



Full wwPDB EM Validation Report ⓘ

Nov 10, 2025 – 10:10 AM EST

PDB ID : 9NNP / pdb_00009nnp
EMDB ID : EMD-49585
Title : Composite structure of HSV-1 helicase-primase in complex with a forked DNA
Authors : He, Q.; Baranovskiy, A.G.; Morstadt, L.M.; Babayeva, N.D.; Lim, C.; Tahirov, T.H.
Deposited on : 2025-03-05
Resolution : 3.20 Å(reported)
Based on initial model : .

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:

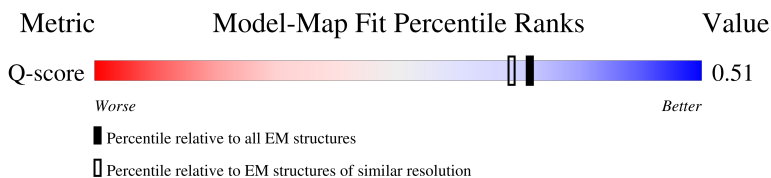
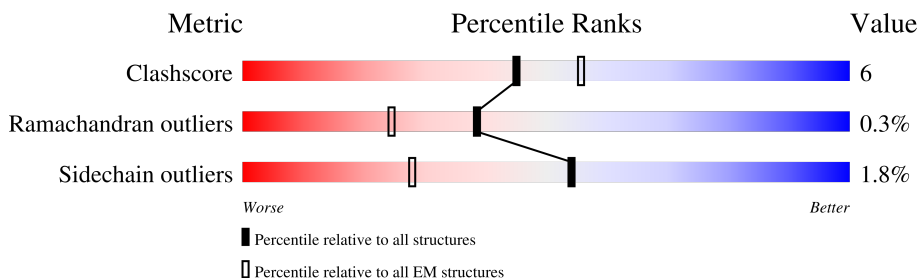
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 3.20 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	852	<div> <div>16%</div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div>
2	B	1058	<div> <div>9%</div> <div>77%</div> <div>13%</div> <div>9%</div> </div>
3	C	750	<div> <div>5%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
4	D	25	<div> <div>12%</div> <div>16%</div> <div>72%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19498 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 replication helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6344	4042	1109	1166	27		

- Molecule 2 is a protein called DNA primase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	963	Total	C	N	O	S	0	0
			7361	4651	1339	1337	34		

- Molecule 3 is a protein called DNA helicase/primase complex-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	750	Total	C	N	O	S	0	0
			5648	3625	1000	1003	20		

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*AP*CP*AP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	7	Total	C	N	O	P	0	0
			143	69	27	40	7		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	B	2	Total	Zn	0
			2	2	

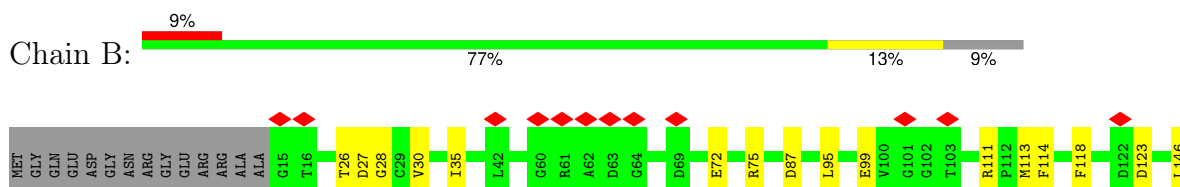
3 Residue-property plots

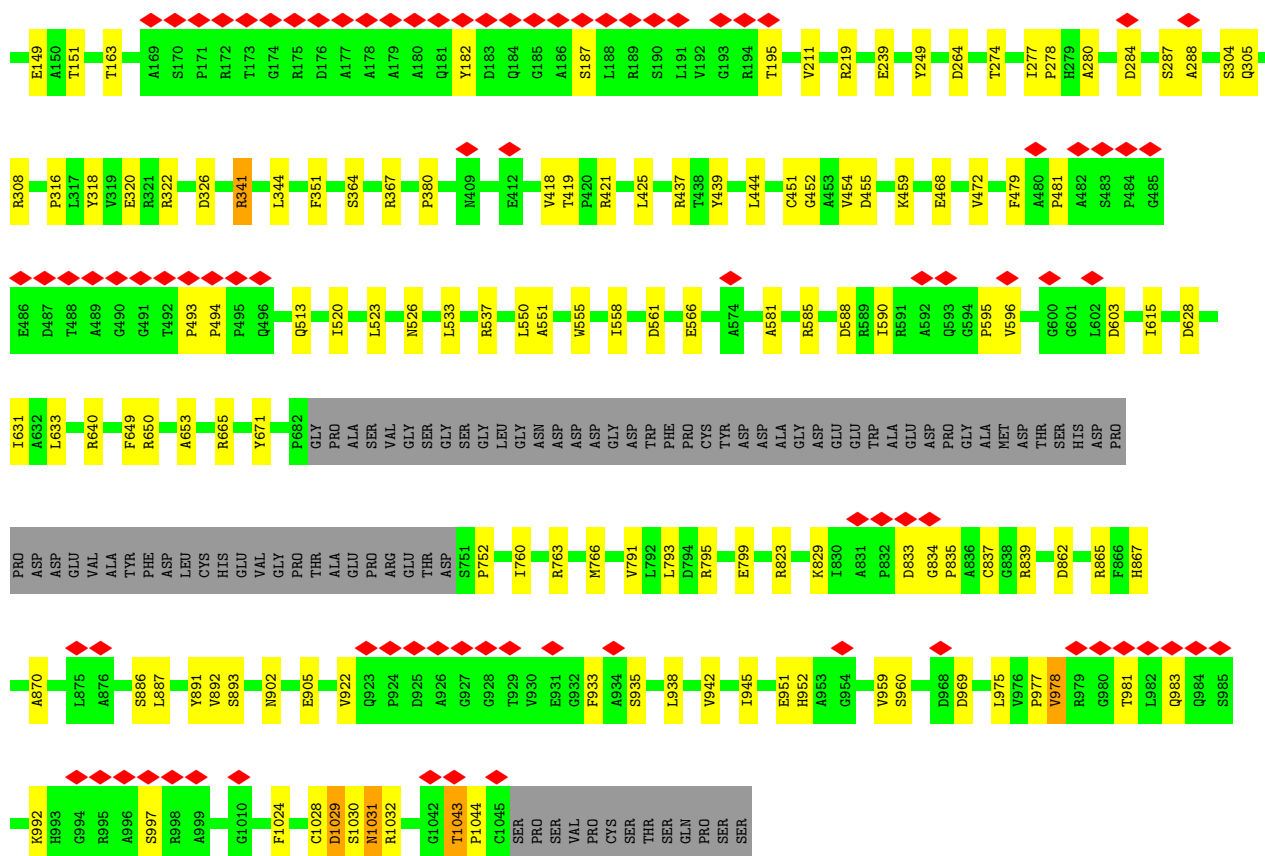
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA replication helicase

