Full wwPDB EM Validation Report

Sep 17, 2024 – 08:30 PM JST

PDB ID	:	8WH4
EMDB ID	:	EMD-37528
Title	:	MPOX E5 hexamer ssDNA bound apo conformation
Authors	:	Zhang, Z.; Dong, C.
Deposited on	:	2023-09-22
Resolution	:	3.03 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

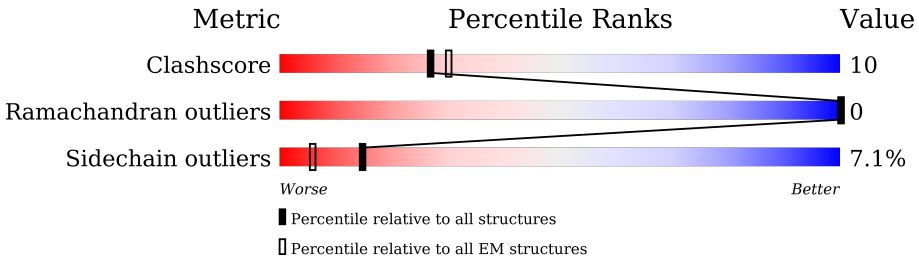
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.03 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	8% 42% 15% • 41%
1	B	785	7% 49% 10% • 41%
1	C	785	• 46% 12% • 41%
1	D	785	9% 44% 13% • 41%
1	E	785	16% 38% 19% • 41%
1	F	785	8% 42% 16% • 41%
2	T	4	100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22354 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
1	A	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		
1	B	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		
1	C	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		
1	D	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		
1	E	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		
1	F	463	Total	C	N	O	S	0	0
			3713	2378	628	691	16		

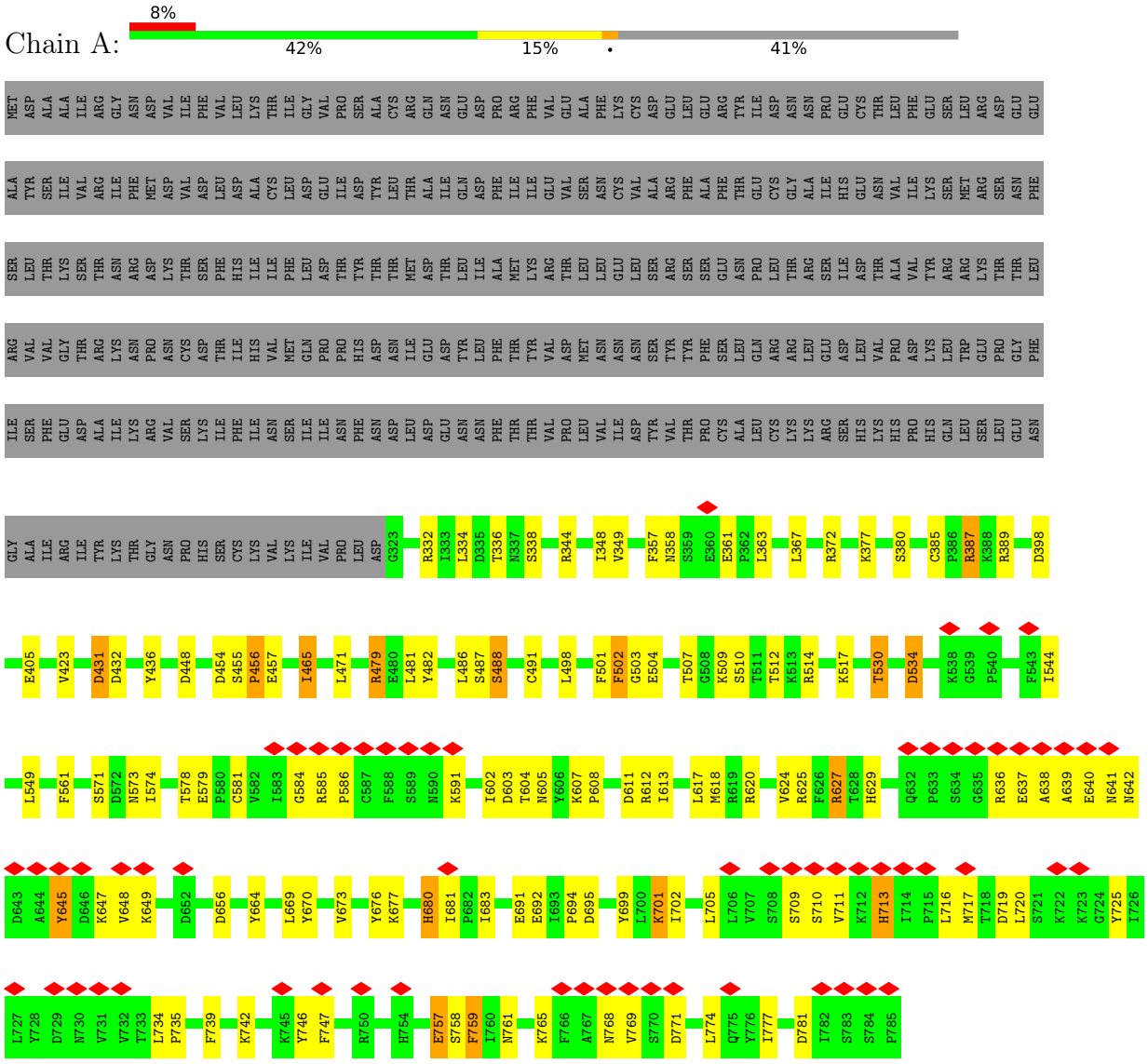
- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	4	Total	C	N	O	P	0	0
			76	36	12	24	4		

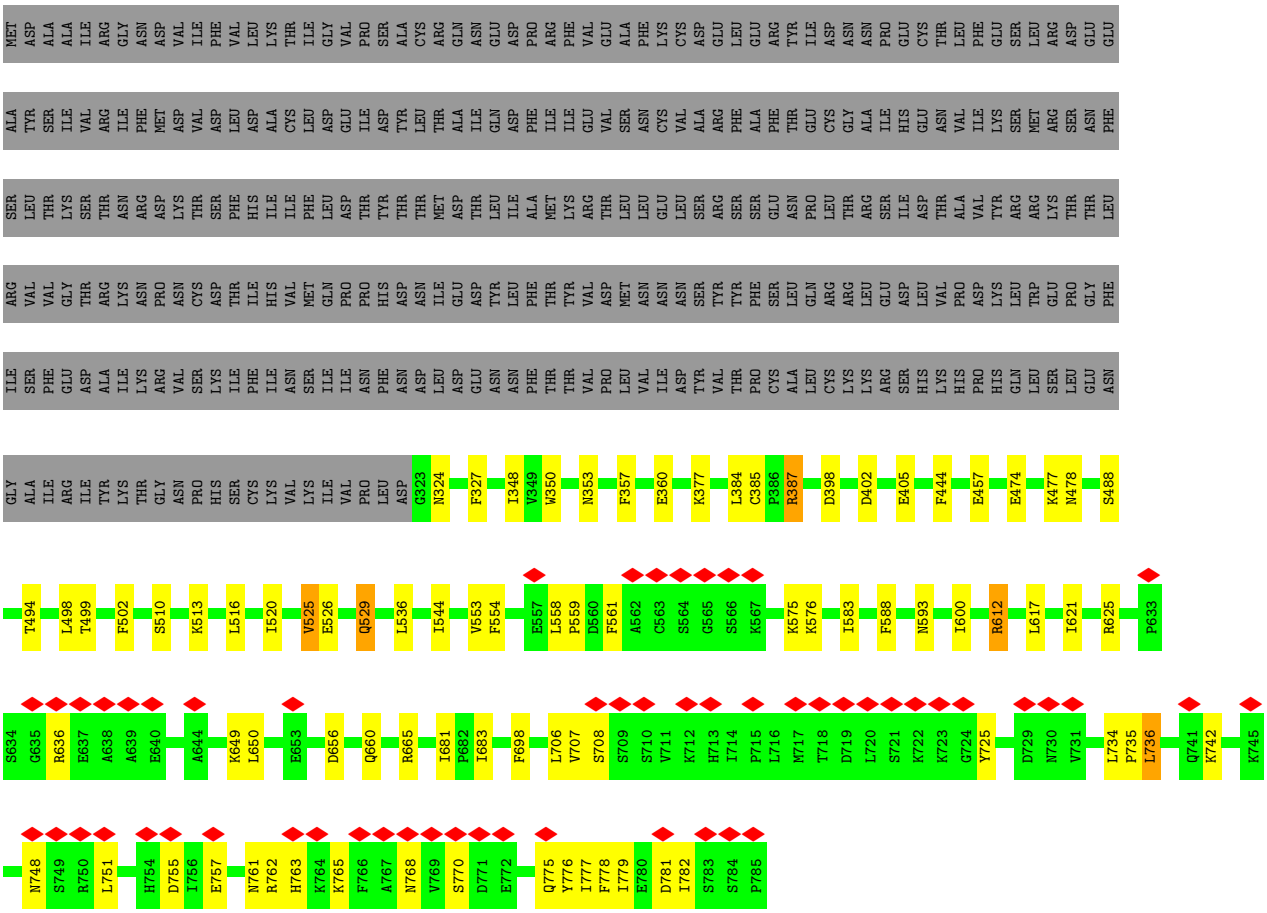
3 Residue-property plots (i)

