



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:56 PM UTC

PDB ID : 9C47 / pdb_00009c47
EMDB ID : EMD-45176
Title : TRRAP module of the human TIP60 complex
Authors : Yang, Z.; Mameri, A.; Florez Ariza, A.J.; Cote, J.; Nogales, E.
Deposited on : 2024-06-03
Resolution : 3.40 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

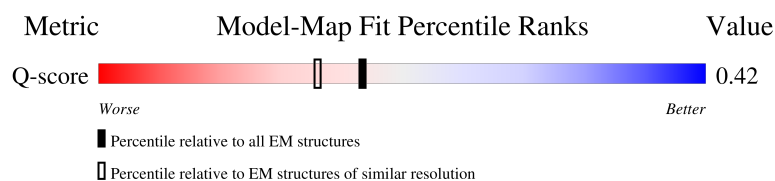
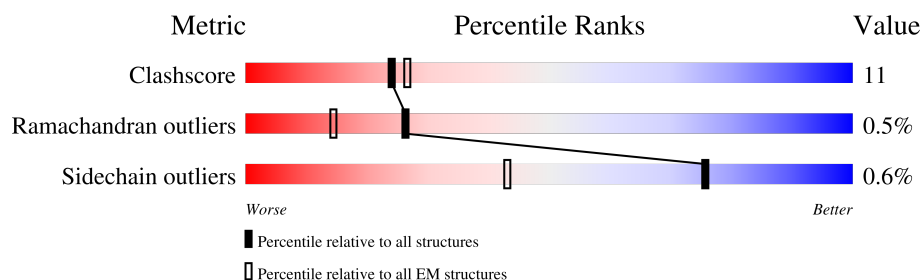
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	C	3859	9% 60% 19% 20%
2	G	3159	.. 96%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 52167 atoms, of which 26380 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 Transformation/transcription domain-associated protein.

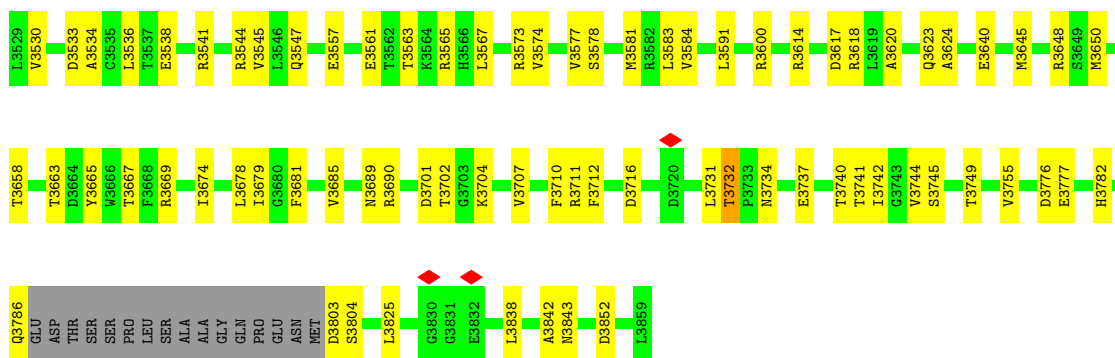
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	3079	50044	15891	25317	4263	4390	183	0	0

- Molecule 2 is a protein called E1A-binding protein p400.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	G	133	2123	669	1063	186	201	4	0	0

