



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:29 PM UTC

PDB ID : 8IZR / pdb_00008izr
EMDB ID : EMD-35869
Title : Multidrug resistance-associated protein 3
Authors : Yun, C.H.; Gao, H.M.
Deposited on : 2023-04-07
Resolution : 3.62 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

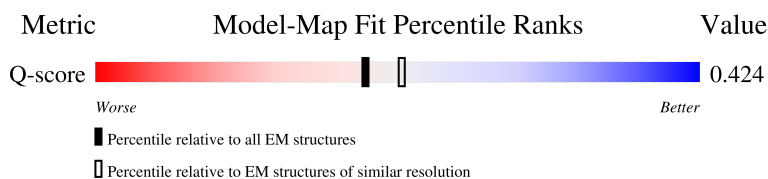
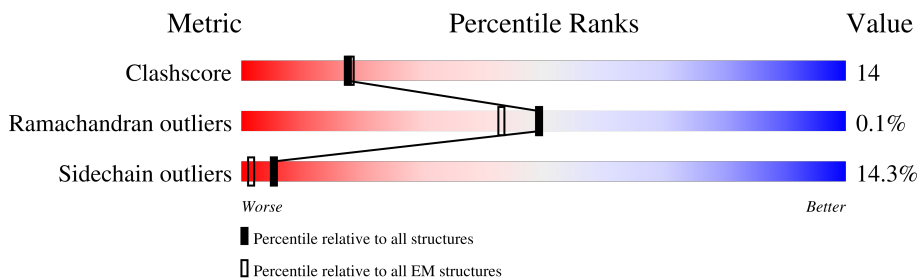
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 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	11773 (3.12 - 4.12)

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	A	1589	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11116 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 ATP-binding cassette sub-family C member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11116	7213	1842	2004	57		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	TYR	variant	UNP Q92887
A	1546	LEU	-	expression tag	UNP Q92887
A	1547	GLU	-	expression tag	UNP Q92887
A	1548	GLU	-	expression tag	UNP Q92887
A	1549	ASN	-	expression tag	UNP Q92887
A	1550	LEU	-	expression tag	UNP Q92887
A	1551	TYR	-	expression tag	UNP Q92887
A	1552	PHE	-	expression tag	UNP Q92887
A	1553	GLN	-	expression tag	UNP Q92887
A	1554	GLY	-	expression tag	UNP Q92887
A	1555	SER	-	expression tag	UNP Q92887
A	1556	GLY	-	expression tag	UNP Q92887
A	1557	GLY	-	expression tag	UNP Q92887
A	1558	GLY	-	expression tag	UNP Q92887
A	1559	GLY	-	expression tag	UNP Q92887
A	1560	GLY	-	expression tag	UNP Q92887
A	1561	GLY	-	expression tag	UNP Q92887
A	1562	ASP	-	expression tag	UNP Q92887
A	1563	TYR	-	expression tag	UNP Q92887
A	1564	LYS	-	expression tag	UNP Q92887
A	1565	ASP	-	expression tag	UNP Q92887
A	1566	HIS	-	expression tag	UNP Q92887
A	1567	ASP	-	expression tag	UNP Q92887
A	1568	GLY	-	expression tag	UNP Q92887
A	1569	ASP	-	expression tag	UNP Q92887
A	1570	TYR	-	expression tag	UNP Q92887
A	1571	LYS	-	expression tag	UNP Q92887
A	1572	ASP	-	expression tag	UNP Q92887

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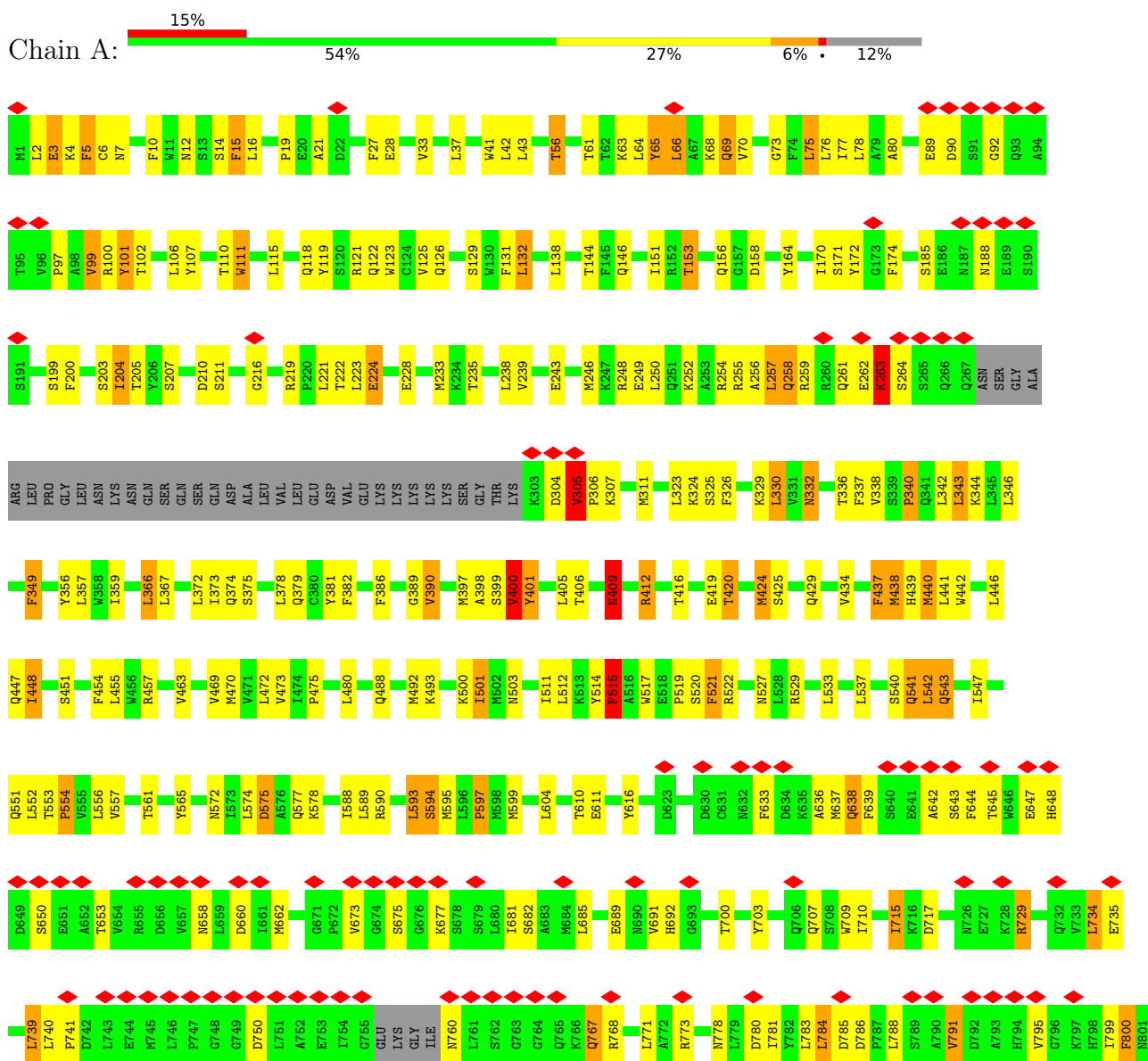
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1573	HIS	-	expression tag	UNP Q92887
A	1574	ASP	-	expression tag	UNP Q92887
A	1575	ILE	-	expression tag	UNP Q92887
A	1576	ASP	-	expression tag	UNP Q92887
A	1577	TYR	-	expression tag	UNP Q92887
A	1578	LYS	-	expression tag	UNP Q92887
A	1579	ASP	-	expression tag	UNP Q92887
A	1580	ASP	-	expression tag	UNP Q92887
A	1581	ASP	-	expression tag	UNP Q92887
A	1582	ASP	-	expression tag	UNP Q92887
A	1583	LYS	-	expression tag	UNP Q92887
A	1584	HIS	-	expression tag	UNP Q92887
A	1585	HIS	-	expression tag	UNP Q92887
A	1586	HIS	-	expression tag	UNP Q92887
A	1587	HIS	-	expression tag	UNP Q92887
A	1588	HIS	-	expression tag	UNP Q92887
A	1589	HIS	-	expression tag	UNP Q92887