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

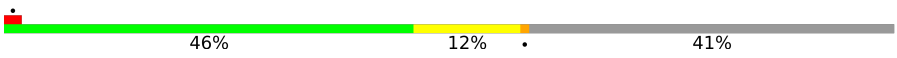


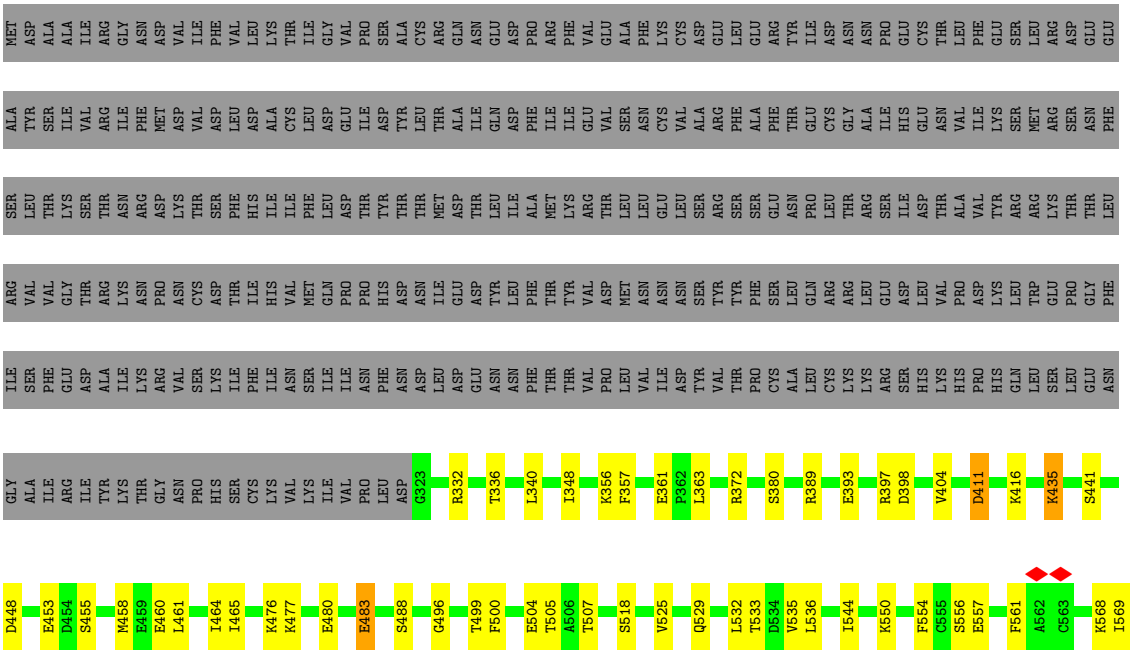
• Molecule 1: Uncoating factor OPG117

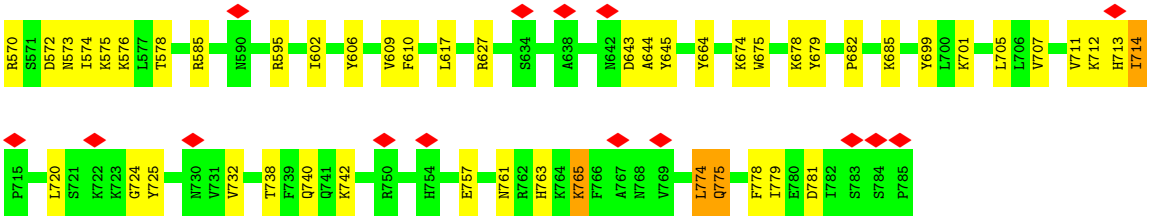


• Molecule 1: Uncoating factor OPG117

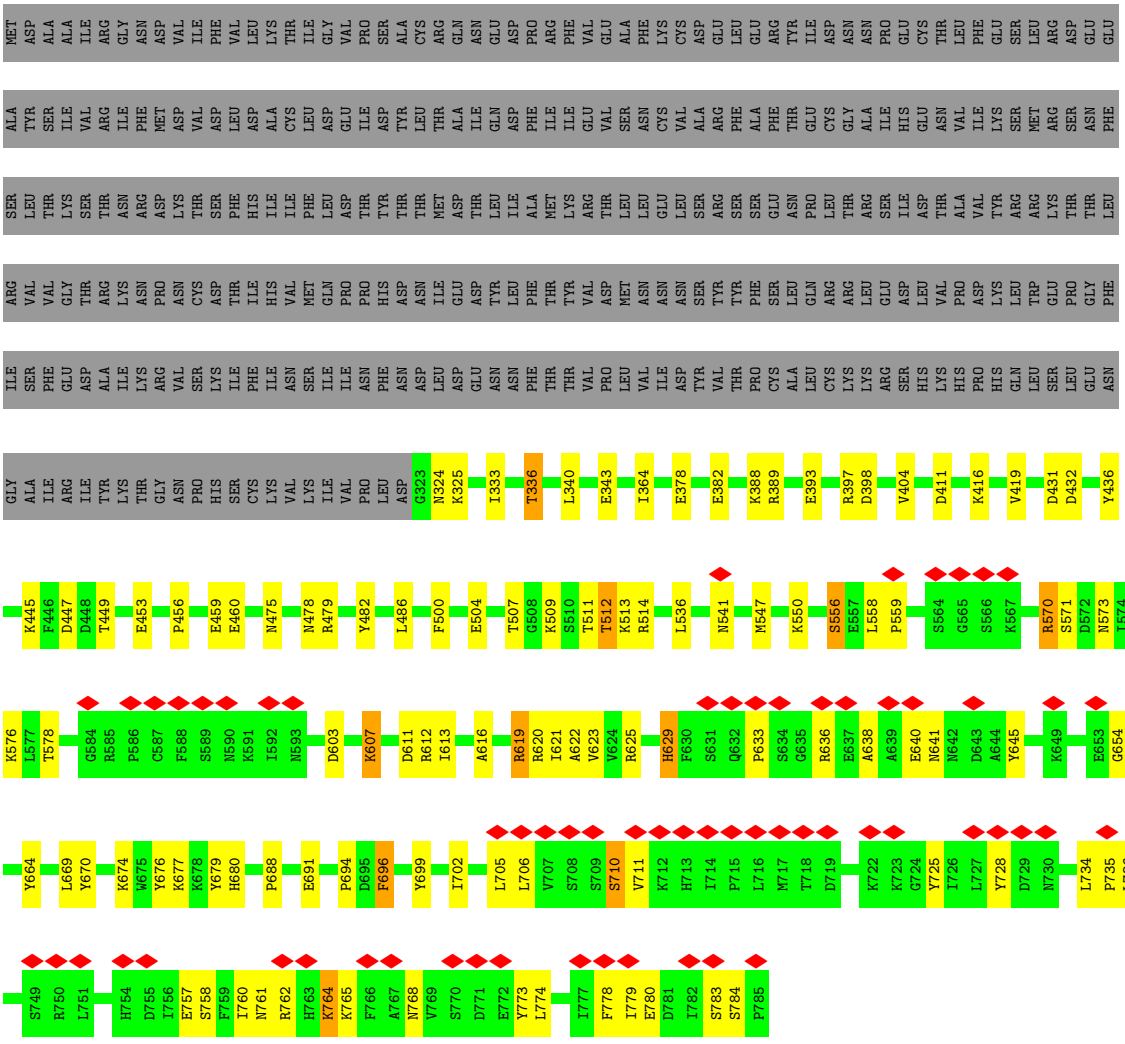
Chain C:



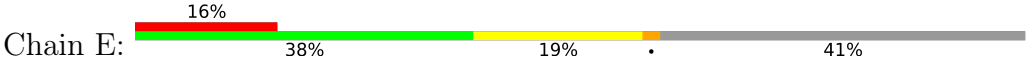


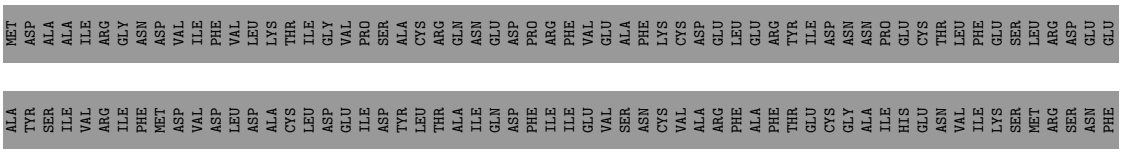


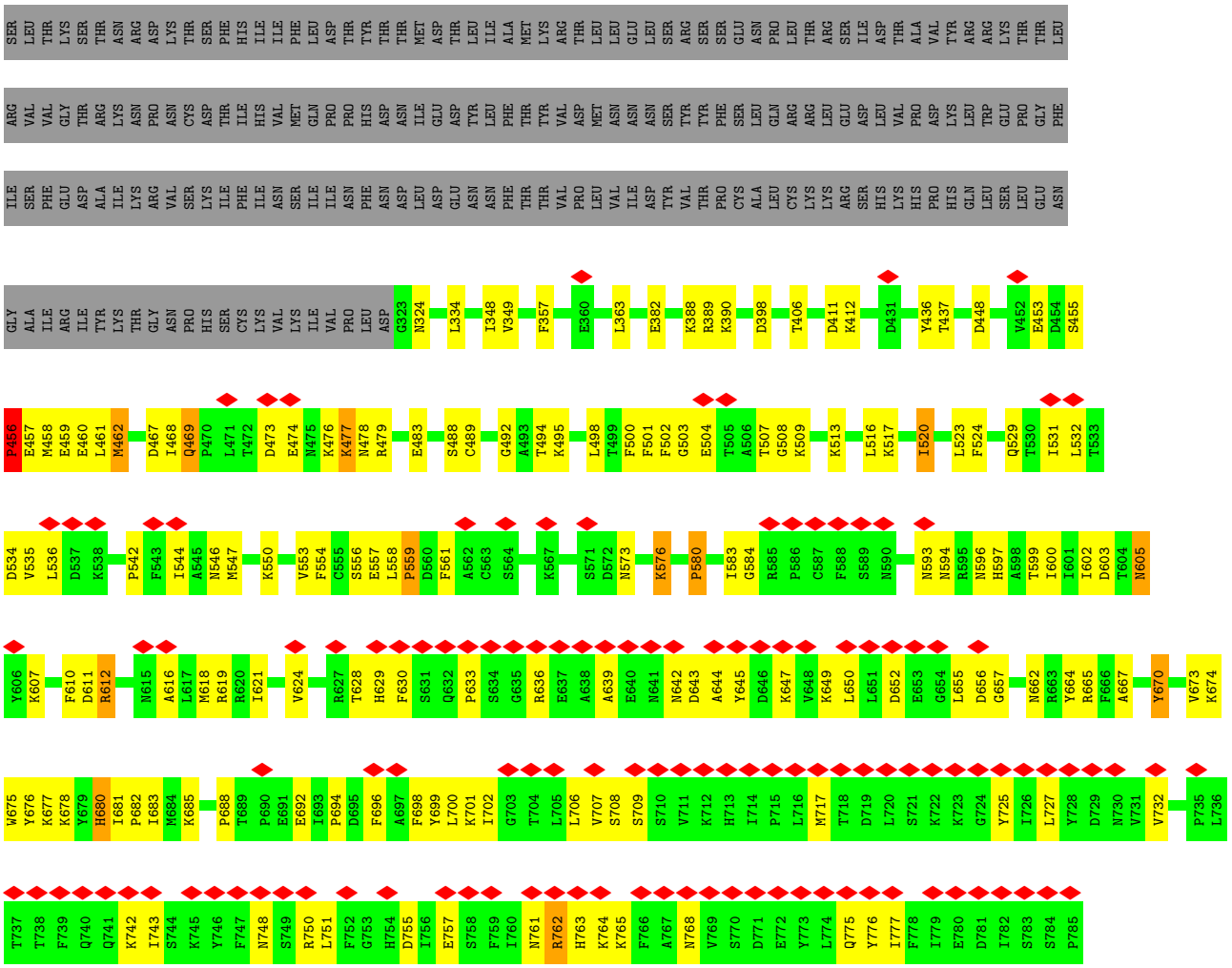
• Molecule 1: Uncoating factor OPG117



• Molecule 1: Uncoating factor OPG117

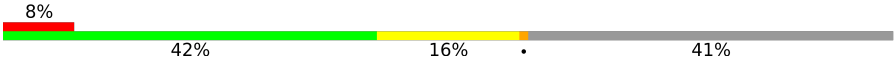


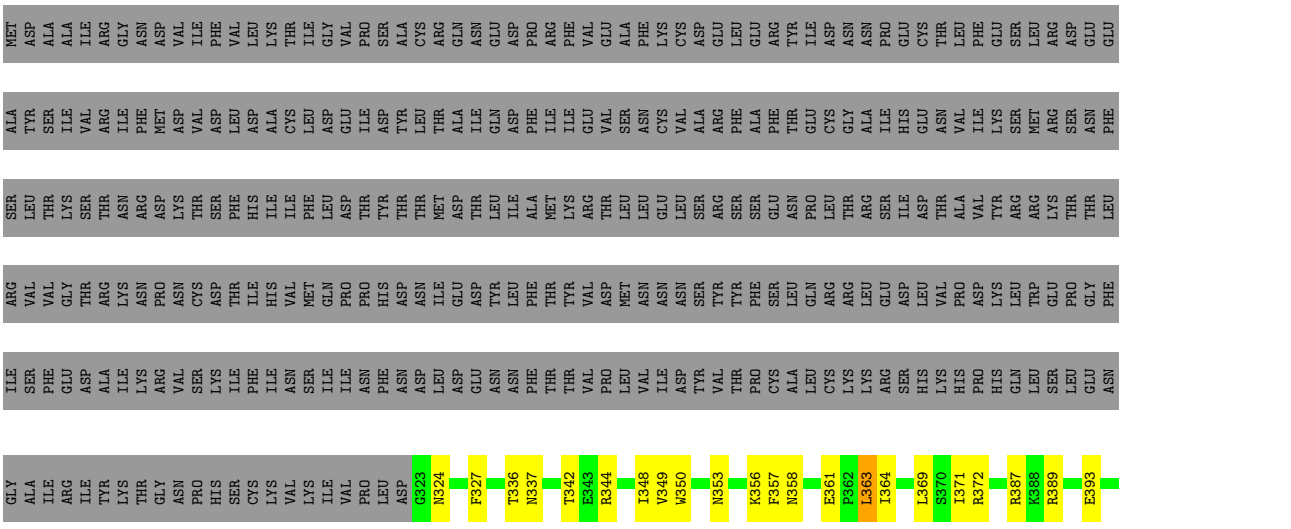


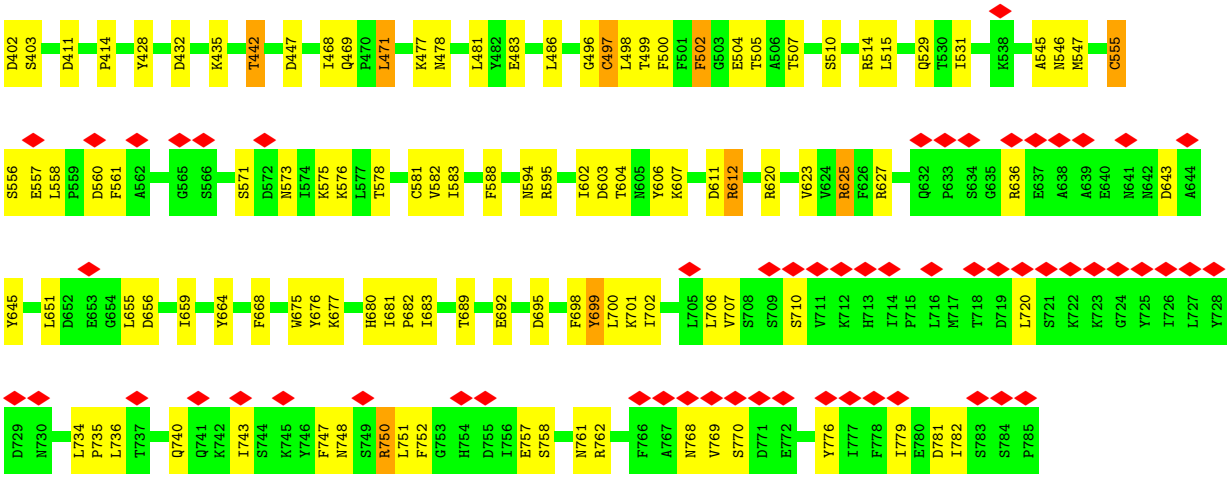


• Molecule 1: Uncoating factor OPG117

Chain F:

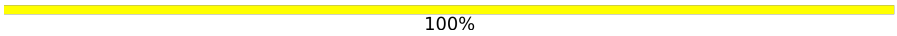






- Molecule 2: DNA (5'-D(P*CP*CP*CP*C)-3')

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263224	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 ($e^-/Å^2$)	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	1.406	Depositor
Minimum map value	-0.865	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.06	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	0.38	2/3793 (0.1%)	0.60	4/5128 (0.1%)
1	B	0.26	0/3793	0.48	0/5128
1	C	0.28	0/3793	0.55	3/5128 (0.1%)
1	D	0.26	0/3793	0.48	0/5128
1	E	0.52	4/3793 (0.1%)	0.85	14/5128 (0.3%)
1	F	0.26	0/3793	0.49	0/5128
2	T	0.63	0/83	0.96	0/124
All	All	0.34	6/22841 (0.0%)	0.59	21/30892 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	559	PRO	CG-CD	-19.89	0.85	1.50
1	A	456	PRO	CG-CD	-15.65	0.99	1.50
1	E	559	PRO	CB-CG	11.83	2.09	1.50
1	E	456	PRO	CG-CD	-8.51	1.22	1.50
1	A	456	PRO	N-CD	7.14	1.57	1.47
1	E	694	PRO	CG-CD	-6.70	1.28	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	559	PRO	N-CD-CG	-24.57	66.34	103.20
1	E	559	PRO	CA-CB-CG	-19.70	66.56	104.00
1	A	456	PRO	N-CD-CG	-17.10	77.55	103.20
1	E	694	PRO	CA-N-CD	-13.49	92.62	111.50
1	E	559	PRO	N-CA-CB	-13.37	87.25	103.30
1	E	456	PRO	N-CD-CG	-13.01	83.69	103.20
1	C	682	PRO	CA-N-CD	-12.23	94.37	111.50
1	A	456	PRO	CA-N-CD	-11.26	95.73	111.50
1	E	456	PRO	CA-CB-CG	-10.58	83.90	104.00
1	A	456	PRO	CA-CB-CG	-10.44	84.16	104.00
1	E	580	PRO	CA-N-CD	-9.94	97.59	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	559	PRO	CB-CG-CD	-9.59	69.11	106.50
1	E	694	PRO	N-CD-CG	-9.53	88.91	103.20
1	E	559	PRO	CA-N-CD	-8.12	100.14	111.50
1	C	682	PRO	N-CD-CG	-7.90	91.35	103.20
1	E	688	PRO	N-CD-CG	-7.85	91.42	103.20
1	E	456	PRO	N-CA-CB	-7.43	94.38	103.30
1	E	688	PRO	CA-N-CD	-6.35	102.61	111.50
1	E	694	PRO	CA-CB-CG	-5.55	93.45	104.00
1	C	572	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	456	PRO	CB-CG-CD	5.13	126.50	106.50

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	106	0
1	B	3713	0	3706	41	0
1	C	3713	0	3706	52	0
1	D	3713	0	3706	83	0
1	E	3713	0	3706	106	0
1	F	3713	0	3706	80	0
2	T	76	0	45	4	0
All	All	22354	0	22281	432	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 10.

