Full wwPDB EM Validation Report (i)

Sep 17, 2024 – 08:29 PM JST

PDB ID	:	8WH3
EMDB ID	:	EMD-37527
Title	:	MPOX E5 hexamer apo form
Authors	:	Zhang, Z.; Dong, C.
Deposited on	:	2023-09-22
Resolution	:	2.87 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 (i) 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 (i)) were used in the production of this report:

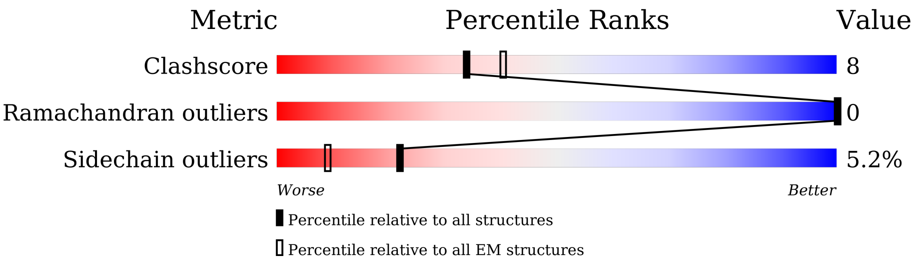
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	785	11% / 49% 10% 41%
1	B	785	17% / 45% 13% • 41%
1	C	785	8% / 48% 10% • 41%
1	D	785	30% / 41% 16% • 41%
1	E	785	18% / 46% 13% 41%
1	F	785	17% / 46% 12% • 41%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22278 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.

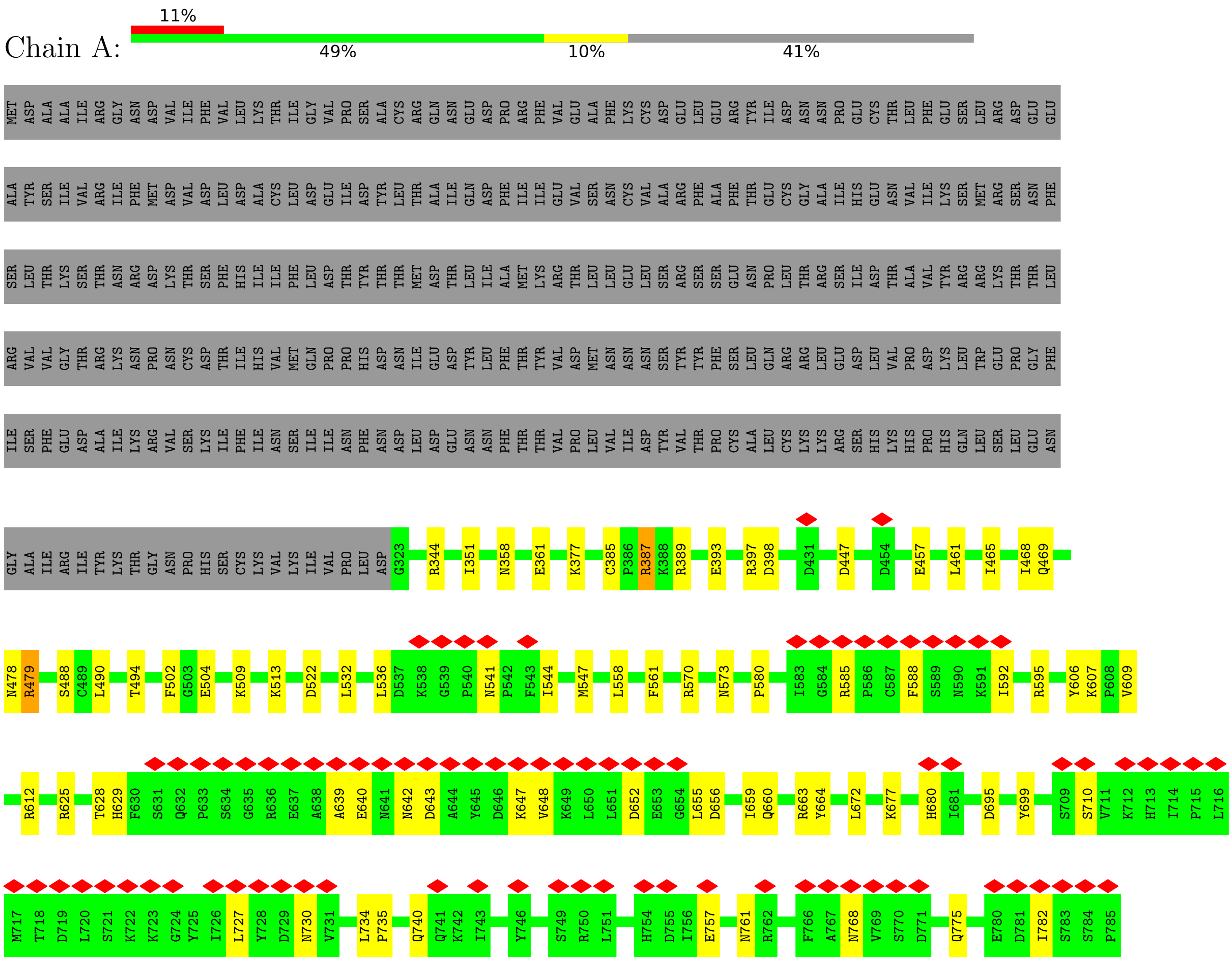
- Molecule 1 is a protein called Uncoating factor OPG117.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	463	3713	2378	628	691	16	0	0
1	B	463	3713	2378	628	691	16	0	0
1	C	463	3713	2378	628	691	16	0	0
1	D	463	3713	2378	628	691	16	0	0
1	E	463	3713	2378	628	691	16	0	0
1	F	463	3713	2378	628	691	16	0	0

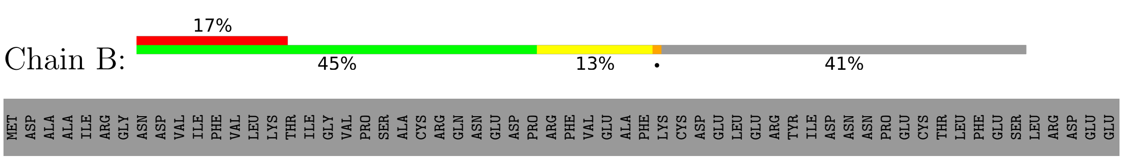
3 Residue-property plots (i)

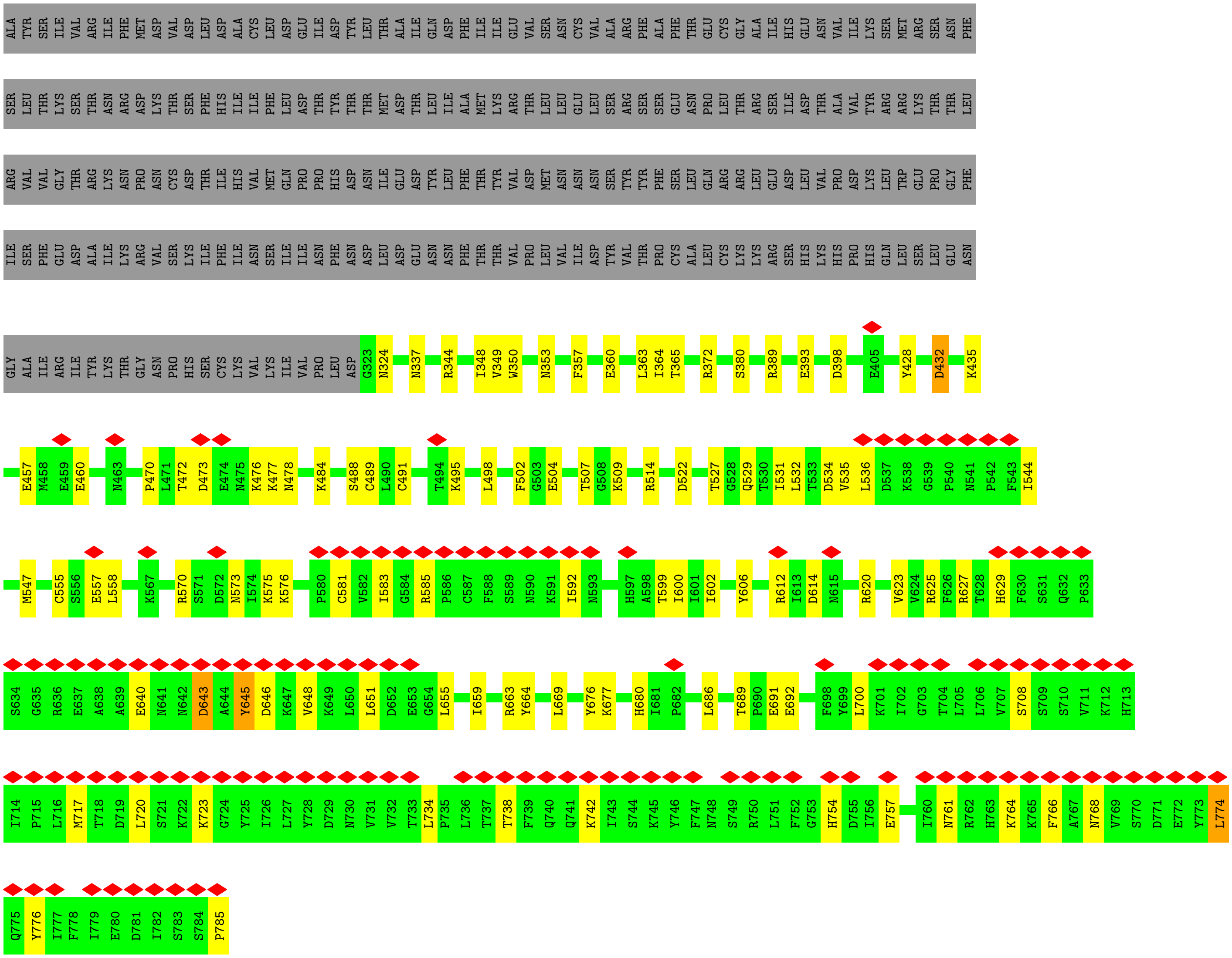
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Uncoating factor OPG117



