Full wwPDB EM Validation Report ⓘ

Nov 2, 2026 – 05:06 PM JST

PDB ID	:	46IP / pdb_000046ip
EMDB ID	:	EMD-83829
Title	:	Bacillus subtilis topoisomerase IV ParC-ParE complex
Authors	:	Zhou, Y.; Su, N.; Ma, Z.; Chen, Y.
Deposited on	:	2026-09-24
Resolution	:	3.10 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:

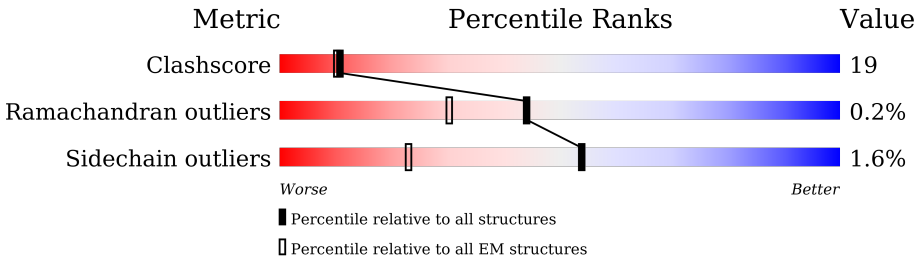
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

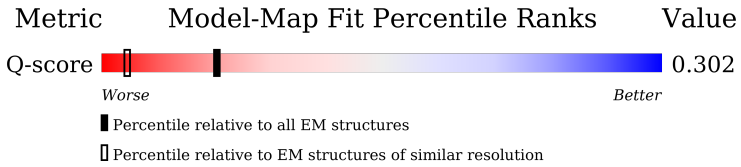
1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	B	696	5% 19% 8% 72%
1	C	696	5% 19% 9% 72%
2	A	847	34% 20% 45%
2	D	847	36% 18% 45%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10370 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 DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	194	Total	C	N	O	S	0	0
			1522	971	261	285	5		
1	C	194	Total	C	N	O	S	0	0
			1522	971	261	285	5		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	656	LEU	-	expression tag	UNP Q59192
B	657	GLU	-	expression tag	UNP Q59192
B	658	LEU	-	expression tag	UNP Q59192
B	659	VAL	-	expression tag	UNP Q59192
B	660	PRO	-	expression tag	UNP Q59192
B	661	ARG	-	expression tag	UNP Q59192
B	662	GLY	-	expression tag	UNP Q59192
B	663	SER	-	expression tag	UNP Q59192
B	664	ASP	-	expression tag	UNP Q59192
B	665	TYR	-	expression tag	UNP Q59192
B	666	LYS	-	expression tag	UNP Q59192
B	667	ASP	-	expression tag	UNP Q59192
B	668	ASP	-	expression tag	UNP Q59192
B	669	ASP	-	expression tag	UNP Q59192
B	670	ASP	-	expression tag	UNP Q59192
B	671	LYS	-	expression tag	UNP Q59192
B	672	TRP	-	expression tag	UNP Q59192
B	673	SER	-	expression tag	UNP Q59192
B	674	HIS	-	expression tag	UNP Q59192
B	675	PRO	-	expression tag	UNP Q59192
B	676	GLN	-	expression tag	UNP Q59192
B	677	PHE	-	expression tag	UNP Q59192
B	678	GLU	-	expression tag	UNP Q59192
B	679	LYS	-	expression tag	UNP Q59192
B	680	GLY	-	expression tag	UNP Q59192
B	681	GLY	-	expression tag	UNP Q59192

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	GLY	-	expression tag	UNP Q59192
B	683	GLY	-	expression tag	UNP Q59192
B	684	SER	-	expression tag	UNP Q59192
B	685	GLY	-	expression tag	UNP Q59192
B	686	GLY	-	expression tag	UNP Q59192
B	687	SER	-	expression tag	UNP Q59192
B	688	ALA	-	expression tag	UNP Q59192
B	689	TRP	-	expression tag	UNP Q59192
B	690	SER	-	expression tag	UNP Q59192
B	691	HIS	-	expression tag	UNP Q59192
B	692	PRO	-	expression tag	UNP Q59192
B	693	GLN	-	expression tag	UNP Q59192
B	694	PHE	-	expression tag	UNP Q59192
B	695	GLU	-	expression tag	UNP Q59192
B	696	LYS	-	expression tag	UNP Q59192
C	656	LEU	-	expression tag	UNP Q59192
C	657	GLU	-	expression tag	UNP Q59192
C	658	LEU	-	expression tag	UNP Q59192
C	659	VAL	-	expression tag	UNP Q59192
C	660	PRO	-	expression tag	UNP Q59192
C	661	ARG	-	expression tag	UNP Q59192
C	662	GLY	-	expression tag	UNP Q59192
C	663	SER	-	expression tag	UNP Q59192
C	664	ASP	-	expression tag	UNP Q59192
C	665	TYR	-	expression tag	UNP Q59192
C	666	LYS	-	expression tag	UNP Q59192
C	667	ASP	-	expression tag	UNP Q59192
C	668	ASP	-	expression tag	UNP Q59192
C	669	ASP	-	expression tag	UNP Q59192
C	670	ASP	-	expression tag	UNP Q59192
C	671	LYS	-	expression tag	UNP Q59192
C	672	TRP	-	expression tag	UNP Q59192
C	673	SER	-	expression tag	UNP Q59192
C	674	HIS	-	expression tag	UNP Q59192
C	675	PRO	-	expression tag	UNP Q59192
C	676	GLN	-	expression tag	UNP Q59192
C	677	PHE	-	expression tag	UNP Q59192
C	678	GLU	-	expression tag	UNP Q59192
C	679	LYS	-	expression tag	UNP Q59192
C	680	GLY	-	expression tag	UNP Q59192
C	681	GLY	-	expression tag	UNP Q59192
C	682	GLY	-	expression tag	UNP Q59192

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Chain	Residue	Modelled	Actual	Comment	Reference
C	683	GLY	-	expression tag	UNP Q59192
C	684	SER	-	expression tag	UNP Q59192
C	685	GLY	-	expression tag	UNP Q59192
C	686	GLY	-	expression tag	UNP Q59192
C	687	SER	-	expression tag	UNP Q59192
C	688	ALA	-	expression tag	UNP Q59192
C	689	TRP	-	expression tag	UNP Q59192
C	690	SER	-	expression tag	UNP Q59192
C	691	HIS	-	expression tag	UNP Q59192
C	692	PRO	-	expression tag	UNP Q59192
C	693	GLN	-	expression tag	UNP Q59192
C	694	PHE	-	expression tag	UNP Q59192
C	695	GLU	-	expression tag	UNP Q59192
C	696	LYS	-	expression tag	UNP Q59192

- Molecule 2 is a protein called DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	464	Total	C	N	O	S	0	0
			3663	2305	644	700	14		
2	D	464	Total	C	N	O	S	0	0
			3663	2305	644	700	14		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	807	LEU	-	expression tag	UNP Q45066
A	808	GLU	-	expression tag	UNP Q45066
A	809	LEU	-	expression tag	UNP Q45066
A	810	VAL	-	expression tag	UNP Q45066
A	811	PRO	-	expression tag	UNP Q45066
A	812	ARG	-	expression tag	UNP Q45066
A	813	GLY	-	expression tag	UNP Q45066
A	814	SER	-	expression tag	UNP Q45066
A	815	ASP	-	expression tag	UNP Q45066
A	816	TYR	-	expression tag	UNP Q45066
A	817	LYS	-	expression tag	UNP Q45066
A	818	ASP	-	expression tag	UNP Q45066
A	819	ASP	-	expression tag	UNP Q45066
A	820	ASP	-	expression tag	UNP Q45066
A	821	ASP	-	expression tag	UNP Q45066
A	822	LYS	-	expression tag	UNP Q45066

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Chain	Residue	Modelled	Actual	Comment	Reference
A	823	TRP	-	expression tag	UNP Q45066
A	824	SER	-	expression tag	UNP Q45066
A	825	HIS	-	expression tag	UNP Q45066
A	826	PRO	-	expression tag	UNP Q45066
A	827	GLN	-	expression tag	UNP Q45066
A	828	PHE	-	expression tag	UNP Q45066
A	829	GLU	-	expression tag	UNP Q45066
A	830	LYS	-	expression tag	UNP Q45066
A	831	GLY	-	expression tag	UNP Q45066
A	832	GLY	-	expression tag	UNP Q45066
A	833	GLY	-	expression tag	UNP Q45066
A	834	GLY	-	expression tag	UNP Q45066
A	835	SER	-	expression tag	UNP Q45066
A	836	GLY	-	expression tag	UNP Q45066
A	837	GLY	-	expression tag	UNP Q45066
A	838	SER	-	expression tag	UNP Q45066
A	839	ALA	-	expression tag	UNP Q45066
A	840	TRP	-	expression tag	UNP Q45066
A	841	SER	-	expression tag	UNP Q45066
A	842	HIS	-	expression tag	UNP Q45066
A	843	PRO	-	expression tag	UNP Q45066
A	844	GLN	-	expression tag	UNP Q45066
A	845	PHE	-	expression tag	UNP Q45066
A	846	GLU	-	expression tag	UNP Q45066
A	847	LYS	-	expression tag	UNP Q45066
D	807	LEU	-	expression tag	UNP Q45066
D	808	GLU	-	expression tag	UNP Q45066
D	809	LEU	-	expression tag	UNP Q45066
D	810	VAL	-	expression tag	UNP Q45066
D	811	PRO	-	expression tag	UNP Q45066
D	812	ARG	-	expression tag	UNP Q45066
D	813	GLY	-	expression tag	UNP Q45066
D	814	SER	-	expression tag	UNP Q45066
D	815	ASP	-	expression tag	UNP Q45066
D	816	TYR	-	expression tag	UNP Q45066
D	817	LYS	-	expression tag	UNP Q45066
D	818	ASP	-	expression tag	UNP Q45066
D	819	ASP	-	expression tag	UNP Q45066
D	820	ASP	-	expression tag	UNP Q45066
D	821	ASP	-	expression tag	UNP Q45066
D	822	LYS	-	expression tag	UNP Q45066
D	823	TRP	-	expression tag	UNP Q45066

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Chain	Residue	Modelled	Actual	Comment	Reference
D	824	SER	-	expression tag	UNP Q45066
D	825	HIS	-	expression tag	UNP Q45066
D	826	PRO	-	expression tag	UNP Q45066
D	827	GLN	-	expression tag	UNP Q45066
D	828	PHE	-	expression tag	UNP Q45066
D	829	GLU	-	expression tag	UNP Q45066
D	830	LYS	-	expression tag	UNP Q45066
D	831	GLY	-	expression tag	UNP Q45066
D	832	GLY	-	expression tag	UNP Q45066
D	833	GLY	-	expression tag	UNP Q45066
D	834	GLY	-	expression tag	UNP Q45066
D	835	SER	-	expression tag	UNP Q45066
D	836	GLY	-	expression tag	UNP Q45066
D	837	GLY	-	expression tag	UNP Q45066
D	838	SER	-	expression tag	UNP Q45066
D	839	ALA	-	expression tag	UNP Q45066
D	840	TRP	-	expression tag	UNP Q45066
D	841	SER	-	expression tag	UNP Q45066
D	842	HIS	-	expression tag	UNP Q45066
D	843	PRO	-	expression tag	UNP Q45066
D	844	GLN	-	expression tag	UNP Q45066
D	845	PHE	-	expression tag	UNP Q45066
D	846	GLU	-	expression tag	UNP Q45066
D	847	LYS	-	expression tag	UNP Q45066

