



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:15 PM UTC

PDB ID : 8W9C / pdb_00008w9c
EMDB ID : EMD-37364
Title : Cryo-EM structure of the Rpd3S complex from budding yeast
Authors : Wang, C.; Zhan, X.
Deposited on : 2023-09-05
Resolution : 3.30 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:

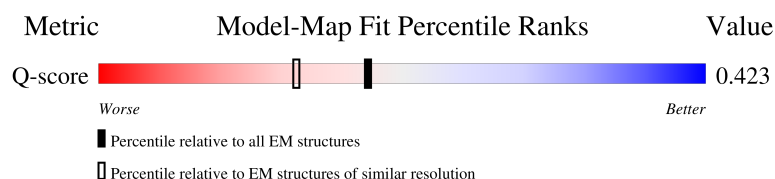
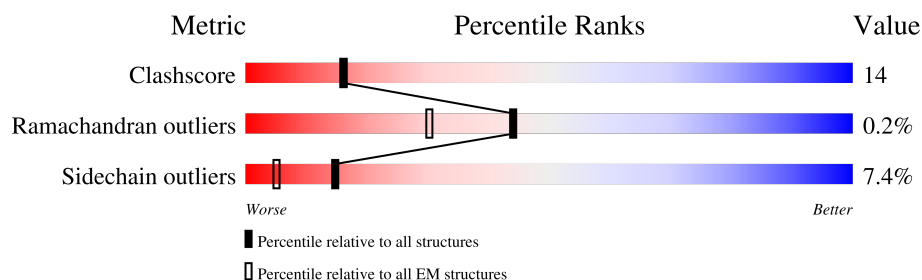
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	15087 (2.80 - 3.80)

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	1536	 8% 24% 13% • 61%
2	E	684	 8% 31% 18% • 48%
2	F	684	 7% 15% 7% 77%
3	B	433	 • 61% 25% • 11%

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Mol	Chain	Length	Quality of chain
4	C	401	28%16%54%
4	D	401	11%27%17%54%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15278 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			5066	3253	860	938	15		

- Molecule 2 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	353	Total	C	N	O	S	0	0
			2884	1837	493	536	18		
2	F	156	Total	C	N	O	S	0	0
			1282	822	211	239	10		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 4 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	183	Total	C	N	O	S	0	0
			1483	950	239	285	9		
4	D	185	Total	C	N	O	S	0	0
			1497	959	241	288	9		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	E	4	Total	Zn	0
			4	4	
5	B	1	Total	Zn	0
			1	1	

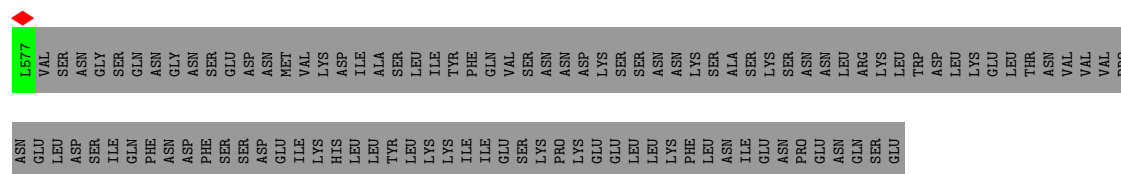
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Mol	Chain	Residues	Atoms		AltConf
5	F	2	Total	Zn	0
			2	2	

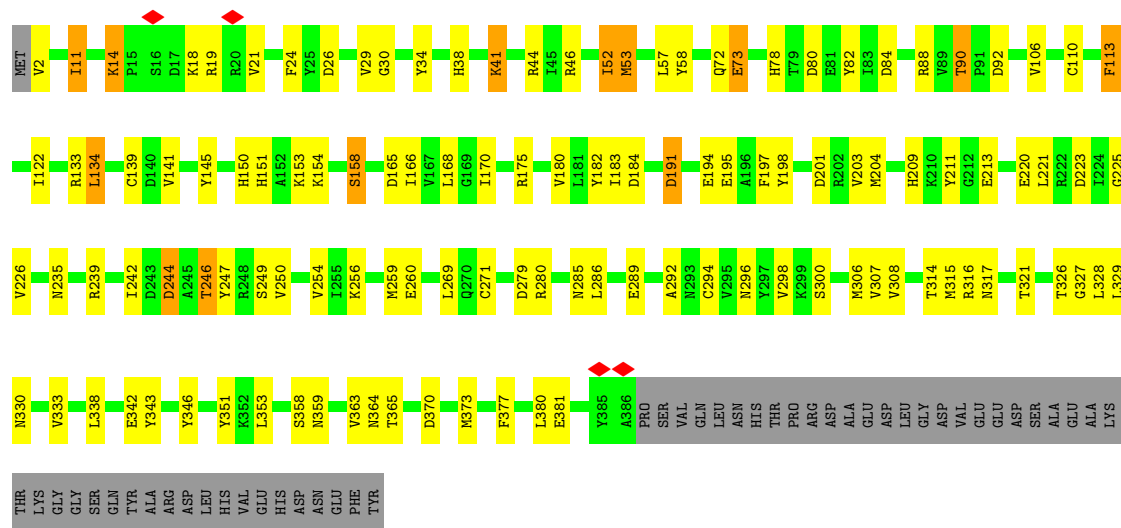
- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	K	0
			2	2	



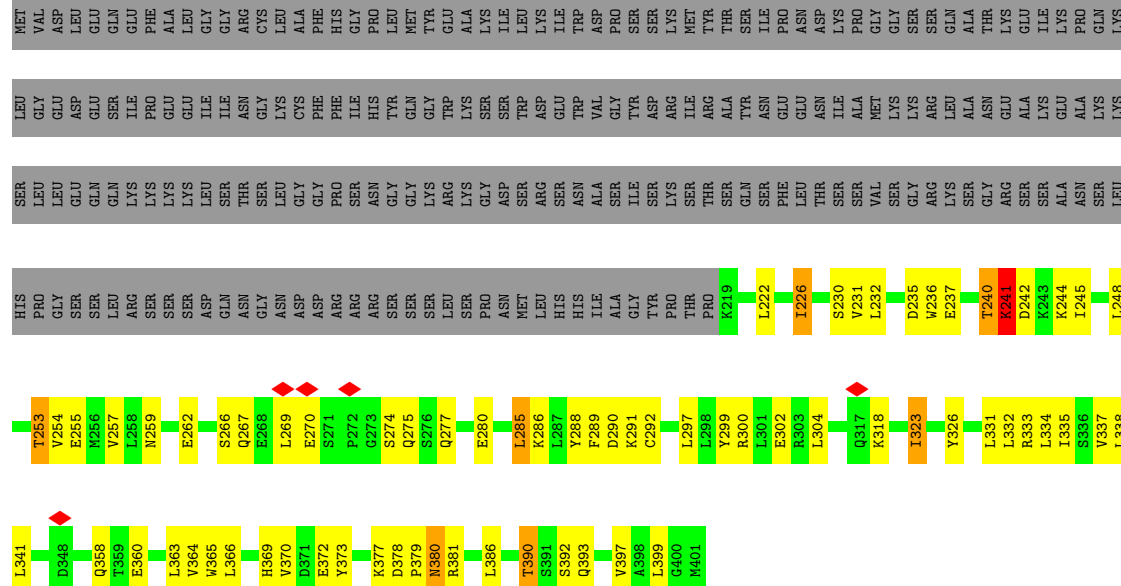
• Molecule 3: Histone deacetylase RPD3

Chain B:

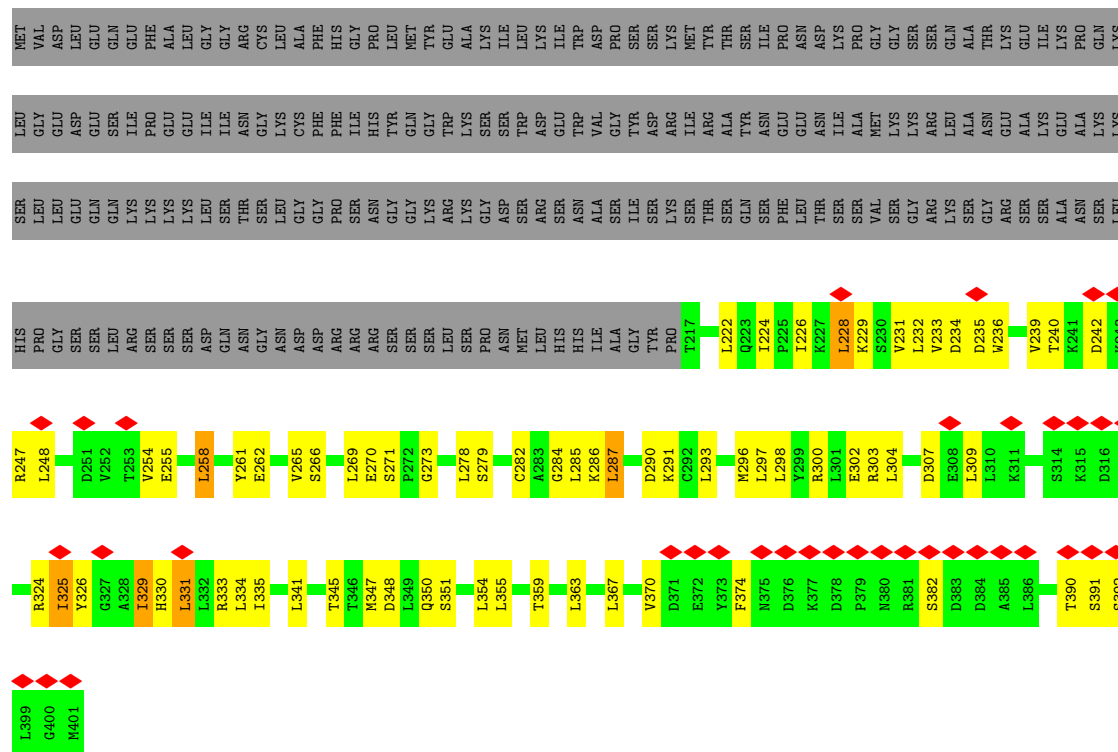


• Molecule 4: Chromatin modification-related protein EAF3

Chain C:



• Molecule 4: Chromatin modification-related protein EAF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	378011	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)	1700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.968	Depositor
Minimum map value	-3.542	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	301.56, 301.56, 301.56	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/5180	0.42	2/6984 (0.0%)
2	E	0.49	7/2952 (0.2%)	0.75	18/3978 (0.5%)
2	F	0.13	0/1313	0.38	0/1763
3	B	0.20	0/3137	0.41	0/4246
4	C	0.21	0/1509	0.43	0/2039
4	D	0.16	0/1524	0.41	0/2061
All	All	0.27	7/15615 (0.0%)	0.49	20/21071 (0.1%)

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
4	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	469	HIS	CE1-NE2	-10.60	1.22	1.32
2	E	471	PRO	C-O	-9.53	1.12	1.23
2	E	469	HIS	CG-ND1	-6.87	1.30	1.38
2	E	517	ASN	N-CA	6.71	1.54	1.46
2	E	518	GLY	CA-C	-5.63	1.44	1.51
2	E	469	HIS	CG-CD2	-5.18	1.30	1.35
2	E	518	GLY	C-O	-5.00	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	469	HIS	CA-C-N	11.68	137.08	120.49
2	E	469	HIS	C-N-CA	11.68	137.08	120.49
2	E	471	PRO	N-CA-C	9.43	125.55	111.41
2	E	518	GLY	N-CA-C	-9.07	91.69	113.18
2	E	517	ASN	CA-CB-CG	-7.92	104.68	112.60
2	E	472	THR	CA-C-O	-7.56	111.40	120.55
2	E	469	HIS	CA-CB-CG	7.50	121.30	113.80
2	E	516	ASN	CA-C-N	7.03	134.97	121.54
2	E	516	ASN	C-N-CA	7.03	134.97	121.54
2	E	517	ASN	N-CA-C	6.33	124.28	110.80
2	E	470	SER	CA-C-O	-6.23	113.52	120.25
1	A	787	VAL	N-CA-C	-6.02	107.99	113.71
2	E	468	LEU	CA-C-N	-5.83	113.53	122.62
2	E	468	LEU	C-N-CA	-5.83	113.53	122.62
2	E	472	THR	O-C-N	5.61	129.38	122.20
2	E	472	THR	N-CA-CB	5.20	119.69	111.17
1	A	696	ILE	N-CA-C	-5.15	107.79	112.12
2	E	515	GLN	CA-C-N	5.05	131.18	121.54
2	E	515	GLN	C-N-CA	5.05	131.18	121.54
2	E	470	SER	N-CA-C	-5.04	103.43	109.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	241	LYS	Peptide

