B	1015	GLN
1	B	1045	ASN
1	B	1058	GLN
1	B	1106	ASN
1	B	1334	GLN
1	B	1446	GLN
1	B	1525	GLN
1	B	1727	GLN
1	B	1808	ASN
1	B	1959	GLN
1	B	2003	ASN
1	B	2028	HIS
1	B	2071	ASN
1	B	2124	GLN
1	B	2223	GLN
1	B	2385	ASN
1	B	2428	ASN
2	E	39	GLN
2	E	41	GLN

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Mol	Chain	Res	Type
2	E	321	ASN
3	Y	67	ASN
3	Y	107	GLN
3	Y	114	GLN
3	Y	212	GLN
3	Y	392	GLN
3	Y	405	HIS
3	Y	426	ASN
3	Y	531	HIS
3	Y	669	HIS
3	Y	995	ASN
3	Y	1061	HIS
3	Y	1098	ASN
3	Y	1105	ASN
3	Y	1113	GLN
3	Y	1159	GLN
3	Y	1226	HIS
3	Y	1233	ASN
3	Y	1264	GLN
3	Y	1289	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	32,33,33	1.62	7 (21%)	48,52,52	1.76	11 (22%)
5	ATP	B	3000	6	32,33,33	1.63	7 (21%)	48,52,52	1.80	11 (22%)

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	-	3/22/38/38	0/3/3/3
5	ATP	B	3000	6	-	4/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3000	ATP	C5-C4	5.01	1.48	1.39
5	A	3000	ATP	C5-C4	4.71	1.47	1.39
5	B	3000	ATP	C5-C6	3.28	1.50	1.41
5	A	3000	ATP	C5-C6	3.23	1.50	1.41
5	A	3000	ATP	PB-O3A	3.20	1.62	1.59
5	B	3000	ATP	PB-O3A	3.05	1.62	1.59
5	A	3000	ATP	PA-O3A	2.95	1.62	1.59
5	B	3000	ATP	PA-O3A	2.83	1.62	1.59
5	B	3000	ATP	C8-N7	2.62	1.36	1.31
5	A	3000	ATP	C8-N7	2.44	1.36	1.31
5	A	3000	ATP	C4-N9	-2.19	1.33	1.37
5	A	3000	ATP	PB-O3B	2.15	1.61	1.59
5	B	3000	ATP	PB-O3B	2.06	1.61	1.59
5	B	3000	ATP	C4-N9	-2.03	1.33	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3000	ATP	C5-C4-N3	-4.94	119.92	126.72
5	A	3000	ATP	C5-C4-N3	-4.90	119.96	126.72
5	A	3000	ATP	N3-C4-N9	3.92	133.83	127.17
5	B	3000	ATP	N3-C2-N1	-3.89	122.70	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3000	ATP	N3-C2-N1	-3.86	122.73	128.58
5	B	3000	ATP	N3-C4-N9	3.85	133.71	127.17
5	B	3000	ATP	C2-N3-C4	3.81	121.15	111.83
5	A	3000	ATP	C2-N3-C4	3.79	121.10	111.83
5	B	3000	ATP	C4-C5-N7	-3.75	106.29	110.58
5	A	3000	ATP	C4-C5-N7	-3.60	106.47	110.58
5	A	3000	ATP	C4-N9-C8	3.39	109.30	105.74
5	B	3000	ATP	C4-N9-C8	3.26	109.16	105.74
5	B	3000	ATP	C5-N7-C8	2.81	107.87	103.45
5	B	3000	ATP	C6-C5-N7	2.74	137.37	132.09
5	A	3000	ATP	C6-C5-N7	2.63	137.17	132.09
5	A	3000	ATP	C5-N7-C8	2.63	107.58	103.45
5	B	3000	ATP	N9-C8-N7	-2.57	110.30	113.94
5	A	3000	ATP	N9-C8-N7	-2.46	110.45	113.94
5	B	3000	ATP	C2-N1-C6	2.27	122.46	118.73
5	A	3000	ATP	O2B-PB-O3A	2.17	113.14	107.27
5	A	3000	ATP	C2-N1-C6	2.14	122.25	118.73
5	B	3000	ATP	O2B-PB-O3A	2.10	112.96	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

