



Full wwPDB EM Validation Report ⓘ

Apr 29, 2024 – 01:43 am BST

PDB ID : 5FVM
EMDB ID : EMD-3329
Title : Cryo electron microscopy of a complex of Tor and Lst8
Authors : Baretic, D.; Berndt, A.; Ohashi, Y.; Johnson, C.M.; Williams, R.L.
Deposited on : 2016-02-09
Resolution : 6.70 Å(reported)
Based on initial model : 4JSV

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.dev92
MolProbity : 4.02b-467
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) : 2.36.2

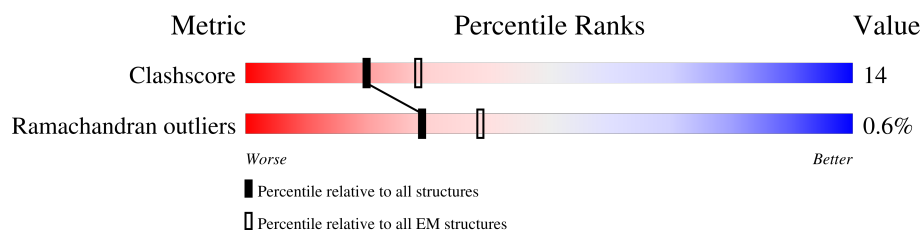
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 6.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	2471	
1	B	2471	
2	C	303	
2	D	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERINE/THREONINE-PROTEIN KINASE TOR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2117	Total 10508	C 6274	N 2117	O 2117	0	0
1	B	2117	Total 10508	C 6274	N 2117	O 2117	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLU	-	expression tag	UNP A0A090BKR
A	-19	LEU	-	expression tag	UNP A0A090BKR
A	-18	LEU	-	expression tag	UNP A0A090BKR
A	-17	GLU	-	expression tag	UNP A0A090BKR
A	-16	GLY	-	expression tag	UNP A0A090BKR
A	-15	GLU	-	expression tag	UNP A0A090BKR
A	-14	LEU	-	expression tag	UNP A0A090BKR
A	-13	LYS	-	expression tag	UNP A0A090BKR
A	-12	THR	-	expression tag	UNP A0A090BKR
A	-11	ALA	-	expression tag	UNP A0A090BKR
A	-10	ALA	-	expression tag	UNP A0A090BKR
A	-9	LEU	-	expression tag	UNP A0A090BKR
A	-8	ALA	-	expression tag	UNP A0A090BKR
A	-7	GLN	-	expression tag	UNP A0A090BKR
A	-6	HIS	-	expression tag	UNP A0A090BKR
A	-5	ASP	-	expression tag	UNP A0A090BKR
A	-4	GLU	-	expression tag	UNP A0A090BKR
A	-3	ALA	-	expression tag	UNP A0A090BKR
A	-2	MET	-	expression tag	UNP A0A090BKR
A	-1	GLY	-	expression tag	UNP A0A090BKR
A	0	GLY	-	expression tag	UNP A0A090BKR
A	1	SER	-	expression tag	UNP A0A090BKR
A	34	ALA	THR	conflict	UNP A0A090BKR
A	44	ALA	PRO	conflict	UNP A0A090BKR
A	48	MET	ILE	conflict	UNP A0A090BKR
A	125	ASP	GLU	conflict	UNP A0A090BKR

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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	ARG	THR	conflict	UNP A0A090BKR
A	998	LEU	VAL	conflict	UNP A0A090BKR
A	1063	VAL	ALA	conflict	UNP A0A090BKR
B	-20	GLU	-	expression tag	UNP A0A090BKR
B	-19	LEU	-	expression tag	UNP A0A090BKR
B	-18	LEU	-	expression tag	UNP A0A090BKR
B	-17	GLU	-	expression tag	UNP A0A090BKR
B	-16	GLY	-	expression tag	UNP A0A090BKR
B	-15	GLU	-	expression tag	UNP A0A090BKR
B	-14	LEU	-	expression tag	UNP A0A090BKR
B	-13	LYS	-	expression tag	UNP A0A090BKR
B	-12	THR	-	expression tag	UNP A0A090BKR
B	-11	ALA	-	expression tag	UNP A0A090BKR
B	-10	ALA	-	expression tag	UNP A0A090BKR
B	-9	LEU	-	expression tag	UNP A0A090BKR
B	-8	ALA	-	expression tag	UNP A0A090BKR
B	-7	GLN	-	expression tag	UNP A0A090BKR
B	-6	HIS	-	expression tag	UNP A0A090BKR
B	-5	ASP	-	expression tag	UNP A0A090BKR
B	-4	GLU	-	expression tag	UNP A0A090BKR
B	-3	ALA	-	expression tag	UNP A0A090BKR
B	-2	MET	-	expression tag	UNP A0A090BKR
B	-1	GLY	-	expression tag	UNP A0A090BKR
B	0	GLY	-	expression tag	UNP A0A090BKR
B	1	SER	-	expression tag	UNP A0A090BKR
B	34	ALA	THR	conflict	UNP A0A090BKR
B	44	ALA	PRO	conflict	UNP A0A090BKR
B	48	MET	ILE	conflict	UNP A0A090BKR
B	125	ASP	GLU	conflict	UNP A0A090BKR
B	557	ARG	THR	conflict	UNP A0A090BKR
B	998	LEU	VAL	conflict	UNP A0A090BKR
B	1063	VAL	ALA	conflict	UNP A0A090BKR

- Molecule 2 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	299	Total	C	N	O	0	0
			1479	881	299	299		
2	D	299	Total	C	N	O	0	0
			1479	881	299	299		

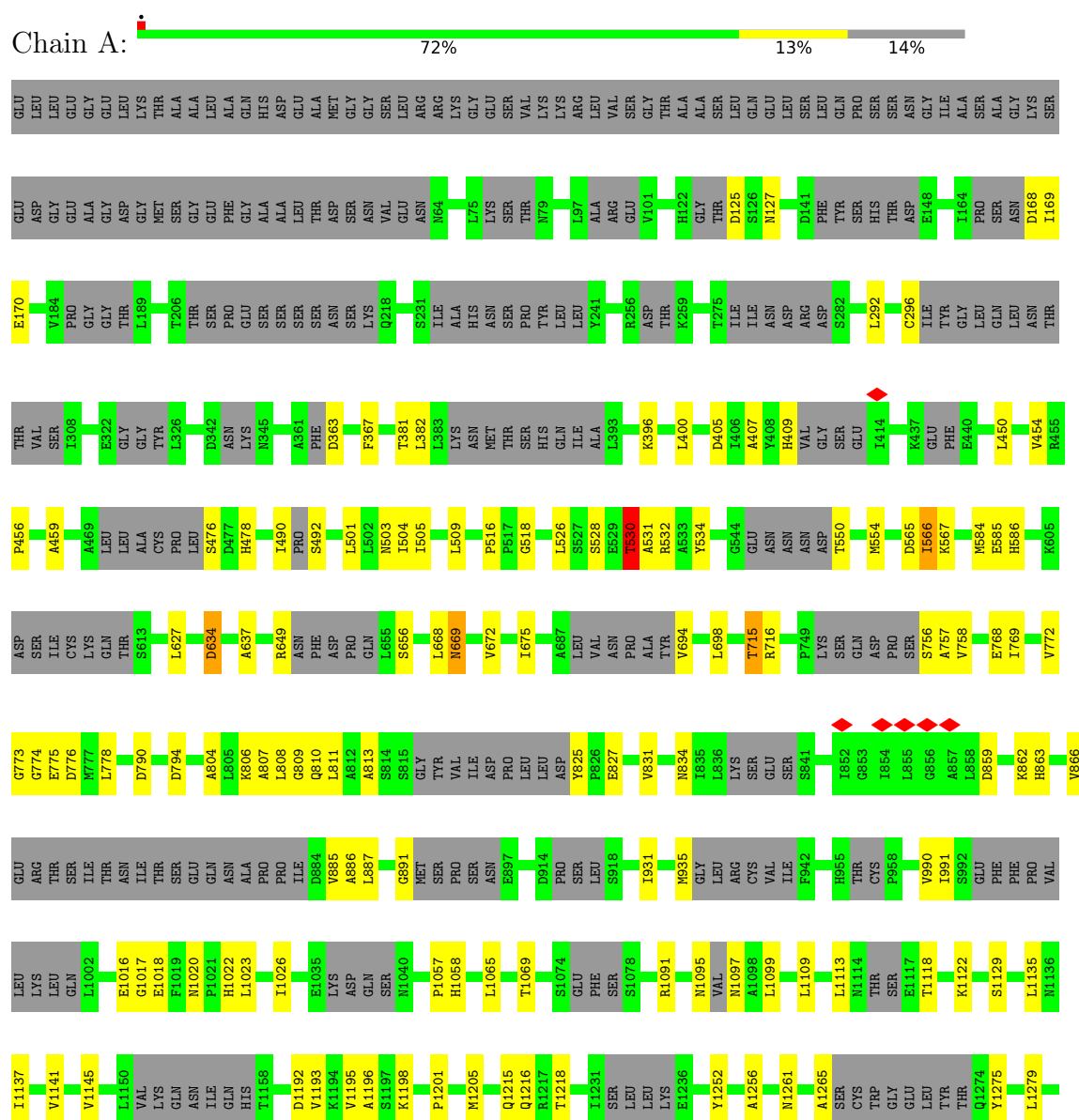
There are 2 discrepancies between the modelled and reference sequences:

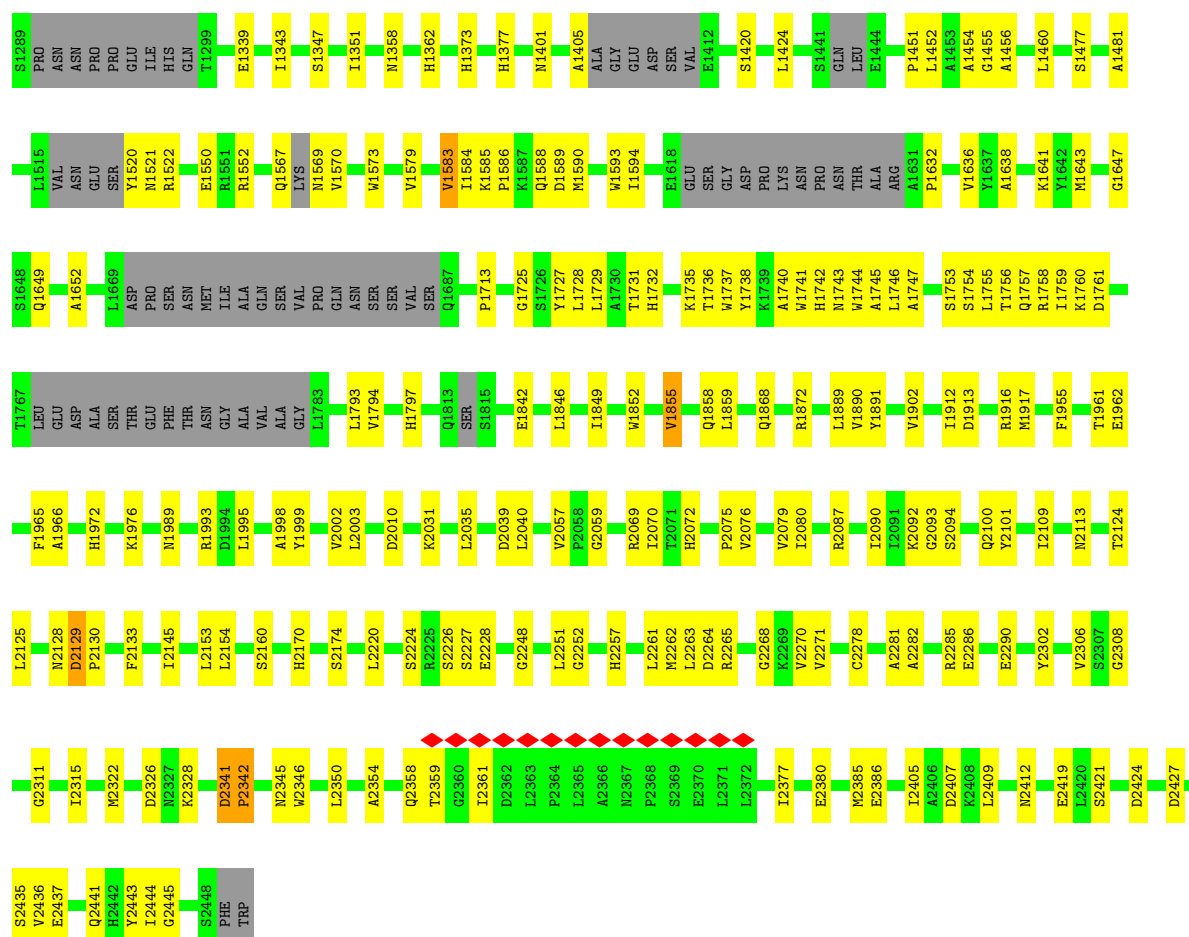
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	ASN	HIS	conflict	UNP A0A090BJK
D	221	ASN	HIS	conflict	UNP A0A090BJK

