Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 08:07 am GMT

PDB ID	:	5A9K
EMDB ID	:	EMD-3087
Title	:	Structural basis for DNA strand separation by a hexameric replicative helicase
Authors	:	Chaban, Y.; Stead, J.A.; Ryzhenkova, K.; Whelan, F.; Lamber, K.; Antson, F.; Sanders, C.M.; Orlova, E.V.
Deposited on	:	2015-07-21
Resolution	:	19.00 Å(reported)
Based on initial model	:	2V9P

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:

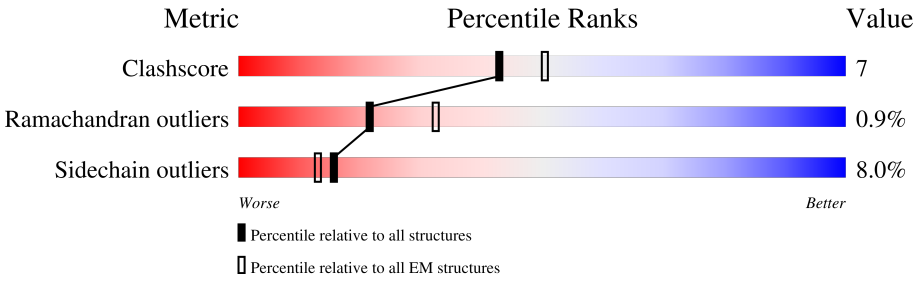
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 19.00 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
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	26% 69% 19% • 11%
1	B	305	25% 71% 14% • 12%
1	C	305	27% 70% 16% • 12%
1	D	305	28% 73% 14% • 10%
1	E	305	23% 68% 20% • 11%
1	F	305	21% 64% 22% •• 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1580	-	-	X	-
2	PO4	C	1579	-	X	-	-

2 Entry composition (i)

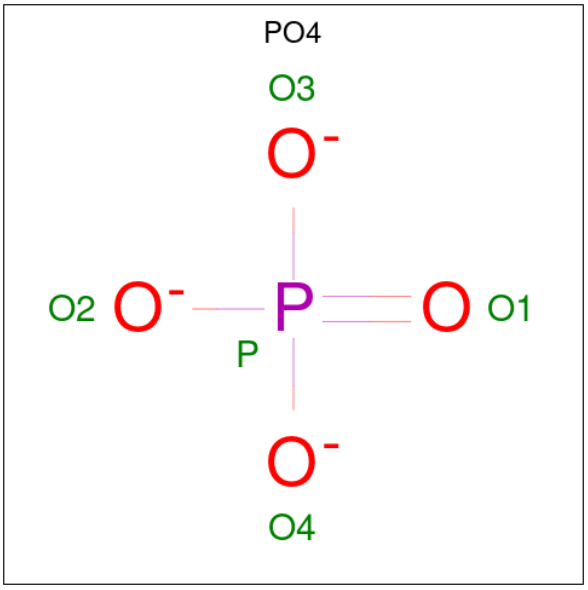
There are 4 unique types of molecules in this entry. The entry contains 13059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 REPLICATION PROTEIN E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	272	Total	C	N	O	S	0	0
			2183	1404	375	394	10		
1	B	268	Total	C	N	O	S	0	0
			2149	1386	370	383	10		
1	C	267	Total	C	N	O	S	0	0
			2142	1382	369	381	10		
1	D	274	Total	C	N	O	S	0	0
			2191	1409	377	395	10		
1	E	270	Total	C	N	O	S	0	0
			2170	1398	373	389	10		
1	F	269	Total	C	N	O	S	0	0
			2158	1392	372	384	10		

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	O	P	0
			10	8	2	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total O P 10 8 2	0
2	B	1	Total O P 10 8 2	0
2	B	1	Total O P 10 8 2	0
2	C	1	Total O P 10 8 2	0
2	C	1	Total O P 10 8 2	0
2	D	1	Total O P 5 4 1	0
2	E	1	Total O P 5 4 1	0
2	F	1	Total O P 5 4 1	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0

- Molecule 4 is water.

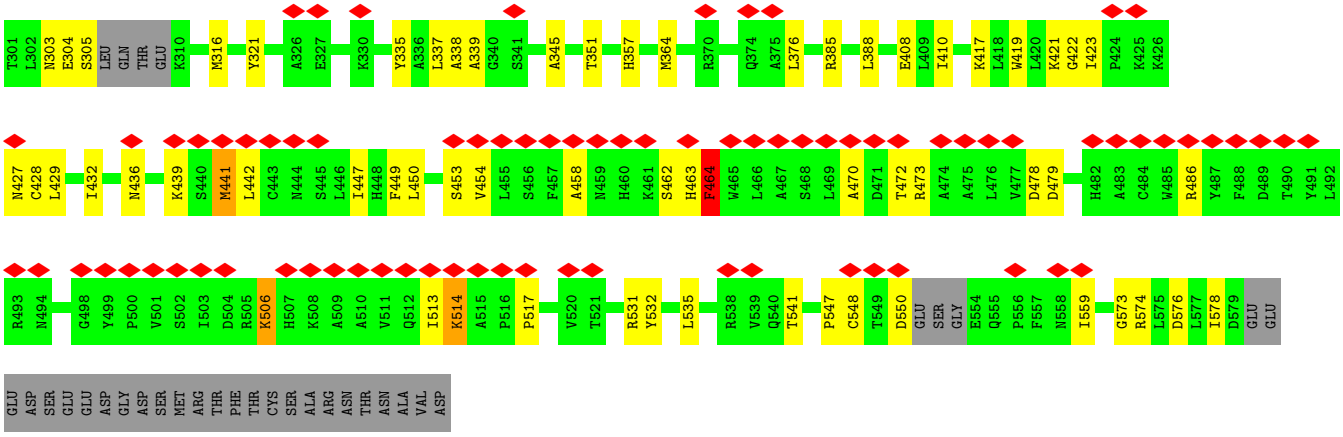
Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total O 3 3	0
4	B	3	Total O 3 3	0
4	C	3	Total O 3 3	0
4	D	4	Total O 4 4	0
4	E	2	Total O 2 2	0
4	F	3	Total O 3 3	0

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.

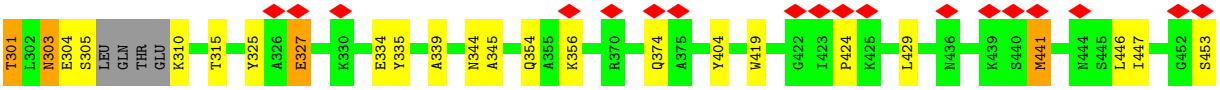
• Molecule 1: REPLICATION PROTEIN E1

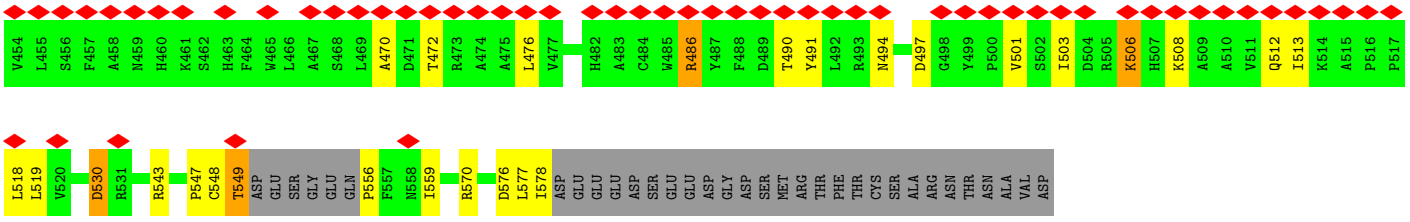
Chain A:



• Molecule 1: REPLICATION PROTEIN E1

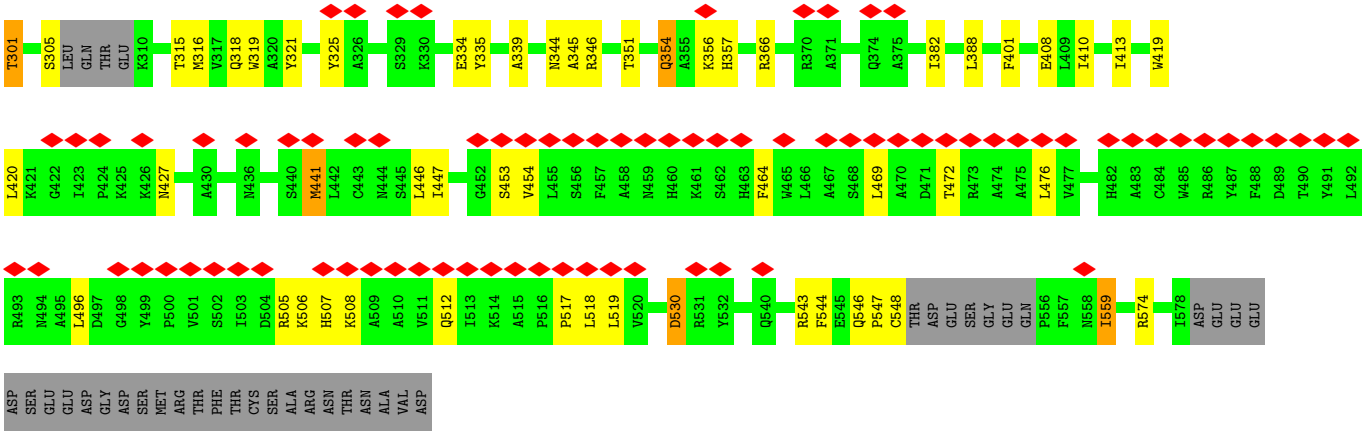
Chain B:





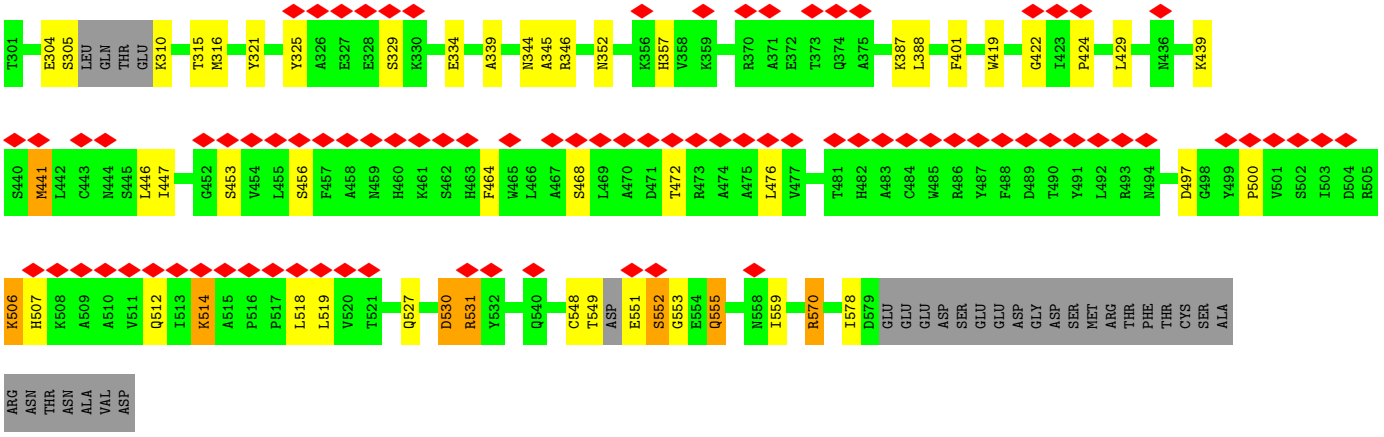
• Molecule 1: REPLICATION PROTEIN E1

Chain C:



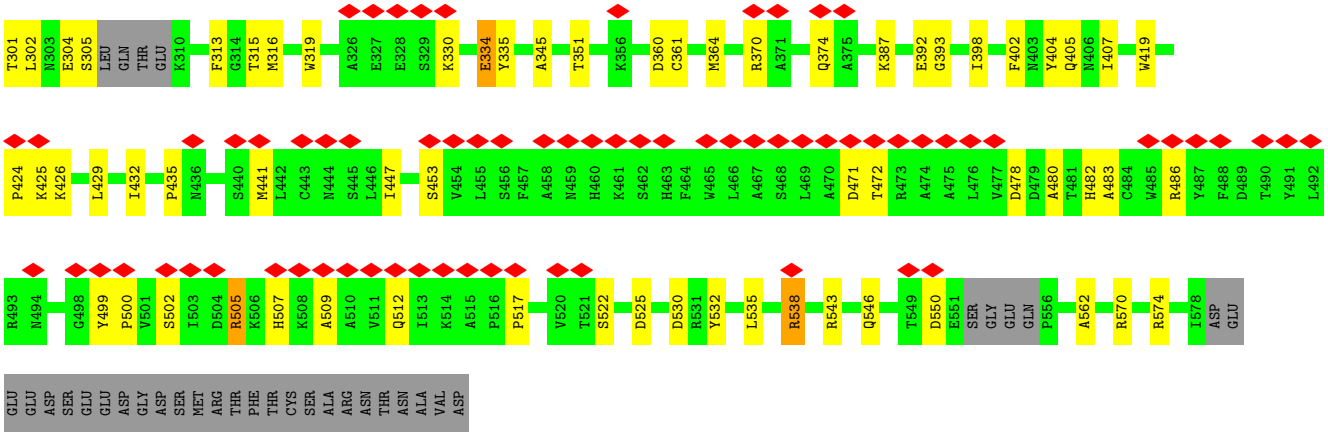
• Molecule 1: REPLICATION PROTEIN E1

Chain D:



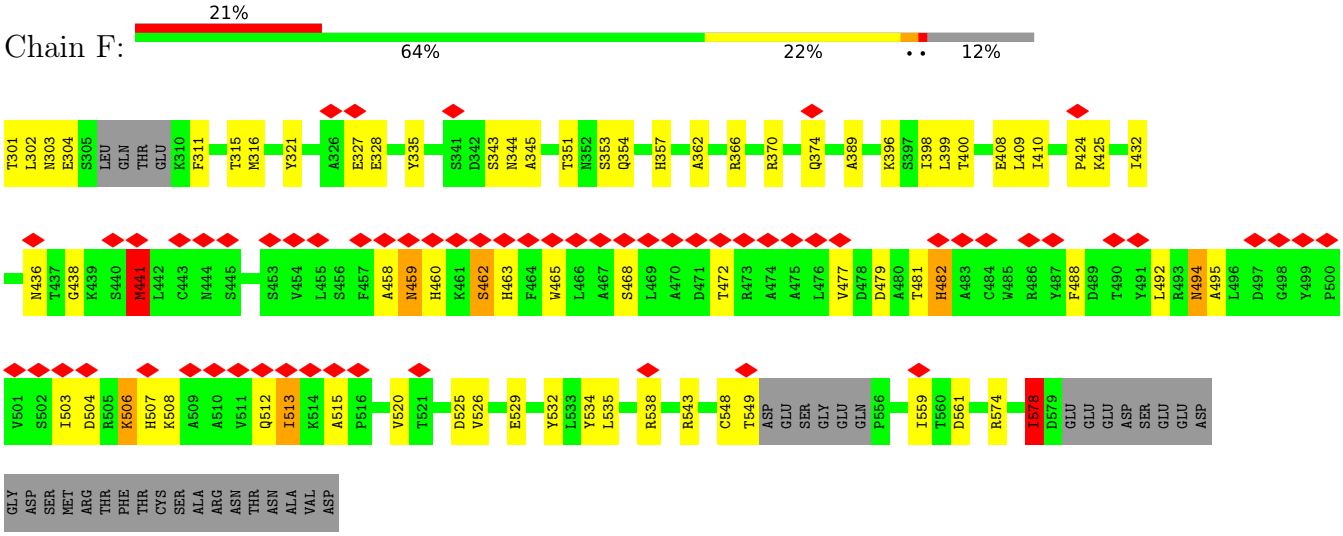
• Molecule 1: REPLICATION PROTEIN E1

Chain E:



• Molecule 1: REPLICATION PROTEIN E1

Chain F:


21%
64%
22%
12%
T301 L302 N303 E304 S305 LEU GLN THR GLU K310 F311 T315 M316 Y321 A326 E327 E328 Y335 S341 D342 S343 N344 A345 T351 N352 S353 Q354 H357 A362 R366 R370 Q374 A389 K396 S397 I398 L399 T400 E408 L409 I410 P424 K425 I432
N436 T437 G438 K439 S440 M441 L442 C443 N444 S445 S453 V454 L455 S456 F457 A458 N459 H460 K461 S462 H463 F464 W465 L466 A467 S468 L469 A470 D471 T472 R473 A474 A475 L476 V477 D478 D479 A480 T481 H482 A483 C484 W485 R486 Y487 F488 D489 T490 Y491 L492 R493 N494 A495 L496 D497 G498 Y499 P500
V501 S502 I503 D504 R505 K506 H507 K508 A509 A510 V511 Q512 I513 K514 A515 P516 V520 T521 D525 V526 E529 Y532 L533 Y534 L535 R538 R543 C548 T549 ASP GLU SER GLY GLU GLN P556 I559 T560 D561 R574 I578 D579 GLU GLU GLU ASP SER GLU GLU ASP
GLY ASP SER MET ARG THR PHE THR CYS SER ALA ARG ASN THR ASN ALA VAL ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	8265	Depositor
Resolution determination method	Not provided	
CTF correction method	FRAMES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	67000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.431	Depositor
Minimum map value	-0.168	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	320.0, 320.0, 320.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	0.48	0/2240	0.59	0/3037
1	B	0.50	1/2206 (0.0%)	0.62	2/2990 (0.1%)
1	C	0.49	0/2199	0.61	0/2980
1	D	0.47	0/2248	0.64	4/3047 (0.1%)
1	E	0.48	0/2227	0.59	0/3017
1	F	0.49	0/2215	0.62	0/3001
All	All	0.48	1/13335 (0.0%)	0.61	6/18072 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE1	5.96	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	486	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	486	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	531	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	570	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	531	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	570	ARG	NE-CZ-NH2	-5.46	117.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2183	0	2132	40	0
1	B	2149	0	2110	28	0
1	C	2142	0	2103	28	0
1	D	2191	0	2140	32	0
1	E	2170	0	2132	43	0
1	F	2158	0	2124	35	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
All	All	13059	0	12741	183	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 7.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:GLU:HG2	1:D:305:SER:H	1.18	1.06
1:E:453:SER:HB2	1:F:512:GLN:HE22	1.32	0.94
1:A:441:MET:HE1	1:A:559:ILE:H	1.32	0.92
1:A:304:GLU:HG2	1:A:305:SER:H	1.41	0.83
2:A:1580:PO4:O1	2:A:1581:PO4:O2	1.97	0.82
1:F:503:ILE:HD12	1:F:513:ILE:CD1	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:MET:HE3	1:C:559:ILE:H	1.51	0.74
1:A:464:PHE:H	1:A:464:PHE:HD1	1.35	0.74
1:F:370:ARG:O	1:F:374:GLN:HG2	1.88	0.73
1:A:421:LYS:HB2	1:A:423:ILE:HD12	1.71	0.71
2:B:1579:PO4:O1	2:B:1580:PO4:O2	2.09	0.71
1:A:376:LEU:O	1:A:473:ARG:NH2	2.24	0.71
1:A:458:ALA:HA	1:B:491:TYR:CD1	2.26	0.70
1:E:505:ARG:HH11	1:E:505:ARG:HB2	1.56	0.70
1:A:573:GLY:HA2	1:A:578:ILE:HD11	1.73	0.69
1:D:352:ASN:OD1	1:E:313:PHE:HB2	1.93	0.69
1:D:439:LYS:NZ	2:D:1580:PO4:O4	2.24	0.68
1:D:304:GLU:HG2	1:D:305:SER:N	1.98	0.68
1:B:303:ASN:HD22	1:C:318:GLN:HA	1.57	0.67
1:B:549:THR:HB	1:B:556:PRO:HD2	1.78	0.66
1:F:462:SER:O	1:F:465:TRP:HD1	1.81	0.63
1:F:482:HIS:ND1	1:F:532:TYR:OH	2.32	0.62
1:A:453:SER:HA	1:B:512:GLN:HE22	1.65	0.62
1:A:385:ARG:HD3	1:A:449:PHE:O	2.00	0.61
1:B:303:ASN:ND2	1:C:318:GLN:HA	2.15	0.61
1:D:507:HIS:HE1	1:E:507:HIS:O	1.85	0.59
1:F:503:ILE:HD12	1:F:513:ILE:HD11	1.84	0.59
1:F:362:ALA:O	1:F:366:ARG:HG2	2.02	0.59
1:F:462:SER:O	1:F:465:TRP:CD1	2.56	0.59
1:C:453:SER:HA	1:D:512:GLN:HE22	1.68	0.58
1:A:532:TYR:HB3	1:A:535:LEU:HD12	1.85	0.58
1:A:432:ILE:CD1	1:A:541:THR:HG23	2.34	0.58
1:E:419:TRP:CD1	1:E:429:LEU:HG	2.39	0.57
1:B:506:LYS:NZ	1:C:508:LYS:O	2.36	0.57
1:F:399:LEU:HD13	1:F:409:LEU:HD22	1.86	0.57
1:D:441:MET:HE3	1:D:559:ILE:H	1.68	0.57
1:A:316:MET:HE1	1:A:357:HIS:HB3	1.86	0.57
1:D:419:TRP:CD1	1:D:429:LEU:HG	2.40	0.56
1:D:441:MET:HA	1:E:499:TYR:OH	2.06	0.56
1:D:401:PHE:HE1	1:D:548:CYS:HG	1.52	0.56
1:E:453:SER:HB3	1:E:472:THR:HG21	1.88	0.56
1:A:464:PHE:CD1	1:A:464:PHE:N	2.73	0.55
1:A:453:SER:HB3	1:A:472:THR:HG21	1.87	0.55
1:A:304:GLU:HG2	1:A:305:SER:N	2.17	0.55
1:F:424:PRO:O	1:F:425:LYS:HB2	2.06	0.55
1:F:578:ILE:O	1:F:578:ILE:HG13	2.06	0.55
1:D:551:GLU:HG3	1:D:552:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:PHE:HA	1:F:492:LEU:HB2	1.89	0.55
1:E:478:ASP:OD2	1:F:494:ASN:ND2	2.40	0.54
1:A:432:ILE:HD12	1:A:541:THR:HG23	1.90	0.54
1:F:438:GLY:O	1:F:441:MET:HB3	2.08	0.54
1:B:447:ILE:HG13	1:B:476:LEU:HB2	1.89	0.54
1:D:304:GLU:CG	1:D:305:SER:H	2.02	0.54
1:B:453:SER:HB3	1:B:472:THR:HG21	1.90	0.54
1:C:325:TYR:CE2	1:C:334:GLU:HG2	2.43	0.54
1:F:432:ILE:HD13	1:F:525:ASP:HA	1.90	0.53
1:B:301:THR:HG22	1:C:321:TYR:CE2	2.43	0.53
1:F:353:SER:O	1:F:357:HIS:CD2	2.60	0.53
1:C:453:SER:HB3	1:C:472:THR:HG21	1.91	0.53
1:A:436:ASN:O	1:A:547:PRO:HA	2.08	0.53
1:E:505:ARG:HH11	1:E:505:ARG:CB	2.22	0.53
1:A:385:ARG:HD2	1:A:450:LEU:O	2.08	0.53
1:B:453:SER:HA	1:C:512:GLN:HE22	1.74	0.53
1:B:304:GLU:HG2	1:B:305:SER:H	1.74	0.52
1:E:319:TRP:HH2	1:E:334:GLU:HB3	1.74	0.52
1:E:425:LYS:HG2	1:E:538:ARG:HG3	1.92	0.52
1:E:505:ARG:NH1	1:E:509:ALA:O	2.44	0.51
1:A:486:ARG:NH2	1:A:531:ARG:HH11	2.09	0.51
1:A:321:TYR:CE2	1:F:301:THR:HG22	2.46	0.50
1:D:453:SER:HB2	1:E:512:GLN:OE1	2.10	0.50
1:F:389:ALA:HB1	1:F:561:ASP:HB3	1.94	0.50
1:D:315:THR:HB	1:D:344:ASN:ND2	2.28	0.49