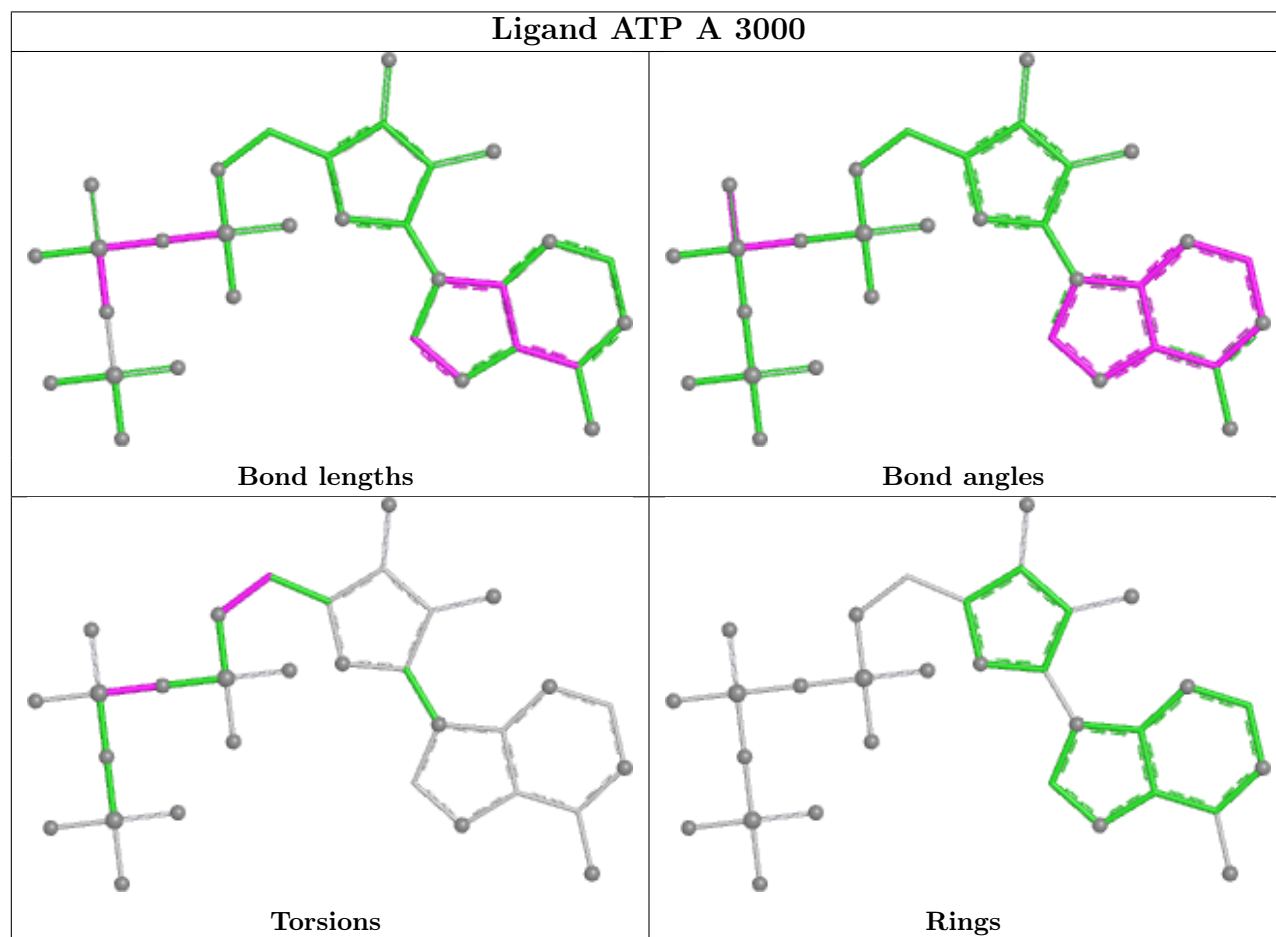
Mol	Chain	Res	Type	Atoms
5	B	3000	ATP	PG-O3B-PB-O1B
5	B	3000	ATP	PA-O3A-PB-O1B
5	A	3000	ATP	PA-O3A-PB-O2B
5	B	3000	ATP	PA-O3A-PB-O2B
5	A	3000	ATP	C4'-C5'-O5'-PA
5	B	3000	ATP	PG-O3B-PB-O2B
5	A	3000	ATP	PA-O3A-PB-O1B