3 Residue-property plots

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: ATP-binding cassette sub-family C member 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.612	Depositor
Minimum map value	-0.379	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.103	Depositor
Map size ($\text{\AA}$)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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	A	0.98	2/11350 (0.0%)	1.56	99/15389 (0.6%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	SER	CA-CB	-5.11	1.47	1.54
1	A	1111	SER	CA-CB	-5.09	1.45	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1291	PRO	N-CA-C	-8.83	99.93	110.70
1	A	1350	ILE	N-CA-C	-8.22	102.23	110.62
1	A	994	ILE	N-CA-C	-8.22	102.23	110.62
1	A	597	PRO	CB-CA-C	-8.02	100.31	113.06
1	A	561	THR	CB-CA-C	-8.00	98.26	110.90
1	A	1359	ILE	N-CA-C	7.93	118.04	110.42
1	A	129	SER	N-CA-C	7.87	118.35	108.19
1	A	340	PRO	CB-CA-C	-7.54	101.08	113.06
1	A	399	SER	N-CA-C	-7.48	104.04	113.02
1	A	1047	PHE	N-CA-C	-7.39	103.22	111.71
1	A	970	TYR	N-CA-C	-7.23	103.40	111.28
1	A	989	ASN	N-CA-C	-6.92	102.96	111.40
1	A	412	ARG	N-CA-C	-6.80	104.24	112.54
1	A	326	PHE	N-CA-C	-6.79	103.81	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1185	HIS	N-CA-C	-6.78	105.16	113.50
1	A	515	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	541	GLN	N-CA-C	-6.66	104.03	111.28
1	A	420	THR	CB-CA-C	6.65	121.83	110.79
1	A	401	TYR	N-CA-C	-6.65	104.03	111.28
1	A	1158	PRO	CB-CA-C	-6.49	101.92	112.62
1	A	1281	GLU	N-CA-C	6.44	118.10	111.14
1	A	205	THR	CB-CA-C	-6.41	99.73	110.56
1	A	1410	LEU	N-CA-C	-6.32	104.40	111.28
1	A	437	PHE	CB-CA-C	-6.31	101.31	111.28
1	A	106	LEU	N-CA-C	-6.20	104.58	111.71
1	A	1240	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	324	LYS	N-CA-C	-6.16	103.93	112.30
1	A	69	GLN	CA-C-N	-6.15	116.86	123.08
1	A	69	GLN	C-N-CA	-6.15	116.86	123.08
1	A	336	THR	CB-CA-C	-6.12	100.62	110.79
1	A	519	PRO	N-CA-C	-6.08	105.07	113.53
1	A	1309	TYR	N-CA-C	-6.03	104.71	111.28
1	A	1011	ASN	CB-CA-C	-5.98	101.49	110.88
1	A	90	ASP	N-CA-C	-5.97	104.77	111.28
1	A	501	ILE	N-CA-C	-5.96	104.54	110.62
1	A	64	LEU	N-CA-C	-5.94	104.80	111.28
1	A	493	LYS	CB-CA-C	-5.88	101.66	110.88
1	A	1009	ILE	N-CA-C	5.87	116.64	110.72
1	A	800	PHE	N-CA-C	-5.80	104.96	111.28
1	A	543	GLN	N-CA-C	-5.77	104.99	111.28
1	A	75	LEU	N-CA-C	-5.75	105.01	111.28
1	A	527	ASN	N-CA-C	-5.73	105.12	111.71
1	A	1083	ARG	N-CA-C	-5.72	105.05	111.28
1	A	65	TYR	CA-C-N	-5.70	113.03	120.44
1	A	65	TYR	C-N-CA	-5.70	113.03	120.44
1	A	254	ARG	N-CA-C	-5.70	105.07	111.28
1	A	519	PRO	CB-CA-C	-5.68	103.25	112.62
1	A	400	VAL	N-CA-C	-5.66	106.94	111.81
1	A	258	GLN	N-CA-C	-5.62	105.16	111.28
1	A	604	LEU	N-CA-C	-5.62	106.97	113.88
1	A	1165	GLU	CA-C-N	-5.61	112.76	120.28
1	A	1165	GLU	C-N-CA	-5.61	112.76	120.28
1	A	1176	PHE	N-CA-C	-5.56	98.97	110.80
1	A	440	MET	N-CA-C	-5.54	105.34	111.71
1	A	1076	PRO	N-CA-C	-5.53	102.51	111.14
1	A	68	LYS	N-CA-C	-5.50	106.40	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	ASP	N-CA-C	5.48	116.93	111.07
1	A	995	GLY	CA-C-N	-5.46	112.97	120.28
1	A	995	GLY	C-N-CA	-5.46	112.97	120.28
1	A	257	LEU	N-CA-C	-5.46	105.33	111.28
1	A	343	LEU	CA-C-N	-5.46	112.97	120.28
1	A	343	LEU	C-N-CA	-5.46	112.97	120.28
1	A	767	GLN	N-CA-C	-5.45	105.34	111.28
1	A	1283	PRO	CB-CA-C	-5.45	104.78	111.64
1	A	305	VAL	N-CA-C	-5.45	101.80	107.84
1	A	1042	HIS	CB-CA-C	5.45	120.11	110.85
1	A	739	LEU	N-CA-C	-5.40	106.67	113.20
1	A	1058	LYS	CA-C-N	-5.37	112.66	120.29
1	A	1058	LYS	C-N-CA	-5.37	112.66	120.29
1	A	349	PHE	CB-CA-C	-5.36	101.90	110.79
1	A	102	THR	CB-CA-C	-5.31	101.82	110.85
1	A	3	GLU	N-CA-C	-5.30	105.51	111.28
1	A	409	ASN	N-CA-C	-5.29	106.66	113.01
1	A	1034	GLN	N-CA-C	-5.28	105.53	111.28
1	A	773	ARG	N-CA-C	-5.25	105.55	111.28
1	A	27	PHE	CB-CA-C	-5.24	102.62	110.90
1	A	164	TYR	N-CA-C	-5.23	105.58	111.28
1	A	1240	PHE	CA-C-N	-5.22	113.98	120.56
1	A	1240	PHE	C-N-CA	-5.22	113.98	120.56
1	A	1218	THR	CA-C-N	-5.21	113.32	120.46
1	A	1218	THR	C-N-CA	-5.21	113.32	120.46
1	A	616	TYR	N-CA-C	-5.21	105.60	111.28
1	A	188	ASN	N-CA-C	-5.20	101.98	110.20
1	A	448	ILE	N-CA-C	-5.20	107.34	111.81
1	A	263	LYS	N-CA-C	-5.19	105.74	111.71
1	A	119	TYR	CB-CA-C	-5.18	102.75	110.88
1	A	806	PRO	N-CA-C	-5.16	106.68	113.65
1	A	1061	LEU	N-CA-C	-5.15	105.66	111.28
1	A	151	ILE	N-CA-C	-5.10	105.41	110.62
1	A	1479	ILE	N-CA-C	-5.07	105.45	110.62
1	A	1163	PHE	N-CA-C	-5.06	105.77	111.28
1	A	1021	ASP	CB-CA-C	5.05	119.44	110.85
1	A	480	LEU	N-CA-C	-5.03	105.79	111.28
1	A	1084	PHE	CB-CA-C	-5.03	100.96	110.01
1	A	250	LEU	N-CA-C	-5.02	105.81	111.28
1	A	1127	VAL	CA-C-N	-5.01	116.32	120.33
1	A	1127	VAL	C-N-CA	-5.01	116.32	120.33
1	A	1095	LEU	N-CA-C	-5.01	106.05	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	ILE	CA-C-O	-5.00	115.50	121.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1230	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11116	0	11376	304	0
All	All	11116	0	11376	304	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 (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:ILE:HG13	1:A:1373:LEU:HD22	1.52	0.90
1:A:1358:ILE:HG23	1:A:1363:VAL:H	1.40	0.86
1:A:78:LEU:CD1	1:A:170:ILE:HG22	2.09	0.82
1:A:1303:ASN:O	1:A:1356:GLY:HA2	1.80	0.82
1:A:97:PRO:HD2	1:A:100:ARG:HD2	1.63	0.80
1:A:1335:ARG:HH21	1:A:1495:LEU:HB2	1.47	0.79
1:A:1305:TYR:HB3	1:A:1320:ILE:HB	1.65	0.79
1:A:1327:MET:HE3	1:A:1485:HIS:O	1.82	0.79
1:A:1359:ILE:HG13	1:A:1360:ILE:HG13	1.65	0.78
1:A:1357:GLN:HB2	1:A:1364:ASP:HB2	1.68	0.75
1:A:537:LEU:HB2	1:A:1050:VAL:HG21	1.69	0.75
1:A:822:MET:HA	1:A:825:LEU:HG	1.69	0.74
1:A:1138:GLN:HB2	1:A:1256:VAL:HG22	1.68	0.74
1:A:1146:ARG:HA	1:A:1149:ARG:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:VAL:HB	1:A:1506:VAL:HG13	1.69	0.73
1:A:999:TRP:HZ2	1:A:1023:ARG:HA	1.54	0.73
1:A:1305:TYR:HA	1:A:1356:GLY:HA3	1.72	0.72
1:A:78:LEU:HD11	1:A:170:ILE:HG22	1.72	0.72
1:A:675:SER:HB2	1:A:836:ASN:H	1.54	0.72
1:A:1308:ARG:HA	1:A:1315:LEU:HA	1.71	0.72
1:A:455:LEU:HB3	1:A:463:VAL:HG11	1.73	0.71
1:A:1335:ARG:NH2	1:A:1495:LEU:H	1.90	0.70
1:A:78:LEU:HD11	1:A:170:ILE:CG2	2.20	0.70
1:A:1334:GLY:HA3	1:A:1340:LYS:HB3	1.74	0.70
1:A:61:THR:HA	1:A:122:GLN:HE22	1.57	0.70
1:A:1335:ARG:CZ	1:A:1493:HIS:O	2.41	0.69
1:A:810:LEU:HB3	1:A:813:LYS:HB2	1.75	0.68
1:A:643:SER:HB2	1:A:691:VAL:HB	1.76	0.68
1:A:1170:LEU:HD21	1:A:1174:ARG:HH22	1.60	0.67
1:A:329:LYS:HB3	1:A:442:TRP:HH2	1.59	0.67
1:A:740:LEU:HB2	1:A:741:PRO:HD3	1.77	0.66
1:A:1508:ASP:HB3	1:A:1513:ILE:HG13	1.77	0.66
1:A:1508:ASP:N	1:A:1513:ILE:HB	2.12	0.65
1:A:257:LEU:HD11	1:A:304:ASP:HB3	1.80	0.64
1:A:1358:ILE:HG23	1:A:1363:VAL:N	2.13	0.63
1:A:28:GLU:HB3	1:A:146:GLN:HG2	1.79	0.63
1:A:256:ALA:HA	1:A:259:ARG:HB2	1.80	0.63
1:A:1327:MET:HE1	1:A:1456:LYS:HG2	1.82	0.62
1:A:636:ALA:HB1	1:A:781:ILE:HD11	1.81	0.61
1:A:803:VAL:HG23	1:A:804:LEU:HG	1.80	0.61
1:A:78:LEU:CD1	1:A:170:ILE:CG2	2.77	0.61
1:A:259:ARG:HA	1:A:262:GLU:HB2	1.81	0.61
1:A:78:LEU:HD13	1:A:170:ILE:HG22	1.80	0.61
1:A:1358:ILE:C	1:A:1364:ASP:H	2.07	0.61
1:A:470:MET:HE2	1:A:557:VAL:HG21	1.82	0.60
1:A:1359:ILE:HA	1:A:1364:ASP:C	2.26	0.60
1:A:1358:ILE:H	1:A:1364:ASP:H	1.50	0.59
1:A:329:LYS:HB3	1:A:442:TRP:CH2	2.38	0.59
1:A:1309:TYR:HB2	1:A:1316:VAL:HG23	1.84	0.59
1:A:1358:ILE:HG23	1:A:1362:GLY:HA3	1.84	0.59
1:A:996:SER:HB2	1:A:1027:TYR:HE1	1.67	0.58
1:A:970:TYR:HE1	1:A:1091:VAL:HG13	1.68	0.58
1:A:739:LEU:HD21	1:A:768:ARG:HD3	1.85	0.58
1:A:999:TRP:CZ2	1:A:1023:ARG:HA	2.39	0.58
1:A:1099:LEU:HA	1:A:1262:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:ILE:HA	1:A:1364:ASP:O	2.04	0.57
1:A:1358:ILE:H	1:A:1364:ASP:N	2.02	0.57
1:A:800:PHE:CD1	1:A:824:PHE:HB3	2.39	0.57
1:A:647:GLU:HB2	1:A:650:SER:HB3	1.87	0.56
1:A:993:PHE:HA	1:A:1034:GLN:HE21	1.69	0.56
1:A:1258:MET:C	1:A:1260:SER:N	2.62	0.56
1:A:397:MET:HG2	1:A:424:MET:HG2	1.86	0.56
1:A:223:LEU:HD21	1:A:1192:THR:HG21	1.86	0.56
1:A:800:PHE:CE2	1:A:827:GLN:HB2	2.41	0.56
1:A:332:ASN:HD22	1:A:374:GLN:HG3	1.70	0.56
1:A:675:SER:HB2	1:A:836:ASN:N	2.20	0.56
1:A:56:THR:O	1:A:123:TRP:HD1	1.89	0.55
1:A:43:LEU:HB2	1:A:131:PHE:CE1	2.41	0.55
1:A:1358:ILE:HG13	1:A:1362:GLY:HA3	1.88	0.55
1:A:1469:LEU:HA	1:A:1472:ASP:HB3	1.89	0.55
1:A:1365:ILE:HG21	1:A:1373:LEU:HD13	1.88	0.55
1:A:398:ALA:HB2	1:A:1190:ILE:HD12	1.89	0.55
1:A:1357:GLN:HB2	1:A:1364:ASP:CB	2.37	0.55
1:A:709:TRP:CE2	1:A:1169:GLY:HA3	2.43	0.54
1:A:19:PRO:HB3	1:A:356:TYR:HD1	1.72	0.54
1:A:337:PHE:HB3	1:A:454:PHE:HE2	1.73	0.54
1:A:1411:GLU:HB2	1:A:1416:LYS:HD3	1.90	0.54
1:A:16:LEU:HA	1:A:21:ALA:HB1	1.89	0.53
1:A:644:PHE:HA	1:A:689:GLU:O	2.08	0.53
1:A:455:LEU:CB	1:A:463:VAL:HG11	2.37	0.53
1:A:1407:TRP:HA	1:A:1410:LEU:HD12	1.89	0.53
1:A:1359:ILE:HB	1:A:1367:SER:HB3	1.90	0.53
1:A:153:THR:HG23	1:A:158:ASP:HB3	1.89	0.53
1:A:1066:ARG:NH2	1:A:1282:ALA:O	2.41	0.53
1:A:1088:ILE:HD13	1:A:1272:ILE:HD13	1.89	0.53
1:A:1391:LEU:HB2	1:A:1426:LEU:O	2.09	0.52
1:A:1457:ILE:HA	1:A:1487:THR:HB	1.91	0.52
1:A:565:TYR:CZ	1:A:572:ASN:HB3	2.45	0.52
1:A:37:LEU:HD22	1:A:110:THR:HG21	1.90	0.52
1:A:1446:CYS:O	1:A:1449:ARG:HB2	2.10	0.52
1:A:639:PHE:HB2	1:A:658:ASN:HA	1.92	0.52
1:A:437:PHE:HD2	1:A:599:MET:HE3	1.75	0.52
1:A:520:SER:HB3	1:A:1398:PHE:CZ	2.45	0.52
1:A:2:LEU:HB3	1:A:5:PHE:HB3	1.92	0.51
1:A:1392:ARG:HH21	1:A:1399:ASN:HB3	1.74	0.51
1:A:1306:GLN:HA	1:A:1317:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:ILE:O	1:A:1364:ASP:N	2.41	0.51