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	5066	0	5024	161	0
2	E	2884	0	2833	108	0
2	F	1282	0	1244	40	0
3	B	3057	0	2933	82	0
4	C	1483	0	1510	46	0
4	D	1497	0	1524	50	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	4	0	0	0	0
5	F	2	0	0	0	0
6	B	2	0	0	0	0
All	All	15278	0	15068	433	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 (433) 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:794:GLY:HA2	2:E:460:LEU:HD13	1.58	0.83
4:D:265:VAL:HG23	4:D:278:LEU:HD11	1.61	0.81
2:E:476:LYS:HB3	2:E:490:LYS:HG2	1.68	0.76
3:B:44:ARG:HB3	3:B:315:MET:HG2	1.68	0.76
4:C:240:THR:O	4:C:242:ASP:N	2.18	0.75
3:B:244:ASP:OD1	3:B:244:ASP:N	2.20	0.74
3:B:113:PHE:HD2	3:B:114:ASP:H	1.35	0.73
3:B:2:VAL:N	3:B:370:ASP:OD2	2.21	0.73
4:D:240:THR:HG21	2:F:372:TYR:HB2	1.70	0.73
4:D:293:LEU:HA	4:D:297:LEU:HD12	1.69	0.72
2:E:372:TYR:OH	2:E:496:ARG:NH1	2.22	0.72
1:A:815:HIS:HB2	3:B:315:MET:HE1	1.72	0.71
1:A:1294:MET:HE1	1:A:1300:MET:HG3	1.73	0.71
3:B:326:THR:O	3:B:330:ASN:ND2	2.23	0.70
2:F:332:ASN:OD1	2:F:332:ASN:N	2.21	0.70
2:E:266:CYS:SG	4:C:300:ARG:NH1	2.65	0.70
2:E:371:GLN:HA	4:C:240:THR:HG21	1.74	0.70
2:E:171:LEU:O	2:E:172:THR:OG1	2.09	0.69
4:D:255:GLU:OE1	4:D:324:ARG:NH1	2.24	0.69
4:C:259:ASN:OD1	4:C:286:LYS:NZ	2.20	0.69
1:A:768:SER:OG	3:B:80:ASP:OD1	2.10	0.69
2:E:384:ARG:HA	2:E:387:PHE:HB3	1.74	0.69
4:D:303:ARG:NH1	2:F:286:CYS:SG	2.65	0.69
2:E:512:ILE:HG23	2:E:549:TYR:HB3	1.75	0.68
2:E:362:PRO:HG3	2:E:499:ASN:HB2	1.76	0.68
4:C:378:ASP:OD2	4:C:381:ARG:NH2	2.27	0.67
1:A:1302:ARG:NH2	1:A:1304:GLU:OE2	2.28	0.67
2:E:452:VAL:HG21	2:E:464:TRP:HZ2	1.59	0.66
1:A:1178:VAL:HG22	1:A:1180:PHE:H	1.60	0.66
3:B:153:LYS:NZ	3:B:191:ASP:OD2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:507:GLU:HB2	2:E:541:GLN:HE21	1.61	0.66
3:B:53:MET:HG2	3:B:58:TYR:HD1	1.61	0.65
1:A:1223:TRP:O	1:A:1227:SER:OG	2.14	0.65
3:B:145:TYR:OH	3:B:326:THR:OG1	2.14	0.65
2:E:516:ASN:HD21	2:E:520:ILE:HG22	1.62	0.65
1:A:959:GLN:OE1	1:A:974:GLN:NE2	2.30	0.64
2:E:493:LYS:HE2	2:E:517:ASN:HB3	1.79	0.64
3:B:209:HIS:HE1	3:B:235:ASN:HB3	1.61	0.64
1:A:831:LEU:HB3	1:A:895:LEU:HD13	1.78	0.64
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.79	0.63
1:A:813:GLU:HG2	2:E:111:THR:HG22	1.80	0.63
2:E:343:ILE:HG21	4:C:291:LYS:HD3	1.80	0.63
1:A:799:ARG:HH21	2:E:390:SER:HB3	1.64	0.63
2:E:495:GLN:NE2	2:E:519:ASN:OD1	2.31	0.63
3:B:29:VAL:HG22	3:B:122:ILE:HG21	1.81	0.63
4:C:236:TRP:CD1	4:C:299:TYR:HH	2.17	0.63
4:D:370:VAL:HG23	4:D:374:PHE:HD2	1.64	0.63
2:F:302:HIS:HB3	2:F:306:CYS:HB2	1.80	0.63
1:A:868:ARG:HD2	1:A:873:LYS:HE3	1.81	0.62
1:A:1163:GLN:O	1:A:1167:ARG:NH2	2.32	0.62
2:E:414:PHE:HB3	2:E:423:THR:HG21	1.82	0.62
1:A:665:GLU:HB3	2:E:552:PHE:CZ	2.35	0.61
1:A:941:LYS:HG2	1:A:942:LEU:HD23	1.82	0.61
1:A:1168:VAL:HG11	1:A:1232:TYR:CE1	2.35	0.61
4:D:345:THR:HG21	2:F:339:LEU:HD23	1.81	0.61
2:F:355:ASN:HD22	2:F:358:LYS:HE2	1.65	0.61
2:E:184:THR:OG1	3:B:73:GLU:OE1	2.19	0.61
3:B:90:THR:HG23	3:B:92:ASP:H	1.66	0.60
2:E:447:TRP:NE1	2:E:466:CYS:SG	2.75	0.60
1:A:977:PHE:CD2	1:A:1152:THR:HG21	2.37	0.59
2:F:263:CYS:O	2:F:267:ASN:N	2.30	0.59
1:A:698:ASP:OD2	1:A:699:LEU:N	2.29	0.59
4:D:235:ASP:OD1	4:D:333:ARG:NH2	2.35	0.59
2:E:489:TYR:OH	4:C:377:LYS:O	2.21	0.59
2:E:491:VAL:HG12	2:E:492:TRP:H	1.67	0.59
1:A:912:TRP:HH2	2:E:113:LEU:HD13	1.66	0.58
4:C:365:TRP:O	4:C:369:HIS:ND1	2.26	0.58
2:F:275:CYS:SG	2:F:276:ASP:N	2.75	0.58
4:C:253:THR:OG1	4:C:323:ILE:O	2.18	0.58
4:D:296:MET:HE1	4:D:341:LEU:HD21	1.85	0.58
1:A:871:TYR:HE2	1:A:894:VAL:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASN:O	2:F:329:GLN:HG2	2.03	0.58
1:A:1161:ILE:HD13	1:A:1239:LEU:HD21	1.85	0.58
2:E:381:LEU:HB3	2:E:384:ARG:HB2	1.86	0.57
2:F:571:GLU:HA	2:F:574:ILE:HD12	1.86	0.57
4:C:300:ARG:NH2	4:C:399:LEU:O	2.36	0.57
3:B:338:LEU:HD21	3:B:353:LEU:HD13	1.87	0.57
4:D:222:LEU:HD11	4:D:363:LEU:HD21	1.86	0.57
1:A:1141:ASN:HD21	1:A:1262:THR:HG23	1.70	0.57
1:A:875:ARG:HA	1:A:878:GLU:HG2	1.87	0.56
3:B:11:ILE:HD11	3:B:289:GLU:HB3	1.88	0.56
4:D:300:ARG:H	2:F:350:GLN:HE21	1.52	0.56
1:A:675:TYR:CE2	1:A:713:ASN:HB2	2.41	0.56
1:A:841:MET:O	1:A:846:LYS:NZ	2.39	0.56
1:A:1079:ARG:HE	1:A:1079:ARG:HA	1.71	0.56
1:A:1290:VAL:HA	1:A:1293:HIS:HD2	1.71	0.56
1:A:1219:LEU:HD11	1:A:1223:TRP:HB2	1.88	0.56
1:A:1300:MET:O	1:A:1317:ILE:HB	2.06	0.56
1:A:878:GLU:HA	1:A:881:ASP:OD1	2.06	0.55
2:E:449:LEU:HD11	2:E:457:PHE:CE2	2.41	0.55
2:E:472:THR:HB	2:E:494:LYS:HD3	1.88	0.55
1:A:782:TRP:CE2	3:B:226:VAL:HG21	2.41	0.55
2:E:324:SER:O	2:E:328:LYS:HG3	2.06	0.55
1:A:771:ASP:OD1	3:B:175:ARG:NH2	2.39	0.55
1:A:1335:LYS:HA	1:A:1338:VAL:HG22	1.87	0.55
3:B:279:ASP:OD2	3:B:280:ARG:N	2.35	0.55
2:E:472:THR:O	2:E:472:THR:OG1	2.06	0.55
1:A:779:ASN:O	1:A:779:ASN:ND2	2.40	0.55
2:E:452:VAL:O	2:E:454:ARG:N	2.39	0.55
3:B:57:LEU:HD11	3:B:327:GLY:HA2	1.89	0.55
4:D:287:LEU:O	4:D:291:LYS:HB2	2.06	0.54
2:F:353:LEU:H	2:F:353:LEU:HD23	1.72	0.54
1:A:872:ASP:O	1:A:875:ARG:N	2.40	0.54
2:E:169:THR:OG1	3:B:342:GLU:OE2	2.20	0.54
4:C:269:LEU:HD13	4:C:274:SER:HB2	1.89	0.54
2:E:189:GLY:HA2	3:B:72:GLN:HB2	1.88	0.54
2:E:450:ASP:OD2	3:B:365:THR:OG1	2.25	0.54
4:C:248:LEU:HD11	4:C:326:TYR:CE1	2.42	0.54
1:A:911:GLU:HG2	2:E:119:PRO:HD2	1.89	0.54
2:E:440:CYS:SG	2:E:441:ASP:N	2.80	0.54
2:E:449:LEU:HD11	2:E:457:PHE:HE2	1.73	0.54
1:A:831:LEU:HD22	1:A:895:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:211:TYR:HE1	3:B:220:GLU:HG3	1.72	0.54
4:C:245:ILE:HG22	4:C:302:GLU:HB3	1.90	0.54
2:E:460:LEU:HD12	3:B:213:GLU:HG2	1.89	0.53
1:A:754:SER:OG	3:B:223:ASP:OD2	2.24	0.53
1:A:664:GLU:O	1:A:667:THR:OG1	2.27	0.53
2:E:498:ILE:HG21	4:C:226:ILE:HD13	1.91	0.53
2:F:274:CYS:HB2	2:F:281:SER:HB2	1.90	0.53
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.09	0.53
2:E:543:ASP:OD1	2:E:543:ASP:N	2.40	0.53
3:B:285:ASN:ND2	3:B:285:ASN:O	2.42	0.53
1:A:1318:ALA:O	1:A:1321:ASP:N	2.40	0.53
2:F:265:ALA:HA	2:F:349:LYS:HA	1.90	0.52
3:B:285:ASN:OD1	3:B:358:SER:OG	2.16	0.52
4:D:229:LYS:O	4:D:233:VAL:HG23	2.08	0.52
2:F:326:PHE:O	2:F:330:ASN:ND2	2.35	0.52
1:A:1065:LEU:HD21	1:A:1266:MET:HE1	1.91	0.52
1:A:972:LYS:HA	1:A:1325:LYS:HE2	1.91	0.52
3:B:239:ARG:HB3	3:B:363:VAL:HG23	1.90	0.52
4:D:229:LYS:HD2	2:F:357:ILE:HG23	1.91	0.52
4:D:261:TYR:O	4:D:265:VAL:HG22	2.10	0.52
3:B:307:VAL:HG21	3:B:329:LEU:HD11	1.92	0.52
4:C:288:TYR:O	4:C:292:CYS:HB2	2.10	0.52
4:D:390:THR:HB	4:D:394:TYR:HB2	1.92	0.52
1:A:959:GLN:HE21	1:A:971:PRO:HB2	1.75	0.52
1:A:1300:MET:HE2	1:A:1317:ILE:HG21	1.92	0.52
1:A:750:ALA:HB2	1:A:782:TRP:HZ3	1.74	0.52
4:D:298:LEU:HD22	4:D:302:GLU:HG3	1.92	0.51
1:A:816:GLU:OE2	2:E:115:LEU:HD11	2.11	0.51
2:F:543:ASP:OD1	2:F:544:GLU:N	2.43	0.51
2:E:361:PHE:CD1	2:E:496:ARG:HD3	2.46	0.51
3:B:26:ASP:O	3:B:29:VAL:HG23	2.11	0.51
1:A:675:TYR:CZ	1:A:713:ASN:HB2	2.45	0.51
1:A:1203:ALA:O	1:A:1207:VAL:HG23	2.10	0.51
2:E:567:PHE:O	2:E:570:GLN:HG2	2.10	0.51
1:A:1151:TRP:HE3	1:A:1249:LEU:HD11	1.74	0.51
4:D:247:ARG:NH2	4:D:382:SER:O	2.43	0.51
2:E:387:PHE:O	2:E:390:SER:HB2	2.10	0.51
2:E:570:GLN:O	2:E:574:ILE:HG12	2.11	0.51
1:A:952:ILE:HA	1:A:955:ILE:HG22	1.93	0.51
1:A:1327:PRO:HG2	1:A:1333:LYS:HG3	1.91	0.51
2:E:316:MET:O	2:E:320:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:LYS:O	2:F:325:ASN:ND2	2.44	0.51
1:A:989:LEU:HD11	1:A:1018:ILE:HD11	1.92	0.50
1:A:1165:ASN:OD1	1:A:1204:TYR:N	2.43	0.50
1:A:1144:ILE:HD11	1:A:1266:MET:HG2	1.92	0.50
4:D:236:TRP:HA	4:D:239:VAL:HG12	1.93	0.50
2:E:402:ASN:ND2	2:E:405:THR:OG1	2.45	0.50
4:C:366:LEU:O	4:C:370:VAL:HG23	2.12	0.50
4:D:304:LEU:HA	4:D:307:ASP:OD2	2.11	0.50
2:E:172:THR:O	2:E:176:THR:OG1	2.26	0.50
3:B:279:ASP:CG	3:B:280:ARG:H	2.20	0.49
3:B:317:ASN:O	3:B:321:THR:OG1	2.25	0.49
2:F:552:PHE:O	2:F:555:ILE:HG13	2.13	0.49
1:A:812:GLU:OE2	3:B:280:ARG:NH2	2.38	0.49
3:B:21:VAL:HG13	3:B:141:VAL:HB	1.95	0.49
3:B:191:ASP:OD1	3:B:191:ASP:N	2.38	0.49
1:A:684:GLU:O	1:A:688:ILE:HG13	2.13	0.49
2:F:274:CYS:SG	2:F:275:CYS:N	2.86	0.49
1:A:755:TYR:OH	3:B:194:GLU:OE1	2.25	0.49
1:A:919:LEU:HD22	2:E:127:SER:OG	2.12	0.49
1:A:953:SER:O	1:A:957:VAL:HG13	2.13	0.49
3:B:294:CYS:O	3:B:298:VAL:HG23	2.12	0.49
2:F:275:CYS:SG	2:F:277:THR:N	2.78	0.49
2:E:493:LYS:CE	2:E:517:ASN:HB3	2.43	0.49
1:A:663:ASN:OD1	1:A:664:GLU:N	2.46	0.49
1:A:851:LEU:HD13	1:A:855:LEU:HG	1.94	0.49
2:E:424:ARG:HD3	2:E:435:ARG:HG3	1.94	0.49
3:B:182:TYR:OH	3:B:184:ASP:OD1	2.21	0.49
1:A:984:ILE:O	1:A:988:ILE:HG13	2.13	0.49
1:A:1016:TYR:CD1	1:A:1065:LEU:HB2	2.48	0.49
1:A:1009:ARG:HE	1:A:1075:GLN:HE22	1.59	0.48
1:A:696:ILE:HG22	2:E:474:VAL:HG21	1.94	0.48
1:A:1199:VAL:HG22	1:A:1200:GLY:H	1.79	0.48
3:B:84:ASP:OD1	3:B:88:ARG:NH1	2.27	0.48
4:C:360:GLU:O	4:C:364:VAL:HG13	2.13	0.48
1:A:956:LYS:O	1:A:960:THR:HG23	2.13	0.48
3:B:11:ILE:HG22	3:B:296:ASN:HD22	1.77	0.48
1:A:690:ASN:CG	2:E:520:ILE:HD13	2.39	0.48
4:C:381:ARG:HH21	4:C:381:ARG:HB2	1.78	0.48
4:C:393:GLN:O	4:C:397:VAL:HG23	2.13	0.48
4:C:222:LEU:HD21	4:C:363:LEU:HD11	1.95	0.48
1:A:770:ARG:HG3	1:A:774:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:ARG:HE	1:A:1300:MET:HE1	1.79	0.48
2:E:402:ASN:N	2:E:403:PRO:HD3	2.29	0.48
4:D:325:ILE:HG13	4:D:326:TYR:CD2	2.49	0.48
4:D:393:GLN:O	4:D:397:VAL:HG23	2.13	0.48
4:D:242:ASP:OD2	4:D:242:ASP:N	2.37	0.47
4:D:347:MET:HG2	4:D:351:SER:HB2	1.95	0.47
4:D:228:LEU:HD21	4:D:367:LEU:HB2	1.95	0.47
2:F:323:GLU:O	2:F:327:ILE:HG23	2.15	0.47
2:E:367:GLY:HA3	2:E:371:GLN:HG3	1.97	0.47
4:C:245:ILE:HG12	4:C:390:THR:HG23	1.97	0.47
4:C:266:SER:O	4:C:275:GLN:NE2	2.36	0.47
2:E:325:ASN:HA	2:E:328:LYS:HE2	1.97	0.47
1:A:1214:LEU:HD11	1:A:1221:HIS:CE1	2.50	0.47
1:A:1286:TYR:O	1:A:1290:VAL:HG12	2.15	0.47
2:E:417:CYS:HA	2:E:446:PRO:O	2.14	0.47
1:A:811:GLU:OE2	3:B:315:MET:N	2.33	0.47
1:A:1144:ILE:HG12	1:A:1256:LEU:HD21	1.97	0.47
1:A:1325:LYS:HD2	1:A:1325:LYS:HA	1.63	0.47
1:A:831:LEU:O	1:A:834:ILE:HG13	2.15	0.47
1:A:945:THR:O	1:A:949:ILE:HG12	2.14	0.47
2:E:339:LEU:HB3	4:C:288:TYR:CE2	2.50	0.47
3:B:204:MET:HE1	3:B:380:LEU:HD21	1.97	0.47
4:D:232:LEU:HD21	4:D:333:ARG:HG2	1.96	0.47
