Full wwPDB EM Validation Report ⓘ

Sep 17, 2023 – 12:20 PM JST

PDB ID	:	7X6V
EMDB ID	:	EMD-33028
Title	:	lymphocytic choriomeningitis virus polymerase- Matrix Z Protein Complex (LCMV L-Z Complex)
Authors	:	Liu, L.; Lou, Z.
Deposited on	:	2022-03-08
Resolution	:	3.60 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:

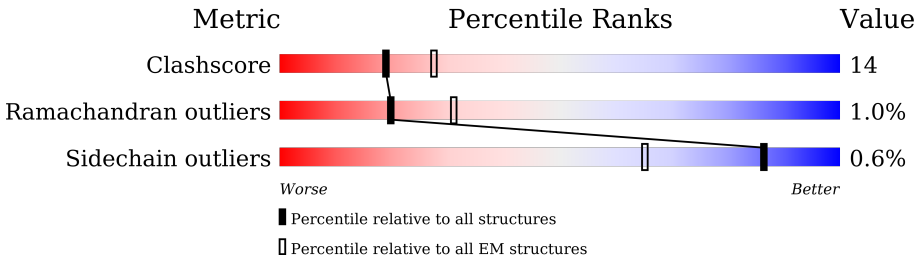
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

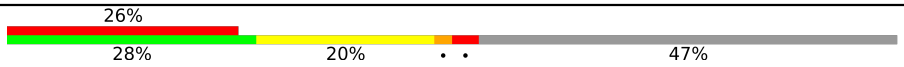
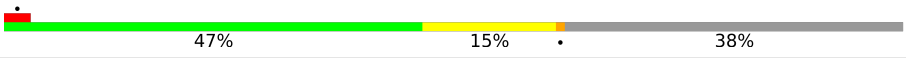
The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	90	
2	A	2210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	B	101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10903 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 RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	48	360	225	69	59	7	0	0

- Molecule 2 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1381	10540	6716	1775	1986	63	1	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

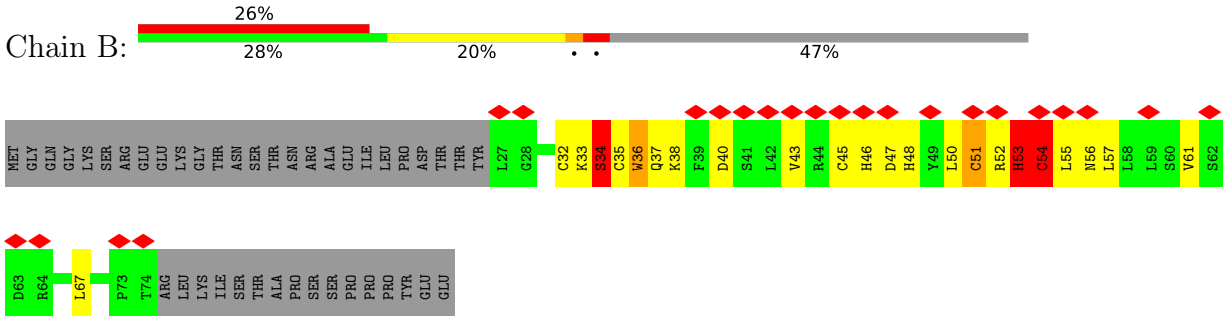
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
4	A	1	1	1	0

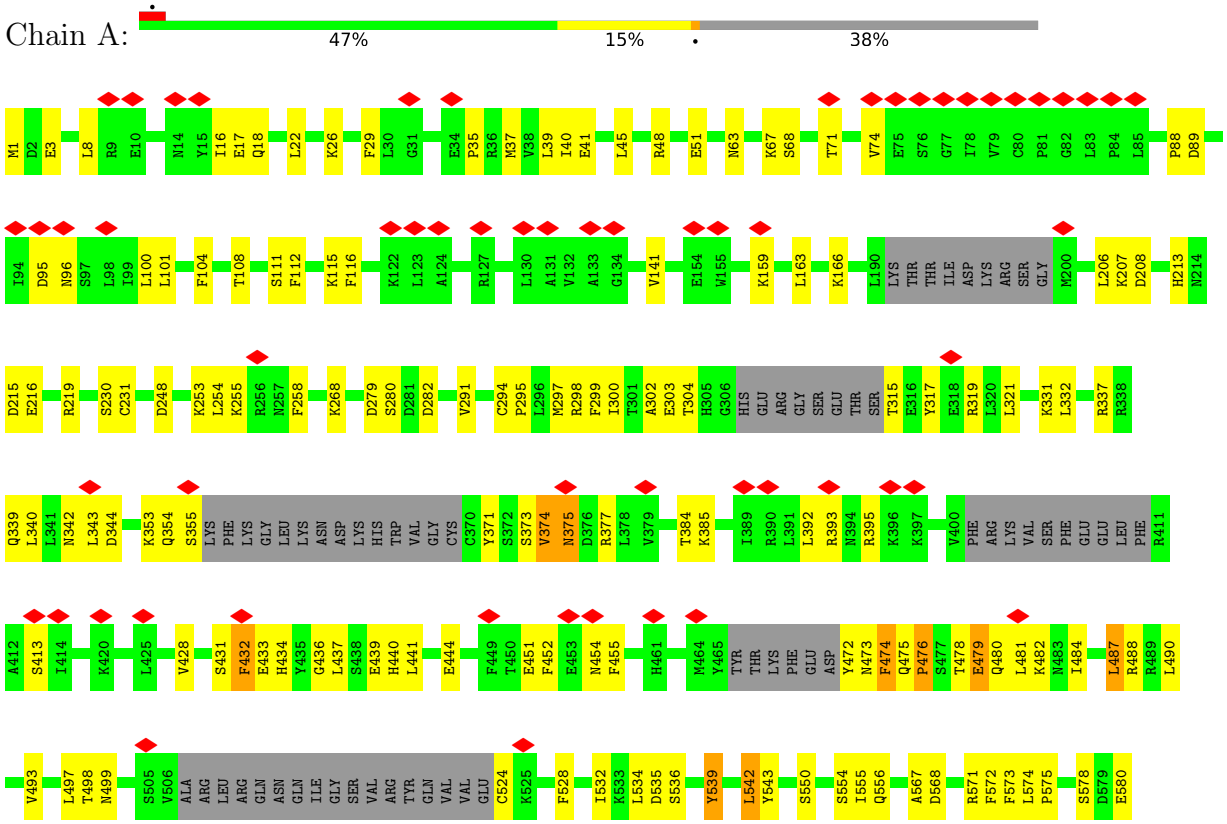
3 Residue-property plots (i)

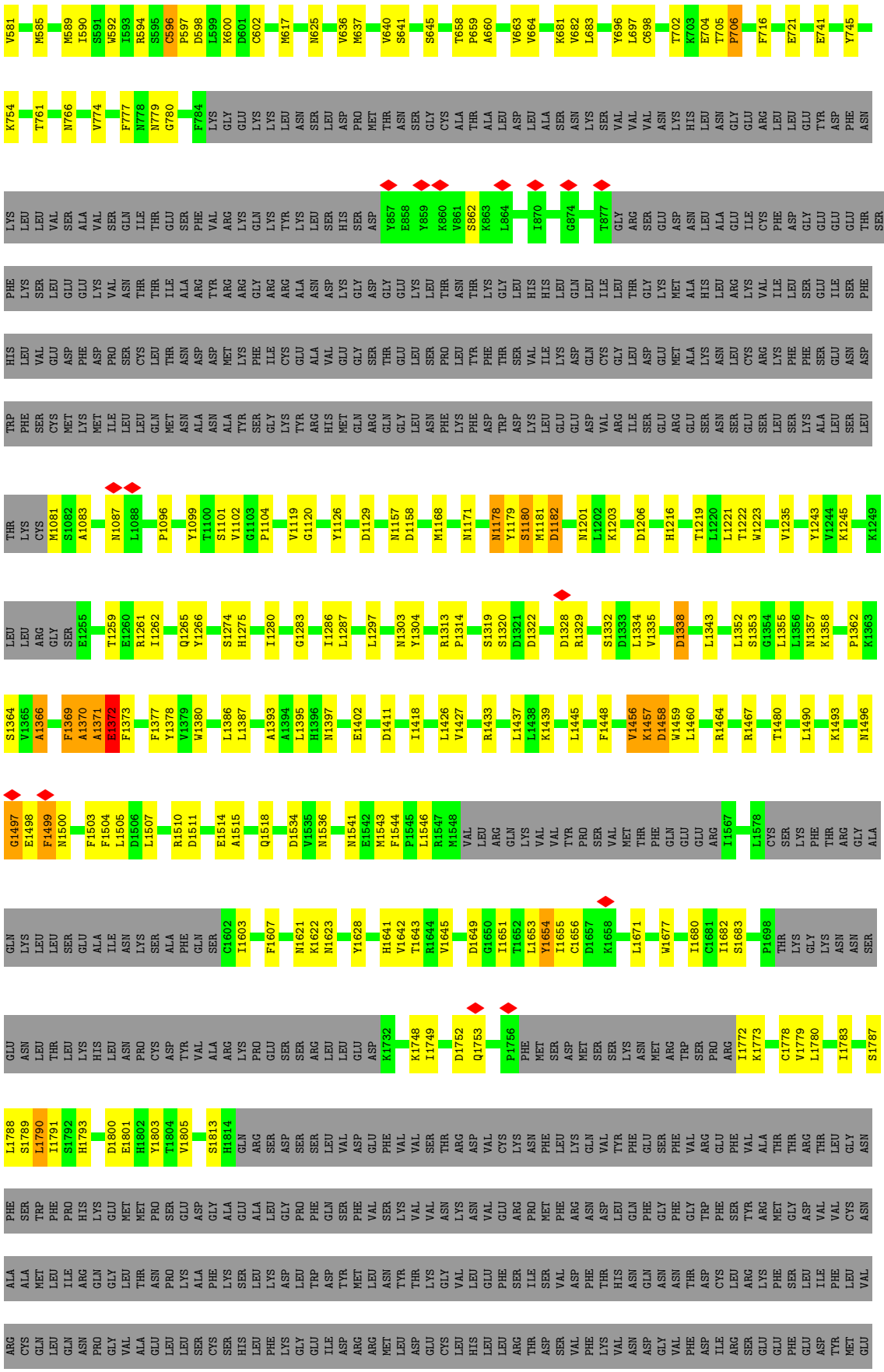
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