All (432) 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:E:456:PRO:HG2	1:E:457:GLU:H	1.43	0.81
1:E:456:PRO:HG2	1:E:457:GLU:N	1.94	0.80
1:B:575:LYS:HE3	1:C:557:GLU:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:GLU:HG3	1:D:664:TYR:HE1	1.50	0.75
1:E:456:PRO:HA	1:E:459:GLU:HG2	1.67	0.74
1:E:534:ASP:O	1:E:573:ASN:ND2	2.23	0.72
1:F:531:ILE:O	1:F:573:ASN:ND2	2.22	0.72
1:A:710:SER:OG	1:E:639:ALA:O	2.08	0.70
1:A:647:LYS:HE2	1:A:649:LYS:HE3	1.74	0.70
1:C:724:GLY:HA3	1:C:738:THR:HG21	1.74	0.69
1:D:728:TYR:HD2	1:D:765:LYS:HE3	1.57	0.69
1:E:556:SER:HA	1:E:603:ASP:HB3	1.74	0.69
1:D:478:ASN:ND2	1:D:625:ARG:O	2.26	0.69
1:A:642:ASN:HB2	1:C:713:HIS:H	1.58	0.68
1:E:504:GLU:O	1:E:509:LYS:NZ	2.25	0.68
1:A:642:ASN:HA	1:C:714:ILE:HG13	1.75	0.68
1:A:713:HIS:HB2	1:E:643:ASP:HA	1.76	0.68
1:A:768:ASN:OD1	1:A:771:ASP:N	2.27	0.68
1:A:498:LEU:HD23	1:A:602:ILE:HD11	1.76	0.67
1:A:680:HIS:O	1:A:680:HIS:ND1	2.26	0.67
1:A:385:CYS:SG	1:A:387:ARG:NH2	2.66	0.67
1:A:713:HIS:HD2	1:A:716:LEU:HD21	1.58	0.67
1:B:385:CYS:SG	1:B:387:ARG:NH2	2.66	0.66
1:F:324:ASN:HD22	1:F:327:PHE:HB2	1.60	0.66
1:F:432:ASP:HA	1:F:435:LYS:HE3	1.78	0.65
1:C:536:LEU:HD12	1:C:576:LYS:HG2	1.79	0.65
1:E:536:LEU:HD22	1:E:544:ILE:HD13	1.77	0.65
1:D:514:ARG:HG3	1:D:659:ILE:HG21	1.77	0.65
1:D:661:ASN:O	1:D:661:ASN:ND2	2.30	0.65
1:C:348:ILE:HG22	1:C:357:PHE:HB3	1.80	0.65
1:E:748:ASN:HB3	1:E:751:LEU:HB2	1.80	0.64
1:D:398:ASP:OD2	1:F:389:ARG:NH2	2.27	0.64
1:D:613:ILE:O	1:D:762:ARG:NH1	2.26	0.64
1:D:633:PRO:HA	1:D:636:ARG:HG3	1.79	0.64
1:E:502:PHE:N	1:E:624:VAL:O	2.30	0.64
1:D:734:LEU:HD12	1:D:735:PRO:HD2	1.80	0.63
1:E:498:LEU:HD23	1:E:602:ILE:HD11	1.79	0.63
1:F:558:LEU:HG	1:F:604:THR:HG23	1.80	0.63
1:A:481:LEU:HD12	1:A:624:VAL:HG22	1.80	0.63
1:F:768:ASN:ND2	1:F:770:SER:OG	2.29	0.63
1:A:349:VAL:HG21	1:A:363:LEU:HB2	1.80	0.63
1:B:777:ILE:HB	1:B:782:ILE:HD11	1.81	0.63
1:E:455:SER:OG	1:E:457:GLU:OE1	2.16	0.62
1:E:494:THR:HG21	1:E:580:PRO:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ARG:HD2	1:A:627:ARG:HD3	1.81	0.62
1:E:652:ASP:HB3	1:E:655:LEU:HB2	1.80	0.62
1:E:698:PHE:HZ	1:E:743:ILE:HD11	1.65	0.62
1:A:504:GLU:O	1:A:509:LYS:NZ	2.33	0.62
1:C:765:LYS:HE2	1:C:775:GLN:HG3	1.82	0.62
1:A:641:ASN:N	1:C:711:VAL:O	2.32	0.62
1:B:478:ASN:ND2	1:B:625:ARG:O	2.28	0.62
1:C:507:THR:HG23	1:C:645:TYR:HE2	1.65	0.61
1:F:625:ARG:NH1	1:F:692:GLU:OE2	2.33	0.61
1:A:765:LYS:HD3	1:A:774:LEU:HA	1.82	0.61
1:D:504:GLU:HG2	1:D:507:THR:HG21	1.82	0.61
1:D:556:SER:HA	1:D:603:ASP:HB3	1.82	0.61
1:C:460:GLU:O	1:C:464:ILE:HG13	2.01	0.61
1:E:607:LYS:NZ	1:E:692:GLU:O	2.33	0.60
1:C:500:PHE:HD1	1:C:602:ILE:HB	1.66	0.60
1:D:616:ALA:HA	1:D:619:ARG:HH21	1.66	0.60
1:E:349:VAL:HG21	1:E:363:LEU:HB2	1.82	0.60
1:C:742:LYS:NZ	1:C:781:ASP:OD1	2.35	0.60
1:F:677:LYS:O	1:F:680:HIS:ND1	2.35	0.60
1:E:382:GLU:HG3	1:E:388:LYS:HD3	1.84	0.60
1:A:534:ASP:O	1:A:573:ASN:ND2	2.29	0.60
1:D:710:SER:OG	1:D:711:VAL:N	2.35	0.60
1:B:768:ASN:ND2	1:B:770:SER:OG	2.35	0.59
1:D:459:GLU:N	1:D:459:GLU:OE1	2.32	0.59
1:D:779:ILE:O	1:D:783:SER:N	2.27	0.59
1:F:604:THR:HG22	1:F:606:TYR:H	1.68	0.59
1:A:642:ASN:HB3	1:C:711:VAL:HA	1.83	0.59
1:B:765:LYS:HD3	1:B:775:GLN:HG3	1.82	0.59
1:D:504:GLU:HG3	1:D:645:TYR:HE1	1.66	0.59
1:D:578:THR:HG21	1:D:620:ARG:HE	1.68	0.59
1:D:705:LEU:HA	1:D:779:ILE:HB	1.84	0.59
1:D:504:GLU:O	1:D:507:THR:OG1	2.18	0.58
1:F:510:SER:OG	1:F:514:ARG:NH2	2.33	0.58
1:A:504:GLU:HG2	1:A:645:TYR:CE1	2.38	0.58
1:E:500:PHE:HE1	1:E:621:ILE:HG23	1.68	0.58
1:E:553:VAL:HB	1:E:600:ILE:HD13	1.86	0.57
1:A:702:ILE:HA	1:A:705:LEU:HB2	1.85	0.57
1:A:768:ASN:HB3	1:E:751:LEU:HA	1.86	0.57
1:D:760:ILE:HA	1:D:774:LEU:HD21	1.85	0.57
1:E:709:SER:H	1:E:775:GLN:HB3	1.70	0.57
1:F:545:ALA:HA	1:F:594:ASN:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LYS:NZ	1:A:694:PRO:HD2	2.20	0.57
1:B:742:LYS:NZ	1:B:781:ASP:OD1	2.38	0.57
1:E:677:LYS:HA	1:E:680:HIS:HB2	1.86	0.57
1:A:709:SER:HB2	1:E:644:ALA:H	1.70	0.56
1:A:454:ASP:OD1	1:A:454:ASP:N	2.38	0.56
1:F:702:ILE:HB	1:F:706:LEU:HD12	1.86	0.56
1:F:414:PRO:O	1:F:442:THR:OG1	2.23	0.56
1:A:389:ARG:NH2	1:C:398:ASP:OD2	2.35	0.56
1:C:535:VAL:HG13	1:C:570:ARG:HH22	1.70	0.56
1:E:584:GLY:O	1:E:594:ASN:ND2	2.32	0.56
1:D:622:ALA:HB2	1:D:688:PRO:HA	1.87	0.56
1:E:469:GLN:OE1	1:E:478:ASN:ND2	2.39	0.55
1:F:342:THR:HG22	1:F:344:ARG:H	1.71	0.55
1:A:471:LEU:HD21	1:A:479:ARG:HH21	1.71	0.55
1:A:702:ILE:HG12	1:A:759:PHE:CE2	2.42	0.55
1:D:419:VAL:HG21	1:D:436:TYR:CD2	2.42	0.55
1:B:398:ASP:OD2	1:C:389:ARG:NH2	2.39	0.55
1:D:636:ARG:NH2	1:D:640:GLU:OE1	2.40	0.55
1:E:696:PHE:O	1:E:700:LEU:N	2.26	0.54
1:D:536:LEU:O	1:D:541:ASN:ND2	2.35	0.54
1:A:713:HIS:CE1	1:E:642:ASN:HA	2.42	0.54
1:D:419:VAL:HG21	1:D:436:TYR:HD2	1.73	0.54
1:F:707:VAL:HG13	1:F:782:ILE:HD12	1.89	0.54
1:D:340:LEU:HD13	1:D:404:VAL:HG21	1.89	0.54
1:D:676:TYR:O	1:D:680:HIS:N	2.41	0.54
1:A:456:PRO:HD2	1:A:457:GLU:H	1.72	0.53
1:C:568:LYS:HG2	1:C:609:VAL:HG12	1.89	0.53
1:D:765:LYS:N	1:D:773:TYR:O	2.40	0.53
1:D:536:LEU:HD12	1:D:576:LYS:HD2	1.90	0.53
1:A:571:SER:OG	1:A:612:ARG:O	2.23	0.53
1:C:525:VAL:HG21	1:C:550:LYS:HG3	1.89	0.53
1:C:361:GLU:HG3	1:C:361:GLU:O	2.08	0.53
1:D:702:ILE:HA	1:D:705:LEU:HB2	1.89	0.53
1:E:459:GLU:HA	1:E:462:MET:SD	2.48	0.53
1:E:529:GLN:NE2	1:E:557:GLU:O	2.40	0.53
1:A:629:HIS:HB2	1:A:648:VAL:HA	1.91	0.53
1:D:382:GLU:HG3	1:D:388:LYS:HD3	1.90	0.53
1:D:482:TYR:HH	1:D:512:THR:HG1	1.55	0.53
1:A:607:LYS:HE2	1:A:607:LYS:HA	1.91	0.53
1:E:630:PHE:HD1	1:E:649:LYS:HB2	1.74	0.53
1:A:742:LYS:NZ	1:A:781:ASP:OD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:OE2	1:D:397:ARG:NH1	2.42	0.53
1:F:504:GLU:HG3	1:F:645:TYR:HE1	1.74	0.53
1:E:681:ILE:O	1:E:683:ILE:N	2.42	0.53
1:D:325:LYS:NZ	1:D:378:GLU:O	2.40	0.52
1:F:348:ILE:HG22	1:F:357:PHE:HB3	1.92	0.52
1:F:502:PHE:HD1	1:F:607:LYS:HZ3	1.55	0.52
1:A:757:GLU:O	1:A:761:ASN:ND2	2.41	0.52
1:D:706:LEU:HD23	1:D:778:PHE:HA	1.90	0.52
1:C:411:ASP:OD1	1:C:411:ASP:N	2.37	0.52
1:F:336:THR:HG21	1:F:371:ILE:HD11	1.92	0.52
1:C:340:LEU:HD13	1:C:404:VAL:HG21	1.90	0.52
1:D:570:ARG:NH2	1:D:573:ASN:OD1	2.41	0.52
1:A:734:LEU:HD12	1:A:735:PRO:HD2	1.92	0.52
1:C:505:THR:O	1:C:645:TYR:OH	2.28	0.52
1:D:696:PHE:CD1	1:D:699:TYR:HB2	2.45	0.52
1:E:513:LYS:HG3	1:E:554:PHE:CD2	2.45	0.52
1:A:710:SER:HB3	1:E:642:ASN:HB3	1.91	0.51
1:D:677:LYS:O	1:D:680:HIS:ND1	2.41	0.51
1:E:670:TYR:O	1:E:674:LYS:HG2	2.10	0.51
1:E:732:VAL:HB	1:E:777:ILE:HD11	1.92	0.51
1:E:656:ASP:OD2	1:E:657:GLY:N	2.43	0.51
1:C:532:LEU:HB3	1:C:569:ILE:HG23	1.93	0.51
1:D:504:GLU:O	1:D:509:LYS:NZ	2.44	0.51
1:E:467:ASP:OD1	1:E:647:LYS:NZ	2.44	0.51
1:E:701:LYS:HZ1	1:E:706:LEU:HD12	1.76	0.51
1:F:758:SER:O	1:F:762:ARG:HB2	2.10	0.51
1:A:611:ASP:OD1	1:A:612:ARG:HG3	2.10	0.51
1:D:504:GLU:N	1:D:504:GLU:OE1	2.44	0.51
1:D:780:GLU:O	1:D:784:SER:OG	2.22	0.51
1:E:498:LEU:HG	1:E:600:ILE:HB	1.93	0.51
1:B:348:ILE:HG22	1:B:357:PHE:HB3	1.92	0.51
1:B:612:ARG:HH21	1:C:606:TYR:HE2	1.59	0.51
1:D:504:GLU:HG3	1:D:645:TYR:CE1	2.45	0.51
1:D:710:SER:HA	1:F:643:ASP:HB3	1.93	0.51
1:C:461:LEU:O	1:C:465:ILE:HG12	2.10	0.51
1:D:389:ARG:NH2	1:E:398:ASP:OD2	2.41	0.51
1:D:500:PHE:HD2	1:D:623:VAL:HG12	1.76	0.51
1:F:701:LYS:HB3	1:F:747:PHE:HZ	1.75	0.51
1:A:640:GLU:HG2	1:A:648:VAL:HG21	1.93	0.50
1:C:763:HIS:HB3	1:C:774:LEU:HD11	1.91	0.50
1:E:629:HIS:O	1:E:649:LYS:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:GLU:O	1:E:761:ASN:ND2	2.44	0.50
1:A:510:SER:O	1:A:514:ARG:HG3	2.11	0.50
1:F:496:GLY:HA2	1:F:578:THR:HG23	1.92	0.50
1:B:525:VAL:HG12	1:B:553:VAL:HG22	1.94	0.50
1:C:393:GLU:OE2	1:C:397:ARG:NH2	2.44	0.50
1:D:482:TYR:OH	1:D:512:THR:OG1	2.27	0.50
1:E:520:ILE:HG23	1:E:523:LEU:HB2	1.94	0.50
1:E:503:GLY:O	1:E:605:ASN:HA	2.12	0.49
1:F:588:PHE:HE2	2:T:3:DC:H1'	1.78	0.49
1:B:516:LEU:O	1:B:520:ILE:HG12	2.11	0.49
1:E:531:ILE:HG13	1:E:532:LEU:HG	1.94	0.49
1:F:369:LEU:O	1:F:372:ARG:NH1	2.43	0.49
2:T:4:DC:H2"	2:T:5:DC:O4'	2.13	0.49
1:B:736:LEU:HD23	1:B:736:LEU:H	1.78	0.49
1:E:616:ALA:HA	1:E:619:ARG:HE	1.77	0.49
1:A:504:GLU:HG2	1:A:645:TYR:CD1	2.48	0.49
1:A:607:LYS:HD3	1:A:608:PRO:HD2	1.94	0.49
1:D:696:PHE:HD1	1:D:699:TYR:HB2	1.78	0.49
1:A:503:GLY:O	1:A:605:ASN:HA	2.13	0.49
1:A:710:SER:HA	1:E:645:TYR:CG	2.47	0.49
1:A:398:ASP:OD2	1:E:389:ARG:NH2	2.44	0.49
1:D:558:LEU:HD22	1:D:559:PRO:HD2	1.94	0.49
1:E:494:THR:HG23	1:E:596:ASN:HD21	1.77	0.49
1:F:734:LEU:HD12	1:F:735:PRO:HD2	1.94	0.49
1:A:456:PRO:HD2	1:A:457:GLU:N	2.28	0.49
1:A:709:SER:HB2	1:E:644:ALA:N	2.27	0.49
1:E:699:TYR:O	1:E:702:ILE:HG12	2.12	0.49
1:F:576:LYS:HE3	1:F:583:ILE:H	1.78	0.49
1:A:637:GLU:HA	1:A:640:GLU:HB2	1.94	0.48
1:A:711:VAL:HA	1:E:645:TYR:HB2	1.95	0.48
1:B:757:GLU:O	1:B:761:ASN:ND2	2.45	0.48
1:C:476:LYS:HG3	1:C:477:LYS:H	1.77	0.48
1:D:641:ASN:HB3	1:E:708:SER:O	2.13	0.48
1:E:762:ARG:HD2	1:E:763:HIS:CD2	2.47	0.48
1:F:560:ASP:HA	1:F:606:TYR:CZ	2.48	0.48
1:A:710:SER:N	1:E:642:ASN:HB3	2.27	0.48
1:F:478:ASN:ND2	1:F:625:ARG:O	2.38	0.48
1:A:769:VAL:H	1:E:750:ARG:HE	1.61	0.48
1:E:473:ASP:OD1	1:E:473:ASP:N	2.47	0.48
1:E:670:TYR:O	1:E:673:VAL:HG12	2.14	0.48
1:E:460:GLU:HB2	1:E:664:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:LEU:HD21	1:F:689:THR:HG21	1.95	0.48
1:C:574:ILE:HG21	1:C:617:LEU:HD12	1.96	0.48
1:F:558:LEU:HD23	1:F:603:ASP:O	2.14	0.48
1:A:710:SER:HA	1:E:645:TYR:CD2	2.49	0.48
1:B:536:LEU:HD12	1:B:576:LYS:HD2	1.96	0.47
1:F:497:CYS:SG	1:F:498:LEU:N	2.87	0.47
1:A:702:ILE:HG12	1:A:759:PHE:HE2	1.79	0.47
1:A:544:ILE:HG21	1:A:584:GLY:HA3	1.96	0.47
1:F:477:LYS:HD2	1:F:477:LYS:HA	1.63	0.47
1:B:707:VAL:HG12	1:B:779:ILE:HG12	1.95	0.47
1:A:603:ASP:OD1	1:A:604:THR:N	2.48	0.47
1:B:529:GLN:HE22	1:B:558:LEU:HD12	1.78	0.47
1:F:555:CYS:HB3	1:F:602:ILE:HG23	1.96	0.47
1:A:701:LYS:HD3	1:A:747:PHE:CZ	2.49	0.47
1:C:496:GLY:HA2	1:C:578:THR:HG23	1.97	0.47
1:F:748:ASN:O	1:F:750:ARG:NH1	2.43	0.47