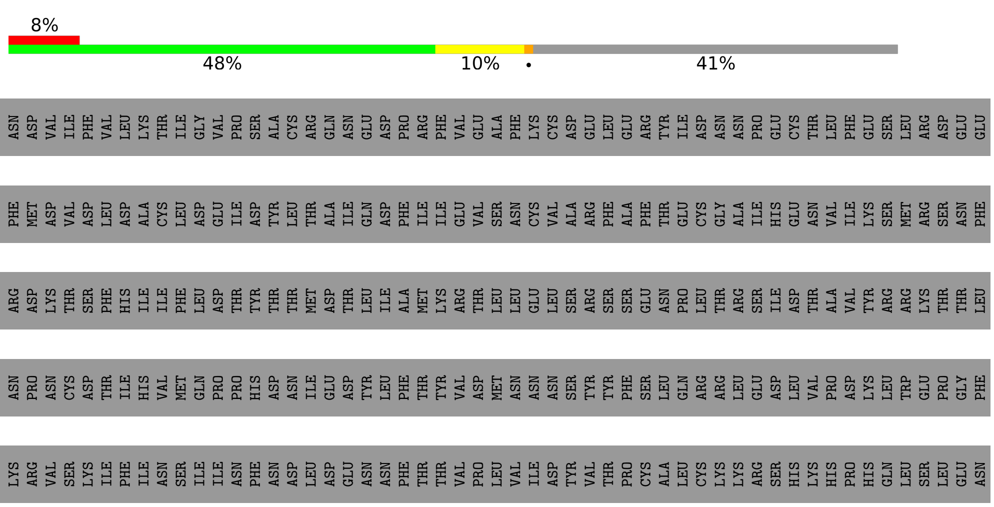
- Molecule 1: Uncoating factor OPG117

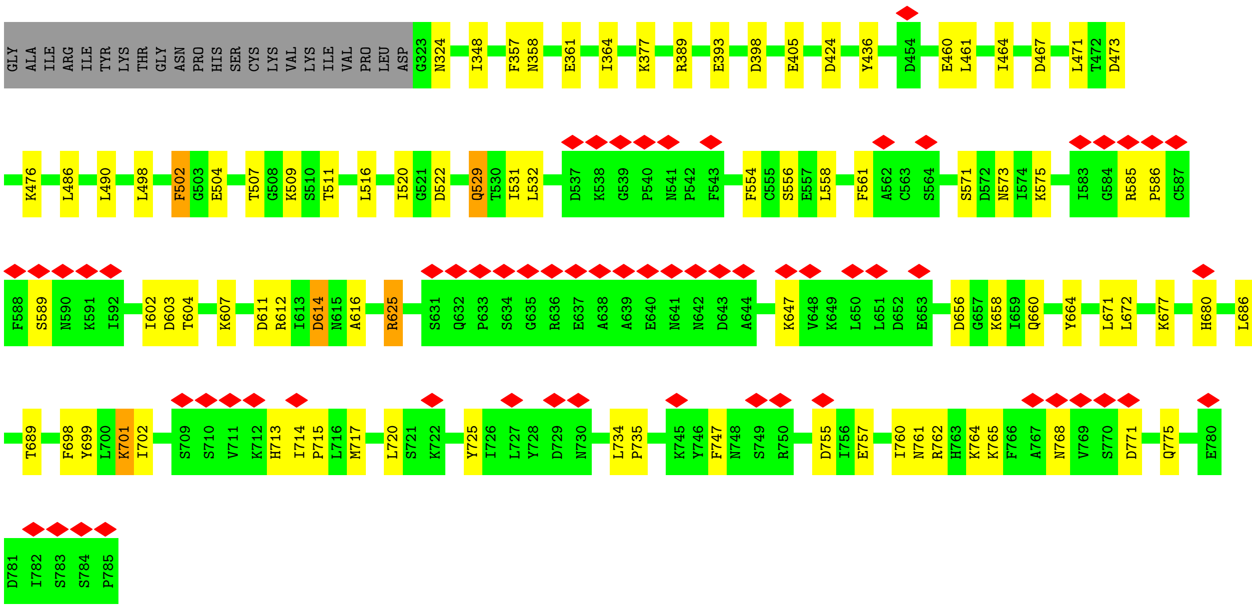




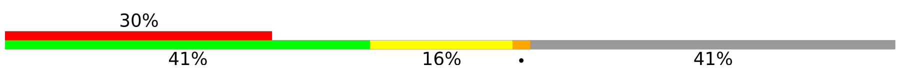
• Molecule 1: Uncoating factor OPG117

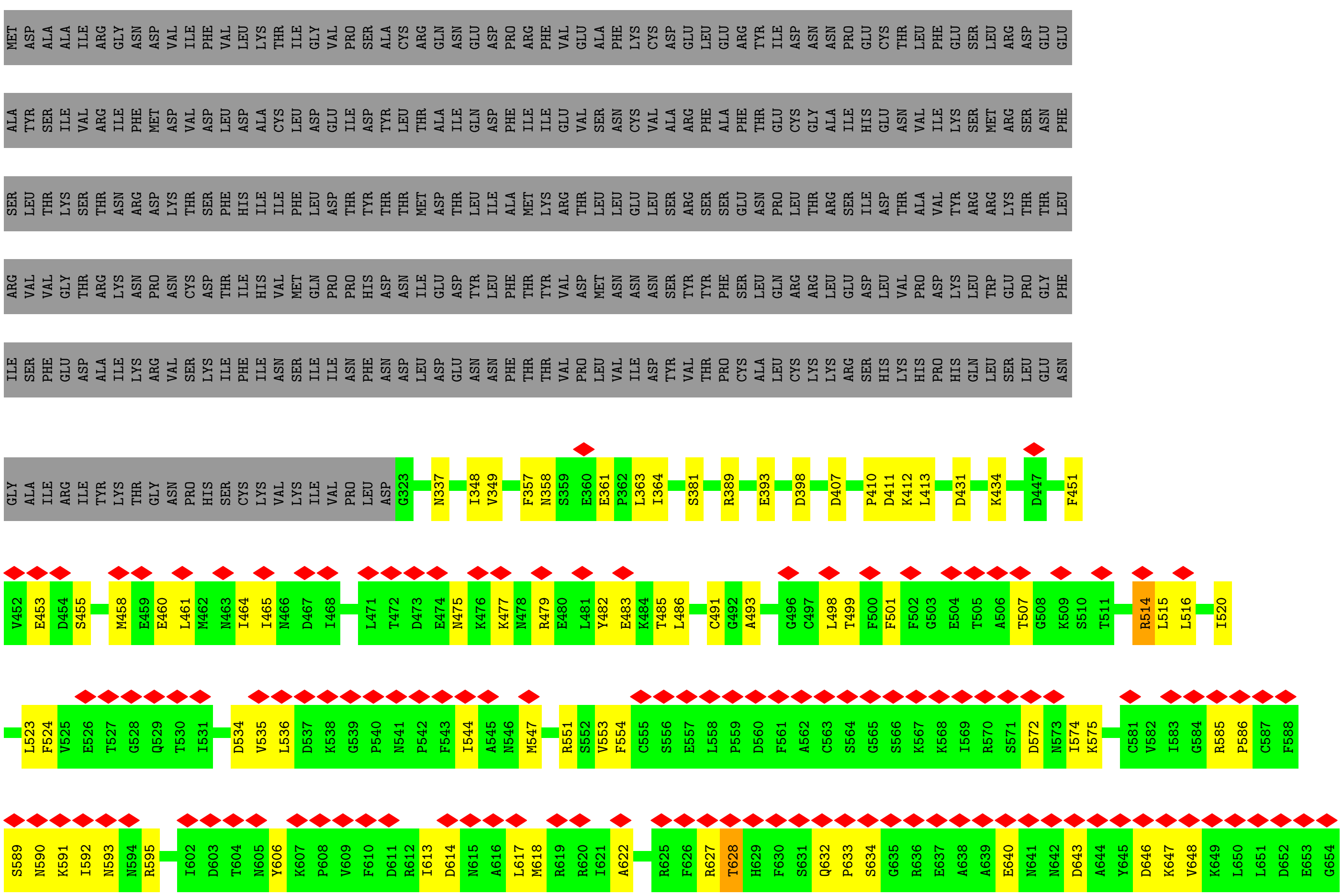
Chain C:

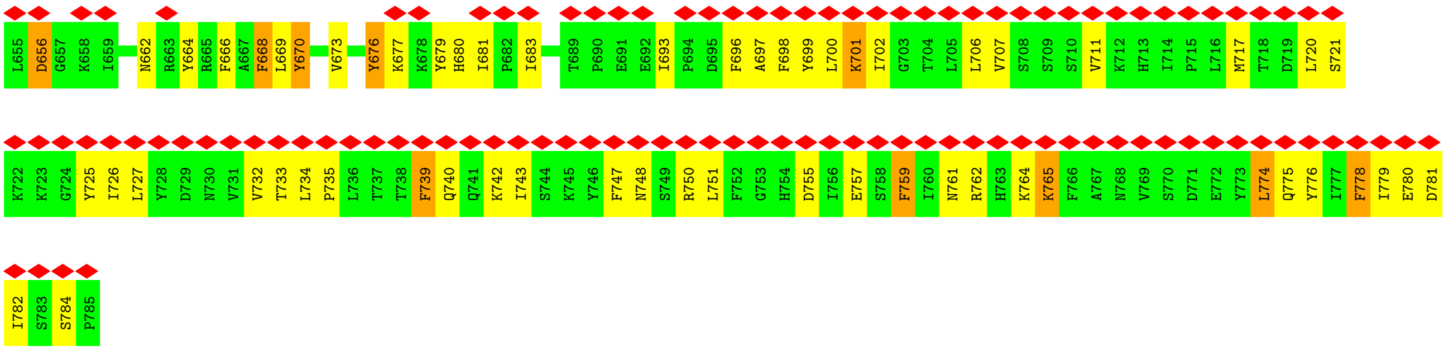




- Molecule 1: Uncoating factor OPG117

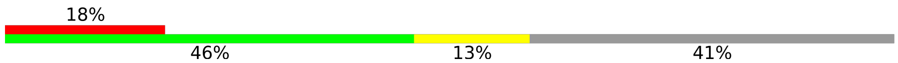
Chain D:


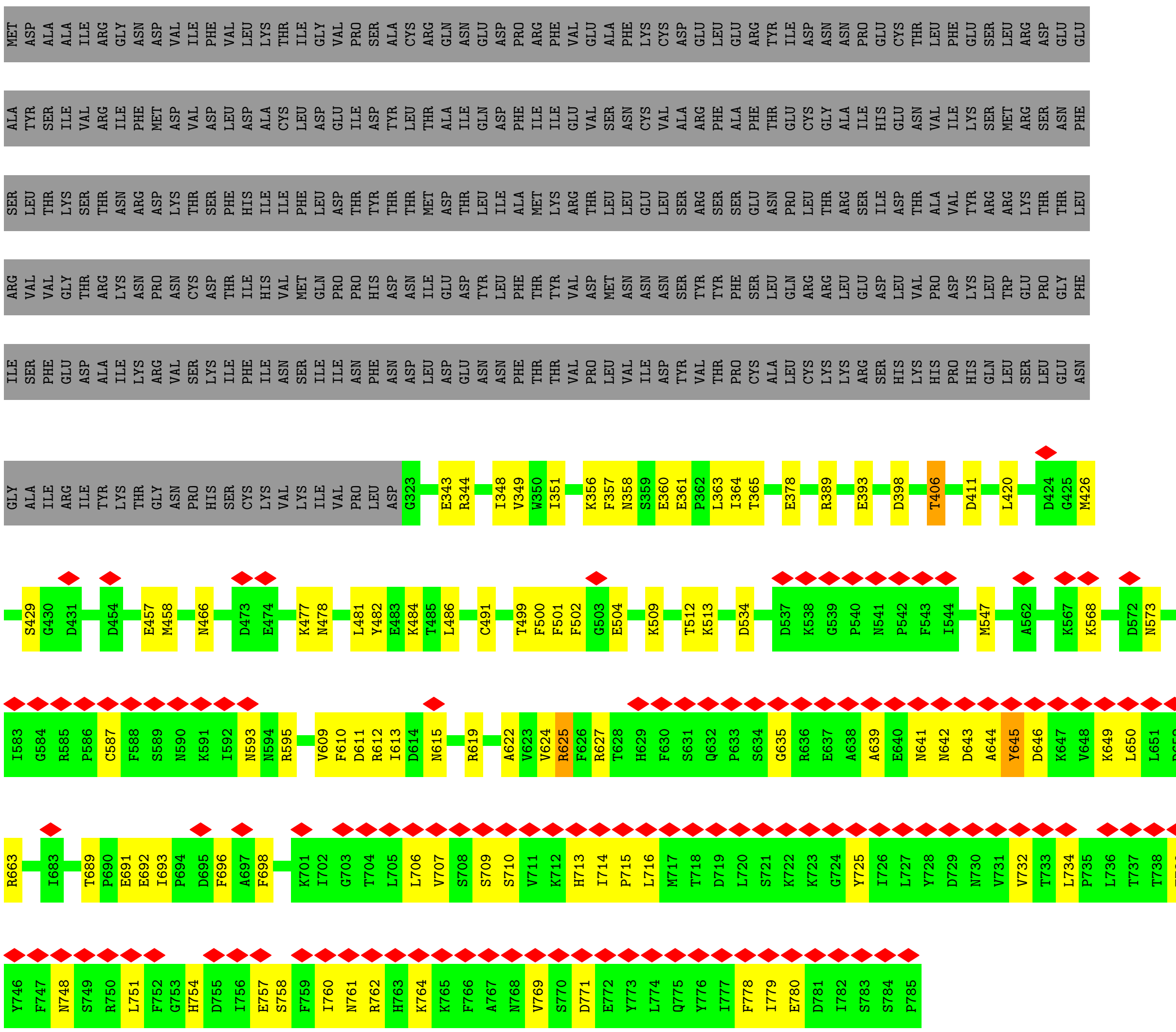




- Molecule 1: Uncoating factor OPG117

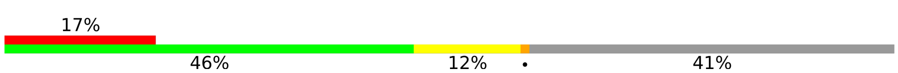
Chain E:

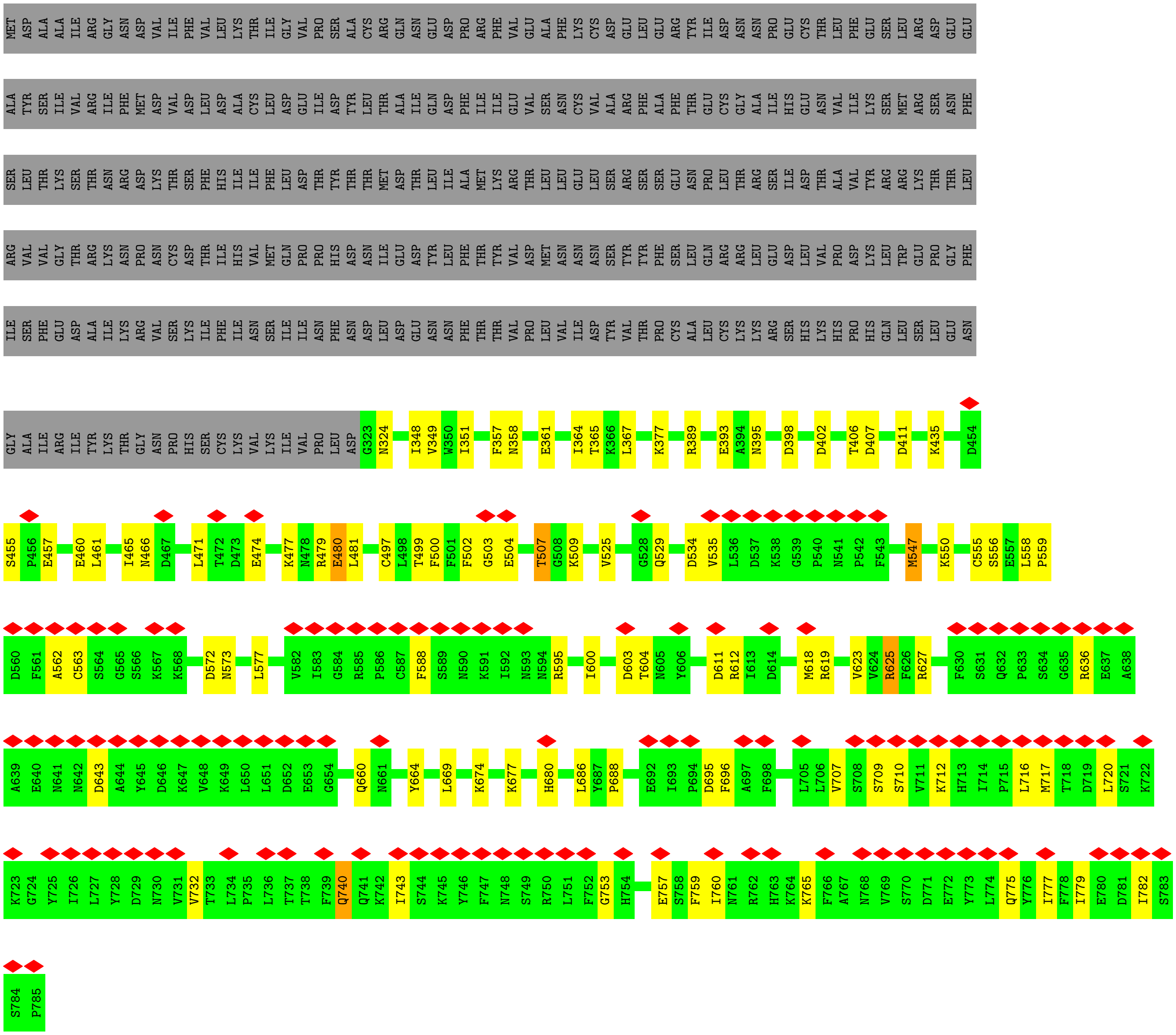




- Molecule 1: Uncoating factor OPG117

Chain F:




MET ASP ALA ALA ILE ARG GLY ASN ASP VAL ILE PHE VAL LEU LYS THR ILE GLY VAL PRO SER ALA CYS ARG GLN ASN GLU ASP PRO ARG PHE VAL GLU ALA PHE LYS CYS ASP GLU LEU GLU ARG TYR ILE ASP ASN ASN PRO GLU CYS THR LEU PHE GLU SER LEU ARG ASP GLU GLU
ALA TYR SER ILE VAL ARG ILE PHE MET ASP VAL ASP LEU ASP ALA CYS LEU ASP GLU ILE ASP TYR LEU THR ALA ILE GLN ASP PHE ILE ILE GLU VAL SER ASN CYS VAL ALA ARG PHE ALA PHE THR GLU CYS GLY ALA ILE HIS GLU ASN VAL ILE LYS SER MET ARG SER ASN PHE
SER LEU THR LYS SER THR ASN ARG ARG ASP LYS THR SER PHE HIS ILE ILE PHE LEU ASP THR TYR THR THR MET ASP THR LEU ILE ALA MET LYS ARG THR LEU LEU GLU LEU SER ARG SER SER GLU ASN PRO LEU THR ARG SER ILE ASP THR ALA VAL TYR ARG ARG LYS THR THR LEU
ARG VAL VAL GLY THR ARG LYS ASN PRO ASN CYS ASP THR ILE HIS HIS VAL MET GLN PRO PRO HIS ASP ASN ILE GLU ASP TYR LEU PHE THR TYR VAL ASP MET ASN ASN ASN SER TYR TYR PHE SER LEU GLN ARG ARG LEU GLU ASP LEU VAL PRO ASP LYS LEU TRP GLU PRO GLY PHE
ILE SER PHE GLU ASP ALA ILE LYS ARG VAL SER LYS ILE PHE ILE ASN SER ILE ILE ASN PHE ASN ASP LEU ASP GLU ASN ASN PHE THR THR VAL PRO LEU VAL ILE ASP TYR VAL THR PRO CYS ALA LEU CYS LYS LYS ARG SER HIS LYS HIS PRO HIS GLN LEU SER LEU GLU ASN
GLY ALA ILE ARG ILE TYR LYS THR GLY ASN PRO HIS SER CYS LYS VAL LYS ILE VAL PRO LEU ASP G323 N324 I348 V349 W350 I351 F357 N358 E361 I364 T365 K366 L367 K377 R389 E393 A394 N395 D398 D402 T406 D407 D411 K435 D454
S455 P456 E457 E460 L461 I465 N466 D467 L471 T472 D473 E474 K477 N478 R479 E480 L481 C497 L498 T499 F500 F501 F502 G503 E504 T507 G508 K509 V525 G528 Q529 D534 V535 L536 D537 K538 G539 P540 N541 P542 F543 M547 K550 C555 S556 E557 L558 P559
D560 F561 A562 C563 S564 G565 S566 K567 K568 D572 N573 L577 V582 I583 G584 R585 P586 C587 F588 S589 N590 K591 I592 N593 N594 R595 I600 D603 T604 N605 Y606 D611 R612 I613 D614 M618 R619 V623 V624 R625 F626 R627 F630 S631 Q632 P633 S634 G635 R636 E637 A638
A639 E640 N641 N642 D643 A644 Y645 D646 K647 V648 K649 L650 L651 D652 E653 G654 Q660 N661 Y664 L669 K674 K677 H680 L686 Y687 P688 E692 I693 P694 D695 F696 A697 F698 L705 L706 V707 S708 S709 S710 V711 K712 H713 I714 P715 L716 M717 T718 D719 L720 S721 K722
K723 G724 Y725 I726 L727 Y728 D729 N730 V731 V732 T733 L734 P735 L736 T737 T738 F739 Q740 Q741 K742 I743 S744 K745 Y746 F747 N748 S749 R750 L751 F752 G753 H754 E757 S758 F759 I760 N761 R762 H763 K764 K765 F766 A767 N768 V769 S770 D771 E772 Y773 L774 Q775 Y776 I777 F778 I779 E780 D781 I782 S783
S784 P785

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	552202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^{-}/\text{Å}^{2}$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.742	Depositor
Minimum map value	-1.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.25	0/3793	0.48	0/5128
1	B	0.26	0/3793	0.48	0/5128
1	C	0.26	0/3793	0.49	0/5128
1	D	0.25	0/3793	0.53	2/5128 (0.0%)
1	E	0.25	0/3793	0.49	0/5128
1	F	0.25	0/3793	0.48	0/5128
All	All	0.25	0/22758	0.49	2/30768 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	515	LEU	CA-CB-CG	7.53	132.63	115.30
1	D	774	LEU	CA-CB-CG	5.07	126.95	115.30

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	3713	0	3706	51	0
1	B	3713	0	3706	59	0
1	C	3713	0	3706	58	0
1	D	3713	0	3706	104	0
1	E	3713	0	3706	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3713	0	3706	58	0
All	All	22278	0	22236	356	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 8.