3 Residue-property plots

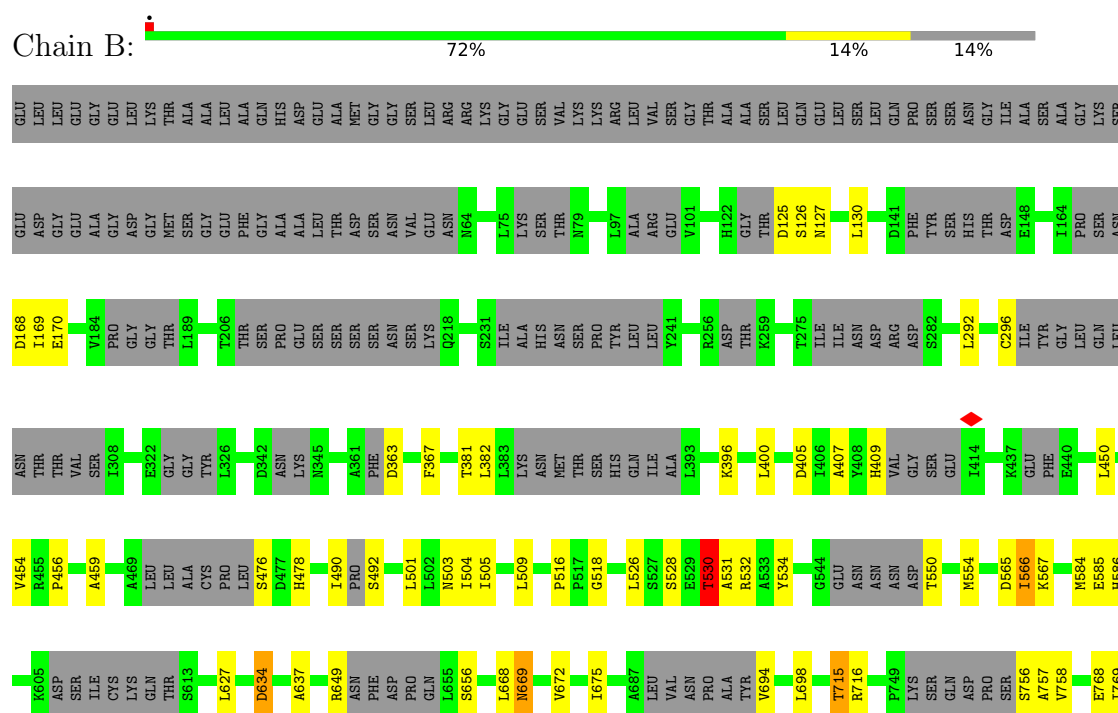
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

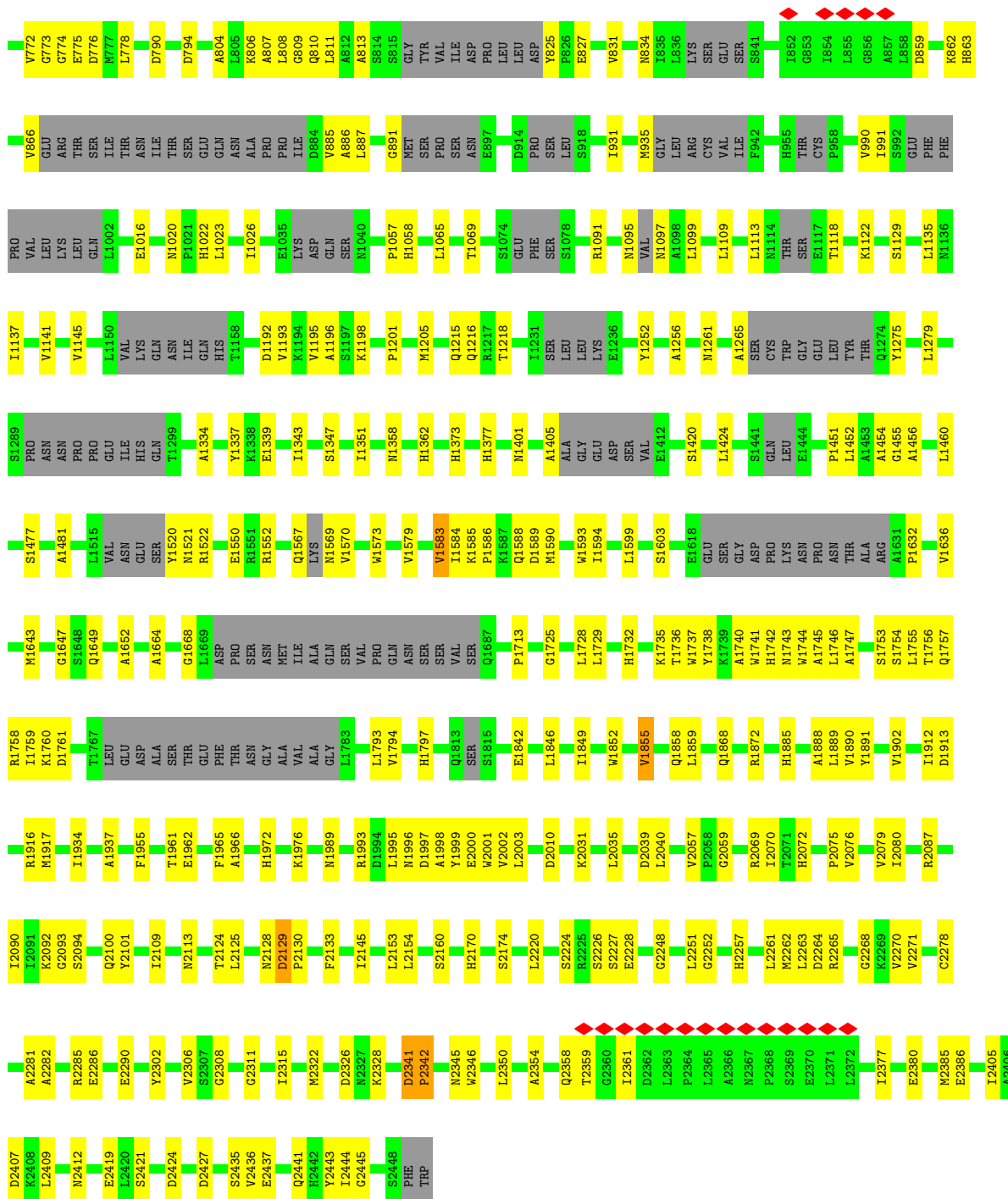
• Molecule 1: SERINE/THREONINE-PROTEIN KINASE TOR2





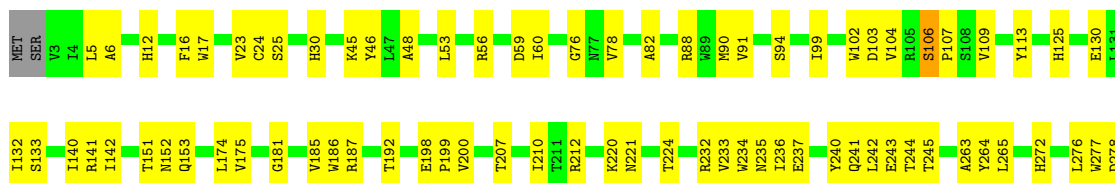
● Molecule 1: SERINE/THREONINE-PROTEIN KINASE TOR2





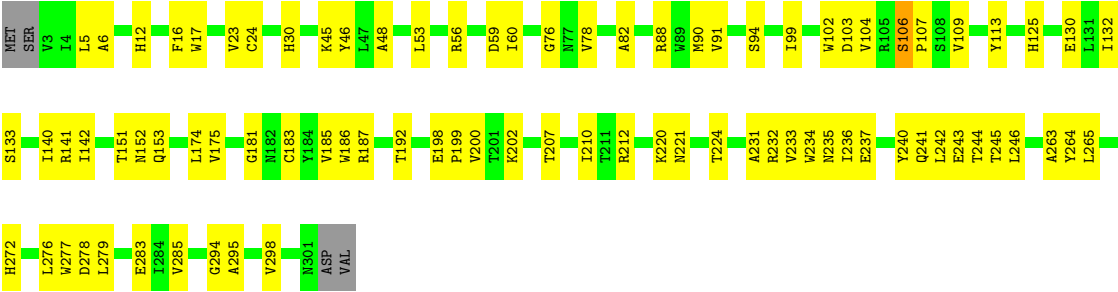
● Molecule 2: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain C: 72% 27% .





● Molecule 2: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	28877	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE (GCTF)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.044	Depositor
Map size (\AA)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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	0.40	0/10457	0.62	4/14512 (0.0%)
1	B	0.40	0/10457	0.62	4/14512 (0.0%)
2	C	0.29	0/1478	0.60	1/2058 (0.0%)
2	D	0.29	0/1478	0.60	1/2058 (0.0%)
All	All	0.39	0/23870	0.61	10/33140 (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	19
1	B	0	19
2	C	0	3
2	D	0	3
All	All	0	44

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	106	SER	C-N-CA	8.81	158.99	122.00
2	C	106	SER	C-N-CA	8.80	158.97	122.00
1	B	2341	ASP	C-N-CA	7.80	154.77	122.00
1	A	2341	ASP	C-N-CA	7.79	154.74	122.00
1	A	530	THR	C-N-CA	5.91	136.47	121.70
1	B	530	THR	C-N-CA	5.88	136.40	121.70
1	A	2129	ASP	C-N-CA	5.41	144.70	122.00
1	B	2129	ASP	C-N-CA	5.40	144.67	122.00
1	B	669	ASN	N-CA-C	5.38	125.53	111.00
1	A	669	ASN	N-CA-C	5.36	125.48	111.00

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1192	ASP	Peptide
1	A	1198	LYS	Peptide
1	A	1522	ARG	Peptide
1	A	1713	PRO	Peptide
1	A	1735	LYS	Peptide
1	A	2010	ASP	Peptide
1	A	2341	ASP	Peptide
1	A	2342	PRO	Peptide
1	A	2359	THR	Peptide
1	A	509	LEU	Peptide
1	A	530	THR	Peptide
1	A	566	ILE	Peptide
1	A	567	LYS	Peptide
1	A	627	LEU	Peptide
1	A	634	ASP	Peptide
1	A	668	LEU	Peptide
1	A	669	ASN	Peptide
1	A	715	THR	Peptide
1	B	1016	GLU	Peptide
1	B	1192	ASP	Peptide
1	B	1198	LYS	Peptide
1	B	1522	ARG	Peptide
1	B	1713	PRO	Peptide
1	B	1735	LYS	Peptide
1	B	2010	ASP	Peptide
1	B	2341	ASP	Peptide
1	B	2342	PRO	Peptide
1	B	2359	THR	Peptide
1	B	509	LEU	Peptide
1	B	530	THR	Peptide
1	B	566	ILE	Peptide
1	B	567	LYS	Peptide
1	B	627	LEU	Peptide
1	B	634	ASP	Peptide
1	B	668	LEU	Peptide
1	B	669	ASN	Peptide
1	B	715	THR	Peptide
2	C	106	SER	Peptide
2	C	192	THR	Peptide

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Mol	Chain	Res	Type	Group
2	C	295	ALA	Peptide
2	D	106	SER	Peptide
2	D	192	THR	Peptide
2	D	295	ALA	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	10508	0	4629	184	0
1	B	10508	0	4629	187	0
2	C	1479	0	673	52	0
2	D	1479	0	673	53	0
All	All	23974	0	10604	476	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 14.