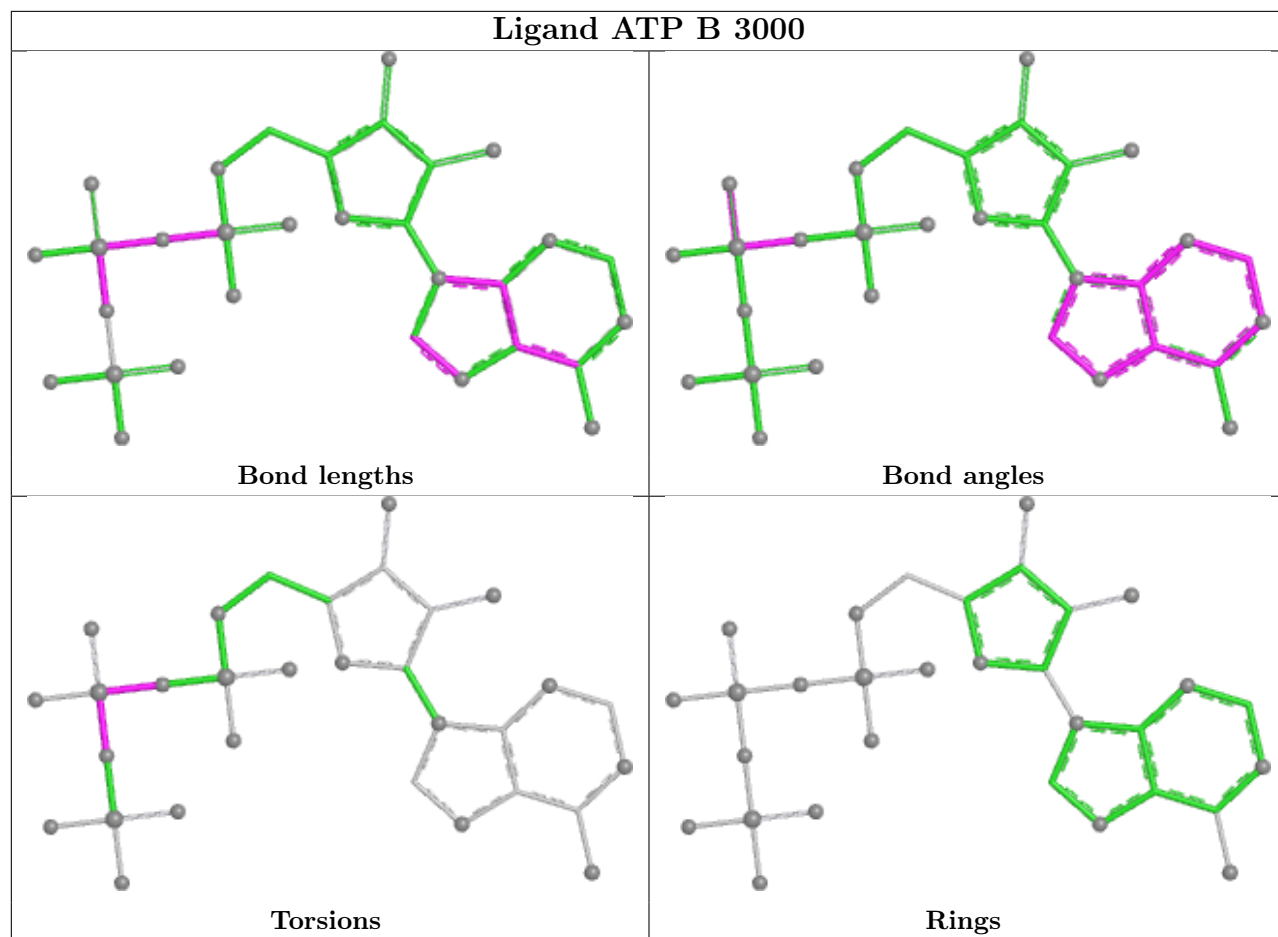
There are no ring outliers.

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.

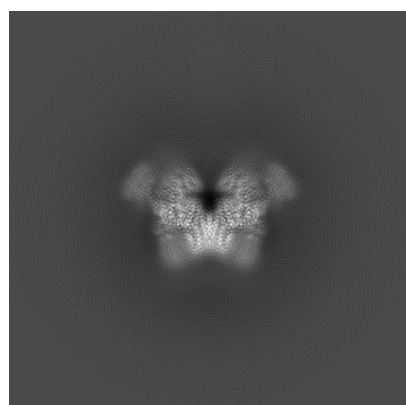
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7087. These allow visual inspection of the internal detail of the map and identification of artifacts.

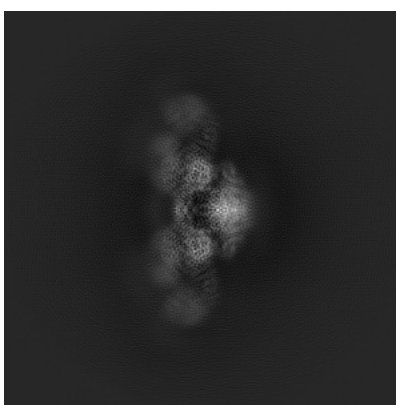
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

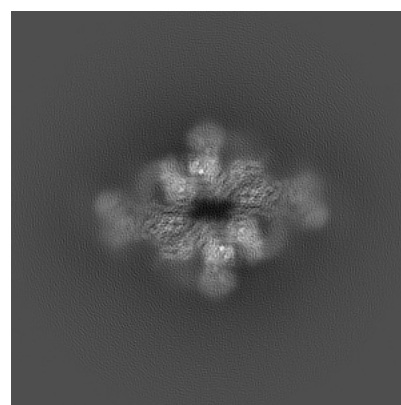
6.1.1 Primary map



X



Y

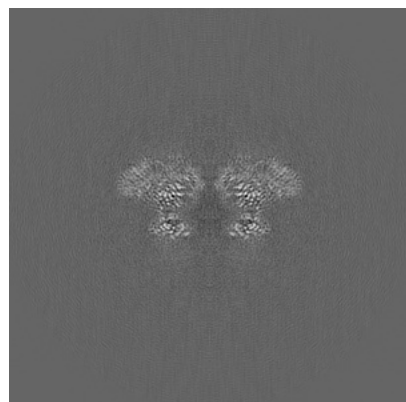


Z

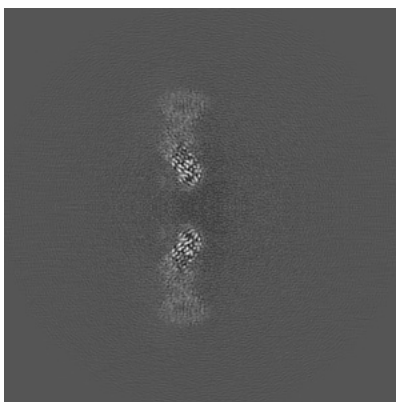
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