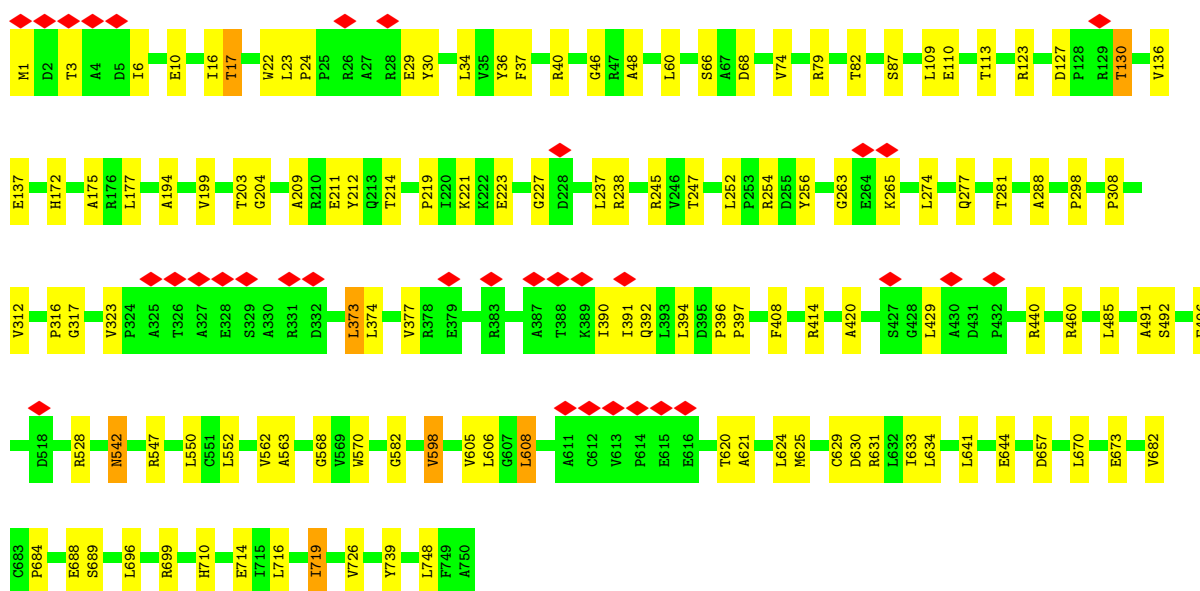
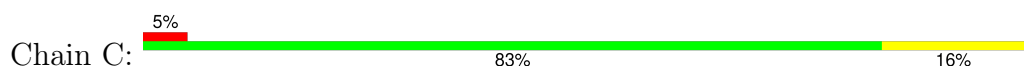


• Molecule 2: DNA primase





• Molecule 3: DNA helicase/primase complex-associated protein



• Molecule 4: DNA (5'-D(P*TP*AP*CP*AP*TP*AP*A)-3')



DC	DC	DA	DC	DG	DG	DC	DA	DC	DC	DC	TS	A9	C10	A11	T12	A13	A14	DT	DA	DC	DA	DT	DA	DC	DA
----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	431843	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.081	Depositor
Minimum map value	-0.640	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.095	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/6483	0.29	0/8802
2	B	0.11	0/7541	0.32	0/10276
3	C	0.12	0/5806	0.31	0/7962
4	D	0.16	0/160	0.32	0/244
All	All	0.11	0/19990	0.31	0/27284

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	396	PRO	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	A	6344	0	6293	78	0
2	B	7361	0	7292	91	0
3	C	5648	0	5621	73	0
4	D	143	0	80	4	0
5	B	2	0	0	0	0
All	All	19498	0	19286	237	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 6.