1:A:1472:ASP:HA	1:A:1475:ILE:HD12	1.92	0.51
1:A:594:SER:O	1:A:597:PRO:HD2	2.10	0.51
1:A:832:VAL:HA	1:A:842:LYS:HA	1.93	0.51
1:A:63:LYS:O	1:A:66:LEU:HB3	2.10	0.51
1:A:1358:ILE:CG1	1:A:1362:GLY:HA3	2.41	0.51
1:A:1258:MET:C	1:A:1260:SER:H	2.19	0.51
1:A:1335:ARG:HH22	1:A:1495:LEU:H	1.58	0.50
1:A:1349:ARG:HE	1:A:1352:GLU:HG2	1.77	0.50
1:A:261:GLN:O	1:A:264:SER:HB3	2.12	0.50
1:A:1275:TYR:HA	1:A:1278:VAL:HG23	1.94	0.50
1:A:647:GLU:HB2	1:A:650:SER:CB	2.42	0.50
1:A:1508:ASP:H	1:A:1513:ILE:HB	1.76	0.50
1:A:799:ILE:HA	1:A:802:LYS:HG2	1.94	0.50
1:A:1116:ILE:HG12	1:A:1241:VAL:HG13	1.93	0.50
1:A:1359:ILE:HG22	1:A:1364:ASP:HB3	1.94	0.50
1:A:144:THR:HG22	1:A:172:TYR:OH	2.12	0.50
1:A:517:TRP:CD1	1:A:1397:PRO:HG3	2.47	0.50
1:A:993:PHE:O	1:A:994:ILE:C	2.54	0.50
1:A:803:VAL:O	1:A:810:LEU:HB2	2.11	0.49
1:A:995:GLY:O	1:A:996:SER:C	2.55	0.49
1:A:343:LEU:O	1:A:344:LYS:C	2.52	0.49
1:A:305:VAL:HG22	1:A:306:PRO:HD2	1.94	0.49
1:A:633:PHE:CE2	1:A:638:GLN:HB2	2.46	0.49
1:A:1305:TYR:HA	1:A:1356:GLY:CA	2.41	0.49
1:A:252:LYS:HA	1:A:255:ARG:HD2	1.95	0.49
1:A:599:MET:HA	1:A:599:MET:HE2	1.94	0.49
1:A:1333:VAL:HG22	1:A:1498:ILE:HG21	1.95	0.49
1:A:645:THR:HG23	1:A:689:GLU:HB2	1.95	0.48
1:A:999:TRP:CZ2	1:A:1026:VAL:HB	2.47	0.48
1:A:673:VAL:HA	1:A:677:LYS:HD3	1.95	0.48
1:A:389:GLY:O	1:A:390:VAL:C	2.55	0.48
1:A:1236:ASP:O	1:A:1237:THR:C	2.51	0.48
1:A:1335:ARG:HD3	1:A:1493:HIS:CD2	2.49	0.48
1:A:258:GLN:O	1:A:262:GLU:N	2.42	0.48
1:A:398:ALA:HB2	1:A:1190:ILE:CD1	2.43	0.48
1:A:222:THR:C	1:A:224:GLU:N	2.69	0.48
1:A:259:ARG:O	1:A:263:LYS:N	2.42	0.48
1:A:1450:ALA:HA	1:A:1453:ARG:HG3	1.96	0.48
1:A:110:THR:O	1:A:111:TRP:C	2.57	0.47
1:A:207:SER:O	1:A:210:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:TYR:O	1:A:1016:PRO:C	2.57	0.47
1:A:1035:GLY:O	1:A:1036:ILE:C	2.58	0.47
1:A:1401:TYR:CE2	1:A:1452:LEU:HB3	2.49	0.47
1:A:511:ILE:HG23	1:A:515:PHE:CE1	2.50	0.47
1:A:111:TRP:HA	1:A:111:TRP:CE3	2.49	0.47
1:A:346:LEU:HD12	1:A:346:LEU:HA	1.81	0.47
1:A:12:ASN:O	1:A:15:PHE:HB2	2.14	0.47
1:A:1107:LEU:HD13	1:A:1107:LEU:HA	1.73	0.47
1:A:28:GLU:OE2	1:A:146:GLN:HA	2.15	0.47
1:A:833:VAL:HB	1:A:841:GLU:HB2	1.96	0.47
1:A:735:GLU:HA	1:A:740:LEU:HD11	1.97	0.47
1:A:788:LEU:HA	1:A:791:VAL:HG23	1.96	0.47
1:A:1289:ARG:H	1:A:1289:ARG:HG2	1.48	0.47
1:A:43:LEU:HB2	1:A:131:PHE:HE1	1.79	0.47
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.74	0.47
1:A:703:TYR:HA	1:A:783:LEU:O	2.14	0.47
1:A:409:ASN:HD21	1:A:412:ARG:HH21	1.64	0.46
1:A:400:VAL:O	1:A:401:TYR:C	2.56	0.46
1:A:540:SER:O	1:A:541:GLN:C	2.55	0.46
1:A:1410:LEU:HD11	1:A:1426:LEU:HD21	1.96	0.46
1:A:69:GLN:HE22	1:A:115:LEU:HA	1.81	0.46
1:A:845:TYR:O	1:A:848:LEU:HB2	2.15	0.46
1:A:1468:ASP:OD2	1:A:1470:GLU:HB3	2.16	0.46
1:A:472:LEU:O	1:A:475:PRO:HD2	2.14	0.46
1:A:729:ARG:HE	1:A:778:ASN:HD21	1.63	0.46
1:A:1201:ILE:HD12	1:A:1201:ILE:HA	1.87	0.46
1:A:1294:TRP:N	1:A:1295:PRO:HD2	2.31	0.46
1:A:993:PHE:HA	1:A:1034:GLN:NE2	2.31	0.46
1:A:1206:TRP:CE2	1:A:1210:ARG:HD3	2.50	0.46
1:A:785:ASP:O	1:A:786:ASP:C	2.58	0.46
1:A:3:GLU:O	1:A:7:ASN:N	2.48	0.46
1:A:1230:ARG:O	1:A:1231:ASP:C	2.58	0.46
1:A:1365:ILE:CG1	1:A:1373:LEU:HD22	2.34	0.45
1:A:488:GLN:HB3	1:A:492:MET:HE2	1.97	0.45
1:A:1358:ILE:CG2	1:A:1362:GLY:HA3	2.45	0.45
1:A:834:LEU:HA	1:A:839:ILE:HA	1.98	0.45
1:A:1370:LEU:HD23	1:A:1370:LEU:HA	1.82	0.45
1:A:199:SER:O	1:A:200:PHE:C	2.60	0.45
1:A:89:GLU:C	1:A:92:GLY:H	2.25	0.45
1:A:517:TRP:CG	1:A:1397:PRO:HG3	2.52	0.45
1:A:521:PHE:O	1:A:522:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:GLN:H	1:A:1423:GLN:CD	2.24	0.45
1:A:1457:ILE:HA	1:A:1487:THR:O	2.17	0.45
1:A:235:THR:O	1:A:239:VAL:HG23	2.17	0.44
1:A:511:ILE:O	1:A:512:LEU:C	2.59	0.44
1:A:804:LEU:HA	1:A:815:ARG:HE	1.82	0.44
1:A:200:PHE:O	1:A:204:ILE:HB	2.17	0.44
1:A:99:VAL:C	1:A:101:TYR:N	2.72	0.44
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.84	0.44
1:A:1274:GLU:O	1:A:1277:LYS:HG2	2.18	0.44
1:A:1403:ASP:C	1:A:1405:GLU:N	2.73	0.44
1:A:1426:LEU:HD23	1:A:1426:LEU:HA	1.84	0.44
1:A:1212:GLU:O	1:A:1213:LEU:C	2.60	0.44
1:A:349:PHE:CZ	1:A:1230:ARG:HD2	2.52	0.44
1:A:378:LEU:O	1:A:379:GLN:C	2.61	0.44
1:A:111:TRP:HA	1:A:111:TRP:HE3	1.82	0.44
1:A:522:ARG:HE	1:A:522:ARG:HB3	1.53	0.44
1:A:1068:PRO:HB3	1:A:1281:GLU:HB2	2.00	0.44
1:A:1146:ARG:HA	1:A:1149:ARG:HD3	1.99	0.44
1:A:366:LEU:HD22	1:A:366:LEU:HA	1.84	0.44
1:A:767:GLN:HG2	1:A:791:VAL:HG22	2.00	0.44
1:A:243:GLU:O	1:A:246:MET:HG2	2.18	0.44
1:A:438:MET:HE3	1:A:438:MET:HB3	1.60	0.44
1:A:804:LEU:HA	1:A:815:ARG:NE	2.33	0.44
1:A:1406:ILE:HA	1:A:1452:LEU:HD21	2.00	0.44
1:A:969:GLU:O	1:A:970:TYR:C	2.60	0.43
1:A:1505:MET:HE2	1:A:1505:MET:HB3	1.86	0.43
1:A:405:LEU:HD21	1:A:1166:THR:HG21	2.00	0.43
1:A:575:ASP:N	1:A:575:ASP:OD1	2.51	0.43
1:A:305:VAL:O	1:A:307:LYS:HG2	2.18	0.43
1:A:675:SER:CB	1:A:836:ASN:H	2.28	0.43
1:A:514:TYR:CZ	1:A:1350:ILE:HD11	2.53	0.43
1:A:542:LEU:O	1:A:543:GLN:C	2.58	0.43
1:A:553:THR:N	1:A:554:PRO:CD	2.82	0.43
1:A:593:LEU:HD23	1:A:593:LEU:HA	1.79	0.43
1:A:1324:ILE:HD12	1:A:1324:ILE:HA	1.77	0.43
1:A:1316:VAL:HG12	1:A:1317:LEU:HG	2.00	0.43
1:A:1365:ILE:HD13	1:A:1365:ILE:H	1.84	0.43
1:A:1415:LEU:HD22	1:A:1415:LEU:HA	1.79	0.43
1:A:637:MET:O	1:A:660:ASP:HA	2.18	0.43
1:A:842:LYS:H	1:A:851:LYS:NZ	2.16	0.43
1:A:1344:THR:HG22	1:A:1491:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ALA:HB1	1:A:781:ILE:CD1	2.48	0.43
1:A:1130:LEU:HD23	1:A:1130:LEU:HA	1.82	0.43
1:A:382:PHE:HD2	1:A:1205:ARG:NH1	2.17	0.43
1:A:41:TRP:HE1	1:A:110:THR:HA	1.83	0.43
1:A:1448:GLY:HA2	1:A:1451:LEU:HD12	1.99	0.43
1:A:660:ASP:OD1	1:A:660:ASP:N	2.51	0.43
1:A:1456:LYS:HD2	1:A:1456:LYS:H	1.84	0.42
1:A:204:ILE:HD12	1:A:204:ILE:HA	1.74	0.42
1:A:469:VAL:HG11	1:A:556:LEU:HD22	2.01	0.42
1:A:734:LEU:HB3	1:A:740:LEU:HD21	2.00	0.42
1:A:1082:ASN:HA	1:A:1085:ALA:HB3	2.00	0.42
1:A:1083:ARG:HG3	1:A:1275:TYR:CE2	2.54	0.42
1:A:1365:ILE:CG2	1:A:1373:LEU:HD13	2.48	0.42
1:A:73:GLY:O	1:A:76:LEU:HB3	2.19	0.42
1:A:132:LEU:HD22	1:A:132:LEU:HA	1.84	0.42
1:A:1328:GLU:HG2	1:A:1329:LYS:N	2.34	0.42
1:A:1461:ASP:O	1:A:1462:GLU:C	2.61	0.42
1:A:15:PHE:O	1:A:21:ALA:HB1	2.20	0.42
1:A:69:GLN:HE21	1:A:118:GLN:HB2	1.84	0.42
1:A:529:ARG:HE	1:A:1057:HIS:CG	2.37	0.42
1:A:1445:LEU:HD12	1:A:1445:LEU:HA	1.92	0.42
1:A:715:ILE:HD13	1:A:715:ILE:HA	1.86	0.42
1:A:1258:MET:O	1:A:1260:SER:N	2.52	0.42
1:A:1335:ARG:NH2	1:A:1495:LEU:N	2.62	0.42
1:A:1460:LEU:HB2	1:A:1490:THR:HG23	2.02	0.42
1:A:1479:ILE:H	1:A:1479:ILE:HG13	1.51	0.42
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.84	0.42
1:A:846:SER:O	1:A:849:LEU:HB2	2.19	0.42
1:A:1101:SER:O	1:A:1102:TRP:C	2.62	0.42
1:A:386:PHE:HD2	1:A:1201:ILE:HD11	1.85	0.42
1:A:992:ALA:CB	1:A:1034:GLN:HG3	2.49	0.42
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.91	0.42
1:A:771:LEU:HD11	1:A:784:LEU:HD22	2.01	0.42
1:A:992:ALA:HB3	1:A:1034:GLN:HG3	2.01	0.42
1:A:1226:MET:HE1	1:A:1241:VAL:HG11	2.02	0.42
1:A:1469:LEU:O	1:A:1473:ASN:N	2.50	0.42
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.78	0.42
1:A:813:LYS:HA	1:A:813:LYS:HD3	1.74	0.42
1:A:998:LEU:HD21	1:A:1118:MET:HE1	2.02	0.42
1:A:1178:HIS:HB3	1:A:1181:ARG:HH21	1.84	0.42
1:A:1312:GLU:H	1:A:1312:GLU:HG3	1.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:10:PHE:HB2	2.01	0.42
1:A:28:GLU:HB3	1:A:146:GLN:CG	2.49	0.42
1:A:1301:GLN:HA	1:A:1323:ASP:HA	2.01	0.42
1:A:424:MET:HG2	1:A:424:MET:O	2.20	0.41
1:A:1358:ILE:HG23	1:A:1362:GLY:CA	2.49	0.41
1:A:1479:ILE:HA	1:A:1483:PHE:HD2	1.85	0.41
1:A:500:LYS:HA	1:A:503:ASN:ND2	2.35	0.41
1:A:1098:SER:O	1:A:1099:LEU:C	2.60	0.41
1:A:1236:ASP:O	1:A:1239:GLY:N	2.52	0.41
1:A:799:ILE:O	1:A:800:PHE:C	2.62	0.41
1:A:470:MET:HE1	1:A:590:ARG:HB2	2.02	0.41
1:A:642:ALA:HA	1:A:692:HIS:O	2.21	0.41
1:A:343:LEU:HD12	1:A:343:LEU:HA	1.92	0.41
1:A:216:GLY:HA2	1:A:221:LEU:HD21	2.02	0.41
1:A:249:GLU:H	1:A:249:GLU:HG2	1.64	0.41
1:A:381:TYR:OH	1:A:439:HIS:HB2	2.21	0.41
1:A:446:LEU:C	1:A:448:ILE:N	2.78	0.41
1:A:707:GLN:CD	1:A:707:GLN:H	2.29	0.41
1:A:810:LEU:O	1:A:815:ARG:NH1	2.54	0.41
1:A:1310:ARG:HB2	1:A:1313:LEU:HB2	2.01	0.41
1:A:1220:PHE:O	1:A:1221:PHE:C	2.64	0.41
1:A:520:SER:HB3	1:A:1398:PHE:CE1	2.55	0.41
1:A:575:ASP:OD1	1:A:578:LYS:HD3	2.21	0.41
1:A:643:SER:CB	1:A:691:VAL:HB	2.48	0.41
1:A:1046:ALA:O	1:A:1047:PHE:C	2.64	0.41
1:A:1049:PHE:O	1:A:1052:ALA:HB3	2.21	0.41
1:A:1224:LEU:O	1:A:1227:VAL:N	2.54	0.41
1:A:1359:ILE:HA	1:A:1364:ASP:HB3	2.03	0.41
1:A:1376:LYS:HA	1:A:1376:LYS:HD3	1.83	0.41
1:A:75:LEU:HD21	1:A:174:PHE:HB2	2.02	0.41
1:A:446:LEU:C	1:A:448:ILE:H	2.29	0.41
1:A:1368:ILE:H	1:A:1368:ILE:HG12	1.81	0.40
1:A:1408:LYS:O	1:A:1412:LEU:HG	2.21	0.40
1:A:65:TYR:O	1:A:69:GLN:HB2	2.21	0.40
1:A:77:ILE:O	1:A:80:ALA:HB3	2.20	0.40
1:A:1110:ILE:O	1:A:1111:SER:C	2.63	0.40
1:A:1125:ILE:O	1:A:1129:PRO:HD2	2.21	0.40
1:A:1358:ILE:N	1:A:1364:ASP:H	2.18	0.40
1:A:1446:CYS:HA	1:A:1449:ARG:HD2	2.02	0.40
1:A:256:ALA:O	1:A:259:ARG:HB2	2.22	0.40
1:A:511:ILE:HD12	1:A:1385:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:LEU:HD23	1:A:1252:LEU:HA	1.97	0.40
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.87	0.40
1:A:1146:ARG:O	1:A:1149:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1392/1589 (88%)	1347 (97%)	43 (3%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	TYR
1	A	1231	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1241/1408 (88%)	1063 (86%)	178 (14%)	3 16