All (476) 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:D:264:TYR:HA	2:D:278:ASP:HA	1.57	0.87
2:C:264:TYR:HA	2:C:278:ASP:HA	1.57	0.84
1:B:2407:ASP:O	1:B:2412:ASN:N	2.11	0.82
1:A:2407:ASP:O	1:A:2412:ASN:N	2.10	0.82
1:A:1955:PHE:HA	1:A:1961:THR:H	1.45	0.82
1:B:1738:TYR:O	1:B:1742:HIS:N	2.13	0.81
1:B:2405:ILE:O	1:B:2409:LEU:N	2.14	0.81
1:A:1738:TYR:O	1:A:1742:HIS:N	2.13	0.81
1:A:1989:ASN:O	1:A:1993:ARG:N	2.13	0.81
2:D:235:ASN:N	2:D:241:GLN:O	2.13	0.81
1:B:2109:ILE:O	1:B:2113:ASN:N	2.14	0.81
1:B:1955:PHE:HA	1:B:1961:THR:H	1.45	0.80
1:A:2109:ILE:O	1:A:2113:ASN:N	2.14	0.79
1:A:2405:ILE:O	1:A:2409:LEU:N	2.14	0.79
1:B:1590:MET:O	1:B:1594:ILE:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1989:ASN:O	1:B:1993:ARG:N	2.13	0.78
1:A:1590:MET:O	1:A:1594:ILE:N	2.16	0.77
1:B:1868:GLN:O	1:B:1872:ARG:N	2.18	0.77
1:A:1756:THR:O	1:A:1760:LYS:N	2.19	0.76
2:C:235:ASN:N	2:C:241:GLN:O	2.13	0.76
1:A:1643:MET:O	1:A:1647:GLY:N	2.18	0.76
1:A:1868:GLN:O	1:A:1872:ARG:N	2.18	0.76
1:B:1118:THR:O	1:B:1122:LYS:N	2.13	0.75
1:B:1756:THR:O	1:B:1760:LYS:N	2.19	0.75
1:A:1118:THR:O	1:A:1122:LYS:N	2.13	0.74
1:B:2160:SER:HA	1:B:2265:ARG:H	1.53	0.74
1:B:1373:HIS:O	1:B:1377:HIS:N	2.20	0.74
1:B:1643:MET:O	1:B:1647:GLY:N	2.18	0.73
1:A:1741:TRP:O	1:A:1745:ALA:N	2.22	0.73
1:A:2248:GLY:O	1:A:2252:GLY:N	2.22	0.72
1:A:2160:SER:HA	1:A:2265:ARG:H	1.53	0.72
1:A:1373:HIS:O	1:A:1377:HIS:N	2.20	0.72
1:B:1741:TRP:O	1:B:1745:ALA:N	2.22	0.72
1:B:2248:GLY:O	1:B:2252:GLY:N	2.22	0.72
1:B:634:ASP:O	1:B:637:ALA:N	2.22	0.72
1:B:2130:PRO:O	1:B:2133:PHE:N	2.21	0.71
1:B:2437:GLU:O	1:B:2441:GLN:N	2.24	0.71
1:A:634:ASP:O	1:A:637:ALA:N	2.22	0.71
1:B:2070:ILE:HA	1:B:2093:GLY:HA2	1.74	0.70
1:A:2070:ILE:HA	1:A:2093:GLY:HA2	1.74	0.70
1:A:2437:GLU:O	1:A:2441:GLN:N	2.24	0.70
1:A:1742:HIS:O	1:A:1746:LEU:N	2.25	0.70
1:A:2130:PRO:O	1:A:2133:PHE:N	2.21	0.70
1:B:1742:HIS:O	1:B:1746:LEU:N	2.25	0.69
2:C:272:HIS:HA	2:C:294:GLY:HA2	1.74	0.69
1:B:1022:HIS:O	1:B:1026:ILE:N	2.24	0.69
2:D:272:HIS:HA	2:D:294:GLY:HA2	1.74	0.69
1:A:1755:LEU:O	1:A:1759:ILE:N	2.26	0.68
2:D:220:LYS:O	2:D:237:GLU:N	2.26	0.68
1:A:2057:VAL:O	1:A:2059:GLY:N	2.26	0.68
1:B:887:LEU:O	1:B:891:GLY:N	2.23	0.68
1:B:2057:VAL:O	1:B:2059:GLY:N	2.26	0.67
1:A:1998:ALA:O	1:A:2002:VAL:N	2.28	0.67
2:C:220:LYS:O	2:C:237:GLU:N	2.26	0.67
1:A:1252:TYR:O	1:A:1256:ALA:N	2.25	0.67
1:A:887:LEU:O	1:A:891:GLY:N	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:SER:N	2:C:141:ARG:O	2.29	0.66
2:C:142:ILE:H	2:C:152:ASN:H	1.43	0.66
2:D:133:SER:O	2:D:141:ARG:N	2.27	0.66
2:D:133:SER:N	2:D:141:ARG:O	2.29	0.66
2:C:265:LEU:N	2:C:277:TRP:O	2.28	0.66
1:A:2311:GLY:O	1:A:2315:ILE:N	2.28	0.66
2:D:5:LEU:O	2:D:17:TRP:N	2.28	0.66
2:C:5:LEU:O	2:C:17:TRP:N	2.28	0.65
1:B:694:VAL:O	1:B:698:LEU:N	2.30	0.65
1:B:1998:ALA:O	1:B:2002:VAL:N	2.28	0.65
2:C:82:ALA:O	2:C:91:VAL:N	2.28	0.65
1:A:866:VAL:O	1:A:885:VAL:N	2.29	0.65
1:B:2262:MET:O	1:B:2271:VAL:N	2.26	0.65
2:D:82:ALA:O	2:D:91:VAL:N	2.28	0.65
1:A:1420:SER:O	1:A:1424:LEU:N	2.30	0.65
2:D:236:ILE:HA	2:D:240:TYR:HA	1.78	0.65
1:A:1401:ASN:O	1:A:1405:ALA:N	2.30	0.65
2:C:236:ILE:HA	2:C:240:TYR:HA	1.78	0.65
2:D:142:ILE:H	2:D:152:ASN:H	1.43	0.65
1:A:2262:MET:O	1:A:2271:VAL:N	2.26	0.65
1:B:866:VAL:O	1:B:885:VAL:N	2.29	0.65
1:B:1755:LEU:O	1:B:1759:ILE:N	2.26	0.65
1:B:1736:THR:C	1:B:1738:TYR:H	1.99	0.64
1:B:2311:GLY:O	1:B:2315:ILE:N	2.28	0.64
1:B:1738:TYR:HA	1:B:1741:TRP:H	1.62	0.64
1:A:1736:THR:C	1:A:1738:TYR:H	1.99	0.64
1:A:1738:TYR:HA	1:A:1741:TRP:H	1.62	0.64
1:B:1401:ASN:O	1:B:1405:ALA:N	2.30	0.64
1:A:694:VAL:O	1:A:698:LEU:N	2.29	0.64
1:B:1097:ASN:O	1:B:1099:LEU:N	2.29	0.64
1:B:1252:TYR:O	1:B:1256:ALA:N	2.25	0.63
1:B:1999:TYR:O	1:B:2003:LEU:N	2.32	0.63
1:A:1567:GLN:O	1:A:1569:ASN:N	2.32	0.63
2:C:133:SER:O	2:C:141:ARG:N	2.27	0.63
2:D:132:ILE:HA	2:D:142:ILE:HA	1.80	0.62
2:C:132:ILE:HA	2:C:142:ILE:HA	1.80	0.62
1:A:1999:TYR:O	1:A:2003:LEU:N	2.32	0.62
1:B:531:ALA:H	1:B:534:TYR:CB	2.12	0.62
1:A:531:ALA:H	1:A:534:TYR:CB	2.13	0.62
1:A:756:SER:O	1:A:758:VAL:N	2.32	0.62
1:B:1567:GLN:O	1:B:1569:ASN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:HIS:O	1:A:1026:ILE:N	2.24	0.62
1:A:2072:HIS:O	1:A:2092:LYS:N	2.33	0.62
1:B:1420:SER:O	1:B:1424:LEU:N	2.30	0.62
1:B:1754:SER:O	1:B:1758:ARG:N	2.33	0.62
2:D:276:LEU:O	2:D:285:VAL:N	2.27	0.62
1:A:1261:ASN:O	1:A:1265:ALA:N	2.33	0.62
2:C:263:ALA:O	2:C:279:LEU:N	2.33	0.62
2:C:276:LEU:O	2:C:285:VAL:N	2.27	0.62
1:B:756:SER:O	1:B:758:VAL:N	2.32	0.61
1:A:2251:LEU:O	1:A:2278:CYS:HA	1.99	0.61
1:B:2251:LEU:O	1:B:2278:CYS:HA	1.99	0.61
2:D:46:TYR:HA	2:D:59:ASP:HA	1.82	0.61
1:B:1753:SER:O	1:B:1757:GLN:N	2.28	0.61
2:C:46:TYR:HA	2:C:59:ASP:HA	1.83	0.61
1:B:1261:ASN:O	1:B:1265:ALA:N	2.33	0.61
2:D:263:ALA:O	2:D:279:LEU:N	2.33	0.61
1:B:2072:HIS:O	1:B:2092:LYS:N	2.33	0.61
2:D:181:GLY:HA2	2:D:210:ILE:H	1.65	0.61
1:A:1097:ASN:O	1:A:1099:LEU:N	2.29	0.61
2:D:265:LEU:N	2:D:277:TRP:O	2.28	0.61
1:A:768:GLU:O	1:A:772:VAL:N	2.34	0.60
1:B:1793:LEU:H	1:B:1794:VAL:HA	1.65	0.60
1:A:2342:PRO:O	1:A:2346:TRP:N	2.23	0.60
1:B:768:GLU:O	1:B:772:VAL:N	2.34	0.60
1:B:1961:THR:O	1:B:1965:PHE:N	2.31	0.60
2:D:17:TRP:HA	2:D:24:CYS:HA	1.83	0.60
1:A:1793:LEU:H	1:A:1794:VAL:HA	1.65	0.60
2:C:181:GLY:HA2	2:C:210:ILE:H	1.65	0.60
2:C:17:TRP:HA	2:C:24:CYS:HA	1.83	0.60
1:A:1753:SER:O	1:A:1757:GLN:N	2.28	0.60
1:A:804:ALA:O	1:A:808:LEU:N	2.27	0.60
1:A:1477:SER:O	1:A:1481:ALA:N	2.35	0.60
1:B:1728:LEU:O	1:B:1732:HIS:N	2.33	0.60
1:B:2342:PRO:O	1:B:2346:TRP:N	2.23	0.59
1:B:1477:SER:O	1:B:1481:ALA:N	2.35	0.59
2:C:232:ARG:HA	2:C:245:THR:HA	1.84	0.59
1:B:2350:LEU:O	1:B:2354:ALA:HA	2.03	0.59
1:A:866:VAL:HA	1:A:886:ALA:HB2	1.85	0.59
1:A:1091:ARG:O	1:A:1095:ASN:N	2.33	0.59
1:A:1972:HIS:O	1:A:1976:LYS:N	2.35	0.59
1:A:1754:SER:O	1:A:1758:ARG:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:ARG:HA	2:D:245:THR:HA	1.84	0.59
1:A:2350:LEU:O	1:A:2354:ALA:HA	2.03	0.59
1:B:1972:HIS:O	1:B:1976:LYS:N	2.35	0.59
1:A:1961:THR:O	1:A:1965:PHE:N	2.31	0.58
1:A:2170:HIS:O	1:A:2174:SER:N	2.37	0.58
1:B:866:VAL:HA	1:B:886:ALA:HB2	1.85	0.58
1:A:807:ALA:O	1:A:811:LEU:N	2.26	0.58
1:B:1632:PRO:O	1:B:1636:VAL:N	2.37	0.58
1:B:2069:ARG:O	1:B:2094:SER:N	2.36	0.58
1:B:1757:GLN:O	1:B:1761:ASP:N	2.36	0.58
1:B:1456:ALA:O	1:B:1460:LEU:N	2.25	0.58
1:B:1913:ASP:O	1:B:1917:MET:N	2.37	0.58
1:A:1590:MET:O	1:A:1593:TRP:N	2.37	0.58
1:A:1757:GLN:O	1:A:1761:ASP:N	2.36	0.58
1:A:1913:ASP:O	1:A:1917:MET:N	2.37	0.58
1:A:1141:VAL:O	1:A:1145:VAL:N	2.36	0.58
1:B:807:ALA:O	1:B:811:LEU:N	2.26	0.58
1:B:2039:ASP:HA	1:B:2076:VAL:HA	1.86	0.58
1:B:1583:VAL:CB	1:B:1584:ILE:HA	2.34	0.58
1:B:2424:ASP:O	1:B:2427:ASP:N	2.37	0.58
1:A:1583:VAL:CB	1:A:1584:ILE:HA	2.34	0.57
2:D:233:VAL:N	2:D:244:THR:O	2.22	0.57
1:B:804:ALA:O	1:B:808:LEU:N	2.27	0.57