All (237) 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)
3:C:397:PRO:HA	3:C:563:ALA:O	1.74	0.87
2:B:561:ASP:HB2	2:B:595:PRO:HD2	1.69	0.72
2:B:763:ARG:NH1	2:B:823:ARG:O	2.22	0.72
2:B:1031:ASN:O	2:B:1031:ASN:ND2	2.24	0.71
2:B:935:SER:HA	2:B:938:LEU:HD12	1.74	0.69
3:C:644:GLU:OE2	3:C:699:ARG:NH2	2.25	0.68
1:A:485:LEU:HD11	1:A:751:ASN:HB3	1.76	0.67
1:A:541:ALA:O	1:A:545:LEU:HD12	1.95	0.66
2:B:26:THR:HG22	2:B:28:GLY:H	1.59	0.66
3:C:60:LEU:HD21	3:C:74:VAL:HG21	1.76	0.66
1:A:513:PHE:HB3	1:A:773:MET:HG2	1.78	0.64
1:A:744:ARG:NH2	1:A:757:GLU:OE2	2.29	0.64
1:A:373:ASP:OD1	1:A:853:ASN:ND2	2.30	0.64
2:B:938:LEU:O	2:B:942:VAL:HG23	1.99	0.63
3:C:23:LEU:HD12	3:C:24:PRO:HD2	1.80	0.63
3:C:633:ILE:HD11	3:C:716:LEU:HD11	1.82	0.62
3:C:390:ILE:HD11	3:C:485:LEU:HG	1.82	0.62
1:A:110:ILE:HG23	1:A:114:LEU:HD12	1.80	0.62
2:B:451:CYS:SG	2:B:526:ASN:ND2	2.70	0.61
1:A:512:GLY:HA2	1:A:548:LEU:HD11	1.82	0.60
2:B:650:ARG:NH2	2:B:671:TYR:O	2.33	0.60
1:A:875:ASP:O	2:B:341:ARG:NH2	2.35	0.60
2:B:113:MET:HG3	2:B:114:PHE:HD2	1.65	0.60
1:A:232:ALA:O	2:B:219:ARG:NH1	2.35	0.60
4:D:13:DA:H2''	4:D:14:DA:H5'	1.83	0.60
1:A:511:PHE:HE2	1:A:775:VAL:HG23	1.66	0.60
2:B:274:THR:OG1	2:B:318:TYR:OH	2.16	0.60
3:C:621:ALA:O	3:C:625:MET:HG3	2.02	0.59
1:A:835:ALA:O	1:A:839:MET:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:568:GLY:HA2	3:C:582:GLY:O	2.02	0.59
2:B:322:ARG:NE	2:B:326:ASP:OD2	2.34	0.58
2:B:969:ASP:OD1	2:B:969:ASP:N	2.36	0.58
3:C:110:GLU:OE2	3:C:440:ARG:NH2	2.37	0.58
2:B:468:GLU:O	2:B:472:VAL:HG23	2.03	0.57
3:C:391:ILE:HD11	3:C:485:LEU:HD23	1.85	0.57
2:B:304:SER:O	2:B:308:ARG:NH1	2.38	0.57
2:B:533:LEU:HD22	2:B:551:ALA:HA	1.85	0.57
2:B:595:PRO:O	2:B:839:ARG:NH1	2.38	0.57
2:B:27:ASP:OD1	2:B:27:ASP:N	2.38	0.57
3:C:562:VAL:HG11	3:C:726:VAL:HG22	1.86	0.57
1:A:504:ALA:HB3	1:A:506:LEU:HG	1.87	0.56
1:A:233:THR:HG1	1:A:234:HIS:HD1	1.52	0.56
3:C:277:GLN:O	3:C:281:THR:HG23	2.04	0.56
2:B:239:GLU:OE2	2:B:304:SER:OG	2.20	0.56
2:B:588:ASP:HB2	2:B:752:PRO:HD3	1.87	0.56
2:B:628:ASP:OD1	2:B:763:ARG:NH2	2.31	0.56
3:C:66:SER:OG	3:C:68:ASP:OD1	2.17	0.56
3:C:374:LEU:HB2	3:C:542:ASN:HD22	1.70	0.56
3:C:29:GLU:HG2	3:C:30:TYR:HD1	1.70	0.56
1:A:368:HIS:O	1:A:372:VAL:HG23	2.06	0.56
1:A:513:PHE:N	1:A:695:THR:O	2.38	0.55
2:B:833:ASP:OD1	2:B:833:ASP:N	2.35	0.55
3:C:127:ASP:OD2	3:C:130:THR:OG1	2.25	0.55
1:A:562:ARG:HB2	1:A:565:LEU:HD11	1.88	0.55
3:C:209:ALA:HB3	3:C:223:GLU:HB3	1.89	0.55
1:A:754:GLU:HA	1:A:757:GLU:HB2	1.87	0.55
2:B:30:VAL:HG21	2:B:95:LEU:HD21	1.90	0.54
2:B:513:GLN:HG2	3:C:641:LEU:HB3	1.89	0.54
3:C:630:ASP:OD1	3:C:739:TYR:OH	2.18	0.54
1:A:159:GLN:OE1	1:A:162:GLN:NE2	2.36	0.54
1:A:676:ARG:NH1	1:A:676:ARG:HB3	2.23	0.54
2:B:421:ARG:HB2	2:B:886:SER:HB3	1.90	0.54
3:C:620:THR:O	3:C:624:LEU:HG	2.08	0.53
3:C:684:PRO:HD2	3:C:688:GLU:HB2	1.90	0.53
1:A:210:ARG:NH1	1:A:272:LEU:O	2.41	0.53
2:B:520:ILE:HG21	2:B:533:LEU:HD11	1.89	0.53
1:A:417:GLU:HB2	1:A:420:PHE:HZ	1.72	0.53
1:A:580:LEU:HD22	1:A:679:ILE:HD12	1.91	0.53
2:B:146:LEU:HD21	2:B:151:THR:HG21	1.90	0.53
2:B:603:ASP:OD1	2:B:603:ASP:N	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:HG23	1:A:647:PHE:HD1	1.73	0.53
3:C:390:ILE:HG23	3:C:391:ILE:H	1.74	0.53
3:C:408:PHE:HB3	3:C:552:LEU:HD11	1.90	0.53
1:A:422:VAL:HG22	1:A:495:VAL:HG22	1.91	0.52
3:C:570:TRP:HZ3	3:C:606:LEU:HD12	1.74	0.52
1:A:812:ARG:NH1	4:D:11:DA:OP1	2.42	0.52
3:C:392:GLN:O	3:C:394:LEU:N	2.38	0.52
1:A:784:VAL:HG22	1:A:793:ALA:HA	1.91	0.52
3:C:682:VAL:O	3:C:689:SER:HA	2.09	0.52
2:B:834:GLY:H	2:B:835:PRO:CD	2.22	0.52
1:A:500:ILE:HD11	1:A:766:LEU:HD21	1.92	0.52
3:C:87:SER:O	3:C:87:SER:OG	2.26	0.51
3:C:211:GLU:HB3	3:C:221:LYS:HB3	1.92	0.51
2:B:981:THR:O	2:B:983:GLN:N	2.42	0.51
2:B:1024:PHE:HA	2:B:1030:SER:HB2	1.92	0.51
1:A:51:ARG:NH1	1:A:54:GLU:OE2	2.44	0.51
2:B:942:VAL:HA	2:B:945:ILE:HG22	1.92	0.51
3:C:528:ARG:HG2	3:C:552:LEU:HD23	1.91	0.51
2:B:113:MET:HG3	2:B:114:PHE:CD2	2.44	0.51
3:C:605:VAL:HA	3:C:608:LEU:HD23	1.93	0.51
2:B:640:ARG:HH11	2:B:640:ARG:HB3	1.76	0.51
3:C:227:GLY:O	3:C:254:ARG:NH1	2.43	0.51
2:B:834:GLY:H	2:B:835:PRO:HD2	1.76	0.50
1:A:433:VAL:HB	1:A:484:GLN:HG3	1.93	0.50
2:B:555:TRP:HA	2:B:558:ILE:HD12	1.94	0.50
3:C:247:THR:HG23	3:C:288:ALA:HA	1.94	0.49
3:C:79:ARG:O	3:C:82:THR:OG1	2.28	0.49
3:C:194:ALA:HA	3:C:214:THR:HG23	1.94	0.49
3:C:491:ALA:HB1	3:C:496:PHE:HD2	1.77	0.49
3:C:17:THR:HG21	3:C:317:GLY:HA2	1.93	0.49
1:A:94:LEU:HD12	1:A:333:LEU:HD11	1.94	0.49
1:A:165:TYR:OH	1:A:176:ASP:OD1	2.31	0.49
1:A:676:ARG:O	1:A:680:LEU:HG	2.13	0.49
1:A:543:ARG:O	1:A:547:ARG:HG3	2.13	0.49
1:A:529:PHE:O	1:A:532:THR:OG1	2.30	0.49
1:A:254:LEU:HD22	1:A:258:LEU:HD13	1.94	0.49
1:A:61:ASP:OD2	1:A:64:GLN:NE2	2.44	0.49
2:B:649:PHE:CD2	2:B:791:VAL:HG21	2.48	0.49
3:C:238:ARG:HH21	3:C:245:ARG:HD2	1.78	0.49
2:B:581:ALA:HB1	2:B:585:ARG:HH12	1.77	0.48
1:A:377:VAL:O	1:A:851:ASN:HA	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:598:VAL:HG23	3:C:719:ILE:HD13	1.94	0.48
3:C:203:THR:OG1	3:C:204:GLY:N	2.46	0.48
2:B:665:ARG:HB3	2:B:665:ARG:CZ	2.43	0.48
2:B:862:ASP:HB3	2:B:865:ARG:HG2	1.95	0.48
3:C:177:LEU:HD13	3:C:670:LEU:HD22	1.96	0.48
3:C:263:GLY:N	3:C:323:VAL:O	2.46	0.48
1:A:417:GLU:HB2	1:A:420:PHE:CZ	2.48	0.47
1:A:133:LEU:HD12	1:A:142:ILE:HD11	1.96	0.47
1:A:325:ARG:NH2	1:A:328:ARG:HD3	2.29	0.47
3:C:420:ALA:HA	3:C:547:ARG:HH21	1.79	0.47
2:B:640:ARG:HB3	2:B:640:ARG:NH1	2.30	0.47
2:B:344:LEU:HD23	2:B:351:PHE:HD1	1.80	0.47
3:C:40:ARG:NH2	3:C:256:TYR:O	2.48	0.47
1:A:554:ILE:HG22	1:A:555:SER:H	1.79	0.47
1:A:739:PHE:HE2	1:A:775:VAL:HG12	1.80	0.47
2:B:959:VAL:HA	2:B:977:PRO:HA	1.97	0.47
2:B:1028:CYS:O	2:B:1029:ASP:HB2	2.14	0.47
3:C:212:TYR:CE2	3:C:219:PRO:HG3	2.50	0.47
1:A:123:ARG:HH21	1:A:505:ARG:HE	1.62	0.46
1:A:502:VAL:HG13	1:A:506:LEU:HD12	1.96	0.46
3:C:46:GLY:C	3:C:252:LEU:HD21	2.40	0.46
2:B:493:PRO:N	2:B:494:PRO:HD2	2.30	0.46
2:B:437:ARG:NH2	3:C:748:LEU:O	2.40	0.46