All (356) 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:725:TYR:HB3	1:D:732:VAL:HG22	1.60	0.82
1:A:710:SER:H	1:E:642:ASN:HB3	1.47	0.80
1:A:642:ASN:HD22	1:C:713:HIS:H	1.30	0.78
1:B:389:ARG:NH1	1:F:398:ASP:OD2	2.19	0.75
1:A:640:GLU:HG2	1:A:648:VAL:HG21	1.71	0.72
1:D:717:MET:HA	1:D:720:LEU:HB2	1.70	0.71
1:A:710:SER:O	1:E:644:ALA:N	2.24	0.71
1:E:378:GLU:OE2	1:E:378:GLU:N	2.23	0.70
1:E:504:GLU:OE2	1:E:504:GLU:N	2.25	0.69
1:D:774:LEU:HD12	1:D:775:GLN:H	1.56	0.69
1:A:536:LEU:O	1:A:541:ASN:ND2	2.25	0.68
1:A:710:SER:N	1:E:642:ASN:HB3	2.07	0.68
1:E:713:HIS:HA	1:E:716:LEU:HG	1.74	0.68
1:D:748:ASN:HB3	1:D:751:LEU:HB2	1.75	0.68
1:E:748:ASN:HB3	1:E:751:LEU:HB2	1.75	0.68
1:C:757:GLU:O	1:C:761:ASN:ND2	2.27	0.67
1:E:426:MET:SD	1:E:426:MET:N	2.68	0.67
1:B:514:ARG:HB3	1:B:659:ILE:HG21	1.77	0.67
1:D:733:THR:HG21	1:D:774:LEU:HG	1.77	0.67
1:A:625:ARG:HH11	1:A:625:ARG:HG2	1.60	0.67
1:A:677:LYS:O	1:A:680:HIS:ND1	2.27	0.66
1:D:693:ILE:HB	1:D:696:PHE:HB2	1.78	0.66
1:E:706:LEU:HD23	1:E:778:PHE:HA	1.78	0.66
1:F:618:MET:HG2	1:F:696:PHE:HE1	1.60	0.66
1:F:534:ASP:OD2	1:F:535:VAL:N	2.29	0.65
1:E:710:SER:HB2	1:E:713:HIS:H	1.61	0.65
1:F:529:GLN:HG2	1:F:559:PRO:HD3	1.80	0.64
1:D:643:ASP:N	1:E:709:SER:O	2.30	0.64
1:B:534:ASP:OD1	1:B:535:VAL:N	2.31	0.64
1:B:643:ASP:N	1:F:710:SER:OG	2.31	0.63
1:D:765:LYS:HB2	1:D:774:LEU:HA	1.81	0.63
1:E:534:ASP:O	1:E:573:ASN:ND2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:777:ILE:HD12	1:F:782:ILE:HD11	1.80	0.62
1:E:504:GLU:O	1:E:509:LYS:NZ	2.24	0.62
1:D:676:TYR:C	1:D:680:HIS:HD1	2.02	0.62
1:D:507:THR:HG23	1:D:628:THR:H	1.63	0.62
1:D:739:PHE:HE1	1:D:778:PHE:HD2	1.46	0.62
1:A:536:LEU:HD22	1:A:544:ILE:HD12	1.81	0.61
1:C:765:LYS:HD3	1:C:775:GLN:HE21	1.65	0.61
1:B:764:LYS:HZ3	1:B:766:PHE:HZ	1.49	0.61
1:D:482:TYR:O	1:D:486:LEU:HG	2.00	0.61
1:C:502:PHE:HE2	1:C:607:LYS:HD3	1.65	0.61
1:E:691:GLU:OE1	1:E:691:GLU:N	2.26	0.61
1:F:348:ILE:HG22	1:F:357:PHE:HB3	1.81	0.61
1:D:547:MET:HG2	1:D:553:VAL:HG21	1.83	0.61
1:B:585:ARG:HB3	1:B:592:ILE:HG22	1.82	0.60
1:D:677:LYS:HA	1:D:680:HIS:CE1	2.36	0.60
1:A:775:GLN:NE2	1:E:643:ASP:OD2	2.35	0.60
1:C:461:LEU:HD23	1:C:664:TYR:HB3	1.82	0.60
1:D:734:LEU:HD12	1:D:735:PRO:HD2	1.83	0.59
1:A:652:ASP:HB3	1:A:655:LEU:HB2	1.84	0.59
1:C:348:ILE:HG22	1:C:357:PHE:HB3	1.85	0.59
1:C:471:LEU:O	1:C:476:LYS:NZ	2.37	0.58
1:D:698:PHE:CD2	1:D:755:ASP:HB3	2.37	0.58
1:D:640:GLU:HG2	1:D:648:VAL:HG21	1.86	0.58
1:B:470:PRO:HB2	1:B:472:THR:HG23	1.86	0.58
1:A:465:ILE:HG22	1:A:479:ARG:HH12	1.68	0.58
1:D:727:LEU:HA	1:D:732:VAL:HA	1.85	0.57
1:F:556:SER:HA	1:F:603:ASP:HB3	1.86	0.57
1:C:677:LYS:O	1:C:680:HIS:ND1	2.37	0.57
1:F:504:GLU:O	1:F:507:THR:OG1	2.19	0.57
1:B:349:VAL:HG21	1:B:363:LEU:HB2	1.86	0.57
1:B:570:ARG:HG3	1:B:573:ASN:HB2	1.86	0.57
1:D:407:ASP:O	1:D:595:ARG:NH2	2.38	0.57
1:D:779:ILE:HA	1:D:782:ILE:HD12	1.87	0.56
1:A:468:ILE:HG22	1:A:469:GLN:HG2	1.86	0.56
1:D:349:VAL:HG21	1:D:363:LEU:HB2	1.87	0.56
1:D:398:ASP:OD2	1:F:389:ARG:NH2	2.37	0.56
1:F:474:GLU:OE1	1:F:474:GLU:N	2.32	0.56
1:C:531:ILE:O	1:C:573:ASN:ND2	2.38	0.56
1:D:707:VAL:HG13	1:D:779:ILE:HD11	1.88	0.56
1:B:398:ASP:OD2	1:C:389:ARG:NH2	2.36	0.56
1:F:525:VAL:HB	1:F:550:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:HG22	1:B:357:PHE:HB3	1.87	0.55
1:F:740:GLN:HA	1:F:743:ILE:HG22	1.89	0.55
1:D:778:PHE:HD1	1:D:779:ILE:N	2.04	0.55
1:B:372:ARG:O	1:B:380:SER:OG	2.24	0.55
1:A:385:CYS:SG	1:A:387:ARG:NH2	2.79	0.55
1:A:504:GLU:O	1:A:509:LYS:NZ	2.40	0.55
1:F:500:PHE:HB2	1:F:623:VAL:HG12	1.88	0.55
1:B:365:THR:HG23	1:B:389:ARG:HB3	1.87	0.55
1:D:681:ILE:HD12	1:D:683:ILE:H	1.72	0.55
1:E:635:GLY:O	1:E:639:ALA:N	2.37	0.55
1:F:461:LEU:HD13	1:F:664:TYR:HB3	1.88	0.55
1:F:717:MET:HA	1:F:720:LEU:HG	1.87	0.55
1:B:360:GLU:OE2	1:B:360:GLU:N	2.26	0.55
1:D:523:LEU:HD13	1:D:551:ARG:HG3	1.88	0.55
1:D:613:ILE:HG23	1:D:617:LEU:HD23	1.88	0.55
1:D:697:ALA:HA	1:D:700:LEU:HB3	1.88	0.54
1:A:625:ARG:HG2	1:A:625:ARG:NH1	2.23	0.54
1:D:411:ASP:OD2	1:D:412:LYS:NZ	2.38	0.54
1:E:625:ARG:NH1	1:E:692:GLU:OE1	2.40	0.54
1:D:348:ILE:HG22	1:D:357:PHE:HB3	1.90	0.54
1:C:502:PHE:CE2	1:C:607:LYS:HD3	2.43	0.54
1:B:774:LEU:HD23	1:B:776:TYR:HB2	1.90	0.54
1:D:707:VAL:HG22	1:D:779:ILE:HG12	1.89	0.54
1:E:707:VAL:HG22	1:E:779:ILE:HG12	1.90	0.53
1:E:713:HIS:HD2	1:E:716:LEU:HD21	1.71	0.53
1:B:761:ASN:HA	1:B:764:LYS:HZ2	1.73	0.53
1:A:734:LEU:HD12	1:A:735:PRO:HD2	1.89	0.53
1:C:467:ASP:OD1	1:C:647:LYS:NZ	2.41	0.53
1:B:495:LYS:HB3	1:B:686:LEU:HD12	1.90	0.53
1:A:478:ASN:ND2	1:A:625:ARG:O	2.37	0.53
1:D:733:THR:HG22	1:D:776:TYR:H	1.74	0.53
1:C:498:LEU:HD23	1:C:602:ILE:HD11	1.90	0.53
1:C:699:TYR:HE2	1:C:762:ARG:HH22	1.56	0.53
1:B:723:LYS:NZ	1:B:785:PRO:O	2.41	0.53
1:D:711:VAL:N	1:F:643:ASP:HB3	2.24	0.52
1:F:680:HIS:O	1:F:680:HIS:ND1	2.42	0.52
1:B:677:LYS:O	1:B:680:HIS:ND1	2.41	0.52
1:D:475:ASN:O	1:D:479:ARG:N	2.37	0.52
1:D:669:LEU:O	1:D:673:VAL:HG13	2.09	0.52
1:E:757:GLU:O	1:E:761:ASN:ND2	2.43	0.52
1:C:689:THR:O	1:C:689:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:HA	1:C:714:ILE:HG22	1.91	0.52
1:A:393:GLU:OE2	1:A:397:ARG:NH1	2.42	0.52
1:A:710:SER:OG	1:E:642:ASN:N	2.43	0.52
1:D:460:GLU:O	1:D:464:ILE:HD12	2.10	0.52
1:E:348:ILE:HG22	1:E:357:PHE:HB3	1.92	0.52
1:C:701:LYS:HG2	1:C:747:PHE:CZ	2.45	0.52
1:C:760:ILE:HG22	1:C:764:LYS:NZ	2.24	0.52
1:F:455:SER:OG	1:F:457:GLU:OE1	2.28	0.52
1:F:577:LEU:HD13	1:F:600:ILE:HD13	1.92	0.51
1:D:499:THR:HG22	1:D:622:ALA:HB3	1.92	0.51
1:F:572:ASP:OD1	1:F:573:ASN:N	2.43	0.51
1:A:655:LEU:O	1:A:659:ILE:HG12	2.10	0.51
1:B:757:GLU:O	1:B:761:ASN:ND2	2.44	0.51
1:E:568:LYS:HG2	1:E:609:VAL:HG12	1.91	0.51
1:B:428:TYR:HB3	1:B:432:ASP:HB2	1.93	0.51
1:B:764:LYS:HB3	1:B:774:LEU:HD12	1.92	0.51
1:C:504:GLU:O	1:C:507:THR:OG1	2.21	0.50
1:A:558:LEU:HD12	1:A:561:PHE:HZ	1.76	0.50
1:C:698:PHE:CD2	1:C:755:ASP:HB3	2.46	0.50
1:F:477:LYS:O	1:F:480:GLU:HG3	2.11	0.50
1:D:739:PHE:HE1	1:D:778:PHE:CD2	2.28	0.50
1:E:734:LEU:HD23	1:E:739:PHE:HD1	1.75	0.50
1:C:717:MET:HA	1:C:720:LEU:HB2	1.92	0.50
1:D:627:ARG:NH2	1:D:643:ASP:O	2.44	0.50
1:D:676:TYR:O	1:D:680:HIS:ND1	2.42	0.50
1:E:725:TYR:HB3	1:E:732:VAL:HG12	1.94	0.50
1:B:457:GLU:OE2	1:B:663:ARG:NH2	2.44	0.50
1:D:711:VAL:H	1:F:643:ASP:HB3	1.77	0.50
1:E:478:ASN:ND2	1:E:625:ARG:O	2.38	0.50
1:D:717:MET:O	1:D:721:SER:N	2.40	0.50
1:D:726:ILE:N	1:D:733:THR:O	2.29	0.50
1:E:481:LEU:HD22	1:E:624:VAL:HG22	1.94	0.50
1:B:432:ASP:O	1:B:435:LYS:NZ	2.37	0.49
1:F:358:ASN:HB3	1:F:361:GLU:O	2.12	0.49
1:F:625:ARG:HD3	1:F:627:ARG:HH11	1.77	0.49
1:F:558:LEU:HD12	1:F:604:THR:HB	1.94	0.49
1:A:757:GLU:O	1:A:761:ASN:ND2	2.45	0.49
1:A:768:ASN:HA	1:E:754:HIS:NE2	2.27	0.49
1:C:558:LEU:HD12	1:C:604:THR:HB	1.94	0.49
1:D:585:ARG:HB3	1:D:592:ILE:HG22	1.94	0.49
1:D:699:TYR:HA	1:D:702:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:GLU:HG2	1:C:761:ASN:HD21	1.77	0.49
1:D:757:GLU:O	1:D:761:ASN:ND2	2.44	0.49
1:D:699:TYR:HA	1:D:702:ILE:HB	1.94	0.49
1:D:389:ARG:NH2	1:E:398:ASP:OD2	2.43	0.49
1:D:762:ARG:NE	1:F:562:ALA:O	2.43	0.49
1:E:714:ILE:HB	1:E:715:PRO:HD3	1.95	0.49
1:F:407:ASP:O	1:F:595:ARG:NH2	2.46	0.49
1:F:503:GLY:O	1:F:509:LYS:NZ	2.45	0.49
1:B:389:ARG:NH2	1:F:395:ASN:OD1	2.45	0.49
1:C:714:ILE:HG22	1:C:715:PRO:HD3	1.95	0.49
1:C:761:ASN:HA	1:C:764:LYS:NZ	2.27	0.49
1:F:709:SER:HB2	1:F:732:VAL:HG13	1.94	0.49
1:B:504:GLU:O	1:B:509:LYS:NZ	2.46	0.48
1:B:478:ASN:ND2	1:B:625:ARG:O	2.45	0.48
1:D:632:GLN:NE2	1:D:633:PRO:HD2	2.28	0.48
1:C:571:SER:OG	1:C:575:LYS:NZ	2.46	0.48
1:D:742:LYS:NZ	1:D:781:ASP:OD1	2.40	0.48
1:E:351:ILE:HB	1:E:356:LYS:HZ1	1.77	0.48
1:E:406:THR:O	1:E:595:ARG:NH2	2.35	0.48
1:E:710:SER:HB2	1:E:713:HIS:N	2.27	0.48
1:F:457:GLU:OE1	1:F:457:GLU:N	2.33	0.48
1:D:750:ARG:NH2	1:E:771:ASP:O	2.46	0.48
1:D:780:GLU:O	1:D:784:SER:OG	2.30	0.48
1:B:677:LYS:HA	1:B:680:HIS:HB3	1.95	0.48
1:D:740:GLN:HA	1:D:743:ILE:HG22	1.95	0.48
1:E:509:LYS:HE2	1:E:509:LYS:HB2	1.53	0.48
1:A:727:LEU:HD11	1:A:730:ASN:HA	1.96	0.48
1:E:611:ASP:OD1	1:E:612:ARG:N	2.47	0.48
1:F:364:ILE:HB	1:F:393:GLU:HG3	1.95	0.48
1:F:547:MET:HA	1:F:550:LYS:HG3	1.96	0.48
1:E:482:TYR:HH	1:E:512:THR:HG1	1.54	0.47
1:E:649:LYS:HD3	1:E:650:LEU:H	1.78	0.47
1:A:490:LEU:HD11	1:A:672:LEU:HB3	1.96	0.47
1:E:364:ILE:HB	1:E:393:GLU:HG3	1.95	0.47
1:F:619:ARG:HA	1:F:688:PRO:HG3	1.96	0.47
1:D:762:ARG:NE	1:F:563:CYS:HA	2.29	0.47
1:D:482:TYR:CE2	1:D:486:LEU:HD11	2.50	0.47
1:A:710:SER:HB2	1:E:639:ALA:C	2.34	0.47
1:D:410:PRO:HB3	1:D:493:ALA:HB2	1.95	0.47
1:E:482:TYR:O	1:E:486:LEU:HD23	2.15	0.47
1:C:516:LEU:O	1:C:520:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ARG:HB2	1:B:646:ASP:HB2	1.97	0.47
1:D:591:LYS:NZ	1:D:593:ASN:O	2.35	0.47
1:F:509:LYS:NZ	1:F:604:THR:O	2.48	0.47
1:F:707:VAL:HG22	1:F:779:ILE:HG12	1.96	0.47
1:C:586:PRO:HD2	1:C:589:SER:HB3	1.98	0.46
1:D:750:ARG:HB2	1:E:769:VAL:HA	1.97	0.46
1:D:483:GLU:HB3	1:D:679:TYR:HE2	1.80	0.46
1:B:708:SER:HA	1:B:776:TYR:HA	1.98	0.46
1:D:668:PHE:HD1	1:D:668:PHE:O	1.98	0.46
1:B:460:GLU:HB2	1:B:664:TYR:HE1	1.81	0.46
1:C:761:ASN:HA	1:C:764:LYS:HZ1	1.80	0.46
1:D:670:TYR:O	1:D:673:VAL:HG22	2.16	0.46
1:D:702:ILE:O	1:D:706:LEU:N	2.49	0.46
1:F:775:GLN:OE1	1:F:775:GLN:N	2.36	0.46
1:C:699:TYR:OH	1:C:762:ARG:NH1	2.45	0.46
1:A:561:PHE:HB2	1:A:609:VAL:HG22	1.98	0.46
1:B:629:HIS:HB2	1:B:645:TYR:CB	2.46	0.46
1:D:590:ASN:HA	1:F:588:PHE:CE2	2.51	0.46
1:F:460:GLU:HB2	1:F:664:TYR:HE1	1.80	0.46
1:A:710:SER:HA	1:E:645:TYR:CE1	2.51	0.46
1:B:738:THR:HG22	1:B:742:LYS:HD2	1.98	0.46
1:C:504:GLU:O	1:C:509:LYS:NZ	2.48	0.45
1:D:477:LYS:HD2	1:D:477:LYS:HA	1.72	0.45
1:B:364:ILE:HB	1:B:393:GLU:HG3	1.98	0.45
1:C:701:LYS:HD2	1:C:702:ILE:N	2.31	0.45
1:A:532:LEU:HD12	1:A:558:LEU:HD11	1.98	0.45
1:D:706:LEU:HD22	1:D:759:PHE:HZ	1.80	0.45
1:D:765:LYS:HD3	1:D:774:LEU:HD12	1.98	0.45
1:B:527:THR:HG23	1:B:555:CYS:HB3	1.99	0.45
1:E:725:TYR:HB3	1:E:732:VAL:CG1	2.47	0.45
1:C:358:ASN:HB3	1:C:361:GLU:O	2.17	0.45
1:A:461:LEU:HD13	1:A:664:TYR:HB3	1.99	0.45
1:B:576:LYS:HE2	1:B:583:ILE:HB	1.98	0.45
1:B:643:ASP:HB2	1:F:712:LYS:N	2.32	0.45
1:E:610:PHE:HB2	1:E:613:ILE:HG22	1.99	0.45
1:D:720:LEU:HB3	1:D:725:TYR:HB2	1.99	0.45
1:B:350:TRP:CZ2	1:B:353:ASN:HA	2.51	0.45
1:C:377:LYS:HD3	1:C:377:LYS:N	2.31	0.45
1:B:536:LEU:HD13	1:B:544:ILE:HG12	1.99	0.44
1:C:671:LEU:HD12	1:C:671:LEU:HA	1.84	0.44
1:D:706:LEU:HD22	1:D:759:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:753:GLY:O	1:F:757:GLU:HG2	2.17	0.44
1:B:629:HIS:HB2	1:B:645:TYR:CG	2.52	0.44
1:E:358:ASN:HB3	1:E:361:GLU:O	2.17	0.44
1:F:716:LEU:HD23	1:F:716:LEU:HA	1.83	0.44
1:A:642:ASN:HA	1:C:715:PRO:HD3	1.99	0.44
1:C:364:ILE:HB	1:C:393:GLU:HG3	1.98	0.44
1:C:734:LEU:HD12	1:C:735:PRO:HD2	1.99	0.44
1:E:500:PHE:N	1:E:622:ALA:O	2.34	0.44
1:F:411:ASP:OD1	1:F:411:ASP:N	2.41	0.44
1:D:701:LYS:HD2	1:D:701:LYS:N	2.33	0.44
1:D:358:ASN:HB3	1:D:361:GLU:O	2.17	0.44
1:F:465:ILE:HG22	1:F:479:ARG:HH12	1.82	0.44
1:D:676:TYR:O	1:D:680:HIS:N	2.31	0.44
1:C:532:LEU:HD11	1:C:602:ILE:HD13	1.99	0.44
1:C:760:ILE:HG22	1:C:764:LYS:HZ2	1.83	0.44
1:C:725:TYR:CD2	1:C:734:LEU:HD13	2.53	0.43
1:D:700:LEU:HD23	1:D:701:LYS:NZ	2.32	0.43
1:E:693:ILE:HB	1:E:696:PHE:HD1	1.83	0.43
1:F:477:LYS:HB2	1:F:477:LYS:HE2	1.77	0.43
1:B:734:LEU:HD12	1:B:734:LEU:HA	1.87	0.43
1:D:431:ASP:HA	1:D:434:LYS:HB2	2.00	0.43
1:E:457:GLU:OE1	1:E:663:ARG:NE	2.51	0.43
1:C:486:LEU:HD23	1:C:486:LEU:HA	1.88	0.43
1:D:575:LYS:HE3	1:D:575:LYS:HB3	1.72	0.43
1:D:412:LYS:O	1:D:551:ARG:NH1	2.45	0.43
1:D:670:TYR:O	1:D:670:TYR:HD1	2.01	0.43
1:A:782:ILE:HG23	1:E:641:ASN:OD1	2.19	0.43
1:D:698:PHE:CD1	1:D:747:PHE:HE2	2.36	0.43
1:B:491:CYS:HB2	1:B:676:TYR:HE2	1.84	0.43
1:D:534:ASP:OD2	1:D:535:VAL:N	2.52	0.43
1:A:629:HIS:CE1	1:A:639:ALA:HB1	2.54	0.43
1:C:509:LYS:HB2	1:C:509:LYS:HE2	1.81	0.43
1:F:406:THR:O	1:F:595:ARG:NH2	2.38	0.43
1:C:476:LYS:HD3	1:C:476:LYS:HA	1.92	0.43
1:D:516:LEU:HD23	1:D:524:PHE:HE2	1.84	0.43
1:E:593:ASN:N	1:E:593:ASN:OD1	2.52	0.43
1:F:466:ASN:OD1	1:F:471:LEU:HD13	2.19	0.43
1:A:494:THR:HG21	1:A:580:PRO:HA	2.00	0.43
1:C:625:ARG:HE	1:C:625:ARG:HB3	1.67	0.43
1:D:451:PHE:HD1	1:D:666:PHE:HB3	1.84	0.43
1:F:497:CYS:HB2	1:F:686:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:PHE:HZ	1:C:585:ARG:HD3	1.83	0.42
1:B:477:LYS:HB3	1:B:477:LYS:HE3	1.76	0.42
1:D:586:PRO:HD2	1:D:589:SER:HB3	2.00	0.42
1:D:627:ARG:HB2	1:D:646:ASP:HB2	2.01	0.42
1:F:677:LYS:HA	1:F:680:HIS:HB3	2.00	0.42
1:B:498:LEU:HD22	1:B:600:ILE:HB	2.01	0.42
1:D:680:HIS:CG	1:D:680:HIS:O	2.72	0.42
1:A:509:LYS:HB2	1:A:509:LYS:HE2	1.77	0.42
1:A:457:GLU:OE1	1:A:663:ARG:NH2	2.52	0.42
1:A:628:THR:HG23	1:A:647:LYS:HB3	2.02	0.42
1:D:698:PHE:HZ	1:D:759:PHE:HB2	1.83	0.42
1:B:504:GLU:O	1:B:507:THR:OG1	2.26	0.42
1:B:531:ILE:O	1:B:573:ASN:ND2	2.50	0.42
1:B:700:LEU:HD23	1:B:700:LEU:HA	1.87	0.42
1:C:460:GLU:O	1:C:464:ILE:HG22	2.19	0.42
1:C:529:GLN:H	1:C:529:GLN:HG3	1.54	0.42
1:C:556:SER:HA	1:C:603:ASP:HB3	2.00	0.42
1:A:358:ASN:HB3	1:A:361:GLU:O	2.20	0.42
1:D:520:ILE:HD12	1:D:523:LEU:HB2	2.02	0.42
1:D:762:ARG:CZ	1:F:563:CYS:HA	2.50	0.42
1:A:588:PHE:CZ	1:C:585:ARG:HD3	2.54	0.42
1:B:640:GLU:HG2	1:B:648:VAL:HG21	2.00	0.42
1:D:574:ILE:HD11	1:D:617:LEU:HD12	2.02	0.42
1:D:693:ILE:N	1:D:693:ILE:HD12	2.35	0.42
1:F:481:LEU:HD12	1:F:481:LEU:HA	1.87	0.42
1:A:570:ARG:HB2	1:A:573:ASN:HB2	2.00	0.42
1:D:613:ILE:HB	1:D:699:TYR:CE2	2.55	0.42
1:E:477:LYS:HB3	1:E:477:LYS:HE3	1.78	0.42
1:C:768:ASN:OD1	1:C:771:ASP:N	2.53	0.41
1:B:655:LEU:HD12	1:B:655:LEU:HA	1.87	0.41
1:D:453:GLU:HA	1:D:670:TYR:HE2	1.85	0.41
1:D:514:ARG:HH22	1:D:656:ASP:HA	1.85	0.41
1:F:351:ILE:HG23	1:F:367:LEU:HD12	2.01	0.41
1:A:629:HIS:NE2	1:A:639:ALA:HB1	2.34	0.41
1:A:398:ASP:OD2	1:E:389:ARG:NH2	2.50	0.41
1:F:349:VAL:HB	1:F:367:LEU:HD13	2.01	0.41
1:A:377:LYS:HD2	1:A:377:LYS:O	2.19	0.41
1:D:461:LEU:HD22	1:D:664:TYR:HB3	2.03	0.41
1:B:754:HIS:O	1:B:757:GLU:HG3	2.20	0.41
1:C:611:ASP:OD1	1:C:612:ARG:N	2.53	0.41
1:D:364:ILE:HB	1:D:393:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:TYR:HA	1:D:485:THR:HG22	2.03	0.41
1:D:498:LEU:O	1:D:622:ALA:N	2.54	0.41
1:D:536:LEU:HD22	1:D:544:ILE:HD11	2.02	0.41
1:E:627:ARG:HG2	1:E:646:ASP:HB2	2.01	0.41
1:A:358:ASN:HD22	1:A:361:GLU:HB3	1.85	0.41
1:B:575:LYS:HA	1:B:620:ARG:HH11	1.86	0.41
1:C:614:ASP:OD1	1:C:616:ALA:N	2.52	0.41
1:C:714:ILE:HD12	1:C:714:ILE:HA	1.88	0.41
1:F:402:ASP:OD1	1:F:402:ASP:N	2.48	0.41
1:B:489:CYS:HA	1:B:599:THR:HG21	2.02	0.41
1:C:490:LEU:HD11	1:C:672:LEU:HB3	2.02	0.41
1:D:465:ILE:HD13	1:D:465:ILE:HA	1.95	0.41
1:A:592:ILE:HD13	1:E:587:CYS:HB2	2.03	0.41
1:B:768:ASN:OD1	1:B:768:ASN:N	2.54	0.41
1:C:686:LEU:HD23	1:C:686:LEU:HA	1.95	0.41
1:D:483:GLU:HB3	1:D:679:TYR:CE2	2.56	0.41
1:D:725:TYR:CD1	1:D:734:LEU:HD13	2.56	0.41
1:E:349:VAL:HG21	1:E:363:LEU:HB2	2.01	0.41
1:E:760:ILE:O	1:E:764:LYS:HB3	2.21	0.41
1:F:611:ASP:OD1	1:F:611:ASP:N	2.53	0.41
1:A:642:ASN:OD1	1:A:643:ASP:N	2.37	0.41
1:B:532:LEU:HD11	1:B:602:ILE:HG12	2.03	0.41
1:C:464:ILE:HD11	1:C:511:THR:HG21	2.03	0.41
1:F:757:GLU:O	1:F:760:ILE:HG22	2.20	0.41
1:D:701:LYS:HD2	1:D:701:LYS:H	1.86	0.40
1:E:758:SER:O	1:E:762:ARG:HB2	2.20	0.40
1:B:509:LYS:HE2	1:B:509:LYS:HB2	1.77	0.40
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.85	0.40
1:B:669:LEU:HD12	1:B:669:LEU:HA	1.90	0.40
1:A:585:ARG:HB3	1:A:592:ILE:HG22	2.02	0.40
1:D:640:GLU:HA	1:D:648:VAL:HG21	2.03	0.40
1:E:689:THR:O	1:E:689:THR:OG1	2.33	0.40
1:A:389:ARG:NH2	1:C:398:ASP:OD2	2.53	0.40
1:B:484:LYS:HB3	1:B:484:LYS:HE3	1.83	0.40
1:B:717:MET:HA	1:B:720:LEU:HB2	2.02	0.40
1:D:764:LYS:HA	1:D:774:LEU:HD13	2.03	0.40
1:D:628:THR:HG23	1:D:647:LYS:HB3	2.03	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	461/785 (59%)	447 (97%)	14 (3%)	0	100	100
1	B	461/785 (59%)	438 (95%)	23 (5%)	0	100	100
1	C	461/785 (59%)	441 (96%)	20 (4%)	0	100	100
1	D	461/785 (59%)	441 (96%)	20 (4%)	0	100	100
1	E	461/785 (59%)	440 (95%)	21 (5%)	0	100	100
1	F	461/785 (59%)	448 (97%)	13 (3%)	0	100	100
All	All	2766/4710 (59%)	2655 (96%)	111 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	414/725 (57%)	395 (95%)	19 (5%)	23	52
1	B	414/725 (57%)	390 (94%)	24 (6%)	17	43
1	C	414/725 (57%)	398 (96%)	16 (4%)	27	59
1	D	414/725 (57%)	389 (94%)	25 (6%)	16	41
1	E	414/725 (57%)	390 (94%)	24 (6%)	17	43
1	F	414/725 (57%)	394 (95%)	20 (5%)	21	51
All	All	2484/4350 (57%)	2356 (95%)	128 (5%)	22	47