1:B:1590:MET:O	1:B:1593:TRP:N	2.37	0.57
1:B:2170:HIS:O	1:B:2174:SER:N	2.37	0.57
2:C:6:ALA:HB2	2:C:16:PHE:HA	1.86	0.57
1:A:363:ASP:O	1:A:367:PHE:N	2.34	0.57
1:A:672:VAL:O	1:A:675:ILE:N	2.38	0.57
2:D:6:ALA:HB2	2:D:16:PHE:HA	1.86	0.57
1:A:1109:LEU:O	1:A:1113:LEU:N	2.34	0.57
2:D:234:TRP:HA	2:D:242:LEU:HA	1.87	0.57
1:B:1141:VAL:O	1:B:1145:VAL:N	2.36	0.57
1:A:2039:ASP:HA	1:A:2076:VAL:HA	1.86	0.57
1:A:2424:ASP:O	1:A:2427:ASP:N	2.37	0.57
1:B:2160:SER:HA	1:B:2264:ASP:HA	1.87	0.57
1:B:672:VAL:O	1:B:675:ILE:N	2.38	0.56
2:C:265:LEU:O	2:C:277:TRP:N	2.38	0.56
2:D:78:VAL:HA	2:D:94:SER:HA	1.87	0.56
1:A:1728:LEU:O	1:A:1732:HIS:N	2.33	0.56
1:B:2080:ILE:H	1:B:2087:ARG:HA	1.69	0.56
1:A:2090:ILE:HA	1:A:2100:GLN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ARG:O	1:B:1095:ASN:N	2.33	0.56
1:B:1358:ASN:O	1:B:1362:HIS:N	2.39	0.56
1:B:2090:ILE:HA	1:B:2100:GLN:HA	1.88	0.56
2:D:265:LEU:O	2:D:277:TRP:N	2.37	0.56
1:A:2080:ILE:H	1:A:2087:ARG:HA	1.69	0.56
2:C:234:TRP:HA	2:C:242:LEU:HA	1.87	0.56
2:C:78:VAL:HA	2:C:94:SER:HA	1.88	0.56
1:A:2069:ARG:O	1:A:2094:SER:N	2.36	0.56
2:C:187:ARG:O	2:C:198:GLU:N	2.38	0.55
1:A:2160:SER:HA	1:A:2264:ASP:HA	1.87	0.55
2:D:187:ARG:O	2:D:198:GLU:N	2.39	0.55
1:A:1358:ASN:O	1:A:1362:HIS:N	2.39	0.55
2:C:233:VAL:O	2:C:243:GLU:N	2.33	0.55
1:A:931:ILE:O	1:A:935:MET:N	2.38	0.55
1:A:1632:PRO:O	1:A:1636:VAL:N	2.37	0.55
1:B:363:ASP:O	1:B:367:PHE:N	2.34	0.55
1:B:2145:ILE:O	1:B:2153:LEU:N	2.28	0.55
1:B:2031:LYS:O	1:B:2035:LEU:N	2.40	0.55
1:A:2031:LYS:O	1:A:2035:LEU:N	2.40	0.54
2:C:233:VAL:N	2:C:244:THR:O	2.22	0.54
1:B:1855:VAL:O	1:B:1859:LEU:N	2.39	0.54
2:D:187:ARG:N	2:D:198:GLU:O	2.36	0.54
1:A:516:PRO:C	1:A:518:GLY:HA3	2.28	0.54
2:C:45:LYS:O	2:C:60:ILE:N	2.40	0.54
1:A:1995:LEU:O	1:A:1999:TYR:N	2.32	0.54
1:B:1109:LEU:O	1:B:1113:LEU:N	2.34	0.54
2:D:45:LYS:O	2:D:60:ILE:N	2.40	0.54
1:A:806:LYS:O	1:A:810:GLN:N	2.28	0.54
1:A:1456:ALA:O	1:A:1460:LEU:N	2.25	0.54
1:B:516:PRO:C	1:B:518:GLY:HA3	2.28	0.54
1:A:2124:THR:O	1:A:2128:ASN:N	2.38	0.54
2:C:82:ALA:N	2:C:91:VAL:O	2.36	0.54
1:B:1962:GLU:O	1:B:1966:ALA:N	2.41	0.53
1:A:516:PRO:O	1:A:518:GLY:HA3	2.08	0.53
1:B:1520:TYR:HA	1:B:1521:ASN:CB	2.38	0.53
1:B:1737:TRP:O	1:B:1740:ALA:N	2.28	0.53
1:B:516:PRO:O	1:B:518:GLY:HA3	2.08	0.53
1:B:1855:VAL:O	1:B:1858:GLN:N	2.42	0.53
1:A:1520:TYR:HA	1:A:1521:ASN:CB	2.38	0.53
1:A:1201:PRO:O	1:A:1205:MET:N	2.42	0.53
2:C:185:VAL:O	2:C:200:VAL:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2377:ILE:O	1:B:2380:GLU:N	2.39	0.53
1:A:1912:ILE:O	1:A:1916:ARG:N	2.28	0.53
1:A:1962:GLU:O	1:A:1966:ALA:N	2.41	0.53
1:A:2285:ARG:HA	1:A:2286:GLU:CB	2.39	0.52
1:A:1855:VAL:O	1:A:1858:GLN:N	2.41	0.52
1:B:2285:ARG:HA	1:B:2286:GLU:CB	2.38	0.52
1:A:1347:SER:O	1:A:1351:ILE:N	2.37	0.52
1:B:1912:ILE:O	1:B:1916:ARG:N	2.28	0.52
1:B:1743:ASN:O	1:B:1747:ALA:N	2.43	0.52
1:B:2281:ALA:O	1:B:2285:ARG:N	2.24	0.52
1:A:1737:TRP:O	1:A:1740:ALA:N	2.28	0.52
1:B:1201:PRO:O	1:B:1205:MET:N	2.42	0.52
1:B:405:ASP:O	1:B:409:HIS:N	2.41	0.52
1:B:407:ALA:HA	1:B:450:LEU:HA	1.92	0.52
2:D:125:HIS:N	2:D:130:GLU:O	2.33	0.52
1:A:407:ALA:HA	1:A:450:LEU:HA	1.92	0.52
1:A:2377:ILE:O	1:A:2380:GLU:N	2.39	0.52
1:B:806:LYS:O	1:B:810:GLN:N	2.28	0.52
2:C:90:MET:H	2:C:103:ASP:HA	1.75	0.51
2:C:99:ILE:N	2:C:113:TYR:O	2.40	0.51
1:A:2326:ASP:C	1:A:2328:LYS:H	2.14	0.51
2:C:12:HIS:O	2:C:30:HIS:N	2.44	0.51
1:A:1743:ASN:O	1:A:1747:ALA:N	2.43	0.51
2:D:90:MET:H	2:D:103:ASP:HA	1.75	0.51
1:A:1855:VAL:O	1:A:1859:LEU:N	2.39	0.51
1:B:1842:GLU:O	1:B:1846:LEU:N	2.44	0.51
2:D:233:VAL:O	2:D:243:GLU:N	2.33	0.51
1:B:1995:LEU:O	1:B:1999:TYR:N	2.32	0.51
2:C:88:ARG:O	2:C:104:VAL:N	2.44	0.51
1:A:584:MET:H	1:A:586:HIS:CB	2.24	0.51
1:B:931:ILE:O	1:B:935:MET:N	2.38	0.51
1:B:2419:GLU:C	1:B:2421:SER:H	2.15	0.51
1:A:1842:GLU:O	1:A:1846:LEU:N	2.44	0.50
1:B:584:MET:H	1:B:586:HIS:CB	2.24	0.50
2:D:186:TRP:HA	2:D:200:VAL:H	1.76	0.50
1:B:396:LYS:O	1:B:400:LEU:N	2.45	0.50
1:B:2125:LEU:O	1:B:2129:ASP:N	2.44	0.50
1:A:2281:ALA:O	1:A:2285:ARG:N	2.24	0.50
2:D:12:HIS:O	2:D:30:HIS:N	2.44	0.50
1:A:1215:GLN:CB	1:A:1218:THR:HA	2.42	0.50
1:B:476:SER:C	1:B:478:HIS:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:TRP:HA	2:C:200:VAL:H	1.76	0.50
1:B:1215:GLN:CB	1:B:1218:THR:HA	2.42	0.50
1:A:2125:LEU:O	1:A:2129:ASP:N	2.44	0.50
1:B:1275:TYR:O	1:B:1279:LEU:N	2.41	0.50
1:B:2326:ASP:C	1:B:2328:LYS:H	2.14	0.50
2:C:187:ARG:N	2:C:198:GLU:O	2.36	0.50
1:B:2224:SER:O	1:B:2227:SER:N	2.41	0.49
1:B:530:THR:N	1:B:531:ALA:HB3	2.27	0.49
2:D:99:ILE:N	2:D:113:TYR:O	2.40	0.49
1:B:1347:SER:O	1:B:1351:ILE:N	2.37	0.49
1:B:1997:ASP:O	1:B:2001:TRP:N	2.40	0.49
2:D:88:ARG:O	2:D:104:VAL:N	2.44	0.49
1:A:396:LYS:O	1:A:400:LEU:N	2.45	0.49
1:A:530:THR:N	1:A:531:ALA:HB3	2.27	0.49
1:A:2419:GLU:C	1:A:2421:SER:H	2.15	0.49
1:A:381:THR:HA	1:A:382:LEU:HA	1.51	0.49
1:A:769:ILE:O	1:A:773:GLY:N	2.46	0.49
1:A:1585:LYS:O	1:A:1588:GLN:N	2.46	0.49
1:A:2145:ILE:O	1:A:2153:LEU:N	2.28	0.49
1:A:476:SER:C	1:A:478:HIS:H	2.15	0.49
2:D:220:LYS:O	2:D:236:ILE:N	2.46	0.49
1:A:1741:TRP:HA	1:A:1744:TRP:CB	2.43	0.48
1:B:769:ILE:O	1:B:773:GLY:N	2.46	0.48
1:B:1585:LYS:O	1:B:1588:GLN:N	2.46	0.48
2:C:125:HIS:N	2:C:130:GLU:O	2.33	0.48
1:A:2354:ALA:O	1:A:2358:GLN:N	2.46	0.48
1:B:2354:ALA:O	1:B:2358:GLN:N	2.46	0.48
1:A:405:ASP:O	1:A:409:HIS:N	2.41	0.48
1:B:2257:HIS:O	1:B:2261:LEU:N	2.47	0.48
2:C:220:LYS:O	2:C:236:ILE:N	2.46	0.48
2:D:185:VAL:O	2:D:200:VAL:N	2.39	0.48
1:A:565:ASP:HA	1:A:566:ILE:HA	1.54	0.48
1:A:1744:TRP:HA	1:A:1747:ALA:HB2	1.96	0.48
2:C:140:ILE:O	2:C:153:GLN:HA	2.14	0.48
1:B:1741:TRP:HA	1:B:1744:TRP:CB	2.44	0.48
1:B:2124:THR:O	1:B:2128:ASN:N	2.38	0.48
1:A:2257:HIS:O	1:A:2261:LEU:N	2.47	0.47
1:B:1065:LEU:O	1:B:1069:THR:N	2.40	0.47
1:B:1744:TRP:HA	1:B:1747:ALA:HB2	1.96	0.47
1:A:2101:TYR:HA	1:A:2154:LEU:O	2.15	0.47
1:B:1738:TYR:CA	1:B:1741:TRP:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2385:MET:HA	1:B:2386:GLU:C	2.35	0.47
2:D:140:ILE:O	2:D:153:GLN:HA	2.14	0.47
1:A:1057:PRO:HA	1:A:1058:HIS:HA	1.70	0.47
1:A:1725:GLY:O	1:A:1729:LEU:N	2.31	0.47
1:A:1738:TYR:CA	1:A:1741:TRP:H	2.28	0.47
1:A:2040:LEU:N	1:A:2075:PRO:O	2.48	0.47
1:A:2385:MET:HA	1:A:2386:GLU:C	2.35	0.47
1:B:2101:TYR:HA	1:B:2154:LEU:O	2.15	0.47
1:B:2263:LEU:HA	1:B:2270:VAL:HA	1.97	0.47
1:A:773:GLY:O	1:A:776:ASP:N	2.35	0.47
1:A:1097:ASN:C	1:A:1099:LEU:H	2.16	0.47
1:A:1550:GLU:C	1:A:1552:ARG:H	2.17	0.47
1:B:1550:GLU:C	1:B:1552:ARG:H	2.17	0.47
1:A:2220:LEU:O	1:A:2224:SER:N	2.48	0.47
1:B:1793:LEU:N	1:B:1794:VAL:HA	2.28	0.46
1:B:2264:ASP:CB	1:B:2268:GLY:HA2	2.46	0.46
2:D:142:ILE:N	2:D:151:THR:HA	2.30	0.46
2:D:277:TRP:HA	2:D:283:GLU:O	2.15	0.46
1:B:2040:LEU:N	1:B:2075:PRO:O	2.48	0.46
1:B:2220:LEU:O	1:B:2224:SER:N	2.48	0.46
1:B:1097:ASN:C	1:B:1099:LEU:H	2.16	0.46