3:C:22:TRP:HZ3	3:C:34:LEU:HB2	1.81	0.46
1:A:474:HIS:O	1:A:476:ARG:NH2	2.49	0.46
2:B:163:THR:HG21	2:B:195:THR:HG21	1.97	0.46
1:A:112:GLU:OE1	2:B:249:TYR:OH	2.32	0.46
3:C:710:HIS:O	3:C:714:GLU:HG2	2.16	0.46
1:A:516:THR:HG23	1:A:519:ALA:H	1.81	0.46
3:C:10:GLU:OE2	3:C:123:ARG:HG2	2.16	0.45
3:C:420:ALA:HA	3:C:547:ARG:NH2	2.32	0.45
1:A:123:ARG:NH1	4:D:13:DA:OP2	2.42	0.45
1:A:481:SER:C	1:A:483:GLN:H	2.23	0.45
2:B:72:GLU:OE1	2:B:75:ARG:NH2	2.49	0.45
4:D:10:DC:H2"	4:D:11:DA:H5"	1.98	0.45
1:A:858:ARG:NH1	2:B:1029:ASP:OD2	2.49	0.45
1:A:337:TRP:HB3	1:A:878:VAL:HG22	1.99	0.45
2:B:891:TYR:CZ	2:B:893:SER:HB2	2.52	0.45
2:B:1043:THR:H	2:B:1044:PRO:HD2	1.82	0.45
3:C:172:HIS:HB2	3:C:175:ALA:HB2	1.99	0.45
3:C:3:THR:HA	3:C:6:ILE:HG12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:THR:O	2:B:419:THR:OG1	2.29	0.44
3:C:199:VAL:HG21	3:C:274:LEU:HD13	2.00	0.44
3:C:265:LYS:HE3	3:C:265:LYS:HB3	1.79	0.44
3:C:460:ARG:HE	3:C:460:ARG:HA	1.82	0.44
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.84	0.44
1:A:657:GLU:O	1:A:662:VAL:HG23	2.17	0.44
2:B:425:LEU:HD21	3:C:748:LEU:HD21	2.00	0.44
2:B:479:PHE:CE2	2:B:481:PRO:HB3	2.52	0.44
3:C:377:VAL:HG21	3:C:542:ASN:ND2	2.33	0.44
1:A:325:ARG:O	1:A:329:GLU:HG2	2.17	0.44
2:B:118:PHE:CD2	2:B:123:ASP:HB3	2.53	0.44
2:B:631:ILE:HB	2:B:760:ILE:HB	2.00	0.44
3:C:673:GLU:OE1	3:C:696:LEU:HD21	2.17	0.43
3:C:113:THR:HG22	3:C:136:VAL:HG23	2.00	0.43
2:B:537:ARG:HB2	2:B:615:ILE:HD11	2.00	0.43
3:C:373:LEU:HB3	3:C:374:LEU:H	1.46	0.43
3:C:631:ARG:O	3:C:631:ARG:HD3	2.19	0.43
1:A:299:GLU:OE1	1:A:312:ARG:NH2	2.52	0.43
2:B:452:GLY:HA3	2:B:550:LEU:HD23	2.01	0.43
2:B:493:PRO:O	2:B:494:PRO:C	2.61	0.43
1:A:500:ILE:HD12	1:A:802:ILE:HB	2.01	0.43
2:B:284:ASP:OD1	2:B:284:ASP:C	2.61	0.43
1:A:155:HIS:NE2	1:A:191:ASP:OD2	2.34	0.43
1:A:319:THR:HG23	1:A:865:ILE:HD11	2.01	0.43
3:C:16:ILE:HG12	3:C:37:PHE:CD1	2.53	0.43
2:B:459:LYS:H	2:B:459:LYS:HG2	1.60	0.43
2:B:795:ARG:O	2:B:799:GLU:HG2	2.18	0.43
1:A:713:ARG:NH1	1:A:714:GLY:H	2.17	0.43
2:B:596:VAL:HG23	2:B:839:ARG:HD2	2.01	0.43
2:B:951:GLU:OE2	2:B:952:HIS:ND1	2.52	0.43
2:B:1031:ASN:ND2	2:B:1031:ASN:C	2.75	0.43
1:A:378:PRO:HG2	1:A:381:TYR:HB2	2.01	0.42
2:B:118:PHE:HD2	2:B:123:ASP:HB3	1.83	0.42
2:B:149:GLU:OE1	2:B:149:GLU:N	2.46	0.42
3:C:550:LEU:HD23	3:C:550:LEU:HA	1.85	0.42
2:B:364:SER:OG	2:B:367:ARG:HG3	2.19	0.42
3:C:429:LEU:HD23	3:C:429:LEU:HA	1.93	0.42
1:A:250:GLU:HB3	1:A:253:LEU:HD12	2.02	0.42
1:A:729:MET:SD	1:A:773:MET:HE1	2.59	0.42
2:B:277:ILE:HG22	2:B:380:PRO:HD3	2.02	0.42
2:B:867:HIS:HB2	2:B:870:ALA:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:TYR:HE1	3:C:48:ALA:HB1	1.85	0.42
1:A:451:GLU:OE1	1:A:451:GLU:N	2.48	0.42
1:A:511:PHE:CE2	1:A:775:VAL:HG23	2.52	0.42
3:C:634:LEU:HD23	3:C:634:LEU:HA	1.80	0.42
2:B:264:ASP:OD1	2:B:264:ASP:N	2.43	0.41
1:A:767:ARG:HB2	1:A:773:MET:SD	2.60	0.41
2:B:902:ASN:O	2:B:905:GLU:HG3	2.20	0.41
2:B:992:LYS:HE2	2:B:992:LYS:HB2	1.88	0.41
1:A:268:MET:HE3	1:A:268:MET:HB3	1.88	0.41
1:A:777:ASN:OD1	1:A:778:THR:N	2.53	0.41
2:B:439:TYR:HD2	2:B:444:LEU:HD11	1.84	0.41
2:B:960:SER:HB2	2:B:978:VAL:HG12	2.02	0.41
3:C:123:ARG:NH1	3:C:137:GLU:OE1	2.53	0.41
1:A:557:TYR:O	1:A:561:GLN:N	2.54	0.41
3:C:37:PHE:HZ	3:C:109:LEU:HD11	1.84	0.41
2:B:997:SER:O	2:B:997:SER:OG	2.34	0.41
3:C:414:ARG:HE	3:C:414:ARG:HB3	1.57	0.41
2:B:959:VAL:HG11	2:B:975:LEU:HB3	2.03	0.41
3:C:492:SER:O	3:C:492:SER:OG	2.39	0.41
1:A:672:ALA:O	1:A:676:ARG:HG3	2.20	0.41
2:B:280:ALA:O	2:B:305:GLN:NE2	2.54	0.41
2:B:316:PRO:O	2:B:320:GLU:HG2	2.21	0.41
2:B:653:ALA:HB1	2:B:766:MET:HE1	2.03	0.41
1:A:207:ASN:OD1	1:A:207:ASN:N	2.49	0.41
1:A:399:LYS:HE3	1:A:399:LYS:HB3	1.71	0.41
1:A:483:GLN:NE2	1:A:754:GLU:OE2	2.54	0.41
2:B:35:ILE:HD13	2:B:35:ILE:HA	1.99	0.41
2:B:829:LYS:N	2:B:837:CYS:O	2.52	0.41
3:C:298:PRO:HG3	3:C:308:PRO:HA	2.03	0.41
1:A:557:TYR:HA	1:A:560:LEU:HB2	2.03	0.41
1:A:350:GLU:OE1	1:A:374:ARG:NH2	2.54	0.40
1:A:713:ARG:HD2	1:A:713:ARG:HA	1.95	0.40
2:B:418:VAL:HB	2:B:887:LEU:HD22	2.04	0.40
1:A:752:VAL:HG11	1:A:796:ILE:HG21	2.03	0.40
2:B:99:GLU:HG2	2:B:111:ARG:HG3	2.03	0.40
2:B:182:TYR:HD2	2:B:187:SER:HB3	1.87	0.40
1:A:341:ILE:O	1:A:342:ASN:HB3	2.21	0.40
1:A:823:ILE:HD11	1:A:848:LEU:HD11	2.03	0.40
2:B:287:SER:OG	2:B:288:ALA:N	2.54	0.40
2:B:628:ASP:CG	2:B:763:ARG:HH21	2.25	0.40
2:B:922:VAL:HG21	2:B:933:PHE:CG	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1030:SER:C	2:B:1032:ARG:H	2.30	0.40
3:C:312:VAL:HG11	3:C:316:PRO:HD2	2.02	0.40
3:C:629:CYS:O	3:C:633:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	793/852 (93%)	752 (95%)	40 (5%)	1 (0%)	48	80
2	B	959/1058 (91%)	906 (94%)	48 (5%)	5 (0%)	25	60
3	C	748/750 (100%)	717 (96%)	30 (4%)	1 (0%)	48	80
All	All	2500/2660 (94%)	2375 (95%)	118 (5%)	7 (0%)	38	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	ILE
3	C	373	LEU
2	B	1029	ASP
2	B	1043	THR
2	B	278	PRO
2	B	978	VAL
2	B	892	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	680/721 (94%)	665 (98%)	15 (2%)	47	73
2	B	757/832 (91%)	746 (98%)	11 (2%)	60	81
3	C	560/560 (100%)	551 (98%)	9 (2%)	58	79
All	All	1997/2113 (94%)	1962 (98%)	35 (2%)	54	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	98	ASN
1	A	154	ASN
1	A	185	TYR
1	A	207	ASN
1	A	316	ASN
1	A	333	LEU
1	A	377	VAL
1	A	429	THR
1	A	487	VAL
1	A	727	THR
1	A	768	ASP
1	A	775	VAL
1	A	823	ILE
1	A	870	LEU
2	B	87	ASP
2	B	211	VAL
2	B	341	ARG
2	B	454	VAL
2	B	455	ASP
2	B	523	LEU
2	B	566	GLU
2	B	590	ILE
2	B	633	LEU
2	B	793	LEU
2	B	1031	ASN
3	C	1	MET
3	C	17	THR
3	C	130	THR
3	C	237	LEU
3	C	542	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	598	VAL
3	C	608	LEU
3	C	657	ASP
3	C	719	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	484	GLN
2	B	79	GLN
2	B	133	HIS
2	B	199	GLN
2	B	416	HIS
2	B	1012	ASN
3	C	242	HIS
3	C	416	GLN
3	C	515	GLN
3	C	542	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