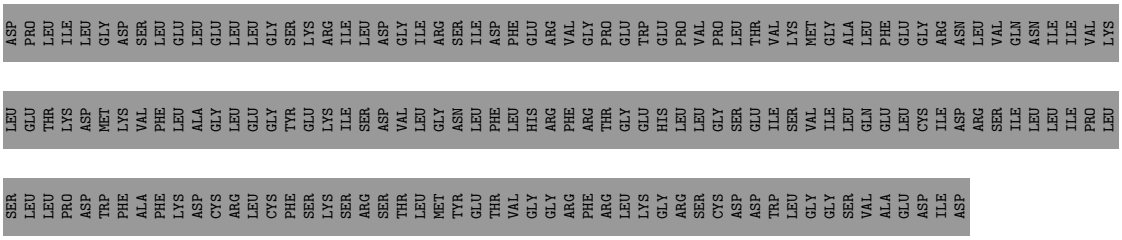
• Molecule 1: RING finger protein Z



• Molecule 2: RNA-directed RNA polymerase L




V581 M585 M589 I590 S591 W592 I593 R594 S595 C596 P597 D598 L599 K600 D601 C602 M617 N625 V636 M637 V640 S641 S645 T658 P659 A660 V663 V664 K681 V682 L683 Y696 L697 C698 T702 K703 E704 T705 P706 F716 E721 E741 Y745
K754 T761 N766 V774 F777 N778 N779 G780 F784
Y857 E858 Y859 K860 V861 S862 K863 L864 I870 G874 T877
P1096 Y1099 T1100 S1101 V1102 G1103 P1104 V1119 G1120 Y1126 D1129 N1157 D1158 M1168 N1171 N1178 Y1179 S1180 M1181 D1182 N1201 L1202 K1203 D1206 H1216 T1219 L1220 L1221 T1222 W1223 V1235 Y1243 V1244 K1245 K1249
T1259 E1260 R1261 I1262 Q1265 Y1266 S1274 H1275 I1280 G1283 I1286 L1287 L1297 N1303 Y1304 R1313 P1314 S1319 S1320 D1321 D1322 D1328 R1329 S1332 D1333 L1334 V1335 D1338 L1343 L1352 S1353 G1354 L1355 L1356 N1357 K1358 P1362 K1363
S1364 V1365 A1366 F1369 A1370 A1371 E1372 F1373 F1377 Y1378 V1379 W1380 L1386 L1387 A1393 A1394 L1395 H1396 N1397 E1402 D1411 I1418 L1426 V1427 R1433 L1437 L1438 K1439 L1445 F1448 V1456 K1457 D1458 W1459 L1460 R1464 R1467 T1480 L1490 K1493 N1496
G1497 E1498 F1499 N1500 F1503 F1504 L1505 D1506 L1507 R1510 D1511 E1514 A1515 Q1518 D1534 V1535 N1536 N1541 E1542 M1543 F1544 P1545 L1546 R1547 M1548 I1567 L1578
C1602 I1603 F1607 N1621 K1622 N1623 Y1628 H1641 V1642 T1643 R1644 V1645 D1649 G1650 I1651 T1652 L1653 Y1654 I1655 C1656 D1657 K1658 L1671 W1677 I1680 C1681 I1682 S1683 P1698
K1732 K1748 I1749 D1752 Q1753 P1756 S1767 I1772 K1773 C1778 V1779 L1780 I1783
L1788 S1789 L1790 I1791 S1792 H1793 D1800 E1801 H1802 Y1803 T1804 V1805 S1813 H1814


ASP PRO LEU ILE LEU GLY ASP SER LEU GLU LEU GLU LEU LEU GLY SER LYS ARG ILE LEU ASP GLY ILE ARG SER ILE ASP PHE GLU ARG VAL GLY PRO GLU TRP GLU PRO VAL PRO LEU THR VAL LYS MET GLY ALA LEU PHE GLU GLY ARG ASN LEU VAL GLN ASN ILE ILE VAL LYS
LEU GLU THR LYS ASP MET LYS VAL PHE LEU ALA GLY LEU GLU GLY TYR GLU LYS ILE SER ASP VAL LEU GLY ASN LEU PHE LEU HIS ARG PHE ARG THR GLY GLU HIS LEU LEU GLY SER GLU ILE SER VAL ILE LEU GLN GLU LEU CYS ILE ASP ARG SER ILE LEU LEU ILE PRO LEU
SER LEU LEU PRO ASP TRP PHE ALA PHE LYS ASP CYS ARG LEU CYS PHE SER LYS SER ARG SER THR LEU MET TYR GLU THR VAL GLY GLY ARG PHE ARG LEU LYS GLY ARG SER CYS ASP ASP TRP LEU GLY GLY SER VAL ALA GLU ASP ILE ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.754	Depositor
Minimum map value	-1.592	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.243	Depositor
Map size (Å)	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.87	4/370 (1.1%)	1.56	4/502 (0.8%)
2	A	0.52	6/10746 (0.1%)	0.75	41/14543 (0.3%)
All	All	0.53	10/11116 (0.1%)	0.79	45/15045 (0.3%)

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
1	B	0	1
2	A	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1371	ALA	C-O	-7.92	1.08	1.23
1	B	53	HIS	C-N	7.12	1.50	1.34
1	B	54	CYS	C-N	7.03	1.50	1.34
2	A	1182	ASP	C-O	-6.49	1.11	1.23
2	A	1182	ASP	CB-CG	6.31	1.65	1.51
2	A	1372	GLU	CG-CD	6.29	1.61	1.51
1	B	36	TRP	CZ3-CH2	-6.04	1.30	1.40
2	A	475	GLN	C-N	5.78	1.45	1.34
1	B	36	TRP	CD2-CE2	-5.72	1.34	1.41
2	A	1322	ASP	C-O	-5.03	1.13	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53	HIS	O-C-N	-25.09	82.56	122.70
1	B	40	ASP	N-CA-C	11.06	140.87	111.00
2	A	539	TYR	CB-CA-C	-9.86	90.68	110.40
1	B	34	SER	CB-CA-C	-9.82	91.44	110.10
2	A	1787	SER	O-C-N	9.81	138.39	122.70
2	A	1369	PHE	N-CA-C	8.24	133.24	111.00
2	A	1370	ALA	C-N-CA	7.81	141.23	121.70
2	A	473	ASN	N-CA-C	-7.77	90.03	111.00
2	A	474	PHE	CB-CA-C	-7.66	95.07	110.40
2	A	596	CYS	CA-CB-SG	-7.56	100.39	114.00
2	A	1372	GLU	OE1-CD-OE2	-7.32	114.52	123.30
2	A	542	LEU	CB-CA-C	7.27	124.00	110.20
2	A	1338	ASP	CB-CA-C	7.22	124.84	110.40
2	A	1338	ASP	N-CA-C	-7.07	91.91	111.00
2	A	472	TYR	O-C-N	7.06	134.00	122.70
2	A	1787	SER	CA-C-N	-6.62	102.63	117.20
2	A	1182	ASP	CB-CG-OD2	6.59	124.23	118.30
2	A	542	LEU	N-CA-C	-6.57	93.26	111.00
2	A	1274	SER	CB-CA-C	-6.48	97.80	110.10
2	A	1180	SER	N-CA-C	-6.45	93.59	111.00
2	A	1370	ALA	CB-CA-C	-6.42	100.46	110.10
2	A	1178	ASN	N-CA-C	-6.32	93.93	111.00
2	A	1671	LEU	CA-CB-CG	6.21	129.58	115.30
2	A	1322	ASP	CB-CA-C	-6.16	98.09	110.40
2	A	1499	PHE	C-N-CA	6.06	136.84	121.70
1	B	47	ASP	CB-CA-C	-5.97	98.46	110.40
2	A	1787	SER	C-N-CA	5.71	135.98	121.70
2	A	1157	ASN	N-CA-C	-5.70	95.60	111.00
2	A	373	SER	N-CA-C	5.68	126.33	111.00
2	A	1456	VAL	O-C-N	-5.68	113.62	122.70
2	A	1203	LYS	N-CA-C	-5.67	95.69	111.00
2	A	1182	ASP	OD1-CG-OD2	-5.66	112.55	123.30
2	A	1275	HIS	N-CA-CB	5.65	120.76	110.60
2	A	375	ASN	CB-CA-C	-5.54	99.33	110.40
2	A	371	TYR	N-CA-C	-5.53	96.07	111.00
2	A	1536	ASN	CB-CA-C	5.47	121.33	110.40
2	A	1511	ASP	C-N-CA	5.46	135.36	121.70
2	A	472	TYR	CA-C-N	-5.43	105.25	117.20
2	A	375	ASN	C-N-CA	5.31	134.98	121.70
2	A	487	LEU	CA-CB-CG	5.30	127.49	115.30
2	A	479	GLU	N-CA-C	5.27	125.23	111.00
2	A	1366	ALA	N-CA-C	-5.21	96.94	111.00
2	A	1158	ASP	CB-CG-OD2	5.14	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1366	ALA	CB-CA-C	5.10	117.76	110.10
2	A	439	GLU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1497	GLY	Mainchain
2	A	478	THR	Mainchain
1	B	53	HIS	Mainchain

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	B	360	0	334	40	0
2	A	10540	0	9843	279	0
3	B	2	0	0	2	0
4	A	1	0	0	0	0
All	All	10903	0	10177	301	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 14.