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	PHE
1	A	6	CYS
1	A	14	SER
1	A	15	PHE
1	A	33	VAL
1	A	56	THR
1	A	66	LEU
1	A	70	VAL
1	A	99	VAL
1	A	101	TYR
1	A	107	TYR
1	A	111	TRP
1	A	125	VAL
1	A	126	GLN
1	A	132	LEU
1	A	138	LEU
1	A	153	THR
1	A	156	GLN
1	A	171	SER
1	A	185	SER
1	A	203	SER
1	A	204	ILE
1	A	211	SER
1	A	219	ARG
1	A	224	GLU
1	A	228	GLU
1	A	233	MET
1	A	238	LEU
1	A	248	ARG
1	A	263	LYS
1	A	305	VAL
1	A	311	MET
1	A	323	LEU
1	A	325	SER
1	A	330	LEU
1	A	332	ASN
1	A	338	VAL
1	A	340	PRO
1	A	357	LEU
1	A	359	ILE
1	A	366	LEU
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	372	LEU
1	A	373	ILE
1	A	375	SER
1	A	390	VAL
1	A	400	VAL
1	A	406	THR
1	A	409	ASN
1	A	416	THR
1	A	419	GLU
1	A	420	THR
1	A	424	MET
1	A	425	SER
1	A	429	GLN
1	A	434	VAL
1	A	438	MET
1	A	440	MET
1	A	447	GLN
1	A	451	SER
1	A	457	ARG
1	A	473	VAL
1	A	501	ILE
1	A	515	PHE
1	A	521	PHE
1	A	542	LEU
1	A	547	ILE
1	A	551	GLN
1	A	552	LEU
1	A	554	PRO
1	A	574	LEU
1	A	575	ASP
1	A	577	GLN
1	A	589	LEU
1	A	593	LEU
1	A	594	SER
1	A	595	MET
1	A	610	THR
1	A	611	GLU
1	A	638	GLN
1	A	648	HIS
1	A	653	THR
1	A	662	MET
1	A	681	ILE