1:A:713:HIS:N	1:E:642:ASN:O	2.47	0.47
1:F:757:GLU:O	1:F:761:ASN:ND2	2.48	0.47
1:A:488:SER:O	1:A:488:SER:OG	2.31	0.47
1:C:453:GLU:O	1:C:458:MET:HG2	2.15	0.47
1:C:757:GLU:O	1:C:761:ASN:ND2	2.48	0.47
1:A:344:ARG:HH21	1:A:591:LYS:HG2	1.80	0.46
1:A:669:LEU:O	1:A:673:VAL:HG23	2.15	0.46
1:D:333:ILE:O	1:D:336:THR:HG22	2.15	0.46
1:F:500:PHE:HB2	1:F:623:VAL:HG22	1.97	0.46
1:B:708:SER:OG	1:C:643:ASP:N	2.48	0.46
1:D:757:GLU:O	1:D:761:ASN:ND2	2.49	0.46
1:F:358:ASN:HB3	1:F:361:GLU:O	2.15	0.46
1:F:681:ILE:O	1:F:683:ILE:N	2.49	0.46
1:B:751:LEU:H	1:F:769:VAL:CB	2.28	0.46
1:E:542:PRO:O	1:E:546:ASN:N	2.39	0.46
1:A:502:PHE:HE2	1:A:607:LYS:HE2	1.80	0.46
1:D:475:ASN:HD21	1:D:478:ASN:HD22	1.64	0.46
1:F:402:ASP:OD2	1:F:403:SER:N	2.48	0.46
1:F:468:ILE:HG22	1:F:469:GLN:HG2	1.98	0.46
1:A:578:THR:HG21	1:A:620:ARG:HD3	1.96	0.46
1:D:725:TYR:CZ	1:D:734:LEU:HD22	2.50	0.46
1:D:728:TYR:CD2	1:D:765:LYS:HE3	2.43	0.46
1:E:348:ILE:HG22	1:E:357:PHE:HB3	1.96	0.46
1:A:710:SER:OG	1:A:711:VAL:N	2.47	0.46
1:E:593:ASN:OD1	1:E:593:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:706:LEU:HB3	1:E:776:TYR:HB3	1.97	0.46
1:A:638:ALA:HA	1:C:712:LYS:CB	2.46	0.46
1:D:654:GLY:O	1:D:658:LYS:HG2	2.15	0.46
1:E:536:LEU:HG	1:E:573:ASN:ND2	2.31	0.46
1:A:502:PHE:HD1	1:A:503:GLY:N	2.13	0.46
1:A:613:ILE:HD13	1:A:699:TYR:CE2	2.50	0.46
1:A:713:HIS:CE1	1:A:777:ILE:HD12	2.51	0.46
1:A:725:TYR:CZ	1:A:734:LEU:HD22	2.51	0.46
1:F:655:LEU:HD12	1:F:659:ILE:HD13	1.97	0.46
1:A:348:ILE:HG22	1:A:357:PHE:HB3	1.97	0.46
1:A:607:LYS:HD2	1:A:694:PRO:HG2	1.98	0.46
1:A:710:SER:HB3	1:E:642:ASN:CB	2.46	0.46
1:D:447:ASP:OD1	1:D:449:THR:OG1	2.27	0.45
1:A:713:HIS:CD2	1:A:716:LEU:HD11	2.51	0.45
1:B:384:LEU:O	1:F:324:ASN:ND2	2.49	0.45
1:B:513:LYS:NZ	1:B:526:GLU:OE2	2.44	0.45
1:D:511:THR:O	1:D:514:ARG:HG2	2.16	0.45
1:B:725:TYR:CE2	1:B:777:ILE:HG23	2.51	0.45
1:F:483:GLU:HG3	1:F:675:TRP:CD2	2.51	0.45
1:A:713:HIS:ND1	1:E:642:ASN:HA	2.31	0.45
1:D:607:LYS:HE2	1:D:694:PRO:HG2	1.97	0.45
1:C:533:THR:HG22	1:C:569:ILE:HA	1.99	0.45
1:C:720:LEU:HD13	1:C:725:TYR:HB2	1.98	0.45
1:E:504:GLU:HB3	1:E:645:TYR:CE1	2.52	0.45
1:F:428:TYR:CD2	1:F:432:ASP:HB3	2.51	0.45
1:B:763:HIS:HB3	1:B:776:TYR:CE2	2.51	0.45
1:E:411:ASP:OD2	1:E:412:LYS:NZ	2.43	0.45
1:E:461:LEU:HD22	1:E:667:ALA:HB1	1.99	0.45
1:F:707:VAL:HG12	1:F:779:ILE:HG22	1.99	0.45
1:C:372:ARG:O	1:C:380:SER:OG	2.28	0.44
1:C:529:GLN:NE2	1:C:532:LEU:HB2	2.32	0.44
1:C:701:LYS:O	1:C:705:LEU:HG	2.17	0.44
1:F:556:SER:HA	1:F:603:ASP:HB3	1.99	0.44
1:F:576:LYS:HE3	1:F:582:VAL:HA	2.00	0.44
1:C:483:GLU:HB2	1:C:675:TRP:CD2	2.52	0.44
1:F:364:ILE:HB	1:F:393:GLU:HG3	2.00	0.44
1:A:691:GLU:HG2	1:A:692:GLU:HG2	1.99	0.44
1:C:707:VAL:HG13	1:C:779:ILE:HG12	1.99	0.44
1:E:611:ASP:OD1	1:E:612:ARG:N	2.51	0.44
1:E:495:LYS:NZ	1:E:597:HIS:O	2.49	0.44
1:E:698:PHE:CZ	1:E:743:ILE:HD11	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LYS:HB3	1:B:477:LYS:HE3	1.59	0.44
1:B:529:GLN:NE2	1:B:558:LEU:HD12	2.32	0.44
1:A:431:ASP:N	1:A:431:ASP:OD1	2.50	0.44
1:E:725:TYR:OH	1:E:742:LYS:NZ	2.51	0.44
1:E:476:LYS:HD2	1:E:476:LYS:HA	1.72	0.44
1:D:760:ILE:O	1:D:764:LYS:N	2.50	0.44
1:F:349:VAL:HG21	1:F:363:LEU:HB2	2.00	0.44
1:A:465:ILE:HG23	1:A:479:ARG:HH12	1.81	0.43
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.87	0.43
1:B:698:PHE:CD2	1:B:755:ASP:HB3	2.53	0.43
1:B:734:LEU:HD12	1:B:735:PRO:HD2	1.99	0.43
1:E:468:ILE:HG13	1:E:508:GLY:HA3	1.99	0.43
1:D:486:LEU:HD12	1:D:486:LEU:HA	1.85	0.43
1:E:676:TYR:O	1:E:680:HIS:N	2.51	0.43
1:A:509:LYS:HB2	1:A:509:LYS:HE2	1.60	0.43
1:A:768:ASN:HB2	1:E:750:ARG:HG3	2.00	0.43
1:E:492:GLY:HA2	1:E:597:HIS:HB3	2.00	0.43
1:E:520:ILE:HD12	1:E:520:ILE:HA	1.78	0.43
1:A:681:ILE:O	1:A:683:ILE:N	2.50	0.43
1:D:669:LEU:HD12	1:D:669:LEU:HA	1.84	0.43
1:E:483:GLU:HG2	1:E:675:TRP:CD2	2.54	0.43
1:F:515:LEU:HD23	1:F:515:LEU:HA	1.86	0.43
1:F:611:ASP:OD1	1:F:612:ARG:N	2.52	0.43
1:C:504:GLU:OE1	1:C:644:ALA:HB1	2.18	0.43
1:B:763:HIS:HD1	1:B:776:TYR:HH	1.55	0.43
1:F:576:LYS:CE	1:F:583:ILE:H	2.32	0.43
1:A:734:LEU:HD23	1:A:739:PHE:HD1	1.83	0.43
1:B:350:TRP:CZ2	1:B:353:ASN:HA	2.53	0.43
1:D:619:ARG:HH12	1:F:505:THR:HG21	1.83	0.43
1:E:762:ARG:HB3	1:E:763:HIS:HD2	1.83	0.43
1:F:699:TYR:HA	1:F:702:ILE:HG12	2.01	0.43
1:B:588:PHE:HE2	2:T:2:DC:H1'	1.83	0.43
1:E:509:LYS:HB2	1:E:509:LYS:HE2	1.61	0.43
1:E:633:PRO:HG3	1:E:650:LEU:HD21	2.01	0.43
1:E:649:LYS:HB3	1:E:649:LYS:HE3	1.82	0.43
1:A:332:ARG:O	1:A:336:THR:HG23	2.18	0.43
1:A:503:GLY:HA3	1:A:509:LYS:HD3	2.01	0.43
1:A:509:LYS:HE3	1:A:603:ASP:OD1	2.19	0.43
1:B:649:LYS:HD3	1:B:649:LYS:HA	1.65	0.43
1:D:343:GLU:OE2	1:D:343:GLU:N	2.45	0.43
1:A:759:PHE:HD1	1:A:759:PHE:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:GLU:OE2	1:C:504:GLU:N	2.34	0.43
1:D:445:LYS:HB2	1:D:445:LYS:HE2	1.75	0.43
1:F:510:SER:O	1:F:514:ARG:HG2	2.19	0.43
1:D:550:LYS:HA	1:D:550:LYS:HD3	1.80	0.42
1:E:500:PHE:CE1	1:E:621:ILE:HG23	2.51	0.42
1:F:681:ILE:HB	1:F:682:PRO:HD2	2.00	0.42
1:A:627:ARG:O	1:A:647:LYS:HB3	2.18	0.42
1:A:677:LYS:HA	1:A:680:HIS:HD2	1.84	0.42
1:D:758:SER:O	1:D:762:ARG:HB2	2.18	0.42
1:A:607:LYS:HZ2	1:A:694:PRO:HD2	1.82	0.42
1:B:536:LEU:HD22	1:B:544:ILE:HD12	2.01	0.42
1:C:585:ARG:HH11	1:C:585:ARG:HG2	1.83	0.42
1:D:736:LEU:HD11	1:D:760:ILE:HD13	2.01	0.42
1:F:529:GLN:NE2	1:F:557:GLU:O	2.47	0.42
1:A:358:ASN:HB3	1:A:361:GLU:O	2.19	0.42
1:A:482:TYR:HH	1:A:512:THR:HG1	1.61	0.42
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.82	0.42
1:D:768:ASN:HB3	1:F:751:LEU:HB2	2.01	0.42
1:E:504:GLU:HB3	1:E:645:TYR:HE1	1.84	0.42
1:C:476:LYS:HG3	1:C:477:LYS:N	2.33	0.42
1:E:628:THR:HG22	1:E:629:HIS:H	1.84	0.42
1:F:676:TYR:O	1:F:680:HIS:HB3	2.19	0.42
1:B:444:PHE:CE1	1:B:665:ARG:HD3	2.54	0.42
1:E:717:MET:HA	1:E:727:LEU:HD22	2.01	0.42
1:F:720:LEU:HD21	1:F:781:ASP:OD1	2.19	0.42
1:D:453:GLU:HB2	1:D:670:TYR:HE2	1.85	0.42
1:D:456:PRO:O	1:D:460:GLU:HG2	2.20	0.42
1:D:500:PHE:HE2	1:D:621:ILE:HG23	1.84	0.42
1:F:504:GLU:O	1:F:507:THR:OG1	2.28	0.42
1:A:579:GLU:HG2	1:A:581:CYS:O	2.19	0.42
1:C:500:PHE:CD1	1:C:602:ILE:HB	2.51	0.42
1:F:651:LEU:HD23	1:F:651:LEU:HA	1.85	0.42
1:A:758:SER:HA	1:A:761:ASN:HD21	1.84	0.42
1:B:748:ASN:HB3	1:F:769:VAL:CB	2.50	0.42
1:F:481:LEU:HD12	1:F:481:LEU:HA	1.92	0.42
1:B:706:LEU:HD23	1:B:778:PHE:HA	2.02	0.42
1:D:629:HIS:HD2	1:D:645:TYR:CE2	2.37	0.42
1:E:768:ASN:OD1	1:E:768:ASN:N	2.53	0.42
1:F:500:PHE:HE1	1:F:602:ILE:HD12	1.85	0.42
1:F:571:SER:HB3	1:F:612:ARG:HH21	1.85	0.42
1:A:372:ARG:O	1:A:380:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ASP:OD1	1:A:720:LEU:N	2.53	0.41
1:E:547:MET:HA	1:E:550:LYS:CG	2.50	0.41
1:A:338:SER:HB3	1:A:367:LEU:HD11	2.02	0.41
1:A:676:TYR:O	1:A:680:HIS:HB3	2.20	0.41
1:B:681:ILE:HG13	1:B:683:ILE:O	2.20	0.41
1:D:364:ILE:HB	1:D:393:GLU:HG3	2.02	0.41
1:D:571:SER:O	1:D:575:LYS:HE3	2.20	0.41
1:F:698:PHE:HB2	1:F:752:PHE:CE1	2.55	0.41
1:F:736:LEU:O	1:F:740:GLN:HG2	2.20	0.41
1:A:571:SER:HB3	1:A:617:LEU:HD23	2.01	0.41
1:A:585:ARG:HA	1:A:586:PRO:HD3	1.95	0.41
1:A:530:THR:O	1:A:534:ASP:HB2	2.20	0.41
1:C:435:LYS:HB2	1:C:435:LYS:HE3	1.77	0.41
1:A:629:HIS:N	1:A:647:LYS:O	2.51	0.41
1:C:678:LYS:HE3	1:C:679:TYR:CZ	2.54	0.41
1:F:546:ASN:OD1	1:F:546:ASN:C	2.59	0.41
1:A:344:ARG:NH2	1:A:591:LYS:HG2	2.35	0.41
1:A:710:SER:C	1:E:645:TYR:H	2.23	0.41
1:C:575:LYS:HB3	1:C:575:LYS:HE3	1.76	0.41
1:F:350:TRP:CZ2	1:F:353:ASN:HA	2.55	0.41
1:F:683:ILE:O	1:F:683:ILE:HD12	2.20	0.41
1:F:740:GLN:HA	1:F:743:ILE:HG22	2.03	0.41
1:D:764:LYS:HA	1:D:774:LEU:HA	2.03	0.41
1:B:529:GLN:OE1	1:B:559:PRO:HD3	2.21	0.41
1:E:479:ARG:O	1:E:483:GLU:HB2	2.21	0.41
1:E:576:LYS:HE3	1:E:583:ILE:HB	2.01	0.41
1:A:498:LEU:HD22	1:A:574:ILE:HG13	2.01	0.41
1:B:725:TYR:OH	1:B:781:ASP:OD2	2.33	0.41
1:C:720:LEU:HD22	1:C:732:VAL:HG11	2.03	0.41
1:D:411:ASP:OD1	1:D:411:ASP:N	2.53	0.41
1:D:416:LYS:HD3	1:D:445:LYS:HG3	2.02	0.41
1:D:638:ALA:HB2	1:E:707:VAL:HG12	2.03	0.41
1:E:477:LYS:HB3	1:E:477:LYS:HE3	1.83	0.41
1:F:575:LYS:HG2	1:F:620:ARG:HH12	1.86	0.41
1:F:748:ASN:HB3	1:F:750:ARG:CD	2.51	0.41
1:A:629:HIS:ND1	1:A:639:ALA:HB1	2.35	0.41
1:D:509:LYS:HB2	1:D:509:LYS:HE2	1.76	0.41
1:D:676:TYR:O	1:D:680:HIS:HB3	2.20	0.41
1:E:619:ARG:H	1:E:619:ARG:HG2	1.55	0.41
1:C:332:ARG:O	1:C:336:THR:HG23	2.21	0.40
1:C:569:ILE:H	1:C:569:ILE:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:516:LEU:HD23	1:E:524:PHE:HE2	1.86	0.40
1:E:529:GLN:OE1	1:E:558:LEU:HA	2.21	0.40
1:F:700:LEU:HD23	1:F:700:LEU:HA	1.94	0.40
1:B:498:LEU:HG	1:B:600:ILE:HB	2.02	0.40
1:D:611:ASP:OD1	1:D:612:ARG:N	2.54	0.40
1:E:406:THR:HA	1:E:437:THR:OG1	2.21	0.40
1:F:751:LEU:HD22	1:F:752:PHE:CD2	2.56	0.40
2:T:2:DC:H2"	2:T:3:DC:C6	2.56	0.40
1:E:535:VAL:HA	1:E:573:ASN:HD21	1.86	0.40
1:B:621:ILE:HD13	1:B:621:ILE:HA	1.93	0.40
1:D:736:LEU:HD11	1:D:760:ILE:HG21	2.03	0.40
1:E:662:ASN:HB3	1:E:665:ARG:CD	2.51	0.40
1:A:710:SER:HG	1:A:711:VAL:H	1.70	0.40
1:A:717:MET:HA	1:A:720:LEU:HG	2.02	0.40
1:B:324:ASN:O	1:B:327:PHE:N	2.53	0.40
1:D:736:LEU:HA	1:D:736:LEU:HD12	1.81	0.40
1:E:507:THR:HG22	1:E:628:THR:H	1.86	0.40
1:F:411:ASP:OD1	1:F:411:ASP:N	2.48	0.40
1:F:471:LEU:H	1:F:471:LEU:HD12	1.87	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%)	436 (95%)	25 (5%)	0	100	100
1	B	461/785 (59%)	449 (97%)	12 (3%)	0	100	100
1	C	461/785 (59%)	440 (95%)	21 (5%)	0	100	100
1	D	461/785 (59%)	440 (95%)	21 (5%)	0	100	100
1	E	461/785 (59%)	438 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	461/785 (59%)	443 (96%)	18 (4%)	0	100	100
All	All	2766/4710 (59%)	2646 (96%)	120 (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%)	378 (91%)	36 (9%)	8	29
1	B	414/725 (57%)	388 (94%)	26 (6%)	15	42
1	C	414/725 (57%)	383 (92%)	31 (8%)	11	35
1	D	414/725 (57%)	393 (95%)	21 (5%)	20	50
1	E	414/725 (57%)	379 (92%)	35 (8%)	8	30
1	F	414/725 (57%)	386 (93%)	28 (7%)	13	39
All	All	2484/4350 (57%)	2307 (93%)	177 (7%)	15	38