2:D:186:TRP:HA	2:D:199:PRO:HA	1.97	0.46
1:A:1889:LEU:C	1:A:1891:TYR:H	2.19	0.46
1:A:456:PRO:HA	1:A:459:ALA:HB3	1.97	0.46
1:A:1339:GLU:O	1:A:1343:ILE:N	2.46	0.46
2:C:142:ILE:N	2:C:151:THR:HA	2.30	0.46
1:A:715:THR:CB	1:A:716:ARG:HA	2.46	0.46
1:B:1135:LEU:C	1:B:1137:ILE:H	2.19	0.46
2:C:277:TRP:HA	2:C:283:GLU:O	2.15	0.46
1:B:715:THR:CB	1:B:716:ARG:HA	2.46	0.46
1:B:1889:LEU:C	1:B:1891:TYR:H	2.19	0.46
1:B:1215:GLN:HA	1:B:1216:GLN:O	2.16	0.46
1:A:862:LYS:O	1:A:866:VAL:N	2.49	0.45
1:A:1135:LEU:C	1:A:1137:ILE:H	2.19	0.45
1:B:456:PRO:HA	1:B:459:ALA:HB3	1.97	0.45
1:A:859:ASP:O	1:A:863:HIS:N	2.41	0.45
1:A:2263:LEU:HA	1:A:2270:VAL:HA	1.97	0.45
1:B:526:LEU:CB	1:B:528:SER:H	2.29	0.45
1:B:859:ASP:O	1:B:863:HIS:N	2.41	0.45
1:B:1744:TRP:HA	1:B:1747:ALA:CB	2.47	0.45
2:C:186:TRP:HA	2:C:199:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1744:TRP:HA	1:A:1747:ALA:CB	2.47	0.45
1:B:1020:ASN:O	1:B:1023:LEU:N	2.49	0.45
1:B:2342:PRO:O	1:B:2345:ASN:N	2.50	0.45
1:A:1020:ASN:O	1:A:1023:LEU:N	2.49	0.45
1:A:1727:TYR:O	1:A:1731:THR:N	2.37	0.45
1:A:2224:SER:O	1:A:2227:SER:N	2.41	0.45
1:A:2342:PRO:O	1:A:2345:ASN:N	2.50	0.45
1:B:550:THR:O	1:B:554:MET:N	2.27	0.45
1:B:2145:ILE:N	1:B:2153:LEU:O	2.50	0.45
1:A:526:LEU:CB	1:A:528:SER:H	2.29	0.45
2:C:221:ASN:HA	2:C:236:ILE:H	1.82	0.45
1:A:1579:VAL:O	1:A:1583:VAL:N	2.50	0.45
1:B:862:LYS:O	1:B:866:VAL:N	2.49	0.45
1:A:809:GLY:O	1:A:813:ALA:N	2.41	0.45
2:D:82:ALA:N	2:D:91:VAL:O	2.36	0.45
1:A:774:GLY:HA2	1:A:775:GLU:HA	1.52	0.45
1:A:1091:ARG:CB	1:A:1129:SER:HA	2.47	0.45
1:A:2264:ASP:CB	1:A:2268:GLY:HA2	2.46	0.45
1:B:1586:PRO:HA	1:B:1589:ASP:O	2.17	0.45
1:B:1725:GLY:O	1:B:1729:LEU:N	2.31	0.45
1:B:2248:GLY:O	1:B:2251:LEU:N	2.50	0.45
1:A:825:TYR:C	1:A:827:GLU:H	2.21	0.44
1:B:2435:SER:HA	1:B:2436:VAL:HA	1.80	0.44
2:C:234:TRP:HA	2:C:243:GLU:N	2.32	0.44
2:D:221:ASN:HA	2:D:236:ILE:H	1.82	0.44
2:D:234:TRP:HA	2:D:243:GLU:N	2.31	0.44
1:A:1215:GLN:HA	1:A:1216:GLN:O	2.16	0.44
1:A:2145:ILE:N	1:A:2153:LEU:O	2.50	0.44
1:B:825:TYR:C	1:B:827:GLU:H	2.20	0.44
1:B:1339:GLU:O	1:B:1343:ILE:N	2.46	0.44
1:A:504:ILE:HA	1:A:505:ILE:HA	1.50	0.44
1:B:530:THR:C	1:B:532:ARG:H	2.20	0.44
1:B:1091:ARG:CB	1:B:1129:SER:HA	2.48	0.44
1:A:1275:TYR:O	1:A:1279:LEU:N	2.41	0.44
1:A:756:SER:O	1:A:757:ALA:N	2.51	0.44
1:A:1586:PRO:HA	1:A:1589:ASP:O	2.18	0.44
1:B:584:MET:HA	1:B:585:GLU:HA	1.70	0.44
1:B:1996:ASN:O	1:B:2000:GLU:N	2.40	0.44
1:A:1849:ILE:O	1:A:1852:TRP:N	2.51	0.44
2:D:181:GLY:HA3	2:D:207:THR:O	2.18	0.44
1:B:2072:HIS:N	1:B:2092:LYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:PRO:HA	1:B:1058:HIS:HA	1.70	0.44
1:B:1579:VAL:O	1:B:1583:VAL:N	2.50	0.44
1:B:1794:VAL:H	1:B:1797:HIS:CB	2.31	0.43
1:A:530:THR:C	1:A:532:ARG:H	2.20	0.43
1:A:1017:GLY:HA2	1:A:1018:GLU:HA	1.72	0.43
1:A:2072:HIS:N	1:A:2092:LYS:O	2.50	0.43
1:A:584:MET:HA	1:A:585:GLU:HA	1.70	0.43
1:B:381:THR:HA	1:B:382:LEU:HA	1.50	0.43
1:B:1649:GLN:O	1:B:1652:ALA:HB3	2.19	0.43
1:B:1599:LEU:O	1:B:1603:SER:N	2.43	0.43
2:C:174:LEU:N	2:C:186:TRP:O	2.52	0.43
1:A:1065:LEU:O	1:A:1069:THR:N	2.40	0.43
1:B:1849:ILE:O	1:B:1852:TRP:N	2.51	0.43
1:A:2248:GLY:O	1:A:2251:LEU:N	2.50	0.43
1:B:125:ASP:C	1:B:127:ASN:H	2.22	0.43
1:B:756:SER:O	1:B:757:ALA:N	2.51	0.43
2:C:181:GLY:HA3	2:C:207:THR:O	2.18	0.43
1:A:1794:VAL:H	1:A:1797:HIS:CB	2.31	0.43
1:B:504:ILE:HA	1:B:505:ILE:HA	1.51	0.43
2:D:186:TRP:HA	2:D:200:VAL:N	2.34	0.43
1:A:501:LEU:C	1:A:503:ASN:H	2.23	0.43
1:A:292:LEU:O	1:A:296:CYS:N	2.51	0.43
1:B:292:LEU:O	1:B:296:CYS:N	2.51	0.43
1:B:2282:ALA:HB2	1:B:2290:GLU:O	2.19	0.43
2:C:16:PHE:O	2:C:25:SER:N	2.44	0.43
2:C:102:TRP:HA	2:C:109:VAL:CB	2.49	0.42
2:D:102:TRP:HA	2:D:109:VAL:CB	2.49	0.42
2:D:231:ALA:O	2:D:246:LEU:N	2.33	0.42
1:A:2079:VAL:HA	1:A:2087:ARG:CB	2.49	0.42
1:A:2282:ALA:HB2	1:A:2290:GLU:O	2.19	0.42
1:A:1195:VAL:CB	1:A:1196:ALA:HA	2.50	0.42
1:A:2443:TYR:C	1:A:2445:GLY:H	2.23	0.42
2:C:53:LEU:HA	2:C:76:GLY:H	1.84	0.42
1:A:125:ASP:C	1:A:127:ASN:H	2.22	0.42
1:A:990:VAL:HA	1:A:991:ILE:HA	1.46	0.42
1:A:1451:PRO:O	1:A:1454:ALA:HB3	2.20	0.42
1:A:1649:GLN:O	1:A:1652:ALA:HB3	2.19	0.42
1:B:990:VAL:HA	1:B:991:ILE:HA	1.46	0.42
1:B:2079:VAL:HA	1:B:2087:ARG:CB	2.49	0.42
1:A:831:VAL:O	1:A:834:ASN:N	2.52	0.42
2:C:17:TRP:HA	2:C:23:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:LEU:HA	2:D:76:GLY:H	1.84	0.42
2:D:234:TRP:HA	2:D:243:GLU:H	1.85	0.42
1:A:550:THR:O	1:A:554:MET:N	2.27	0.42
1:A:2322:MET:O	1:A:2326:ASP:N	2.52	0.42
1:B:1195:VAL:CB	1:B:1196:ALA:HA	2.49	0.42
2:D:212:ARG:O	2:D:224:THR:HA	2.20	0.42
1:A:776:ASP:C	1:A:778:LEU:H	2.23	0.42
1:B:809:GLY:O	1:B:813:ALA:N	2.41	0.42
1:A:1793:LEU:N	1:A:1794:VAL:HA	2.28	0.41
1:B:126:SER:O	1:B:130:LEU:N	2.36	0.41
1:B:649:ARG:HA	1:B:656:SER:N	2.35	0.41
2:C:186:TRP:HA	2:C:200:VAL:N	2.34	0.41
1:A:790:ASP:O	1:A:794:ASP:N	2.53	0.41
1:A:1215:GLN:HA	1:A:1216:GLN:C	2.41	0.41
1:B:1451:PRO:O	1:B:1454:ALA:HB3	2.20	0.41
1:A:2302:TYR:HA	1:A:2308:GLY:HA3	2.03	0.41
1:B:168:ASP:C	1:B:170:GLU:H	2.23	0.41
1:A:2226:SER:C	1:A:2228:GLU:H	2.23	0.41
1:B:776:ASP:C	1:B:778:LEU:H	2.23	0.41
2:D:17:TRP:HA	2:D:23:VAL:O	2.20	0.41
2:D:174:LEU:N	2:D:186:TRP:O	2.52	0.41
1:B:790:ASP:O	1:B:794:ASP:N	2.53	0.41
1:B:2226:SER:C	1:B:2228:GLU:H	2.23	0.41
2:D:48:ALA:HA	2:D:56:ARG:O	2.20	0.41
1:A:168:ASP:C	1:A:170:GLU:H	2.23	0.41
1:B:774:GLY:HA2	1:B:775:GLU:HA	1.52	0.41
1:B:2160:SER:HA	1:B:2265:ARG:N	2.27	0.41
2:C:48:ALA:HA	2:C:56:ARG:O	2.20	0.41
1:A:649:ARG:HA	1:A:656:SER:N	2.35	0.41
1:A:2160:SER:HA	1:A:2265:ARG:N	2.27	0.41
1:B:1215:GLN:HA	1:B:1216:GLN:C	2.41	0.41
1:A:1452:LEU:O	1:A:1455:GLY:N	2.54	0.41
1:A:2435:SER:HA	1:A:2436:VAL:HA	1.80	0.41
1:B:501:LEU:C	1:B:503:ASN:H	2.22	0.41
1:B:565:ASP:HA	1:B:566:ILE:HA	1.54	0.41
2:C:212:ARG:O	2:C:224:THR:HA	2.20	0.41
1:B:2443:TYR:C	1:B:2445:GLY:H	2.23	0.41
1:B:1664:ALA:O	1:B:1668:GLY:N	2.54	0.40
1:B:2322:MET:O	1:B:2326:ASP:N	2.52	0.40
2:D:183:CYS:O	2:D:202:LYS:HA	2.21	0.40
1:B:831:VAL:O	1:B:834:ASN:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1334:ALA:O	1:B:1337:TYR:N	2.54	0.40
1:B:1885:HIS:O	1:B:1888:ALA:HB3	2.22	0.40
2:C:278:ASP:H	2:C:283:GLU:N	2.20	0.40
1:A:1570:VAL:O	1:A:1573:TRP:N	2.55	0.40
1:A:1638:ALA:O	1:A:1641:LYS:N	2.54	0.40
1:B:1570:VAL:O	1:B:1573:TRP:N	2.55	0.40
1:A:1744:TRP:O	1:A:1747:ALA:HB3	2.21	0.40
1:B:1452:LEU:O	1:B:1455:GLY:N	2.54	0.40
1:B:2302:TYR:HA	1:B:2308:GLY:HA3	2.03	0.40
1:B:1934:ILE:O	1:B:1937:ALA:HB2	2.22	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	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	25	66
1	B	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	25	66
2	C	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	15	54
2	D	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	15	54
All	All	4628/5548 (83%)	3694 (80%)	904 (20%)	30 (1%)	29	66