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Mol	Chain	Res	Type
1	A	682	SER
1	A	685	LEU
1	A	700	THR
1	A	710	ILE
1	A	715	ILE
1	A	717	ASP
1	A	729	ARG
1	A	734	LEU
1	A	750	ASP
1	A	760	ASN
1	A	784	LEU
1	A	791	VAL
1	A	795	VAL
1	A	803	VAL
1	A	804	LEU
1	A	816	LEU
1	A	825	LEU
1	A	827	GLN
1	A	831	ILE
1	A	834	LEU
1	A	838	THR
1	A	839	ILE
1	A	848	LEU
1	A	859	LEU
1	A	969	GLU
1	A	984	LEU
1	A	996	SER
1	A	1007	SER
1	A	1032	LEU
1	A	1034	GLN
1	A	1038	VAL
1	A	1044	TRP
1	A	1050	VAL
1	A	1061	LEU
1	A	1064	ILE
1	A	1075	THR
1	A	1080	ILE
1	A	1094	THR
1	A	1099	LEU
1	A	1103	ILE
1	A	1107	LEU
1	A	1110	ILE

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Mol	Chain	Res	Type
1	A	1112	THR
1	A	1143	SER
1	A	1155	THR
1	A	1158	PRO
1	A	1164	SER
1	A	1177	GLU
1	A	1188	VAL
1	A	1193	ASN
1	A	1201	ILE
1	A	1210	ARG
1	A	1213	LEU
1	A	1218	THR
1	A	1236	ASP
1	A	1242	LEU
1	A	1253	ASN
1	A	1257	ARG
1	A	1259	THR
1	A	1260	SER
1	A	1267	VAL
1	A	1300	ILE
1	A	1307	VAL
1	A	1312	GLU
1	A	1315	LEU
1	A	1316	VAL
1	A	1318	ARG
1	A	1323	ASP
1	A	1324	ILE
1	A	1336	THR
1	A	1341	SER
1	A	1344	THR
1	A	1352	GLU
1	A	1358	ILE
1	A	1359	ILE
1	A	1365	ILE
1	A	1368	ILE
1	A	1379	ILE
1	A	1386	LEU
1	A	1408	LYS
1	A	1414	HIS
1	A	1415	LEU
1	A	1423	GLN
1	A	1438	SER

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Mol	Chain	Res	Type
1	A	1456	LYS
1	A	1458	LEU
1	A	1467	VAL
1	A	1474	LEU
1	A	1479	ILE
1	A	1487	THR
1	A	1496	HIS
1	A	1513	ILE
1	A	1514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	122	GLN
1	A	128	ASN
1	A	332	ASN
1	A	383	GLN
1	A	447	GLN
1	A	503	ASN
1	A	577	GLN
1	A	694	HIS
1	A	711	GLN
1	A	731	GLN
1	A	760	ASN
1	A	765	GLN
1	A	778	ASN
1	A	794	HIS
1	A	798	HIS
1	A	827	GLN
1	A	997	ASN
1	A	1057	HIS
1	A	1185	HIS
1	A	1247	ASN
1	A	1443	GLN

5.3.3 RNA ⓘ

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.

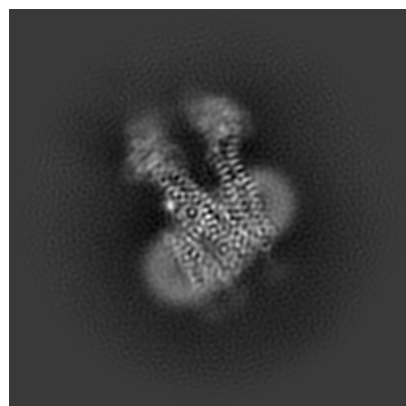
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35869. These allow visual inspection of the internal detail of the map and identification of artifacts.

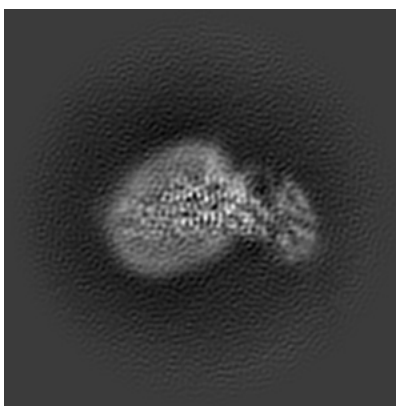
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

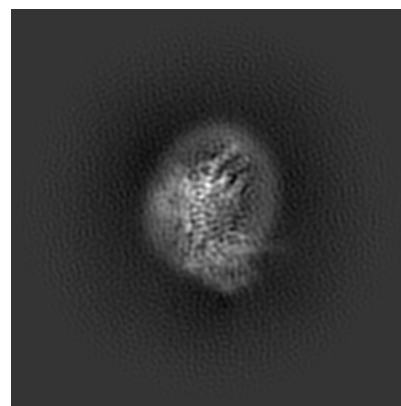
6.1.1 Primary map



X

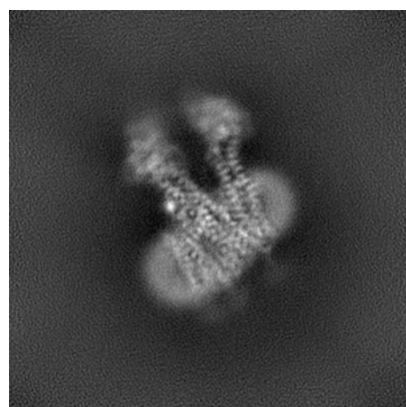


Y

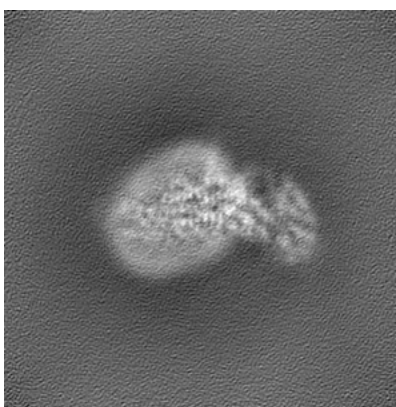


Z

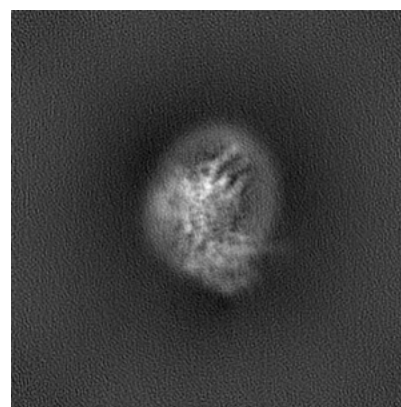
6.1.2 Raw map



X



Y

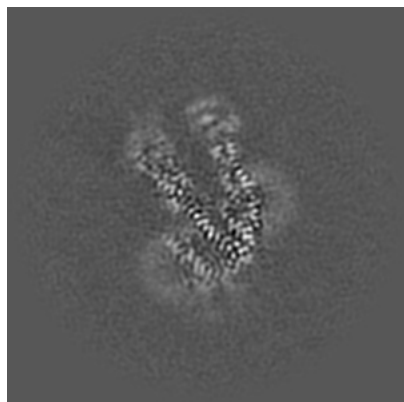


Z

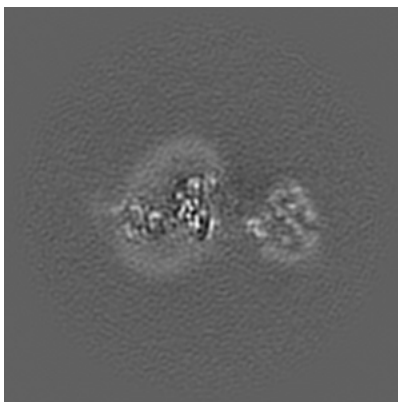
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