All (301) 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:A:596:CYS:HB3	2:A:597:PRO:CD	1.47	1.42
1:B:51:CYS:SG	1:B:54:CYS:HB2	1.67	1.34
2:A:1334:LEU:O	2:A:1338:ASP:O	1.64	1.13
2:A:1448:PHE:CE2	2:A:1788:LEU:HD11	1.86	1.09
2:A:1499:PHE:HD2	2:A:1503:PHE:HB2	1.18	1.05
2:A:596:CYS:HB3	2:A:597:PRO:HD3	1.12	1.05
2:A:596:CYS:HB3	2:A:597:PRO:HD2	1.34	1.04
2:A:434:HIS:CE1	2:A:1628:TYR:CE1	2.49	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:581:VAL:HG23	2:A:1426:LEU:HD11	1.39	1.00
2:A:374:VAL:O	2:A:385:LYS:HA	1.62	1.00
2:A:596:CYS:CB	2:A:597:PRO:CD	2.25	0.99
2:A:1448:PHE:HE2	2:A:1788:LEU:HD11	1.26	0.97
2:A:573:PHE:CE1	2:A:1433:ARG:NH2	2.33	0.95
2:A:596:CYS:CB	2:A:597:PRO:HD3	1.95	0.94
1:B:51:CYS:SG	1:B:54:CYS:CB	2.54	0.94
2:A:573:PHE:HE1	2:A:1433:ARG:HH22	1.13	0.91
1:B:53:HIS:CD2	1:B:54:CYS:H	1.88	0.91
2:A:581:VAL:HG23	2:A:1426:LEU:CD1	2.02	0.90
2:A:574:LEU:HD11	2:A:1395:LEU:HD13	1.54	0.87
1:B:57:LEU:O	2:A:596:CYS:SG	2.32	0.86
2:A:1498:GLU:HG3	2:A:1499:PHE:H	1.37	0.86
2:A:1499:PHE:CD2	2:A:1503:PHE:HB2	2.09	0.85
1:B:35:CYS:HA	2:A:681:LYS:O	1.76	0.84
2:A:1493:LYS:O	2:A:1498:GLU:HB3	1.79	0.83
2:A:434:HIS:HE1	2:A:1628:TYR:CE1	1.93	0.82
1:B:36:TRP:HZ3	2:A:640:VAL:HB	1.43	0.82
2:A:499:ASN:OD1	2:A:543:TYR:OH	1.97	0.82
2:A:1498:GLU:HG3	2:A:1499:PHE:N	1.95	0.81
2:A:1490:LEU:HD21	2:A:1503:PHE:CE1	2.16	0.81
2:A:1490:LEU:HD11	2:A:1499:PHE:CE2	2.16	0.80
2:A:215:ASP:O	2:A:219:ARG:HB2	1.83	0.79
2:A:434:HIS:CE1	2:A:1628:TYR:CZ	2.69	0.79
2:A:1789:SER:O	2:A:1790:LEU:HG	1.81	0.79
1:B:51:CYS:SG	3:B:101:ZN:ZN	1.72	0.78
1:B:67:LEU:HD21	2:A:683:LEU:CD1	2.15	0.77
1:B:61:VAL:CG2	2:A:596:CYS:SG	2.74	0.76
2:A:696:TYR:CE2	2:A:1386:LEU:HD22	2.22	0.74
2:A:704:GLU:OE2	2:A:1603:ILE:HG22	1.86	0.74
2:A:596:CYS:CB	2:A:597:PRO:HD2	2.03	0.73
1:B:61:VAL:HG21	2:A:596:CYS:SG	2.30	0.72
1:B:35:CYS:SG	2:A:681:LYS:O	2.50	0.70
2:A:1490:LEU:CD1	2:A:1499:PHE:CZ	2.75	0.70
2:A:581:VAL:CG2	2:A:1426:LEU:HD11	2.20	0.69
2:A:294:CYS:HB2	2:A:295:PRO:HD3	1.74	0.69
2:A:1456:VAL:C	2:A:1458:ASP:H	1.96	0.67
2:A:1357:ASN:O	2:A:1358:LYS:HG3	1.94	0.67
2:A:1171:ASN:ND2	2:A:1178:ASN:OD1	2.27	0.67
1:B:51:CYS:HG	3:B:101:ZN:ZN	1.09	0.67
2:A:658:THR:O	2:A:660:ALA:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:ILE:O	2:A:18:GLN:NE2	2.28	0.66
2:A:1498:GLU:CG	2:A:1499:PHE:H	2.06	0.66
2:A:1328:ASP:OD2	2:A:1329:ARG:N	2.26	0.66
1:B:53:HIS:CG	1:B:54:CYS:H	2.14	0.65
2:A:1641:HIS:O	2:A:1641:HIS:ND1	2.28	0.65
2:A:1749:ILE:O	2:A:1753:GLN:NE2	2.29	0.65
2:A:353:LYS:HE2	2:A:454:ASN:HD21	1.62	0.65
2:A:451:GLU:O	2:A:455:PHE:HB2	1.95	0.65
1:B:45:CYS:SG	1:B:46:HIS:N	2.69	0.65
1:B:67:LEU:HD21	2:A:683:LEU:HD11	1.78	0.64
2:A:207:LYS:HG2	2:A:208:ASP:H	1.61	0.64
1:B:36:TRP:CZ3	2:A:640:VAL:HB	2.32	0.63
2:A:1496:ASN:OD1	2:A:1497:GLY:N	2.30	0.63
2:A:1682:ILE:HD11	2:A:1788:LEU:HD13	1.81	0.63
2:A:1499:PHE:HE2	2:A:1503:PHE:HD1	1.45	0.62
2:A:375:ASN:HA	2:A:384:THR:O	1.99	0.62
2:A:645:SER:OG	2:A:1362:PRO:O	2.12	0.61
2:A:48:ARG:NH1	2:A:51:GLU:OE2	2.33	0.61
2:A:1083:ALA:O	2:A:1087:ASN:ND2	2.34	0.61
2:A:315:THR:OG1	2:A:319:ARG:NH1	2.33	0.61
2:A:705:THR:HG23	2:A:705:THR:O	2.00	0.61
1:B:35:CYS:HB3	1:B:37:GLN:HG3	1.82	0.60
1:B:32:CYS:HB2	1:B:35:CYS:HB2	1.84	0.60
1:B:35:CYS:O	2:A:681:LYS:CB	2.50	0.60
2:A:474:PHE:O	2:A:476:PRO:HD3	2.02	0.60
2:A:862:SER:O	2:A:1245:LYS:NZ	2.34	0.60
2:A:761:THR:O	2:A:761:THR:HG22	2.03	0.59
1:B:33:LYS:HB2	1:B:48:HIS:HB2	1.85	0.59
2:A:17:GLU:O	2:A:26:LYS:NZ	2.35	0.58
2:A:304:THR:OG1	2:A:476:PRO:HG2	2.03	0.58
2:A:432:PHE:HA	2:A:436:GLY:H	1.69	0.58
2:A:754:LYS:O	2:A:766:ASN:ND2	2.29	0.58
2:A:63:ASN:ND2	2:A:67:LYS:O	2.36	0.58
2:A:1081:MET:SD	2:A:1081:MET:N	2.76	0.58
2:A:332:LEU:O	2:A:332:LEU:HD23	2.04	0.58
2:A:479:GLU:HG2	2:A:479:GLU:O	2.04	0.57
2:A:68[A]:SER:HB3	2:A:71:THR:HG1	1.70	0.57
2:A:108:THR:OG1	2:A:111:SER:OG	2.22	0.57
2:A:590:ILE:O	2:A:594:ARG:NH2	2.36	0.57
2:A:1261:ARG:NH2	2:A:1265:GLN:OE1	2.38	0.57
2:A:1621:ASN:OD1	2:A:1622:LYS:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:279:ASP:O	2:A:280:SER:HB3	2.05	0.57
2:A:600:LYS:O	2:A:602:CYS:N	2.37	0.56
2:A:535:ASP:O	2:A:536:SER:C	2.43	0.56
2:A:1499:PHE:CE2	2:A:1503:PHE:HD1	2.23	0.56
2:A:315:THR:HG1	2:A:319:ARG:NH1	2.04	0.56
2:A:1682:ILE:HD11	2:A:1788:LEU:CD1	2.36	0.56
2:A:497:LEU:C	2:A:499:ASN:H	2.09	0.56
2:A:332:LEU:HD23	2:A:332:LEU:C	2.25	0.56
1:B:61:VAL:HG23	2:A:596:CYS:SG	2.44	0.56
2:A:542:LEU:HD12	2:A:556:GLN:HE21	1.70	0.55
2:A:1490:LEU:HD21	2:A:1503:PHE:HE1	1.71	0.55
2:A:528:PHE:HB2	2:A:543:TYR:CE2	2.42	0.55
2:A:385:LYS:HZ1	2:A:524:CYS:N	2.04	0.55
2:A:1448:PHE:CD2	2:A:1788:LEU:HD11	2.41	0.55
2:A:1505:LEU:O	2:A:1510:ARG:NH2	2.35	0.55
2:A:1179:TYR:O	2:A:1181:MET:N	2.40	0.54
2:A:1370:ALA:HA	2:A:1378:TYR:O	2.07	0.54
2:A:1504:PHE:HD1	2:A:1780:LEU:HD21	1.72	0.54
1:B:67:LEU:HD21	2:A:683:LEU:HD12	1.87	0.54
2:A:696:TYR:CD2	2:A:1386:LEU:HD22	2.42	0.54
2:A:108:THR:HG1	2:A:111:SER:HG	1.53	0.54
2:A:392:LEU:HA	2:A:395:ARG:CZ	2.37	0.54
2:A:585:MET:HG3	2:A:1387:LEU:HD21	1.89	0.53
2:A:1353:SER:HB3	2:A:1358:LYS:O	2.09	0.53
2:A:1779:VAL:O	2:A:1783:ILE:HG12	2.09	0.52
2:A:1789:SER:O	2:A:1790:LEU:CG	2.55	0.52
1:B:67:LEU:CD2	2:A:683:LEU:HD11	2.39	0.52
2:A:777:PHE:CZ	2:A:1297:LEU:HD22	2.44	0.52
2:A:1683:SER:O	2:A:1683:SER:OG	2.27	0.52
2:A:696:TYR:HE2	2:A:1386:LEU:HD13	1.74	0.52
2:A:253:LYS:O	2:A:254:LEU:HB2	2.09	0.52
1:B:51:CYS:SG	1:B:54:CYS:SG	3.07	0.52
2:A:1243:TYR:HA	2:A:1261:ARG:HH11	1.75	0.52
1:B:53:HIS:CG	1:B:54:CYS:N	2.78	0.52
2:A:532:ILE:HB	2:A:539:TYR:O	2.11	0.51
2:A:1393:ALA:O	2:A:1397:ASN:ND2	2.43	0.51
2:A:1642:VAL:CB	2:A:1653:LEU:HD13	2.41	0.51
2:A:1216:HIS:HA	2:A:1219:THR:HG22	1.92	0.51
2:A:625:ASN:OD1	2:A:664:VAL:HG21	2.11	0.51
2:A:375:ASN:OD1	2:A:377:ARG:N	2.44	0.51
2:A:554:SER:OG	2:A:555:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:428:VAL:HG22	2:A:440:HIS:HD2	1.76	0.50
2:A:431:SER:O	2:A:433:GLU:O	2.29	0.50
2:A:1645:VAL:N	2:A:1654:TYR:HE2	2.09	0.50
2:A:637:MET:O	2:A:641:SER:HB3	2.10	0.50
2:A:1439:LYS:HD3	2:A:1445:LEU:HD11	1.93	0.50
2:A:479:GLU:O	2:A:482:LYS:HB2	2.11	0.50
2:A:774:VAL:HG11	2:A:1201:ASN:HB3	1.93	0.50
2:A:1119:VAL:HG23	2:A:1120:GLY:H	1.76	0.50
2:A:1790:LEU:O	2:A:1791:ILE:HD13	2.12	0.50
1:B:33:LYS:HD3	1:B:48:HIS:HB3	1.92	0.50
2:A:22:LEU:HB3	2:A:26:LYS:HE3	1.92	0.50
2:A:258:PHE:O	2:A:1343:LEU:HD11	2.12	0.50
1:B:53:HIS:C	1:B:55:LEU:N	2.65	0.50
2:A:248:ASP:O	2:A:253:LYS:NZ	2.42	0.50
2:A:1677:TRP:O	2:A:1680:ILE:N	2.44	0.49
2:A:480:GLN:C	2:A:482:LYS:N	2.64	0.49
2:A:1541:ASN:OD1	2:A:1541:ASN:O	2.30	0.49
2:A:550:SER:OG	2:A:568:ASP:OD1	2.26	0.49
2:A:302:ALA:HA	2:A:479:GLU:OE1	2.13	0.49
1:B:32:CYS:C	1:B:34:SER:H	2.15	0.49
2:A:216:GLU:OE2	2:A:745:TYR:HD1	1.95	0.49
2:A:617:MET:HE1	2:A:697:LEU:O	2.12	0.49
2:A:1490:LEU:CD1	2:A:1499:PHE:CE2	2.88	0.49
2:A:280:SER:OG	2:A:282:ASP:OD1	2.30	0.48