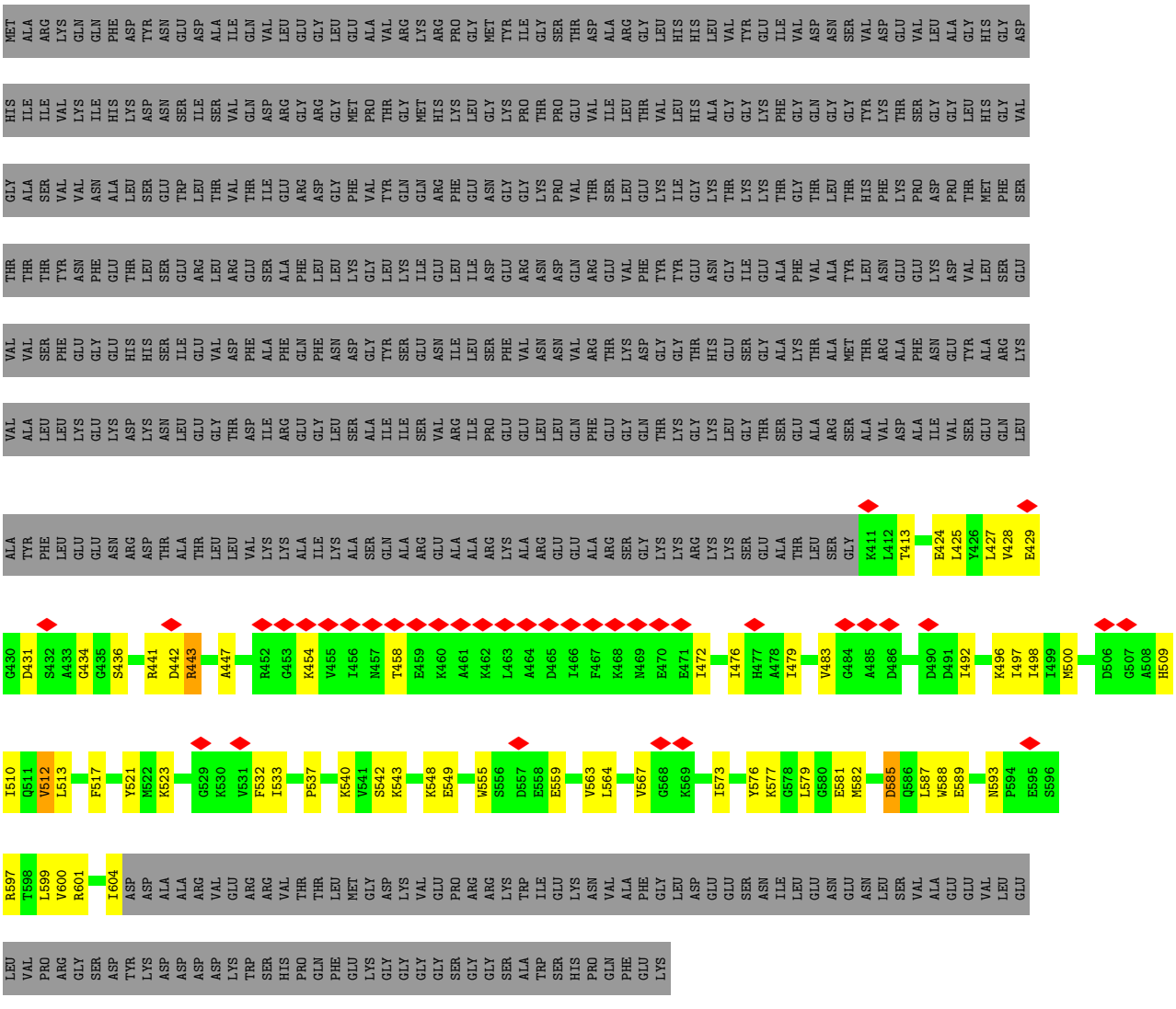
3 Residue-property plots (i)

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: DNA topoisomerase 4 subunit B

Chain B:

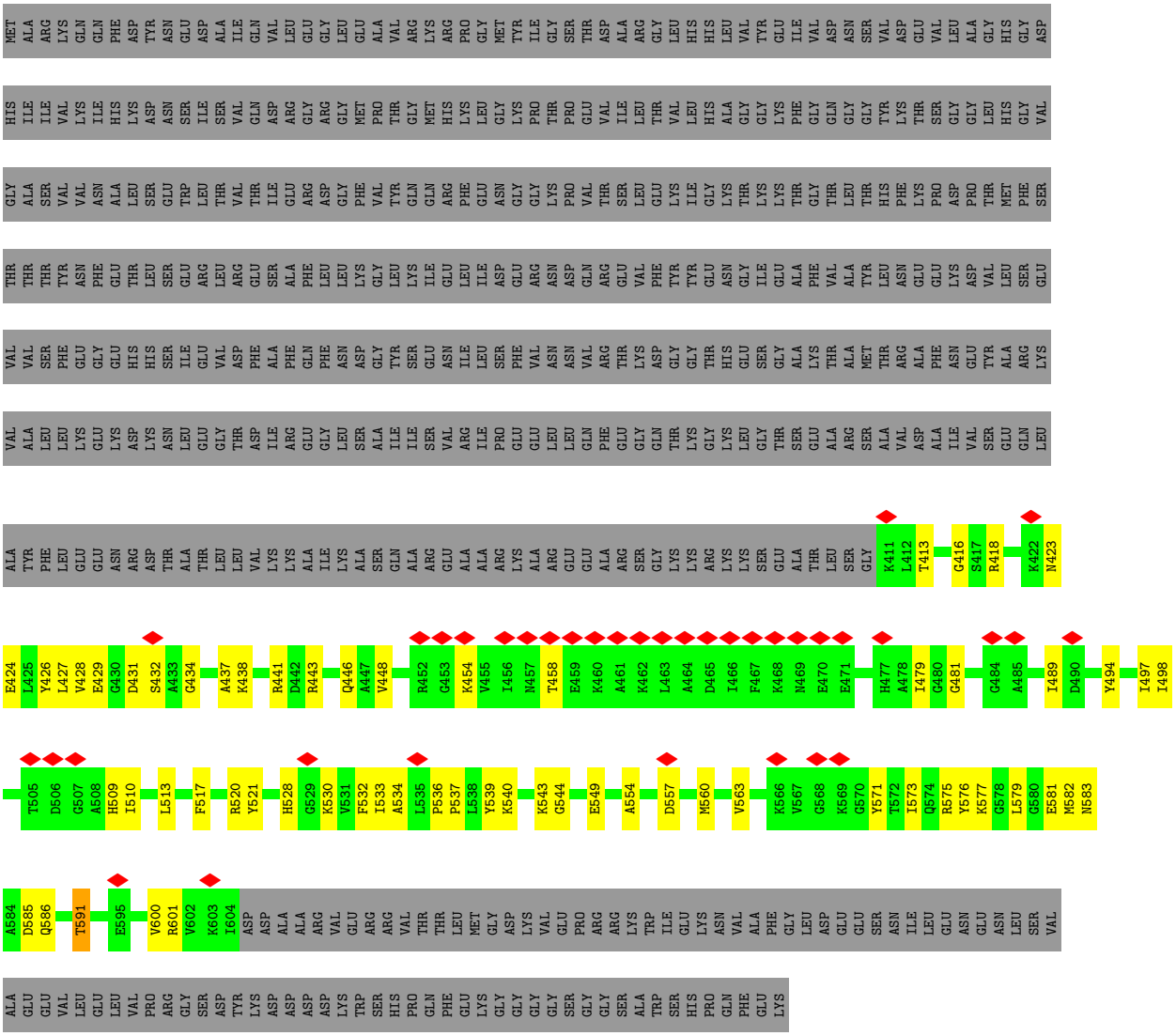




• Molecule 1: DNA topoisomerase 4 subunit B

Chain C:

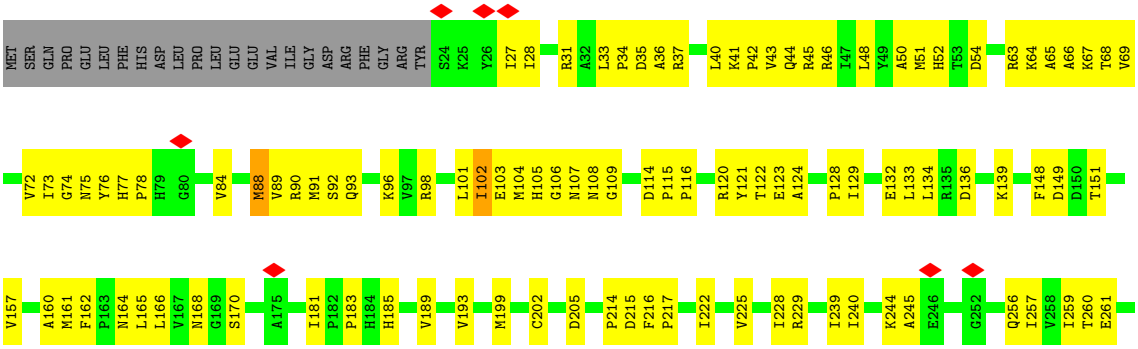


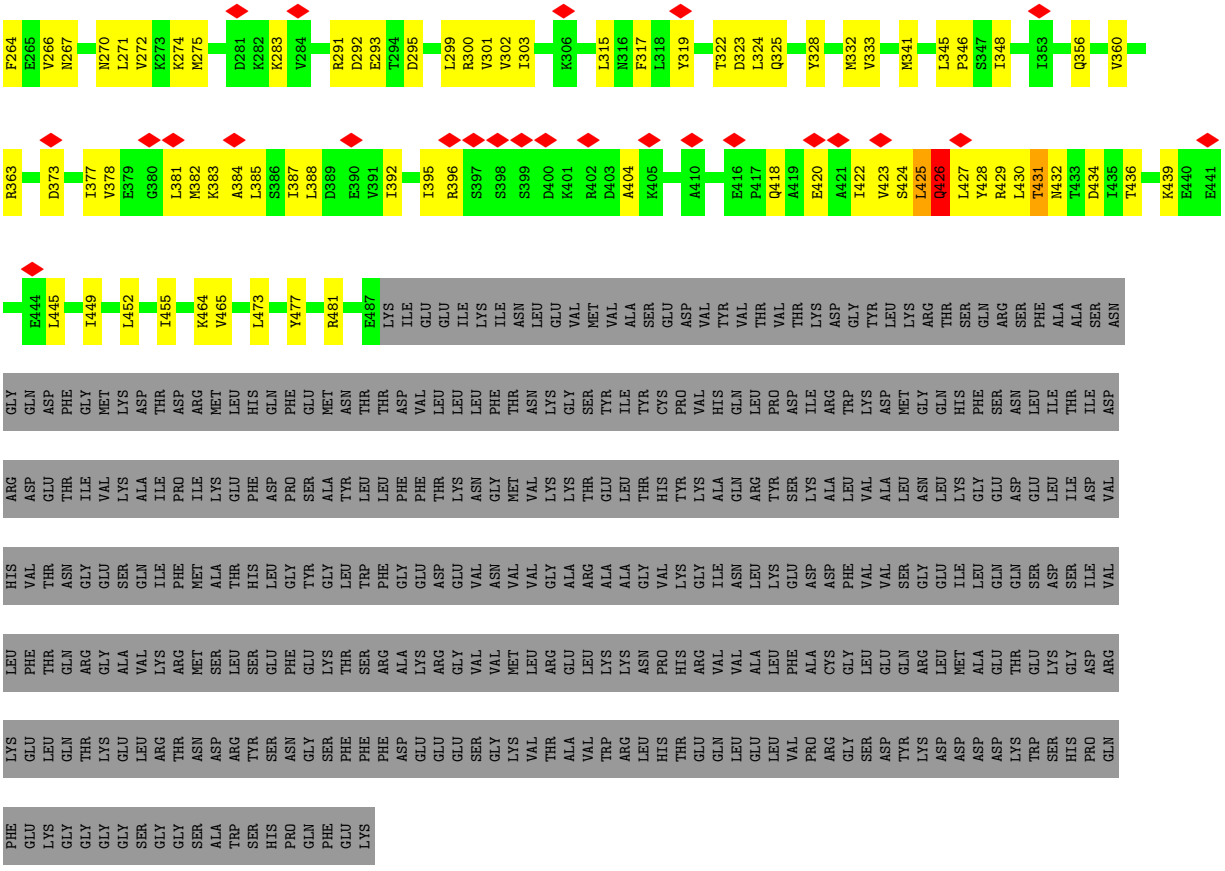


• Molecule 2: DNA topoisomerase 4 subunit A

Chain A:

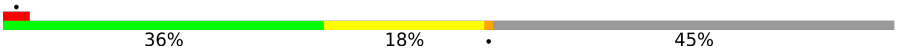


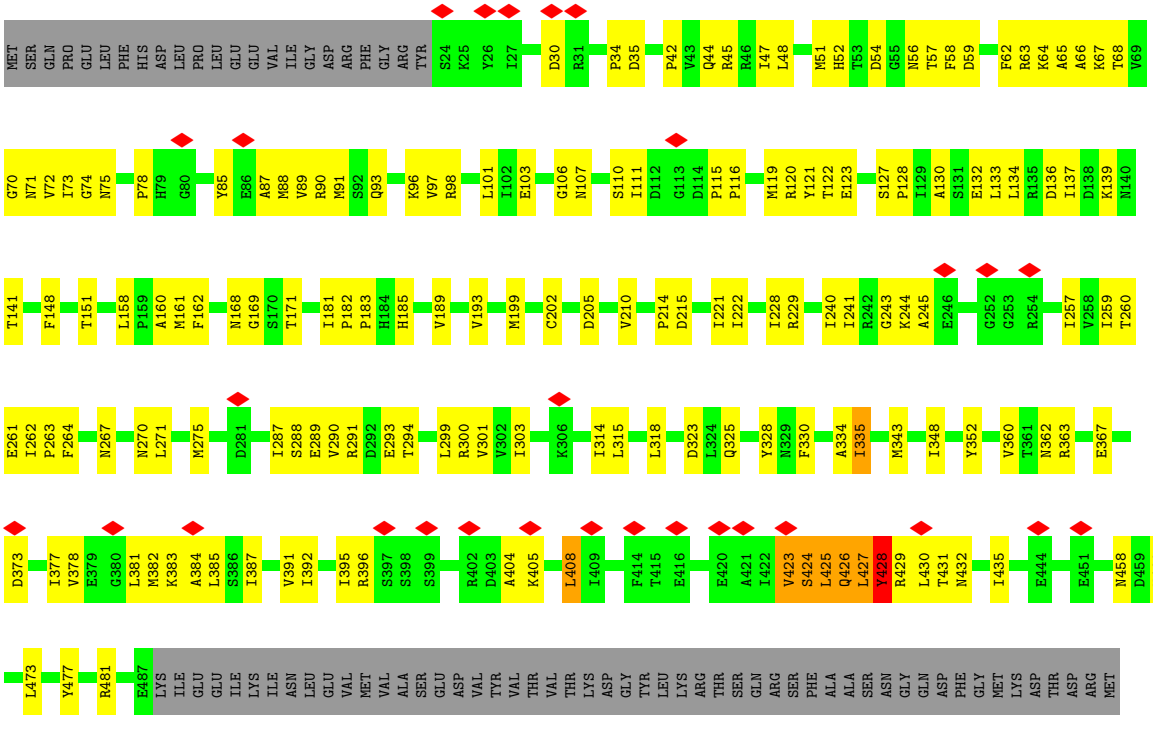




• Molecule 2: DNA topoisomerase 4 subunit A

Chain D:





LEU HIS GLN PHE GLU MET ASN THR THR ASP VAL LEU LEU LEU PHE THR ASN LYS GLY SER TYR ILE TYR CYS PRO VAL HIS GLN LEU PRO ASP ILE ARG TRP LYS ASP MET GLY GLN HIS PHE SER ASN LEU ILE THR ILE ASP ARG ASP GLU THR ILE VAL LYS ALA ILE PRO ILE LYS

GLU PHE ASP PRO SER ALA TYR LEU LEU PHE PHE THR LYS ASN GLY MET VAL LYS LYS THR GLU LEU THR HIS TYR LYS ALA GLN ARG TYR SER LYS ALA LEU VAL ALA LEU ASN LEU LYS GLY GLU ASP GLU LEU ILE ASP VAL HIS VAL THR ASN GLY GLU SER GLN ILE PHE MET ALA

THR HIS LEU GLY TYR GLY LEU TRP PHE GLY GLU ASP GLU VAL ASN VAL VAL GLY ALA ARG ALA ALA GLY VAL LYS GLY ILE ASN LEU LYS GLU ASP ASP PHE VAL VAL SER GLY GLU ILE LEU GLN GLN SER ASP SER ILE VAL LEU PHE THR GLN ARG GLY GLY ALA VAL LYS ARG MET SER

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

ARG TYR SER ASN GLY SER PHE PHE PHE ASP GLU GLU GLU SER GLY LYS VAL THR ALA VAL TRP ARG LEU HIS THR GLU GLN LEU GLU LEU VAL PRO ARG GLY SER ASP TYR LYS ASP ASP ASP ASP LYS TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY GLY SER GLY GLY SER ALA

TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00471	Depositor
Map size (Å)	223.2, 223.2, 223.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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	B	0.16	0/1549	0.44	1/2085 (0.0%)
1	C	0.15	0/1549	0.38	0/2085
2	A	0.21	0/3718	0.52	0/5013
2	D	0.21	0/3718	0.54	4/5013 (0.1%)
All	All	0.20	0/10534	0.50	5/14196 (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
2	A	0	2
2	D	0	4
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	427	LEU	CA-C-N	-9.40	108.47	122.86
2	D	427	LEU	C-N-CA	-9.40	108.47	122.86
2	D	425	LEU	CA-CB-CG	7.73	143.34	116.30
2	D	428	TYR	CA-CB-CG	6.45	125.50	113.90
1	B	443	ARG	CB-CG-CD	5.44	123.82	111.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	426	GLN	Peptide
2	A	431	THR	Peptide

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Mol	Chain	Res	Type	Group
2	D	423	VAL	Peptide
2	D	424	SER	Peptide
2	D	426	GLN	Peptide
2	D	428	TYR	Peptide

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	B	1522	0	1546	55	0
1	C	1522	0	1550	50	0
2	A	3663	0	3746	184	0
2	D	3663	0	3739	185	0
All	All	10370	0	10581	390	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 19.