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	A	454	VAL
1	A	490	ILE
1	A	1855	VAL
1	A	1890	VAL

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Mol	Chain	Res	Type
1	A	2444	ILE
1	B	169	ILE
1	B	454	VAL
1	B	490	ILE
1	B	1855	VAL
1	B	1890	VAL
1	B	2444	ILE
1	A	1583	VAL
1	B	1583	VAL
1	A	492	SER
1	A	1193	VAL
1	A	1902	VAL
1	A	2306	VAL
1	B	492	SER
1	B	1193	VAL
1	B	1902	VAL
1	B	2306	VAL
1	A	2361	ILE
1	B	2361	ILE
2	C	107	PRO
2	D	107	PRO
2	C	298	VAL
2	D	298	VAL
2	C	175	VAL
2	D	175	VAL

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1245:CYS	C	1246:SER	N	4.79
1	B	1245:CYS	C	1246:SER	N	4.79
1	A	1097:ASN	C	1098:ALA	N	4.03
1	B	1097:ASN	C	1098:ALA	N	4.03
1	A	756:SER	C	757:ALA	N	3.62
1	B	756:SER	C	757:ALA	N	3.62

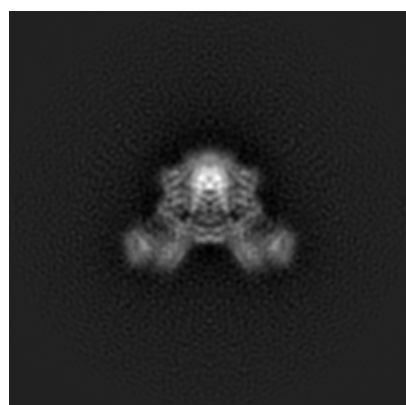
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3329. These allow visual inspection of the internal detail of the map and identification of artifacts.

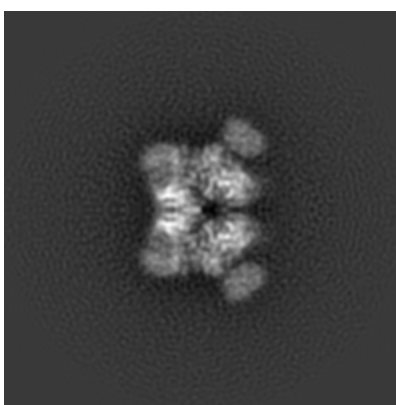
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

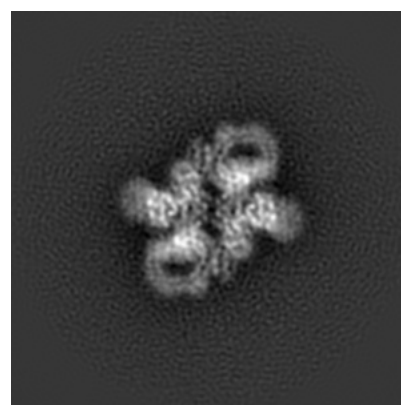
6.1.1 Primary map



X



Y

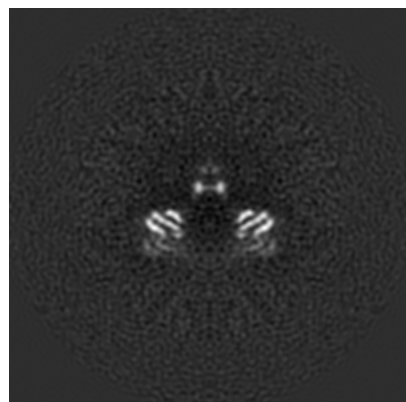


Z

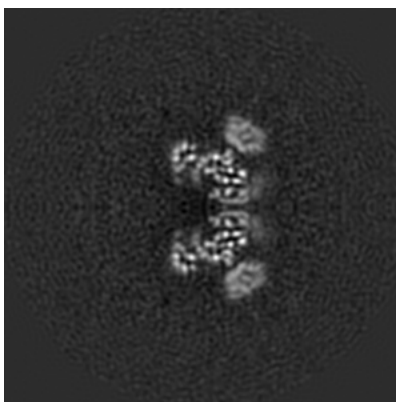
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

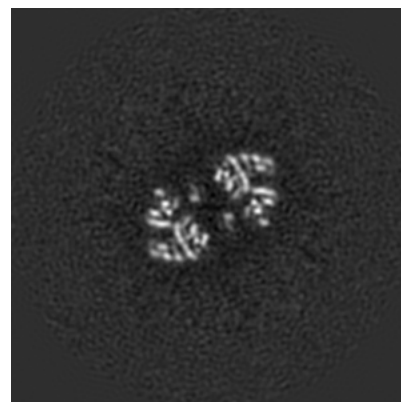
6.2.1 Primary map



X Index: 160



Y Index: 160

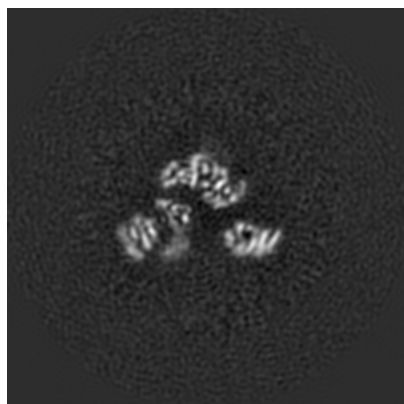


Z Index: 160

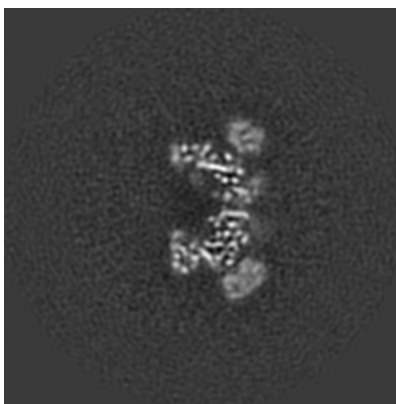
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

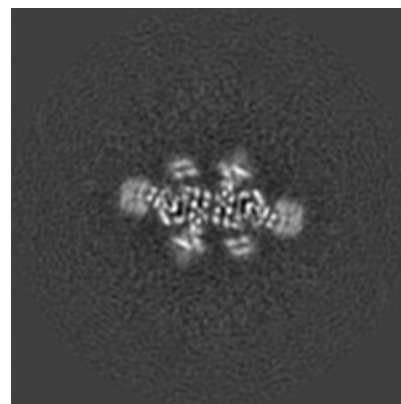
6.3.1 Primary map



X Index: 149



Y Index: 163

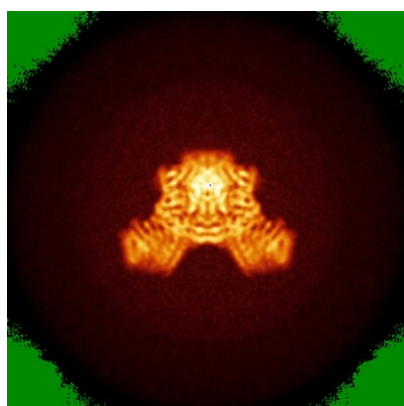


Z Index: 181

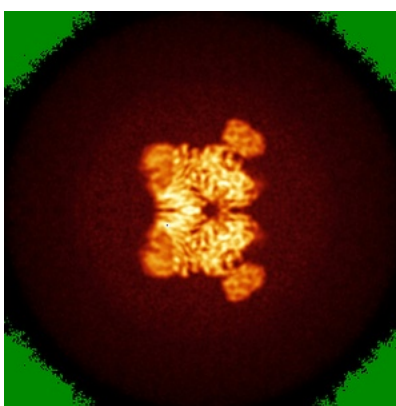
The images above show the largest variance slices of the map in three orthogonal directions.

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

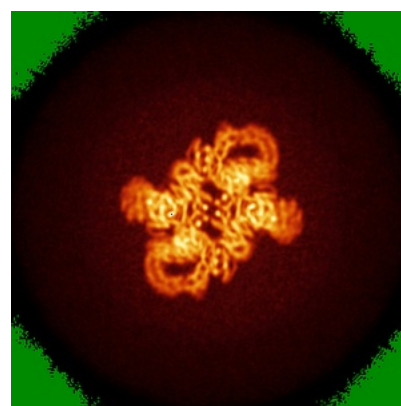
6.4.1 Primary map



X



Y

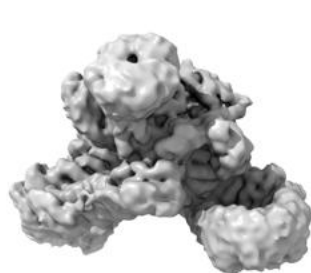


Z

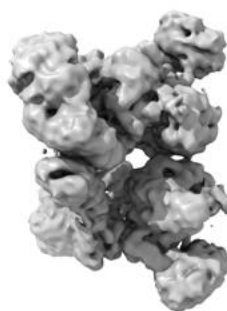
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

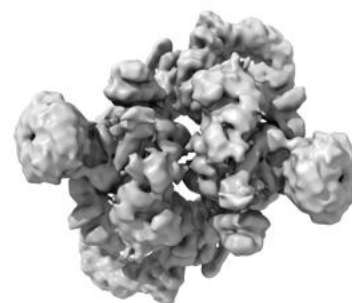
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