1:A:665:GLU:OE1	1:A:665:GLU:N	2.48	0.46
1:A:825:LEU:HD11	1:A:906:ARG:HH22	1.78	0.46
1:A:1299:ASN:ND2	1:A:1299:ASN:H	2.12	0.46
3:B:247:TYR:CD2	3:B:286:LEU:HD11	2.50	0.46
4:C:253:THR:OG1	4:C:254:VAL:N	2.46	0.46
4:D:348:ASP:OD2	4:D:351:SER:OG	2.30	0.46
1:A:957:VAL:HG21	2:E:414:PHE:HD2	1.80	0.46
1:A:1003:SER:O	1:A:1007:LYS:HG3	2.16	0.46
1:A:779:ASN:ND2	3:B:195:GLU:O	2.49	0.46
1:A:823:SER:O	1:A:827:THR:HG23	2.14	0.46
3:B:183:ILE:HB	3:B:269:LEU:HD13	1.96	0.46
4:C:255:GLU:HA	4:C:286:LYS:HE2	1.96	0.46
4:D:391:SER:OG	4:D:392:SER:N	2.49	0.46
1:A:696:ILE:O	2:E:474:VAL:HG11	2.14	0.46
2:E:452:VAL:HG21	2:E:464:TRP:CZ2	2.47	0.46
4:C:297:LEU:HD13	4:C:334:LEU:HB2	1.97	0.46
1:A:690:ASN:ND2	1:A:694:GLN:OE1	2.48	0.46
1:A:900:GLN:O	1:A:903:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:288:ASP:HB2	2:E:348:PRO:HG3	1.96	0.46
2:E:514:TYR:CD1	2:E:516:ASN:HB3	2.51	0.46
3:B:30:GLY:C	3:B:46:ARG:HH21	2.22	0.46
1:A:1009:ARG:NE	1:A:1075:GLN:HE22	2.13	0.46
1:A:817:TYR:HE2	2:E:111:THR:HG21	1.81	0.46
1:A:1147:PHE:HE2	1:A:1253:ALA:HB2	1.80	0.46
4:C:244:LYS:HE2	4:C:379:PRO:HG2	1.98	0.46
1:A:1148:PHE:O	1:A:1152:THR:OG1	2.34	0.45
3:B:256:LYS:O	3:B:260:GLU:HB2	2.15	0.45
4:C:269:LEU:HD23	4:C:270:GLU:H	1.81	0.45
4:C:290:ASP:OD1	4:C:323:ILE:HG23	2.16	0.45
3:B:220:GLU:HG2	3:B:221:LEU:H	1.81	0.45
4:D:297:LEU:HD21	4:D:334:LEU:HB2	1.98	0.45
1:A:853:PRO:HA	1:A:884:HIS:CE1	2.50	0.45
1:A:995:PHE:CE1	1:A:1247:GLN:HA	2.51	0.45
2:E:300:ASP:HB3	2:E:302:HIS:HE1	1.82	0.45
3:B:246:THR:O	3:B:250:VAL:HG23	2.17	0.45
3:B:343:TYR:HB3	3:B:346:TYR:CD2	2.51	0.45
2:E:574:ILE:O	2:E:578:VAL:HG23	2.16	0.45
3:B:34:TYR:HD2	3:B:38:HIS:HD2	1.64	0.45
3:B:134:LEU:HD11	3:B:306:MET:HB2	1.99	0.45
1:A:917:ARG:HD3	3:B:351:TYR:OH	2.16	0.45
4:D:326:TYR:HD1	4:D:330:HIS:CE1	2.34	0.45
1:A:1120:LEU:HD21	1:A:1338:VAL:HB	1.99	0.45
2:E:398:LEU:HD23	2:E:457:PHE:HD1	1.81	0.45
2:E:437:ILE:HG12	2:E:448:HIS:CD2	2.51	0.45
2:E:520:ILE:HD12	2:E:542:ILE:HG21	1.98	0.45
3:B:151:HIS:HB3	3:B:158:SER:O	2.16	0.45
1:A:1264:GLU:O	1:A:1268:LEU:HG	2.17	0.45
2:E:320:LYS:HB2	2:E:320:LYS:HE3	1.76	0.45
4:C:381:ARG:NH2	4:C:381:ARG:HB2	2.31	0.45
4:D:285:LEU:HD23	4:D:285:LEU:HA	1.74	0.45
1:A:1063:MET:HB3	1:A:1064:SER:H	1.54	0.45
2:E:317:ALA:HA	2:E:320:LYS:HE2	1.99	0.45
2:E:351:PHE:HE2	4:C:337:VAL:HB	1.82	0.45
2:E:429:SER:O	2:E:430:HIS:ND1	2.50	0.45
1:A:1009:ARG:HE	1:A:1074:TYR:HD1	1.63	0.44
1:A:1280:ALA:O	1:A:1284:ILE:HG13	2.17	0.44
2:E:287:LEU:HD23	2:E:287:LEU:HA	1.78	0.44
4:D:231:VAL:HA	4:D:234:ASP:OD2	2.17	0.44
1:A:1069:LEU:HD13	1:A:1069:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:LEU:C	2:E:172:THR:HG1	2.16	0.44
2:E:478:ILE:H	2:E:489:TYR:HA	1.81	0.44
3:B:2:VAL:HG13	3:B:373:MET:HE2	1.99	0.44
2:F:355:ASN:O	2:F:359:GLU:HG2	2.17	0.44
3:B:41:LYS:O	3:B:44:ARG:NE	2.50	0.44
4:C:277:GLN:HB3	4:C:358:GLN:HE22	1.81	0.44
3:B:52:ILE:O	3:B:57:LEU:HB2	2.18	0.44
3:B:78:HIS:HD1	3:B:82:TYR:HD1	1.65	0.44
2:E:562:GLN:HA	2:E:565:LYS:HE2	1.99	0.44
4:D:284:GLY:HA3	2:F:336:PHE:CD2	2.52	0.44
2:E:255:ILE:HG13	2:E:255:ILE:O	2.18	0.44
1:A:1183:ASP:OD1	1:A:1184:LEU:N	2.51	0.44
2:E:372:TYR:CE1	4:C:237:GLU:HB2	2.52	0.44
2:E:565:LYS:HE2	2:E:565:LYS:HB3	1.68	0.44
3:B:18:LYS:HD2	3:B:18:LYS:HA	1.84	0.44
3:B:80:ASP:OD2	3:B:80:ASP:N	2.49	0.44
4:C:338:LEU:HA	4:C:341:LEU:HD12	2.00	0.44
1:A:1020:LEU:HG	1:A:1273:ARG:HG2	2.00	0.44
3:B:14:LYS:NZ	3:B:300:SER:OG	2.47	0.44
3:B:150:HIS:HB3	3:B:166:ILE:HD12	2.00	0.44
3:B:377:PHE:O	3:B:381:GLU:HG2	2.18	0.44
2:F:284:PHE:CD2	2:F:293:PRO:HB3	2.53	0.44
2:F:305:GLU:O	2:F:309:LYS:HG2	2.18	0.44
2:E:553:ASP:OD1	4:D:271:SER:OG	2.35	0.43
3:B:30:GLY:O	3:B:46:ARG:NH2	2.50	0.43
3:B:182:TYR:CE1	3:B:184:ASP:HB2	2.53	0.43
1:A:773:MET:HE3	1:A:773:MET:HB2	1.83	0.43
1:A:979:PHE:HD1	1:A:985:PHE:HZ	1.66	0.43
1:A:1225:GLU:O	1:A:1229:ARG:HG3	2.18	0.43
2:E:272:PHE:HB3	2:E:281:SER:HB3	2.00	0.43
2:E:554:LYS:HA	2:E:557:LYS:HE3	2.00	0.43
2:E:569:PHE:O	2:E:573:LEU:HG	2.18	0.43
4:D:335:ILE:HD12	4:D:359:THR:HG23	1.99	0.43
1:A:996:ILE:HA	1:A:999:THR:HG22	2.00	0.43
3:B:165:ASP:HA	3:B:168:LEU:HD12	2.00	0.43
3:B:259:MET:HE2	3:B:259:MET:HB3	1.74	0.43
1:A:959:GLN:NE2	1:A:971:PRO:HB2	2.33	0.43
2:E:324:SER:HA	2:E:327:ILE:HD12	2.00	0.43
3:B:24:PHE:HZ	3:B:133:ARG:HD3	1.83	0.43
2:E:378:LYS:O	2:E:379:ILE:HG23	2.18	0.43
2:E:504:LEU:HD12	2:E:538:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:329:ILE:HD11	4:D:330:HIS:CE1	2.53	0.43
2:F:557:LYS:HB2	2:F:557:LYS:HE3	1.84	0.43
1:A:867:ILE:O	1:A:871:TYR:HB2	2.19	0.43
1:A:877:PHE:O	1:A:880:ILE:HG22	2.19	0.43
1:A:1066:LEU:HB2	1:A:1270:VAL:HG11	1.99	0.43
3:B:92:ASP:OD1	3:B:92:ASP:N	2.52	0.43
4:D:258:LEU:HD23	4:D:286:LYS:HG3	2.00	0.43
4:D:293:LEU:HD11	4:D:326:TYR:CZ	2.52	0.43
1:A:696:ILE:HD11	2:E:517:ASN:O	2.18	0.43
1:A:1204:TYR:CE1	1:A:1208:LEU:HD11	2.54	0.43
1:A:1302:ARG:NH1	1:A:1315:GLN:OE1	2.51	0.43
1:A:1337:TYR:HD2	1:A:1337:TYR:HA	1.71	0.43
2:F:318:THR:O	2:F:322:ILE:HG13	2.19	0.43
1:A:973:SER:OG	1:A:1315:GLN:HB2	2.18	0.43
2:E:323:GLU:OE1	2:E:338:LYS:HG2	2.19	0.43
4:C:254:VAL:HG21	4:C:289:PHE:CZ	2.54	0.43
4:D:262:GLU:O	4:D:266:SER:HB2	2.18	0.43
2:E:512:ILE:HG21	4:D:273:GLY:HA2	2.01	0.43
1:A:688:ILE:HG22	1:A:702:LEU:HD12	2.00	0.42
1:A:992:ALA:O	1:A:996:ILE:HG13	2.19	0.42
1:A:1343:LEU:HB3	1:A:1345:HIS:ND1	2.34	0.42
2:E:166:ASP:N	2:E:166:ASP:OD1	2.52	0.42
4:D:232:LEU:HD13	2:F:353:LEU:HD13	2.01	0.42
4:D:331:LEU:HD22	4:D:331:LEU:HA	1.87	0.42
1:A:853:PRO:HA	1:A:884:HIS:HE1	1.84	0.42
1:A:1019:SER:O	1:A:1024:ILE:N	2.50	0.42
1:A:1194:MET:HG3	1:A:1196:LEU:HG	2.00	0.42
3:B:292:ALA:HB1	3:B:328:LEU:HD21	2.02	0.42
1:A:938:ALA:HA	1:A:941:LYS:HE2	2.02	0.42
1:A:1338:VAL:HA	1:A:1341:TYR:CD1	2.54	0.42
4:C:248:LEU:HD11	4:C:326:TYR:CZ	2.54	0.42
2:F:273:LEU:HD23	2:F:284:PHE:CD1	2.54	0.42
2:E:333:VAL:HA	4:C:280:GLU:HG3	2.01	0.42
2:E:498:ILE:HD13	4:C:226:ILE:HG21	2.01	0.42
1:A:981:ASP:OD2	1:A:984:ILE:HG13	2.19	0.42
1:A:1226:GLU:O	1:A:1230:GLN:HG3	2.18	0.42
3:B:26:ASP:HB3	3:B:29:VAL:HG23	2.01	0.42
2:E:493:LYS:HD2	2:E:493:LYS:HA	1.85	0.42
2:E:553:ASP:O	2:E:557:LYS:HG2	2.20	0.42
2:E:568:GLN:O	2:E:571:GLU:HG3	2.19	0.42
4:D:335:ILE:HD13	4:D:335:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:ASN:HA	2:F:358:LYS:HE2	2.01	0.42
1:A:1003:SER:OG	1:A:1005:PRO:HD2	2.20	0.42
2:E:292:ASP:OD2	2:E:294:ASN:ND2	2.53	0.42
2:E:336:PHE:CE1	2:E:339:LEU:HD12	2.54	0.42
4:D:248:LEU:HD23	4:D:309:LEU:HD22	2.01	0.42
2:F:322:ILE:HA	2:F:325:ASN:HD21	1.85	0.42
4:D:300:ARG:HG3	4:D:303:ARG:NH2	2.34	0.42
1:A:837:LYS:HD2	1:A:840:ASN:HD21	1.84	0.42
2:F:263:CYS:HA	2:F:281:SER:O	2.20	0.42
4:C:262:GLU:O	4:C:266:SER:HB3	2.19	0.42
2:F:292:ASP:OD2	2:F:293:PRO:HD2	2.20	0.42
2:E:292:ASP:HB3	2:E:295:ASN:OD1	2.20	0.41
1:A:949:ILE:O	1:A:953:SER:OG	2.36	0.41
1:A:1129:ILE:O	1:A:1129:ILE:HG13	2.18	0.41
1:A:1137:ASN:HB2	1:A:1283:GLN:HE22	1.85	0.41
1:A:1199:VAL:O	1:A:1201:GLU:N	2.52	0.41
2:E:454:ARG:NH1	2:E:458:LYS:HB2	2.35	0.41
2:E:510:GLN:HG3	4:D:354:LEU:HD22	2.02	0.41
3:B:316:ARG:H	3:B:316:ARG:HG3	1.68	0.41
1:A:936:LYS:HE3	1:A:1225:GLU:OE2	2.20	0.41
2:E:374:ASP:C	2:E:376:ASN:H	2.29	0.41
3:B:198:TYR:CE2	3:B:225:GLY:HA2	2.55	0.41
3:B:271:CYS:SG	3:B:307:VAL:HG13	2.60	0.41
1:A:872:ASP:O	1:A:874:GLU:N	2.54	0.41
1:A:1318:ALA:HB3	1:A:1321:ASP:HB2	2.01	0.41
3:B:197:PHE:CD1	3:B:203:VAL:HG21	2.55	0.41
1:A:875:ARG:HA	1:A:878:GLU:OE1	2.20	0.41
1:A:939:ASP:CG	1:A:1157:ARG:HH22	2.28	0.41
1:A:955:ILE:HG23	1:A:974:GLN:HG3	2.02	0.41
1:A:959:GLN:O	1:A:963:LYS:HB2	2.20	0.41
2:E:351:PHE:CE1	4:C:333:ARG:HB3	2.56	0.41
2:E:381:LEU:HD23	2:E:384:ARG:HG3	2.03	0.41
1:A:950:SER:O	1:A:954:SER:OG	2.30	0.41
1:A:1018:ILE:O	1:A:1022:PHE:HD2	2.04	0.41
1:A:1261:LYS:O	1:A:1265:ILE:HG13	2.21	0.41
2:E:296:LEU:HD12	2:E:297:PRO:HD2	2.01	0.41
2:E:409:SER:OG	2:E:410:ASN:N	2.52	0.41
3:B:239:ARG:H	3:B:364:ASN:HD21	1.68	0.41
4:D:269:LEU:HD23	4:D:269:LEU:HA	1.82	0.41
1:A:1234:ASN:O	3:B:359:ASN:ND2	2.45	0.41
1:A:1284:ILE:HD11	1:A:1336:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:HIS:O	1:A:684:GLU:HG2	2.21	0.41
1:A:928:LEU:HD12	1:A:928:LEU:HA	1.88	0.41
1:A:1284:ILE:HD11	1:A:1336:TYR:HE2	1.85	0.41
1:A:1324:LEU:HD12	1:A:1325:LYS:H	1.86	0.41
3:B:34:TYR:CD2	3:B:38:HIS:HD2	2.39	0.41
3:B:106:VAL:HG13	3:B:110:CYS:O	2.21	0.41
4:C:232:LEU:HD23	4:C:232:LEU:HA	1.96	0.41
4:D:270:GLU:H	4:D:270:GLU:CD	2.28	0.41
4:D:287:LEU:HD13	4:D:287:LEU:HA	1.92	0.41
2:F:364:VAL:O	2:F:365:LYS:HD2	2.21	0.41
1:A:750:ALA:HB3	4:C:380:ASN:HD21	1.85	0.41
1:A:770:ARG:HH12	3:B:154:LYS:HD2	1.86	0.41
1:A:790:SER:O	1:A:790:SER:OG	2.35	0.41
1:A:1233:ASN:HB3	1:A:1235:LYS:HB2	2.03	0.41
3:B:57:LEU:HA	3:B:57:LEU:HD23	1.85	0.41
4:D:265:VAL:CG2	4:D:278:LEU:HD11	2.42	0.41
4:C:318:LYS:HG3	4:C:318:LYS:O	2.21	0.40
2:F:259:ASN:ND2	2:F:274:CYS:SG	2.94	0.40
2:F:305:GLU:CD	2:F:305:GLU:H	2.29	0.40
1:A:830:CYS:SG	1:A:831:LEU:N	2.94	0.40
2:E:336:PHE:CZ	4:C:285:LEU:HD23	2.55	0.40
4:C:257:VAL:HG22	4:C:373:TYR:CZ	2.56	0.40
2:F:326:PHE:CD1	2:F:341:PHE:HB2	2.57	0.40
1:A:1161:ILE:HD13	1:A:1239:LEU:CD2	2.52	0.40
2:E:478:ILE:N	2:E:489:TYR:HA	2.36	0.40
2:F:568:GLN:HA	2:F:571:GLU:OE1	2.22	0.40
1:A:679:LYS:HA	1:A:679:LYS:HD3	1.86	0.40
1:A:841:MET:HB3	1:A:845:GLU:HB2	2.04	0.40
1:A:862:ILE:HD13	1:A:862:ILE:HA	1.90	0.40
1:A:979:PHE:CD1	1:A:985:PHE:HZ	2.40	0.40
1:A:1242:ILE:HD12	1:A:1242:ILE:HA	1.96	0.40
1:A:1343:LEU:HG	1:A:1344:PRO:HD2	2.02	0.40
2:E:275:CYS:SG	2:E:276:ASP:N	2.95	0.40
2:F:349:LYS:HB2	2:F:349:LYS:HE3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	598/1536 (39%)	568 (95%)	29 (5%)	1 (0%)	43	71
2	E	343/684 (50%)	293 (85%)	48 (14%)	2 (1%)	21	52
2	F	152/684 (22%)	151 (99%)	1 (1%)	0	100	100
3	B	383/433 (88%)	365 (95%)	18 (5%)	0	100	100
4	C	181/401 (45%)	171 (94%)	9 (5%)	1 (1%)	21	52
4	D	183/401 (46%)	175 (96%)	8 (4%)	0	100	100
All	All	1840/4139 (44%)	1723 (94%)	113 (6%)	4 (0%)	44	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	517	ASN
4	C	241	LYS
1	A	873	LYS
2	E	518	GLY