2:A:779:ASN:OD1	2:A:780:GLY:N	2.46	0.48
2:A:1456:VAL:C	2:A:1458:ASP:N	2.65	0.48
2:A:1411:ASP:OD1	2:A:1467:ARG:NH1	2.46	0.48
2:A:1643:THR:OG1	2:A:1654:TYR:HB2	2.12	0.48
2:A:567:ALA:HB1	2:A:572:PHE:HE2	1.78	0.48
2:A:696:TYR:HE2	2:A:1386:LEU:HD22	1.76	0.48
2:A:1304:TYR:HD1	2:A:1313:ARG:HH22	1.60	0.48
2:A:163:LEU:HD23	2:A:166:LYS:HZ1	1.77	0.48
2:A:8:LEU:HB3	2:A:29:PHE:HZ	1.79	0.48
2:A:354:GLN:O	2:A:355:SER:OG	2.26	0.48
1:B:57:LEU:O	2:A:596:CYS:CB	2.62	0.47
2:A:1129:ASP:OD1	2:A:1129:ASP:N	2.47	0.47
2:A:1:MET:N	2:A:3:GLU:OE1	2.36	0.47
2:A:696:TYR:HH	2:A:1377:PHE:HE1	1.61	0.47
2:A:721:GLU:OE2	2:A:1259:THR:OG1	2.32	0.47
2:A:331:LYS:HE2	2:A:331:LYS:HB2	1.64	0.47
2:A:1653:LEU:O	2:A:1655:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:437:LEU:O	2:A:440:HIS:ND1	2.48	0.47
2:A:1460:LEU:HG	2:A:1803:TYR:HD2	1.79	0.47
1:B:35:CYS:HA	2:A:681:LYS:C	2.35	0.47
2:A:1332:SER:O	2:A:1335:VAL:HG12	2.15	0.47
2:A:432:PHE:HA	2:A:436:GLY:N	2.30	0.47
2:A:1262:ILE:HG22	2:A:1266:TYR:CE1	2.50	0.47
1:B:32:CYS:C	1:B:34:SER:N	2.69	0.46
1:B:43:VAL:N	1:B:50:LEU:O	2.28	0.46
2:A:1243:TYR:HA	2:A:1261:ARG:NH1	2.31	0.46
2:A:534:LEU:O	2:A:535:ASP:C	2.51	0.46
2:A:1179:TYR:HD1	2:A:1366:ALA:HB2	1.80	0.46
2:A:1402:GLU:HG3	2:A:1546:LEU:HD21	1.96	0.46
2:A:1445:LEU:O	2:A:1649:ASP:HB2	2.15	0.46
2:A:580:GLU:O	2:A:580:GLU:HG2	2.15	0.46
2:A:1168:MET:HE1	2:A:1373:PHE:HB3	1.98	0.46
2:A:1490:LEU:HD12	2:A:1499:PHE:CZ	2.51	0.46
2:A:413:SER:HA	2:A:452:PHE:CD2	2.51	0.46
2:A:1448:PHE:HE2	2:A:1788:LEU:CD1	2.13	0.46
2:A:1645:VAL:O	2:A:1654:TYR:OH	2.17	0.46
2:A:116:PHE:CE2	2:A:141:VAL:HG21	2.51	0.46
2:A:1456:VAL:HG11	2:A:1813:SER:HA	1.97	0.46
2:A:71:THR:HA	2:A:74:VAL:HG12	1.98	0.46
2:A:441:LEU:HA	2:A:444:GLU:HG3	1.98	0.46
2:A:575:PRO:HA	2:A:578:SER:OG	2.16	0.46
2:A:1328:ASP:CG	2:A:1329:ARG:H	2.15	0.46
2:A:636:VAL:O	2:A:640:VAL:HG22	2.16	0.45
2:A:1371:ALA:HB3	2:A:1378:TYR:HB2	1.98	0.45
2:A:1800:ASP:OD1	2:A:1801:GLU:N	2.50	0.45
2:A:353:LYS:HE2	2:A:454:ASN:ND2	2.27	0.45
2:A:159:LYS:O	2:A:163:LEU:HG	2.16	0.45
2:A:1286:ILE:HG22	2:A:1287:LEU:HD23	1.98	0.45
2:A:37:MET:HA	2:A:40:ILE:HG12	1.99	0.45
2:A:1099:TYR:HB2	2:A:1104:PRO:HA	1.97	0.45
2:A:1543:MET:O	2:A:1544:PHE:HD2	1.99	0.45
2:A:493:VAL:O	2:A:497:LEU:N	2.49	0.45
2:A:339:GLN:O	2:A:343:LEU:HD23	2.17	0.45
2:A:1101:SER:OG	2:A:1222:THR:HG21	2.17	0.45
2:A:1498:GLU:HG3	2:A:1499:PHE:HD1	1.82	0.45
2:A:115:LYS:HA	2:A:115:LYS:HD3	1.77	0.45
2:A:1303:ASN:OD1	2:A:1314:PRO:HG2	2.17	0.45
2:A:716:PHE:CD2	2:A:1235:VAL:HG11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1653:LEU:C	2:A:1655:ILE:H	2.20	0.45
2:A:297:MET:O	2:A:299:PHE:N	2.50	0.44
2:A:353:LYS:NZ	2:A:354:GLN:HE22	2.14	0.44
2:A:1319:SER:O	2:A:1320:SER:CB	2.65	0.44
2:A:1505:LEU:HA	2:A:1510:ARG:HH12	1.81	0.44
2:A:342:ASN:OD1	2:A:393:ARG:NE	2.51	0.44
1:B:54:CYS:HA	2:A:682:VAL:HG23	2.00	0.44
2:A:589:MET:HA	2:A:592:TRP:CE3	2.52	0.44
2:A:1102:VAL:O	2:A:1223:TRP:HD1	2.00	0.44
2:A:1457:LYS:C	2:A:1459:TRP:H	2.21	0.44
2:A:705:THR:HA	2:A:706:PRO:HD2	1.63	0.44
2:A:1498:GLU:HG3	2:A:1499:PHE:CD1	2.52	0.44
2:A:374:VAL:O	2:A:385:LYS:CA	2.51	0.44
2:A:490:LEU:HA	2:A:575:PRO:O	2.17	0.44
2:A:1460:LEU:HD11	2:A:1805:VAL:HG11	2.00	0.44
1:B:38:LYS:HD2	1:B:38:LYS:HA	1.88	0.44
2:A:1748:LYS:HD2	2:A:1752:ASP:HB2	1.99	0.44
2:A:41:GLU:O	2:A:45:LEU:HD23	2.18	0.43
2:A:89:ASP:N	2:A:101:LEU:O	2.51	0.43
2:A:1503:PHE:O	2:A:1507:LEU:N	2.48	0.43
2:A:1651:ILE:HG23	2:A:1651:ILE:O	2.17	0.43
2:A:1369:PHE:HE1	2:A:1380:TRP:CB	2.31	0.43
2:A:1649:ASP:OD1	2:A:1649:ASP:N	2.51	0.43
2:A:254:LEU:HD23	2:A:255:LYS:N	2.34	0.43
2:A:696:TYR:C	2:A:698:CYS:H	2.21	0.43
1:B:35:CYS:C	1:B:37:GLN:N	2.69	0.43
2:A:1180:SER:O	2:A:1180:SER:OG	2.37	0.43
2:A:1772:ILE:HG13	2:A:1773:LYS:H	1.83	0.43
2:A:571:ARG:HE	2:A:702:THR:CG2	2.32	0.43
1:B:33:LYS:CB	1:B:48:HIS:HB2	2.49	0.43
2:A:1778:CYS:HB3	2:A:1791:ILE:HD11	2.00	0.43
2:A:88:PRO:HG3	2:A:100:LEU:HD22	2.00	0.42
2:A:253:LYS:HB2	2:A:253:LYS:HE2	1.78	0.42
2:A:1534:ASP:HB3	2:A:1654:TYR:O	2.19	0.42
2:A:1372:GLU:O	2:A:1372:GLU:CG	2.67	0.42
2:A:1418:ILE:CG1	2:A:1427:VAL:HG21	2.48	0.42
2:A:35:PRO:O	2:A:39:LEU:HD23	2.19	0.42
2:A:1181:MET:HA	2:A:1364:SER:HB2	2.00	0.42
2:A:1515:ALA:HA	2:A:1518:GLN:HG2	2.00	0.42
2:A:474:PHE:C	2:A:476:PRO:HD3	2.40	0.42
2:A:1789:SER:C	2:A:1790:LEU:HG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:HIS:O	1:B:56:ASN:N	2.52	0.42
2:A:321:LEU:HD23	2:A:321:LEU:HA	1.68	0.42
2:A:294:CYS:HB2	2:A:295:PRO:CD	2.48	0.42
2:A:1280:ILE:HG13	2:A:1280:ILE:O	2.19	0.42
2:A:95:ASP:OD1	2:A:96:ASN:N	2.53	0.42
2:A:1514:GLU:CD	2:A:1514:GLU:N	2.73	0.42
2:A:295:PRO:HG2	2:A:298:ARG:H	1.85	0.41
2:A:1499:PHE:HB3	2:A:1500:ASN:H	1.47	0.41
2:A:1543:MET:O	2:A:1544:PHE:CD2	2.72	0.41
2:A:1645:VAL:HG12	2:A:1654:TYR:CE2	2.55	0.41
2:A:213:HIS:CD2	2:A:741:GLU:HG2	2.55	0.41
2:A:484:ILE:O	2:A:488:ARG:HG3	2.20	0.41
2:A:499:ASN:OD1	2:A:543:TYR:CZ	2.71	0.41
2:A:1206:ASP:OD1	2:A:1206:ASP:N	2.53	0.41
2:A:268:LYS:HB3	2:A:268:LYS:HE2	1.89	0.41
2:A:1352:LEU:O	2:A:1355:LEU:N	2.53	0.41
2:A:297:MET:C	2:A:299:PHE:N	2.74	0.41
2:A:1749:ILE:H	2:A:1749:ILE:HD12	1.85	0.41
1:B:67:LEU:CD2	2:A:683:LEU:CD1	2.95	0.41
2:A:300:ILE:O	2:A:302:ALA:N	2.52	0.41
2:A:303:GLU:HA	2:A:476:PRO:HD2	2.03	0.41
2:A:207:LYS:HG2	2:A:208:ASP:N	2.32	0.41
2:A:294:CYS:SG	2:A:663:VAL:HG21	2.60	0.41
2:A:337:ARG:HA	2:A:340:LEU:HB3	2.00	0.41
2:A:487:LEU:O	2:A:487:LEU:HD23	2.21	0.41
2:A:1456:VAL:CG1	2:A:1813:SER:HA	2.51	0.41
2:A:230:SER:OG	2:A:231:CYS:N	2.54	0.41
1:B:33:LYS:HB2	1:B:48:HIS:CB	2.49	0.41
2:A:104:PHE:HE2	2:A:112:PHE:HD1	1.67	0.41
2:A:317:TYR:OH	2:A:344:ASP:OD1	2.24	0.41
2:A:392:LEU:HA	2:A:395:ARG:NH1	2.36	0.41
2:A:1126:TYR:CE1	2:A:1283:GLY:HA2	2.55	0.41
2:A:1221:LEU:HA	2:A:1221:LEU:HD23	1.84	0.41
2:A:1426:LEU:HD12	2:A:1426:LEU:HA	1.86	0.41
2:A:1437:LEU:HD22	2:A:1607:PHE:CE1	2.55	0.41
2:A:1653:LEU:CD1	2:A:1656:CYS:H	2.34	0.41
2:A:1791:ILE:C	2:A:1793:HIS:H	2.23	0.41
2:A:596:CYS:C	2:A:598:ASP:N	2.74	0.41
2:A:1343:LEU:HA	2:A:1343:LEU:HD12	1.70	0.41
1:B:34:SER:HB3	2:A:682:VAL:O	2.21	0.40
2:A:206:LEU:HD21	2:A:1096:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1645:VAL:H	2:A:1654:TYR:HE2	1.68	0.40
2:A:1622:LYS:HG3	2:A:1623:ASN:OD1	2.21	0.40
2:A:1682:ILE:HD11	2:A:1788:LEU:CD2	2.51	0.40
2:A:1682:ILE:HD11	2:A:1788:LEU:HD22	2.04	0.40
2:A:596:CYS:C	2:A:598:ASP:H	2.24	0.40
2:A:291:VAL:HA	2:A:294:CYS:SG	2.62	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	B	46/90 (51%)	35 (76%)	9 (20%)	2 (4%)	2 24
2	A	1354/2210 (61%)	1146 (85%)	196 (14%)	12 (1%)	17 57
All	All	1400/2300 (61%)	1181 (84%)	205 (15%)	14 (1%)	20 55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	HIS
1	B	54	CYS
2	A	481	LEU
2	A	1457	LYS
2	A	1458	ASP
2	A	432	PHE
2	A	1790	LEU
2	A	498	THR
2	A	659	PRO
2	A	1654	TYR
2	A	374	VAL
2	A	1480	THR