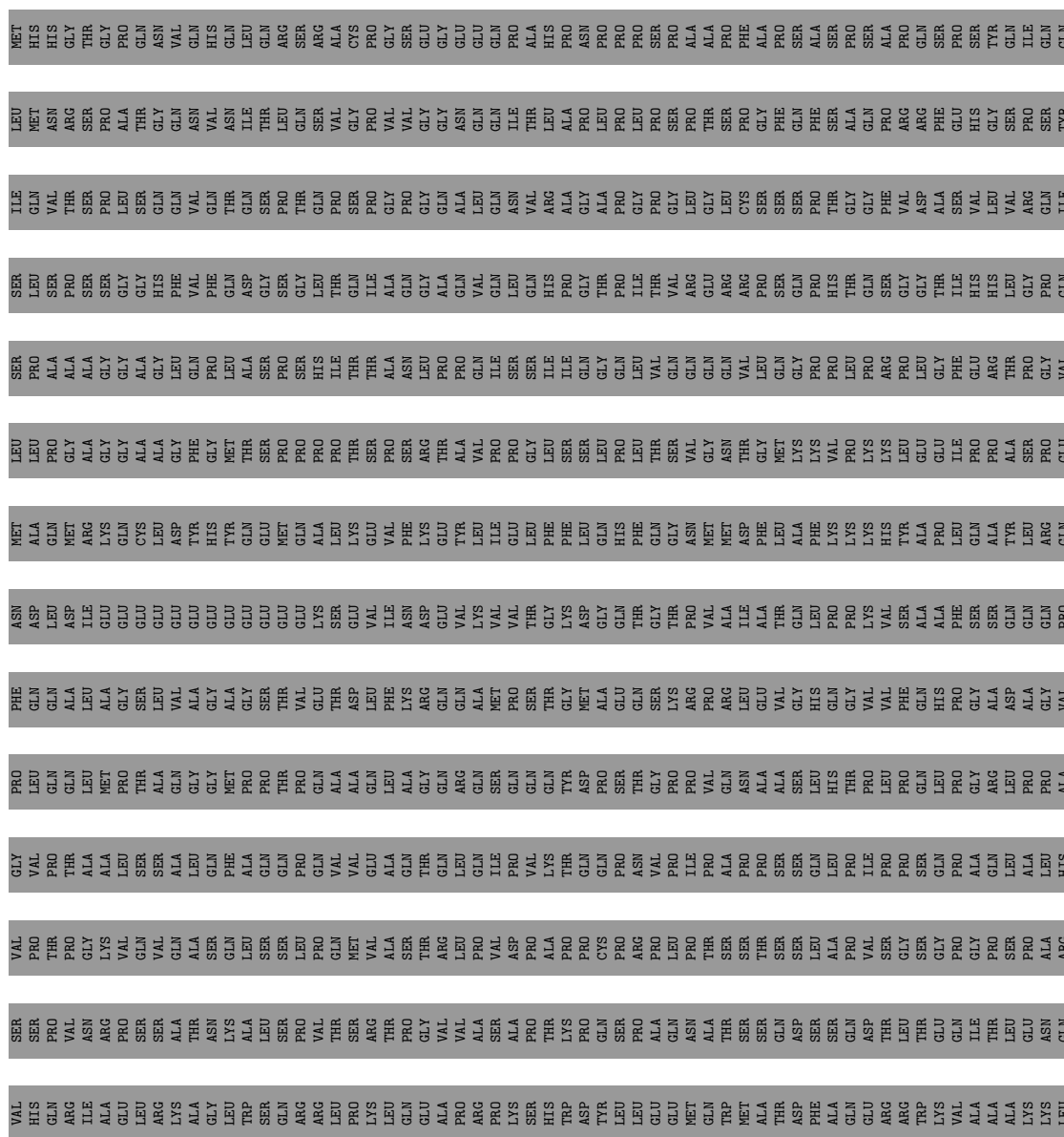






- Molecule 2: E1A-binding protein p400

Chain G: 96%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.397	Depositor
Minimum map value	-1.369	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.451	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.12	0/25236	0.28	3/34128 (0.0%)
2	G	0.64	2/1081 (0.2%)	0.64	5/1468 (0.3%)
All	All	0.17	2/26317 (0.0%)	0.30	8/35596 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2387	PRO	N-CD	16.77	1.71	1.47
2	G	2386	LEU	C-N	7.36	1.51	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1291	PRO	N-CA-C	-10.39	98.02	110.70
1	C	1291	PRO	CB-CA-C	8.68	121.51	110.92
1	C	1295	HIS	CA-C-O	-7.28	113.55	122.36
2	G	2386	LEU	CA-C-N	6.34	127.76	119.84
2	G	2386	LEU	C-N-CA	6.34	127.76	119.84
2	G	2444	ARG	CA-C-N	5.60	127.78	120.28
2	G	2444	ARG	C-N-CA	5.60	127.78	120.28
2	G	2390	LEU	N-CA-C	-5.40	102.47	111.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	2444	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	C	24727	25317	25273	528	0
2	G	1060	1063	1062	46	0
All	All	25787	26380	26335	563	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 11.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2387:PRO:N	2:G:2387:PRO:CD	1.71	1.45
2:G:2433:GLU:O	2:G:2444:ARG:NH1	1.83	1.10
1:C:3578:SER:OG	1:C:3581:MET:N	2.08	0.86
2:G:2378:GLN:NE2	2:G:2382:GLN:OE1	2.09	0.86
1:C:642:MET:HE1	1:C:650:ILE:HD12	1.56	0.84
1:C:2832:ASN:ND2	1:C:3044:TYR:OH	2.13	0.81
1:C:3745:SER:O	1:C:3749:THR:OG1	1.99	0.80
1:C:3617:ASP:OD1	1:C:3618:ARG:N	2.15	0.79
1:C:3544:ARG:NE	1:C:3776:ASP:OD2	2.15	0.79
1:C:3650:MET:HE2	1:C:3650:MET:HA	1.63	0.79
1:C:2743:GLU:OE1	1:C:2743:GLU:N	2.16	0.79
1:C:1400:GLU:N	1:C:1400:GLU:OE1	2.14	0.78
1:C:2293:PHE:O	1:C:2296:SER:OG	2.01	0.78
1:C:446:MET:O	1:C:449:LEU:N	2.15	0.78
1:C:366:THR:O	1:C:370:THR:OG1	1.99	0.78
1:C:2335:LEU:O	1:C:2337:VAL:HG23	1.84	0.78
1:C:1381:GLN:N	1:C:1381:GLN:OE1	2.17	0.77
1:C:2348:GLN:O	1:C:2352:THR:OG1	2.01	0.77
1:C:450:GLU:N	1:C:450:GLU:OE2	2.18	0.77
1:C:411:LEU:HB3	1:C:415:ILE:HD11	1.67	0.76
1:C:1594:HIS:O	1:C:1601:ARG:NH2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2818:GLN:NE2	1:C:2822:ASP:OD1	2.18	0.76
1:C:2189:SER:O	1:C:2191:LYS:N	2.19	0.75
1:C:1136:PRO:O	1:C:1139:SER:OG	2.04	0.74
1:C:1217:CYS:O	1:C:1234:GLN:NE2	2.19	0.74
1:C:2303:GLU:O	1:C:2306:ASN:ND2	2.20	0.74
1:C:2400:MET:SD	1:C:2401:THR:N	2.60	0.74
1:C:1168:MET:O	1:C:1216:ARG:NH1	2.20	0.74
1:C:627:GLU:N	1:C:627:GLU:OE1	2.20	0.74
1:C:1100:MET:O	1:C:1105:LYS:NZ	2.20	0.74
1:C:898:PHE:O	1:C:902:ASN:ND2	2.21	0.73
2:G:2376:LEU:HD22	2:G:2408:VAL:HG11	1.71	0.73
1:C:2393:SER:O	1:C:2397:VAL:HG12	1.88	0.73
1:C:565:THR:HG1	1:C:578:ASN:N	1.86	0.73
1:C:3508:LYS:O	1:C:3510:ASN:N	2.22	0.72
2:G:2367:GLU:O	2:G:2416:ARG:NH2	2.22	0.72
1:C:1081:GLU:N	1:C:1081:GLU:OE1	2.22	0.72
1:C:2788:GLN:OE1	1:C:2788:GLN:N	2.22	0.72
1:C:3701:ASP:OD1	1:C:3702:THR:N	2.23	0.71
1:C:2334:ARG:NE	1:C:2334:ARG:O	2.24	0.71
1:C:561:THR:HG22	1:C:589:TYR:OH	1.92	0.70
1:C:3574:VAL:HG22	1:C:3584:VAL:HG23	1.72	0.69
1:C:651:PHE:O	1:C:655:VAL:N	2.24	0.69
1:C:763:LEU:O	1:C:767:ILE:HG22	1.92	0.69
1:C:3357:ALA:O	1:C:3623:GLN:NE2	2.25	0.69
1:C:2699:THR:HG1	1:C:2700:HIS:HD1	1.41	0.69
1:C:705:GLU:OE1	1:C:705:GLU:N	2.26	0.69
1:C:3479:GLU:OE2	1:C:3495:LYS:NZ	2.18	0.69
1:C:673:ASN:OD1	1:C:674:SER:N	2.27	0.68
1:C:2472:GLU:N	1:C:2472:GLU:OE1	2.25	0.68
1:C:2873:GLU:OE2	1:C:2888:ARG:NE	2.27	0.68
1:C:2479:CYS:SG	1:C:2480:SER:N	2.66	0.68
1:C:1735:TYR:O	1:C:1739:GLU:N	2.26	0.67
1:C:2474:LEU:CD1	1:C:2640:LEU:HD11	2.25	0.67
1:C:557:VAL:HG21	1:C:592:LEU:HD11	1.77	0.67
1:C:2338:MET:SD	1:C:2338:MET:N	2.68	0.67
1:C:1215:MET:O	1:C:1219:THR:OG1	2.09	0.67
1:C:437:GLU:OE1	1:C:439:GLY:N	2.28	0.66
1:C:1668:ARG:NH1	1:C:1712:GLU:OE1	2.28	0.66
2:G:2443:LEU:HD22	2:G:2447:GLN:HB2	1.76	0.66
1:C:2935:GLN:NE2	1:C:2983:ASP:OD1	2.30	0.65
1:C:1295:HIS:O	1:C:1296:LEU:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1373:LEU:HD22	1:C:1386:ILE:HG22	1.78	0.65
1:C:1737:GLU:N	1:C:1737:GLU:OE1	2.30	0.65
1:C:3266:TYR:OH	1:C:3319:GLU:OE1	2.12	0.65
1:C:724:PHE:O	1:C:728:ASN:ND2	2.29	0.65
1:C:2414:ASN:O	1:C:2418:LEU:HD12	1.97	0.65
1:C:2798:ASP:OD2	2:G:2469:LYS:NZ	2.30	0.65
1:C:2172:GLU:O	1:C:2175:SER:OG	2.15	0.64
1:C:1671:TRP:O	1:C:1719:ARG:NH1	2.30	0.64
2:G:2384:LEU:HD13	2:G:2393:VAL:HG23	1.79	0.64
1:C:3360:ASP:OD1	1:C:3361:ALA:N	2.31	0.64
1:C:2340:MET:SD	1:C:2343:ARG:N	2.71	0.64
1:C:3359:SER:N	1:C:3623:GLN:OE1	2.31	0.64
1:C:1048:HIS:O	1:C:1052:VAL:HG23	1.98	0.63
1:C:3838:LEU:O	1:C:3842:ALA:N	2.32	0.63
1:C:1376:CYS:SG	1:C:1379:LEU:HD12	2.37	0.63
1:C:2497:GLU:OE1	1:C:2619:HIS:NE2	2.32	0.63
1:C:1198:VAL:HG11	1:C:1203:VAL:HG22	1.81	0.62
1:C:309:MET:SD	1:C:309:MET:N	2.72	0.62
1:C:2150:ASP:OD1	1:C:2151:LYS:N	2.33	0.62
1:C:1574:MET:HE3	1:C:1574:MET:O	1.99	0.62
1:C:2285:TYR:CD2	1:C:2289:LEU:HD21	2.34	0.62
1:C:372:ARG:NH2	1:C:411:LEU:HD11	2.13	0.62
1:C:2197:ILE:O	1:C:2197:ILE:HG22	1.99	0.62
2:G:2386:LEU:HB3	2:G:2387:PRO:CD	2.29	0.62
1:C:2489:HIS:O	1:C:2664:GLN:NE2	2.33	0.62
1:C:583:PRO:O	1:C:586:THR:OG1	2.16	0.62
1:C:3681:PHE:CE2	1:C:3685:VAL:HG21	2.35	0.62
1:C:3707:VAL:HG21	1:C:3710:PHE:CE2	2.34	0.62
1:C:1433:MET:O	1:C:1439:SER:OG	2.13	0.61
1:C:3190:GLN:OE1	1:C:3191:ASN:N	2.32	0.61
1:C:3142:PHE:O	1:C:3146:VAL:HG12	2.00	0.61
2:G:2387:PRO:O	2:G:2388:LEU:C	2.44	0.61
1:C:3577:VAL:HG23	1:C:3577:VAL:O	2.00	0.61
1:C:1729:MET:SD	1:C:1729:MET:N	2.72	0.61
1:C:1442:LEU:O	1:C:1512:LYS:NZ	2.34	0.61
1:C:1576:GLU:HA	1:C:1579:LEU:HD12	1.83	0.61
1:C:1370:LEU:HA	1:C:1373:LEU:HD12	1.82	0.61
1:C:3481:PRO:O	1:C:3528:TYR:OH	2.10	0.61
1:C:3538:GLU:OE1	1:C:3711:ARG:NH1	2.34	0.61
1:C:3614:ARG:NE	1:C:3645:MET:SD	2.74	0.60
1:C:409:GLU:N	1:C:409:GLU:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2299:LYS:NZ	1:C:2303:GLU:OE1	2.34	0.60
1:C:1199:SER:OG	1:C:1202:ALA:N	2.31	0.60
1:C:3782:HIS:O	1:C:3786:GLN:N	2.34	0.60
1:C:427:VAL:HG11	1:C:560:ILE:HG22	1.82	0.60
1:C:2491:TRP:NE1	1:C:2664:GLN:OE1	2.32	0.59
1:C:252:PRO:O	1:C:256:ASN:ND2	2.35	0.59
1:C:1650:VAL:HG21	1:C:1657:LEU:HD12	1.85	0.59
1:C:783:LEU:HD11	1:C:815:VAL:HG21	1.83	0.59
1:C:1061:PHE:C	1:C:1062:LEU:HD23	2.27	0.59
1:C:2880:MET:O	1:C:2883:LYS:N	2.35	0.59
1:C:1054:VAL:HG11	1:C:1125:ILE:HD13	1.84	0.59
1:C:3731:LEU:O	1:C:3732:THR:HG22	2.03	0.59
2:G:2389:ASN:O	2:G:2390:LEU:C	2.44	0.59
1:C:1015:ARG:NH1	1:C:1088:ASP:OD1	2.36	0.59
1:C:642:MET:HE1	1:C:650:ILE:CD1	2.31	0.58
1:C:642:MET:HE2	1:C:647:PHE:HA	1.84	0.58
1:C:1286:LEU:HG	1:C:1290:VAL:HG23	1.85	0.58
1:C:1454:LEU:H	1:C:1454:LEU:HD23	1.68	0.58
1:C:423:LEU:O	1:C:427:VAL:HG13	2.03	0.58
1:C:549:LEU:O	1:C:552:THR:OG1	2.21	0.58
1:C:2821:GLU:HA	2:G:2468:MET:HE1	1.86	0.58
1:C:1105:LYS:HD2	1:C:1158:LEU:HD23	1.86	0.58
1:C:1325:MET:O	1:C:1379:LEU:HD11	2.04	0.57
1:C:2942:GLU:OE2	1:C:2977:ARG:NH1	2.37	0.57
1:C:3210:ASP:OD1	1:C:3212:LYS:N	2.37	0.57
1:C:348:ILE:HG23	1:C:349:PRO:HD3	1.86	0.57
1:C:2708:LEU:HD11	1:C:3665:TYR:CD1	2.39	0.57
1:C:877:TRP:CE3	1:C:2926:VAL:HG21	2.40	0.57
1:C:2095:ASP:OD1	1:C:2096:THR:N	2.38	0.57
1:C:1221:LEU:O	1:C:1226:ARG:NH1	2.38	0.57
1:C:2169:THR:O	1:C:2173:VAL:HG22	2.04	0.57
1:C:3494:ILE:N	1:C:3494:ILE:HD12	2.19	0.57
1:C:597:MET:HE3	1:C:668:LEU:HD23	1.87	0.57
1:C:2194:GLN:O	1:C:2198:ALA:N	2.38	0.57
1:C:2851:LEU:HD12	1:C:2851:LEU:O	2.04	0.56
1:C:2759:ASP:N	1:C:2759:ASP:OD1	2.39	0.56
1:C:3803:ASP:O	1:C:3804:SER:OG	2.15	0.56
1:C:1080:GLU:N	1:C:1080:GLU:OE1	2.37	0.56
1:C:1419:GLU:N	1:C:1419:GLU:OE1	2.38	0.56
2:G:2388:LEU:HD21	2:G:2401:TRP:HH2	1.70	0.56
2:G:2388:LEU:HD21	2:G:2401:TRP:CH2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2840:TYR:HB2	2:G:2471:THR:HG21	1.88	0.56
1:C:2463:ASP:OD1	1:C:2473:ARG:NH2	2.37	0.56
1:C:2474:LEU:HD13	1:C:2640:LEU:HD11	1.86	0.56
1:C:1391:PHE:CE1	1:C:1409:MET:HE3	2.42	0.55
1:C:2361:ALA:HA	1:C:2364:LEU:HD23	1.87	0.55
1:C:711:LEU:HD12	1:C:711:LEU:O	2.07	0.55
1:C:3237:GLN:OE1	1:C:3547:GLN:NE2	2.38	0.55
1:C:3689:ASN:OD1	1:C:3690:ARG:N	2.40	0.55
1:C:3275:THR:HG23	1:C:3536:LEU:HD11	1.88	0.55
1:C:357:GLU:OE1	1:C:401:LEU:HD23	2.07	0.55
1:C:592:LEU:C	1:C:592:LEU:HD23	2.32	0.55
1:C:1897:HIS:O	1:C:1901:VAL:HG23	2.07	0.55
1:C:3331:ASN:OD1	1:C:3333:HIS:N	2.36	0.55
1:C:1774:GLN:OE1	1:C:1774:GLN:HA	2.07	0.54
1:C:3177:VAL:HG23	1:C:3218:ALA:CB	2.37	0.54
2:G:2386:LEU:HB3	2:G:2387:PRO:HD3	1.90	0.54
1:C:557:VAL:HG21	1:C:592:LEU:CD1	2.37	0.54
1:C:1353:LEU:O	1:C:1357:LYS:N	2.41	0.54
1:C:1343:CYS:O	1:C:1366:ARG:NH2	2.40	0.54
1:C:2201:MET:O	1:C:2205:ASN:N	2.40	0.54
1:C:671:VAL:O	1:C:675:PHE:N	2.40	0.54
1:C:909:SER:OG	1:C:3704:LYS:NZ	2.41	0.54
1:C:1121:VAL:O	1:C:1125:ILE:HG22	2.08	0.54
1:C:2169:THR:O	1:C:2173:VAL:HG13	2.07	0.54
1:C:279:ASP:OD1	1:C:280:PHE:N	2.40	0.54
1:C:979:ASP:OD2	1:C:2521:ILE:HD12	2.08	0.54
1:C:554:VAL:HG21	1:C:631:VAL:HG23	1.89	0.54
1:C:2364:LEU:HD22	1:C:2364:LEU:H	1.71	0.54
1:C:3742:ILE:HD12	1:C:3742:ILE:N	2.22	0.54