All (390) 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:A:93:GLN:HA	2:A:108:ASN:HD22	1.43	0.84
1:B:413:THR:HG23	2:A:292:ASP:HB3	1.60	0.83
1:B:427:LEU:HG	1:B:497:ILE:HD11	1.61	0.83
2:D:51:MET:HB3	2:D:56:ASN:HB3	1.61	0.81
2:D:89:VAL:HG21	2:D:116:PRO:HG3	1.62	0.79
2:D:132:GLU:HB3	2:D:161:MET:HB2	1.65	0.78
2:A:425:LEU:HD13	2:D:427:LEU:HG	1.65	0.78
2:D:360:VAL:HG22	2:D:363:ARG:HH12	1.51	0.76
1:C:498:ILE:HG22	1:C:532:PHE:HB2	1.66	0.76
2:A:427:LEU:HD13	2:D:384:ALA:HB3	1.67	0.76
2:A:133:LEU:HA	2:A:160:ALA:HA	1.68	0.75
2:A:267:ASN:HB3	2:A:270:ASN:HB2	1.69	0.75
2:A:166:LEU:HD21	2:A:345:LEU:HD11	1.68	0.74
2:A:96:LYS:HA	2:A:264:PHE:HE1	1.53	0.74
2:A:432:ASN:HB3	2:D:396:ARG:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:431:THR:HA	2:D:392:ILE:HA	1.69	0.74
2:D:259:ILE:O	2:D:300:ARG:HA	1.86	0.73
1:B:498:ILE:HD12	1:B:532:PHE:HB2	1.70	0.73
2:D:162:PHE:HB3	2:D:473:LEU:HD21	1.69	0.73
2:A:132:GLU:HB3	2:A:161:MET:HB2	1.70	0.72
2:A:162:PHE:HB3	2:A:473:LEU:HD21	1.73	0.69
2:A:52:HIS:HB2	2:A:134:LEU:HD13	1.75	0.68
2:A:259:ILE:HB	2:A:301:VAL:HB	1.75	0.68
2:A:430:LEU:HD11	2:D:430:LEU:HD21	1.75	0.68
2:A:89:VAL:HG21	2:A:116:PRO:HG3	1.75	0.68
1:B:443:ARG:HB3	2:A:295:ASP:HB3	1.74	0.68
2:A:164:ASN:HD21	2:A:168:ASN:HD22	1.40	0.68
1:B:564:LEU:HD21	1:B:573:ILE:HD11	1.76	0.68
2:A:384:ALA:HB3	2:D:427:LEU:HD13	1.75	0.67
2:D:243:GLY:HA3	2:D:261:GLU:O	1.95	0.66
2:A:425:LEU:HG	2:D:425:LEU:HB3	1.76	0.65
2:A:257:ILE:HB	2:A:303:ILE:HB	1.78	0.65
2:A:428:TYR:CD2	2:D:423:VAL:HA	2.30	0.65
1:B:537:PRO:HD2	1:B:582:MET:HE1	1.79	0.65
1:B:543:LYS:O	1:B:549:GLU:HA	1.95	0.65
1:B:442:ASP:HB2	1:B:588:TRP:CH2	2.32	0.65
2:A:418:GLN:O	2:A:422:ILE:HG13	1.96	0.65
2:D:85:TYR:HE1	2:D:119:MET:HA	1.62	0.65
2:A:431:THR:HB	2:D:395:ILE:HB	1.79	0.65
1:C:427:LEU:HG	1:C:497:ILE:HD11	1.79	0.64
1:C:431:ASP:HB2	2:D:115:PRO:HD2	1.79	0.64
2:A:445:LEU:O	2:A:449:ILE:HG13	1.97	0.64
2:A:189:VAL:O	2:A:193:VAL:HG23	1.97	0.64
2:D:334:ALA:HB3	2:D:343:MET:HE2	1.78	0.64
2:A:428:TYR:CD2	2:D:425:LEU:HG	2.32	0.64
1:B:581:GLU:HG2	2:A:121:TYR:HB3	1.80	0.63
2:A:40:LEU:HD11	2:A:48:LEU:HD12	1.80	0.63
1:C:528:HIS:HB2	1:C:530:LYS:HZ2	1.64	0.63
2:D:189:VAL:O	2:D:193:VAL:HG23	1.98	0.62
2:D:35:ASP:HB2	2:D:45:ARG:HH21	1.64	0.62
2:A:427:LEU:C	2:D:425:LEU:HD11	2.25	0.62
2:D:395:ILE:HD11	2:D:408:LEU:HG	1.81	0.62
2:D:290:VAL:HG22	2:D:303:ILE:HG23	1.81	0.61
2:D:133:LEU:HA	2:D:160:ALA:HA	1.82	0.61
2:A:422:ILE:HA	2:D:426:GLN:O	2.00	0.61
1:B:429:GLU:HG3	1:B:510:ILE:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:LEU:HA	2:A:51:MET:HG3	1.81	0.61
2:D:387:ILE:O	2:D:391:VAL:HG23	2.00	0.61
2:D:45:ARG:HG3	2:D:158:LEU:HG	1.82	0.61
2:D:214:PRO:HG3	2:D:330:PHE:HZ	1.65	0.61
2:A:98:ARG:HB2	2:A:183:PRO:HB2	1.82	0.60
2:A:214:PRO:HG2	2:A:222:ILE:HD13	1.83	0.60
1:C:438:LYS:NZ	2:D:111:ILE:HG22	2.17	0.60
2:D:275:MET:HG2	2:D:318:LEU:HD21	1.82	0.60
2:D:98:ARG:HB2	2:D:183:PRO:HB2	1.81	0.60
2:A:428:TYR:CG	2:D:423:VAL:HA	2.36	0.59
2:A:72:VAL:HA	2:A:76:TYR:HD2	1.67	0.59
2:A:93:GLN:NE2	2:A:96:LYS:HG3	2.17	0.59
2:D:405:LYS:HG3	2:D:423:VAL:HG11	1.85	0.59
2:D:427:LEU:O	2:D:430:LEU:HB2	2.02	0.59
1:C:510:ILE:HA	1:C:513:LEU:HD12	1.85	0.59
2:D:185:HIS:O	2:D:189:VAL:HG23	2.02	0.59
1:B:496:LYS:HB3	1:B:498:ILE:HD11	1.85	0.59
2:D:133:LEU:HD23	2:D:160:ALA:HA	1.84	0.59
1:C:537:PRO:HD2	1:C:582:MET:HE1	1.85	0.58
2:D:89:VAL:O	2:D:93:GLN:HG3	2.03	0.58
2:A:42:PRO:O	2:A:46:ARG:HG3	2.04	0.58
1:C:560:MET:HE2	1:C:560:MET:HA	1.84	0.58
2:A:429:ARG:H	2:D:425:LEU:HG	1.69	0.58
2:A:151:THR:HG21	2:D:63:ARG:HD3	1.85	0.58
1:C:533:ILE:HG12	1:C:600:VAL:HB	1.86	0.58
2:A:425:LEU:HG	2:D:425:LEU:HD13	1.84	0.58
1:B:441:ARG:O	2:A:295:ASP:HB2	2.04	0.58
2:A:373:ASP:O	2:A:377:ILE:HG12	2.03	0.58
2:A:429:ARG:HA	2:A:434:ASP:CB	2.34	0.57
2:D:48:LEU:HB3	2:D:134:LEU:HD11	1.86	0.57
2:A:132:GLU:O	2:A:161:MET:HG2	2.04	0.57
1:C:438:LYS:HZ1	2:D:111:ILE:HG22	1.69	0.57
2:D:133:LEU:HG	2:D:162:PHE:CE1	2.40	0.57
2:A:166:LEU:HD23	2:A:189:VAL:HG13	1.85	0.57
1:C:423:ASN:HB3	1:C:494:TYR:HD1	1.68	0.57
2:A:274:LYS:HD3	2:A:322:THR:HG22	1.87	0.57
2:A:345:LEU:HB3	2:A:346:PRO:HD3	1.87	0.56
1:B:582:MET:N	2:A:106:GLY:HA2	2.20	0.56
2:D:378:VAL:O	2:D:382:MET:HG2	2.05	0.56
2:A:222:ILE:HG23	2:A:239:ILE:HD12	1.88	0.56
2:A:73:ILE:HD12	2:D:73:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ILE:HD11	1:C:530:LYS:HZ1	1.71	0.56
1:B:597:ARG:NH1	1:B:599:LEU:HD21	2.19	0.56
2:A:65:ALA:HB1	2:A:88:MET:SD	2.46	0.56
2:D:215:ASP:OD2	2:D:481:ARG:HG3	2.05	0.56
2:A:63:ARG:HG2	2:D:151:THR:HG21	1.88	0.56
2:A:93:GLN:HA	2:A:108:ASN:ND2	2.18	0.56
2:D:385:LEU:HD13	2:D:435:ILE:HG23	1.88	0.56
2:A:473:LEU:HD12	2:A:477:TYR:HD2	1.71	0.56
2:D:30:ASP:HA	2:D:42:PRO:HG2	1.87	0.55
2:A:170:SER:H	2:A:181:ILE:HB	1.71	0.55
2:A:67:LYS:HA	2:D:74:GLY:O	2.07	0.55
2:A:272:VAL:HG21	2:A:292:ASP:CG	2.31	0.55
2:D:271:LEU:HD13	2:D:323:ASP:HB2	1.89	0.55
1:C:454:LYS:HA	1:C:510:ILE:HD11	1.88	0.55
1:C:489:ILE:HD11	1:C:530:LYS:NZ	2.22	0.55
2:A:422:ILE:HG23	2:D:427:LEU:HB2	1.89	0.54
2:A:429:ARG:HB2	2:D:425:LEU:HB2	1.89	0.54
1:C:424:GLU:HB2	1:C:446:GLN:HA	1.90	0.54
2:A:395:ILE:HD13	2:D:431:THR:HG22	1.89	0.54
2:A:65:ALA:O	2:A:69:VAL:HG23	2.08	0.54
2:A:64:LYS:HA	2:A:123:GLU:HA	1.89	0.54
2:A:185:HIS:O	2:A:189:VAL:HG23	2.08	0.54
2:A:377:ILE:O	2:A:381:LEU:HG	2.07	0.54
2:D:182:PRO:HG3	2:D:330:PHE:CZ	2.43	0.54
2:A:96:LYS:HA	2:A:264:PHE:CE1	2.39	0.53
2:A:93:GLN:HE21	2:A:96:LYS:HG3	1.72	0.53
2:A:425:LEU:HD22	2:D:430:LEU:HG	1.90	0.53
2:A:148:PHE:CE1	2:D:66:ALA:HB3	2.44	0.53
2:A:360:VAL:HG22	2:A:363:ARG:NH2	2.24	0.53
2:A:427:LEU:O	2:D:425:LEU:HD11	2.09	0.53
2:A:422:ILE:HG22	2:D:428:TYR:HB3	1.89	0.53
2:D:243:GLY:CA	2:D:261:GLU:O	2.56	0.53
2:A:136:ASP:HB3	2:A:139:LYS:HD2	1.89	0.53
2:A:74:GLY:N	2:D:70:GLY:HA3	2.24	0.53
2:A:425:LEU:CG	2:D:425:LEU:HD13	2.39	0.53
2:A:425:LEU:HA	2:D:426:GLN:N	2.24	0.53
2:D:426:GLN:O	2:D:427:LEU:HB2	2.09	0.53
1:B:413:THR:HG22	1:B:441:ARG:HH12	1.72	0.53
2:A:427:LEU:HD11	2:D:381:LEU:HA	1.91	0.53
2:A:432:ASN:CB	2:D:396:ARG:HD3	2.36	0.53
2:A:149:ASP:HB3	2:D:64:LYS:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:LYS:HB2	2:A:261:GLU:HB2	1.90	0.52
1:C:571:TYR:HE1	1:C:573:ILE:HD11	1.75	0.52
2:D:48:LEU:HA	2:D:51:MET:HE2	1.90	0.52
2:D:221:ILE:HD11	2:D:244:LYS:HD3	1.92	0.52
2:A:429:ARG:HB2	2:D:425:LEU:HD12	1.92	0.52
1:C:582:MET:N	2:D:106:GLY:HA2	2.25	0.52
2:A:428:TYR:CE2	2:D:425:LEU:N	2.77	0.52
2:A:383:LYS:O	2:A:387:ILE:HG12	2.09	0.52
1:C:438:LYS:O	1:C:441:ARG:HG2	2.09	0.52
2:D:139:LYS:NZ	2:D:367:GLU:HG3	2.25	0.52
1:B:510:ILE:HA	1:B:513:LEU:HD12	1.91	0.52
2:A:378:VAL:O	2:A:382:MET:HG2	2.10	0.52
1:B:585:ASP:O	1:B:589:GLU:HG3	2.10	0.52
2:A:429:ARG:H	2:D:425:LEU:CG	2.21	0.52
2:A:396:ARG:HD3	2:D:432:ASN:ND2	2.24	0.52
2:D:35:ASP:HB2	2:D:45:ARG:NH2	2.24	0.52
2:D:85:TYR:HD1	2:D:119:MET:HG2	1.74	0.52
2:D:373:ASP:O	2:D:377:ILE:HG12	2.09	0.51
2:A:425:LEU:HD22	2:D:427:LEU:HA	1.90	0.51
2:A:181:ILE:HD11	2:A:332:MET:HA	1.92	0.51
1:C:520:ARG:HA	1:C:520:ARG:NE	2.24	0.51
2:A:214:PRO:HD2	2:A:228:ILE:HD13	1.93	0.51
2:A:455:ILE:HD11	2:A:465:VAL:HG21	1.93	0.51
2:A:429:ARG:HA	2:A:434:ASP:HB2	1.92	0.51
1:B:454:LYS:HA	1:B:510:ILE:HD11	1.92	0.51
1:C:479:ILE:HG23	1:C:481:GLY:H	1.76	0.51
1:B:443:ARG:HG3	2:A:293:GLU:O	2.10	0.51
2:A:101:LEU:HG	2:A:168:ASN:ND2	2.26	0.51
2:A:291:ARG:NH2	2:A:302:VAL:HG11	2.26	0.51
2:D:44:GLN:NE2	2:D:91:MET:HG2	2.26	0.51
2:A:256:GLN:HA	2:A:303:ILE:O	2.11	0.50
1:C:509:HIS:O	1:C:513:LEU:HG	2.12	0.50
1:C:528:HIS:HB2	1:C:530:LYS:NZ	2.26	0.50
1:C:534:ALA:HB1	1:C:591:THR:HG22	1.93	0.50
2:D:56:ASN:HD21	2:D:63:ARG:HB2	1.76	0.50
2:D:360:VAL:HG22	2:D:363:ARG:NH1	2.23	0.50
2:A:404:ALA:HB1	2:D:431:THR:HG21	1.93	0.50
2:D:139:LYS:HE3	2:D:363:ARG:HB2	1.94	0.50
2:D:257:ILE:HG21	2:D:315:LEU:HD13	1.94	0.50
2:A:275:MET:HG3	2:A:322:THR:HG21	1.94	0.50
2:A:425:LEU:HD13	2:D:427:LEU:CG	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:MET:HG2	2:D:202:CYS:HB3	1.94	0.50
2:D:262:ILE:HG23	2:D:299:LEU:HD21	1.94	0.50
1:B:563:VAL:O	1:B:567:VAL:HG23	2.11	0.49
1:B:577:LYS:H	1:B:581:GLU:CD	2.19	0.49
2:D:48:LEU:HA	2:D:51:MET:CE	2.41	0.49
2:D:52:HIS:HB2	2:D:134:LEU:HD13	1.93	0.49
2:D:103:GLU:OE2	2:D:127:SER:HA	2.12	0.49
2:A:324:LEU:O	2:A:324:LEU:HD23	2.12	0.49
2:D:257:ILE:HB	2:D:303:ILE:HD12	1.94	0.49
2:A:418:GLN:HE22	2:A:422:ILE:HD11	1.77	0.49
1:C:416:GLY:HA2	2:D:293:GLU:HG2	1.95	0.49
2:A:425:LEU:CD2	2:D:427:LEU:HA	2.29	0.49
1:C:443:ARG:HG3	2:D:293:GLU:HB3	1.95	0.49
2:D:267:ASN:HB2	2:D:270:ASN:HB2	1.93	0.49
2:D:139:LYS:CE	2:D:363:ARG:HB2	2.43	0.49
2:D:44:GLN:HA	2:D:47:ILE:HD12	1.94	0.49
2:D:240:ILE:HG21	2:D:325:GLN:HE21	1.78	0.49
2:D:377:ILE:O	2:D:381:LEU:HG	2.12	0.49
1:B:509:HIS:O	1:B:513:LEU:HG	2.13	0.48
2:A:215:ASP:OD1	2:A:481:ARG:HG3	2.13	0.48
2:D:458:ASN:ND2	2:D:460:LYS:HE3	2.28	0.48
1:C:539:TYR:CE1	1:C:575:ARG:HD3	2.48	0.48
2:D:54:ASP:OD1	2:D:67:LYS:HE2	2.13	0.48
2:D:287:ILE:HD11	2:D:314:ILE:HD11	1.94	0.48
2:A:120:ARG:HB3	2:D:78:PRO:HB2	1.96	0.48
2:D:395:ILE:HD13	2:D:404:ALA:HB1	1.94	0.48
1:B:479:ILE:HG23	1:B:492:ILE:HG23	1.94	0.48