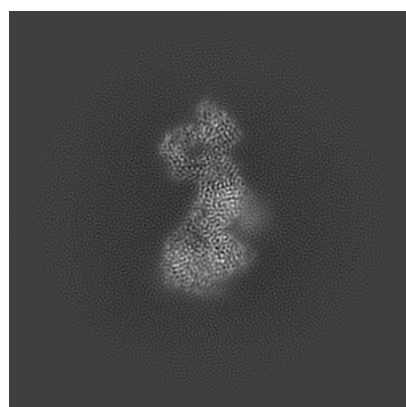
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49585. These allow visual inspection of the internal detail of the map and identification of artifacts.

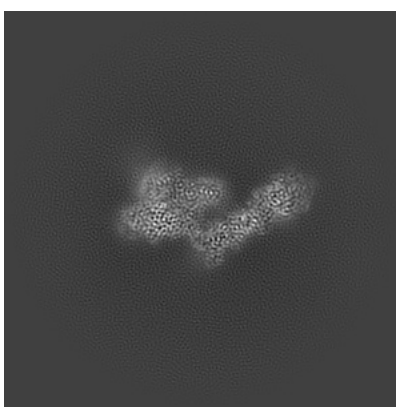
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

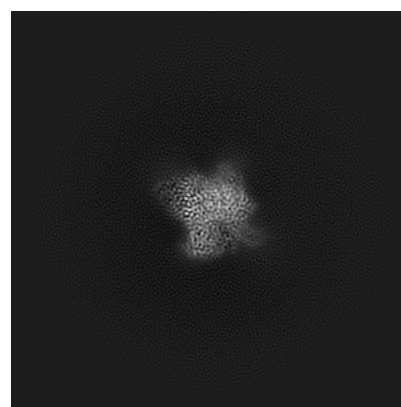
6.1.1 Primary map



X



Y

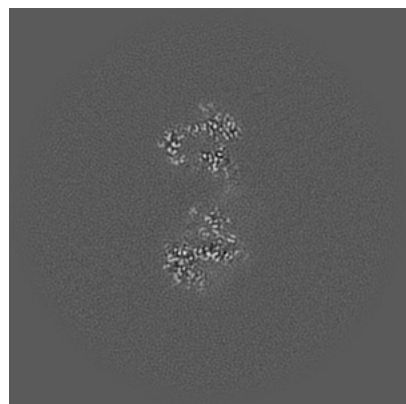


Z

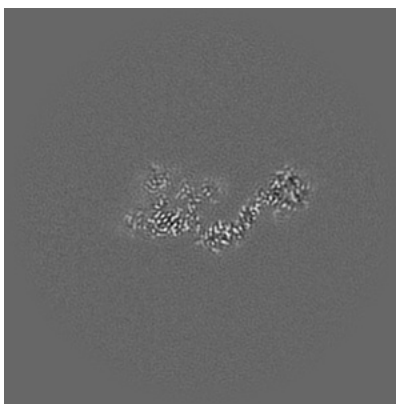
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

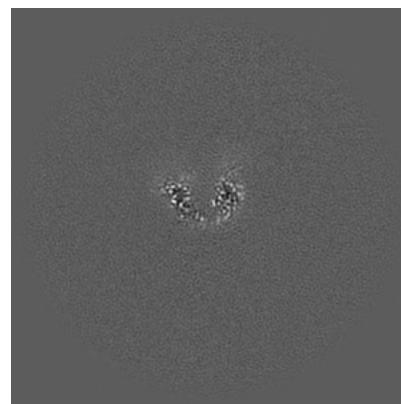
6.2.1 Primary map



X Index: 180



Y Index: 180

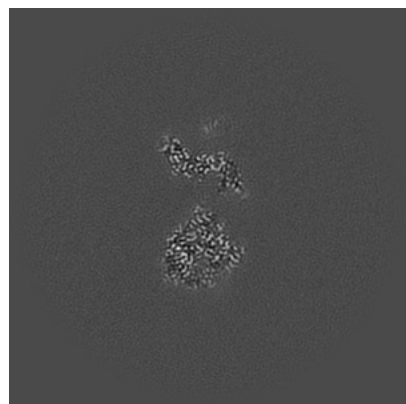


Z Index: 180

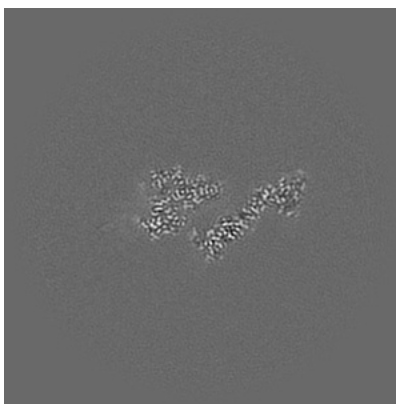
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

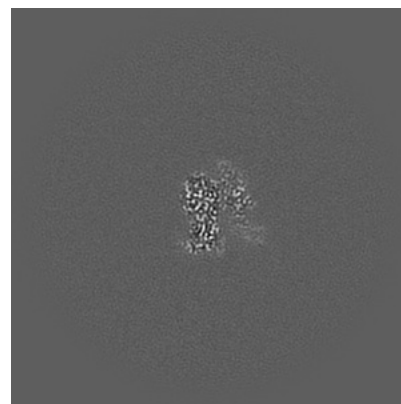
6.3.1 Primary map



X Index: 171



Y Index: 191

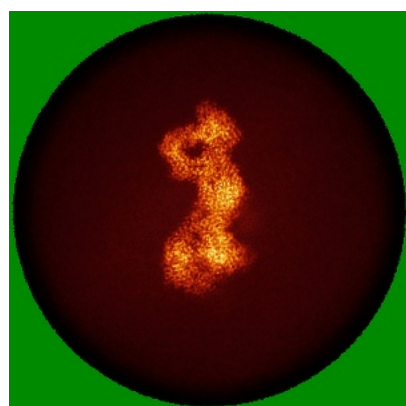


Z Index: 139

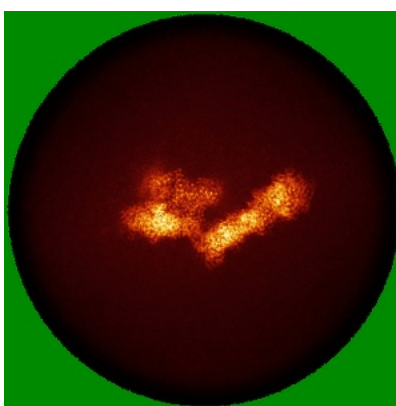
The images above show the largest variance slices of the map in three orthogonal directions.