1:C:1181:GLN:NE2	1:C:1244:ASP:OD2	2.41	0.54
1:C:2683:VAL:HG22	1:C:2684:PRO:HD3	1.89	0.54
1:C:2962:ASN:OD1	1:C:2963:SER:N	2.41	0.54
1:C:2742:GLN:N	1:C:2743:GLU:OE1	2.41	0.54
1:C:2949:ILE:HD13	1:C:2967:MET:SD	2.47	0.53
1:C:2124:ARG:NH1	1:C:2128:ASN:OD1	2.41	0.53
1:C:775:LEU:O	1:C:779:PHE:N	2.41	0.53
1:C:1373:LEU:CD2	1:C:1386:ILE:HG22	2.37	0.53
1:C:3226:VAL:HG13	1:C:3226:VAL:O	2.06	0.53
1:C:635:PHE:O	1:C:638:VAL:HG12	2.09	0.53
1:C:1113:VAL:O	1:C:1117:VAL:HG23	2.09	0.53
1:C:1913:ALA:O	1:C:1917:ARG:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2376:LEU:HD11	2:G:2421:CYS:SG	2.48	0.53
1:C:1180:GLN:NE2	1:C:1217:CYS:SG	2.81	0.53
2:G:2393:VAL:O	2:G:2394:SER:C	2.52	0.53
1:C:2203:CYS:O	1:C:2207:LYS:NZ	2.42	0.52
1:C:3267:PHE:CE1	1:C:3318:LEU:HD22	2.44	0.52
1:C:1592:LEU:O	1:C:1601:ARG:NH1	2.42	0.52
1:C:2418:LEU:HD12	1:C:2418:LEU:H	1.74	0.52
1:C:3600:ARG:HE	1:C:3650:MET:HE1	1.75	0.52
1:C:2640:LEU:O	1:C:2645:GLN:NE2	2.43	0.52
1:C:2676:VAL:HG11	1:C:2702:LEU:HD22	1.92	0.52
1:C:3275:THR:HG23	1:C:3536:LEU:CD1	2.39	0.52
1:C:1198:VAL:HG11	1:C:1203:VAL:CG2	2.40	0.52
1:C:1428:ARG:HD3	1:C:1432:MET:HE3	1.91	0.52
1:C:284:GLN:HE22	1:C:285:ILE:HD13	1.75	0.52
1:C:2781:GLU:OE2	1:C:2823:HIS:ND1	2.42	0.52
1:C:3423:ASP:OD1	1:C:3424:PHE:N	2.41	0.52
1:C:1659:SER:O	1:C:1661:HIS:ND1	2.40	0.52
1:C:3146:VAL:HG11	1:C:3159:TRP:CZ3	2.45	0.52
2:G:2392:ILE:HD11	2:G:2398:THR:HA	1.91	0.52
1:C:401:LEU:HD22	1:C:401:LEU:H	1.74	0.51
1:C:1259:GLN:O	1:C:1263:SER:N	2.37	0.51
1:C:1535:LEU:HD12	1:C:1536:LEU:N	2.25	0.51
1:C:1292:PRO:HG2	1:C:1335:PHE:CG	2.45	0.51
1:C:1377:ASN:OD1	1:C:1378:TYR:N	2.44	0.51
1:C:450:GLU:O	1:C:454:LEU:HD23	2.11	0.51
1:C:1078:HIS:N	1:C:1088:ASP:OD2	2.39	0.51
1:C:2449:CYS:SG	1:C:2450:ALA:N	2.83	0.51
1:C:2661:HIS:CD2	1:C:2672:LEU:HD13	2.45	0.51
2:G:2384:LEU:HD13	2:G:2393:VAL:CG2	2.41	0.51
1:C:2499:LEU:O	1:C:2502:VAL:HG12	2.10	0.51
1:C:2872:VAL:O	1:C:2876:CYS:N	2.43	0.51
1:C:446:MET:O	1:C:450:GLU:OE2	2.29	0.51
1:C:1556:GLU:OE2	1:C:1594:HIS:NE2	2.41	0.51
1:C:2285:TYR:CE2	1:C:2289:LEU:HD21	2.46	0.51
1:C:3544:ARG:NH1	1:C:3777:GLU:OE1	2.40	0.51
1:C:3618:ARG:NH1	1:C:3640:GLU:OE2	2.43	0.51
1:C:292:ALA:O	1:C:295:ILE:HD11	2.11	0.50
1:C:408:ASP:HB3	1:C:411:LEU:HD13	1.93	0.50
1:C:601:ASP:OD1	1:C:602:ILE:N	2.42	0.50
1:C:2375:VAL:HG21	1:C:2417:PHE:CE1	2.46	0.50
1:C:1460:ASN:OD1	1:C:1462:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1834:GLN:O	1:C:1837:THR:OG1	2.28	0.50
1:C:3648:ARG:O	1:C:3734:ASN:ND2	2.45	0.50
1:C:800:GLN:NE2	1:C:804:ASP:OD1	2.45	0.50
1:C:2908:VAL:HG21	1:C:2944:GLN:HB2	1.93	0.50
1:C:1325:MET:N	1:C:1378:TYR:OH	2.38	0.50
1:C:2494:GLN:OE1	1:C:2494:GLN:N	2.44	0.50
1:C:2865:MET:HG3	1:C:2891:LEU:HD21	1.93	0.50
1:C:2946:ALA:HB1	1:C:2998:HIS:NE2	2.27	0.50
1:C:3306:MET:SD	1:C:3307:GLN:N	2.85	0.50
1:C:418:MET:SD	1:C:419:SER:N	2.84	0.50
1:C:851:LEU:C	1:C:851:LEU:HD12	2.37	0.50
1:C:2153:LEU:HD22	1:C:2199:ALA:HB3	1.93	0.50
1:C:3330:GLU:OE1	1:C:3330:GLU:N	2.39	0.50
1:C:1394:LEU:HD23	1:C:1394:LEU:O	2.12	0.50
1:C:581:LEU:H	1:C:646:THR:HG21	1.77	0.49
1:C:952:SER:O	1:C:960:ARG:NH2	2.45	0.49
1:C:1461:ASP:OD1	1:C:1462:LYS:N	2.44	0.49
1:C:1555:ARG:O	1:C:1559:ILE:HG23	2.12	0.49
1:C:1862:MET:CE	1:C:1865:ALA:HB3	2.41	0.49
1:C:2298:GLN:OE1	1:C:2298:GLN:N	2.45	0.49
1:C:1916:ALA:O	1:C:1920:VAL:HG22	2.12	0.49
1:C:3267:PHE:CZ	1:C:3318:LEU:HD22	2.47	0.49
1:C:1527:ALA:HB1	1:C:1531:LEU:HD21	1.93	0.49
1:C:3193:SER:OG	1:C:3194:LYS:N	2.44	0.49
1:C:3133:ASN:OD1	1:C:3134:LYS:N	2.45	0.49
1:C:1981:LEU:O	1:C:1984:HIS:N	2.45	0.49
1:C:2798:ASP:OD1	1:C:2799:LYS:N	2.45	0.49
1:C:3270:ARG:CZ	1:C:3322:VAL:HG11	2.42	0.49
1:C:3494:ILE:HG21	1:C:3526:TYR:HE2	1.78	0.49
1:C:1290:VAL:HG11	1:C:1323:PHE:CB	2.42	0.49
1:C:1934:ARG:O	1:C:1938:GLY:N	2.46	0.49
1:C:2340:MET:HE1	1:C:2342:MET:HB3	1.95	0.49
1:C:2949:ILE:HD11	1:C:2970:VAL:CG1	2.42	0.49
1:C:1391:PHE:CD1	1:C:1427:MET:HE3	2.46	0.49
1:C:1061:PHE:O	1:C:1062:LEU:O	2.29	0.49
1:C:3533:ASP:OD1	1:C:3534:ALA:N	2.44	0.49
1:C:933:ALA:HB1	1:C:2639:ILE:HD12	1.94	0.48
1:C:2659:GLY:N	2:G:2398:THR:O	2.42	0.48
1:C:3058:LEU:O	1:C:3062:SER:OG	2.24	0.48
1:C:678:ASN:OD1	1:C:678:ASN:C	2.56	0.48
1:C:821:LEU:HD11	1:C:856:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1348:SER:O	1:C:1352:LYS:N	2.45	0.48
1:C:1921:ARG:NH2	1:C:1924:MET:SD	2.87	0.48
1:C:2466:MET:CE	1:C:2498:LEU:HD22	2.43	0.48
1:C:2291:SER:OG	1:C:2295:ARG:NH1	2.42	0.48
1:C:3177:VAL:HG23	1:C:3218:ALA:HB2	1.94	0.48
1:C:3428:VAL:O	1:C:3430:GLY:N	2.45	0.48
1:C:1531:LEU:HD11	1:C:1561:PHE:CE2	2.49	0.48
1:C:1058:CYS:SG	1:C:1126:LEU:HD11	2.53	0.48
1:C:671:VAL:O	1:C:675:PHE:HB2	2.13	0.48
1:C:1574:MET:HE3	1:C:1579:LEU:HD11	1.96	0.48
1:C:1610:ARG:O	1:C:1614:LEU:HD12	2.14	0.48
1:C:2695:TYR:CE1	1:C:2699:THR:HG21	2.48	0.48
1:C:3187:CYS:SG	1:C:3199:LEU:HD22	2.53	0.48
1:C:2269:PHE:CE1	1:C:2273:MET:HE1	2.49	0.47
1:C:3054:VAL:HG11	1:C:3089:LEU:HD23	1.96	0.47
1:C:1865:ALA:HB2	1:C:1886:LEU:HD22	1.97	0.47
1:C:3663:THR:O	1:C:3667:THR:HG22	2.14	0.47
1:C:3685:VAL:CG2	1:C:3825:LEU:HD21	2.43	0.47
1:C:1422:GLN:O	1:C:1426:HIS:ND1	2.47	0.47
1:C:2174:LEU:O	1:C:2178:LEU:HD12	2.14	0.47
1:C:2346:PHE:O	1:C:2350:ILE:N	2.46	0.47
1:C:3322:VAL:HG22	1:C:3577:VAL:HG21	1.95	0.47
1:C:427:VAL:HG11	1:C:560:ILE:CG2	2.44	0.47
1:C:2683:VAL:CG2	1:C:2684:PRO:HD3	2.44	0.47
1:C:744:MET:HE3	1:C:744:MET:HA	1.96	0.47
1:C:1862:MET:HA	1:C:1862:MET:HE3	1.96	0.47
1:C:2205:ASN:OD1	1:C:2206:THR:N	2.47	0.47
1:C:3561:GLU:H	1:C:3561:GLU:CD	2.22	0.47
1:C:655:VAL:N	1:C:656:PRO:HD2	2.30	0.47
1:C:1675:ASN:OD1	1:C:1675:ASN:N	2.43	0.47
1:C:3492:TYR:O	1:C:3492:TYR:CD1	2.68	0.47
1:C:1276:THR:O	1:C:1280:GLU:N	2.48	0.47
1:C:1356:TYR:HB3	1:C:1359:LEU:HD12	1.96	0.47
1:C:3679:ILE:HG23	1:C:3707:VAL:HG21	1.96	0.47
1:C:1261:MET:HE2	1:C:1314:PHE:CB	2.44	0.47
1:C:1540:MET:SD	1:C:1587:MET:HE2	2.55	0.47
1:C:557:VAL:O	1:C:561:THR:HG23	2.14	0.47
1:C:991:PRO:O	1:C:992:ASN:HB3	2.15	0.47
1:C:2368:VAL:CG1	1:C:2399:MET:HE1	2.45	0.47
1:C:2711:GLU:OE2	1:C:3669:ARG:NH2	2.38	0.47
1:C:3102:LEU:HA	1:C:3105:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3146:VAL:O	1:C:3150:ASP:N	2.47	0.47
1:C:2988:TRP:CE2	1:C:3047:ILE:HD13	2.50	0.47
1:C:3054:VAL:HG12	1:C:3058:LEU:CD2	2.45	0.47
1:C:336:LYS:O	1:C:340:THR:HG23	2.15	0.46
1:C:1289:MET:O	1:C:1290:VAL:C	2.59	0.46
1:C:659:VAL:HG11	1:C:692:TYR:HE2	1.80	0.46
1:C:1151:GLU:O	1:C:1157:LYS:NZ	2.40	0.46
1:C:2466:MET:HE2	1:C:2498:LEU:HD22	1.97	0.46
1:C:670:ILE:O	1:C:674:SER:OG	2.33	0.46
1:C:797:LEU:HD23	1:C:797:LEU:H	1.81	0.46
1:C:1454:LEU:HD23	1:C:1454:LEU:N	2.30	0.46
1:C:1671:TRP:CE3	1:C:1696:LEU:HD22	2.51	0.46
2:G:2392:ILE:HG23	2:G:2392:ILE:O	2.15	0.46
1:C:2956:THR:O	1:C:2960:ARG:NH2	2.48	0.46
1:C:3561:GLU:O	1:C:3565:ARG:NH1	2.49	0.46
1:C:411:LEU:N	1:C:411:LEU:HD12	2.30	0.46
1:C:3223:CYS:O	1:C:3226:VAL:HG12	2.16	0.46
1:C:1614:LEU:HD12	1:C:1614:LEU:H	1.81	0.46
1:C:2197:ILE:O	1:C:2197:ILE:CG2	2.64	0.46
1:C:2355:ILE:O	1:C:2358:SER:OG	2.32	0.46
1:C:1061:PHE:O	1:C:1062:LEU:HD23	2.14	0.46
1:C:1992:LEU:O	1:C:2002:GLN:NE2	2.47	0.46
1:C:2774:THR:OG1	1:C:2820:TRP:NE1	2.44	0.46
1:C:3491:HIS:O	1:C:3492:TYR:C	2.58	0.46
1:C:1727:CYS:HA	1:C:1729:MET:HE1	1.96	0.46
1:C:2421:VAL:HG12	1:C:2421:VAL:O	2.16	0.46
1:C:2414:ASN:O	1:C:2417:PHE:N	2.49	0.46
1:C:1015:ARG:NH2	1:C:1094:ASP:OD2	2.49	0.45
1:C:1071:GLN:O	1:C:1073:SER:N	2.47	0.45
1:C:1122:ALA:HA	1:C:1125:ILE:HG22	1.99	0.45
1:C:1286:LEU:CG	1:C:1290:VAL:HG23	2.45	0.45
1:C:3150:ASP:OD2	2:G:2521:ARG:NH2	2.49	0.45
2:G:2443:LEU:HD22	2:G:2447:GLN:CB	2.44	0.45
1:C:859:ASP:OD1	1:C:860:PHE:N	2.50	0.45
1:C:1168:MET:SD	1:C:1213:LEU:HA	2.56	0.45
1:C:1467:MET:N	1:C:1467:MET:HE2	2.31	0.45
1:C:868:VAL:HG22	1:C:868:VAL:O	2.16	0.45
1:C:2217:SER:HA	1:C:2220:MET:HE2	1.99	0.45
1:C:3054:VAL:HG11	1:C:3089:LEU:CD2	2.47	0.45
1:C:3530:VAL:HG22	1:C:3583:LEU:CD2	2.45	0.45
1:C:446:MET:O	1:C:447:ARG:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1566:PRO:HA	1:C:1569:THR:HG22	1.99	0.45
1:C:2300:MET:C	1:C:2300:MET:SD	3.00	0.45
1:C:462:TYR:CD1	1:C:462:TYR:N	2.82	0.45
1:C:2294:MET:HG3	1:C:2347:ILE:HD11	1.99	0.45
1:C:2337:VAL:HG12	1:C:2337:VAL:O	2.16	0.45
1:C:424:LEU:HD21	1:C:555:CYS:HB3	1.98	0.45
1:C:917:THR:HG23	1:C:917:THR:O	2.17	0.45
1:C:1268:ALA:HB2	1:C:1275:VAL:HG22	1.99	0.45
1:C:1475:MET:O	1:C:1478:VAL:HG12	2.17	0.45
1:C:3148:MET:HE1	2:G:2498:LEU:HD23	1.98	0.45
1:C:3744:VAL:O	1:C:3749:THR:HG23	2.16	0.45
1:C:348:ILE:N	1:C:349:PRO:HD2	2.32	0.45
1:C:731:MET:C	1:C:731:MET:SD	3.00	0.45
1:C:1327:LEU:HD13	1:C:1379:LEU:HD13	1.98	0.45
1:C:1643:ILE:HD13	1:C:1643:ILE:N	2.32	0.45
1:C:3741:THR:OG1	1:C:3742:ILE:HD12	2.16	0.45
1:C:1290:VAL:O	1:C:1312:ASN:OD1	2.35	0.45
1:C:1535:LEU:HD12	1:C:1535:LEU:C	2.41	0.45
1:C:1537:GLU:O	1:C:1541:LYS:N	2.39	0.45
1:C:2104:VAL:HG21	1:C:2123:SER:HB3	1.98	0.45
1:C:2368:VAL:CG2	1:C:2413:LEU:HD22	2.47	0.45
2:G:2386:LEU:C	2:G:2387:PRO:CD	2.81	0.45
1:C:865:ILE:O	1:C:869:ARG:N	2.50	0.44
1:C:1318:LEU:O	1:C:1321:ARG:N	2.50	0.44