2:A:257:ILE:HG21	2:A:315:LEU:HD13	1.95	0.48
1:C:581:GLU:OE2	2:D:64:LYS:HE2	2.13	0.48
2:D:293:GLU:O	2:D:300:ARG:HB3	2.13	0.48
1:B:443:ARG:HD2	2:A:295:ASP:OD2	2.13	0.48
1:B:577:LYS:HB3	2:A:121:TYR:CD1	2.48	0.48
1:C:577:LYS:HE2	1:C:577:LYS:HB2	1.72	0.48
2:D:294:THR:HG23	2:D:299:LEU:HA	1.96	0.48
2:A:91:MET:SD	2:A:101:LEU:HD12	2.54	0.48
1:B:497:ILE:C	1:B:498:ILE:HD13	2.39	0.48
1:B:559:GLU:O	1:B:563:VAL:HG12	2.14	0.48
2:A:66:ALA:HB3	2:D:148:PHE:CE1	2.48	0.48
2:A:425:LEU:O	2:D:429:ARG:HB2	2.14	0.48
1:C:532:PHE:CE2	1:C:601:ARG:HG2	2.49	0.48
2:A:240:ILE:HG21	2:A:325:GLN:HE21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ILE:HD13	2:D:88:MET:HB2	1.96	0.48
1:B:523:LYS:HZ1	1:B:604:ILE:HG21	1.79	0.48
2:A:473:LEU:HD12	2:A:477:TYR:CD2	2.49	0.48
2:A:43:VAL:HG23	2:A:84:VAL:HG22	1.95	0.47
1:C:543:LYS:O	1:C:549:GLU:HA	2.14	0.47
2:D:259:ILE:HD12	2:D:301:VAL:HB	1.96	0.47
1:B:476:ILE:HD12	1:B:483:VAL:HB	1.96	0.47
2:A:425:LEU:HA	2:D:425:LEU:HB3	1.96	0.47
2:D:141:THR:HA	2:D:362:ASN:HB2	1.97	0.47
1:B:431:ASP:HB3	2:A:114:ASP:HB3	1.96	0.47
1:C:426:TYR:HB2	1:C:448:VAL:HA	1.97	0.47
1:B:537:PRO:HA	1:B:555:TRP:HA	1.97	0.47
2:A:423:VAL:HA	2:D:428:TYR:CZ	2.50	0.47
2:D:132:GLU:HG2	2:D:473:LEU:HD13	1.96	0.47
1:B:431:ASP:HB2	2:A:115:PRO:HD2	1.97	0.47
2:A:101:LEU:HD21	2:A:164:ASN:ND2	2.30	0.47
2:A:183:PRO:HG3	2:A:217:PRO:HD3	1.95	0.47
1:B:532:PHE:CE2	1:B:601:ARG:HB3	2.50	0.47
1:B:436:SER:HB3	1:B:587:LEU:HD23	1.97	0.47
1:B:548:LYS:HD3	1:B:548:LYS:C	2.39	0.47
1:C:554:ALA:HB2	1:C:563:VAL:HG21	1.96	0.47
2:D:35:ASP:HA	2:D:335:ILE:HG13	1.97	0.47
2:D:241:ILE:HB	2:D:263:PRO:HB3	1.97	0.47
2:A:170:SER:N	2:A:181:ILE:HB	2.29	0.46
2:A:436:THR:HG23	2:A:439:LYS:NZ	2.30	0.46
1:B:424:GLU:HG2	1:B:496:LYS:HE2	1.97	0.46
2:A:428:TYR:N	2:D:425:LEU:HD21	2.19	0.46
2:A:452:LEU:O	2:A:455:ILE:HG22	2.16	0.46
2:D:103:GLU:CD	2:D:128:PRO:HD3	2.40	0.46
2:A:428:TYR:CE2	2:D:425:LEU:HG	2.51	0.46
1:C:429:GLU:HG3	1:C:510:ILE:HG13	1.97	0.46
1:C:432:SER:OG	2:D:107:ASN:HB3	2.15	0.46
2:D:182:PRO:HG3	2:D:330:PHE:CE2	2.50	0.46
1:B:500:MET:HE3	1:B:579:LEU:HD13	1.98	0.46
2:A:431:THR:HG21	2:D:391:VAL:HG12	1.96	0.46
2:A:44:GLN:HE22	2:A:91:MET:HE3	1.80	0.46
2:A:245:ALA:HA	2:A:259:ILE:HA	1.98	0.46
2:D:34:PRO:O	2:D:334:ALA:HB1	2.16	0.46
2:D:343:MET:HE3	2:D:348:ILE:HG12	1.98	0.46
1:B:443:ARG:HG3	2:A:293:GLU:C	2.41	0.46
2:A:425:LEU:CD2	2:D:430:LEU:HG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:LYS:HB3	2:D:121:TYR:HD1	1.80	0.46
2:D:64:LYS:HA	2:D:122:THR:O	2.16	0.46
2:D:428:TYR:HD1	2:D:428:TYR:O	1.99	0.46
2:A:72:VAL:HG11	2:A:84:VAL:HG11	1.97	0.45
2:A:183:PRO:CG	2:A:217:PRO:HD3	2.45	0.45
1:C:543:LYS:HD2	1:C:544:GLY:N	2.31	0.45
2:D:221:ILE:HD11	2:D:244:LYS:CD	2.46	0.45
2:D:383:LYS:O	2:D:387:ILE:HG12	2.16	0.45
1:C:583:ASN:HB2	1:C:586:GLN:HG3	1.99	0.45
1:B:441:ARG:NH1	1:B:447:ALA:HA	2.30	0.45
1:B:533:ILE:CG1	1:B:600:VAL:HB	2.47	0.45
1:B:443:ARG:HG2	2:A:293:GLU:HB3	1.98	0.45
2:A:78:PRO:HB2	2:D:120:ARG:HB3	1.99	0.45
1:B:425:LEU:HD23	1:B:497:ILE:HD13	1.99	0.45
2:A:101:LEU:HD21	2:A:162:PHE:HZ	1.82	0.45
2:A:319:TYR:HD1	2:A:324:LEU:HD22	1.82	0.45
2:D:473:LEU:HD12	2:D:477:TYR:CE1	2.51	0.45
2:A:381:LEU:O	2:A:385:LEU:HG	2.17	0.44
2:A:388:LEU:HD13	2:A:430:LEU:HD21	1.99	0.44
1:C:418:ARG:HG2	2:D:291:ARG:HD3	1.99	0.44
2:D:97:VAL:HB	2:D:168:ASN:OD1	2.17	0.44
1:B:548:LYS:HD3	1:B:548:LYS:O	2.17	0.44
2:A:356:GLN:O	2:A:360:VAL:HG23	2.17	0.44
2:A:34:PRO:HA	2:A:41:LYS:HA	1.99	0.44
2:A:35:ASP:HB2	2:A:45:ARG:NH1	2.33	0.44
2:A:293:GLU:OE2	2:A:300:ARG:HG2	2.17	0.44
2:A:396:ARG:HD3	2:D:432:ASN:CG	2.43	0.44
1:C:557:ASP:O	1:C:560:MET:HB2	2.17	0.44
2:D:222:ILE:HG21	2:D:228:ILE:HD11	1.99	0.44
2:D:244:LYS:HB2	2:D:261:GLU:HB2	2.00	0.44
1:B:472:ILE:O	1:B:476:ILE:HG22	2.18	0.44
2:A:216:PHE:CD1	2:A:264:PHE:HB2	2.53	0.44
2:D:44:GLN:HG2	2:D:87:ALA:HB1	2.00	0.44
2:A:392:ILE:HG22	2:D:432:ASN:ND2	2.33	0.44
2:D:205:ASP:OD1	2:D:229:ARG:HD3	2.16	0.44
1:B:597:ARG:HG3	1:B:599:LEU:HD21	2.00	0.44
2:A:73:ILE:HA	2:A:77:HIS:O	2.18	0.44
1:C:418:ARG:HD3	2:D:289:GLU:OE2	2.18	0.44
2:D:66:ALA:HB2	2:D:119:MET:C	2.43	0.44
2:D:134:LEU:HG	2:D:158:LEU:HD13	1.99	0.44
1:B:540:LYS:HE2	1:B:542:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ARG:H	1:B:601:ARG:HG2	1.59	0.44
2:A:102:ILE:HD11	2:A:124:ALA:HB1	2.01	0.43
1:C:458:THR:HG21	1:C:517:PHE:HD1	1.83	0.43
2:A:283:LYS:HZ2	2:A:317:PHE:HE2	1.66	0.43
1:C:458:THR:HB	1:C:521:TYR:HE2	1.84	0.43
2:D:169:GLY:HA3	2:D:181:ILE:O	2.19	0.43
2:D:352:TYR:OH	2:D:470:LEU:HD21	2.19	0.43
1:B:533:ILE:HG12	1:B:600:VAL:HB	2.00	0.43
2:D:57:THR:HG22	2:D:58:PHE:H	1.83	0.43
2:D:132:GLU:O	2:D:161:MET:HG2	2.18	0.43
1:B:509:HIS:O	1:B:512:VAL:HG12	2.18	0.43
2:D:66:ALA:HB2	2:D:119:MET:HB3	2.01	0.43
2:D:130:ALA:O	2:D:133:LEU:HB2	2.18	0.43
2:D:241:ILE:HD11	2:D:328:TYR:HB2	2.01	0.43
2:A:50:ALA:O	2:A:54:ASP:HB2	2.19	0.43
2:D:139:LYS:HE3	2:D:139:LYS:HB2	1.87	0.43
2:D:271:LEU:HG	2:D:275:MET:HE3	2.01	0.43
2:D:473:LEU:HD12	2:D:477:TYR:CD1	2.54	0.43
2:A:74:GLY:O	2:D:67:LYS:HA	2.18	0.42
2:A:423:VAL:HG13	2:D:428:TYR:CE1	2.54	0.42
2:A:27:ILE:HA	2:A:31:ARG:HB3	2.02	0.42
2:A:36:ALA:HA	2:A:165:LEU:HD22	2.01	0.42
2:A:425:LEU:CD2	2:D:425:LEU:HD13	2.49	0.42
2:A:104:MET:HE2	2:A:122:THR:HB	2.01	0.42
2:D:62:PHE:HB3	2:D:123:GLU:HB3	2.00	0.42
1:B:458:THR:HB	1:B:521:TYR:HE2	1.83	0.42
2:A:165:LEU:HD23	2:A:348:ILE:HG23	2.01	0.42
1:C:423:ASN:HB3	1:C:494:TYR:CD1	2.53	0.42
1:C:428:VAL:HG21	1:C:434:GLY:CA	2.49	0.42
1:C:458:THR:HG21	1:C:517:PHE:CD1	2.54	0.42
2:A:69:VAL:HA	2:A:72:VAL:HG12	2.00	0.42
2:A:430:LEU:HD23	2:A:430:LEU:HA	1.93	0.42
2:A:239:ILE:HG12	2:A:328:TYR:HB3	2.02	0.42
2:D:245:ALA:HA	2:D:259:ILE:HA	2.00	0.42
2:A:37:ARG:HB2	2:A:157:VAL:HG21	2.02	0.42
2:A:423:VAL:HA	2:D:428:TYR:CE1	2.54	0.42
2:D:47:ILE:HG23	2:D:68:THR:HG21	2.01	0.42
2:D:111:ILE:HD12	2:D:111:ILE:HA	1.90	0.42
2:A:68:THR:O	2:A:72:VAL:HG12	2.19	0.42
2:A:199:MET:SD	2:A:202:CYS:HB3	2.59	0.42
2:A:260:THR:O	2:A:299:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:464:LYS:HB2	2:A:464:LYS:HE3	1.95	0.42
2:A:40:LEU:HB2	2:A:45:ARG:HG3	2.01	0.42
2:A:424:SER:O	2:D:425:LEU:HA	2.20	0.42
2:A:101:LEU:HD11	2:A:164:ASN:ND2	2.35	0.41
2:A:103:GLU:OE1	2:A:128:PRO:HD3	2.20	0.41
2:A:388:LEU:O	2:A:392:ILE:HG13	2.20	0.41
2:D:56:ASN:ND2	2:D:63:ARG:HB2	2.36	0.41
1:B:458:THR:HG21	1:B:517:PHE:HD1	1.85	0.41
2:A:425:LEU:HA	2:D:426:GLN:H	1.84	0.41
2:D:137:ILE:HA	2:D:141:THR:OG1	2.20	0.41
2:A:129:ILE:HG12	2:A:162:PHE:CE1	2.55	0.41
2:A:264:PHE:O	2:A:266:VAL:HG23	2.19	0.41
2:D:96:LYS:HA	2:D:264:PHE:HE1	1.85	0.41
2:D:318:LEU:HD23	2:D:318:LEU:HA	1.88	0.41
2:A:420:GLU:O	2:A:423:VAL:HG23	2.21	0.41
2:A:423:VAL:HG13	2:D:428:TYR:CZ	2.55	0.41
2:D:71:ASN:O	2:D:75:ASN:HB2	2.20	0.41
1:B:576:TYR:HA	1:B:581:GLU:OE1	2.20	0.41
2:A:75:ASN:HB2	2:A:76:TYR:CE2	2.55	0.41
1:B:458:THR:HG21	1:B:517:PHE:CD1	2.55	0.41
2:A:92:SER:HB3	2:A:102:ILE:HG23	2.02	0.41
2:A:107:ASN:CG	2:A:109:GLY:H	2.29	0.41
2:A:271:LEU:HD13	2:A:323:ASP:HB2	2.03	0.41
2:A:424:SER:HB3	2:D:426:GLN:OE1	2.20	0.41
2:D:56:ASN:ND2	2:D:63:ARG:HD2	2.36	0.41
2:D:65:ALA:HB1	2:D:88:MET:CE	2.51	0.41
2:D:136:ASP:CG	2:D:139:LYS:HE2	2.46	0.41
2:D:199:MET:HE2	2:D:202:CYS:HA	2.03	0.41
1:B:428:VAL:HG21	1:B:434:GLY:CA	2.50	0.41
2:A:205:ASP:OD1	2:A:229:ARG:HD3	2.21	0.41
1:C:539:TYR:HE1	1:C:575:ARG:HD3	1.83	0.41
1:B:593:ASN:C	1:B:597:ARG:HD3	2.46	0.40
2:D:139:LYS:HZ2	2:D:367:GLU:HG3	1.86	0.40
2:A:333:VAL:HA	2:A:341:MET:O	2.21	0.40
2:A:449:ILE:HG22	2:A:449:ILE:O	2.21	0.40
1:C:437:ALA:O	1:C:441:ARG:HB3	2.21	0.40
1:C:532:PHE:HE2	1:C:601:ARG:HG2	1.86	0.40
1:C:540:LYS:HB2	1:C:576:TYR:CE2	2.56	0.40
2:D:48:LEU:HB2	2:D:158:LEU:HD11	2.04	0.40
2:D:90:ARG:HH22	2:D:171:THR:HG23	1.86	0.40
2:D:101:LEU:HD23	2:D:101:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:VAL:HG11	2:D:352:TYR:HE2	1.85	0.40
2:A:28:ILE:HG23	2:A:33:LEU:HD12	2.03	0.40
2:A:225:VAL:HG12	2:A:229:ARG:NH2	2.36	0.40
2:A:426:GLN:HB2	2:D:425:LEU:HD23	1.91	0.40
1:C:536:PRO:HG3	1:C:579:LEU:HD11	2.04	0.40
2:D:68:THR:O	2:D:72:VAL:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	192/696 (28%)	188 (98%)	4 (2%)	0	100	100
1	C	192/696 (28%)	189 (98%)	3 (2%)	0	100	100
2	A	462/847 (54%)	437 (95%)	24 (5%)	1 (0%)	43	73
2	D	462/847 (54%)	442 (96%)	19 (4%)	1 (0%)	43	73
All	All	1308/3086 (42%)	1256 (96%)	50 (4%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	426	GLN
2	D	424	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	161/580 (28%)	159 (99%)	2 (1%)	63	78
1	C	161/580 (28%)	158 (98%)	3 (2%)	50	73
2	A	404/738 (55%)	399 (99%)	5 (1%)	63	78
2	D	404/738 (55%)	396 (98%)	8 (2%)	48	72
All	All	1130/2636 (43%)	1112 (98%)	18 (2%)	54	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	512	VAL
1	B	585	ASP
2	A	88	MET
2	A	90	ARG
2	A	102	ILE
2	A	105	HIS
2	A	425	LEU
1	C	413	THR
1	C	585	ASP
1	C	591	THR
2	D	59	ASP
2	D	110	SER
2	D	210	VAL
2	D	260	THR
2	D	288	SER
2	D	335	ILE
2	D	408	LEU
2	D	428	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	593	ASN
2	A	56	ASN
2	A	79	HIS
2	A	93	GLN
2	A	164	ASN
2	A	316	ASN
2	A	325	GLN