Continued on next page...

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Mol	Chain	Res	Type
2	A	476	PRO
2	A	706	PRO

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	B	40/84 (48%)	36 (90%)	4 (10%)	7 35
2	A	1086/2034 (53%)	1083 (100%)	3 (0%)	92 97
All	All	1126/2118 (53%)	1119 (99%)	7 (1%)	86 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	SER
1	B	51	CYS
1	B	52	ARG
1	B	54	CYS
2	A	1182	ASP
2	A	1372	GLU
2	A	1464	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	HIS
2	A	18	GLN
2	A	354	GLN
2	A	434	HIS
2	A	454	ASN
2	A	480	GLN
2	A	1087	ASN
2	A	1753	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

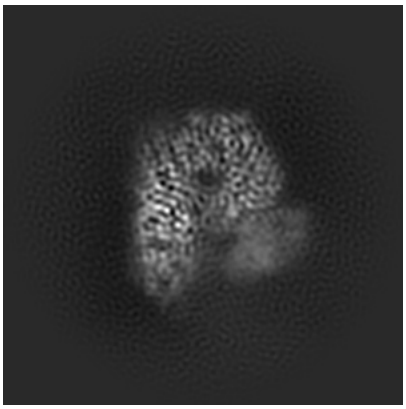
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33028. These allow visual inspection of the internal detail of the map and identification of artifacts.

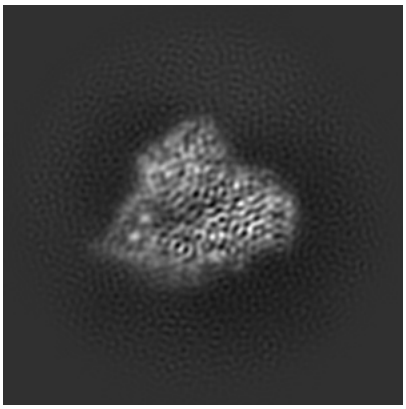
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

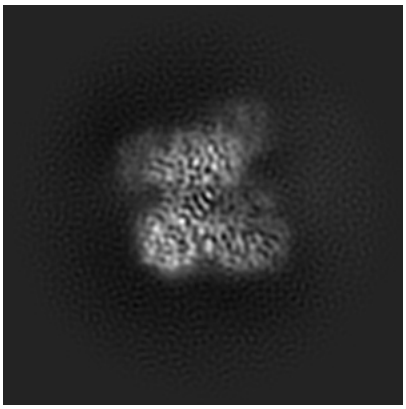
6.1.1 Primary map



X

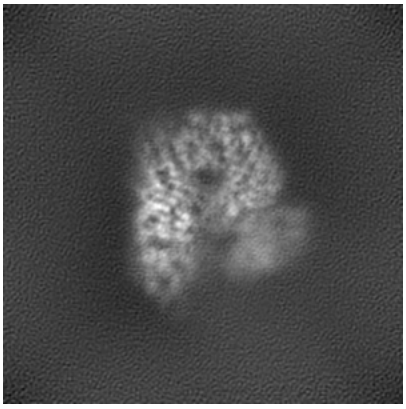


Y

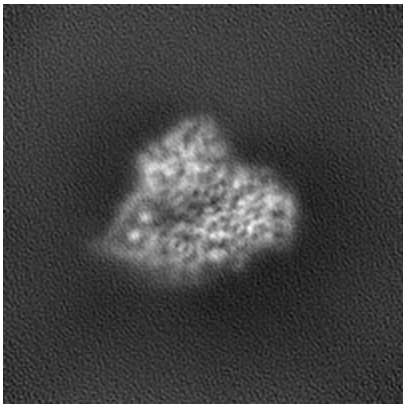


Z

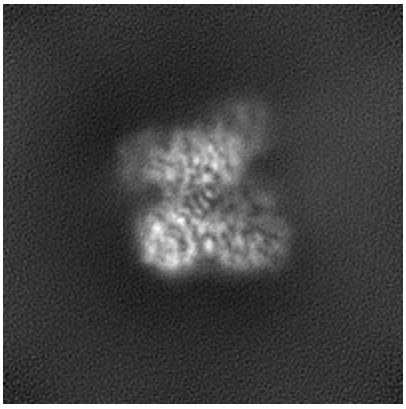
6.1.2 Raw map



X



Y

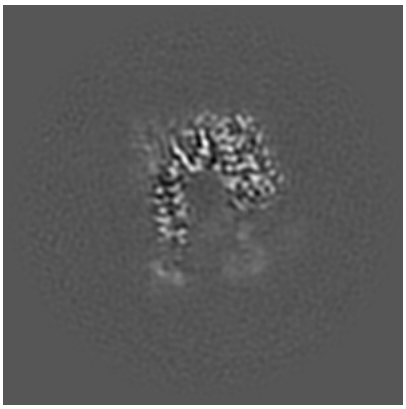


Z

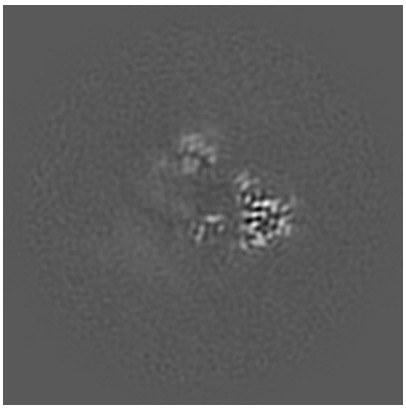
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

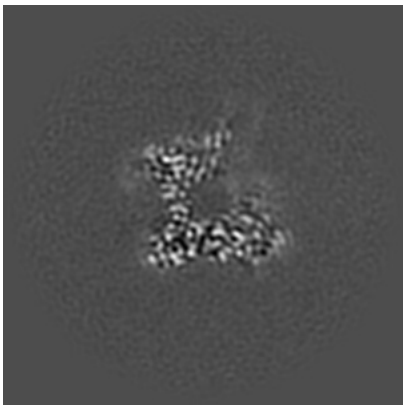
6.2.1 Primary map



X Index: 100

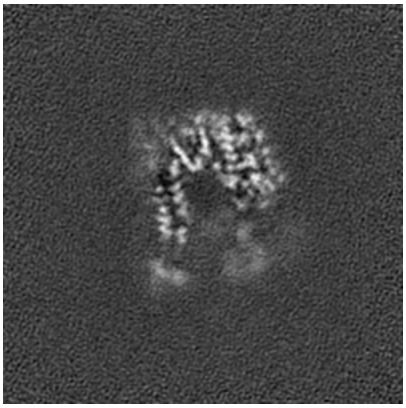


Y Index: 100

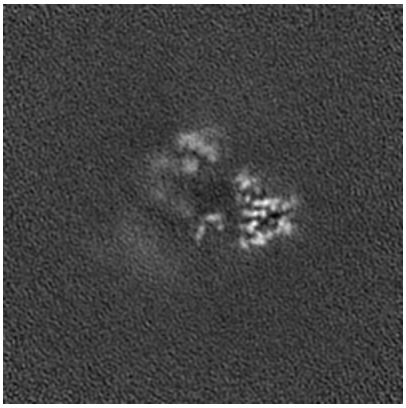


Z Index: 100

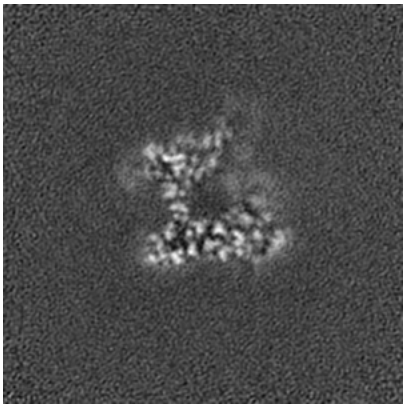
6.2.2 Raw map



X Index: 100



Y Index: 100

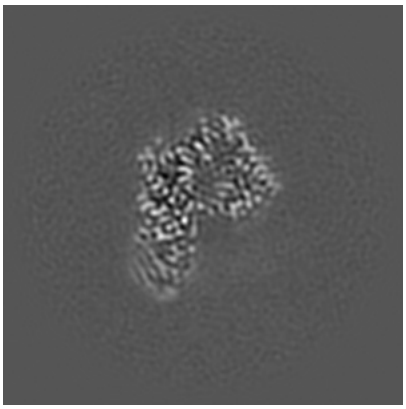


Z Index: 100

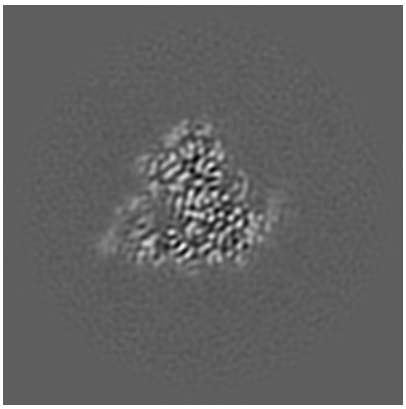
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