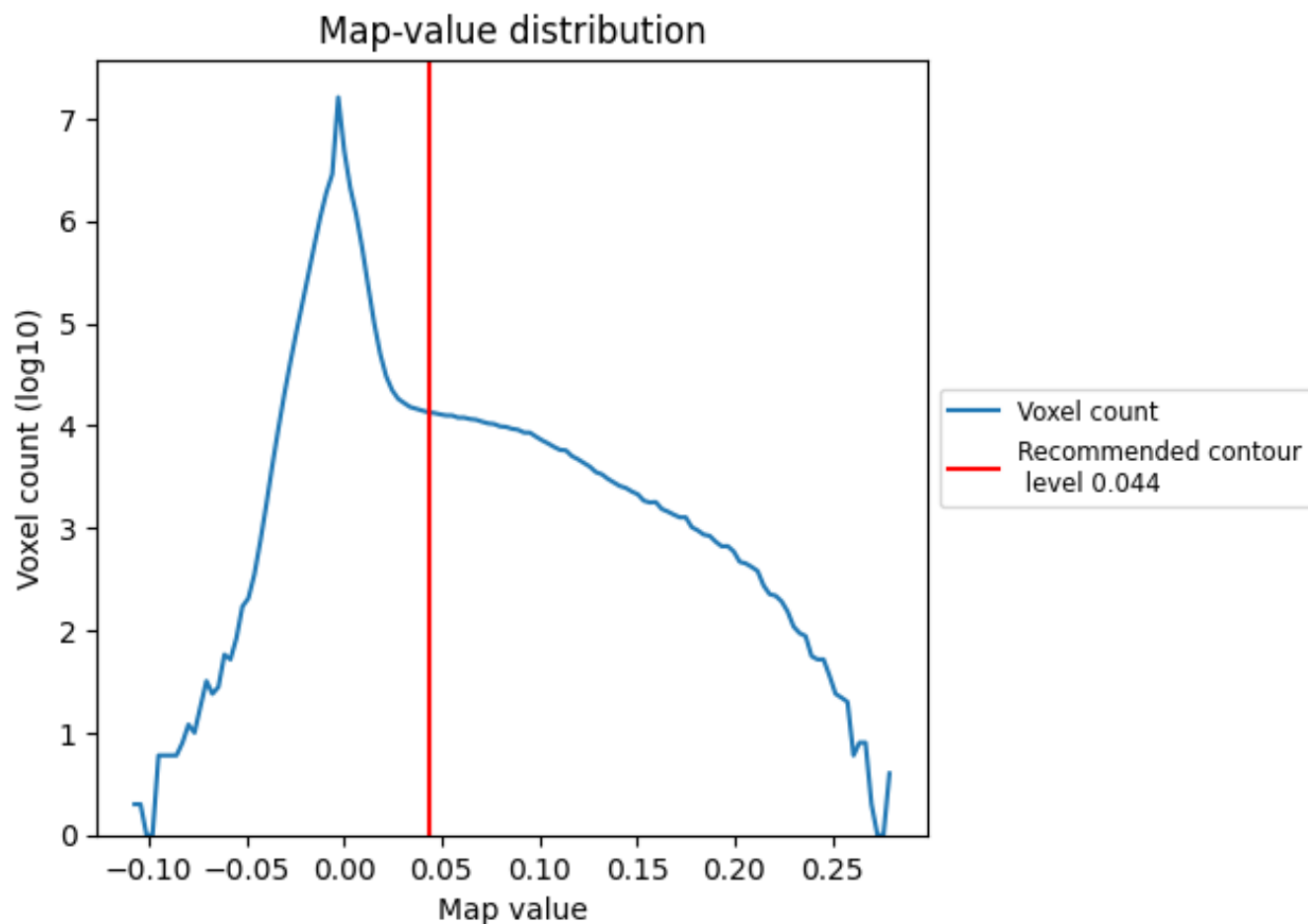
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

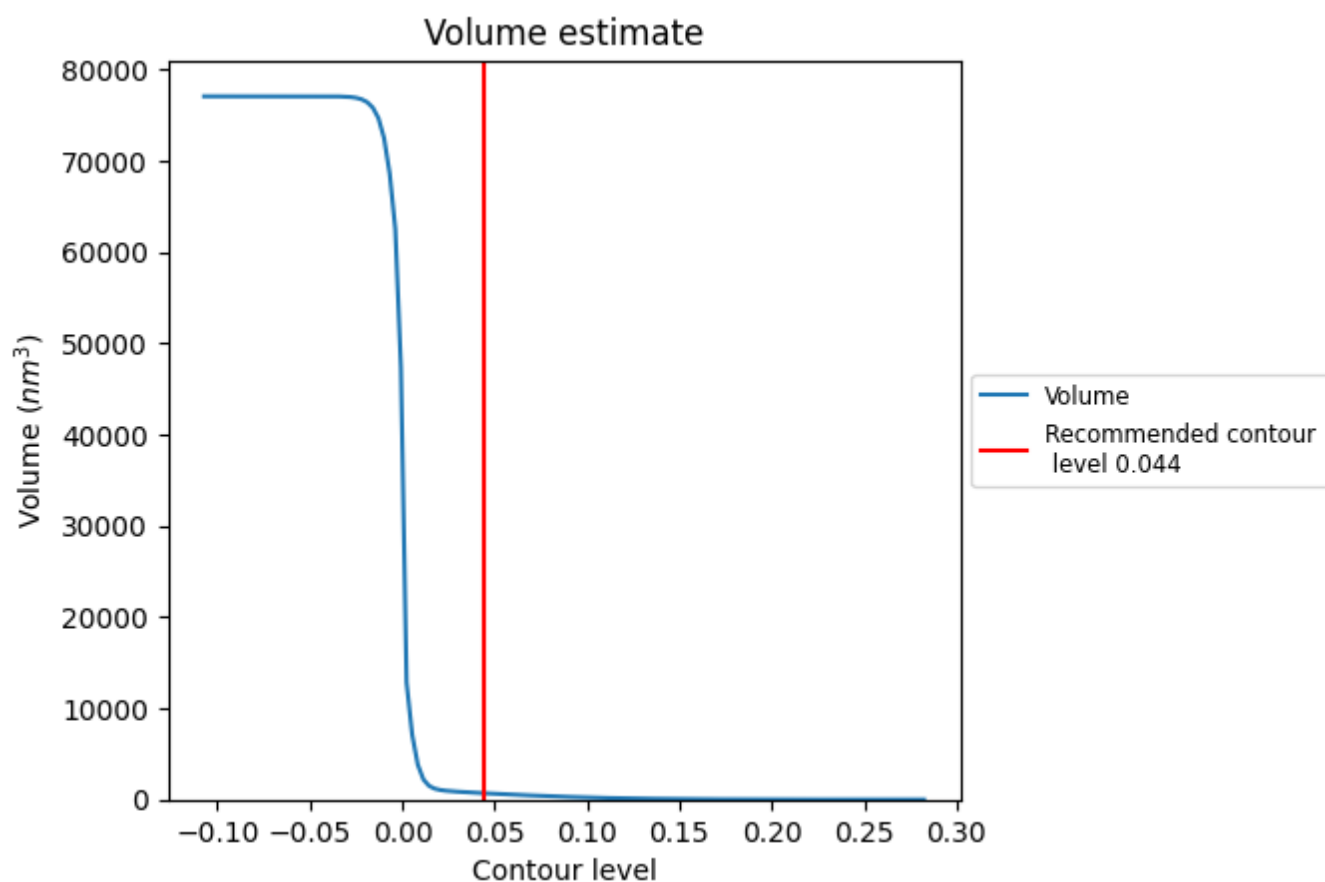
This section contains the results of statistical analysis of the map.

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.

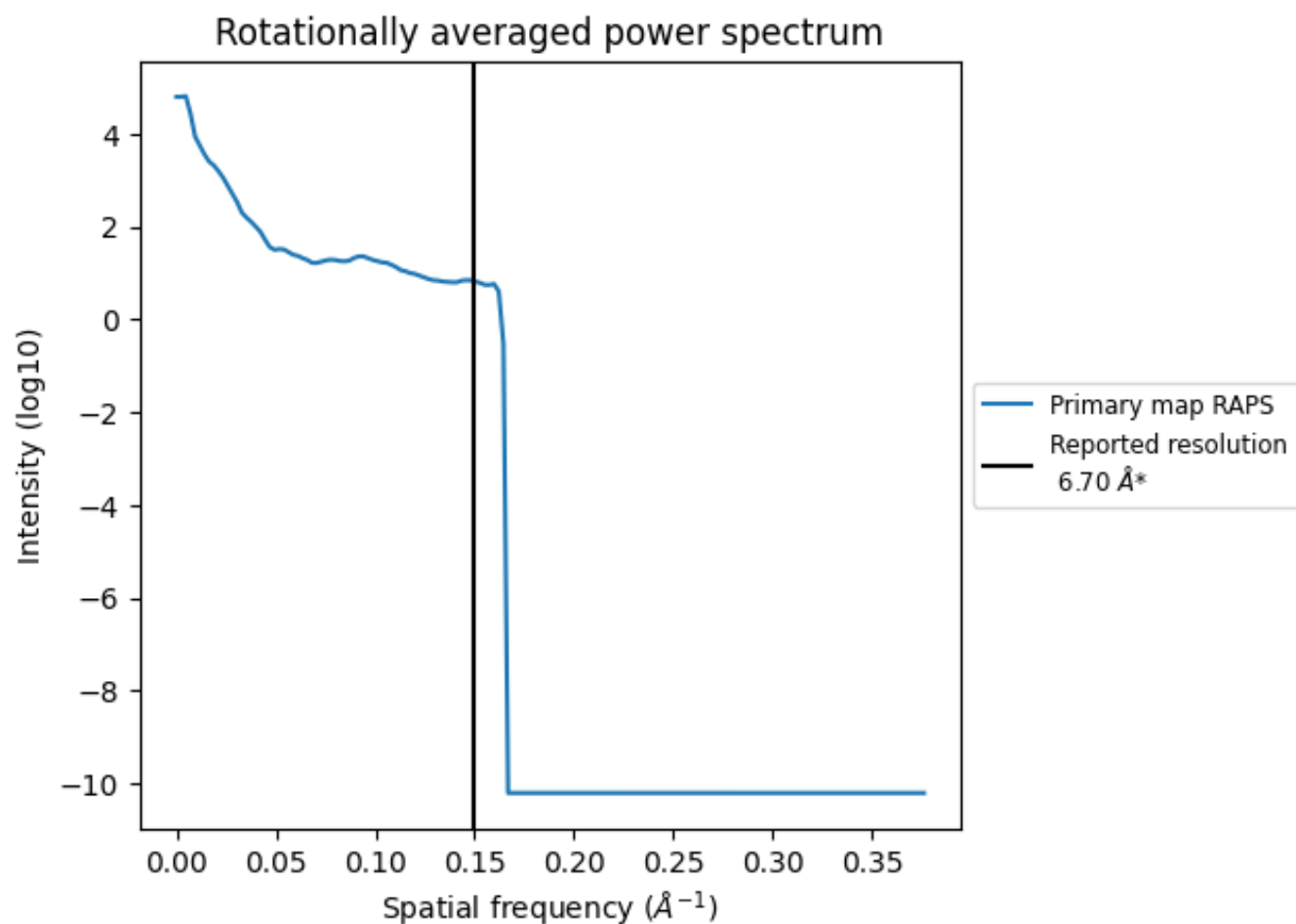
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 631 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 ⓘ