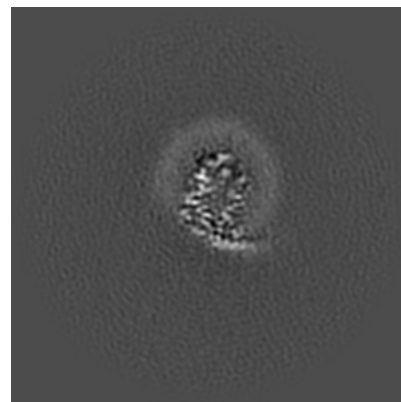
6.2.1 Primary map



X Index: 128

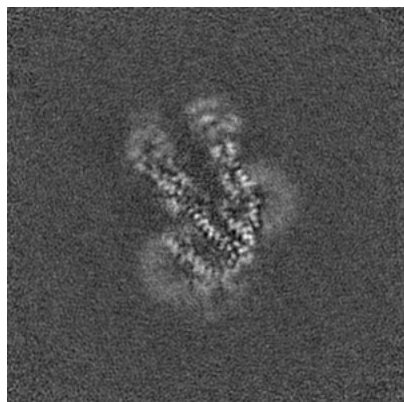


Y Index: 128

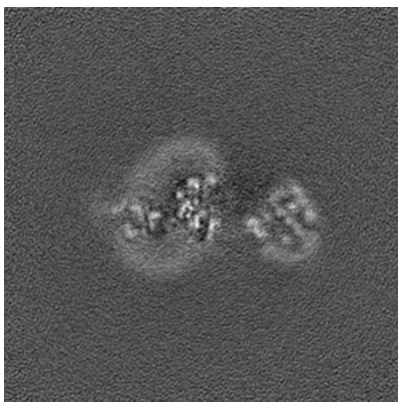


Z Index: 128

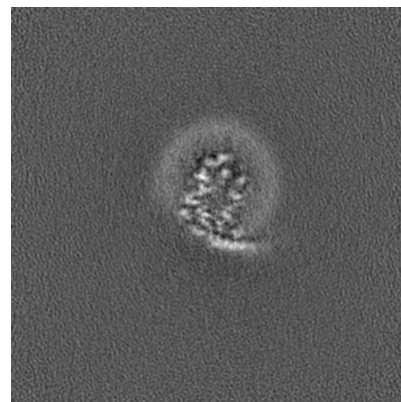
6.2.2 Raw map



X Index: 128



Y Index: 128

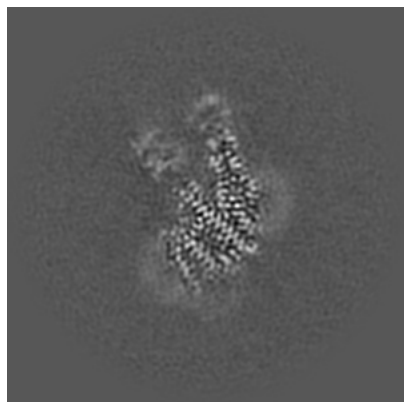


Z Index: 128

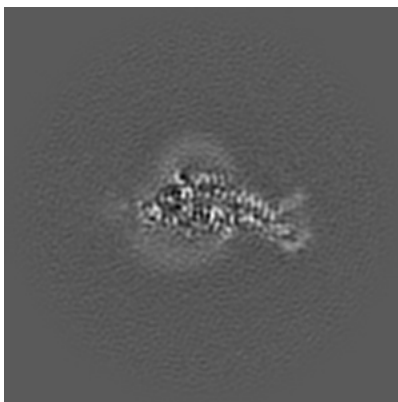
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

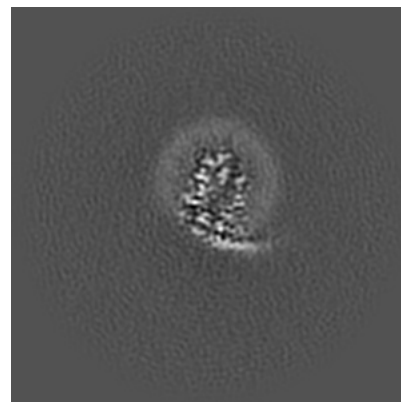
6.3.1 Primary map



X Index: 121

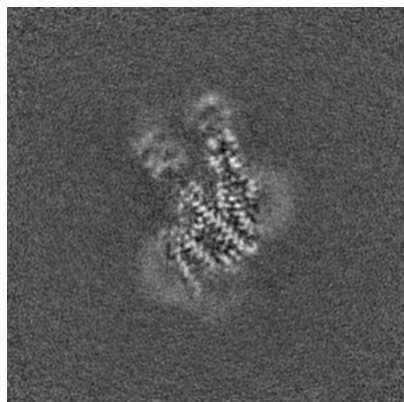


Y Index: 144

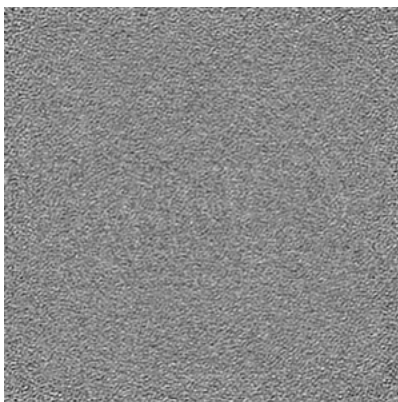


Z Index: 129

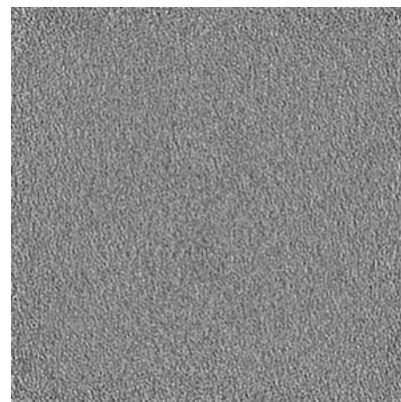
6.3.2 Raw map



X Index: 121



Y Index: 0

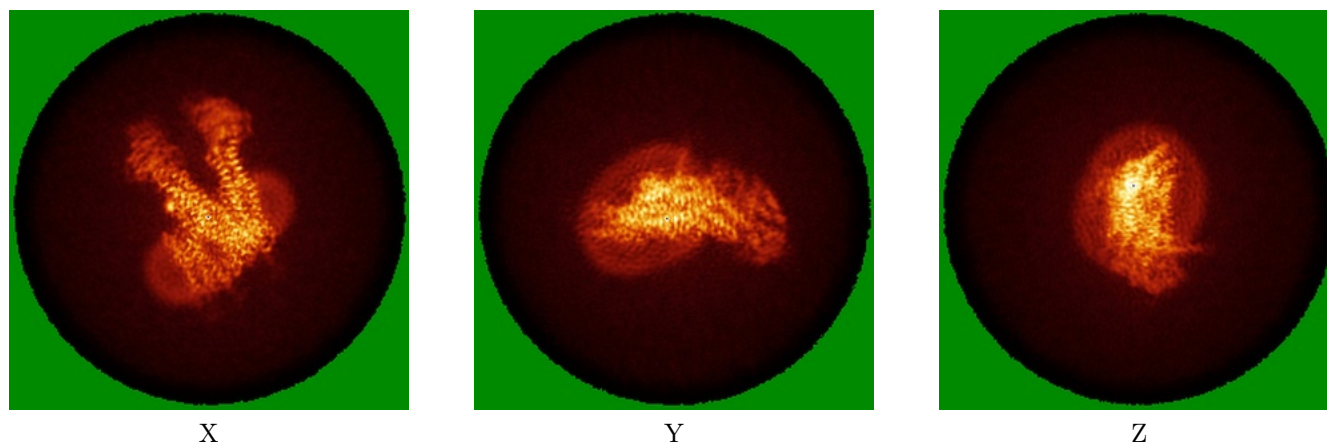


Z Index: 0

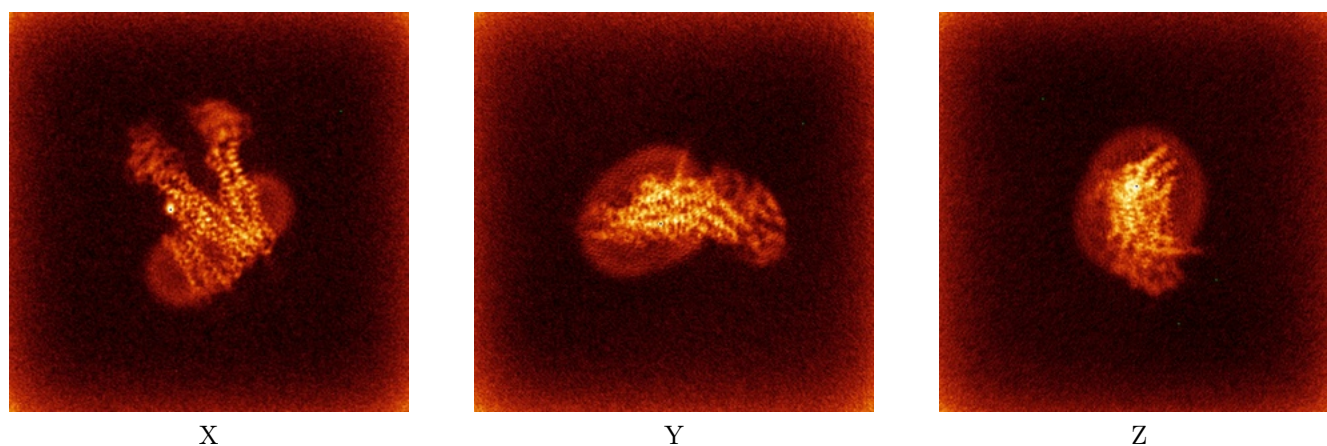
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

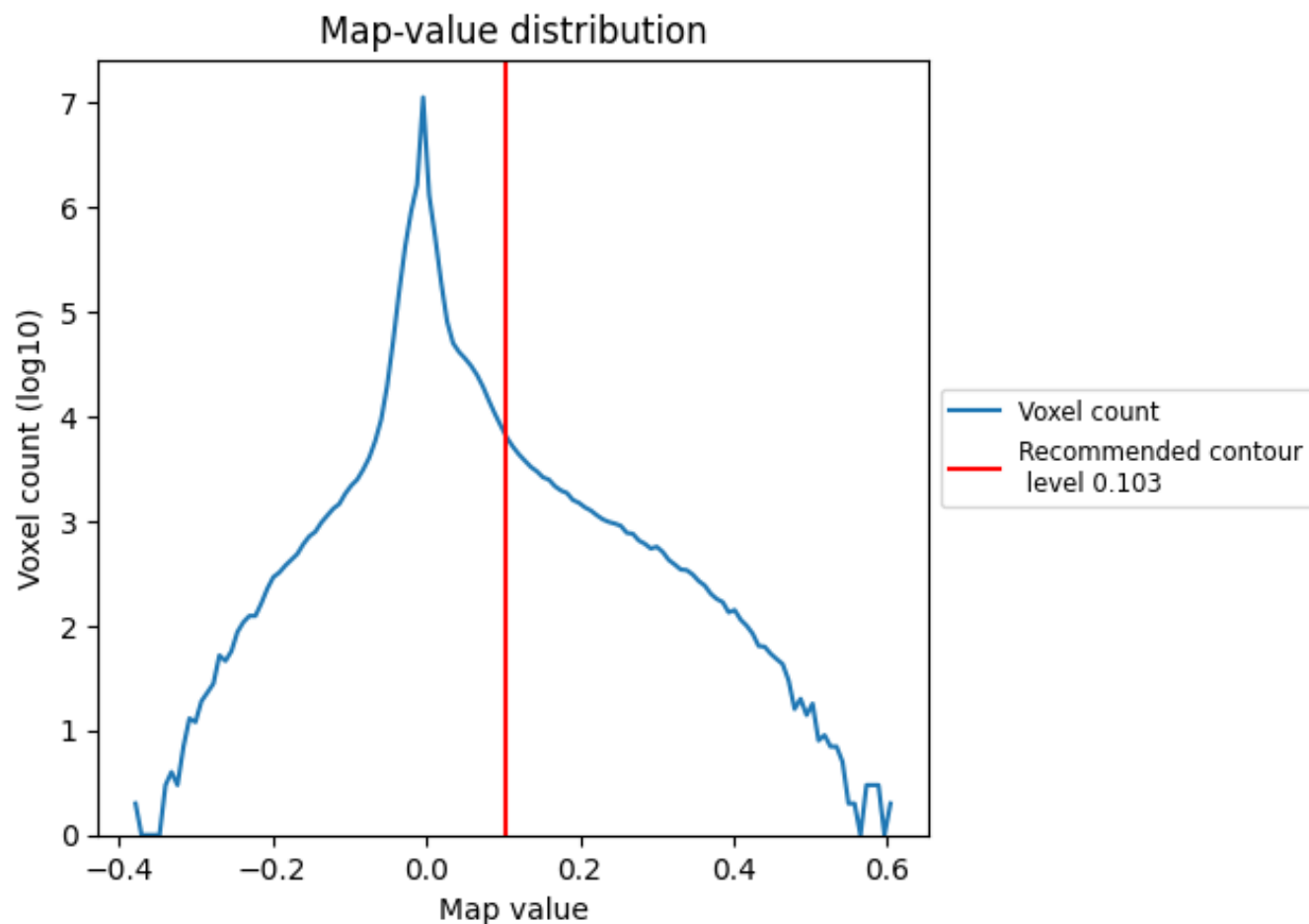
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