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	A	351	ILE
1	A	387	ARG
1	A	447	ASP
1	A	479	ARG
1	A	488	SER
1	A	502	PHE
1	A	513	LYS
1	A	522	ASP
1	A	547	MET
1	A	595	ARG
1	A	606	TYR
1	A	607	LYS
1	A	612	ARG
1	A	656	ASP
1	A	660	GLN
1	A	695	ASP
1	A	699	TYR
1	A	740	GLN
1	B	324	ASN
1	B	337	ASN
1	B	344	ARG
1	B	432	ASP
1	B	473	ASP
1	B	476	LYS
1	B	488	SER
1	B	502	PHE
1	B	522	ASP
1	B	529	GLN
1	B	547	MET
1	B	557	GLU
1	B	581	CYS
1	B	606	TYR
1	B	612	ARG
1	B	614	ASP
1	B	623	VAL
1	B	643	ASP
1	B	645	TYR
1	B	651	LEU
1	B	689	THR
1	B	691	GLU
1	B	692	GLU

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Mol	Chain	Res	Type
1	B	774	LEU
1	C	324	ASN
1	C	405	GLU
1	C	424	ASP
1	C	436	TYR
1	C	473	ASP
1	C	502	PHE
1	C	522	ASP
1	C	529	GLN
1	C	554	PHE
1	C	561	PHE
1	C	614	ASP
1	C	625	ARG
1	C	656	ASP
1	C	658	LYS
1	C	660	GLN
1	C	701	LYS
1	D	337	ASN
1	D	381	SER
1	D	413	LEU
1	D	455	SER
1	D	458	MET
1	D	491	CYS
1	D	501	PHE
1	D	514	ARG
1	D	554	PHE
1	D	572	ASP
1	D	606	TYR
1	D	614	ASP
1	D	618	MET
1	D	628	THR
1	D	634	SER
1	D	656	ASP
1	D	662	ASN
1	D	668	PHE
1	D	670	TYR
1	D	676	TYR
1	D	701	LYS
1	D	739	PHE
1	D	759	PHE
1	D	765	LYS
1	D	778	PHE

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Mol	Chain	Res	Type
1	E	343	GLU
1	E	344	ARG
1	E	360	GLU
1	E	365	THR
1	E	406	THR
1	E	411	ASP
1	E	420	LEU
1	E	429	SER
1	E	458	MET
1	E	466	ASN
1	E	484	LYS
1	E	491	CYS
1	E	499	THR
1	E	501	PHE
1	E	502	PHE
1	E	513	LYS
1	E	547	MET
1	E	615	ASN
1	E	619	ARG
1	E	625	ARG
1	E	645	TYR
1	E	656	ASP
1	E	698	PHE
1	E	780	GLU
1	F	324	ASN
1	F	365	THR
1	F	377	LYS
1	F	435	LYS
1	F	480	GLU
1	F	499	THR
1	F	502	PHE
1	F	507	THR
1	F	547	MET
1	F	555	CYS
1	F	612	ARG
1	F	625	ARG
1	F	636	ARG
1	F	660	GLN
1	F	669	LEU
1	F	674	LYS
1	F	695	ASP
1	F	740	GLN

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Mol	Chain	Res	Type
1	F	759	PHE
1	F	765	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	761	ASN
1	C	761	ASN
1	D	629	HIS
1	E	761	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

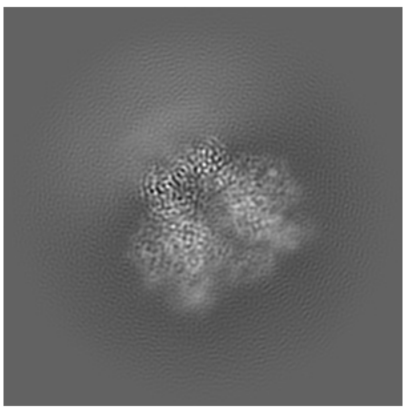
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37527. These allow visual inspection of the internal detail of the map and identification of artifacts.