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	A	560/1391 (40%)	516 (92%)	44 (8%)	11	36
2	E	332/653 (51%)	311 (94%)	21 (6%)	16	44
2	F	148/653 (23%)	144 (97%)	4 (3%)	39	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	326/367 (89%)	301 (92%)	25 (8%)	12	37
4	C	172/359 (48%)	153 (89%)	19 (11%)	6	23
4	D	174/359 (48%)	160 (92%)	14 (8%)	11	36
All	All	1712/3782 (45%)	1585 (93%)	127 (7%)	15	38

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	666	VAL
1	A	690	ASN
1	A	697	LEU
1	A	712	SER
1	A	754	SER
1	A	763	THR
1	A	779	ASN
1	A	783	VAL
1	A	805	GLU
1	A	812	GLU
1	A	815	HIS
1	A	828	ILE
1	A	831	LEU
1	A	836	ASN
1	A	871	TYR
1	A	874	GLU
1	A	907	ARG
1	A	922	LYS
1	A	942	LEU
1	A	943	LEU
1	A	945	THR
1	A	953	SER
1	A	1068	ILE
1	A	1142	THR
1	A	1152	THR
1	A	1153	THR
1	A	1154	ILE
1	A	1161	ILE
1	A	1171	GLU
1	A	1191	LEU
1	A	1227	SER
1	A	1235	LYS
1	A	1241	THR