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Mol	Chain	Res	Type
2	A	407	ASN
1	C	574	GLN
2	D	56	ASN
2	D	99	ASN
2	D	325	GLN
2	D	337	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

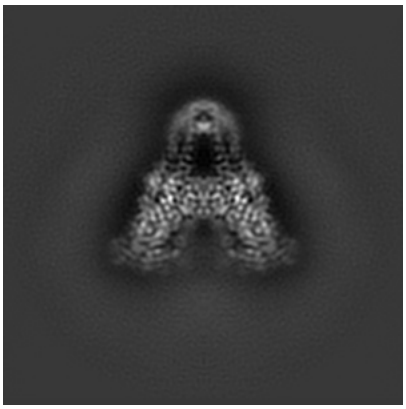
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-83829. These allow visual inspection of the internal detail of the map and identification of artifacts.

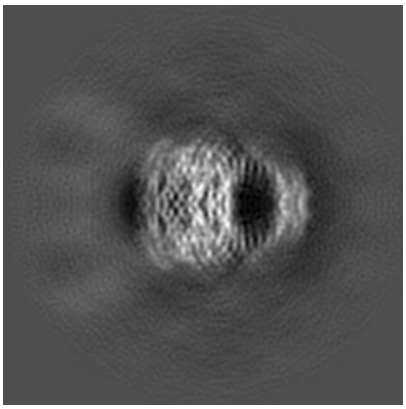
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

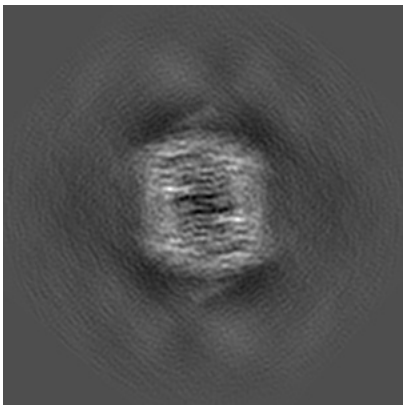
6.1.1 Primary map



X

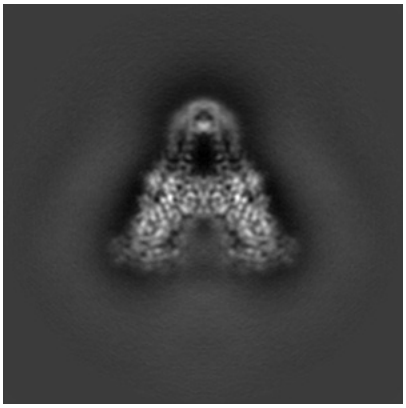


Y

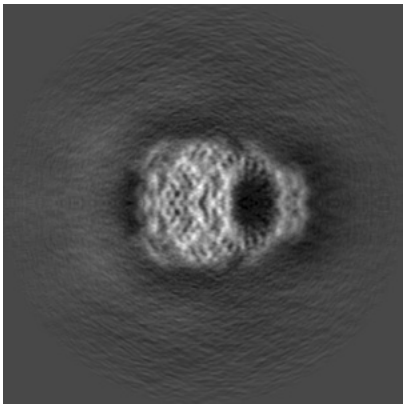


Z

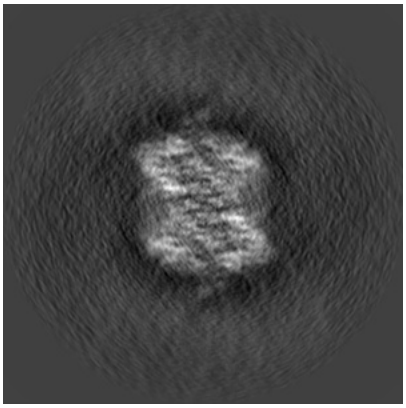
6.1.2 Raw map



X



Y

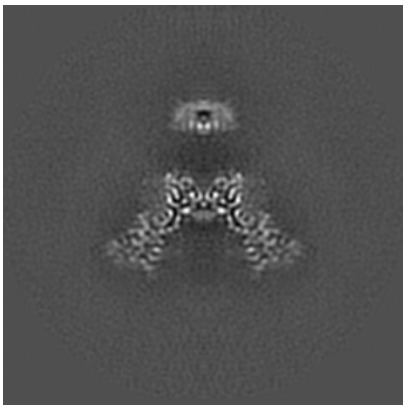


Z

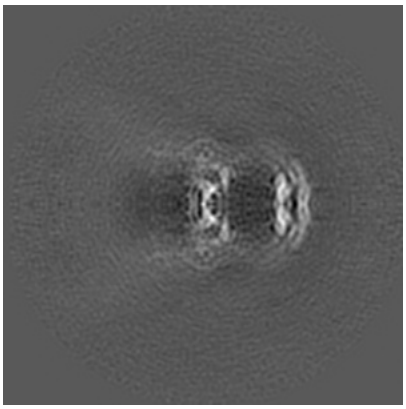
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

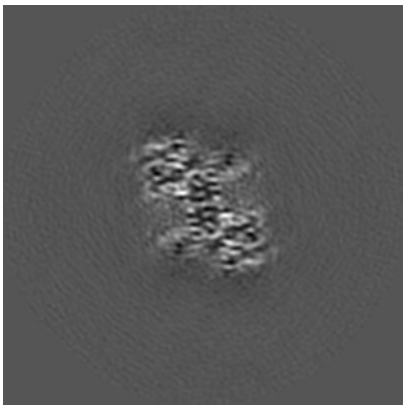
6.2.1 Primary map



X Index: 120

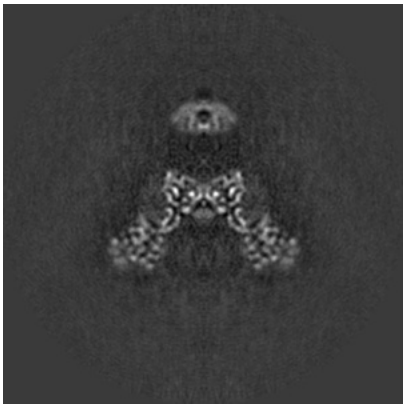


Y Index: 120

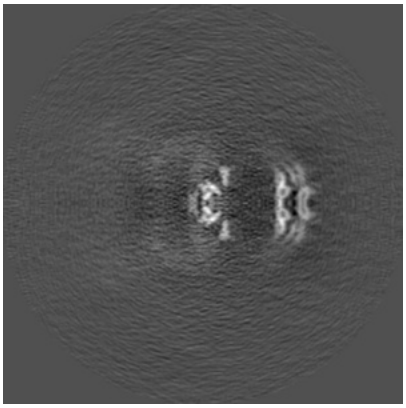


Z Index: 120

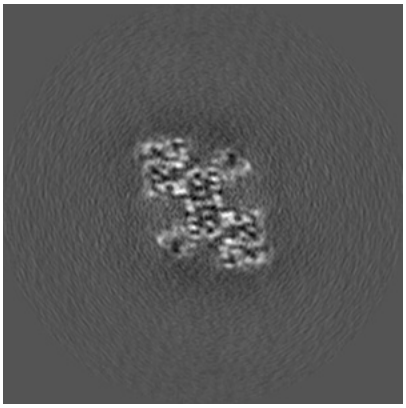
6.2.2 Raw map



X Index: 120



Y Index: 120

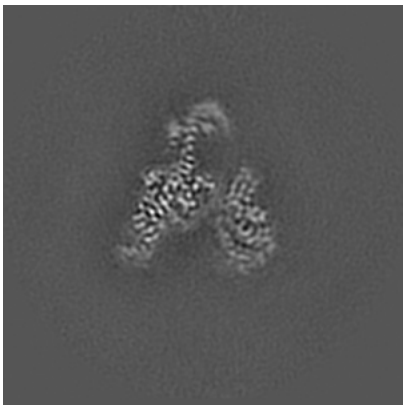


Z Index: 120

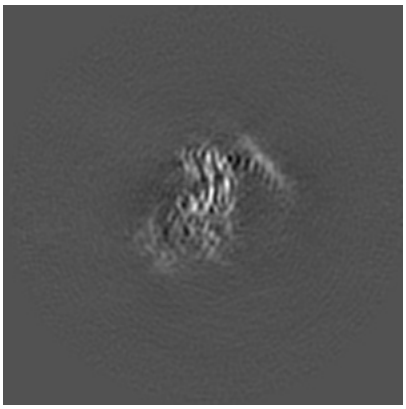
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

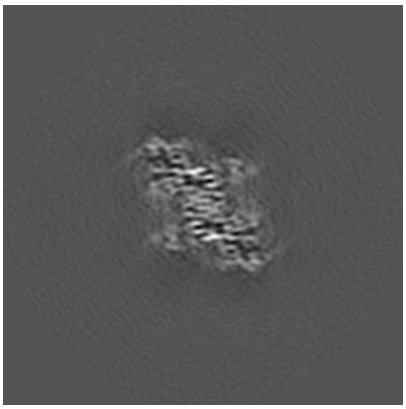
6.3.1 Primary map



X Index: 136

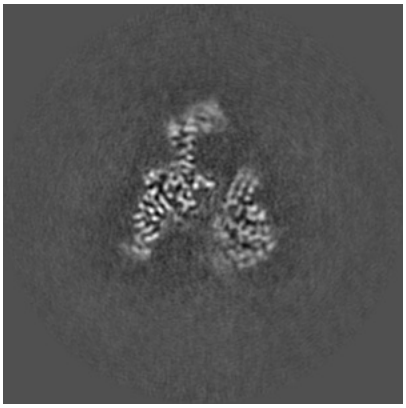


Y Index: 100

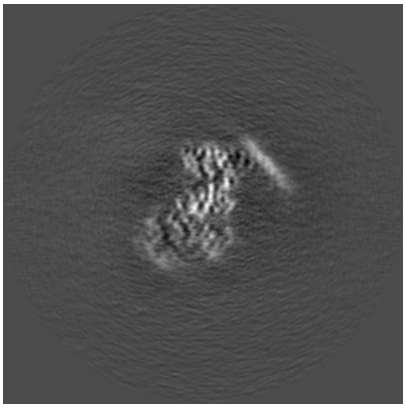


Z Index: 124

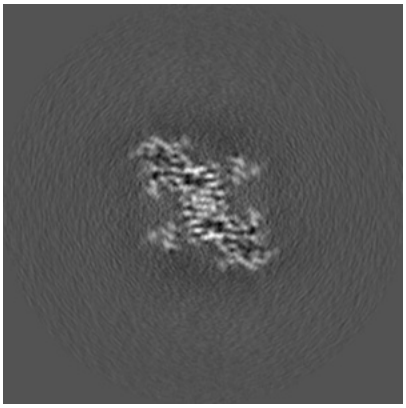
6.3.2 Raw map



X Index: 137



Y Index: 100

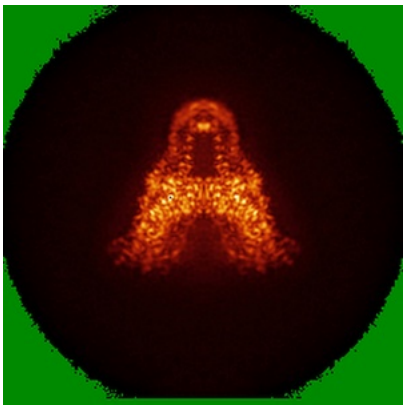


Z Index: 124

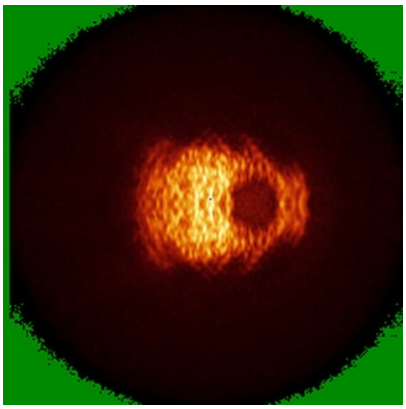
The images above show the largest variance slices of the map in three orthogonal directions.