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

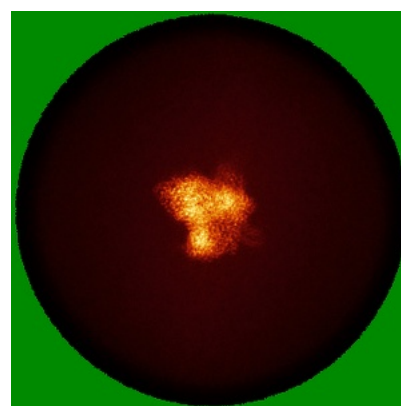
6.4.1 Primary map



X



Y

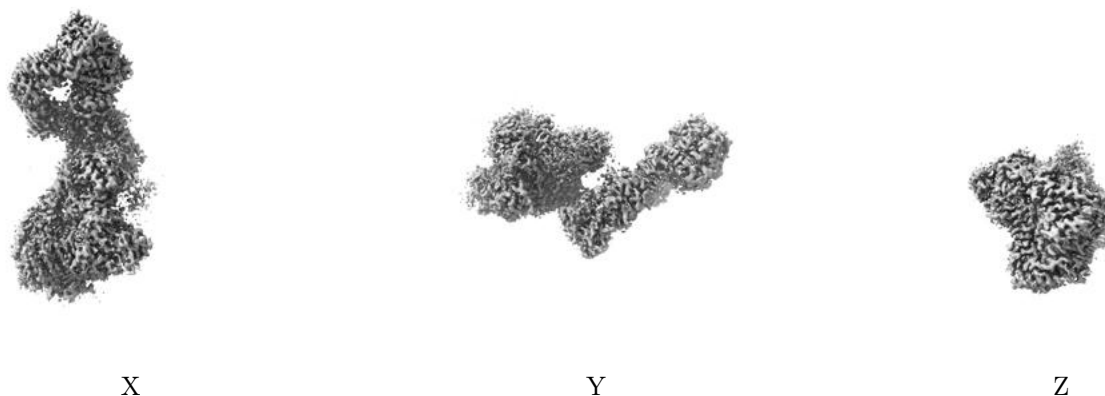


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

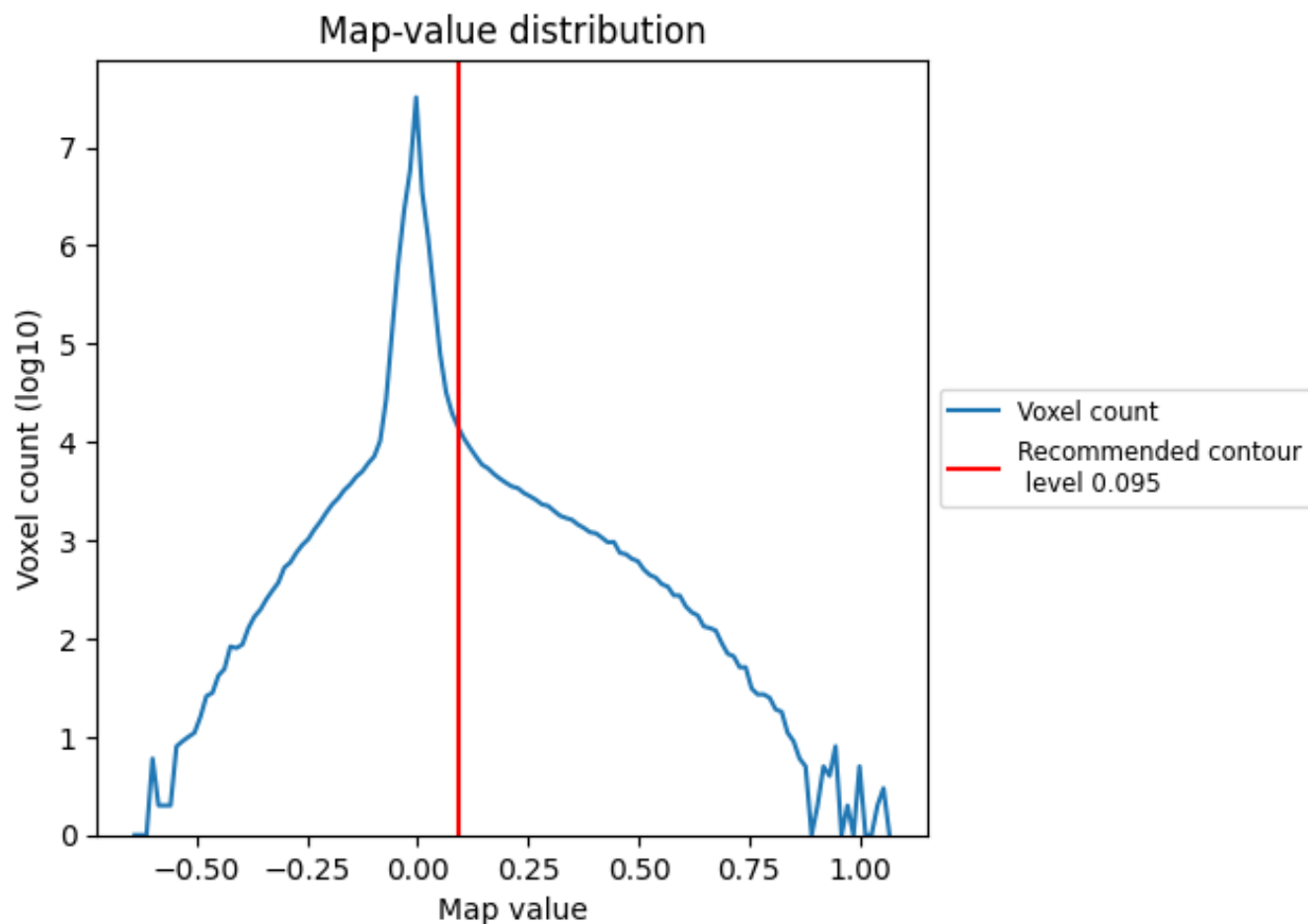
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