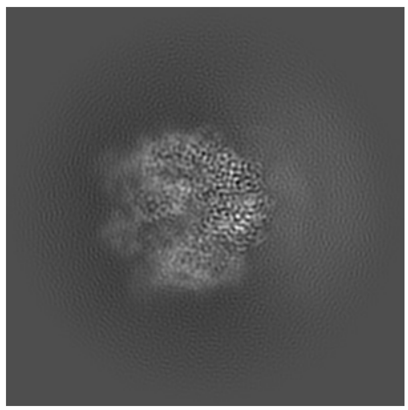
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

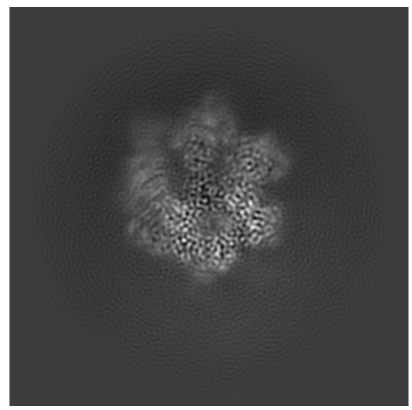
6.1.1 Primary map



X

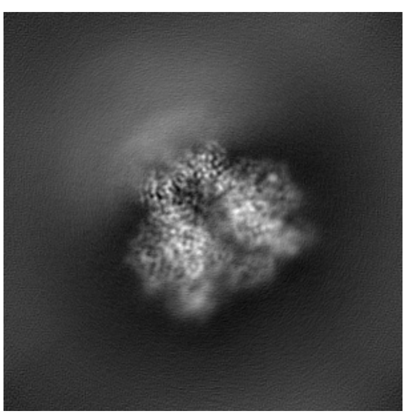


Y

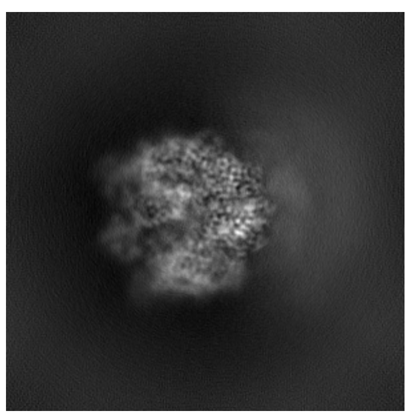


Z

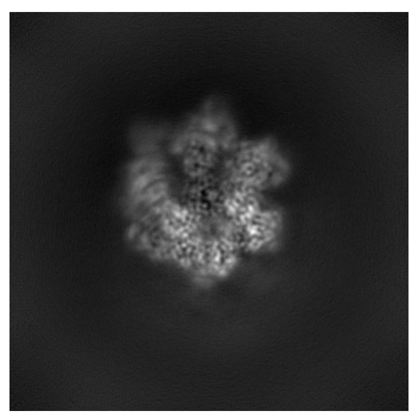
6.1.2 Raw map



X



Y

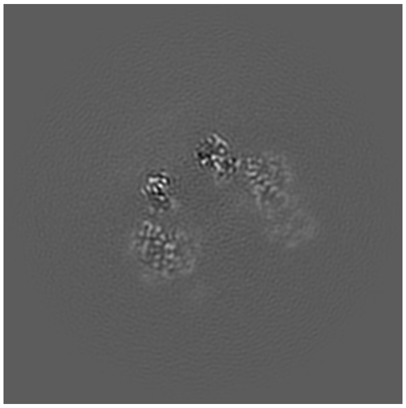


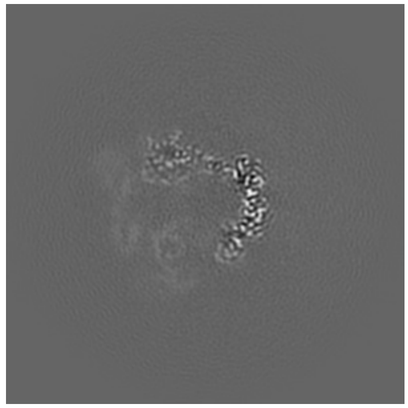
Z

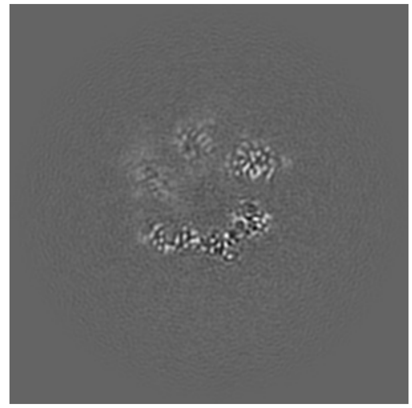
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

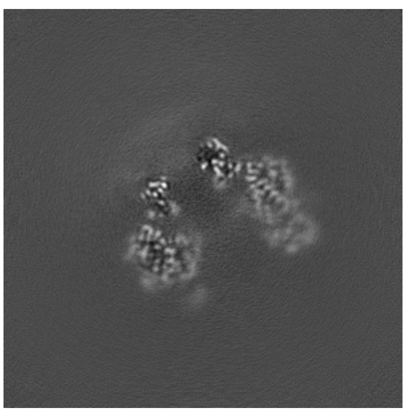
6.2.1 Primary map

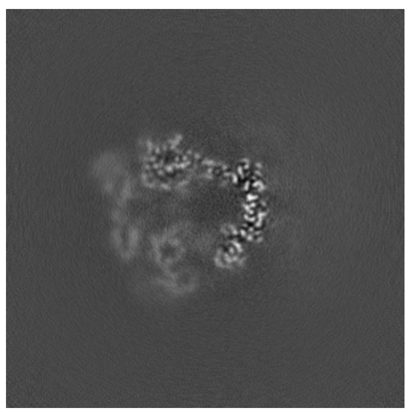

X Index: 160

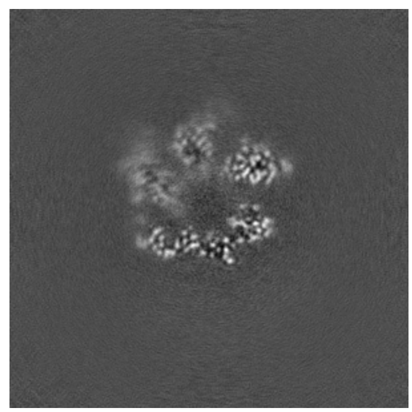

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

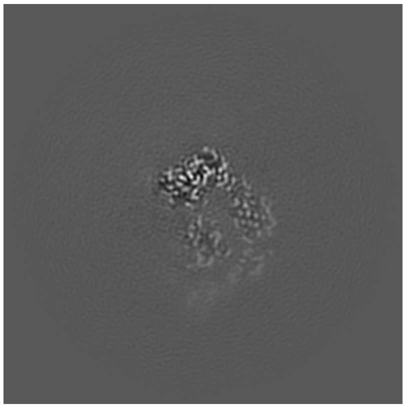

Y Index: 160


Z Index: 160

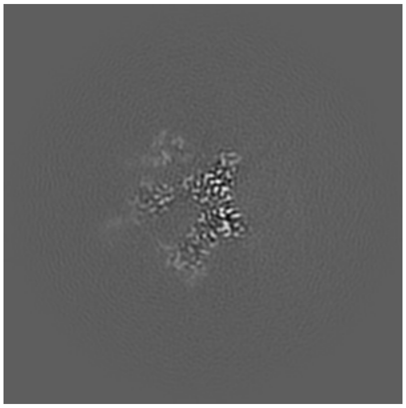
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

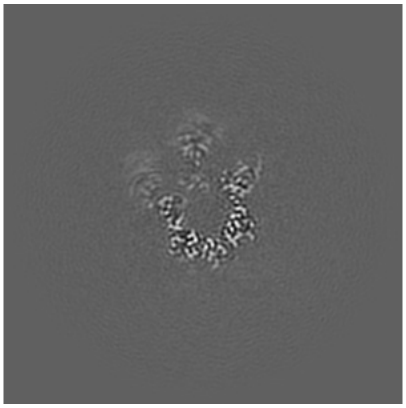
6.3.1 Primary map



X Index: 187

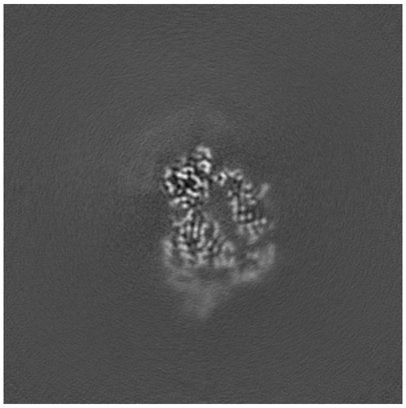


Y Index: 131

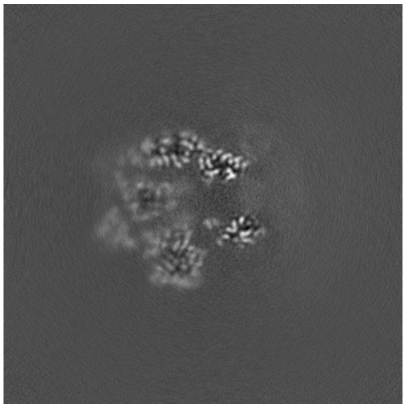


Z Index: 180

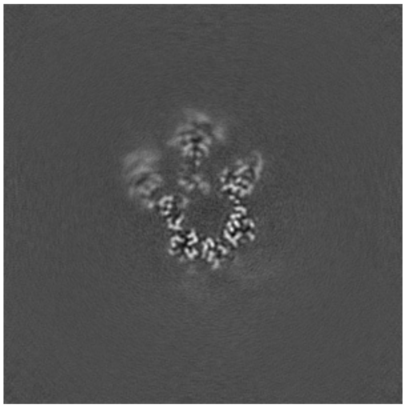
6.3.2 Raw map



X Index: 193



Y Index: 144

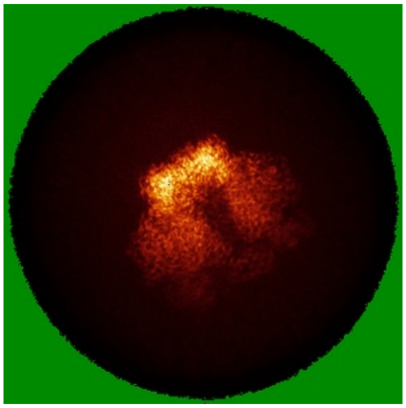


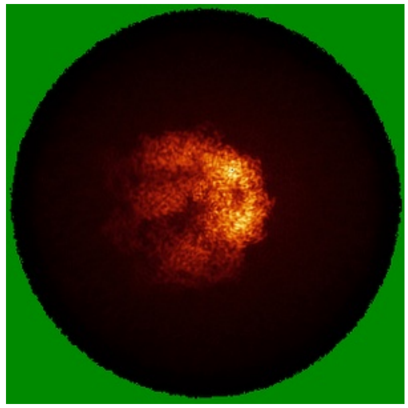
Z Index: 180

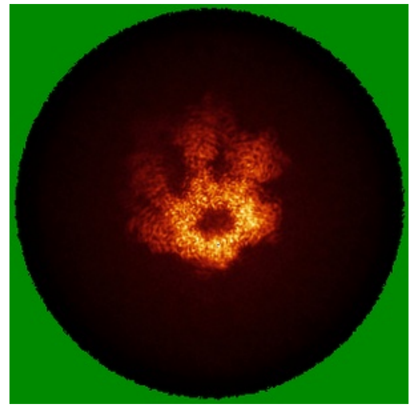
The images above show the largest variance slices of the map in three orthogonal directions.

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

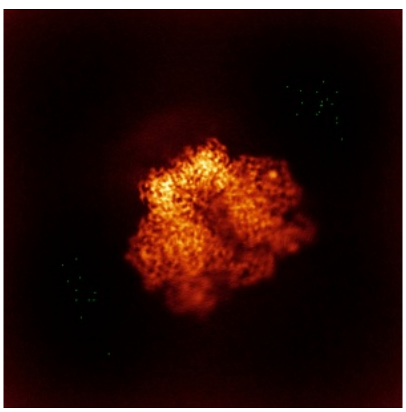
6.4.1 Primary map

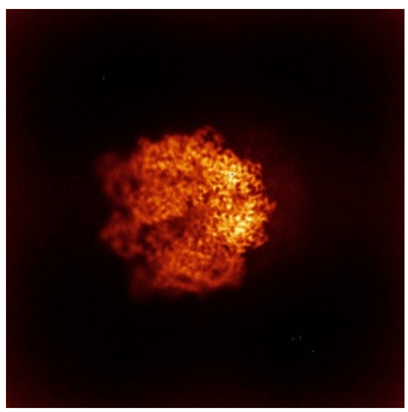

X

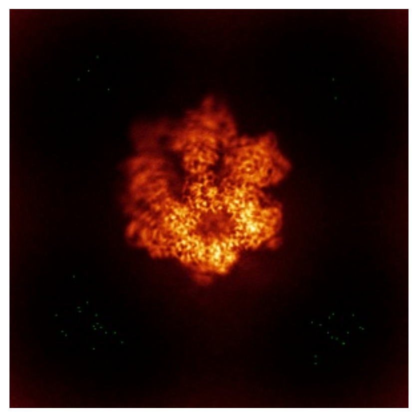

Y


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 0.1. 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.