1:C:1441:THR:O	1:C:1445:VAL:HG22	2.16	0.44
1:C:3001:GLY:O	1:C:3004:THR:OG1	2.35	0.44
1:C:3567:LEU:HD13	1:C:3755:VAL:HG23	2.00	0.44
1:C:3737:GLU:HA	1:C:3740:THR:HG23	1.99	0.44
1:C:1048:HIS:CE1	1:C:2521:ILE:HD11	2.51	0.44
1:C:1862:MET:HE1	1:C:1865:ALA:HB3	1.99	0.44
1:C:2699:THR:OG1	1:C:2700:HIS:ND1	2.34	0.44
1:C:418:MET:C	1:C:418:MET:HE2	2.42	0.44
1:C:838:SER:OG	1:C:840:THR:HG22	2.17	0.44
1:C:2162:VAL:O	1:C:2166:ASN:ND2	2.51	0.44
1:C:3690:ARG:NH2	1:C:3852:ASP:OD2	2.42	0.44
1:C:455:LYS:CG	1:C:553:LEU:HD21	2.48	0.44
1:C:2177:LEU:O	1:C:2181:LEU:HG	2.16	0.44
1:C:2177:LEU:HD22	1:C:2218:ARG:NH2	2.32	0.44
1:C:2375:VAL:HG21	1:C:2417:PHE:HE1	1.81	0.44
2:G:2433:GLU:C	2:G:2433:GLU:OE2	2.60	0.44
1:C:2699:THR:HG1	1:C:2700:HIS:CE1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1293:LYS:O	1:C:1294:LYS:C	2.60	0.44
1:C:1295:HIS:O	1:C:1296:LEU:O	2.36	0.44
1:C:1533:LYS:HB3	1:C:1534:PRO:HD3	2.00	0.44
1:C:1935:MET:HE2	1:C:1935:MET:N	2.32	0.44
1:C:2181:LEU:HD21	1:C:2218:ARG:HG2	1.99	0.44
1:C:2493:LYS:HE3	1:C:2622:THR:HG22	2.00	0.44
1:C:3678:LEU:CD1	1:C:3755:VAL:HG21	2.47	0.44
1:C:1475:MET:CE	1:C:1542:THR:HG21	2.48	0.44
1:C:3235:ILE:HD11	1:C:3257:VAL:HG11	2.00	0.44
1:C:3266:TYR:CD1	1:C:3315:LEU:HD12	2.52	0.44
1:C:3731:LEU:HD23	1:C:3843:ASN:HB3	1.99	0.44
1:C:879:THR:HG23	1:C:891:ALA:HB1	2.00	0.44
1:C:2327:SER:HA	1:C:2330:LEU:HD23	1.99	0.44
2:G:2384:LEU:CD1	2:G:2393:VAL:HG23	2.46	0.44
1:C:824:LEU:HD11	1:C:828:MET:HE1	1.99	0.43
1:C:1033:ASP:C	1:C:1033:ASP:OD1	2.61	0.43
1:C:2189:SER:O	1:C:2192:PRO:HD2	2.18	0.43
1:C:1817:ASP:N	1:C:1818:PRO:CD	2.81	0.43
1:C:2707:THR:HG22	1:C:2751:LEU:HD13	2.01	0.43
1:C:988:LEU:HG	1:C:1125:ILE:HD11	2.00	0.43
1:C:1774:GLN:OE1	1:C:1777:LEU:HD22	2.18	0.43
1:C:1319:GLN:N	1:C:1320:PRO:CD	2.82	0.43
1:C:2652:ILE:HG21	1:C:2679:MET:HE1	2.01	0.43
1:C:3530:VAL:HG22	1:C:3583:LEU:HD21	1.99	0.43
1:C:3617:ASP:OD1	1:C:3617:ASP:C	2.61	0.43
2:G:2506:ASP:OD1	2:G:2506:ASP:N	2.49	0.43
1:C:1170:ARG:C	1:C:1171:LEU:HD22	2.44	0.43
1:C:1291:PRO:HB3	1:C:1332:HIS:NE2	2.34	0.43
1:C:1579:LEU:O	1:C:1585:SER:OG	2.37	0.43
1:C:2368:VAL:HG23	1:C:2413:LEU:HD22	2.01	0.43
1:C:2686:ILE:O	1:C:2688:ILE:HD12	2.18	0.43
1:C:2809:ALA:O	1:C:2810:SER:OG	2.25	0.43
1:C:3169:LYS:O	1:C:3170:GLU:HG2	2.18	0.43
1:C:1736:MET:SD	1:C:1736:MET:N	2.91	0.43
1:C:3199:LEU:HD12	1:C:3231:TRP:CZ3	2.54	0.43
1:C:2417:PHE:CD1	1:C:2417:PHE:C	2.96	0.43
1:C:2707:THR:CG2	1:C:2751:LEU:HD13	2.48	0.43
1:C:3147:GLN:OE1	2:G:2509:LEU:HD13	2.19	0.43
1:C:3578:SER:OG	1:C:3581:MET:O	2.27	0.43
1:C:3716:ASP:OD1	1:C:3716:ASP:N	2.49	0.43
1:C:413:SER:OG	1:C:545:ASP:OD2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1059:GLY:N	1:C:1060:PRO:HD3	2.34	0.43
1:C:3488:LYS:O	1:C:3488:LYS:HG3	2.17	0.43
1:C:1778:ASN:HB2	1:C:1779:PRO:HD3	2.01	0.43
2:G:2379:ALA:HB2	2:G:2407:VAL:HG11	2.01	0.43
1:C:1824:MET:SD	1:C:1824:MET:N	2.91	0.42
1:C:2656:LEU:HD23	1:C:2672:LEU:HD11	2.01	0.42
1:C:1467:MET:HE2	1:C:1467:MET:HA	2.01	0.42
1:C:1762:PRO:C	1:C:1764:PHE:H	2.27	0.42
1:C:2911:ALA:CB	1:C:2940:ILE:HD11	2.49	0.42
1:C:3161:ASP:OD1	1:C:3183:TYR:OH	2.29	0.42
1:C:3304:MET:O	1:C:3308:ARG:N	2.50	0.42
1:C:673:ASN:O	1:C:677:ALA:HB2	2.19	0.42
1:C:2958:LEU:HD11	1:C:3005:TRP:HB2	2.00	0.42
1:C:3516:LEU:HD22	1:C:3530:VAL:HG23	2.00	0.42
2:G:2384:LEU:HD11	2:G:2392:ILE:HA	2.01	0.42
2:G:2393:VAL:HG12	2:G:2394:SER:N	2.34	0.42
1:C:1543:GLU:OE1	1:C:1587:MET:HE1	2.20	0.42
1:C:2323:LEU:HD12	1:C:2323:LEU:O	2.18	0.42
1:C:3541:ARG:NH2	1:C:3712:PHE:O	2.52	0.42
1:C:817:LEU:HD23	1:C:817:LEU:H	1.85	0.42
1:C:951:LYS:CG	1:C:1027:MET:HE1	2.50	0.42
1:C:1293:LYS:HA	1:C:1293:LYS:HD2	1.92	0.42
1:C:1371:ASN:ND2	1:C:1408:CYS:SG	2.93	0.42
1:C:1909:LEU:HA	1:C:1963:ILE:HD13	2.01	0.42
1:C:2297:LEU:O	1:C:2301:VAL:N	2.52	0.42
1:C:3591:LEU:H	1:C:3591:LEU:HD23	1.83	0.42
1:C:1718:LEU:HD11	1:C:1764:PHE:CZ	2.54	0.42
1:C:1761:ASP:O	1:C:1763:ASN:ND2	2.52	0.42
1:C:2851:LEU:HD12	1:C:2851:LEU:C	2.45	0.42
1:C:2932:PRO:O	1:C:2936:ALA:N	2.51	0.42
1:C:3192:GLU:N	1:C:3230:GLN:OE1	2.53	0.42
2:G:2387:PRO:HG2	2:G:2390:LEU:HD12	2.02	0.42
1:C:3545:VAL:HG11	1:C:3710:PHE:C	2.44	0.42
2:G:2384:LEU:HD12	2:G:2388:LEU:O	2.18	0.42
1:C:1406:GLU:OE2	1:C:1450:SER:OG	2.36	0.42
1:C:1728:ASN:HD21	1:C:1732:LEU:HD13	1.85	0.42
2:G:2398:THR:O	2:G:2398:THR:OG1	2.37	0.42
1:C:992:ASN:O	1:C:996:LYS:N	2.34	0.42
1:C:2329:GLU:O	1:C:2333:THR:N	2.46	0.42
1:C:2800:ALA:O	1:C:2804:HIS:ND1	2.42	0.42
1:C:2880:MET:O	1:C:2884:VAL:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3115:LYS:O	1:C:3118:THR:OG1	2.36	0.42
1:C:3741:THR:CB	1:C:3742:ILE:HD12	2.50	0.42
1:C:1574:MET:CE	1:C:1579:LEU:HD11	2.49	0.42
1:C:2368:VAL:HG12	1:C:2399:MET:HE1	2.02	0.42
1:C:2628:THR:O	1:C:2632:LEU:N	2.52	0.42
1:C:2847:ILE:HG22	1:C:2848:ASN:N	2.35	0.42
1:C:2949:ILE:HD11	1:C:2970:VAL:HG13	2.02	0.42
1:C:3509:HIS:CG	1:C:3510:ASN:N	2.87	0.42
2:G:2467:LEU:O	2:G:2471:THR:HG23	2.20	0.42
1:C:1191:MET:HE1	1:C:1259:GLN:CB	2.49	0.41
1:C:1434:LEU:HD21	1:C:1463:PHE:CD1	2.55	0.41
1:C:2474:LEU:HB3	1:C:2648:LEU:HD11	2.02	0.41
1:C:2957:ASN:OD1	1:C:2957:ASN:N	2.50	0.41
1:C:1050:THR:OG1	1:C:1118:ILE:HG22	2.20	0.41
1:C:1052:VAL:HG22	1:C:2521:ILE:HG13	2.01	0.41
1:C:1740:ILE:HB	1:C:1741:PRO:HD3	2.02	0.41
1:C:1865:ALA:O	1:C:1869:LEU:N	2.52	0.41
1:C:2248:LYS:HE3	1:C:2249:VAL:HG13	2.01	0.41
1:C:2773:GLU:HB2	1:C:2796:ALA:HB2	2.02	0.41
1:C:554:VAL:HG23	1:C:555:CYS:N	2.36	0.41
1:C:2199:ALA:O	1:C:2202:THR:OG1	2.36	0.41
1:C:2846:HIS:O	2:G:2413:ARG:NH1	2.51	0.41
1:C:3122:TYR:CZ	2:G:2498:LEU:HD21	2.56	0.41
1:C:3369:ASN:O	1:C:3373:LYS:N	2.48	0.41
1:C:565:THR:OG1	1:C:578:ASN:N	2.50	0.41
1:C:817:LEU:HD23	1:C:817:LEU:N	2.36	0.41
1:C:935:LEU:HD11	1:C:2636:LEU:HB3	2.02	0.41
1:C:1292:PRO:HG2	1:C:1335:PHE:CD1	2.55	0.41
1:C:1881:TYR:HB2	1:C:1919:ILE:HG21	2.02	0.41
1:C:1949:ILE:HG21	1:C:1961:VAL:HG12	2.03	0.41
1:C:2206:THR:O	1:C:2207:LYS:CG	2.68	0.41
1:C:3650:MET:HA	1:C:3650:MET:CE	2.43	0.41
1:C:899:GLY:O	1:C:903:ARG:NH2	2.53	0.41
1:C:1177:LEU:HD13	1:C:1234:GLN:HA	2.00	0.41
1:C:1905:PHE:CD1	1:C:1927:LEU:HD21	2.55	0.41
1:C:3370:PHE:O	1:C:3374:LEU:N	2.54	0.41
1:C:3731:LEU:O	1:C:3732:THR:O	2.39	0.41
1:C:978:GLU:OE1	1:C:2520:SER:OG	2.27	0.41
1:C:1128:SER:OG	1:C:1130:GLU:OE2	2.32	0.41
1:C:2098:VAL:HG12	1:C:2102:ILE:CD1	2.51	0.41
1:C:2821:GLU:HB2	2:G:2468:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3574:VAL:CG2	1:C:3584:VAL:HG23	2.47	0.41
1:C:915:VAL:HG23	1:C:915:VAL:O	2.21	0.41
1:C:2850:TYR:CE1	1:C:2872:VAL:HG23	2.56	0.41
1:C:3105:ILE:HD11	1:C:3125:LYS:HB2	2.02	0.41
2:G:2384:LEU:HD11	2:G:2392:ILE:CA	2.51	0.41
1:C:597:MET:HE3	1:C:668:LEU:CD2	2.50	0.41
1:C:985:TYR:O	1:C:989:ALA:N	2.52	0.41
1:C:1467:MET:HE2	1:C:1467:MET:CA	2.51	0.41
1:C:1524:ILE:O	1:C:1524:ILE:HG23	2.20	0.41
1:C:1575:MET:O	1:C:1578:THR:OG1	2.35	0.41
1:C:1760:ASN:O	1:C:1761:ASP:C	2.63	0.41
1:C:2497:GLU:HB2	1:C:2615:VAL:HG13	2.03	0.41
1:C:2773:GLU:CB	1:C:2796:ALA:HB2	2.51	0.41
1:C:3509:HIS:CG	1:C:3510:ASN:H	2.38	0.41
1:C:3557:GLU:O	1:C:3563:THR:OG1	2.37	0.41
1:C:1290:VAL:HB	1:C:1291:PRO:HD3	2.03	0.41
1:C:1520:LEU:O	1:C:1520:LEU:HD23	2.20	0.41
1:C:2597:LYS:O	1:C:2601:THR:HG23	2.22	0.41
1:C:3485:LEU:HD12	1:C:3573:ARG:HG3	2.04	0.41
2:G:2443:LEU:HB3	2:G:2448:ILE:HG23	2.02	0.41
1:C:648:LYS:O	1:C:652:GLN:HG2	2.20	0.40
1:C:873:MET:HE2	1:C:902:ASN:HA	2.02	0.40
1:C:876:LEU:O	1:C:879:THR:HG22	2.21	0.40
1:C:2219:LEU:HD11	1:C:2243:TYR:CD1	2.56	0.40
1:C:2423:TYR:CD1	1:C:2423:TYR:C	2.97	0.40
1:C:2821:GLU:CB	2:G:2468:MET:HE1	2.51	0.40
1:C:3545:VAL:HG11	1:C:3710:PHE:O	2.21	0.40
1:C:3620:ALA:O	1:C:3624:ALA:N	2.46	0.40
1:C:1709:GLY:O	1:C:1712:GLU:N	2.48	0.40
1:C:2201:MET:HE2	1:C:2201:MET:HB2	1.97	0.40
1:C:3180:ILE:HG21	1:C:3219:VAL:HG23	2.03	0.40
2:G:2389:ASN:C	2:G:2391:THR:N	2.79	0.40
2:G:2398:THR:O	2:G:2399:PRO:C	2.62	0.40
1:C:255:MET:HG3	1:C:256:ASN:H	1.86	0.40
1:C:1917:ARG:HA	1:C:1920:VAL:HG22	2.03	0.40
1:C:2306:ASN:N	1:C:2307:PRO:CD	2.84	0.40
1:C:2368:VAL:O	1:C:2372:GLU:N	2.51	0.40
1:C:3491:HIS:CD2	1:C:3491:HIS:H	2.38	0.40
1:C:972:VAL:HG23	1:C:2509:ILE:HG21	2.03	0.40
1:C:1018:PHE:HE1	1:C:1049:TYR:HH	1.66	0.40
1:C:2858:ARG:NH1	1:C:2989:SER:OG	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3158:MET:HA	1:C:3158:MET:HE2	2.02	0.40
1:C:3567:LEU:CD2	1:C:3674:ILE:HG23	2.52	0.40
1:C:3658:THR:O	1:C:3658:THR:HG22	2.21	0.40
2:G:2433:GLU:O	2:G:2444:ARG:CZ	2.62	0.40
1:C:943:ILE:HD11	1:C:970:PHE:CB	2.51	0.40
1:C:1074:THR:O	1:C:1074:THR:HG22	2.21	0.40
1:C:1968:VAL:HG11	1:C:1985:MET:HE3	2.04	0.40
1:C:2470:VAL:HG22	1:C:2502:VAL:HG11	2.04	0.40
1:C:2746:ASP:OD1	1:C:2768:ARG:NH1	2.45	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	C	3015/3859 (78%)	2824 (94%)	179 (6%)	12 (0%)	30	59
2	G	127/3159 (4%)	114 (90%)	9 (7%)	4 (3%)	3	18
All	All	3142/7018 (45%)	2938 (94%)	188 (6%)	16 (0%)	26	54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1062	LEU
1	C	2190	PHE
1	C	2449	CYS
1	C	3509	HIS
2	G	2393	VAL
1	C	678	ASN
1	C	1296	LEU
2	G	2386	LEU
2	G	2387	PRO