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Mol	Chain	Res	Type
1	A	1246	THR
1	A	1249	LEU
1	A	1255	THR
1	A	1256	LEU
1	A	1262	THR
1	A	1294	MET
1	A	1297	THR
1	A	1299	ASN
1	A	1313	SER
1	A	1314	ILE
1	A	1337	TYR
2	E	107	LYS
2	E	115	LEU
2	E	180	ASN
2	E	360	THR
2	E	371	GLN
2	E	375	GLU
2	E	379	ILE
2	E	387	PHE
2	E	388	ASN
2	E	394	SER
2	E	395	ILE
2	E	398	LEU
2	E	437	ILE
2	E	441	ASP
2	E	454	ARG
2	E	462	SER
2	E	466	CYS
2	E	472	THR
2	E	491	VAL
2	E	543	ASP
2	E	554	LYS
3	B	11	ILE
3	B	14	LYS
3	B	19	ARG
3	B	41	LYS
3	B	52	ILE
3	B	53	MET
3	B	73	GLU
3	B	90	THR
3	B	113	PHE
3	B	114	ASP

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Mol	Chain	Res	Type
3	B	134	LEU
3	B	139	CYS
3	B	158	SER
3	B	170	ILE
3	B	180	VAL
3	B	191	ASP
3	B	201	ASP
3	B	242	ILE
3	B	244	ASP
3	B	246	THR
3	B	249	SER
3	B	254	VAL
3	B	308	VAL
3	B	314	THR
3	B	333	VAL
4	C	226	ILE
4	C	230	SER
4	C	231	VAL
4	C	235	ASP
4	C	240	THR
4	C	241	LYS
4	C	253	THR
4	C	267	GLN
4	C	285	LEU
4	C	304	LEU
4	C	323	ILE
4	C	331	LEU
4	C	332	LEU
4	C	335	ILE
4	C	372	GLU
4	C	380	ASN
4	C	386	LEU
4	C	390	THR
4	C	392	SER
4	D	224	ILE
4	D	226	ILE
4	D	228	LEU
4	D	254	VAL
4	D	258	LEU
4	D	279	SER
4	D	282	CYS
4	D	287	LEU

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Mol	Chain	Res	Type
4	D	290	ASP
4	D	325	ILE
4	D	329	ILE
4	D	331	LEU
4	D	350	GLN
4	D	355	LEU
2	F	275	CYS
2	F	319	LEU
2	F	332	ASN
2	F	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	690	ASN
1	A	694	GLN
1	A	779	ASN
1	A	801	ASN
1	A	802	GLN
1	A	824	ASN
1	A	836	ASN
1	A	959	GLN
1	A	961	ASN
1	A	974	GLN
1	A	983	ASN
1	A	1039	ASN
1	A	1075	GLN
1	A	1081	ASN
1	A	1190	GLN
1	A	1221	HIS
1	A	1247	GLN
1	A	1293	HIS
1	A	1299	ASN
2	E	259	ASN
2	E	331	ASN
2	E	346	HIS
2	E	352	GLN
2	E	376	ASN
2	E	388	ASN
2	E	402	ASN
2	E	433	ASN
2	E	459	ASN

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Mol	Chain	Res	Type
2	E	495	GLN
2	E	516	ASN
2	E	521	GLN
2	E	541	GLN
2	E	580	ASN
3	B	150	HIS
3	B	188	HIS
3	B	235	ASN
3	B	364	ASN
4	C	305	GLN
4	C	353	GLN
4	C	358	GLN
4	C	380	ASN
4	C	393	GLN
4	D	305	GLN
4	D	330	HIS
4	D	350	GLN
4	D	375	ASN
4	D	380	ASN
2	F	259	ASN
2	F	268	GLN
2	F	295	ASN
2	F	302	HIS
2	F	304	ASN
2	F	346	HIS
2	F	355	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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.

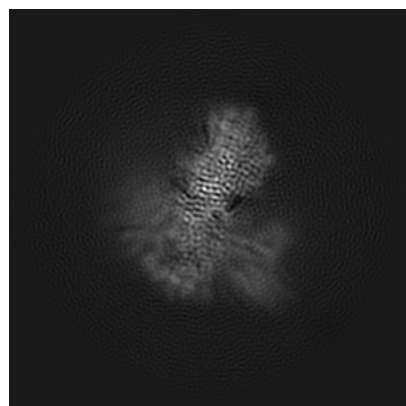
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37364. These allow visual inspection of the internal detail of the map and identification of artifacts.

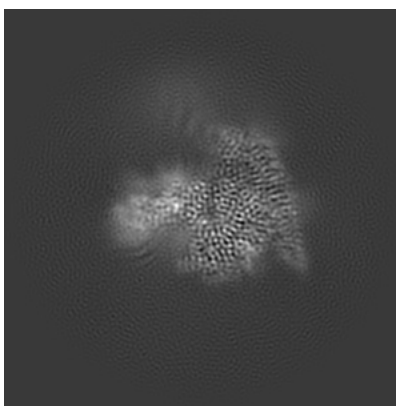
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

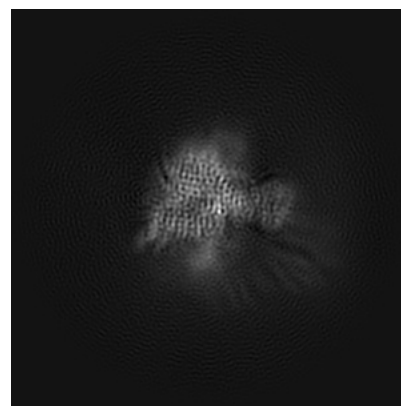
6.1.1 Primary map



X

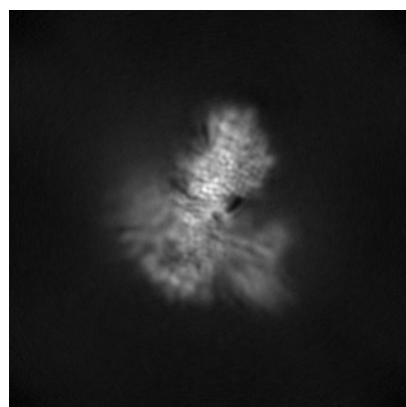


Y

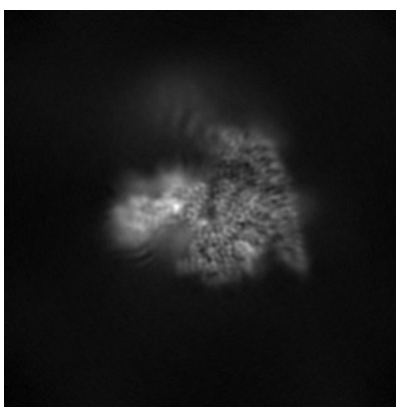


Z

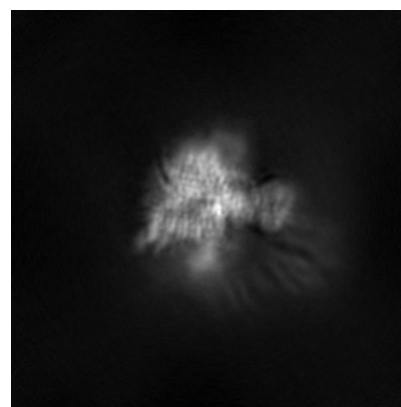
6.1.2 Raw map



X



Y

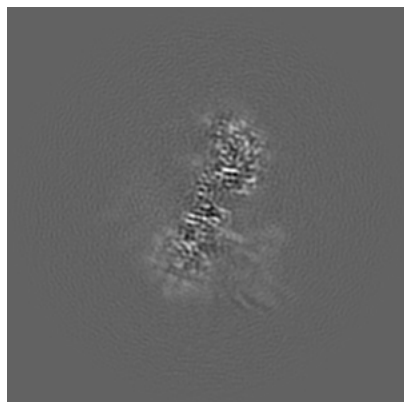


Z

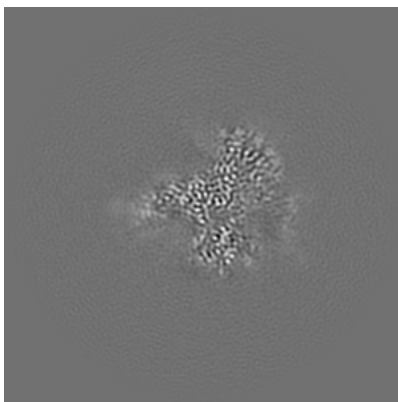
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