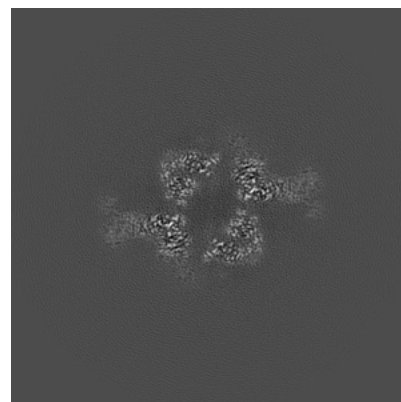
6.2.1 Primary map



X Index: 187



Y Index: 187

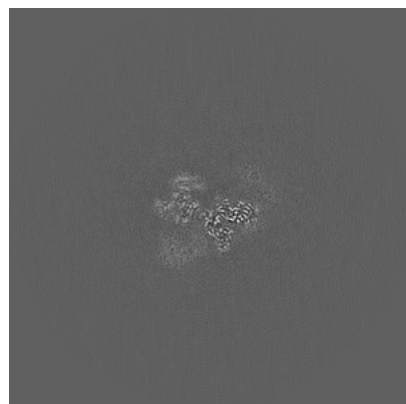


Z Index: 187

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

6.3 Largest variance slices [i](#)

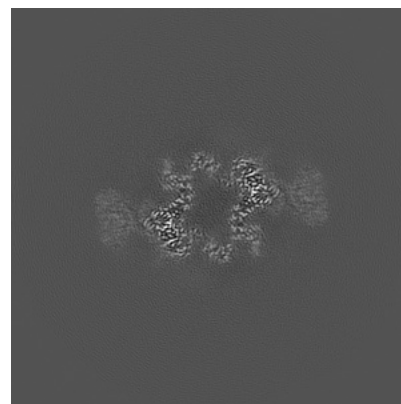
6.3.1 Primary map



X Index: 222



Y Index: 169

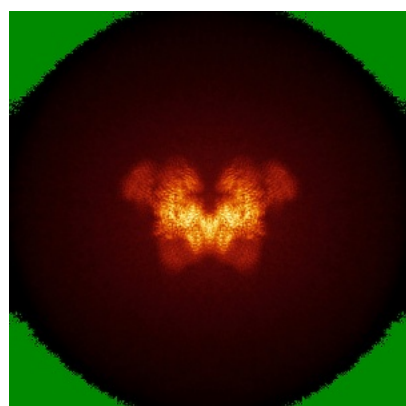


Z Index: 177

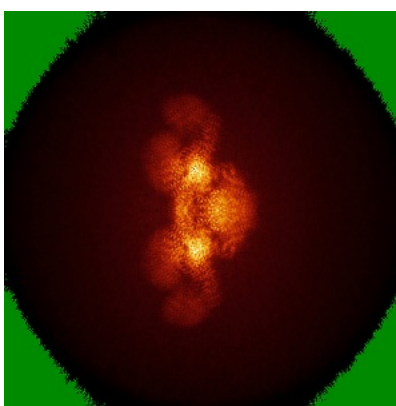
The images above show the largest variance slices of the map in three orthogonal directions.

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

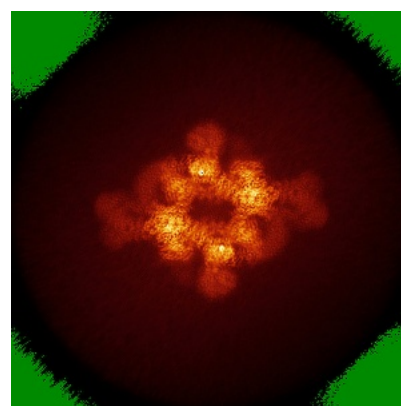
6.4.1 Primary map



X



Y

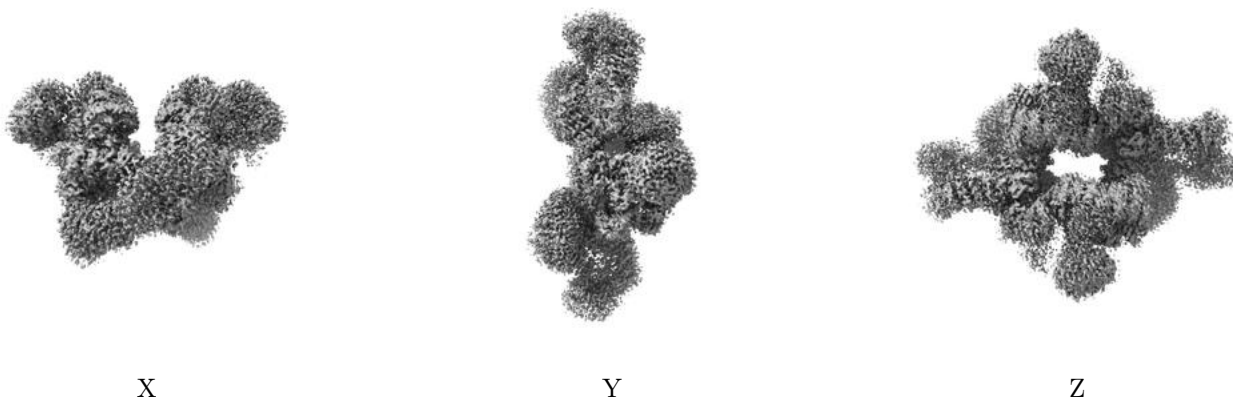


Z

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 [i](#)

6.5.1 Primary map



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.