1:C:351:THR:O	1:C:354:GLN:HG2	2.13	0.49
1:E:335:TYR:CE2	1:E:345:ALA:HA	2.48	0.49
1:A:385:ARG:HD2	1:A:450:LEU:C	2.34	0.49
1:A:419:TRP:CD1	1:A:429:LEU:HG	2.48	0.48
1:C:316:MET:HE1	1:C:357:HIS:HB3	1.94	0.48
1:D:441:MET:CE	1:D:559:ILE:H	2.26	0.48
1:E:505:ARG:HH11	1:E:505:ARG:CG	2.26	0.48
1:B:424:PRO:HA	1:B:497:ASP:O	2.14	0.48
1:A:441:MET:HE1	1:A:559:ILE:N	2.14	0.48
1:A:513:ILE:HG22	1:A:514:LYS:O	2.13	0.48
1:B:325:TYR:CE2	1:B:334:GLU:HG2	2.49	0.48
1:B:530:ASP:OD1	1:B:530:ASP:N	2.43	0.48
1:C:446:LEU:HD23	1:C:519:LEU:HD11	1.96	0.48
1:D:464:PHE:CE1	1:D:506:LYS:HA	2.49	0.47
1:E:393:GLY:H	1:E:562:ALA:HB1	1.79	0.47
1:F:311:PHE:HZ	1:F:316:MET:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ASN:HB3	1:C:496:LEU:O	2.14	0.47
1:A:486:ARG:HH22	1:A:531:ARG:HH11	1.62	0.47
1:B:304:GLU:HG3	1:C:315:THR:HA	1.97	0.47
1:C:301:THR:HG22	1:D:321:TYR:CE2	2.50	0.47
1:F:503:ILE:HD12	1:F:513:ILE:HD13	1.92	0.47
1:D:316:MET:HE1	1:D:357:HIS:HB3	1.96	0.47
1:B:315:THR:HB	1:B:344:ASN:ND2	2.30	0.47
1:E:532:TYR:HB3	1:E:535:LEU:HD12	1.96	0.47
1:E:313:PHE:CZ	1:E:360:ASP:HB3	2.49	0.47
1:C:546:GLN:HA	1:C:547:PRO:HD3	1.71	0.46
1:F:315:THR:HB	1:F:344:ASN:ND2	2.30	0.46
1:E:480:ALA:HB3	1:E:522:SER:HB2	1.97	0.46
1:F:335:TYR:CE2	1:F:345:ALA:HA	2.51	0.46
1:A:304:GLU:CG	1:A:305:SER:H	2.22	0.46
1:A:470:ALA:HA	1:A:513:ILE:HD12	1.97	0.46
1:F:351:THR:O	1:F:354:GLN:HG3	2.15	0.46
1:C:447:ILE:HG13	1:C:476:LEU:HB2	1.97	0.46
1:D:447:ILE:HG13	1:D:476:LEU:HB2	1.97	0.46
1:C:530:ASP:OD1	1:C:530:ASP:N	2.44	0.46
1:D:551:GLU:CG	1:D:552:SER:N	2.79	0.46
1:A:417:LYS:HD2	1:A:576:ASP:HB2	1.97	0.45
1:C:382:ILE:HD11	1:C:420:LEU:HD22	1.98	0.45
1:A:422:GLY:HA2	1:A:427:ASN:HD22	1.81	0.45
1:D:422:GLY:HA3	1:D:514:LYS:NZ	2.32	0.45
1:D:555:GLN:O	1:D:555:GLN:HG3	2.16	0.45
1:E:404:TYR:O	1:E:546:GLN:HG3	2.16	0.45
1:D:453:SER:HB3	1:D:472:THR:HG21	1.99	0.45
1:E:419:TRP:CE2	1:E:517:PRO:HB3	2.51	0.45
1:B:419:TRP:CD1	1:B:429:LEU:HG	2.52	0.45
1:E:301:THR:O	1:E:302:LEU:C	2.55	0.45
1:E:316:MET:HE3	1:E:361:CYS:HB2	1.98	0.45
1:E:432:ILE:HD13	1:E:525:ASP:HA	1.99	0.45
1:C:319:TRP:HH2	1:C:334:GLU:HB3	1.81	0.45
1:B:339:ALA:HA	1:B:345:ALA:HB3	1.98	0.45
1:E:402:PHE:HD1	1:E:407:ILE:HD11	1.82	0.44
1:F:463:HIS:HE1	1:F:504:ASP:OD2	2.00	0.44
1:C:419:TRP:CE2	1:C:517:PRO:HB3	2.53	0.44
1:E:301:THR:HG22	1:F:321:TYR:CZ	2.53	0.44
1:E:370:ARG:O	1:E:374:GLN:HG2	2.18	0.44
1:E:435:PRO:HB3	1:F:534:TYR:CE1	2.53	0.44
1:B:490:THR:HB	1:B:491:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HB2	1:A:423:ILE:CD1	2.44	0.44
1:C:464:PHE:CE1	1:C:506:LYS:HA	2.53	0.44
1:C:339:ALA:HA	1:C:345:ALA:HB3	2.00	0.44
1:D:346:ARG:HE	1:D:346:ARG:HB2	1.65	0.44
1:D:530:ASP:OD1	1:D:530:ASP:N	2.49	0.44
1:E:304:GLU:HB3	1:E:305:SER:H	1.65	0.44
1:C:454:VAL:HG21	1:D:500:PRO:HB2	2.00	0.43
1:F:327:GLU:O	1:F:328:GLU:C	2.56	0.43
1:C:346:ARG:HE	1:C:346:ARG:HB2	1.50	0.43
1:D:339:ALA:HA	1:D:345:ALA:HB3	2.00	0.43
1:E:330:LYS:O	1:E:334:GLU:HB2	2.19	0.43
1:E:499:TYR:HB3	1:E:500:PRO:CD	2.49	0.43
1:A:432:ILE:HD13	1:A:541:THR:HG23	2.00	0.43
1:E:447:ILE:HD13	1:E:447:ILE:HA	1.93	0.43
1:D:424:PRO:HA	1:D:497:ASP:O	2.19	0.43
1:A:464:PHE:HE2	1:A:506:LYS:HA	1.84	0.42
1:E:405:GLN:NE2	1:E:546:GLN:HB2	2.34	0.42
1:B:404:TYR:OH	1:B:547:PRO:O	2.31	0.42
1:B:470:ALA:HB2	1:B:503:ILE:HG21	2.01	0.42
1:E:482:HIS:O	1:E:483:ALA:C	2.56	0.42
1:C:410:ILE:HA	1:C:413:ILE:HD12	2.02	0.42
1:D:325:TYR:CE2	1:D:334:GLU:HG2	2.54	0.42
1:F:534:TYR:CE2	1:F:538:ARG:CZ	3.02	0.42
1:B:441:MET:CE	1:B:559:ILE:H	2.32	0.42
1:A:478:ASP:HB3	1:B:494:ASN:HD22	1.83	0.42
1:D:456:SER:HB2	1:E:502:SER:HB3	2.00	0.42
1:F:459:ASN:HB3	1:F:460:HIS:H	1.54	0.42
1:F:532:TYR:HB3	1:F:535:LEU:HD12	2.00	0.42
1:C:335:TYR:OH	1:C:344:ASN:ND2	2.52	0.42
1:E:301:THR:HG22	1:F:321:TYR:CE2	2.54	0.42
1:B:374:GLN:HE22	1:B:513:ILE:HD11	1.85	0.41
1:B:577:LEU:O	1:B:578:ILE:C	2.59	0.41
1:A:458:ALA:HB2	1:B:491:TYR:HB3	2.03	0.41
1:E:424:PRO:O	1:E:425:LYS:HB2	2.20	0.41
1:D:446:LEU:HD23	1:D:519:LEU:HD11	2.02	0.41
1:E:374:GLN:NE2	1:E:471:ASP:HA	2.35	0.41
1:F:398:ILE:HG12	1:F:559:ILE:HD12	2.02	0.41
1:A:337:LEU:C	1:A:339:ALA:H	2.23	0.41
1:F:477:VAL:HB	1:F:520:VAL:HG13	2.02	0.41
1:A:439:LYS:N	2:A:1580:PO4:O3	2.53	0.41
1:B:335:TYR:OH	1:B:344:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:ALA:HB1	1:F:515:ALA:CB	2.50	0.41
1:A:473:ARG:O	1:A:517:PRO:HD2	2.21	0.41
1:B:446:LEU:HD23	1:B:519:LEU:HD11	2.03	0.41
1:C:401:PHE:HE2	1:C:544:PHE:CE2	2.38	0.41
1:D:555:GLN:HE21	1:D:555:GLN:HB2	1.66	0.41
1:E:374:GLN:HE22	1:E:471:ASP:HA	1.85	0.41
1:E:478:ASP:OD2	1:F:494:ASN:CG	2.60	0.41
1:E:301:THR:O	1:E:301:THR:HG23	2.21	0.41
1:A:335:TYR:CE2	1:A:345:ALA:HA	2.55	0.40
1:A:447:ILE:HD13	1:A:447:ILE:HA	1.93	0.40
1:E:453:SER:HB3	1:E:472:THR:CG2	2.50	0.40
1:E:398:ILE:CG2	1:E:402:PHE:HE2	2.35	0.40
1:A:316:MET:CE	1:A:357:HIS:HB3	2.50	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	266/305 (87%)	244 (92%)	20 (8%)	2 (1%)	19 60
1	B	262/305 (86%)	251 (96%)	10 (4%)	1 (0%)	34 72
1	C	261/305 (86%)	252 (97%)	9 (3%)	0	100 100
1	D	268/305 (88%)	256 (96%)	8 (3%)	4 (2%)	10 46
1	E	264/305 (87%)	246 (93%)	18 (7%)	0	100 100
1	F	263/305 (86%)	239 (91%)	17 (6%)	7 (3%)	5 31
All	All	1584/1830 (87%)	1488 (94%)	82 (5%)	14 (1%)	21 57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	506	LYS
1	D	553	GLY
1	F	479	ASP
1	F	506	LYS
1	B	576	ASP
1	D	552	SER
1	F	458	ALA
1	F	578	ILE
1	A	338	ALA
1	A	464	PHE
1	F	459	ASN
1	F	462	SER
1	F	441	MET
1	D	578	ILE