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	LEU
1	A	377	LYS
1	A	387	ARG
1	A	405	GLU
1	A	423	VAL
1	A	431	ASP
1	A	432	ASP
1	A	436	TYR
1	A	448	ASP
1	A	455	SER
1	A	465	ILE
1	A	479	ARG
1	A	487	SER

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Mol	Chain	Res	Type
1	A	488	SER
1	A	491	CYS
1	A	501	PHE
1	A	502	PHE
1	A	507	THR
1	A	517	LYS
1	A	530	THR
1	A	534	ASP
1	A	561	PHE
1	A	618	MET
1	A	627	ARG
1	A	636	ARG
1	A	645	TYR
1	A	656	ASP
1	A	664	TYR
1	A	670	TYR
1	A	680	HIS
1	A	695	ASP
1	A	701	LYS
1	A	713	HIS
1	A	746	TYR
1	A	757	GLU
1	A	759	PHE
1	B	360	GLU
1	B	377	LYS
1	B	387	ARG
1	B	402	ASP
1	B	405	GLU
1	B	457	GLU
1	B	474	GLU
1	B	488	SER
1	B	494	THR
1	B	499	THR
1	B	502	PHE
1	B	510	SER
1	B	525	VAL
1	B	529	GLN
1	B	554	PHE
1	B	561	PHE
1	B	583	ILE
1	B	593	ASN
1	B	612	ARG

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Mol	Chain	Res	Type
1	B	617	LEU
1	B	636	ARG
1	B	650	LEU
1	B	656	ASP
1	B	660	GLN
1	B	736	LEU
1	B	762	ARG
1	C	356	LYS
1	C	363	LEU
1	C	411	ASP
1	C	416	LYS
1	C	435	LYS
1	C	441	SER
1	C	448	ASP
1	C	455	SER
1	C	480	GLU
1	C	483	GLU
1	C	488	SER
1	C	499	THR
1	C	518	SER
1	C	544	ILE
1	C	554	PHE
1	C	556	SER
1	C	561	PHE
1	C	573	ASN
1	C	595	ARG
1	C	610	PHE
1	C	627	ARG
1	C	664	TYR
1	C	674	LYS
1	C	685	LYS
1	C	699	TYR
1	C	714	ILE
1	C	740	GLN
1	C	765	LYS
1	C	774	LEU
1	C	775	GLN
1	C	778	PHE
1	D	324	ASN
1	D	336	THR
1	D	431	ASP
1	D	432	ASP

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Mol	Chain	Res	Type
1	D	479	ARG
1	D	512	THR
1	D	513	LYS
1	D	547	MET
1	D	556	SER
1	D	570	ARG
1	D	607	LYS
1	D	619	ARG
1	D	629	HIS
1	D	658	LYS
1	D	661	ASN
1	D	674	LYS
1	D	679	TYR
1	D	691	GLU
1	D	696	PHE
1	D	710	SER
1	D	764	LYS
1	E	324	ASN
1	E	334	LEU
1	E	390	LYS
1	E	436	TYR
1	E	448	ASP
1	E	453	GLU
1	E	456	PRO
1	E	458	MET
1	E	462	MET
1	E	469	GLN
1	E	474	GLU
1	E	477	LYS
1	E	488	SER
1	E	489	CYS
1	E	501	PHE
1	E	517	LYS
1	E	520	ILE
1	E	559	PRO
1	E	561	PHE
1	E	576	LYS
1	E	599	THR
1	E	605	ASN
1	E	610	PHE
1	E	612	ARG
1	E	618	MET

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Mol	Chain	Res	Type
1	E	636	ARG
1	E	670	TYR
1	E	678	LYS
1	E	680	HIS
1	E	682	PRO
1	E	685	LYS
1	E	755	ASP
1	E	762	ARG
1	E	764	LYS
1	E	765	LYS
1	F	337	ASN
1	F	356	LYS
1	F	363	LEU
1	F	387	ARG
1	F	442	THR
1	F	447	ASP
1	F	471	LEU
1	F	486	LEU
1	F	497	CYS
1	F	499	THR
1	F	502	PHE
1	F	547	MET
1	F	555	CYS
1	F	561	PHE
1	F	581	CYS
1	F	595	ARG
1	F	612	ARG
1	F	625	ARG
1	F	627	ARG
1	F	636	ARG
1	F	656	ASP
1	F	664	TYR
1	F	668	PHE
1	F	695	ASP
1	F	699	TYR
1	F	710	SER
1	F	750	ARG
1	F	776	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	761	ASN
1	C	741	GLN
1	D	475	ASN
1	D	629	HIS
1	D	641	ASN
1	E	475	ASN
1	E	478	ASN
1	E	713	HIS
1	E	761	ASN
1	F	324	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.