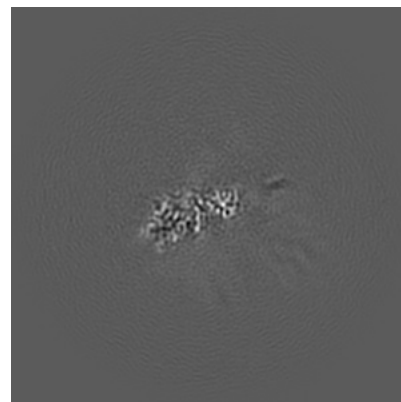
6.2.1 Primary map



X Index: 140

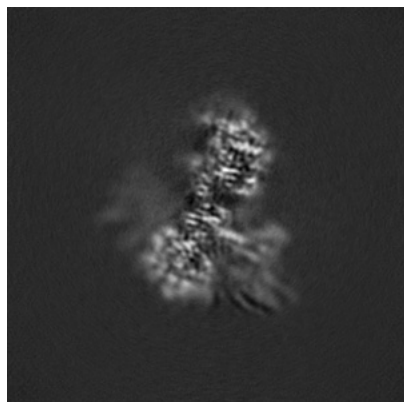


Y Index: 140

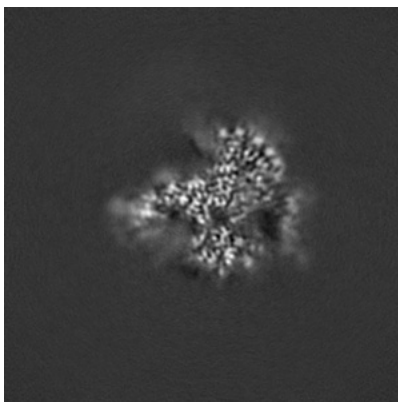


Z Index: 140

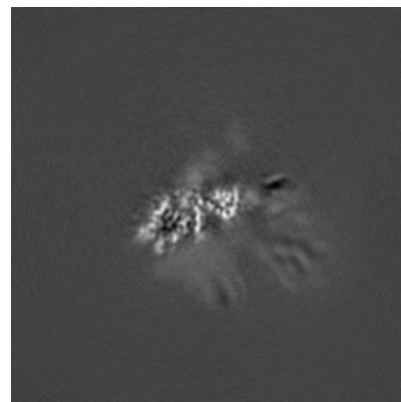
6.2.2 Raw map



X Index: 140



Y Index: 140

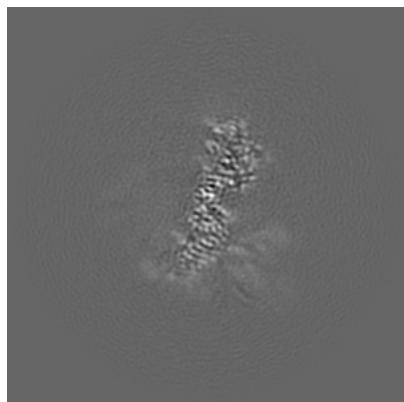


Z Index: 140

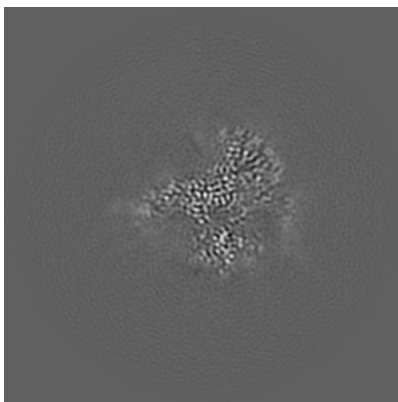
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

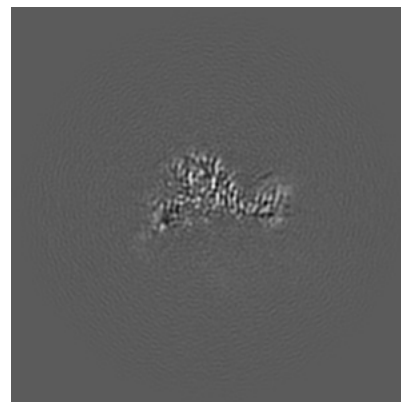
6.3.1 Primary map



X Index: 145

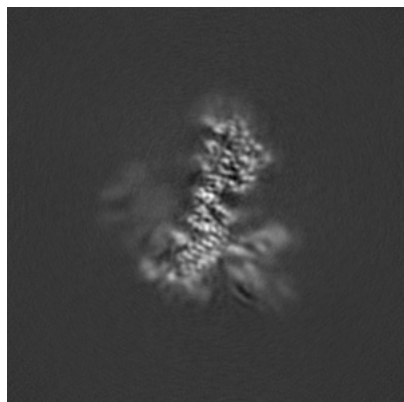


Y Index: 141

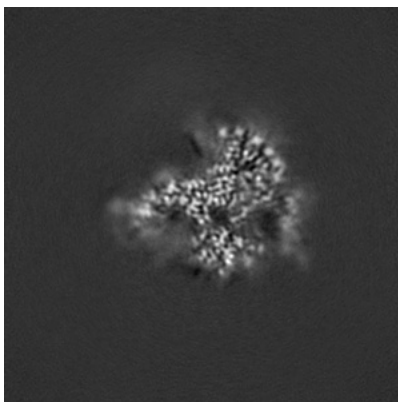


Z Index: 160

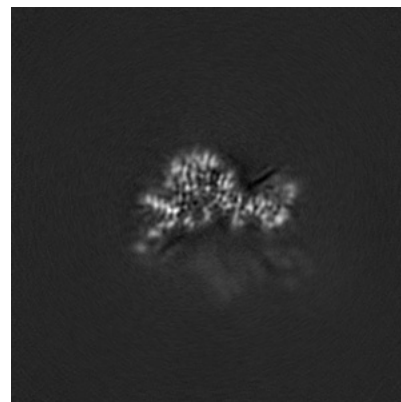
6.3.2 Raw map



X Index: 145



Y Index: 141

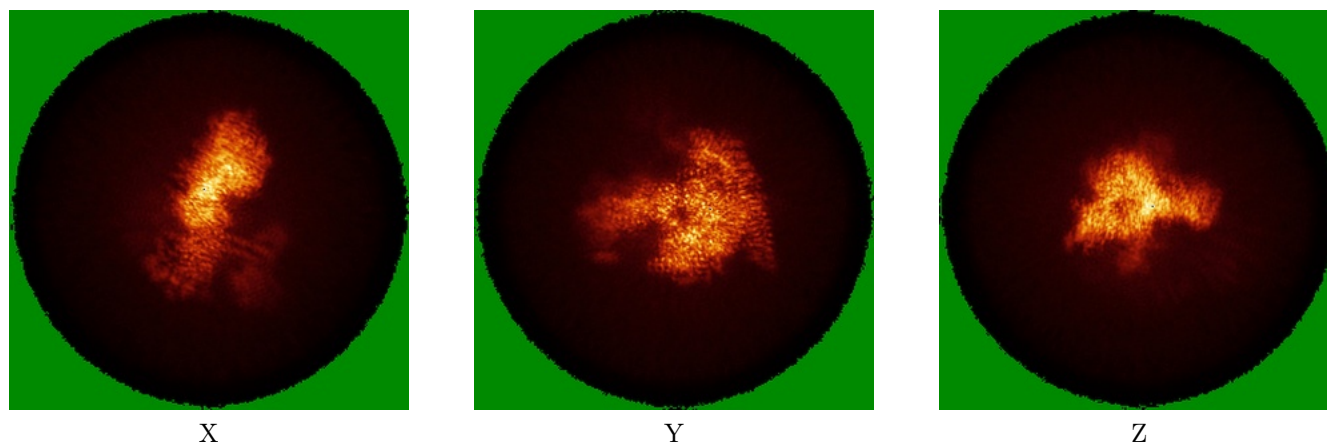


Z Index: 157

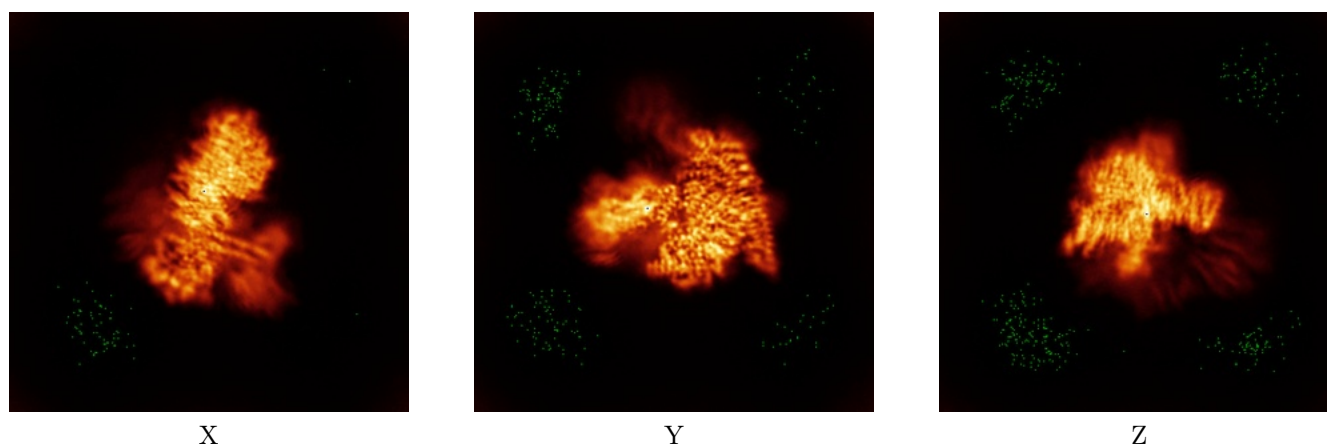
The images above show the largest variance slices of the map in three orthogonal directions.

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.