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	229/259 (88%)	210 (92%)	19 (8%)	11 34
1	B	225/259 (87%)	208 (92%)	17 (8%)	13 37
1	C	224/259 (86%)	207 (92%)	17 (8%)	13 37
1	D	229/259 (88%)	215 (94%)	14 (6%)	18 44
1	E	228/259 (88%)	212 (93%)	16 (7%)	15 40
1	F	226/259 (87%)	200 (88%)	26 (12%)	5 21
All	All	1361/1554 (88%)	1252 (92%)	109 (8%)	16 35

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	351	THR
1	A	364	MET
1	A	388	LEU
1	A	408	GLU

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Mol	Chain	Res	Type
1	A	410	ILE
1	A	428	CYS
1	A	441	MET
1	A	442	LEU
1	A	454	VAL
1	A	462	SER
1	A	463	HIS
1	A	464	PHE
1	A	479	ASP
1	A	506	LYS
1	A	514	LYS
1	A	548	CYS
1	A	550	ASP
1	A	574	ARG
1	B	301	THR
1	B	303	ASN
1	B	310	LYS
1	B	327	GLU
1	B	354	GLN
1	B	356	LYS
1	B	441	MET
1	B	486	ARG
1	B	501	VAL
1	B	506	LYS
1	B	508	LYS
1	B	518	LEU
1	B	530	ASP
1	B	543	ARG
1	B	548	CYS
1	B	549	THR
1	B	570	ARG
1	C	301	THR
1	C	305	SER
1	C	354	GLN
1	C	356	LYS
1	C	366	ARG
1	C	388	LEU
1	C	408	GLU
1	C	441	MET
1	C	469	LEU
1	C	505	ARG
1	C	507	HIS

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Mol	Chain	Res	Type
1	C	518	LEU
1	C	530	ASP
1	C	543	ARG
1	C	548	CYS
1	C	559	ILE
1	C	574	ARG
1	D	310	LYS
1	D	329	SER
1	D	387	LYS
1	D	388	LEU
1	D	441	MET
1	D	468	SER
1	D	514	LYS
1	D	518	LEU
1	D	527	GLN
1	D	530	ASP
1	D	531	ARG
1	D	549	THR
1	D	555	GLN
1	D	570	ARG
1	E	315	THR
1	E	334	GLU
1	E	351	THR
1	E	364	MET
1	E	387	LYS
1	E	392	GLU
1	E	426	LYS
1	E	441	MET
1	E	486	ARG
1	E	505	ARG
1	E	530	ASP
1	E	538	ARG
1	E	543	ARG
1	E	550	ASP
1	E	570	ARG
1	E	574	ARG
1	F	302	LEU
1	F	303	ASN
1	F	304	GLU
1	F	343	SER
1	F	396	LYS
1	F	400	THR

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Mol	Chain	Res	Type
1	F	408	GLU
1	F	410	ILE
1	F	436	ASN
1	F	441	MET
1	F	468	SER
1	F	472	THR
1	F	481	THR
1	F	482	HIS
1	F	494	ASN
1	F	506	LYS
1	F	507	HIS
1	F	508	LYS
1	F	513	ILE
1	F	526	VAL
1	F	529	GLU
1	F	543	ARG
1	F	548	CYS
1	F	549	THR
1	F	574	ARG
1	F	578	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	463	HIS
1	A	512	GLN
1	A	527	GLN
1	B	303	ASN
1	B	374	GLN
1	B	527	GLN
1	C	427	ASN
1	C	459	ASN
1	D	507	HIS
1	D	527	GLN
1	D	555	GLN
1	E	523	ASN
1	F	323	HIS
1	F	427	ASN
1	F	463	HIS
1	F	512	GLN
1	F	546	GLN

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)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	D	1580	-	4,4,4	0.88	0	6,6,6	0.62	0
2	PO4	C	1579	3	4,4,4	1.82	1 (25%)	6,6,6	2.43	4 (66%)
2	PO4	A	1581	3	4,4,4	1.26	0	6,6,6	0.70	0
2	PO4	E	1579	-	4,4,4	0.82	0	6,6,6	0.46	0
2	PO4	F	1580	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	C	1580	3	4,4,4	1.72	1 (25%)	6,6,6	2.54	2 (33%)
2	PO4	A	1580	3	4,4,4	0.97	0	6,6,6	0.91	0
2	PO4	B	1580	3	4,4,4	1.12	0	6,6,6	0.88	0
2	PO4	B	1579	3	4,4,4	1.03	0	6,6,6	1.01	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1579	PO4	P-O3	-2.88	1.45	1.54
2	C	1580	PO4	P-O2	-2.86	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1580	PO4	O2-P-O1	-5.54	90.62	110.89
2	C	1579	PO4	O3-P-O1	-3.73	97.23	110.89
2	C	1579	PO4	O4-P-O3	-2.73	99.21	107.97
2	C	1579	PO4	O3-P-O2	2.61	116.35	107.97
2	C	1579	PO4	O4-P-O1	2.51	120.09	110.89
2	C	1580	PO4	O4-P-O3	2.16	114.89	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1580	PO4	1	0
2	A	1581	PO4	1	0
2	A	1580	PO4	2	0
2	B	1580	PO4	1	0
2	B	1579	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

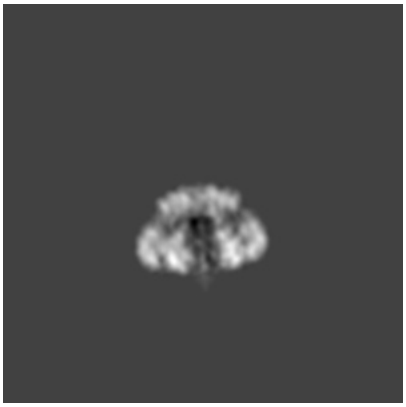
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3087. 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