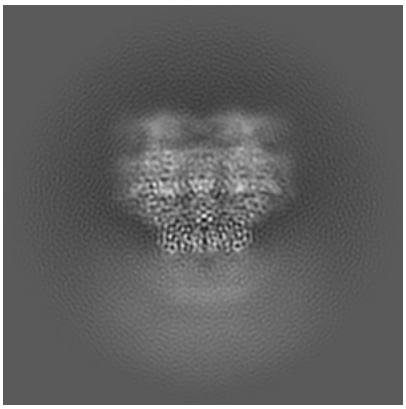
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37528. These allow visual inspection of the internal detail of the map and identification of artifacts.

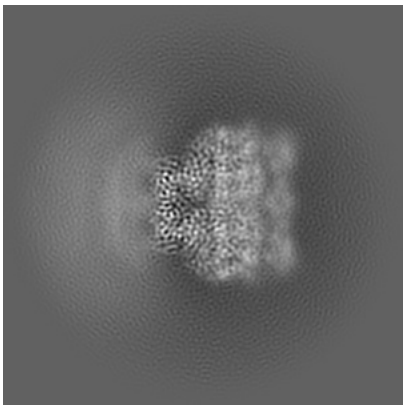
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

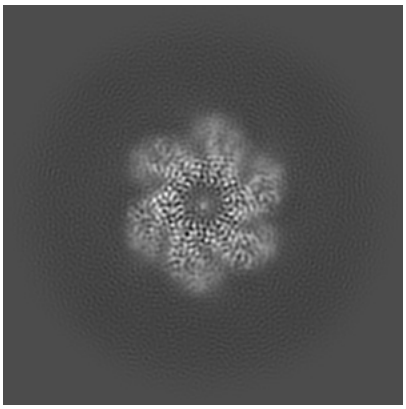
6.1.1 Primary map



X

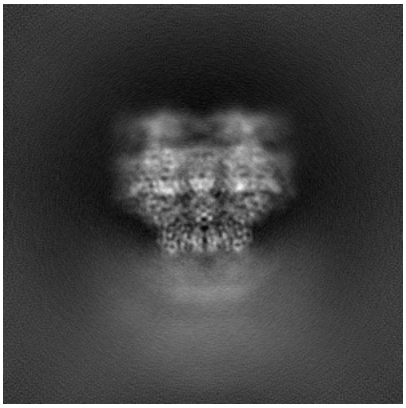


Y

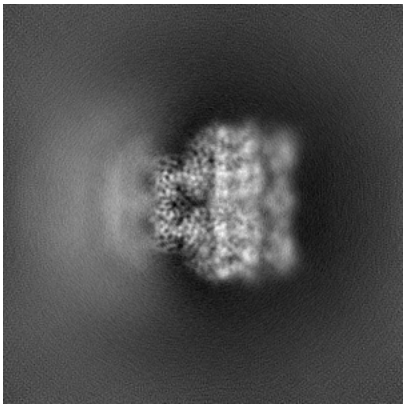


Z

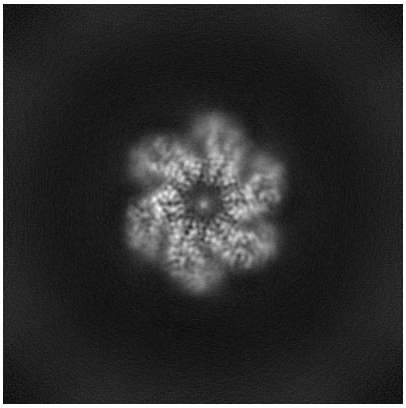
6.1.2 Raw map



X



Y

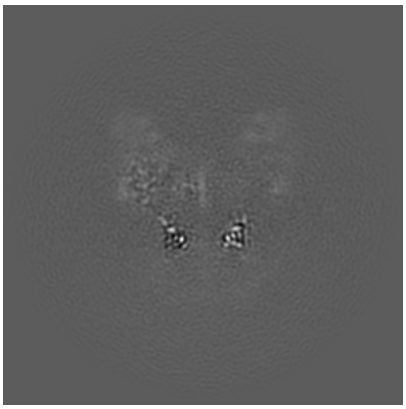


Z

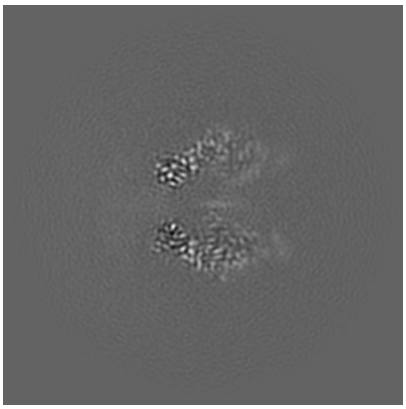
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

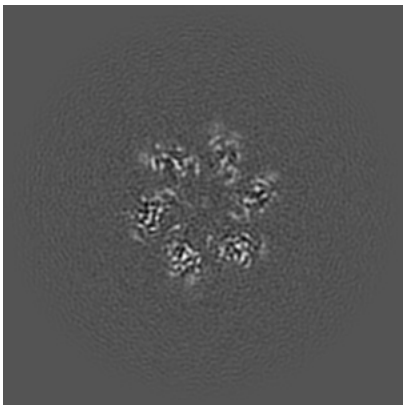
6.2.1 Primary map



X Index: 160

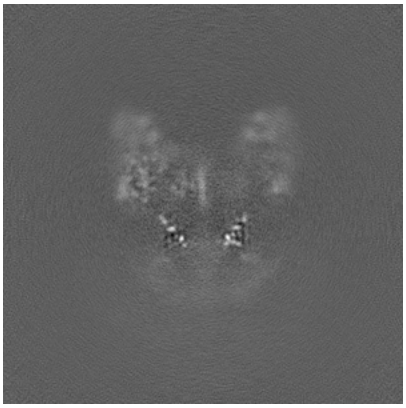


Y Index: 160

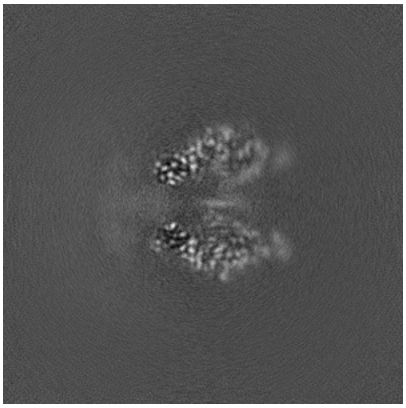


Z Index: 160

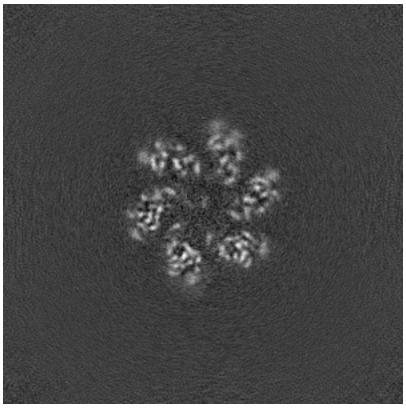
6.2.2 Raw map



X Index: 160



Y Index: 160

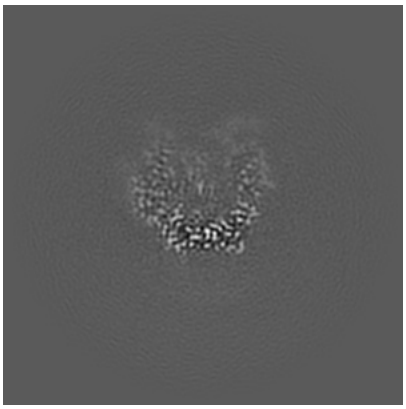


Z Index: 160

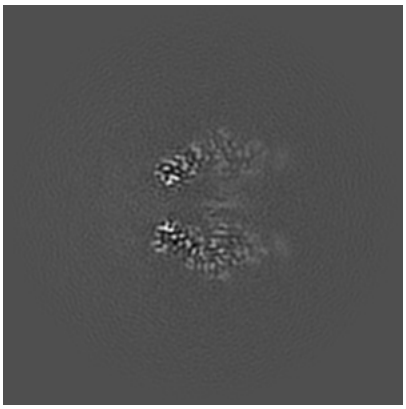
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

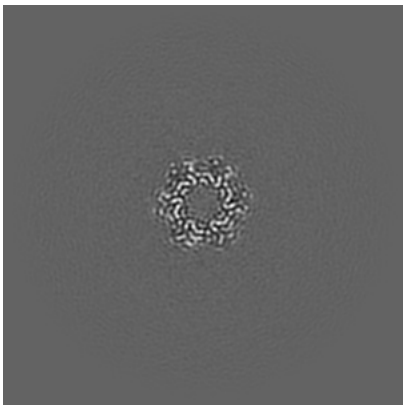
6.3.1 Primary map



X Index: 138

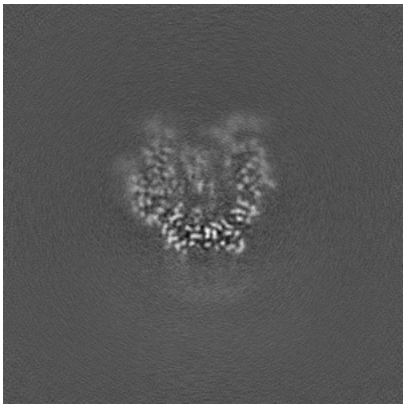


Y Index: 158

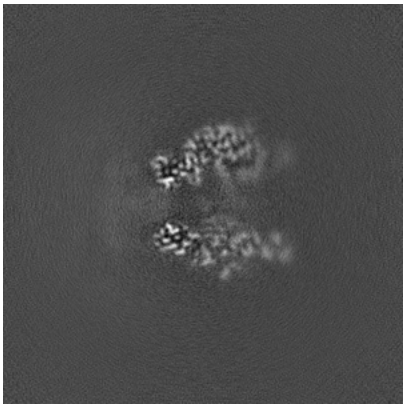


Z Index: 134

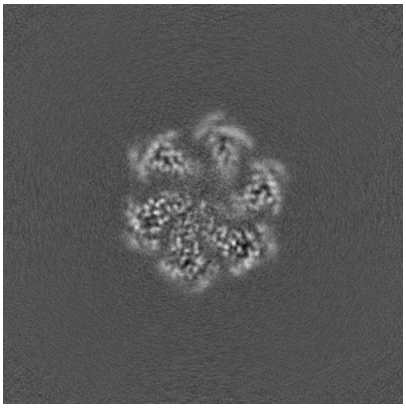
6.3.2 Raw map



X Index: 138



Y Index: 164

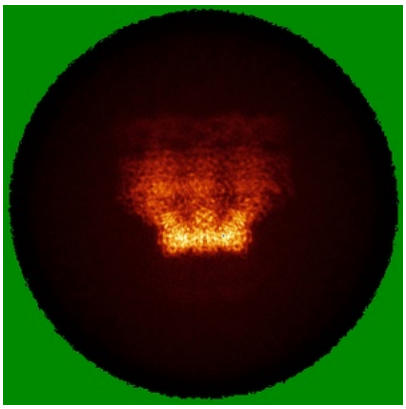


Z Index: 173

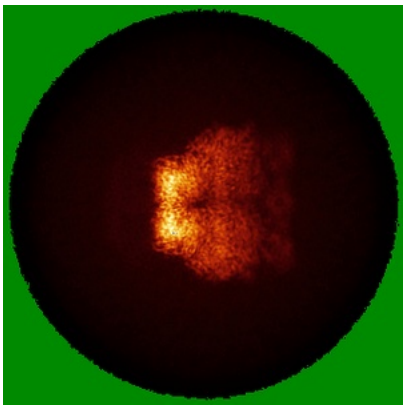
The images above show the largest variance slices of the map in three orthogonal directions.

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

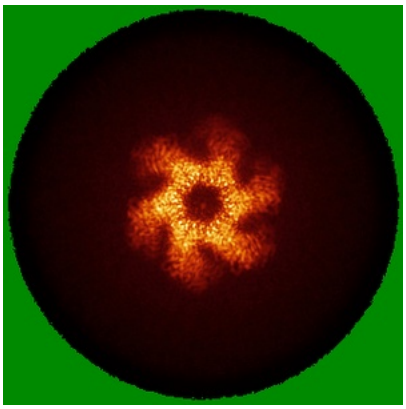
6.4.1 Primary map



X

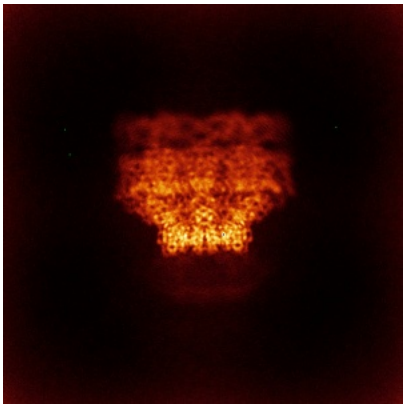


Y

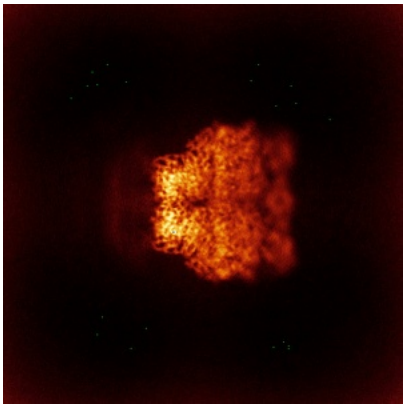


Z

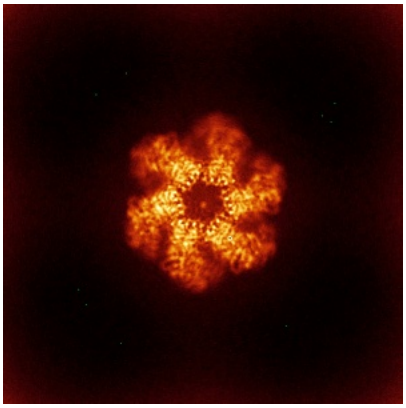
6.4.2 Raw map



X



Y



Z

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

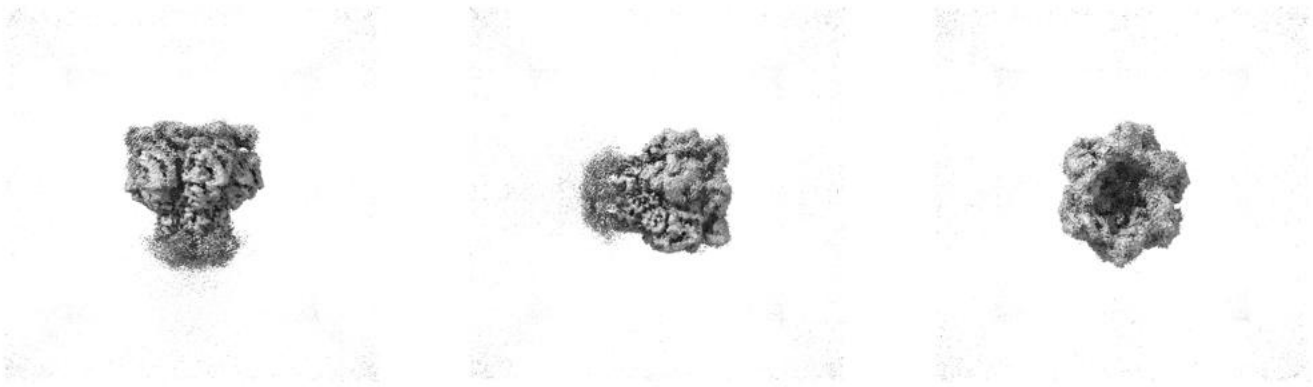
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