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

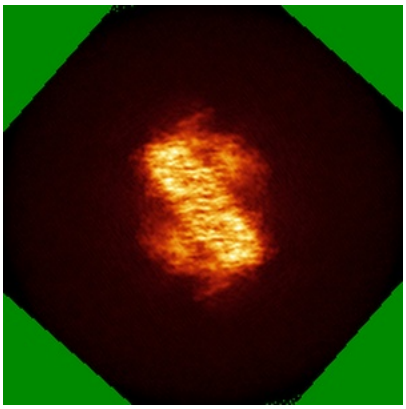
6.4.1 Primary map



X

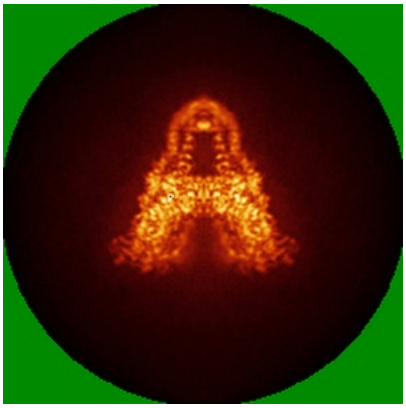


Y

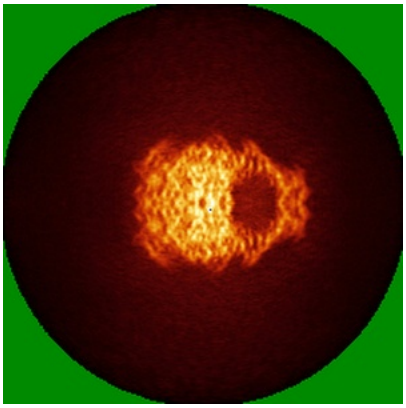


Z

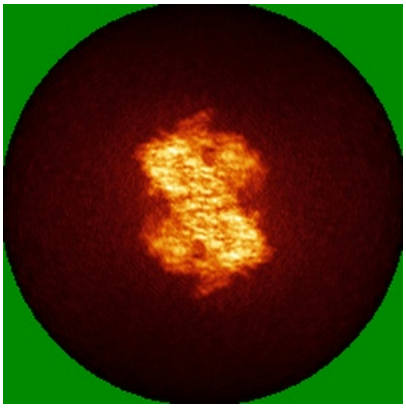
6.4.2 Raw map



X



Y

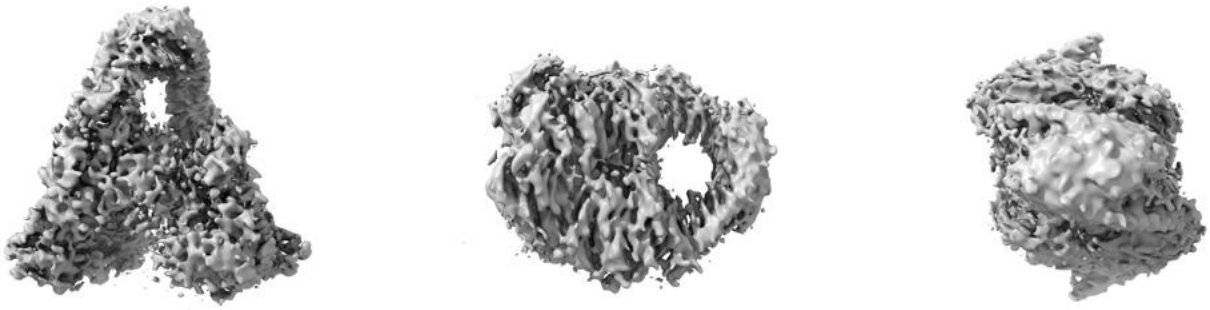


Z

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

6.5 Orthogonal surface views (i)

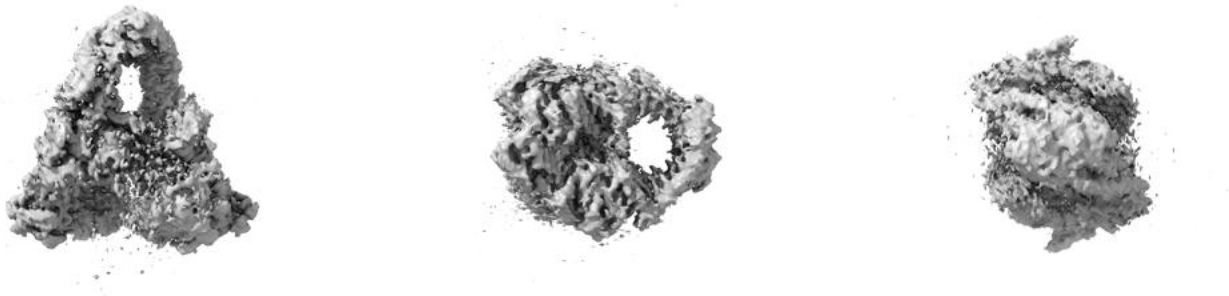
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00471. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

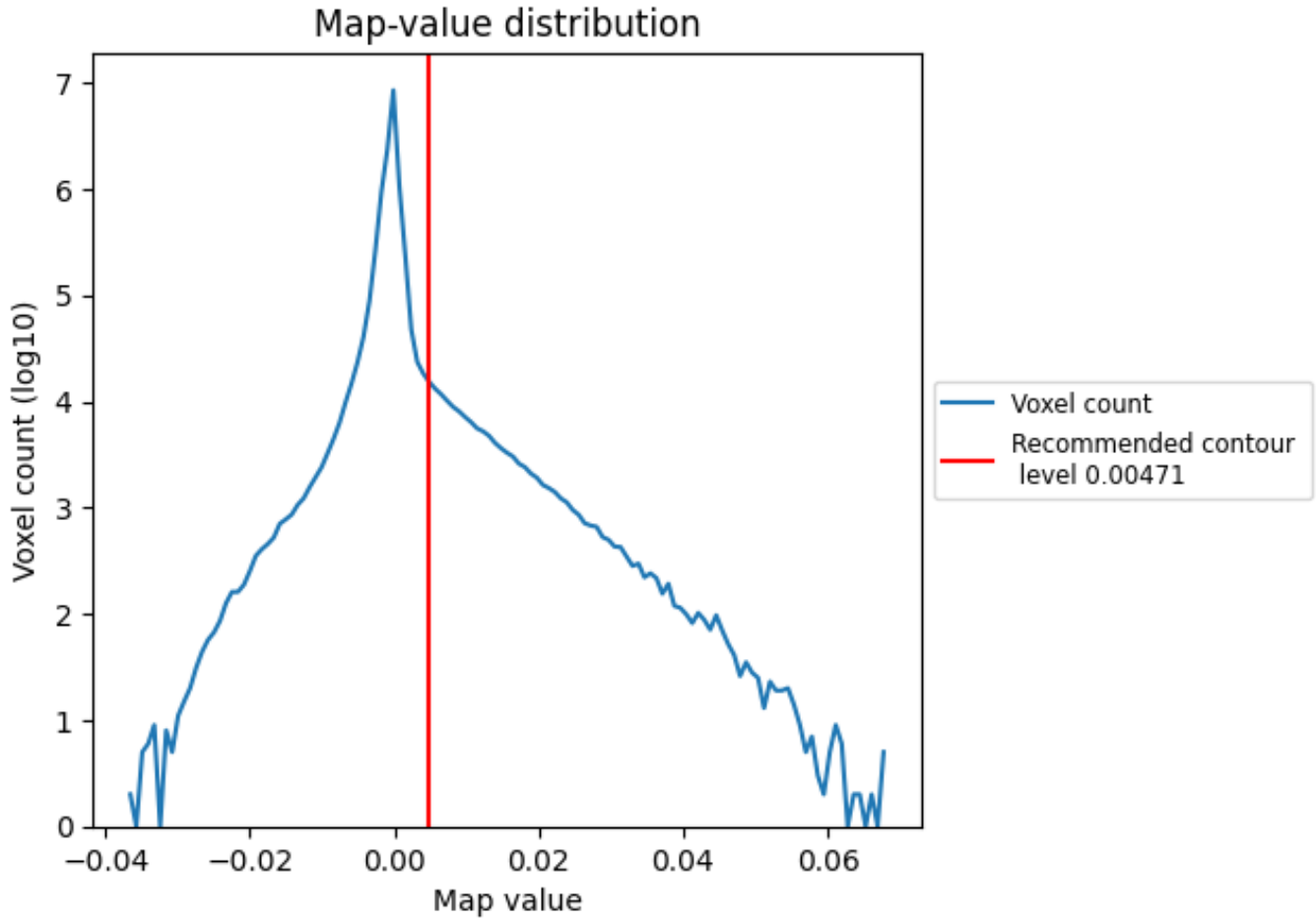
6.6 Mask visualisation (i)

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

7 Map analysis

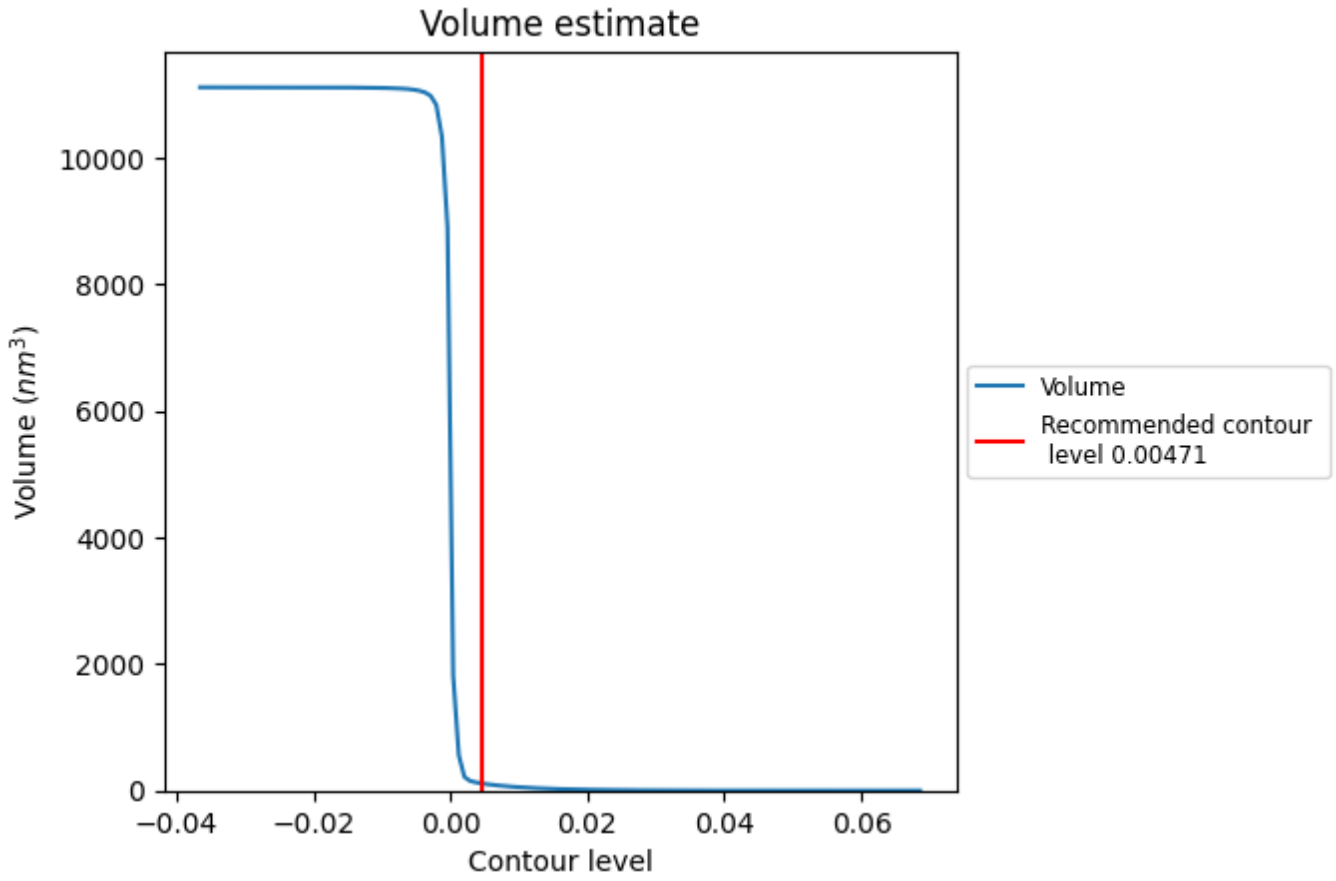
This section contains the results of statistical analysis of the map.

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.

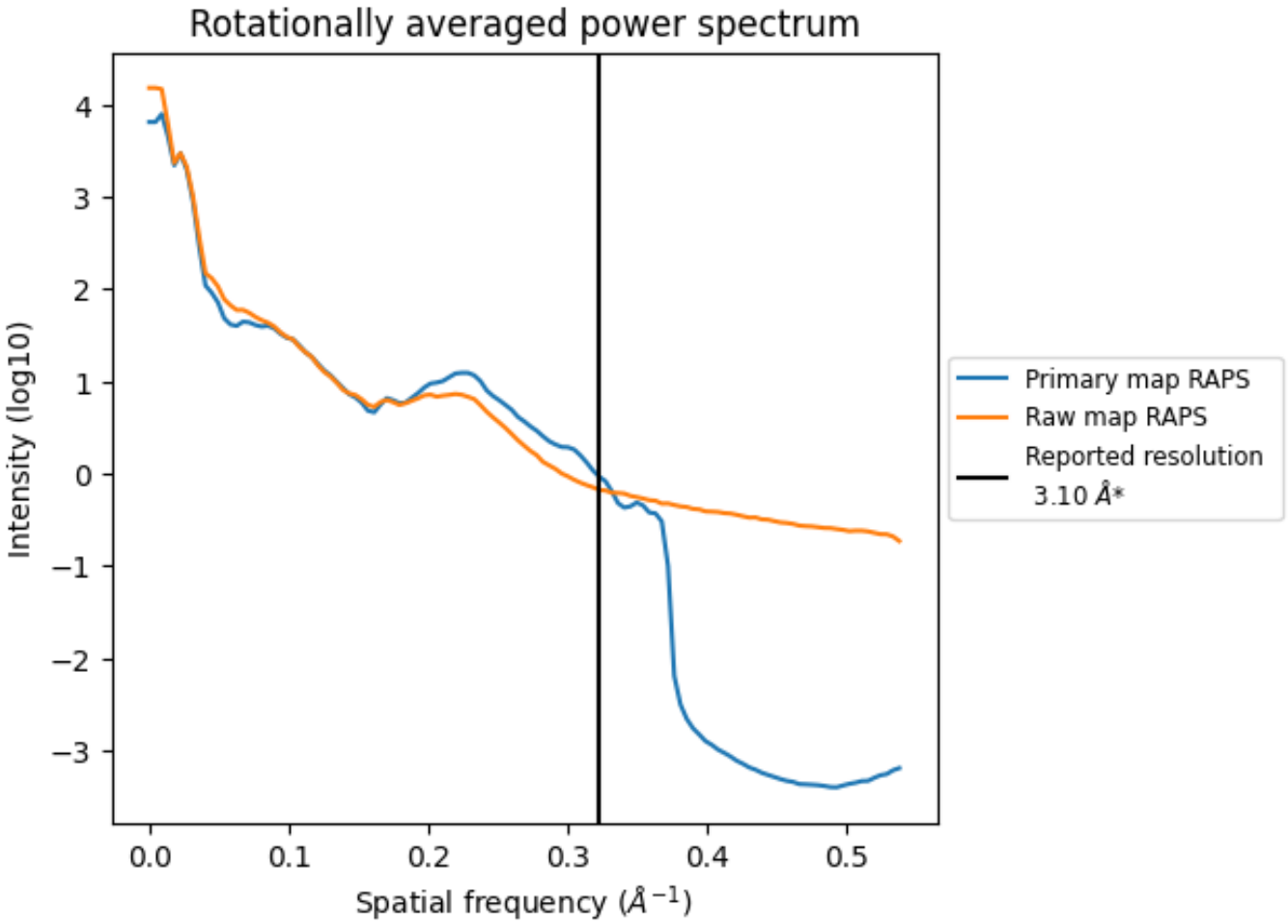
7.2 Volume estimate (i)