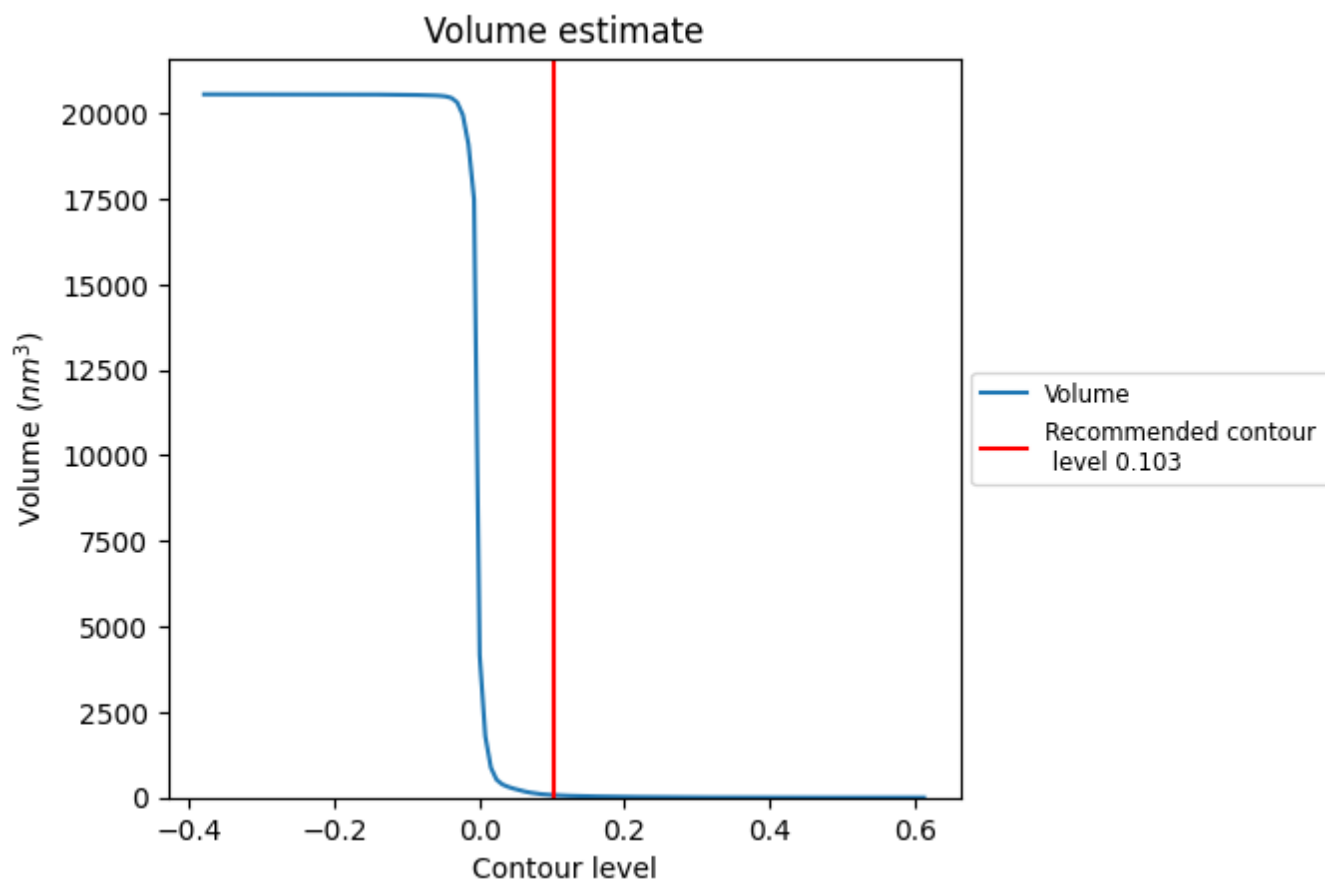
This section contains the results of statistical analysis of the map.

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.

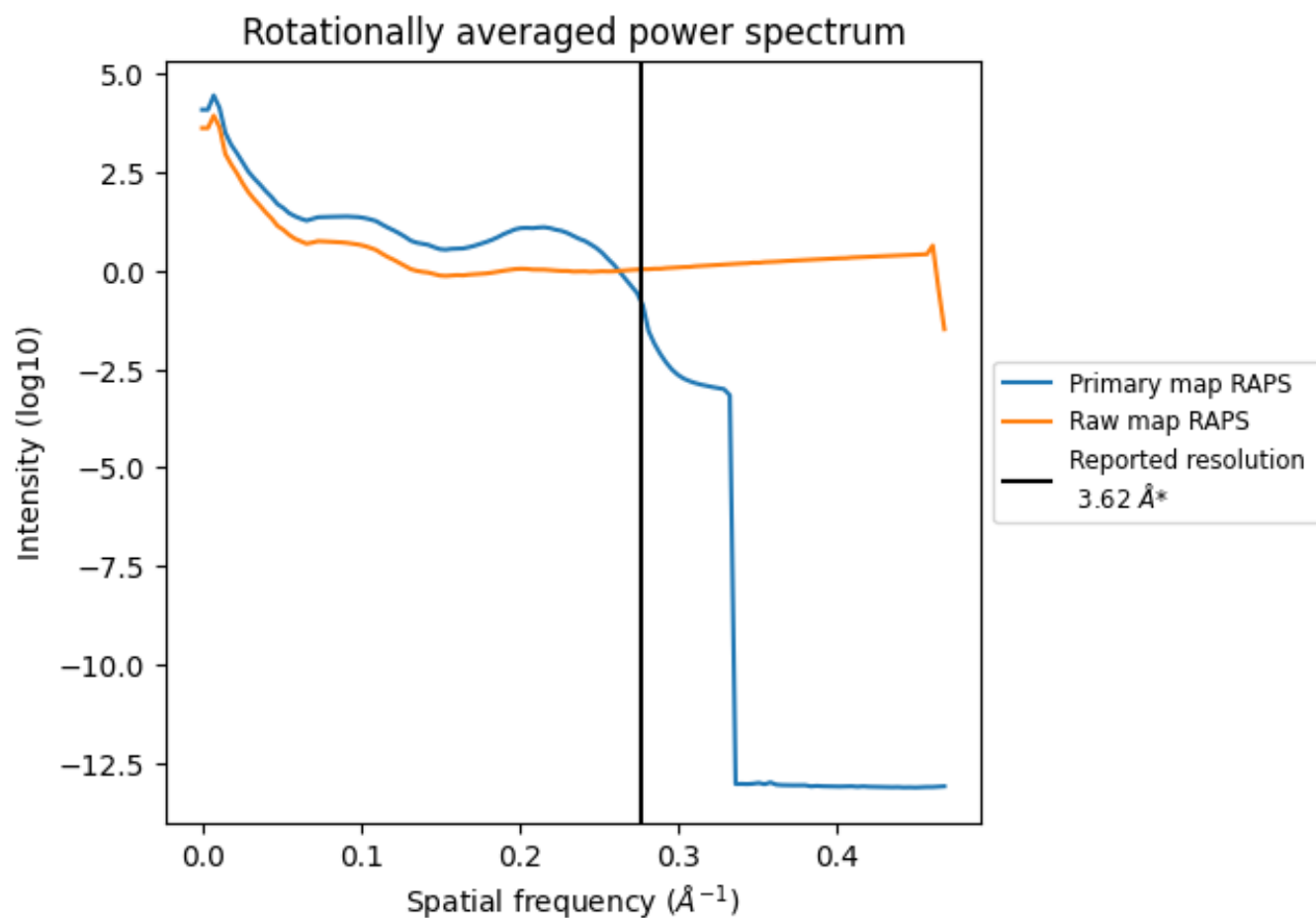
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