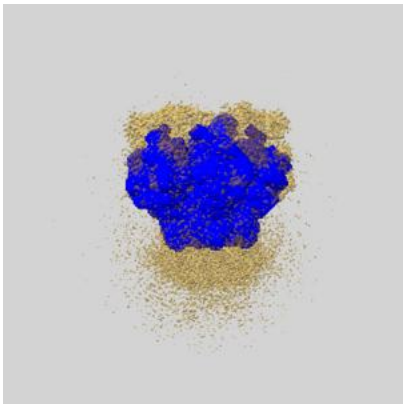
6.6 Mask visualisation (i)

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

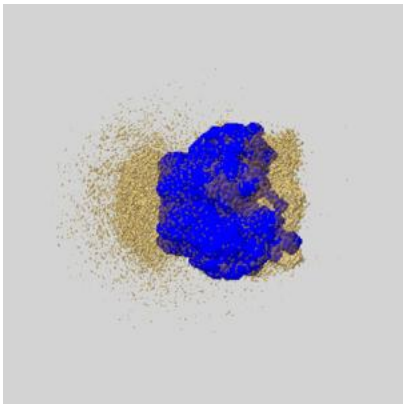
A mask typically either:

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

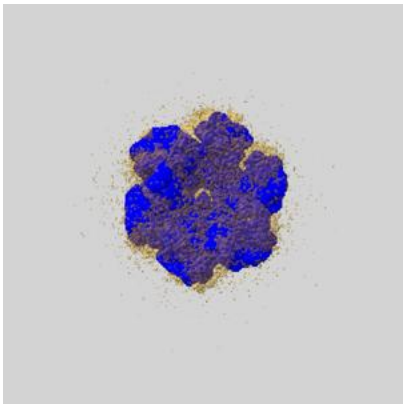
6.6.1 emd_37528_msk_1.map (i)



X



Y

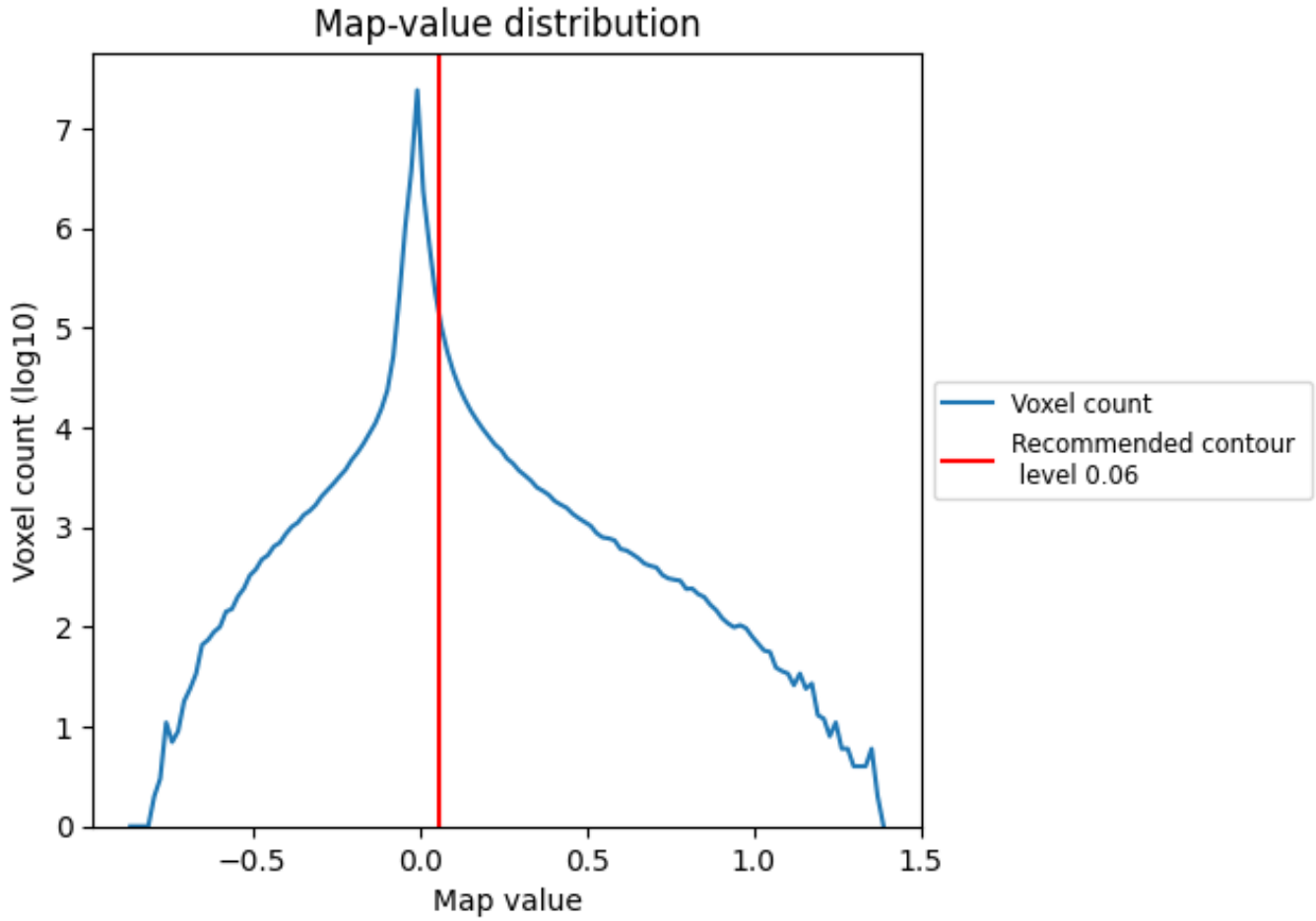


Z

7 Map analysis

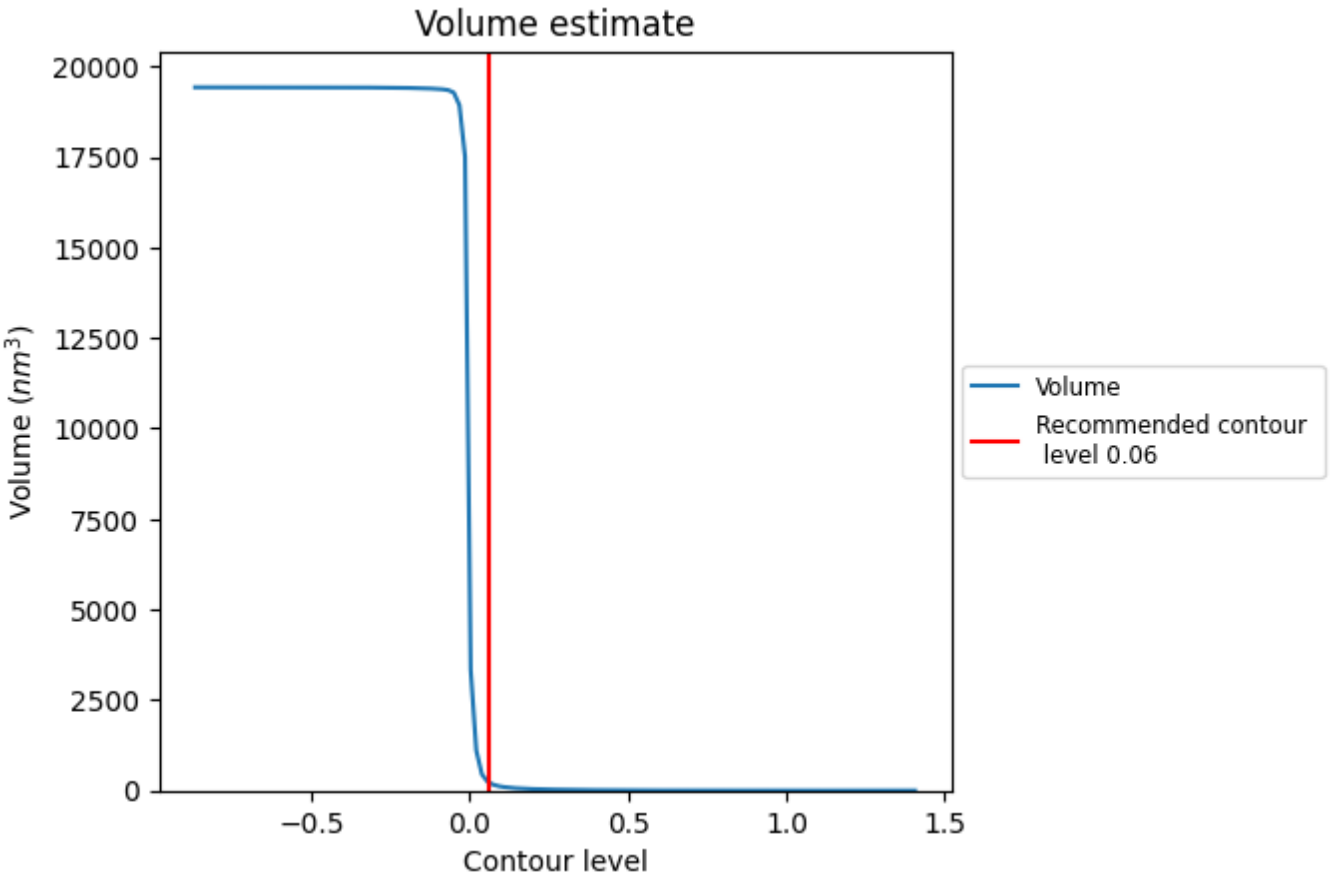
This section contains the results of statistical analysis of the map.

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.

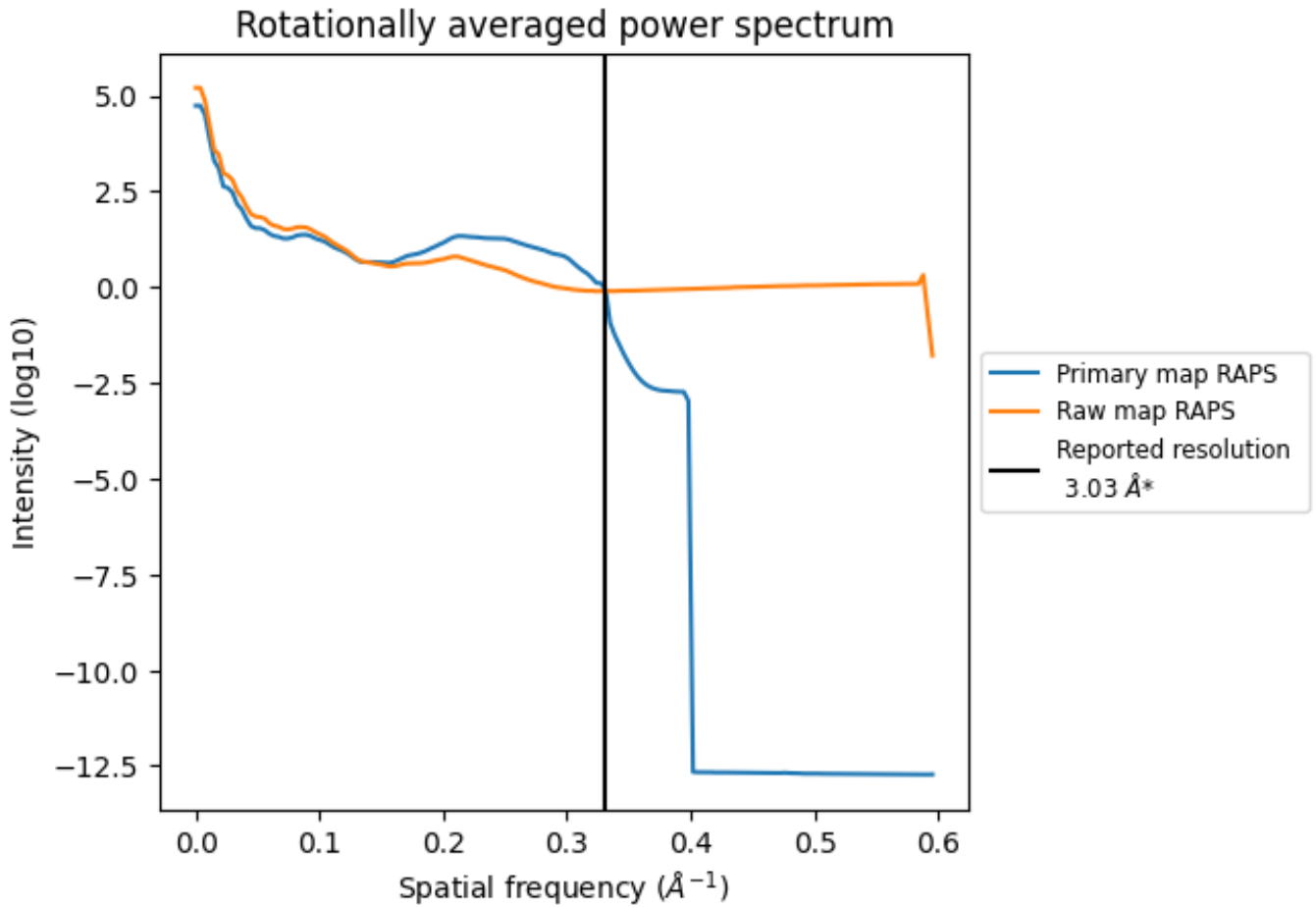
7.2 Volume estimate



The volume at the recommended contour level is 234 nm^3; this corresponds to an approximate mass of 211 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)