The volume at the recommended contour level is 111 nm^3; this corresponds to an approximate mass of 101 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 (i)

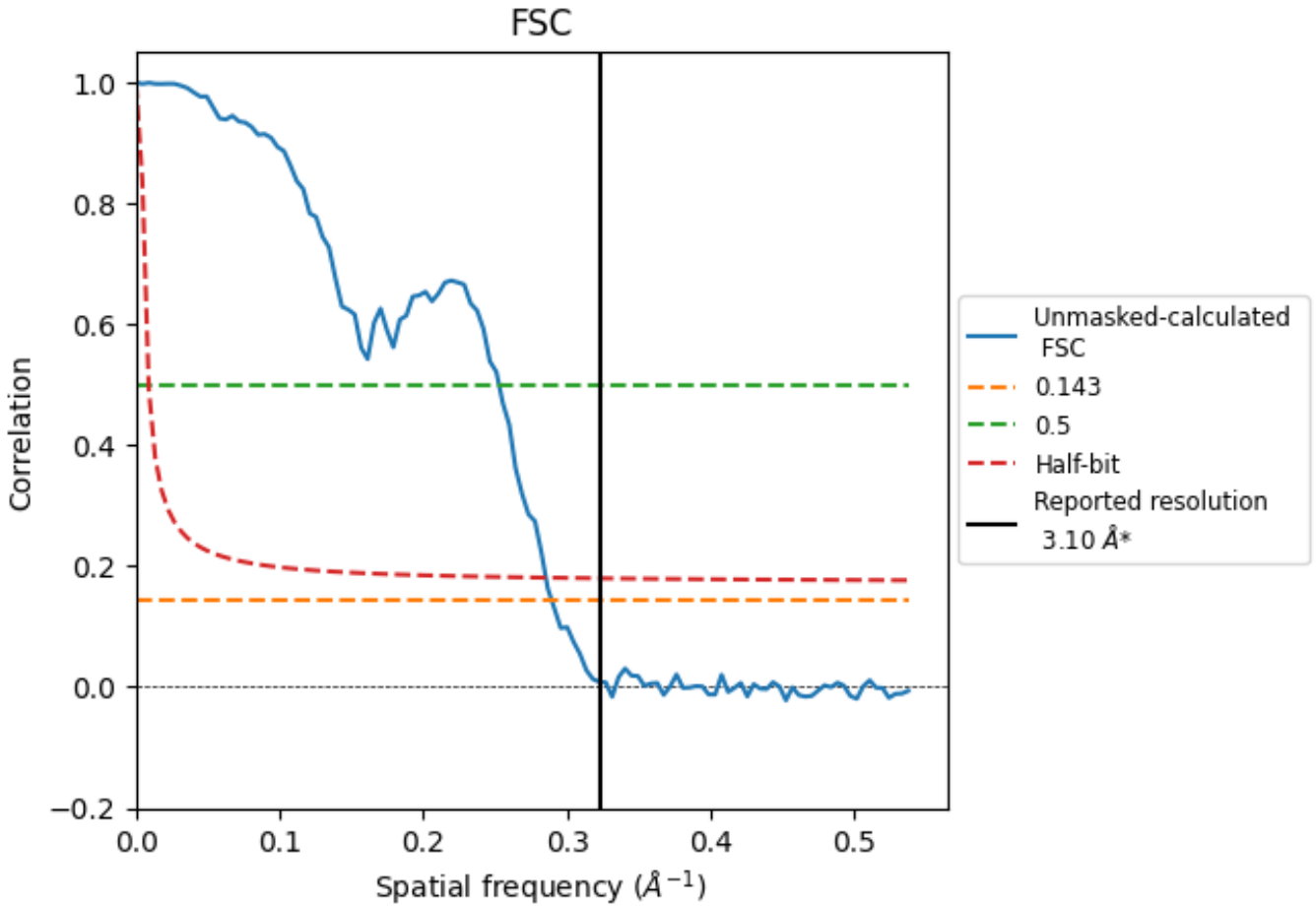


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

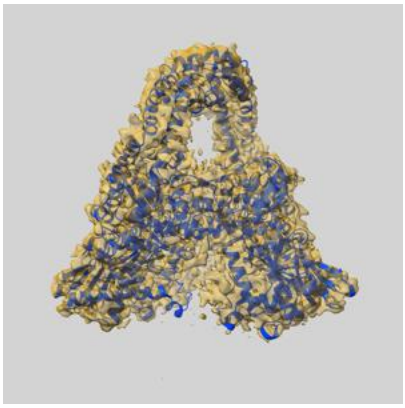
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	3.96	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 3.1 by more than 10 %

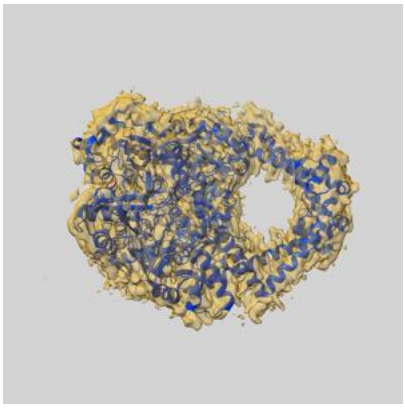
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-83829 and PDB model 46IP. Per-residue inclusion information can be found in section 3 on page 8.

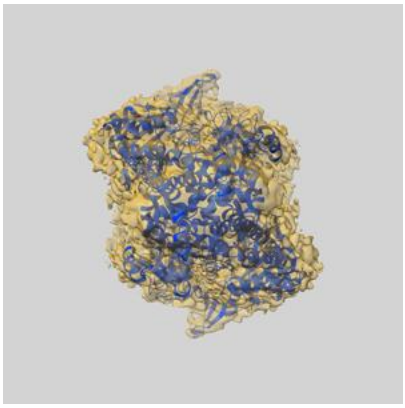
9.1 Map-model overlay



X



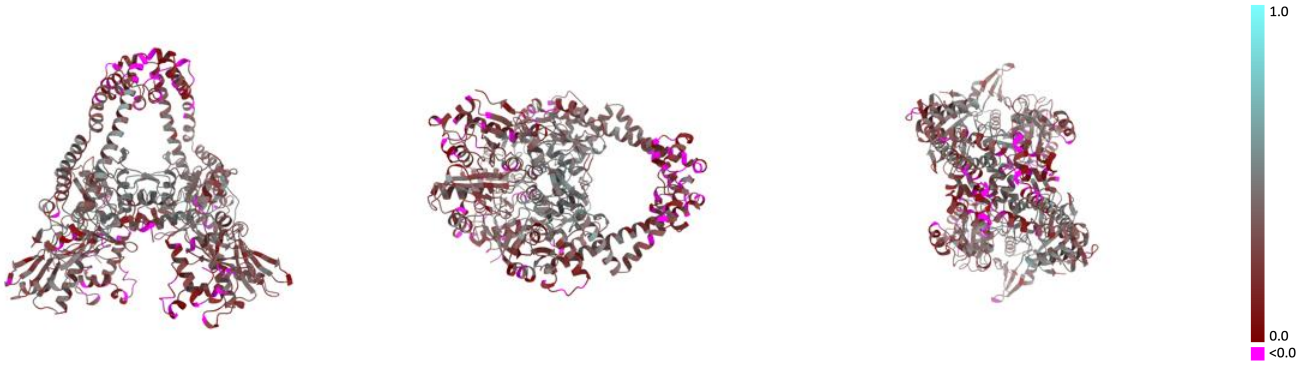
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00471 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.

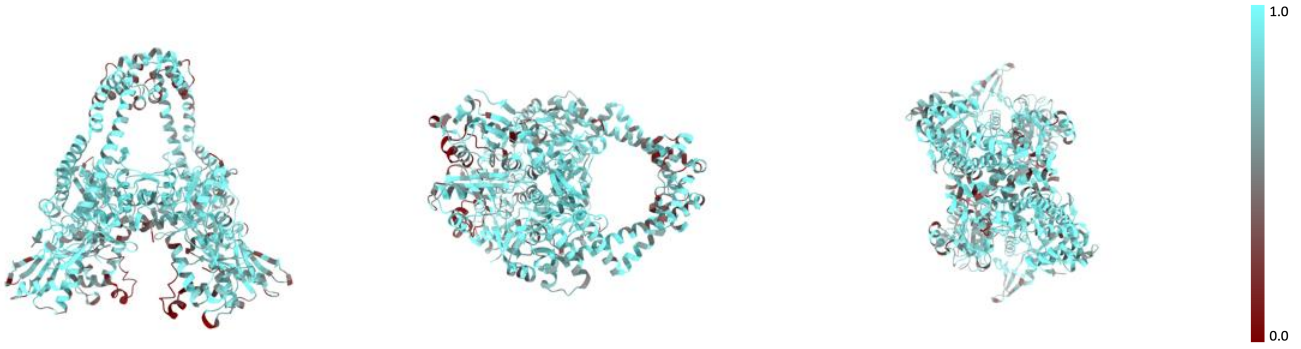
9.2 Q-score mapped to coordinate model (i)



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.

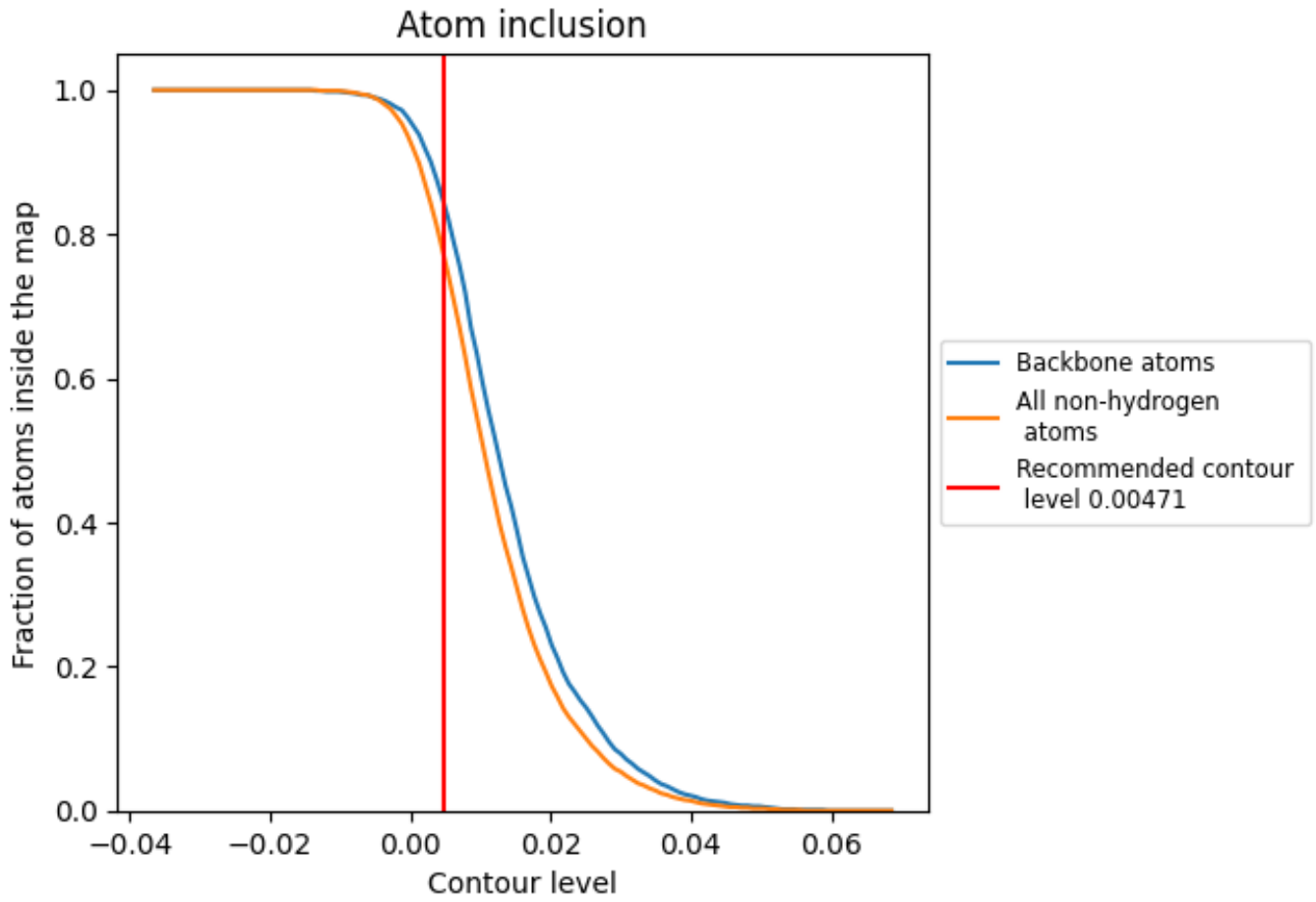
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00471).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.00471) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7720	0.3020
A	0.8040	0.3180
B	0.6800	0.2520
C	0.6700	0.2410
D	0.8210	0.3340