6.1.1 Primary map



X

Y

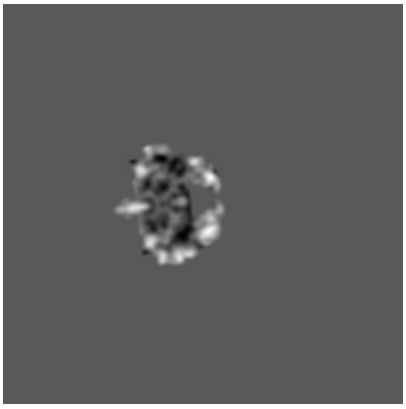
Z

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

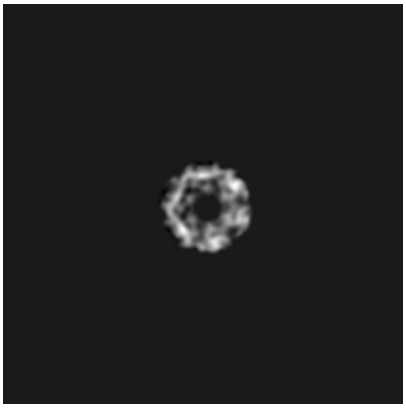
6.2 Central slices

6.2.1 Primary map

X Index: 100



Y Index: 100



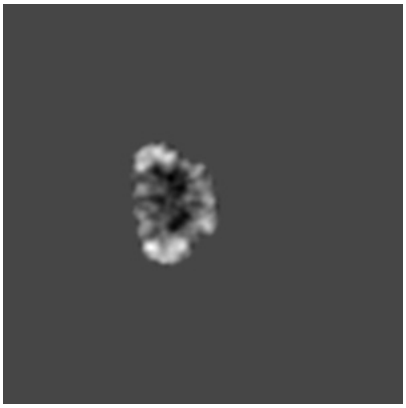
Z Index: 100

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

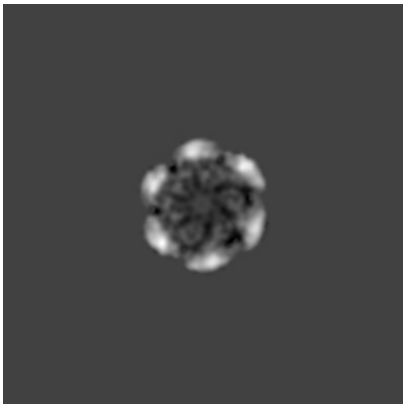
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 122



Y Index: 85

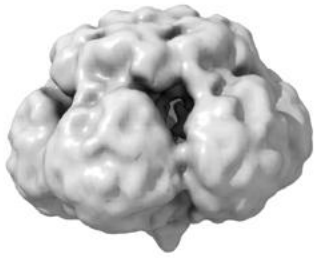


Z Index: 77

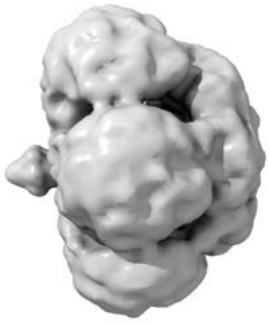
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

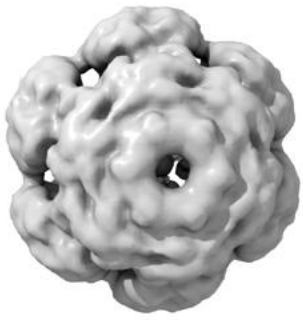
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

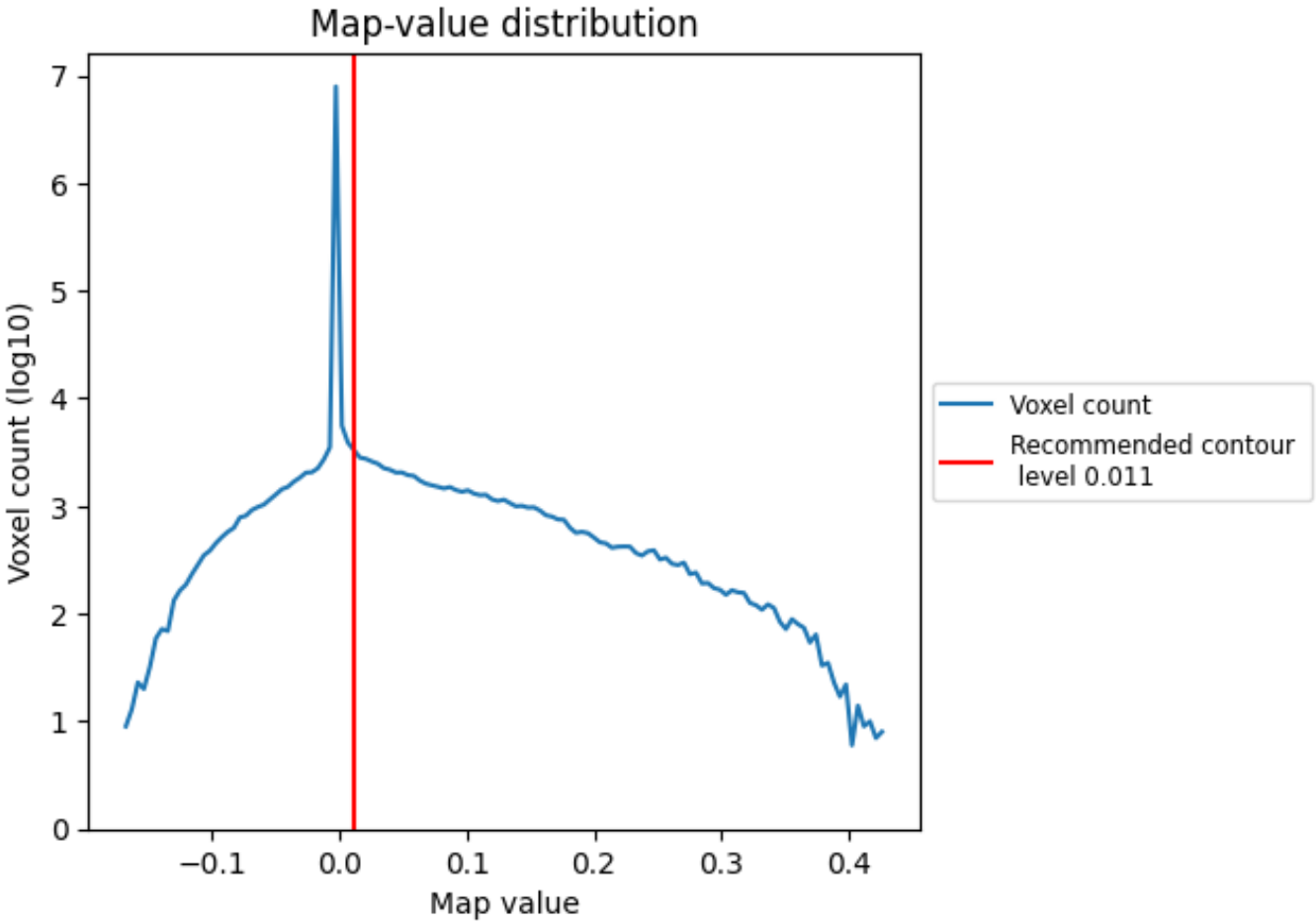
6.5 Mask visualisation (i)