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Mol	Chain	Res	Type
2	G	2388	LEU
1	C	1292	PRO
1	C	857	GLN
1	C	981	LYS
1	C	1285	VAL
1	C	1762	PRO
1	C	3732	THR

5.3.2 Protein sidechains ⓘ

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	C	2742/3423 (80%)	2730 (100%)	12 (0%)	84	83
2	G	119/2663 (4%)	113 (95%)	6 (5%)	22	49
All	All	2861/6086 (47%)	2843 (99%)	18 (1%)	76	80

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

Mol	Chain	Res	Type
1	C	250	PHE
1	C	697	LEU
1	C	758	LEU
1	C	882	ASN
1	C	1287	GLN
1	C	1289	MET
1	C	1290	VAL
1	C	1293	LYS
1	C	2289	LEU
1	C	2466	MET
1	C	2670	SER
1	C	2924	HIS
2	G	2384	LEU
2	G	2386	LEU
2	G	2389	ASN
2	G	2390	LEU

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Mol	Chain	Res	Type
2	G	2392	ILE
2	G	2394	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	284	GLN
1	C	315	GLN
1	C	326	HIS
1	C	405	ASN
1	C	425	ASN
1	C	652	GLN
1	C	836	ASN
1	C	920	GLN
1	C	982	HIS
1	C	1005	HIS
1	C	1048	HIS
1	C	1078	HIS
1	C	1134	GLN
1	C	1287	GLN
1	C	1303	ASN
1	C	1312	ASN
1	C	1371	ASN
1	C	1443	ASN
1	C	1728	ASN
1	C	1803	ASN
1	C	1842	HIS
1	C	2166	ASN
1	C	2377	ASN
1	C	2464	ASN
1	C	2818	GLN
1	C	2832	ASN
1	C	2928	HIS
1	C	2935	GLN
1	C	2950	ASN
1	C	2961	ASN
1	C	2987	HIS
1	C	3088	GLN
1	C	3165	ASN
1	C	3435	HIS
1	C	3474	GLN
1	C	3566	HIS

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Mol	Chain	Res	Type
2	G	2427	ASN
2	G	2457	HIS

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.

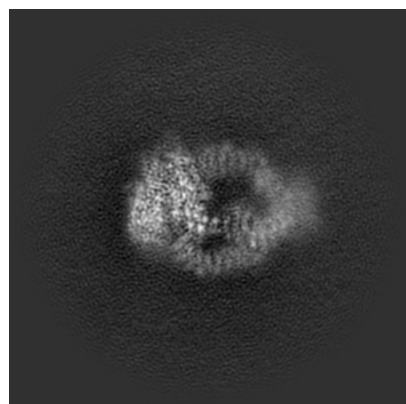
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45176. These allow visual inspection of the internal detail of the map and identification of artifacts.

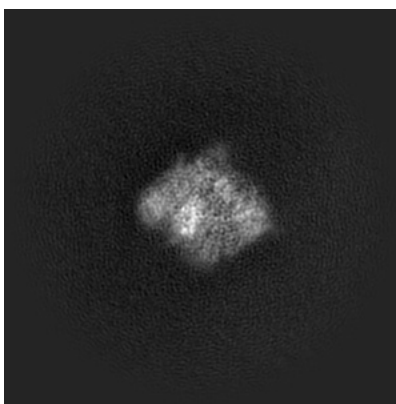
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

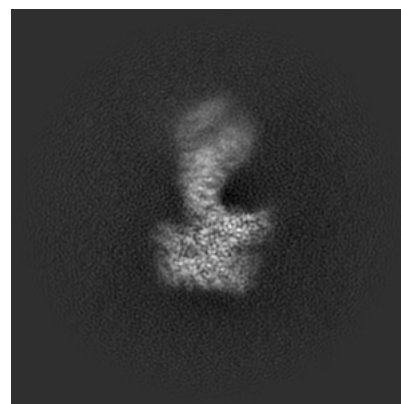
6.1.1 Primary map



X

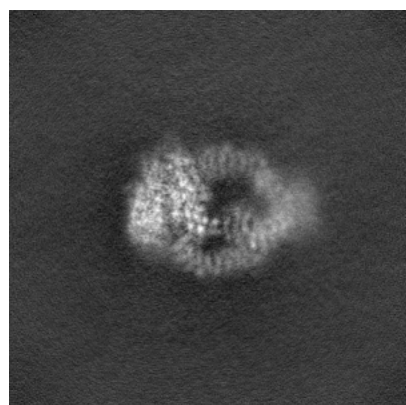


Y

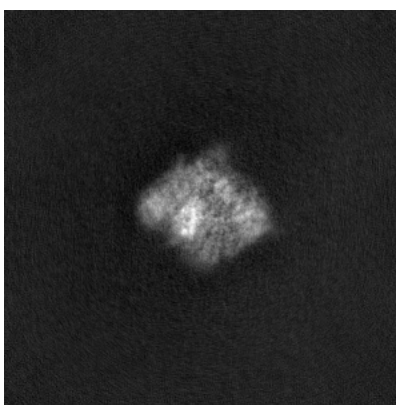


Z

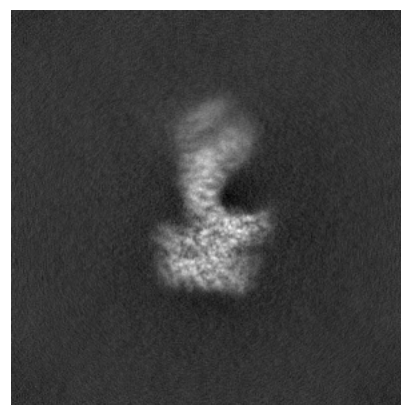
6.1.2 Raw map



X



Y

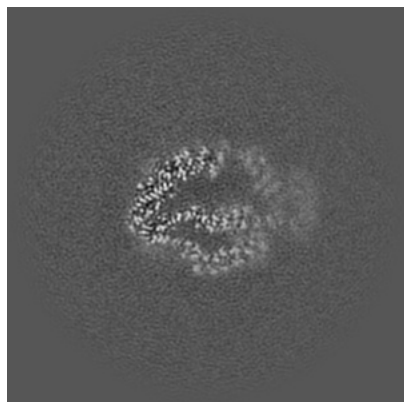


Z

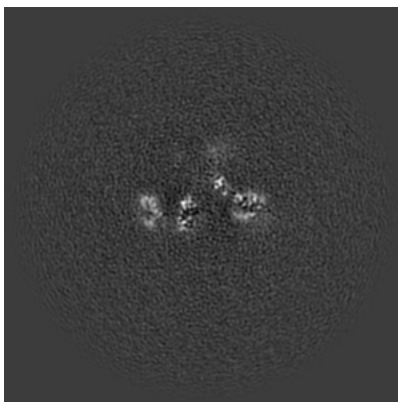
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