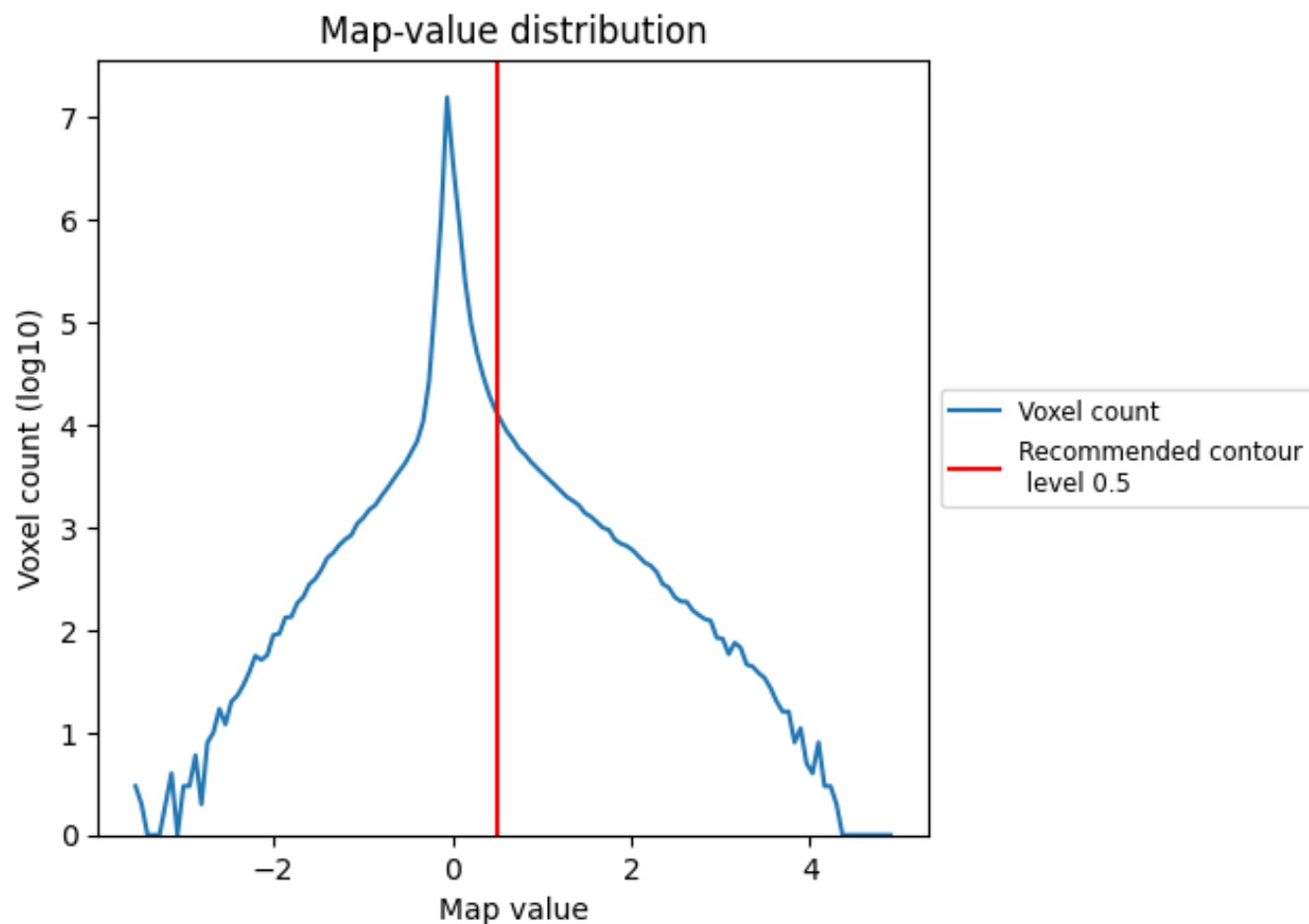
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

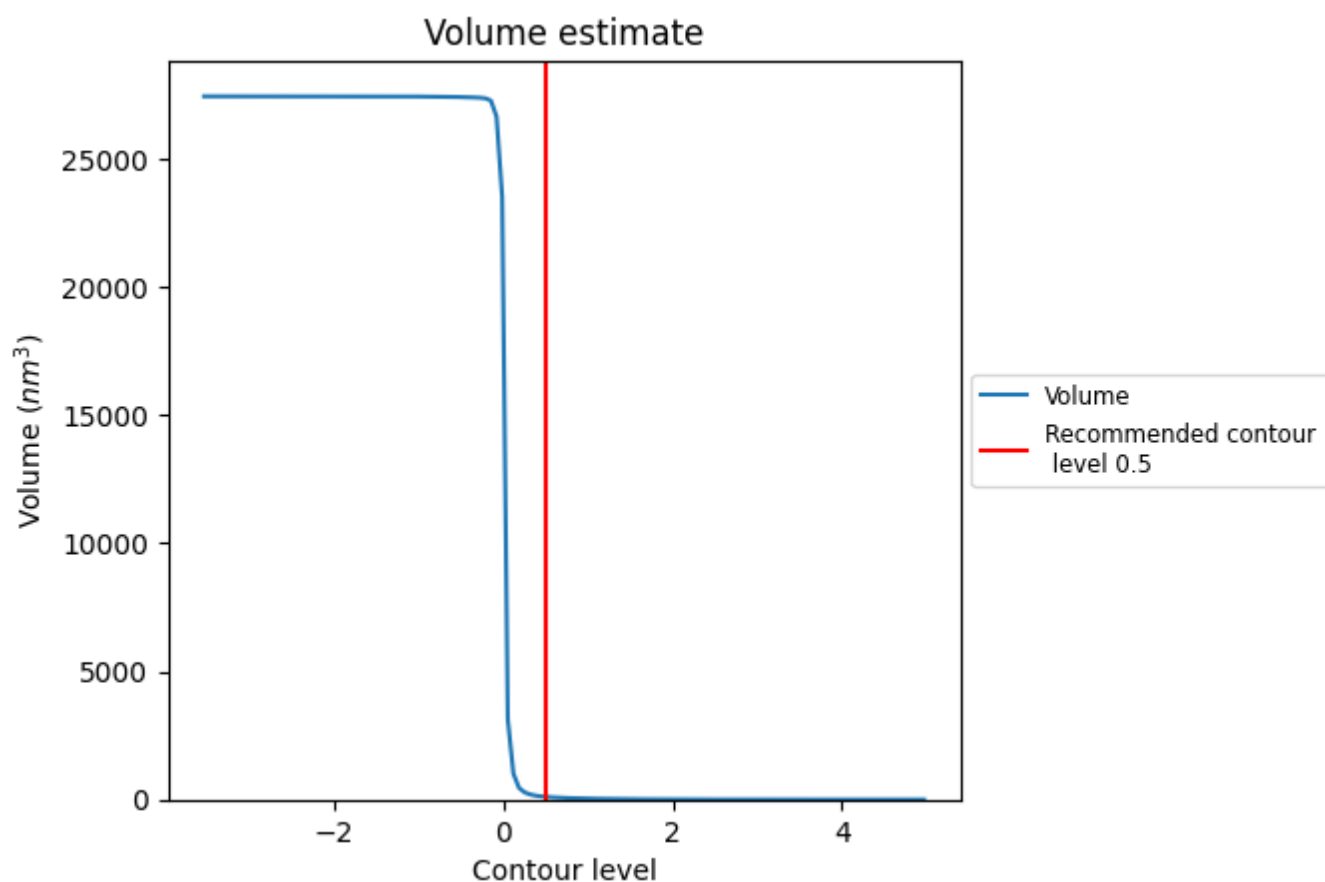
This section contains the results of statistical analysis of the map.

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.

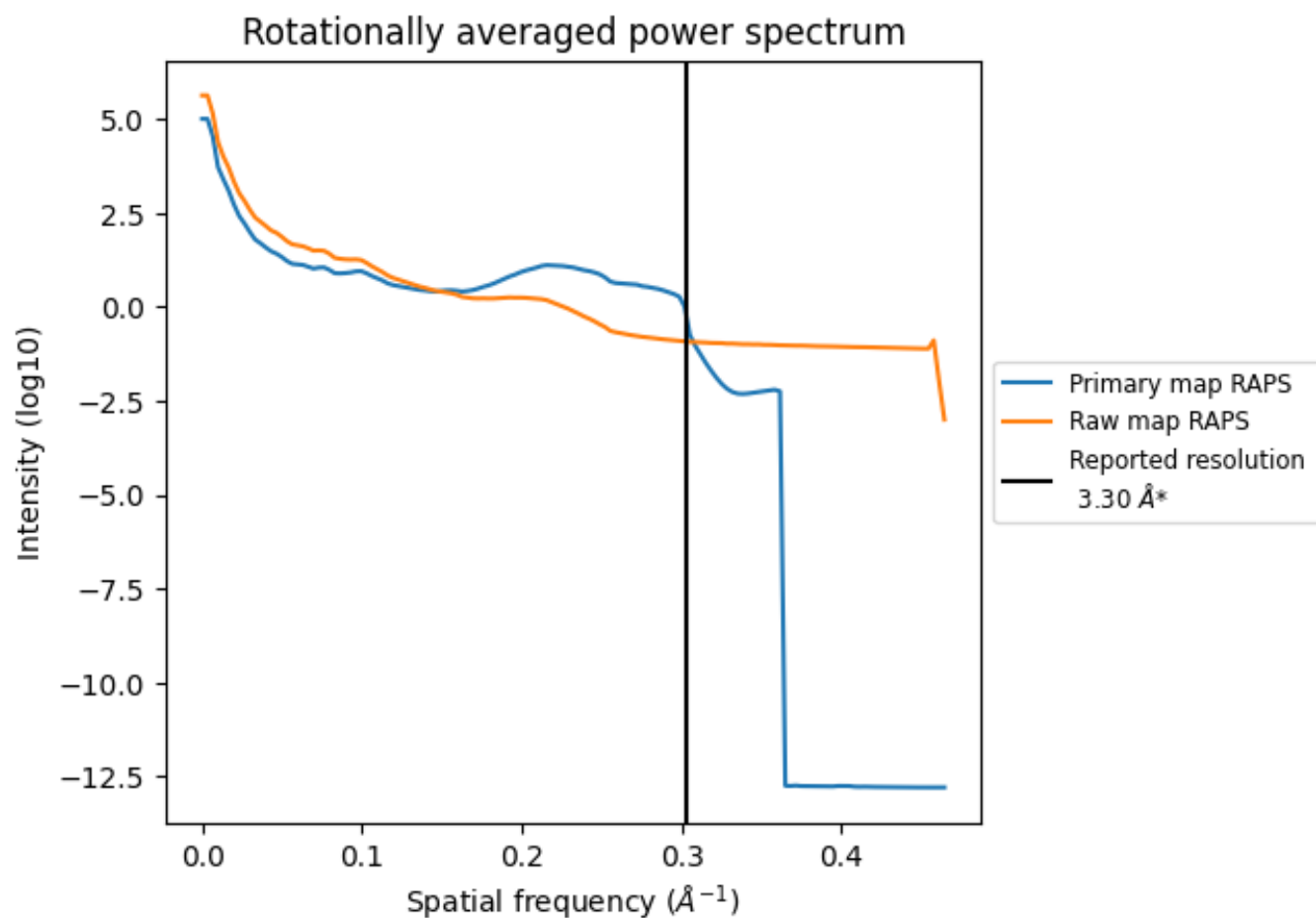
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 95 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 ⓘ