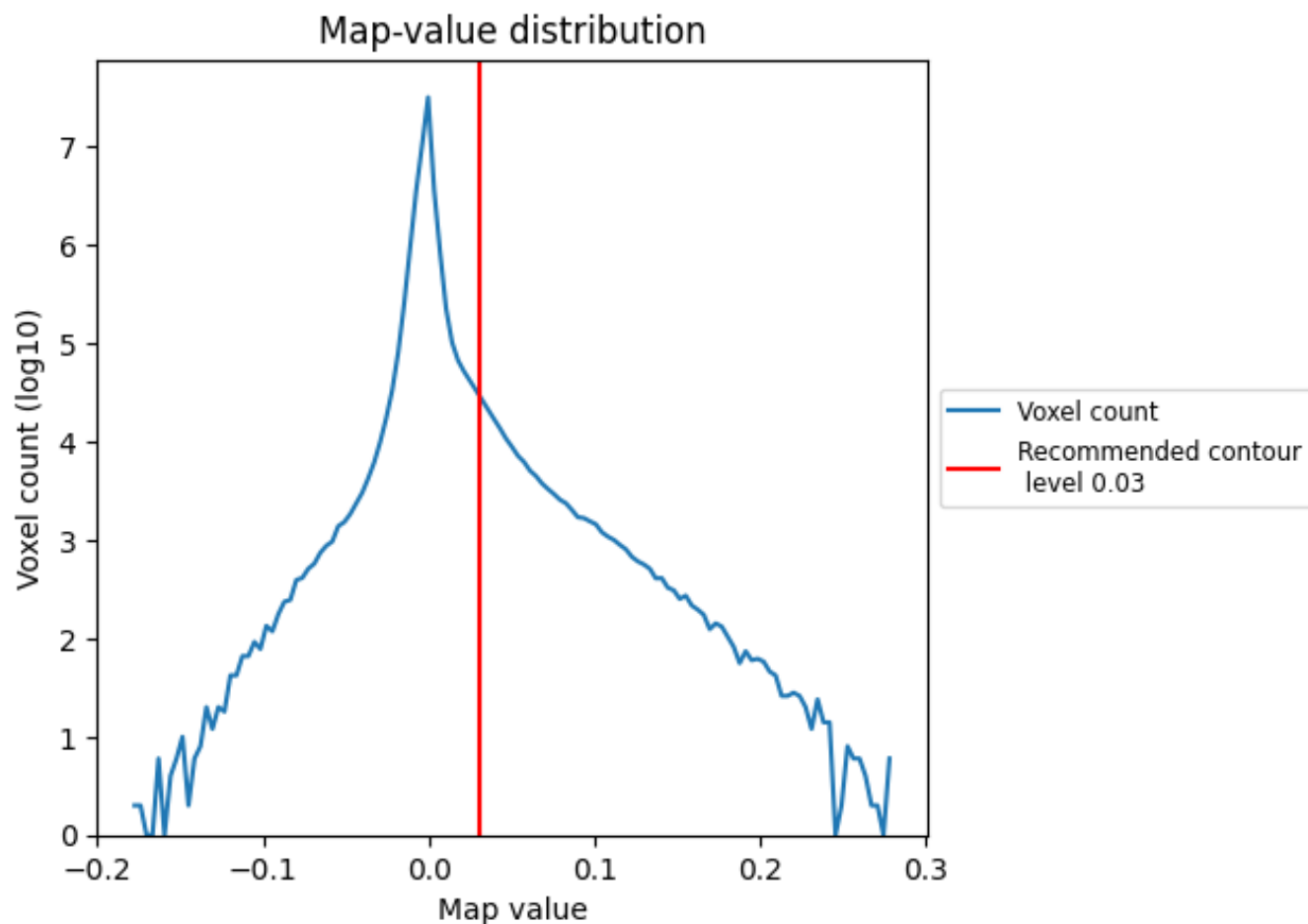
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