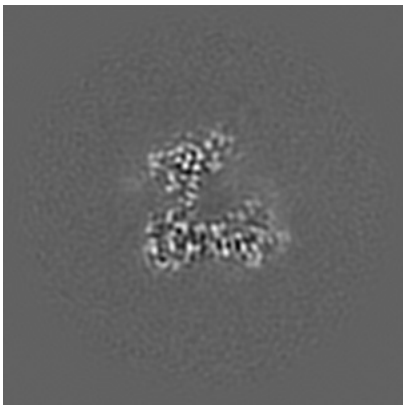
6.3.1 Primary map



X Index: 86

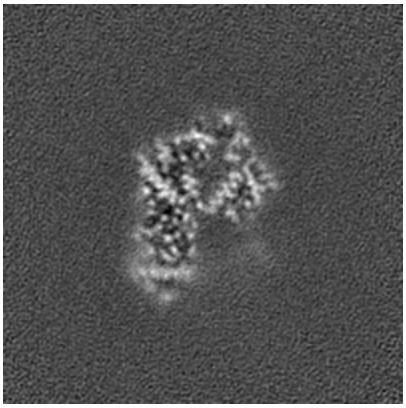


Y Index: 79

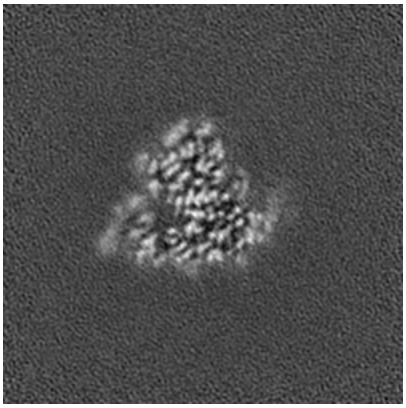


Z Index: 104

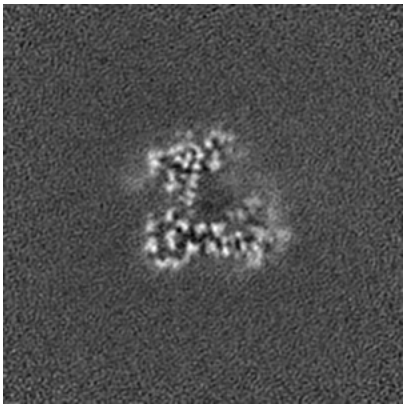
6.3.2 Raw map



X Index: 84



Y Index: 79

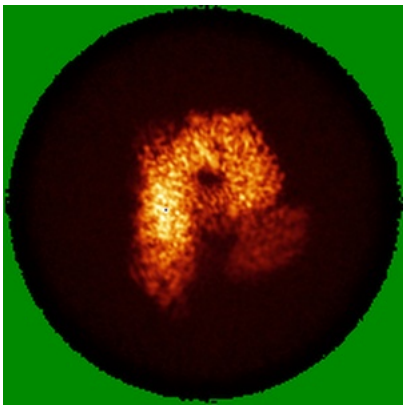


Z Index: 104

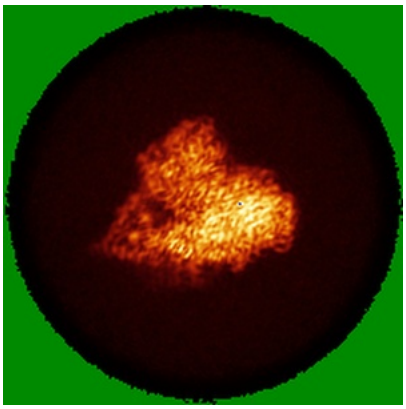
The images above show the largest variance slices of the map in three orthogonal directions.

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

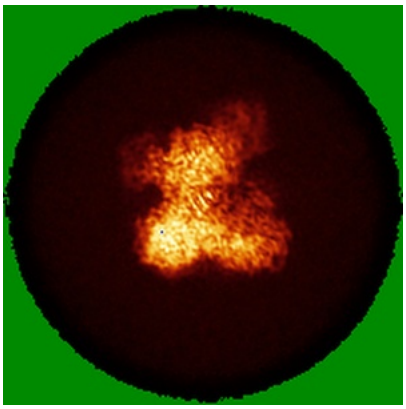
6.4.1 Primary map



X

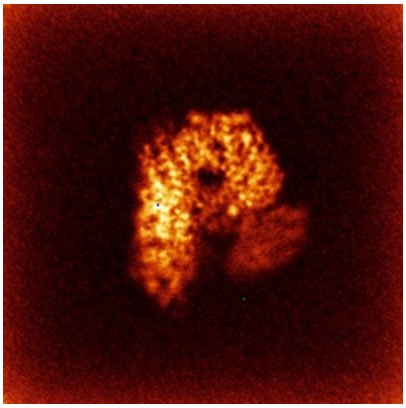


Y

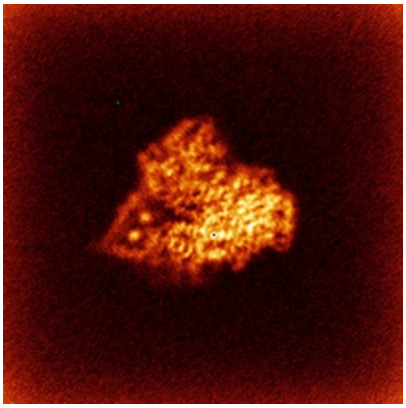


Z

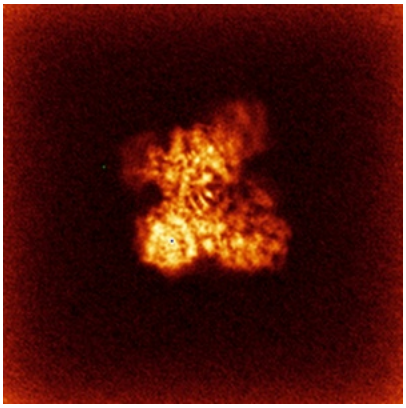
6.4.2 Raw map



X



Y

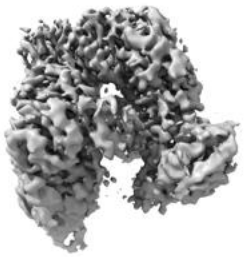


Z

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.

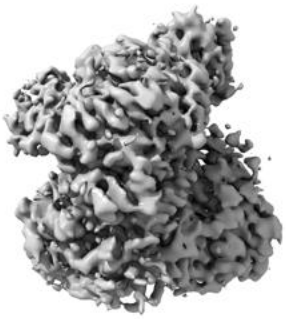
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

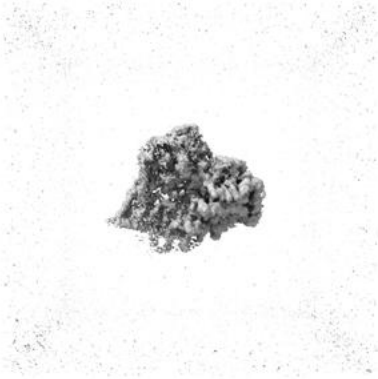


Z

The images above show the 3D surface view of the map at the recommended contour level 0.243. 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.

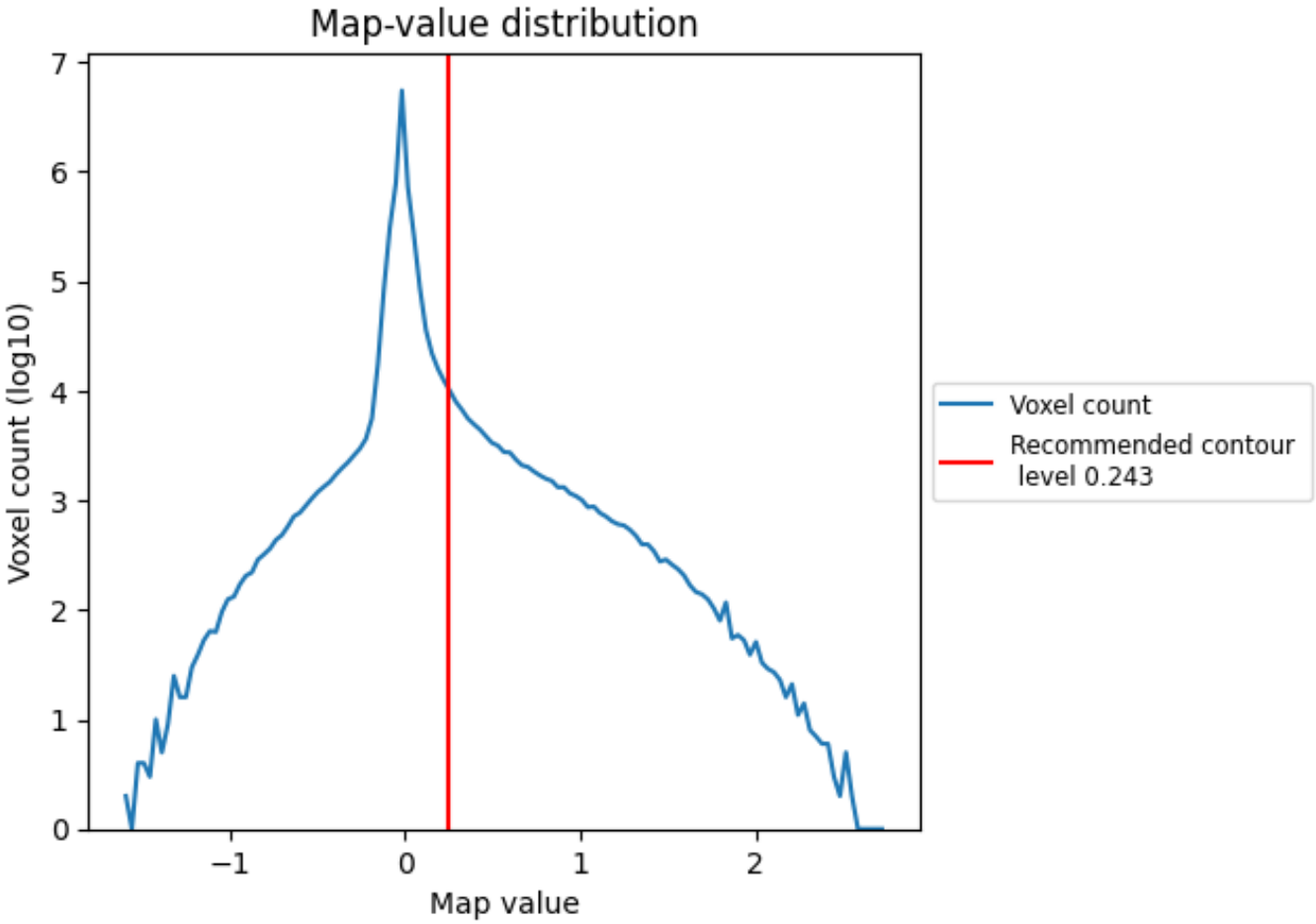
6.6 Mask visualisation (i)