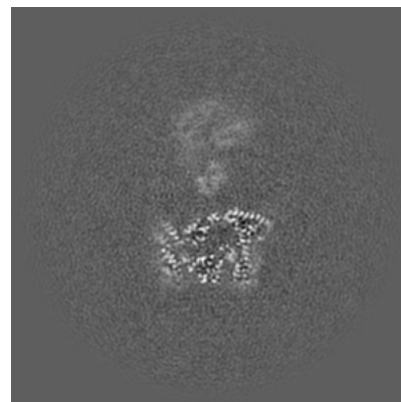
6.2.1 Primary map



X Index: 180

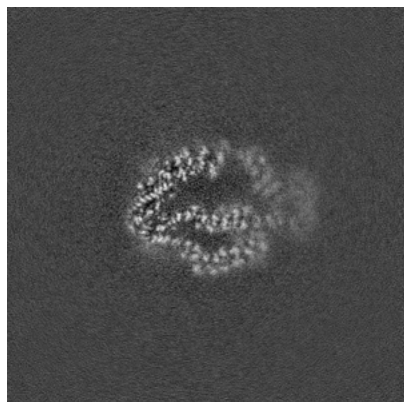


Y Index: 180

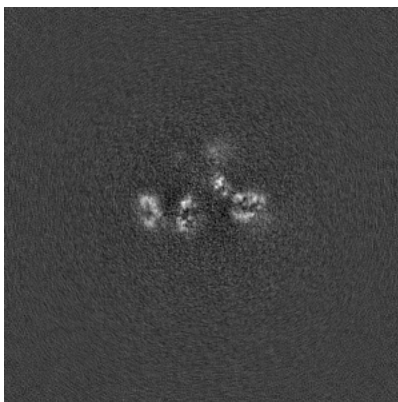


Z Index: 180

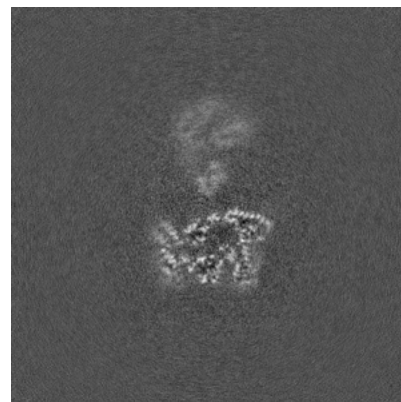
6.2.2 Raw map



X Index: 180



Y Index: 180

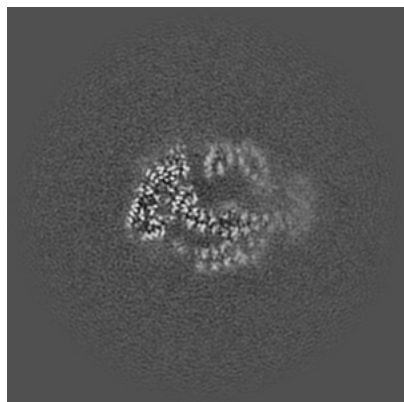


Z Index: 180

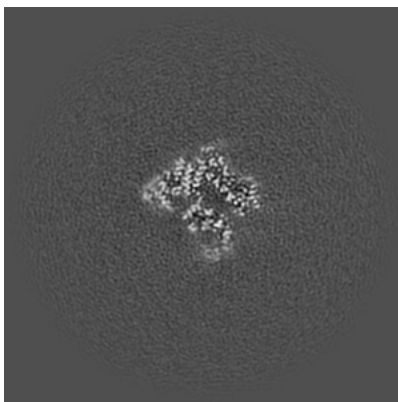
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

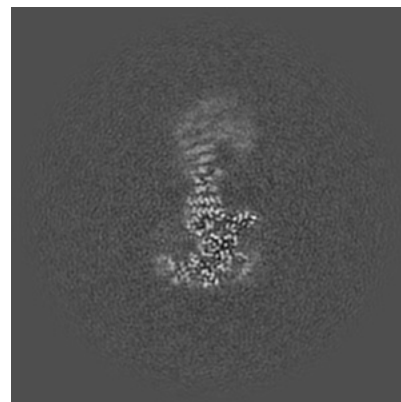
6.3.1 Primary map



X Index: 173

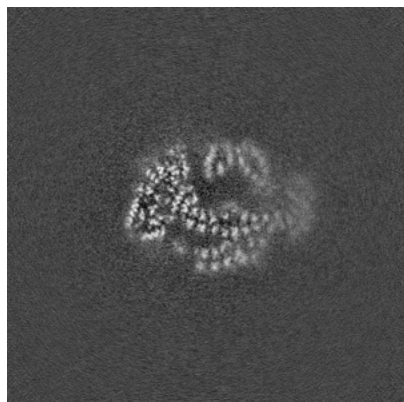


Y Index: 162

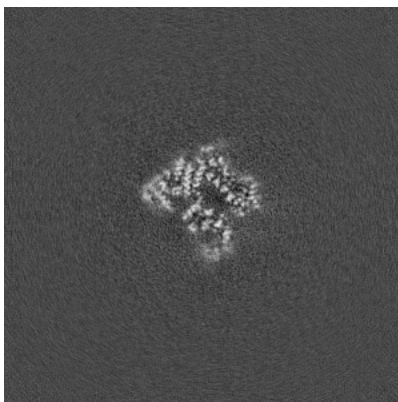


Z Index: 170

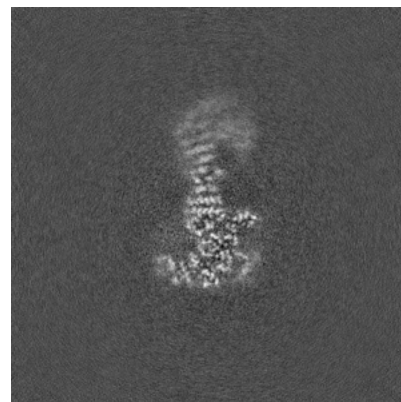
6.3.2 Raw map



X Index: 173



Y Index: 162

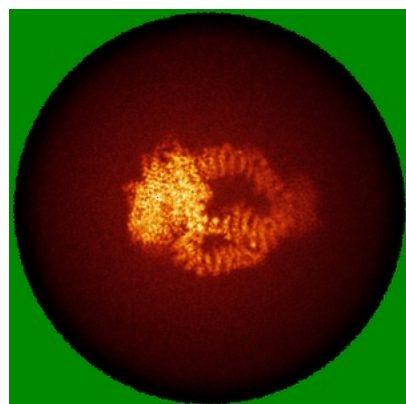


Z Index: 170

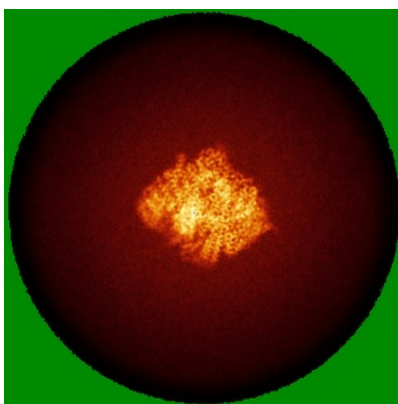
The images above show the largest variance slices of the map in three orthogonal directions.

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

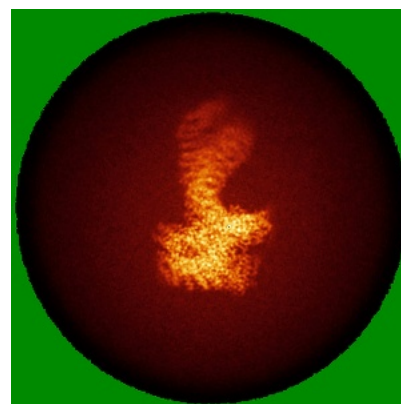
6.4.1 Primary map



X

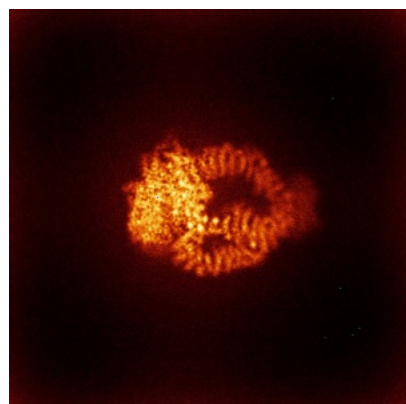


Y

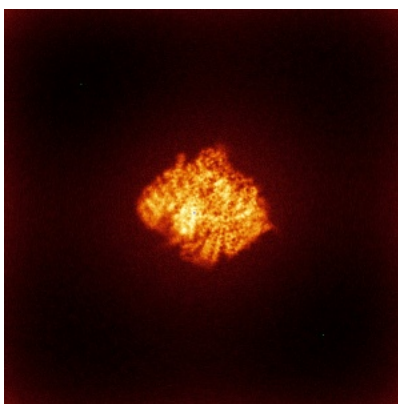


Z

6.4.2 Raw map



X



Y

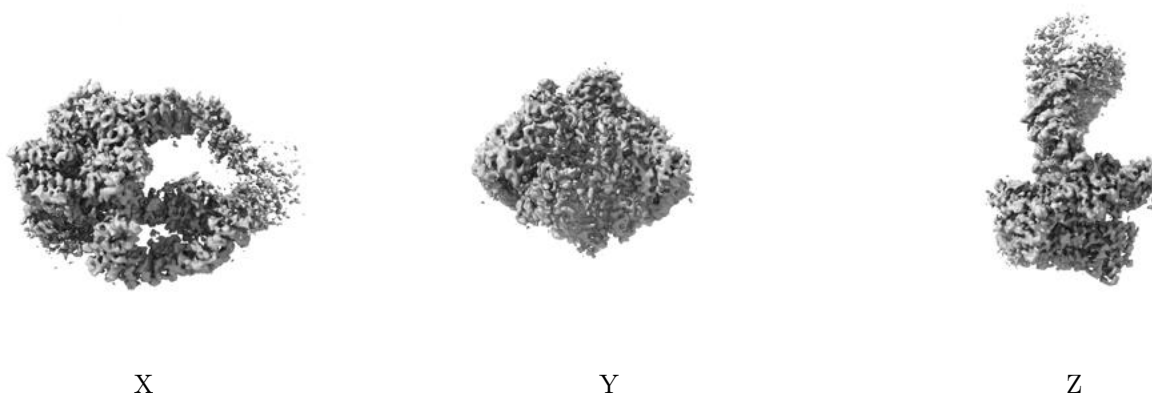


Z

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.