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

7 Map analysis

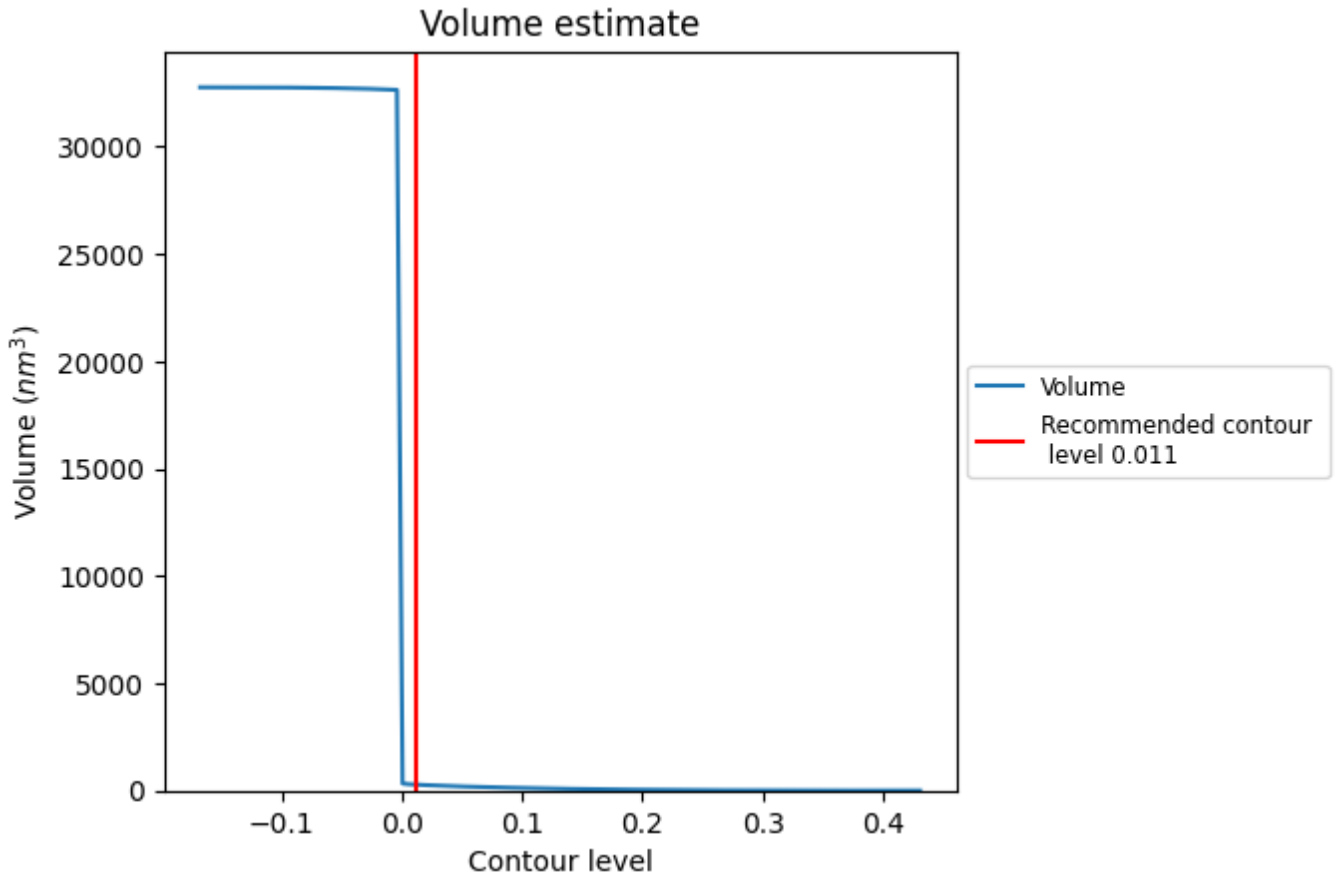
This section contains the results of statistical analysis of the map.

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.

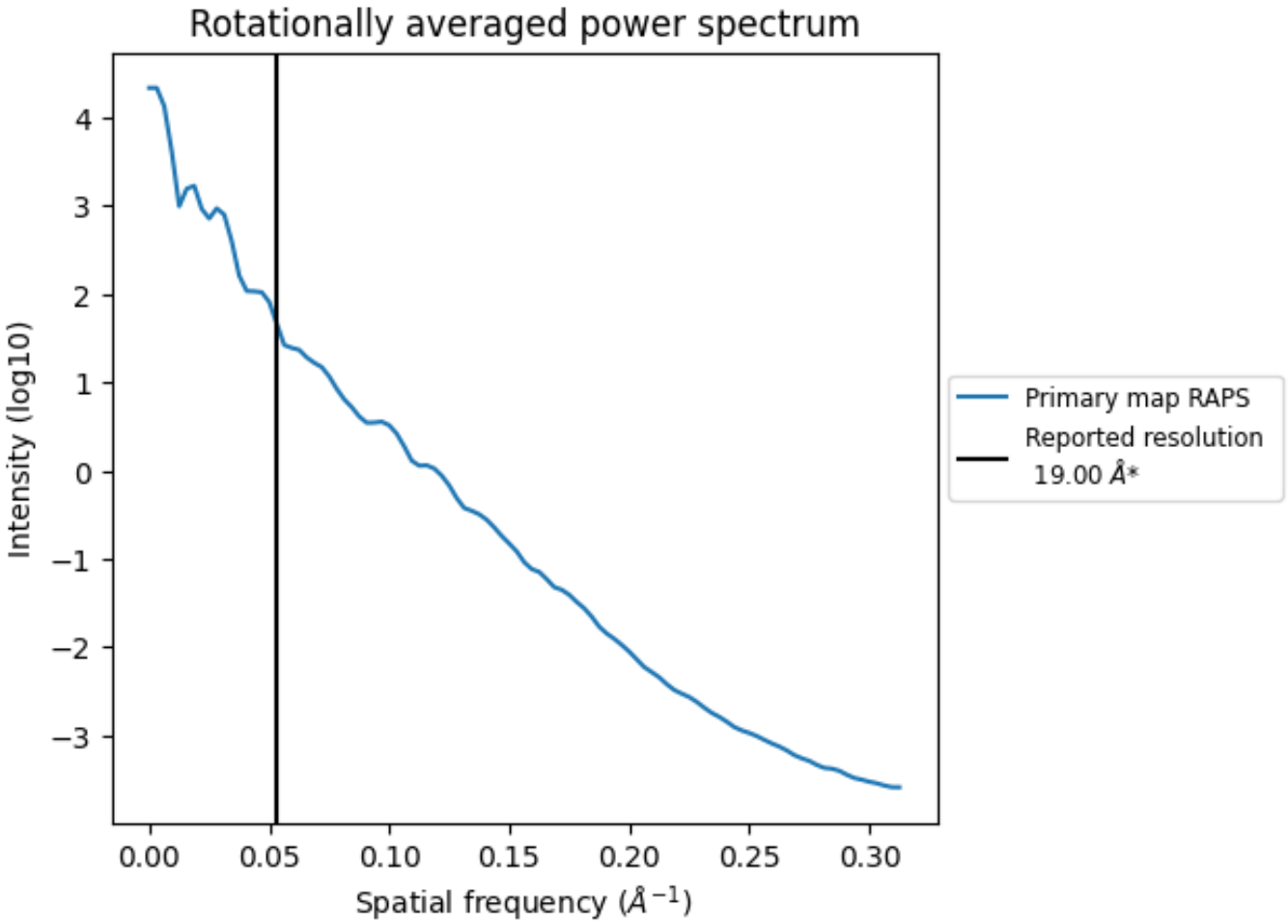
7.2 Volume estimate



The volume at the recommended contour level is 278 nm^3; this corresponds to an approximate mass of 251 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 0.053 Å^{-1}

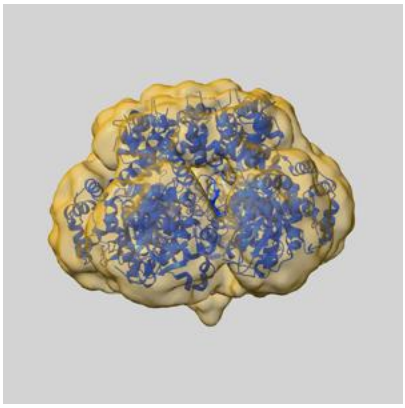
8 Fourier-Shell correlation (i)

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

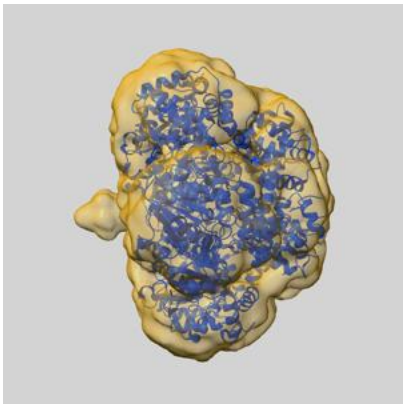
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3087 and PDB model 5A9K. Per-residue inclusion information can be found in section 3 on page 6.