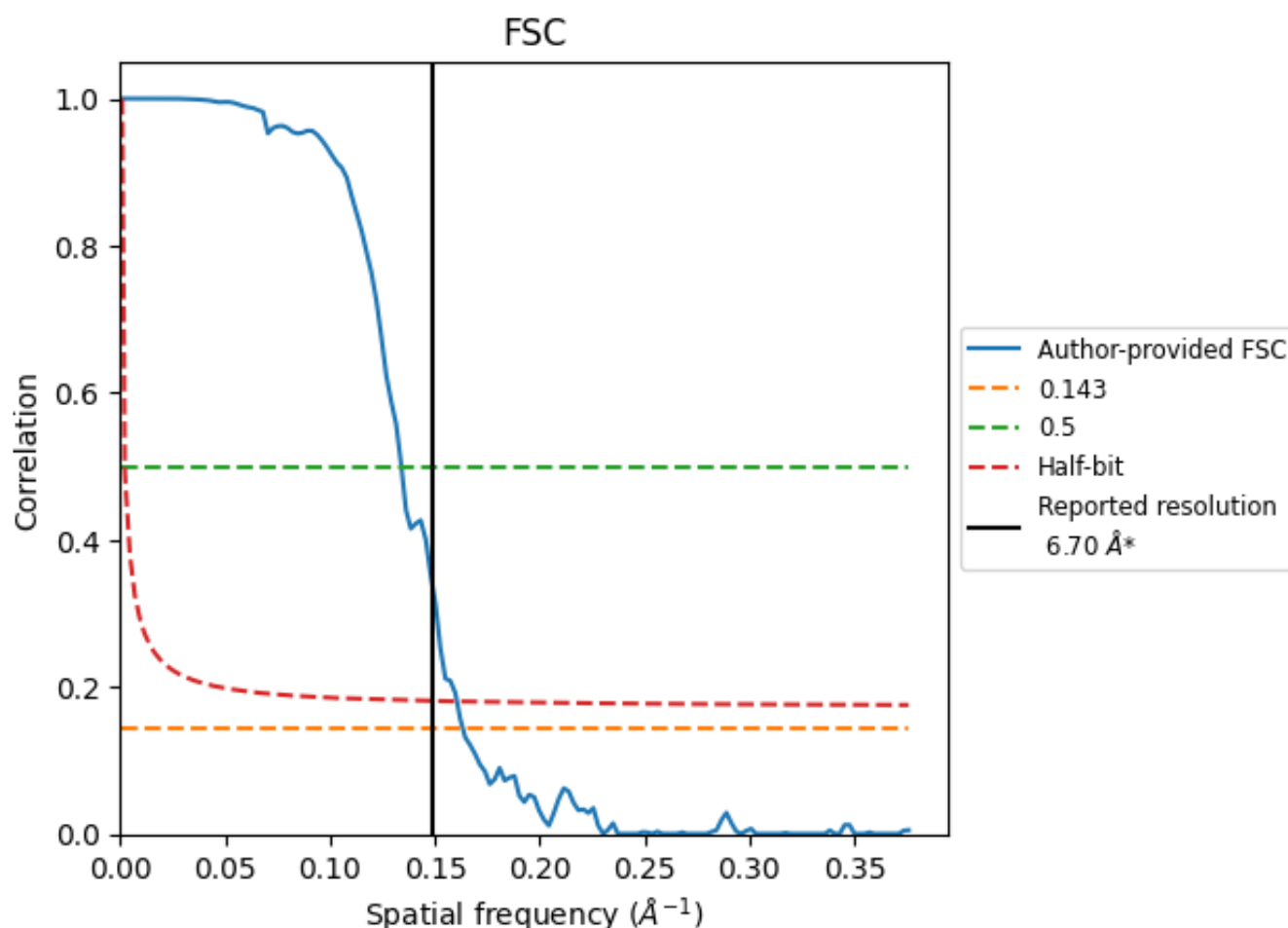


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

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 0.149 Å⁻¹

8.2 Resolution estimates [i](#)

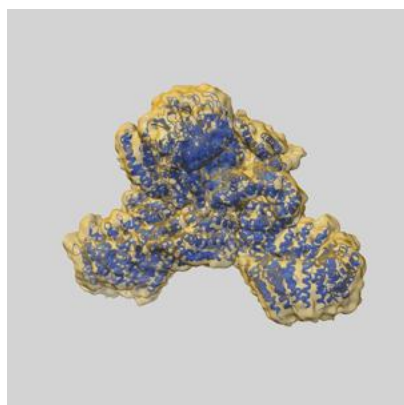
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	6.12	7.46	6.23
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

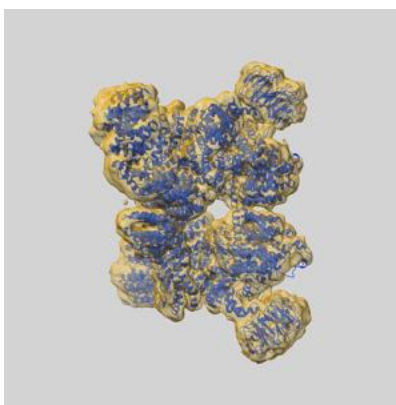
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3329 and PDB model 5FVM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

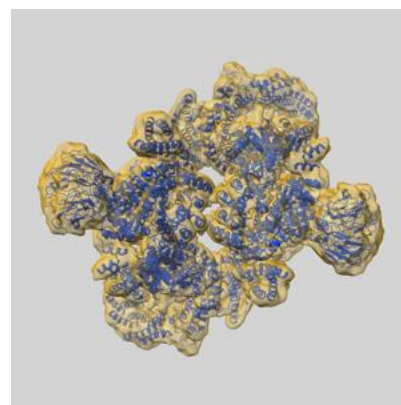
9.1 Map-model overlay [i](#)



X



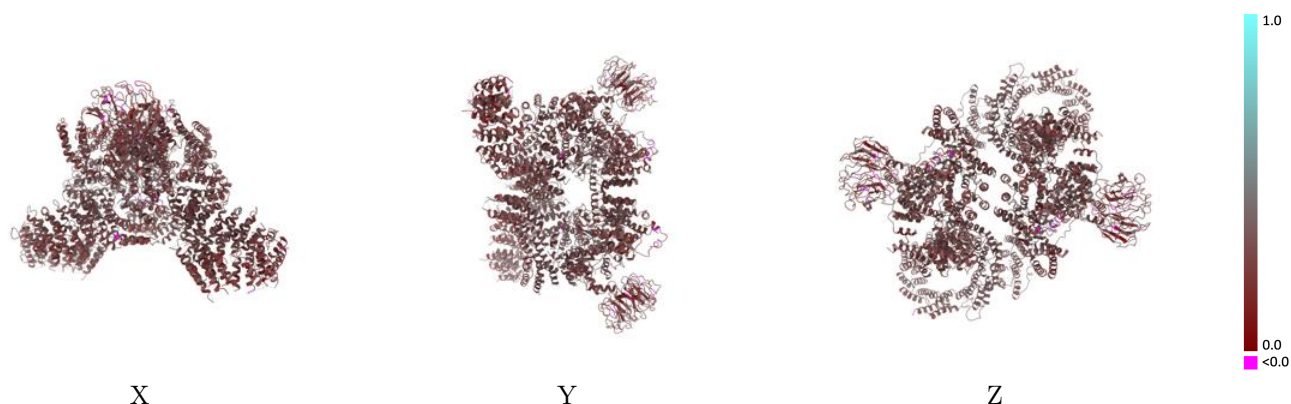
Y



Z

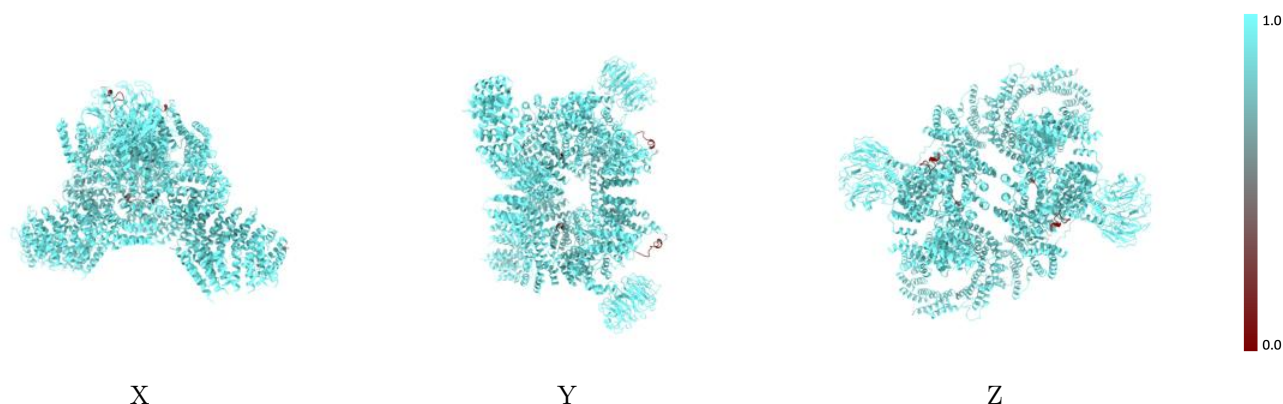
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



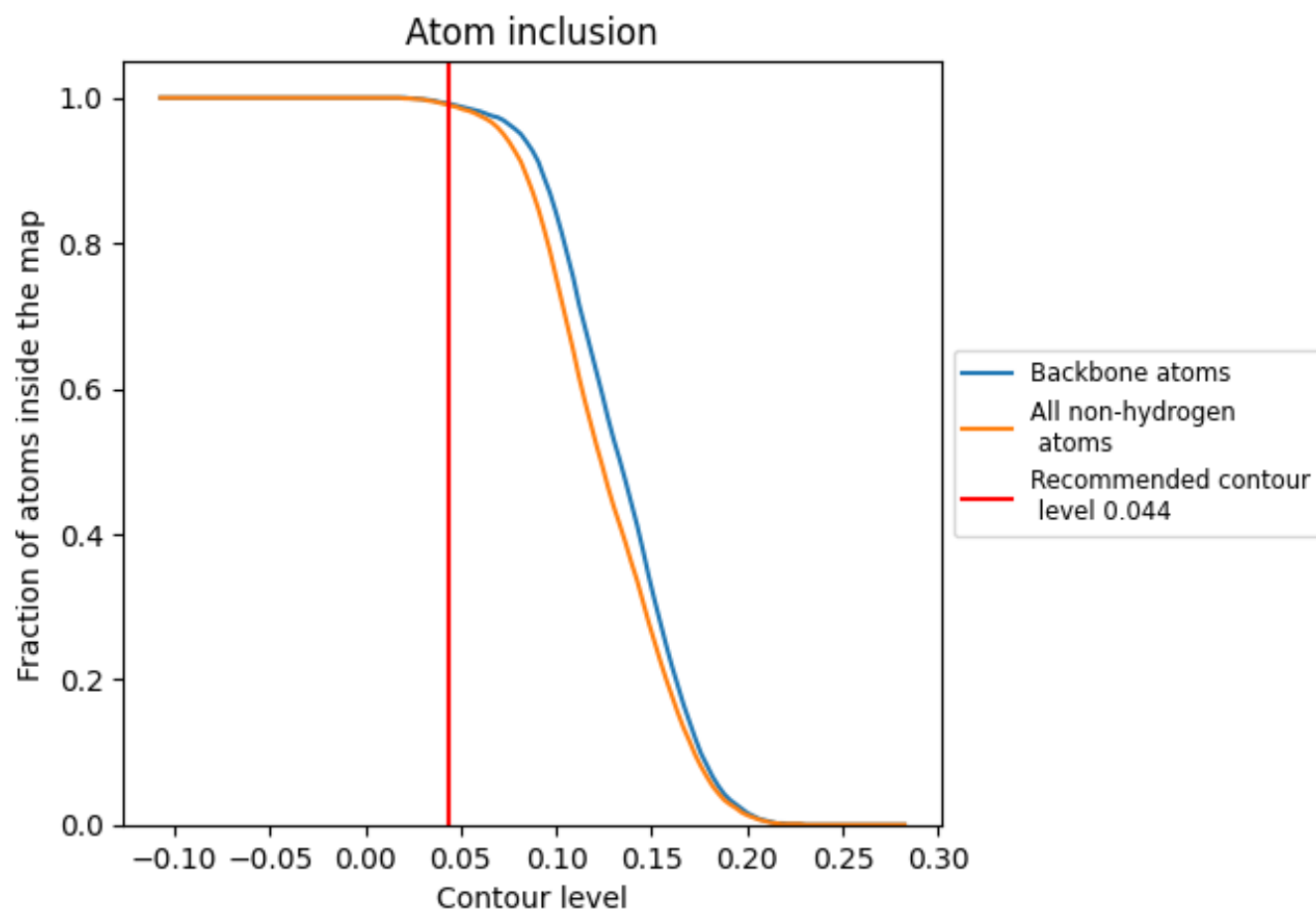
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9900	<div></div> 0.2970
A	<div></div> 0.9890	<div></div> 0.3030
B	<div></div> 0.9890	<div></div> 0.3020
C	<div></div> 1.0000	<div></div> 0.2560
D	<div></div> 1.0000	<div></div> 0.2580