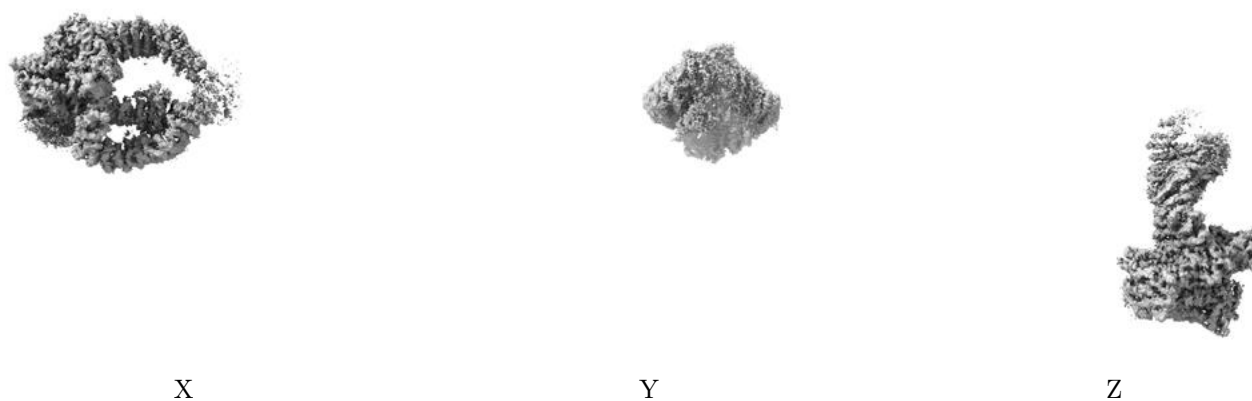
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.451. 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



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

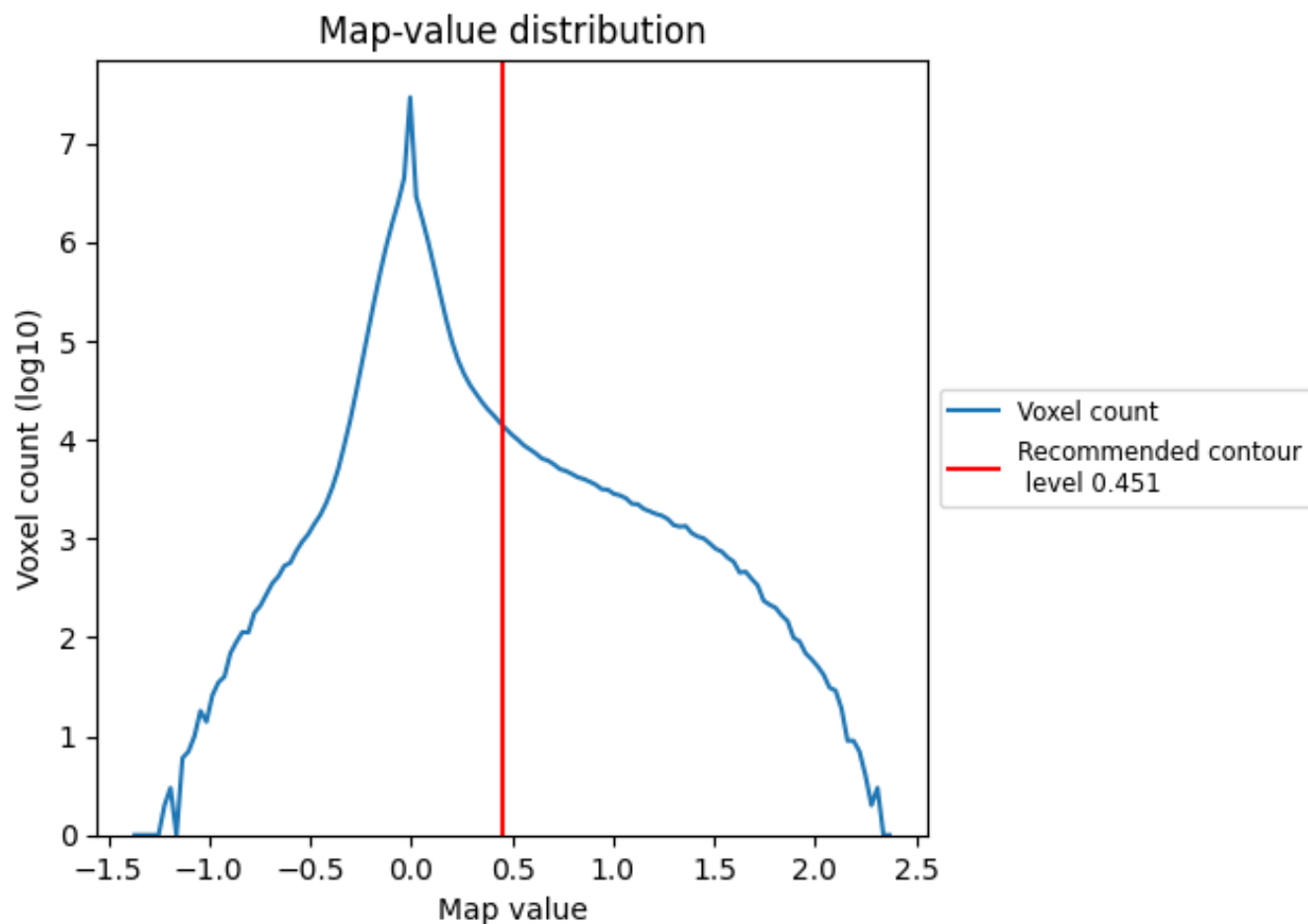
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

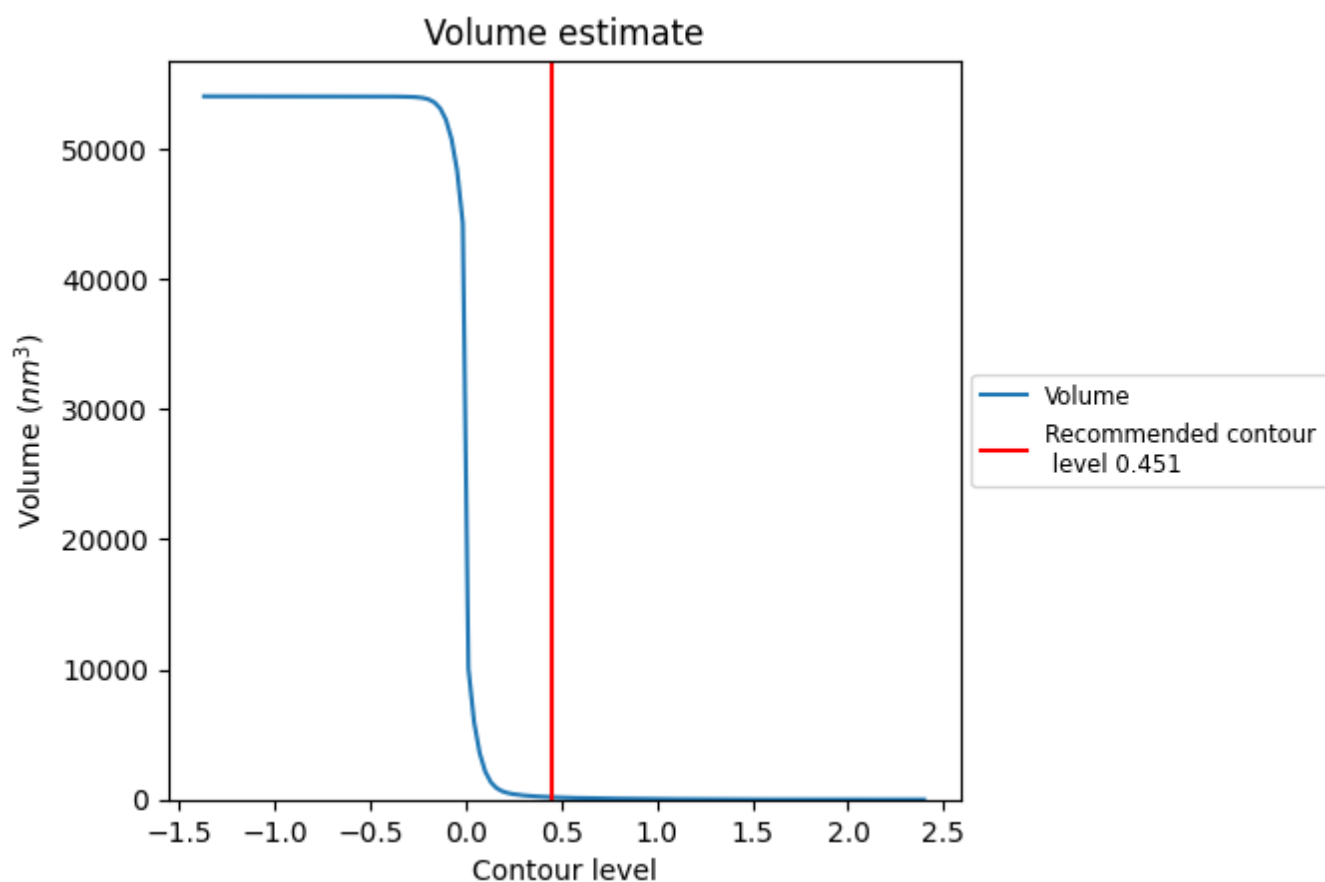
This section contains the results of statistical analysis of the map.

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.

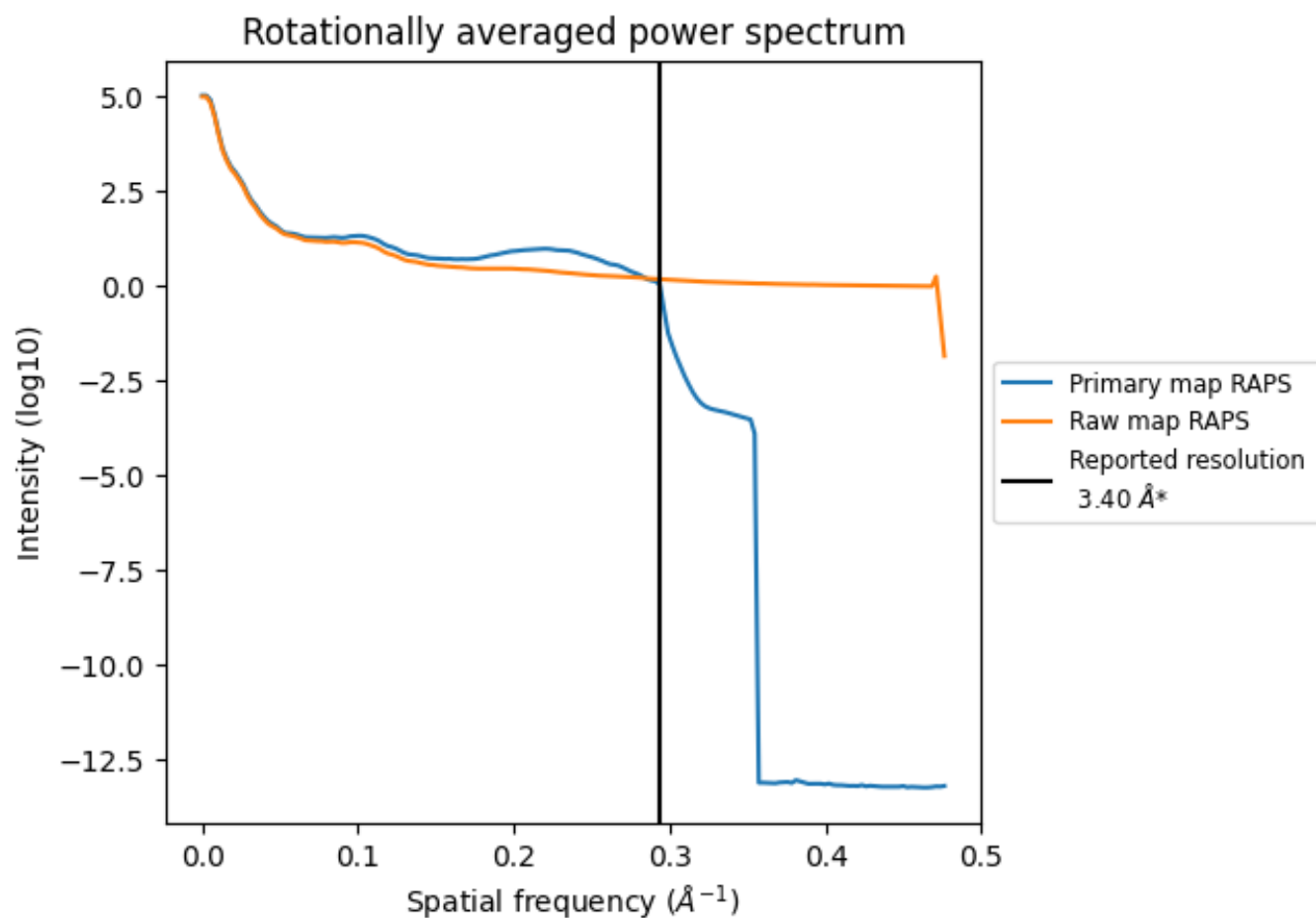
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm³; this corresponds to an approximate mass of 164 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