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

7 Map analysis

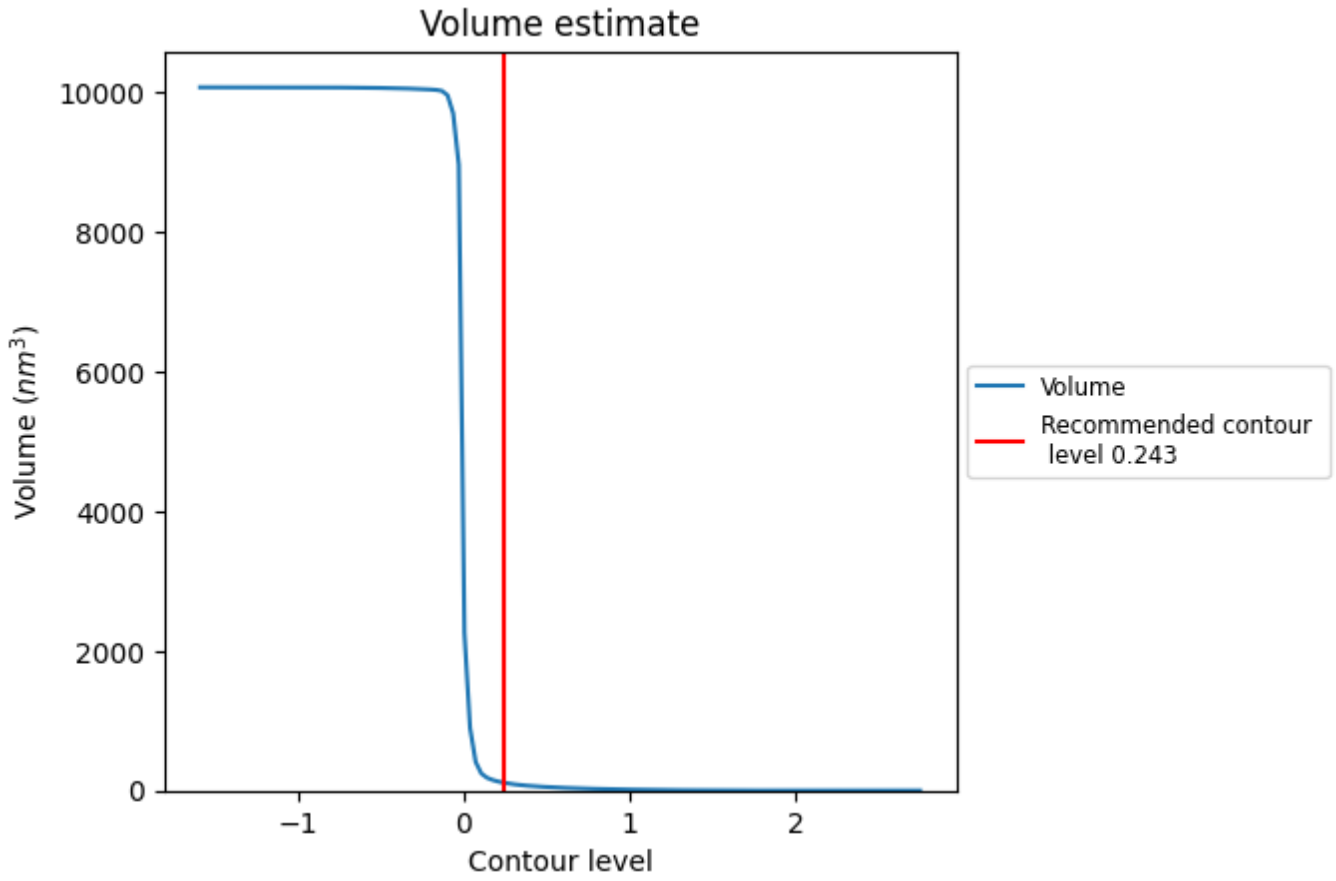
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

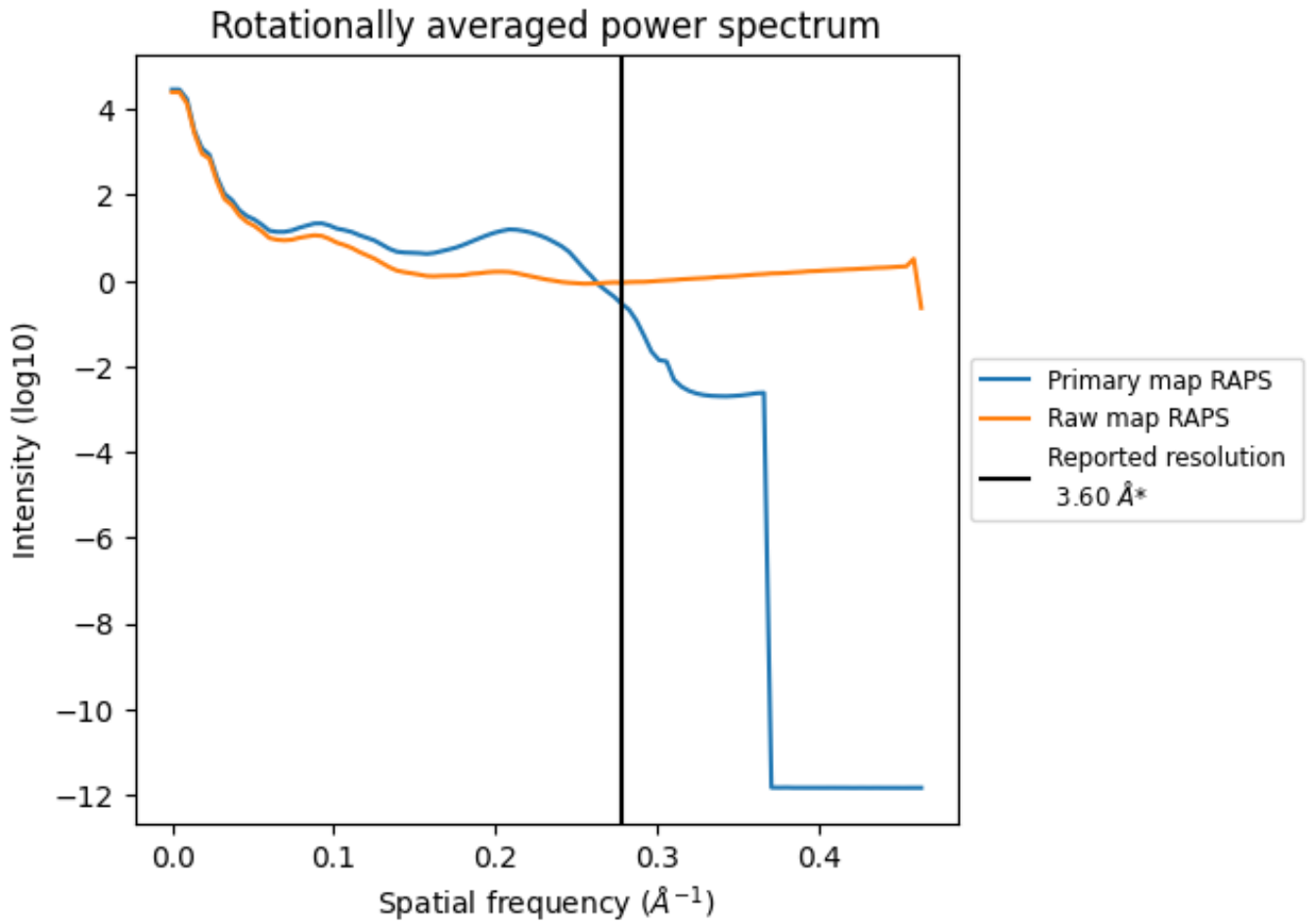
7.2 Volume estimate



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 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)