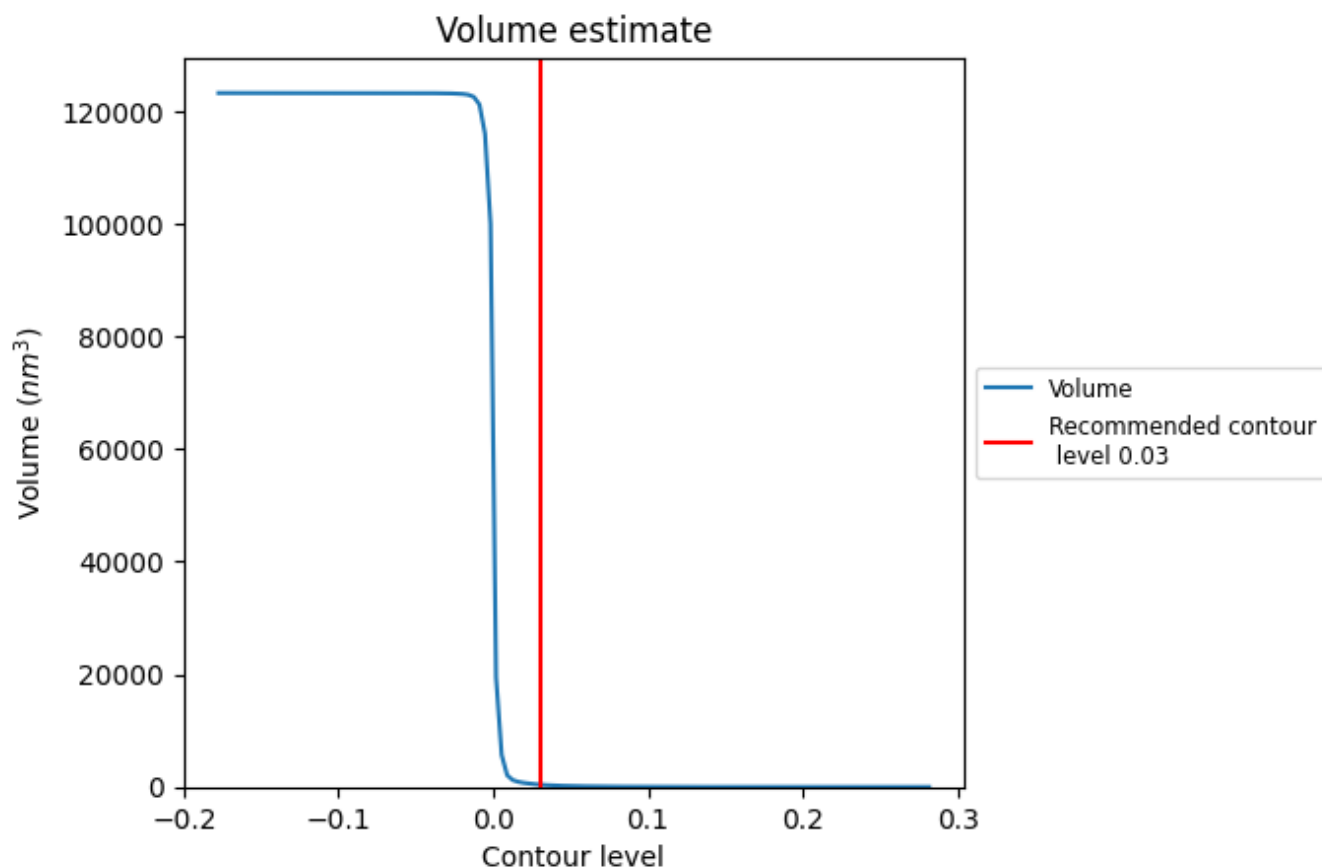
This section contains the results of statistical analysis of the map.

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.

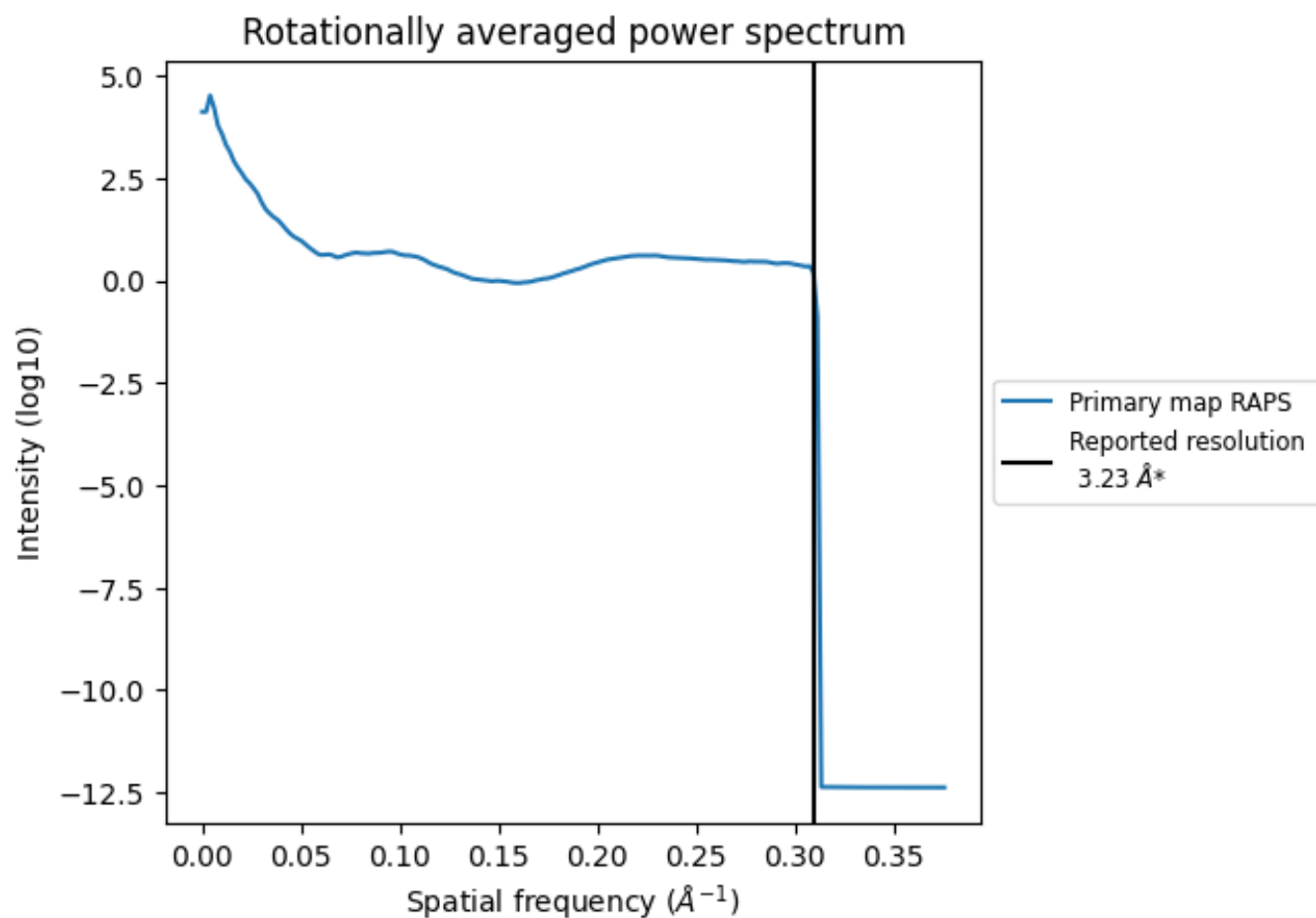
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; 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