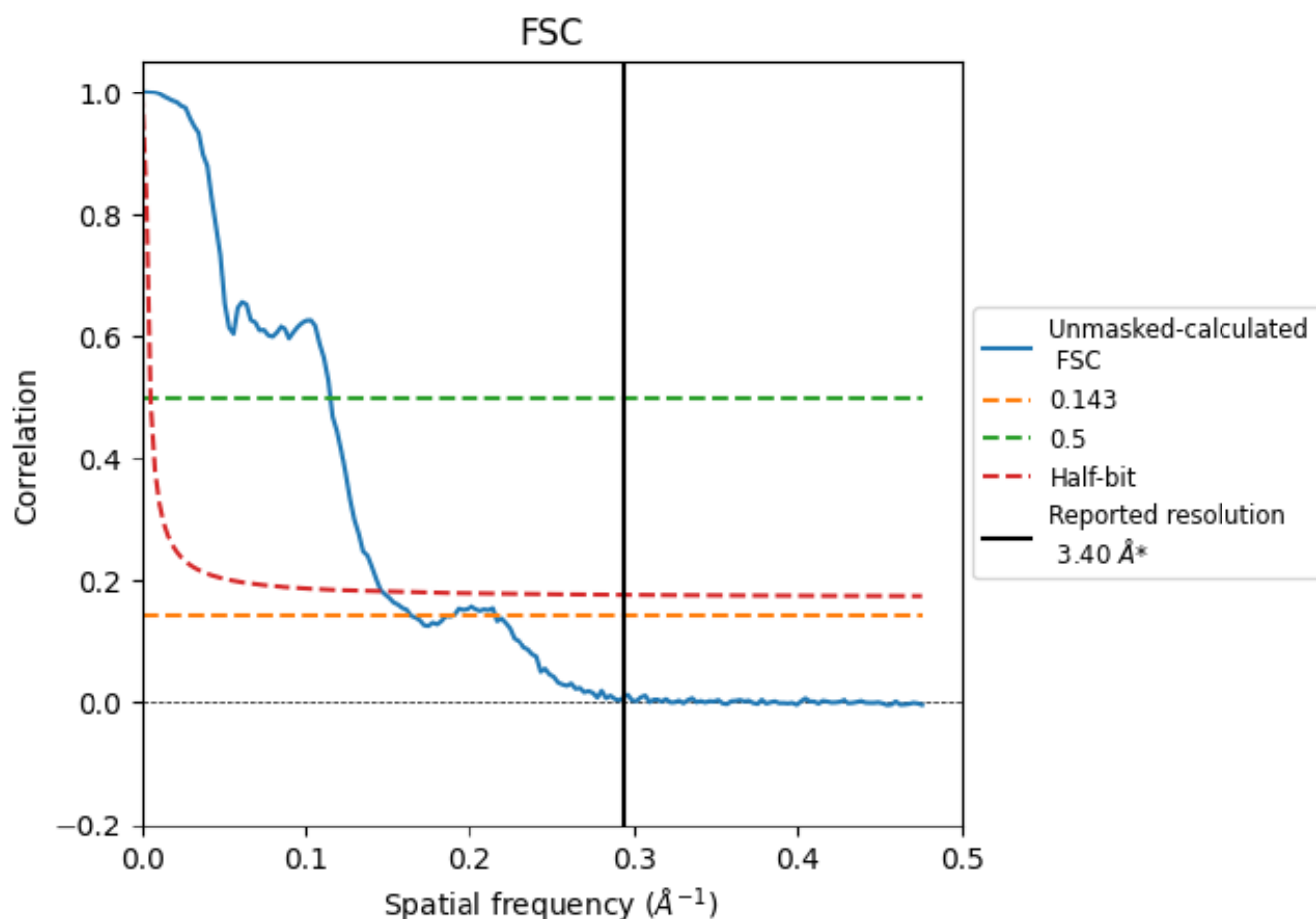


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

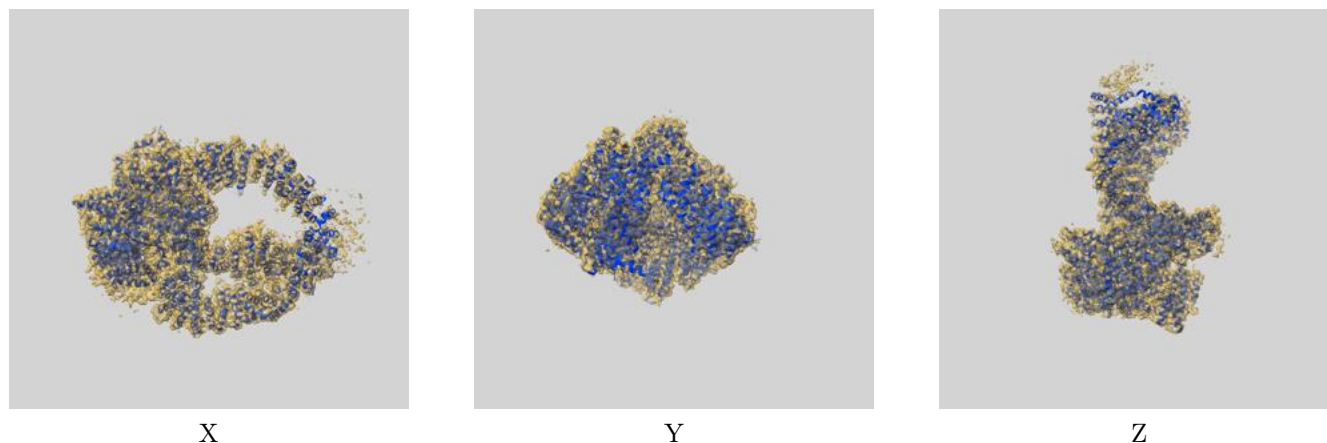
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.10	8.70	6.83

*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 6.10 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

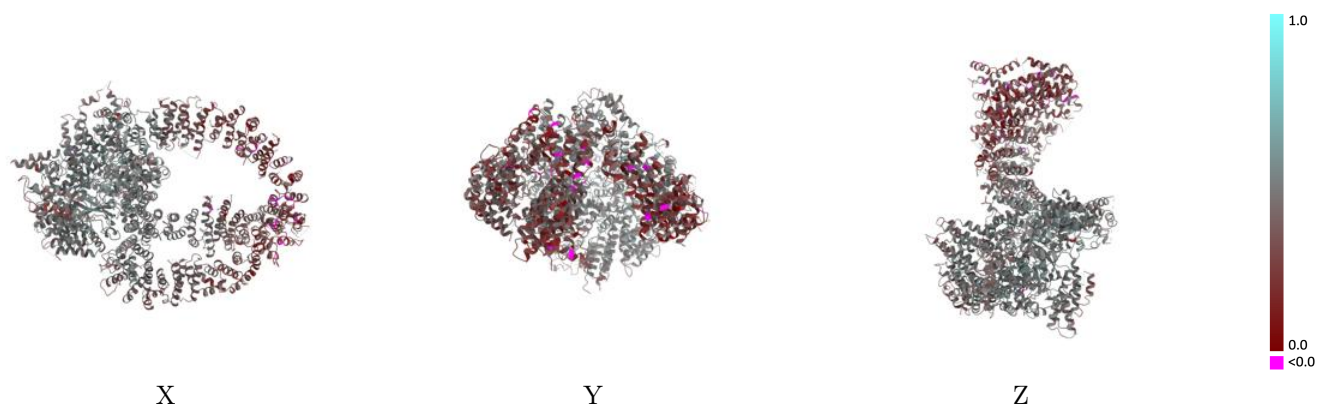
This section contains information regarding the fit between EMDB map EMD-45176 and PDB model 9C47. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



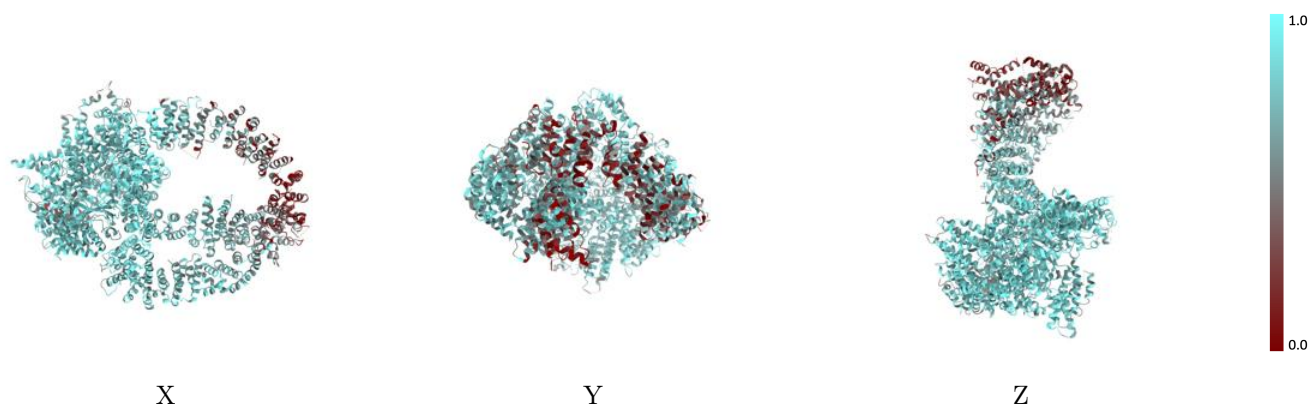
The images above show the 3D surface view of the map at the recommended contour level 0.451 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



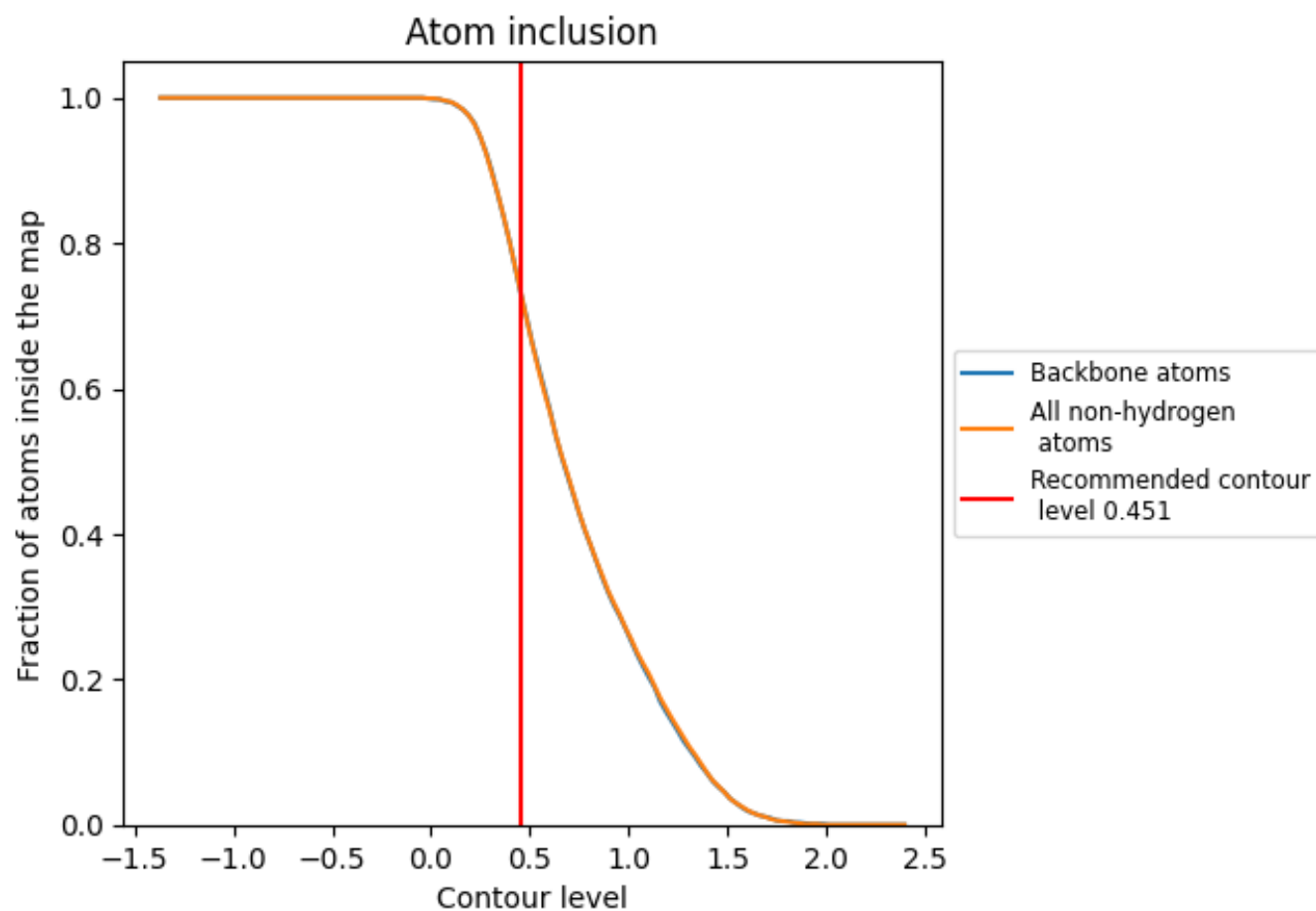
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.451).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 74% 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 (0.451) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.4200
C	0.7460	0.4200
G	0.7250	0.4210