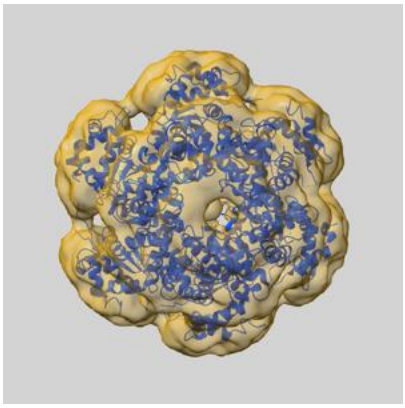
9.1 Map-model overlay



X



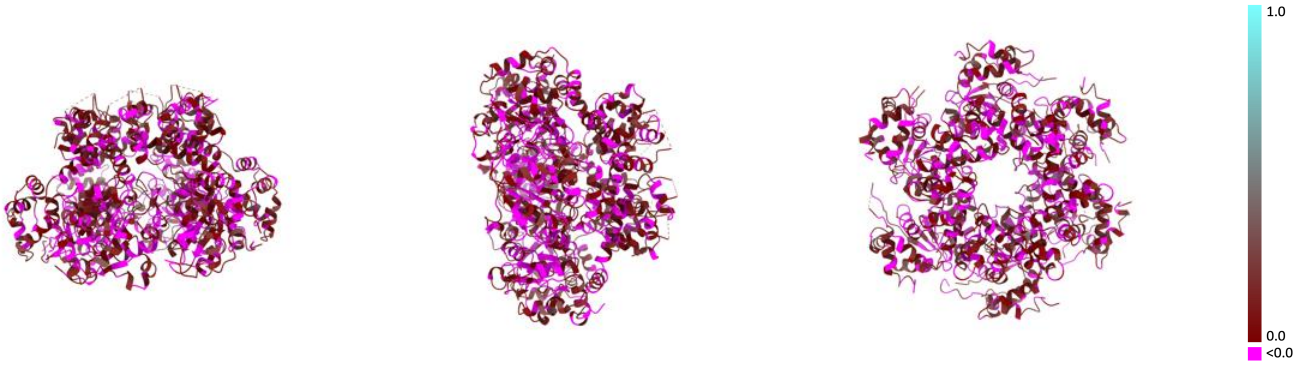
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

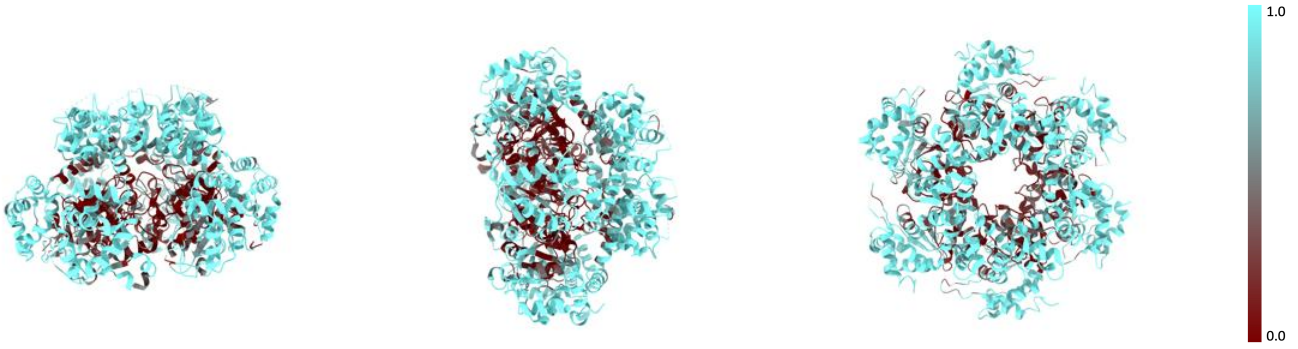
9.2 Q-score mapped to coordinate model (i)



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.

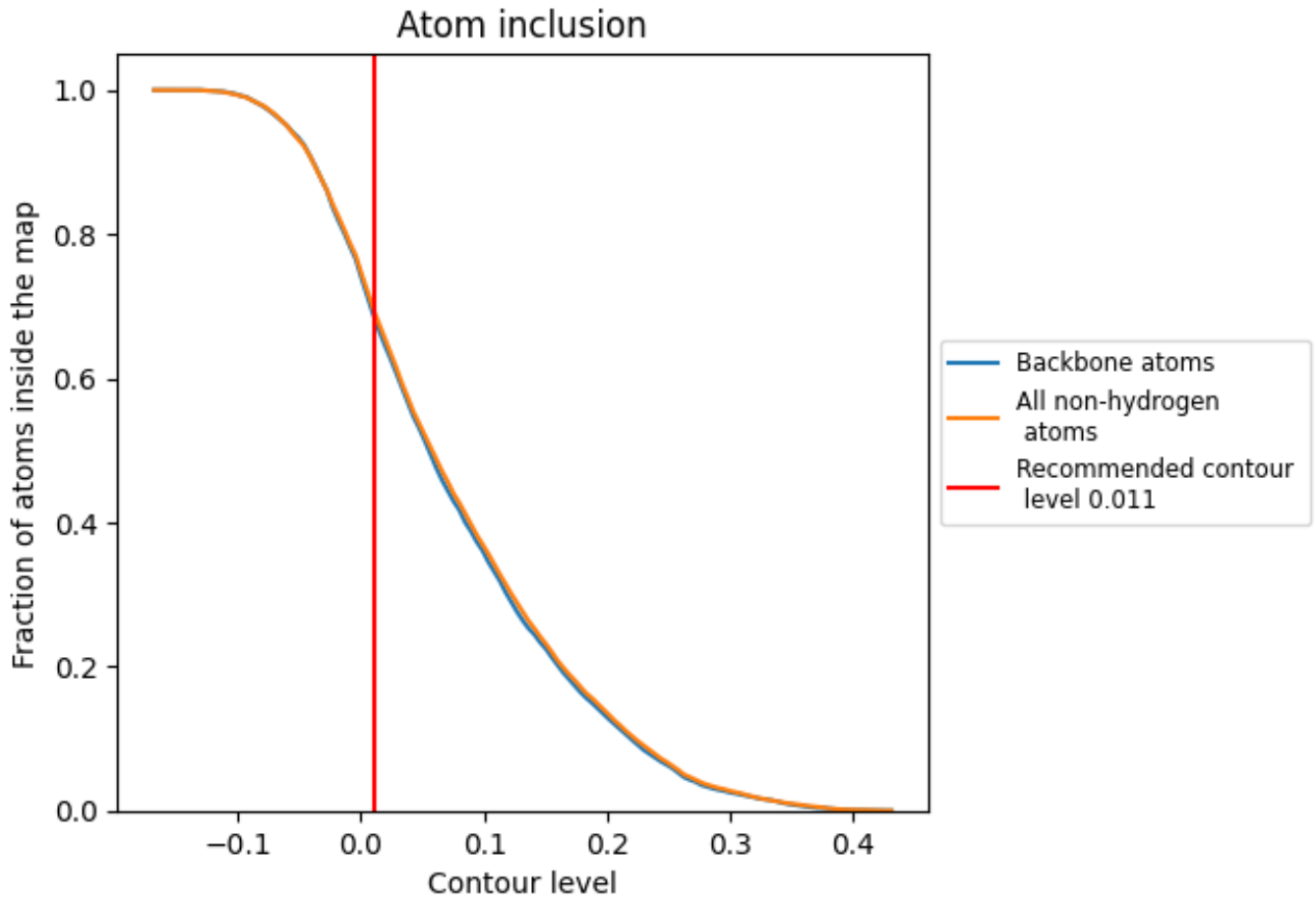
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 69% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6919	0.0420
A	0.6919	0.0370
B	0.6894	0.0420
C	0.6717	0.0460
D	0.6713	0.0430
E	0.7070	0.0420
F	0.7347	0.0400