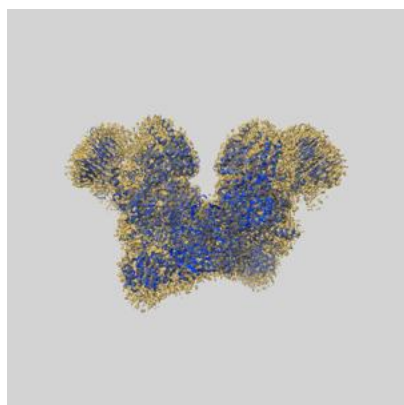
8 Fourier-Shell correlation ⓘ

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

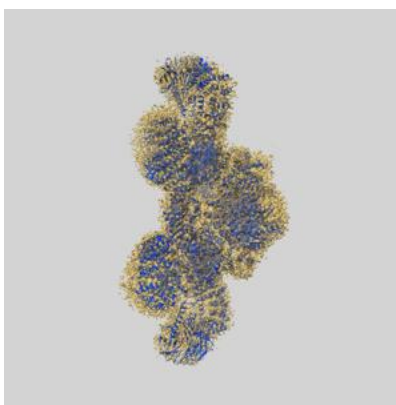
9 Map-model fit [i](#)

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 [7](#).

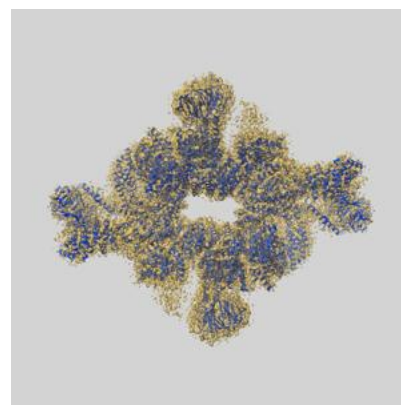
9.1 Map-model overlay [i](#)