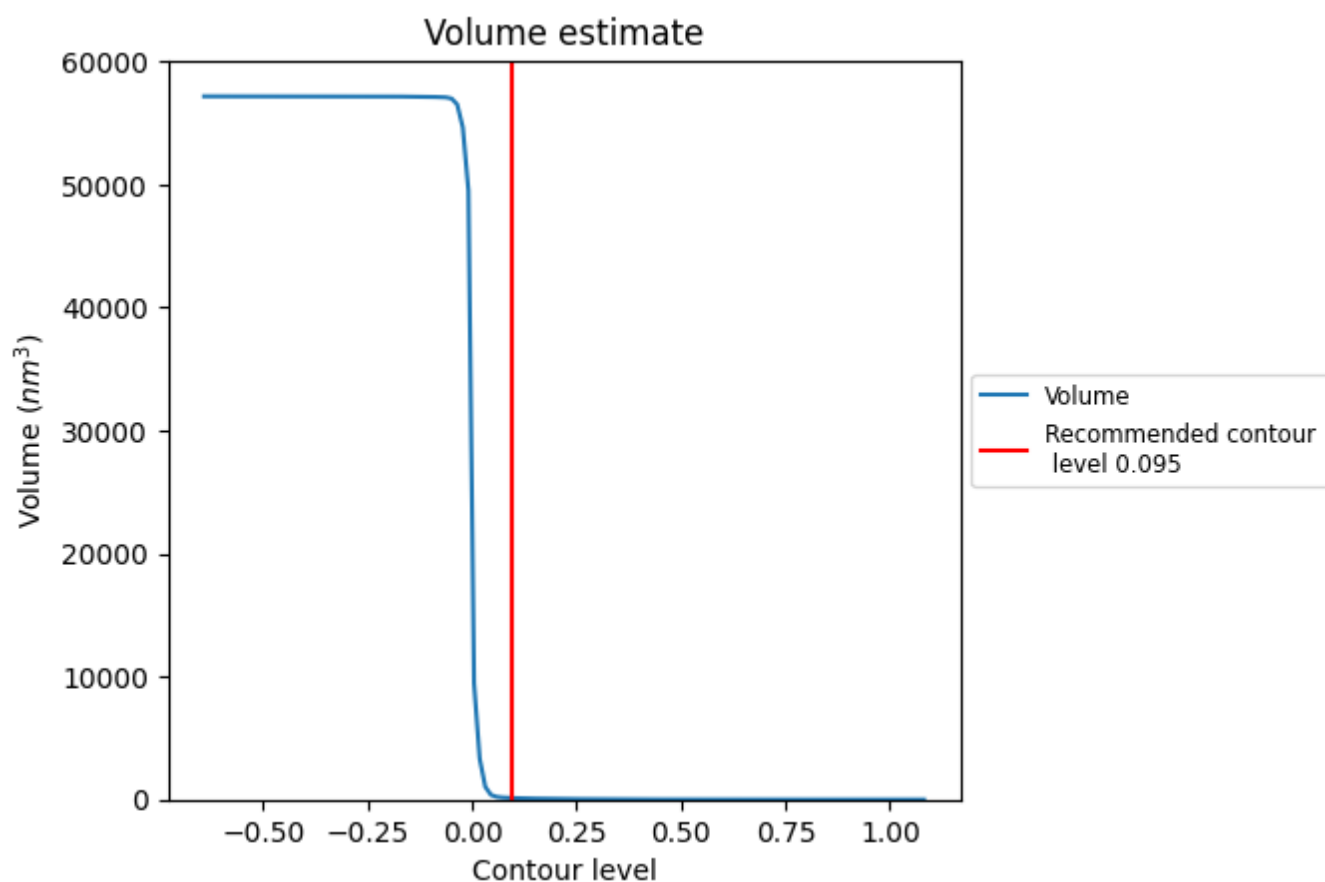
This section contains the results of statistical analysis of the map.

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.

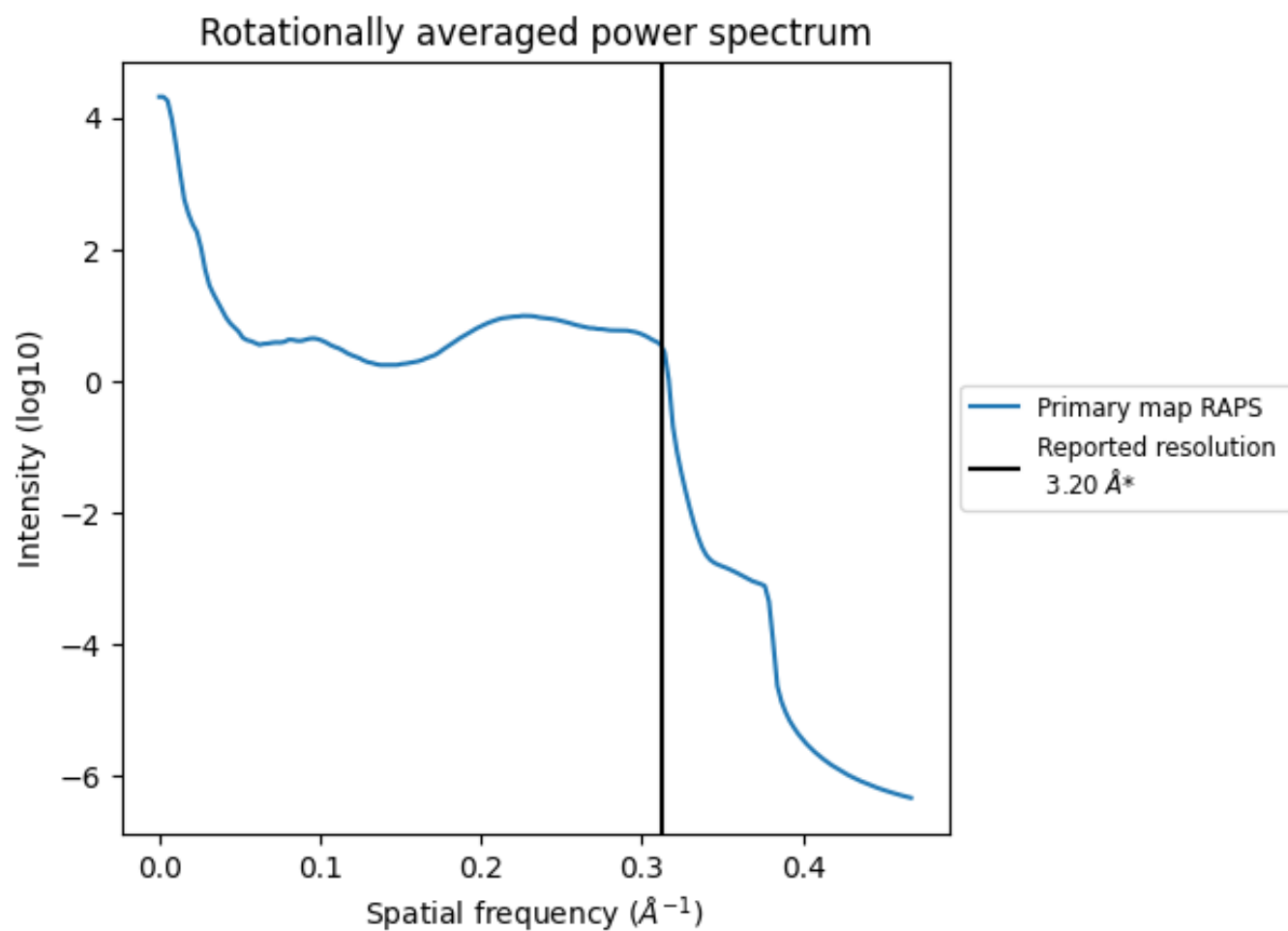
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 0.312 Å⁻¹

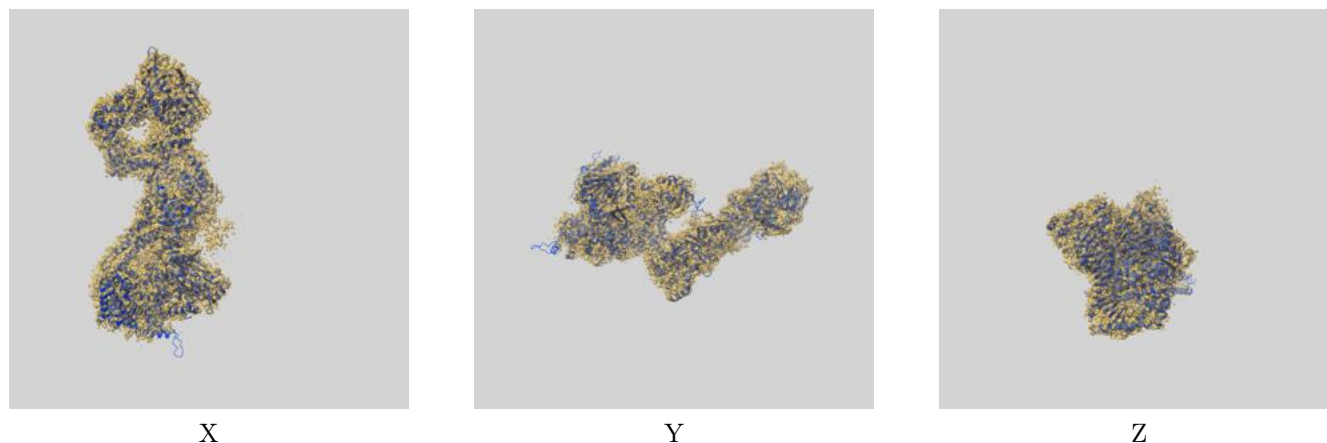
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