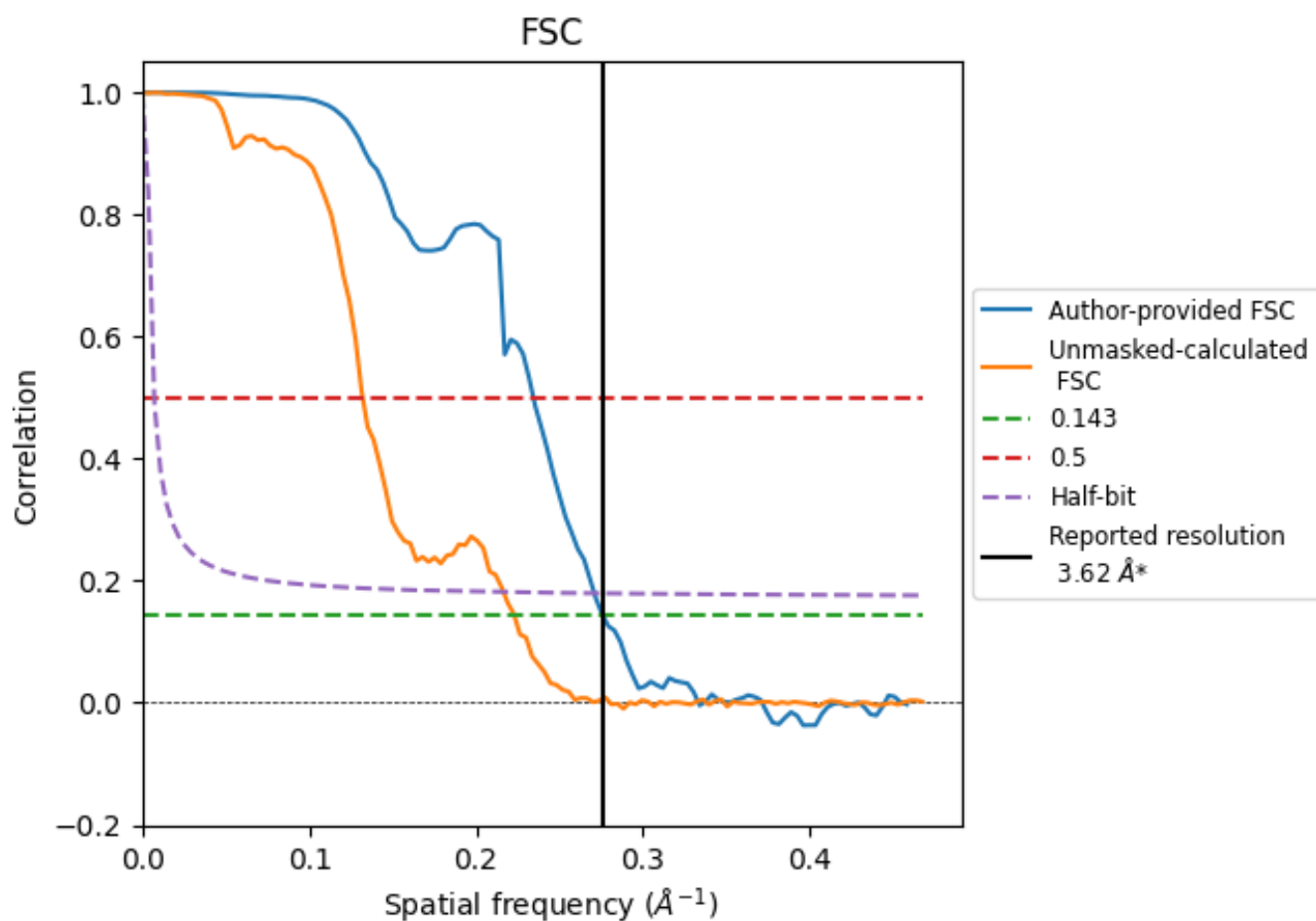


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 0.276 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

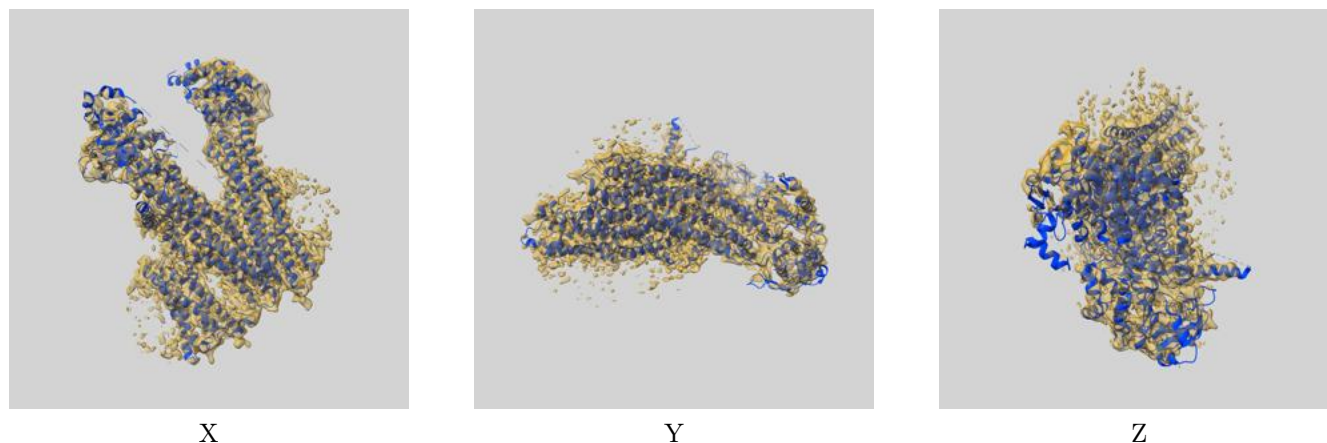
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	4.27	3.69
Unmasked-calculated*	4.48	7.57	4.62

*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 4.48 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

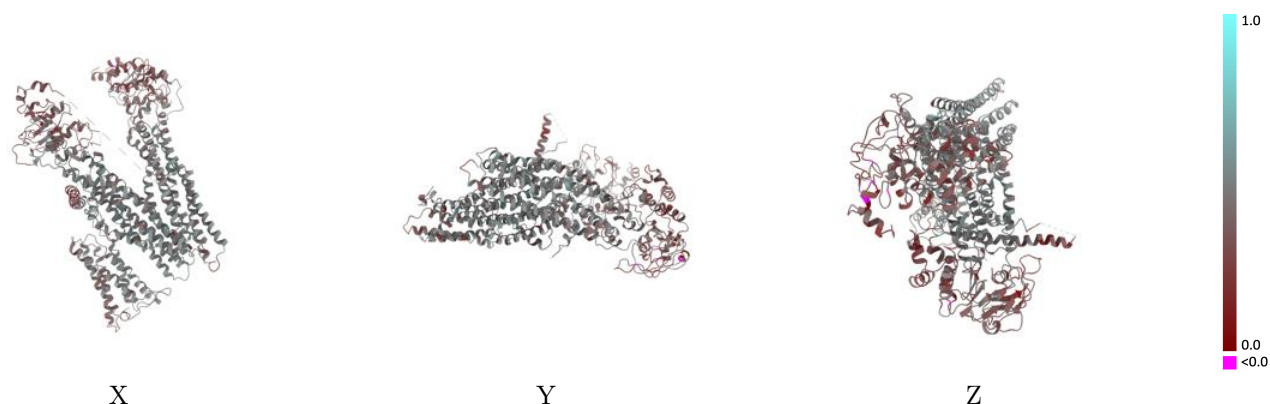
This section contains information regarding the fit between EMDB map EMD-35869 and PDB model 8IZR. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.103 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](#)

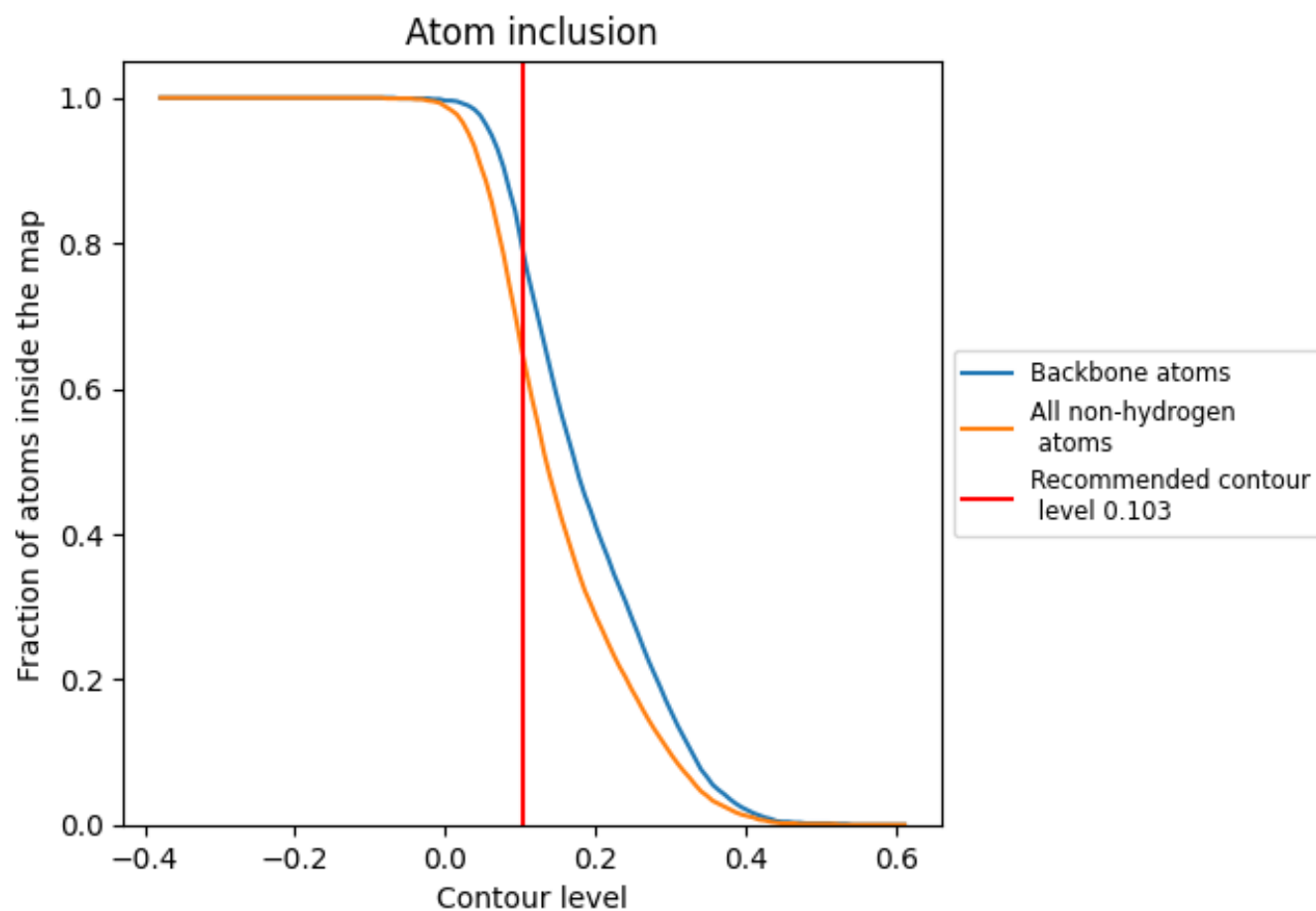


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4240
A	0.6500	0.4240