X



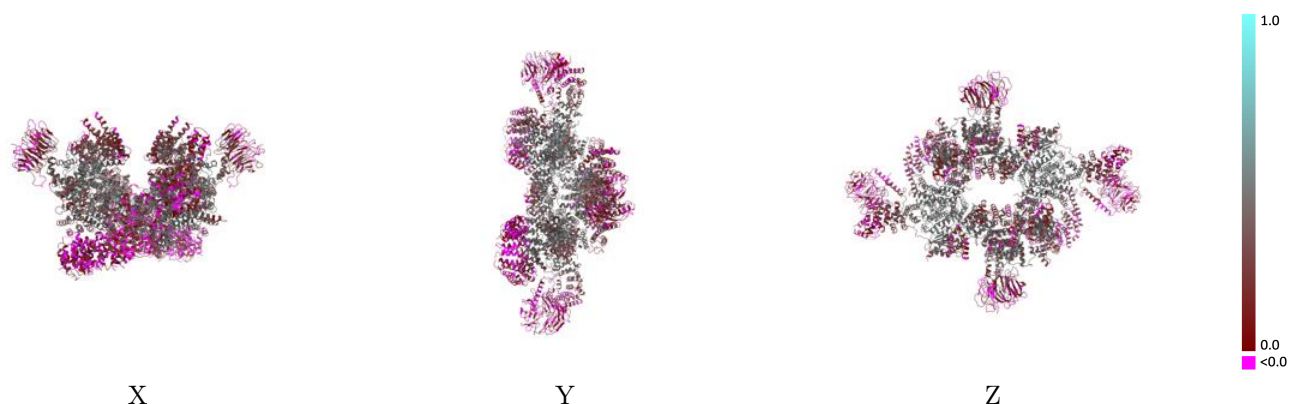
Y



Z

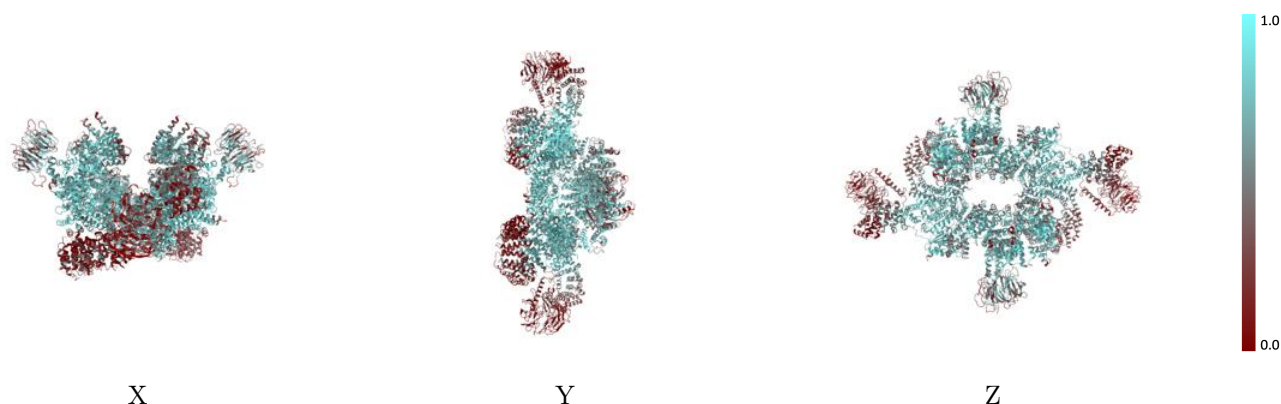
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



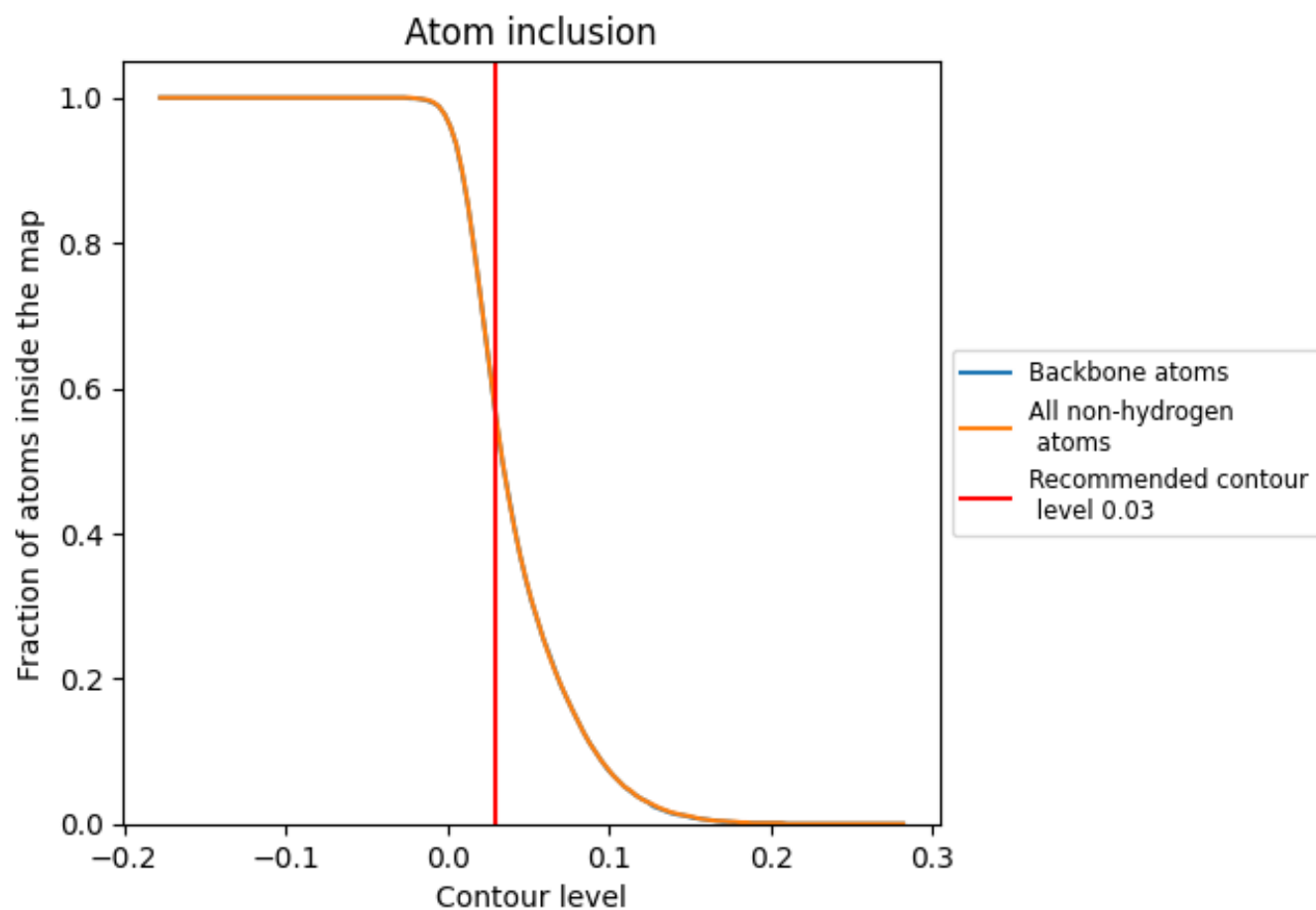
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



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