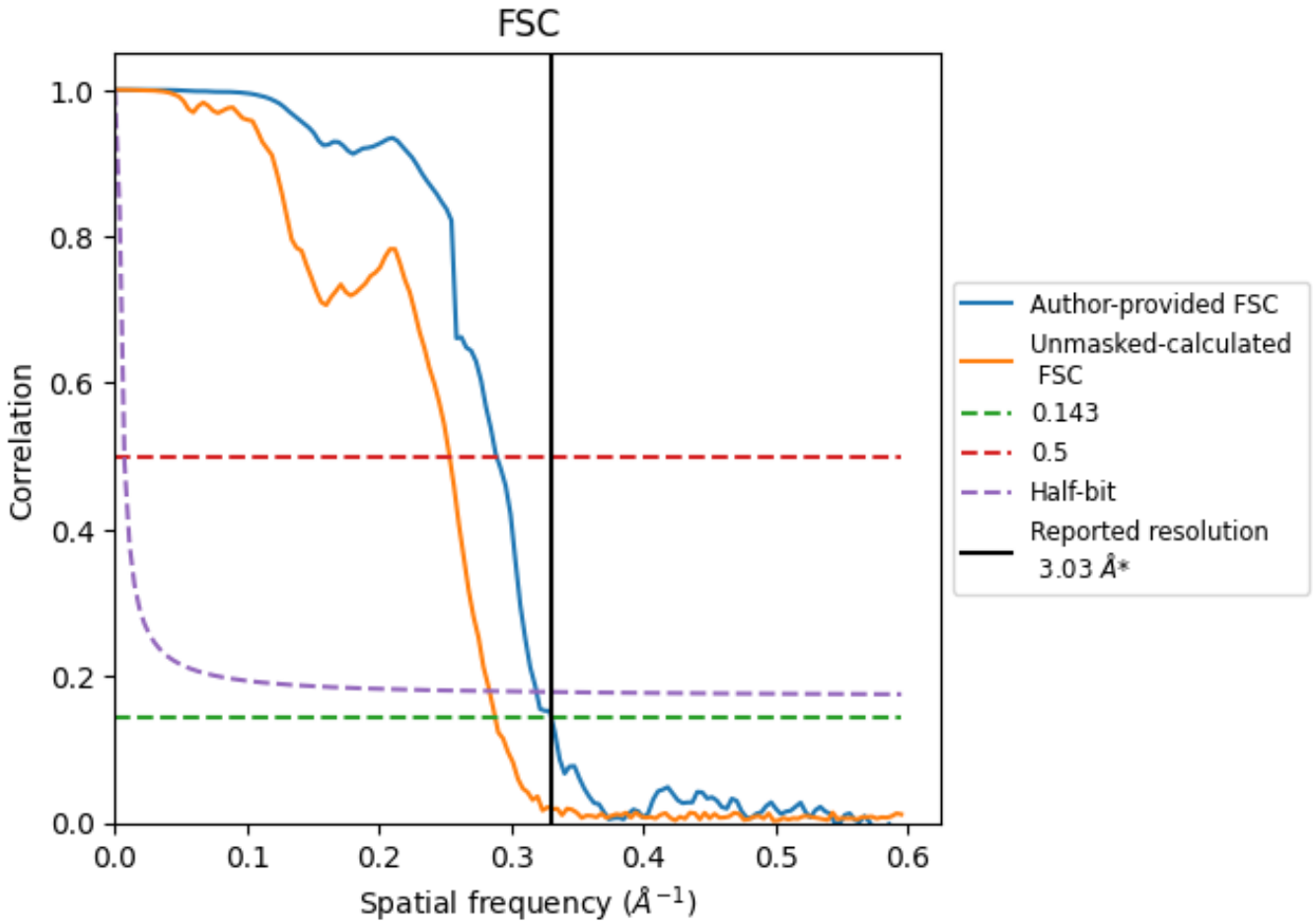


*Reported resolution corresponds to spatial frequency of 0.330 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

8.2 Resolution estimates (i)

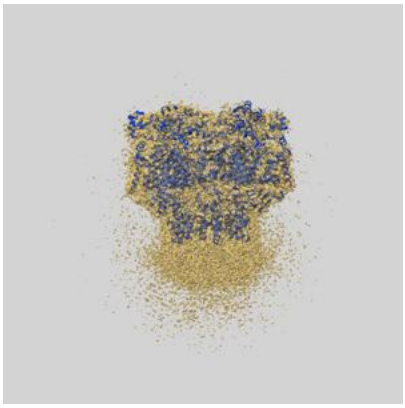
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.46	3.13
Unmasked-calculated*	3.47	3.95	3.53

*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 3.47 differs from the reported value 3.03 by more than 10 %

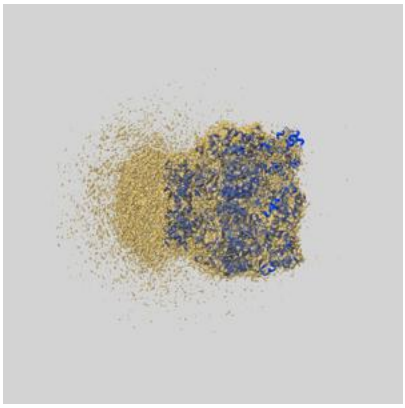
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37528 and PDB model 8WH4. Per-residue inclusion information can be found in section 3 on page 4.

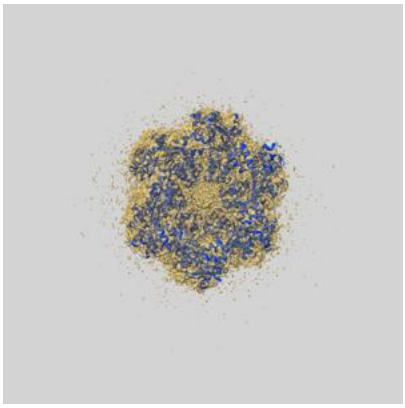
9.1 Map-model overlay



X



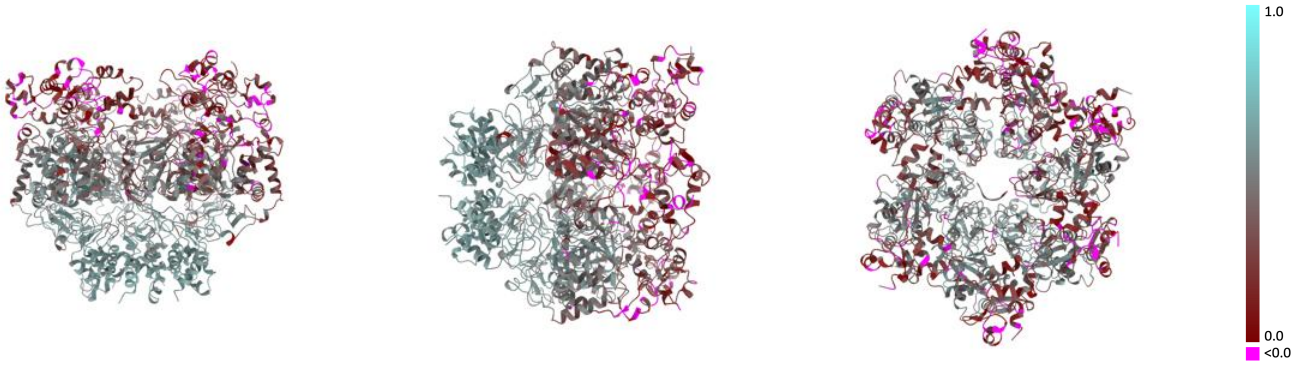
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

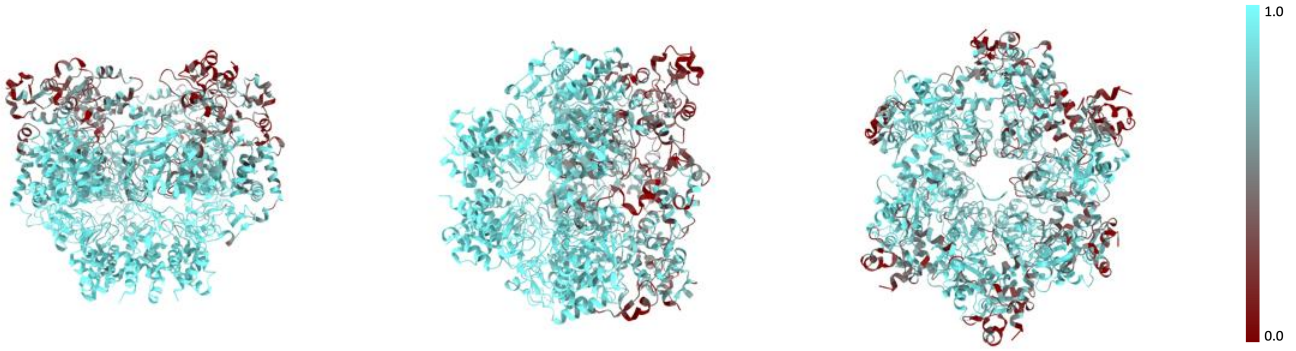
9.2 Q-score mapped to coordinate model (i)



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.

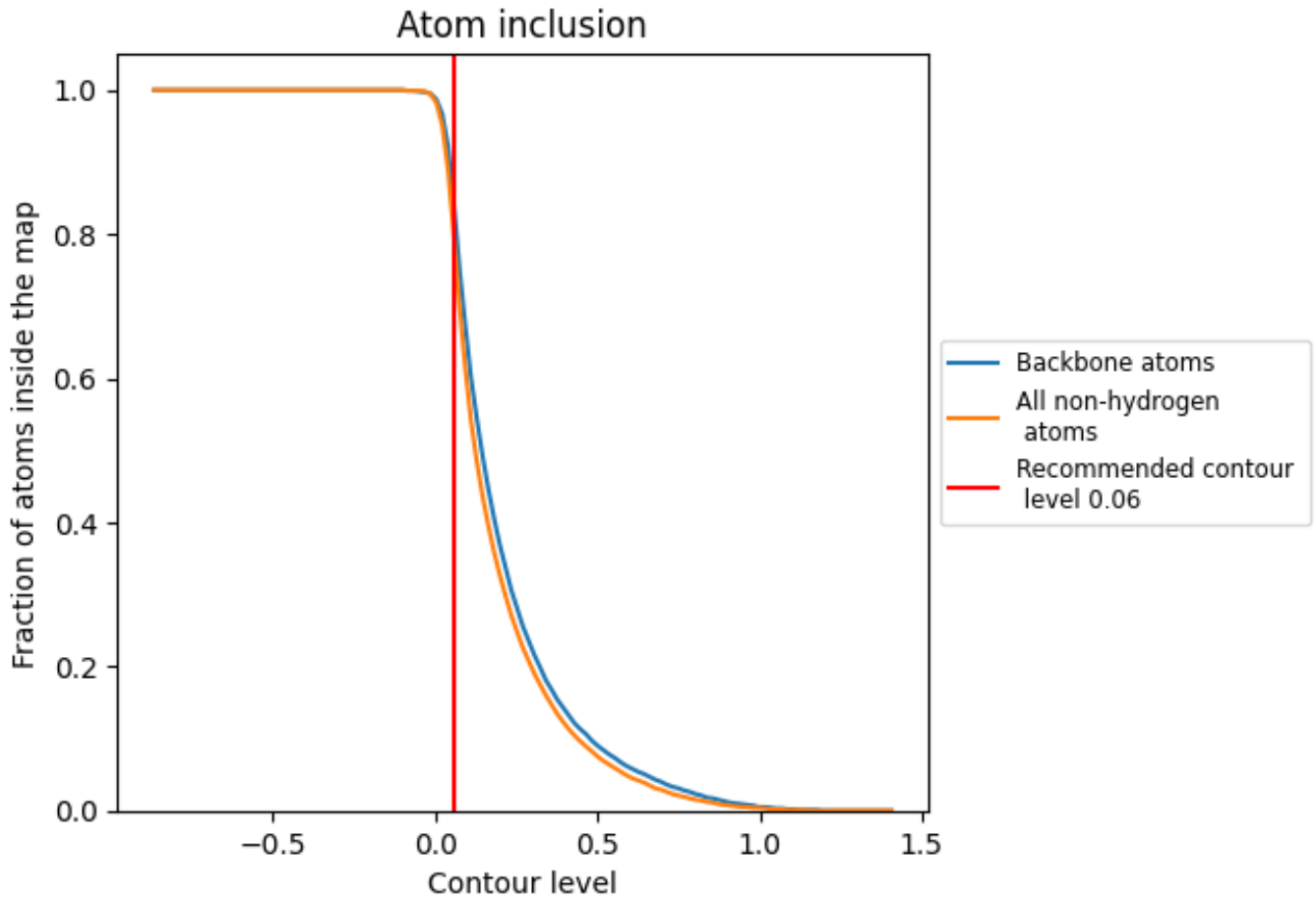
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.4040
A	0.7890	0.3990
B	0.8150	0.4530
C	0.8820	0.4630
D	0.7650	0.3670
E	0.6590	0.3140
F	0.8100	0.4300
T	0.9080	0.3940