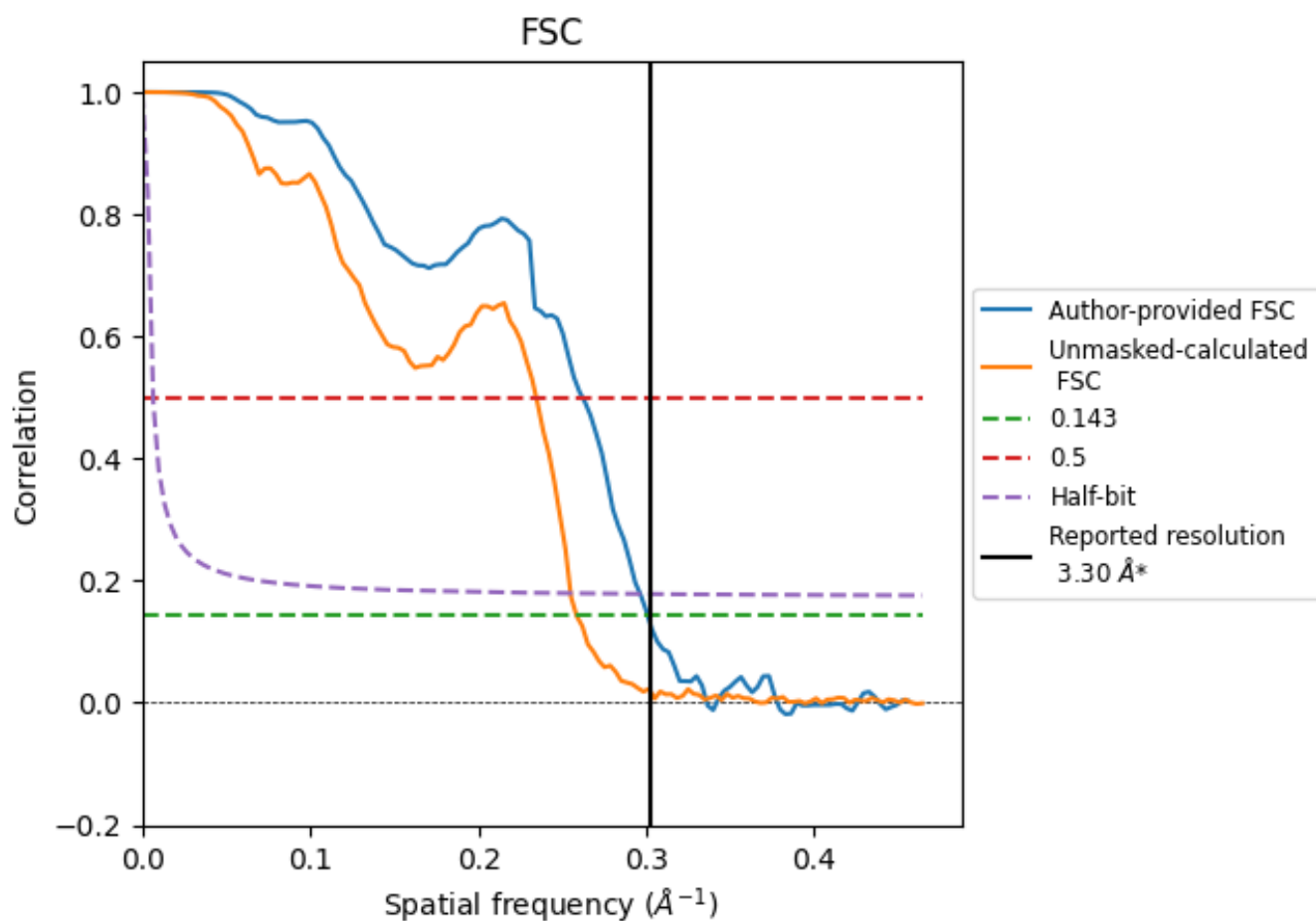


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

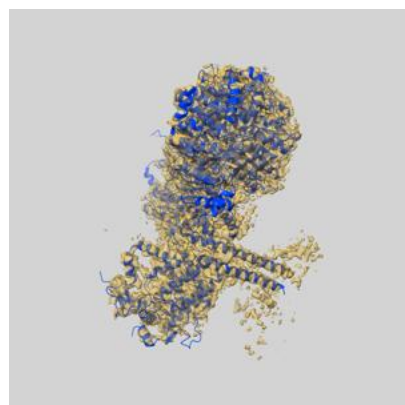
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.82	3.37
Unmasked-calculated*	3.87	4.26	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.3 by more than 10 %

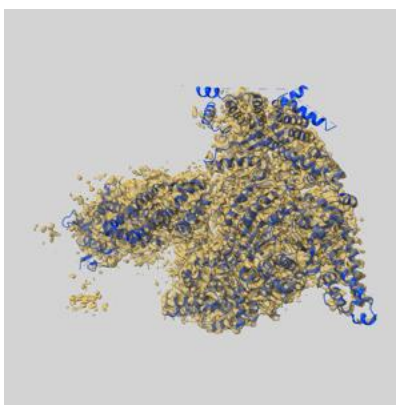
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37364 and PDB model 8W9C. Per-residue inclusion information can be found in section [3](#) on page [6](#).

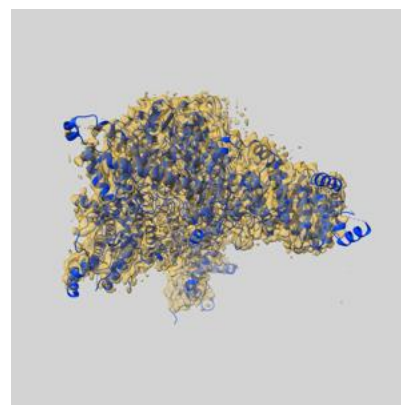
9.1 Map-model overlay [i](#)



X



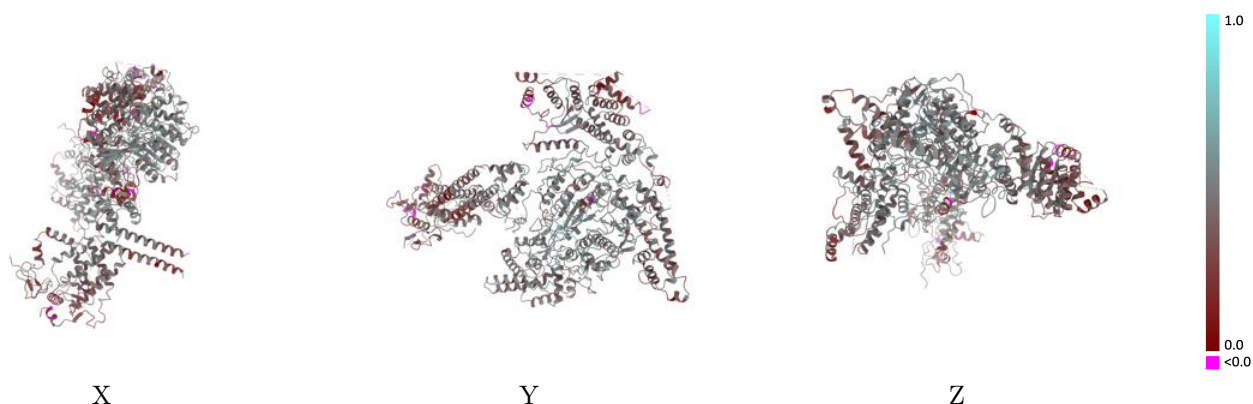
Y



Z

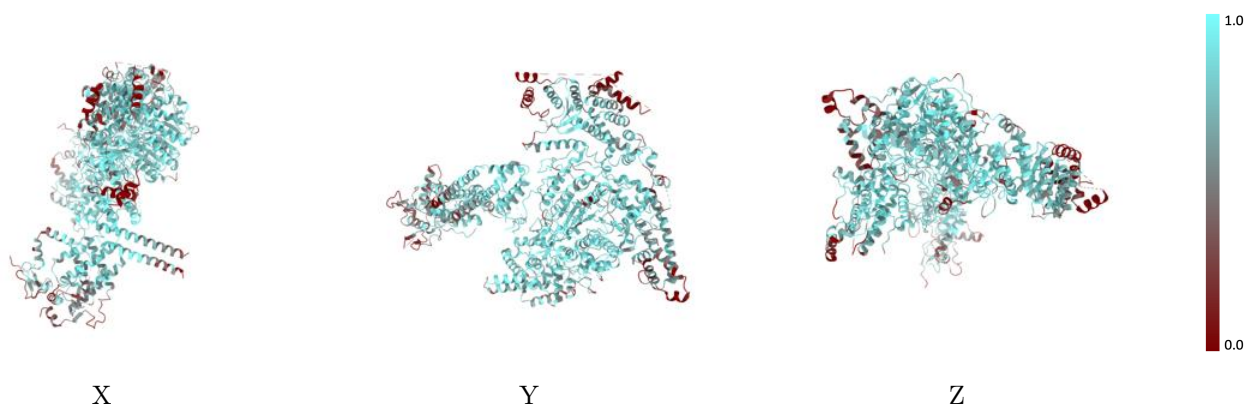
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



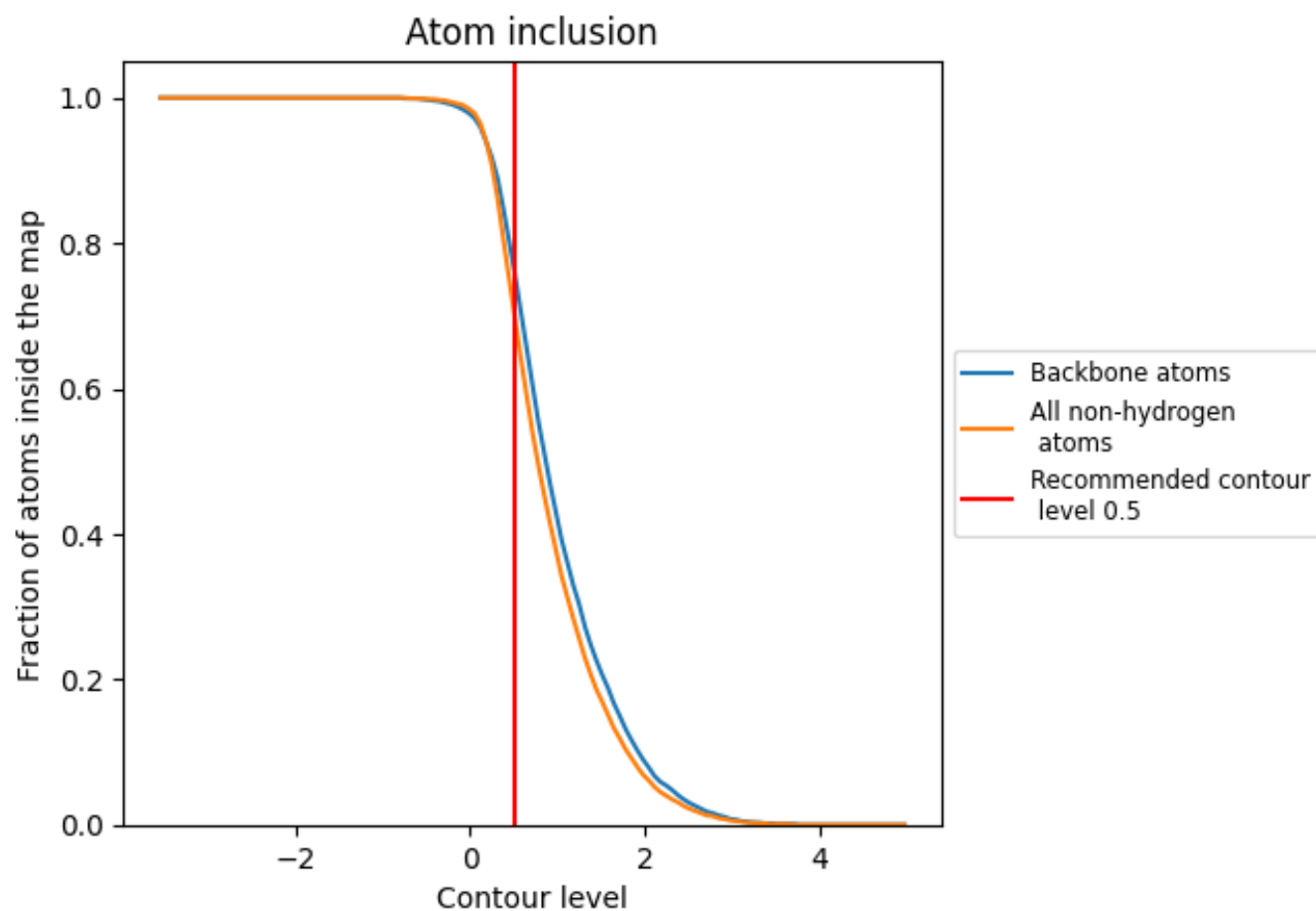
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.4230
A	0.6480	0.4050
B	0.8470	0.4940
C	0.8310	0.4610
D	0.6070	0.3430
E	0.7080	0.4390
F	0.5530	0.3390

1.0

0.0

<0.0