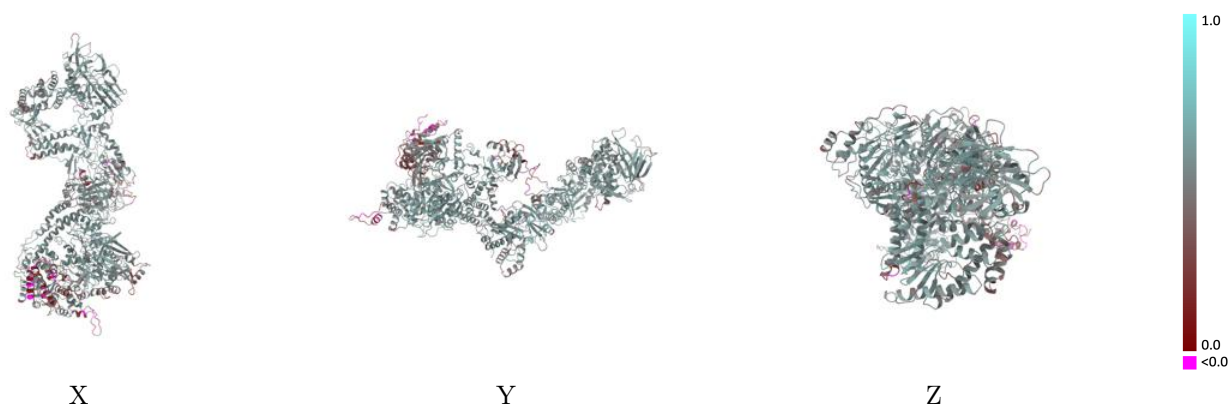
This section contains information regarding the fit between EMDB map EMD-49585 and PDB model 9NNP. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



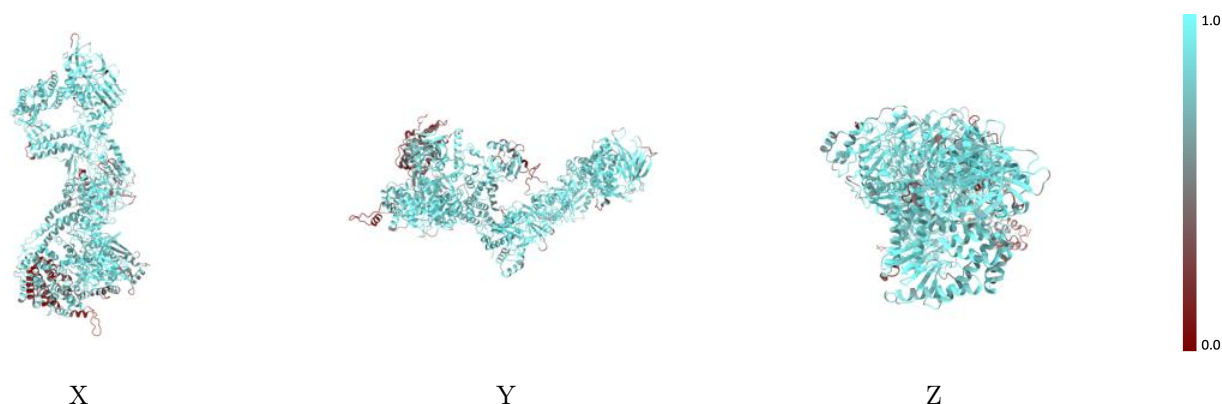
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



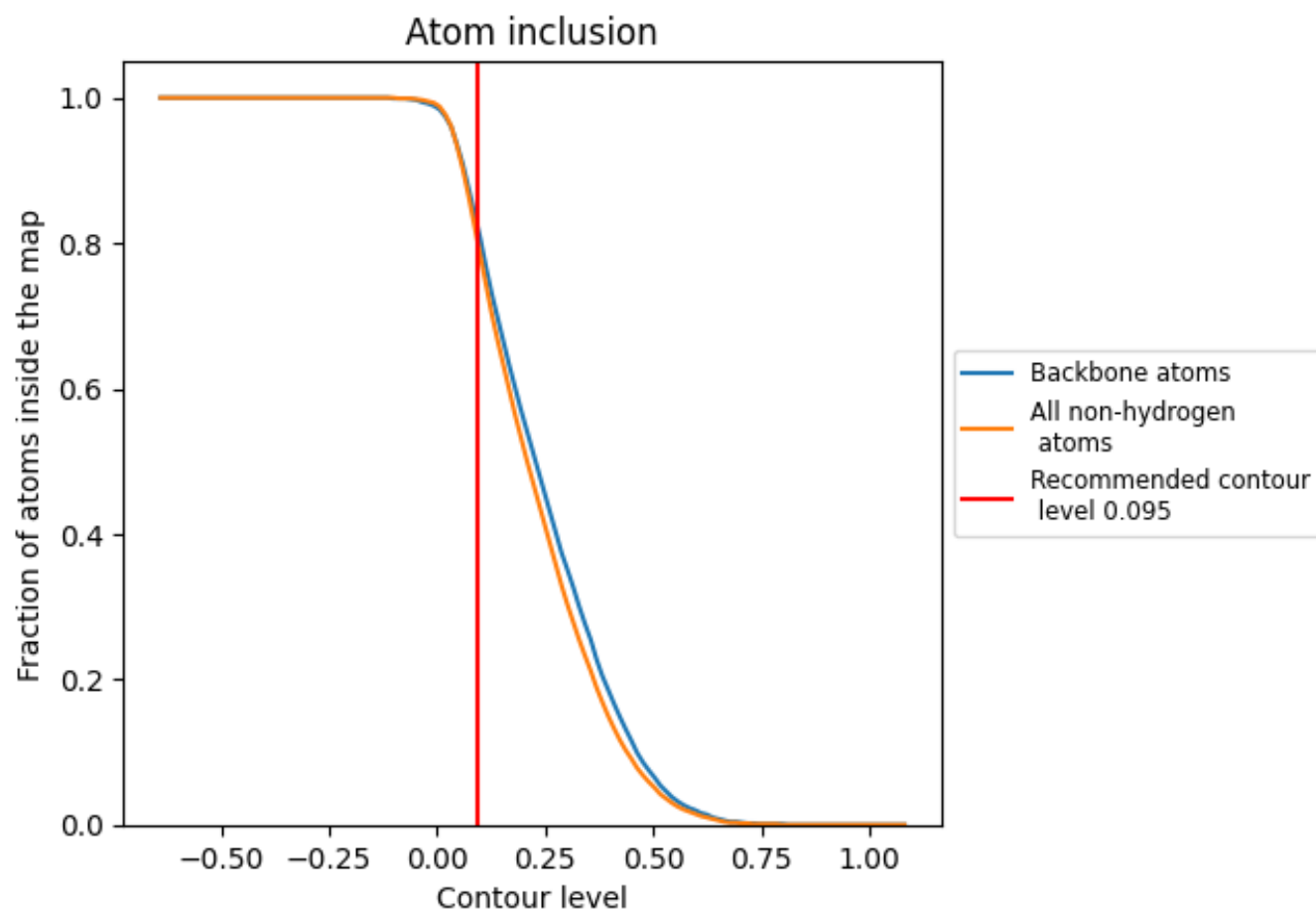
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7970	<div></div> 0.5100
A	<div></div> 0.7400	<div></div> 0.4820
B	<div></div> 0.8000	<div></div> 0.5110
C	<div></div> 0.8550	<div></div> 0.5380
D	<div></div> 0.9510	<div></div> 0.5830