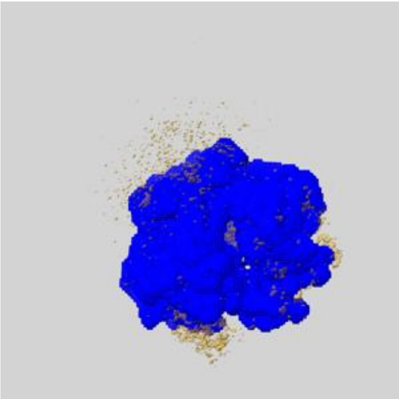
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

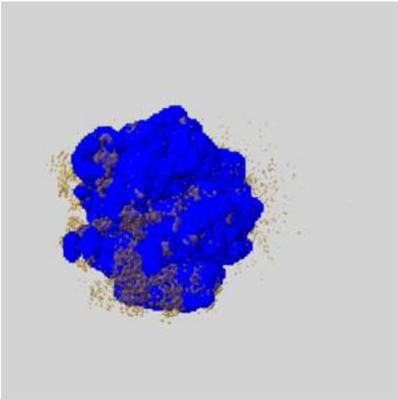
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

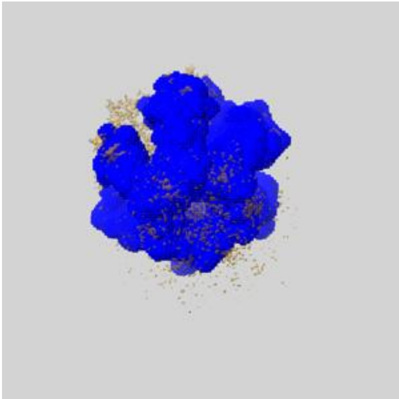
6.6.1 emd_37527_msk_1.map (i)



X



Y

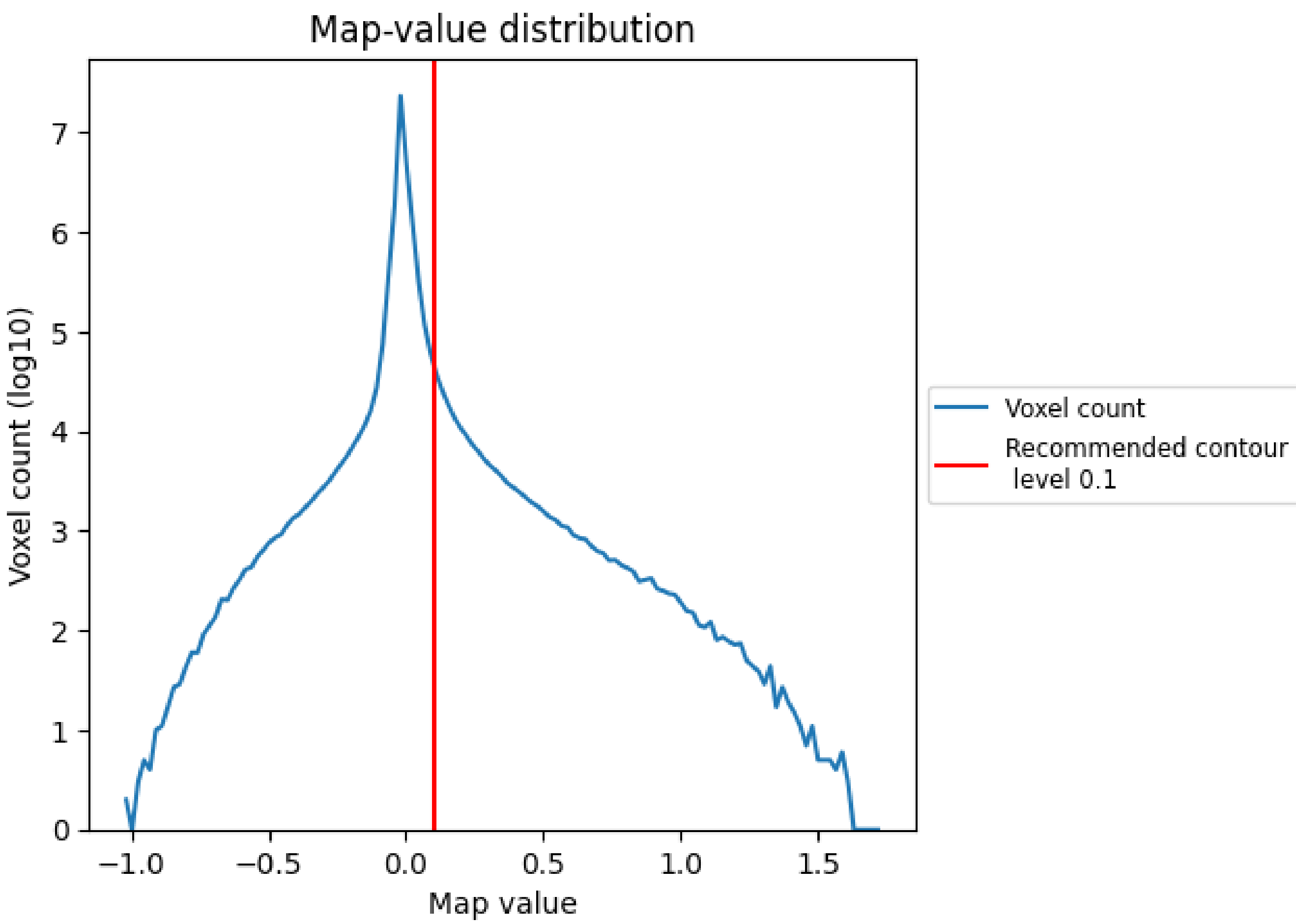


Z

7 Map analysis (i)

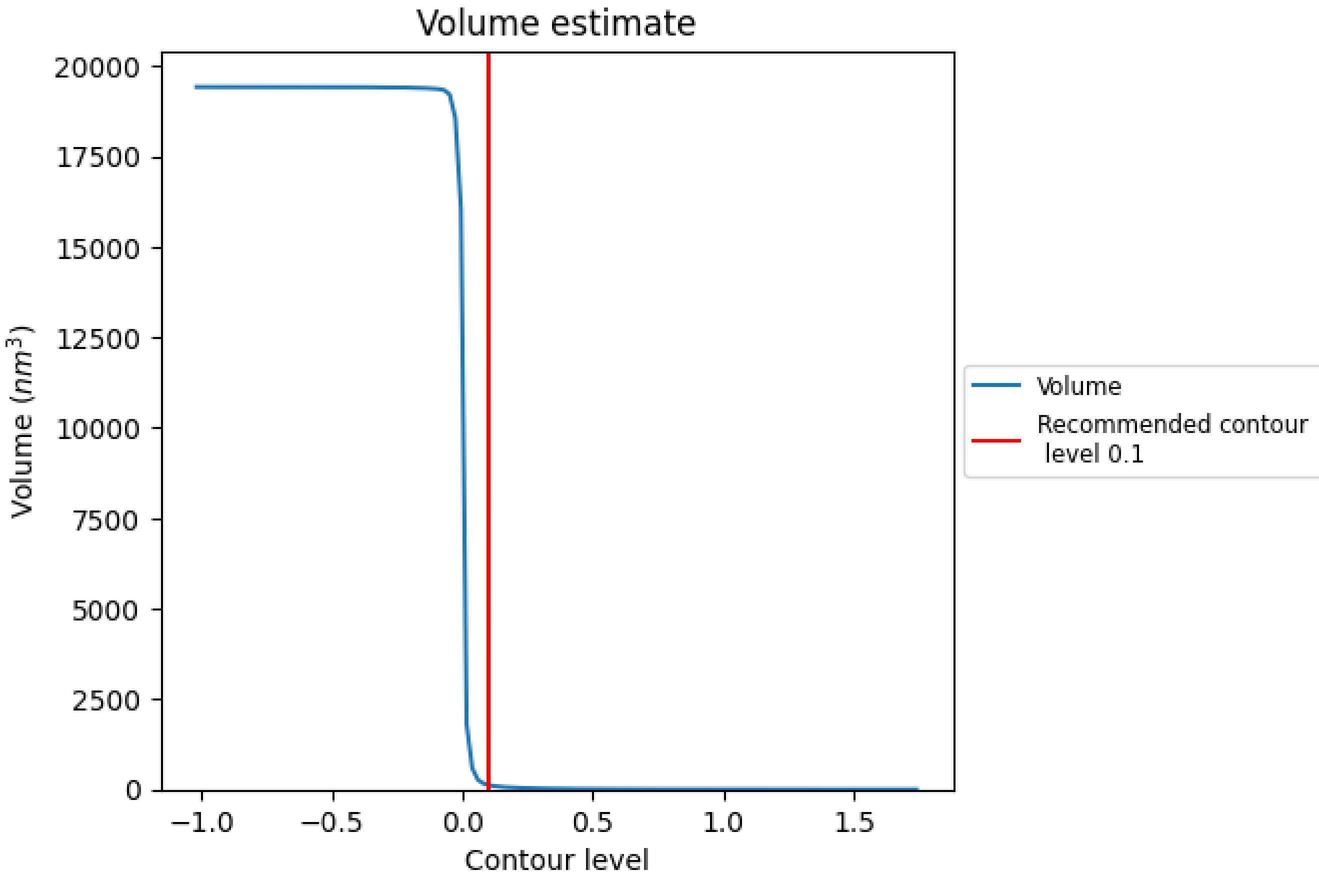
This section contains the results of statistical analysis of the map.

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.

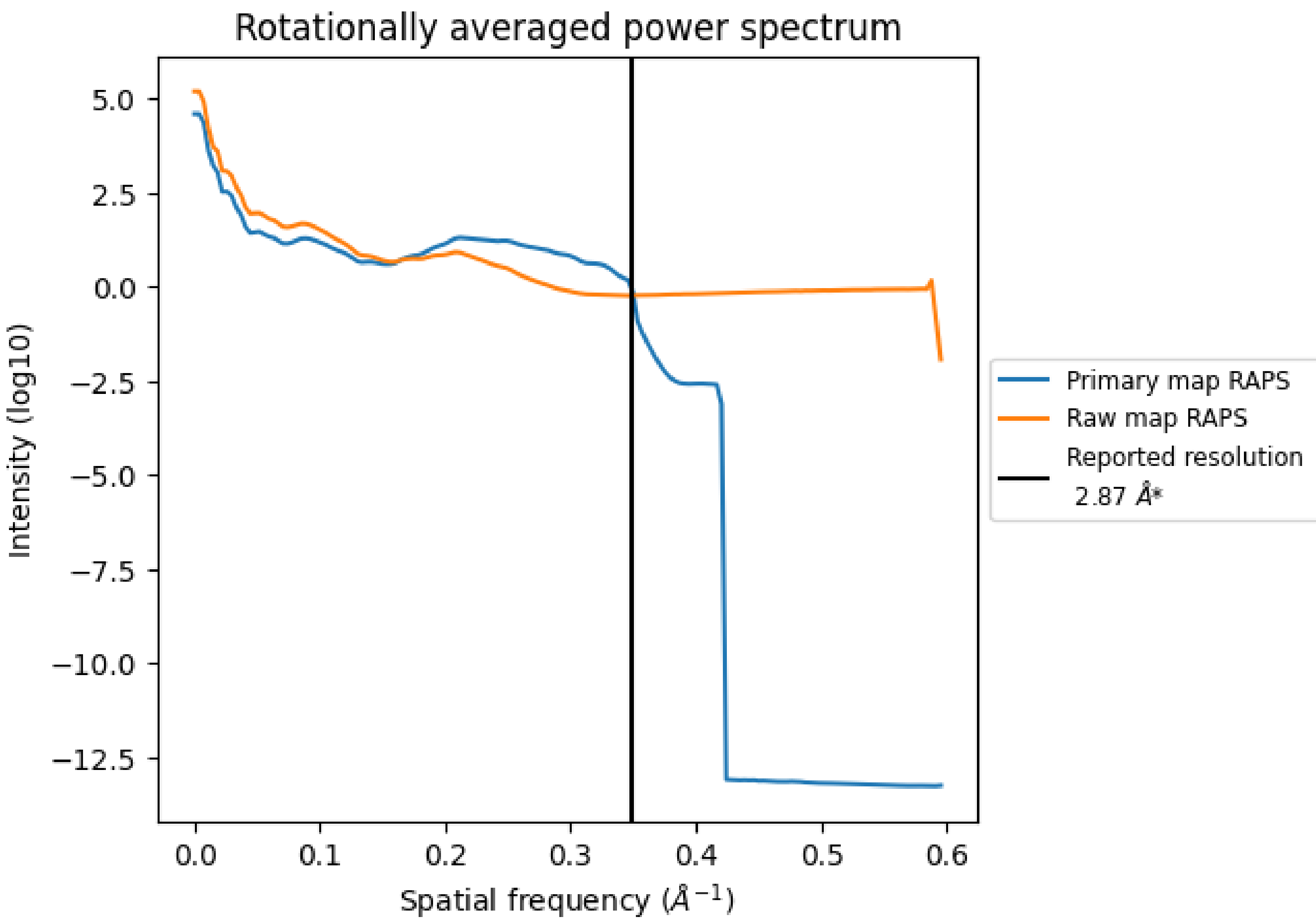
7.2 Volume estimate (i)