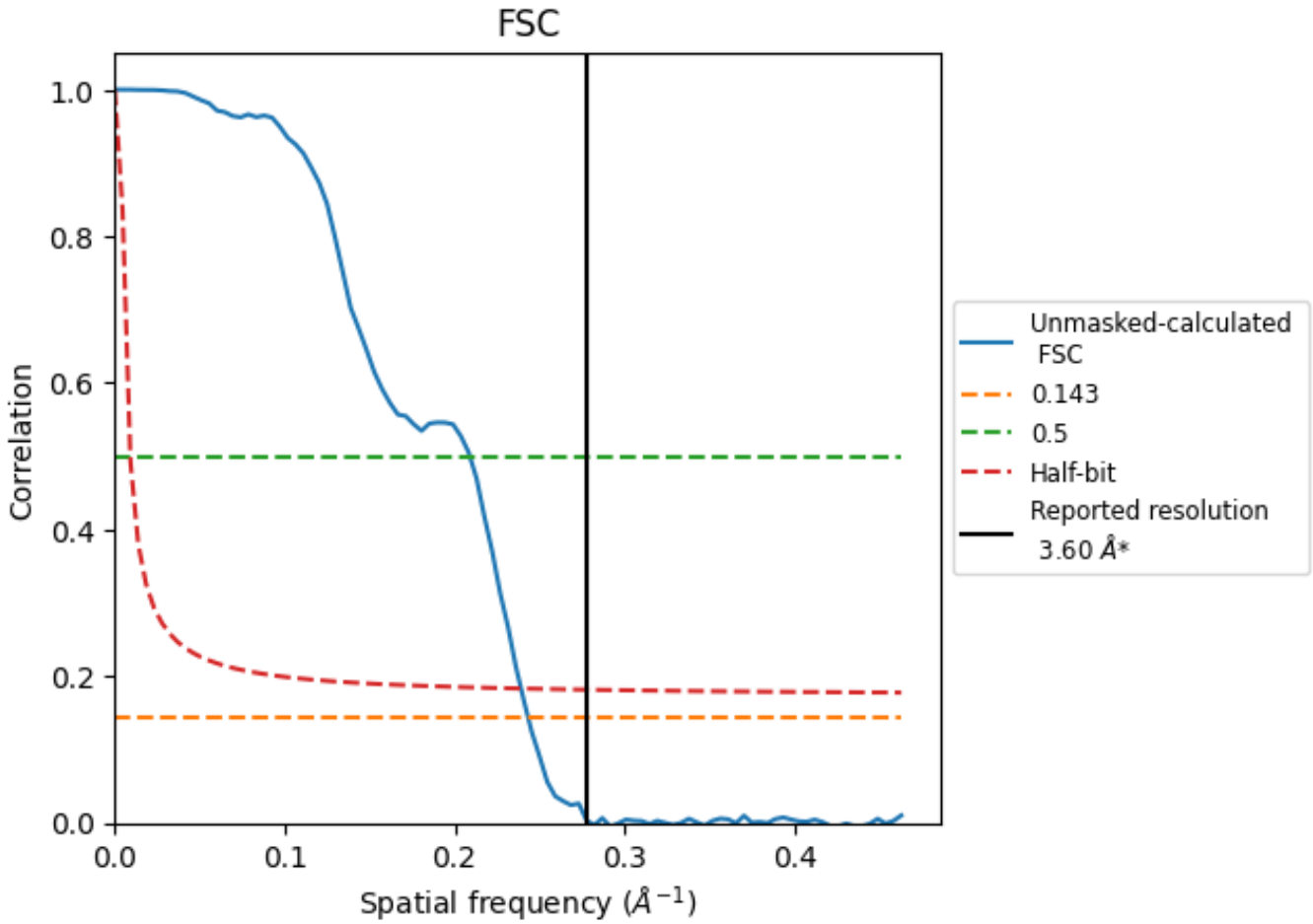


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

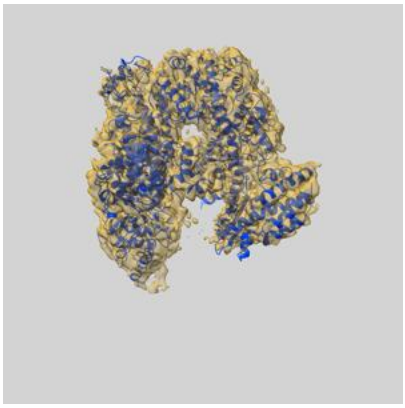
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	4.78	4.18

*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 4.11 differs from the reported value 3.6 by more than 10 %

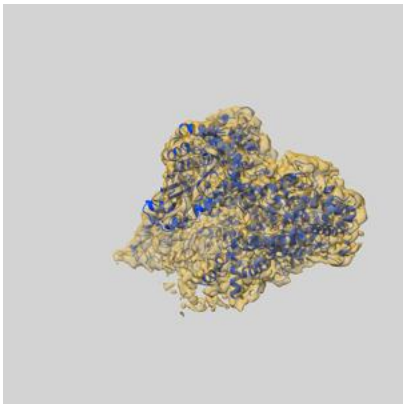
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33028 and PDB model 7X6V. Per-residue inclusion information can be found in section 3 on page 4.

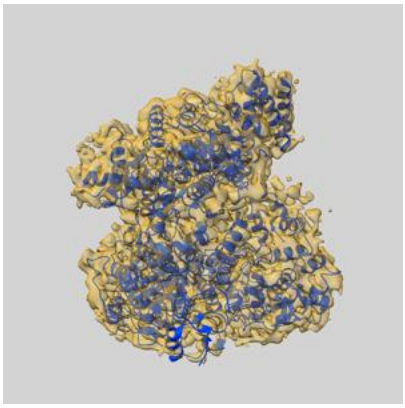
9.1 Map-model overlay



X



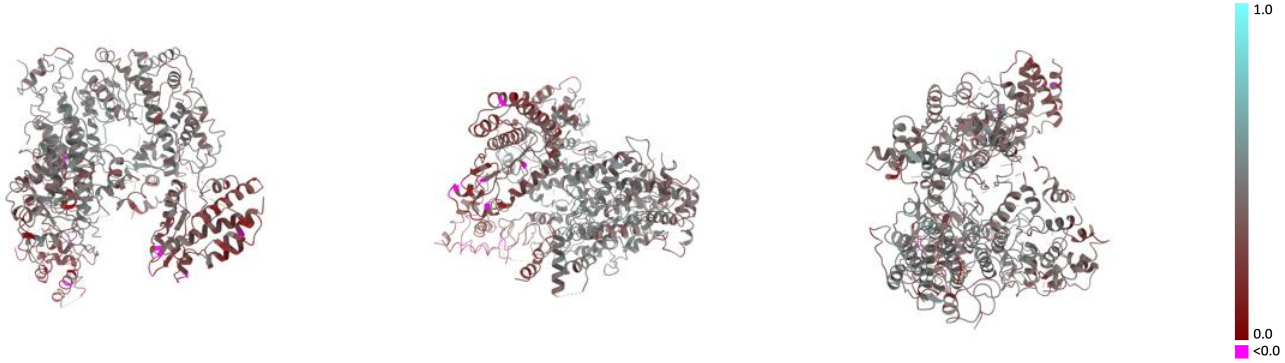
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.243 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.

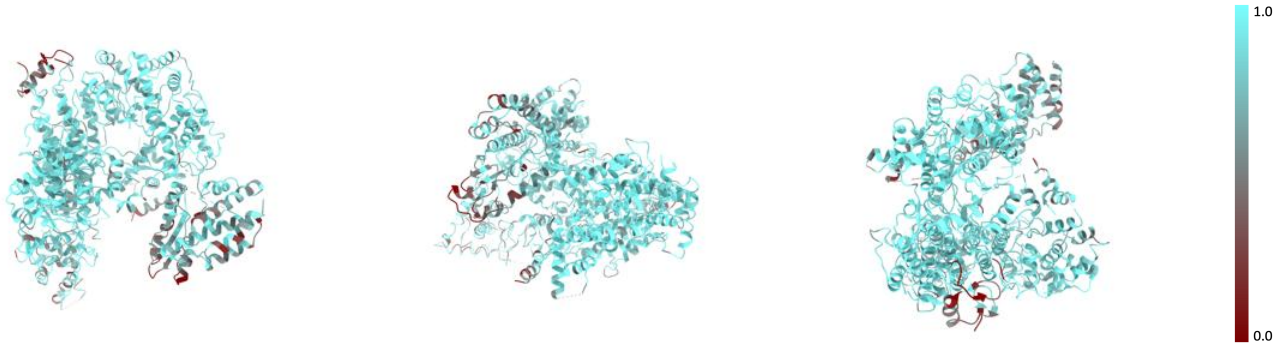
9.2 Q-score mapped to coordinate model (i)



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.

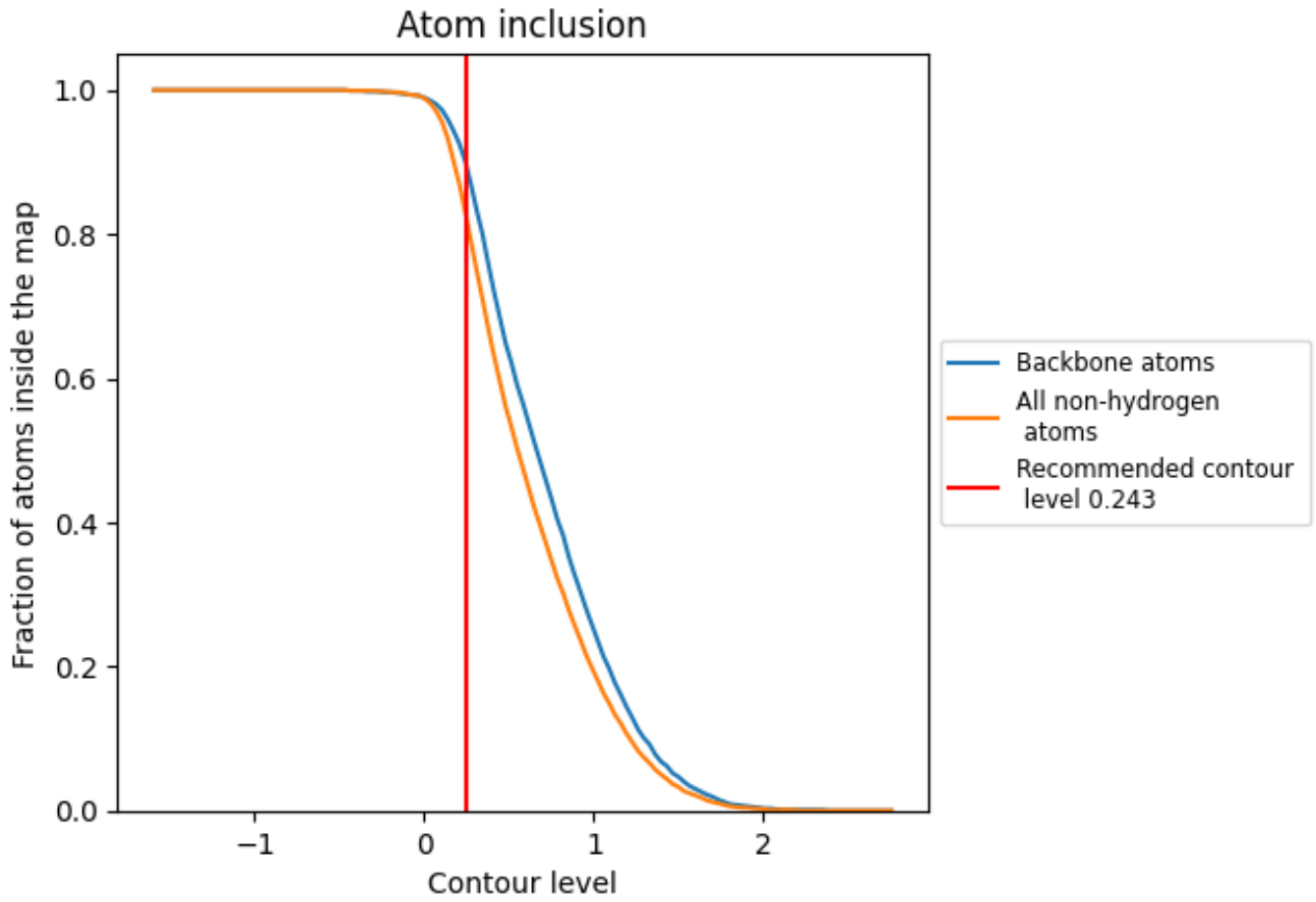
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.243).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.3930
A	0.8410	0.3930
B	0.4630	0.4140