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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)

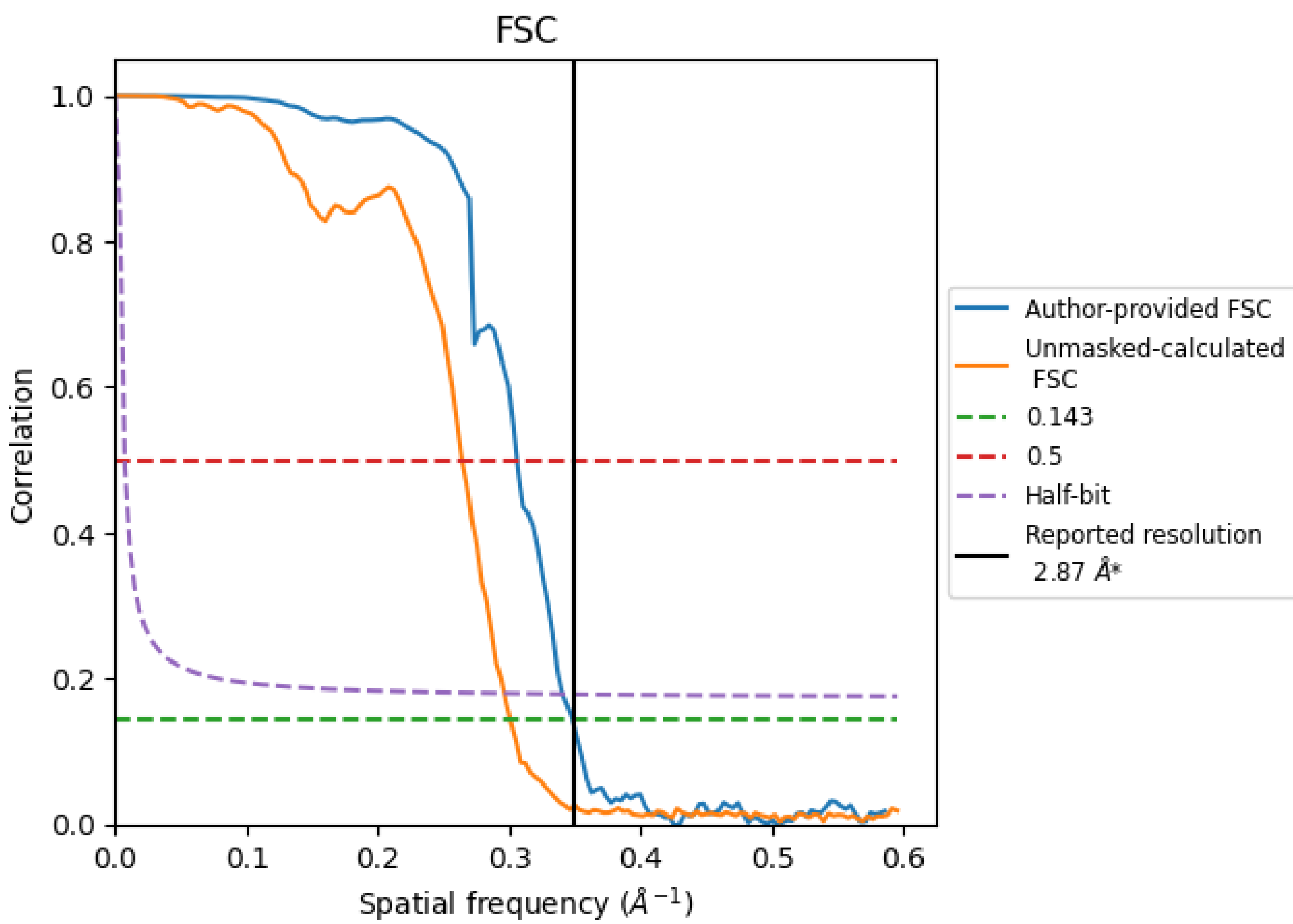


*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

8.2 Resolution estimates ⓘ

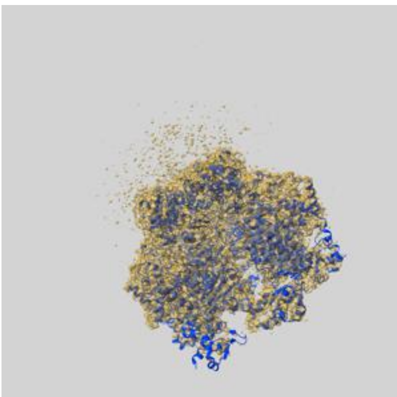
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.27	2.94
Unmasked-calculated*	3.32	3.79	3.37

*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 3.32 differs from the reported value 2.87 by more than 10 %

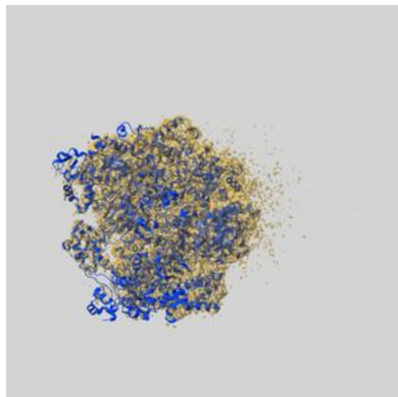
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37527 and PDB model 8WH3. Per-residue inclusion information can be found in section 3 on page 4.

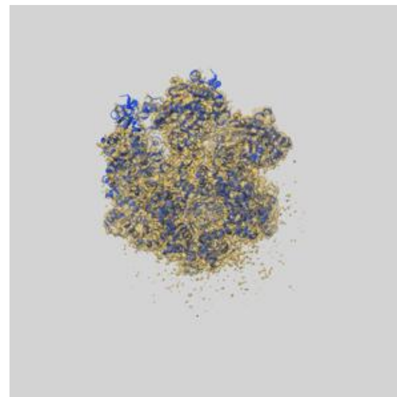
9.1 Map-model overlay (i)



X



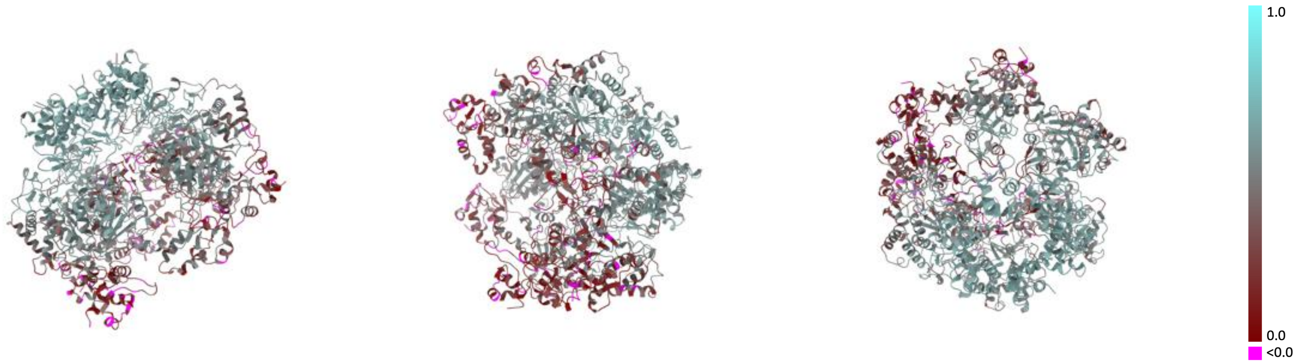
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

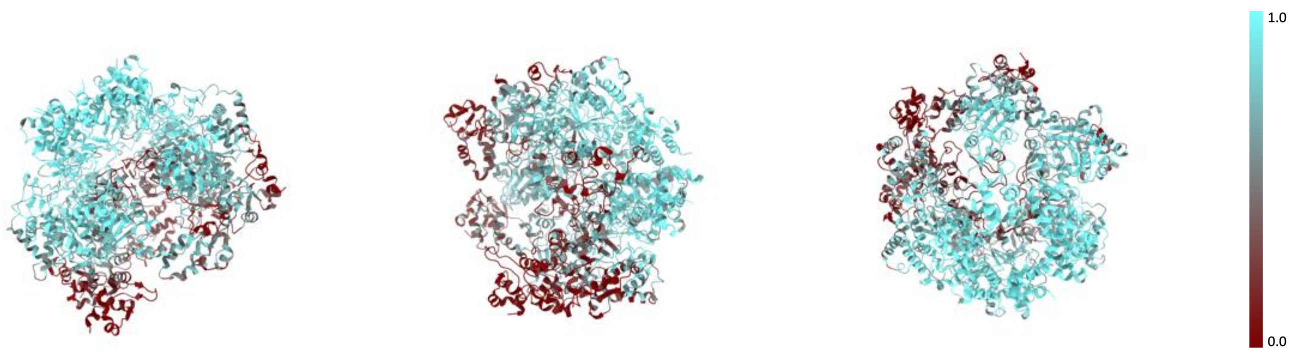
9.2 Q-score mapped to coordinate model (i)



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.

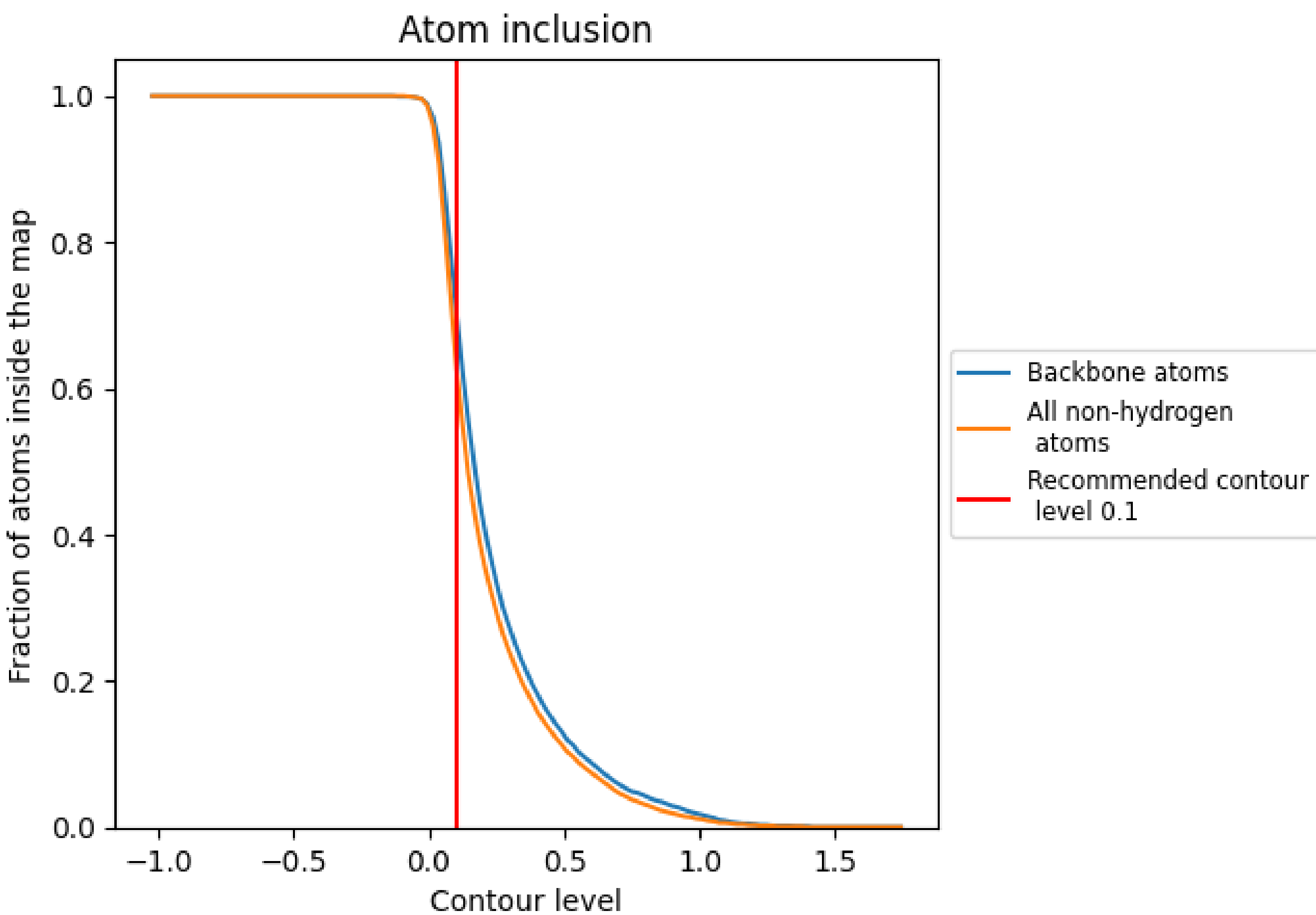
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.4250
A	0.7200	0.4720
B	0.6270	0.4160
C	0.7520	0.4920
D	0.4540	0.3260
E	0.6140	0.4150
F	0.6490	0.4310