



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:18 PM UTC

PDB ID : 8GF6 / pdb_00008gf6
EMDB ID : EMD-29979
Title : Apo-apo MCR assembly intermediate
Authors : Joiner, A.M.N.; Chadwick, G.L.; Nayak, D.D.
Deposited on : 2023-03-07
Resolution : 3.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

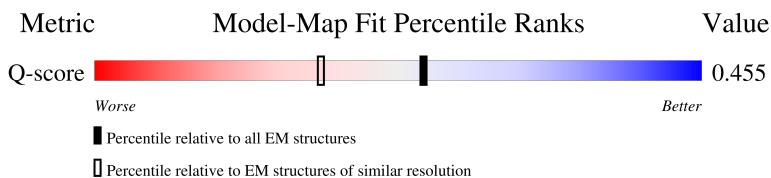
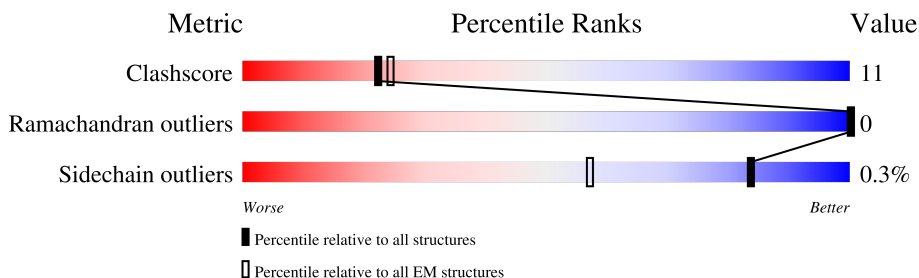
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	570	
1	B	570	
2	C	434	
2	D	434	

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Mol	Chain	Length	Quality of chain
3	E	248	 70% 29%
3	F	248	 73% 27%
4	X	193	 13% 42% 20% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18315 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 Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	461	Total	C	N	O	S	0	0
			3519	2212	600	685	22		
1	B	484	Total	C	N	O	S	0	0
			3693	2322	628	719	24		

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	432	Total	C	N	O	S	0	0
			3148	1971	543	616	18		
2	D	431	Total	C	N	O	S	0	0
			3143	1968	542	615	18		

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	247	Total	C	N	O	S	0	0
			1926	1192	352	369	13		
3	F	247	Total	C	N	O	S	0	0
			1926	1192	352	369	13		

- Molecule 4 is a protein called Methyl coenzyme M reductase, subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	120	Total	C	N	O	S	0	0
			960	608	172	177	3		

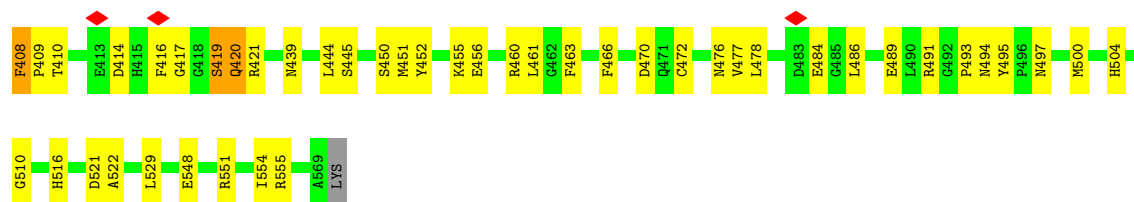
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-22	MET	-	expression tag	UNP Q8THG8
X	-21	ASP	-	expression tag	UNP Q8THG8
X	-20	TYR	-	expression tag	UNP Q8THG8

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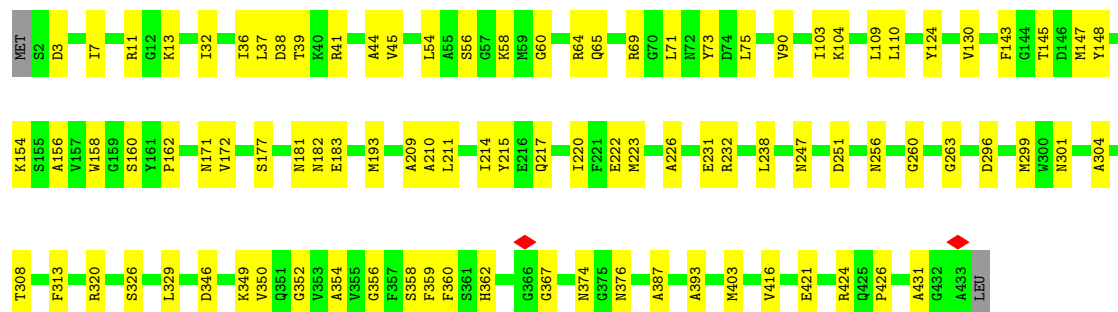
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Chain	Residue	Modelled	Actual	Comment	Reference
X	-19	LYS	-	expression tag	UNP Q8THG8
X	-18	ASP	-	expression tag	UNP Q8THG8
X	-17	ASP	-	expression tag	UNP Q8THG8
X	-16	ASP	-	expression tag	UNP Q8THG8
X	-15	ASP	-	expression tag	UNP Q8THG8
X	-14	LYS	-	expression tag	UNP Q8THG8
X	-13	GLY	-	expression tag	UNP Q8THG8
X	-12	GLY	-	expression tag	UNP Q8THG8
X	-11	GLY	-	expression tag	UNP Q8THG8
X	-10	TRP	-	expression tag	UNP Q8THG8
X	-9	SER	-	expression tag	UNP Q8THG8
X	-8	HIS	-	expression tag	UNP Q8THG8
X	-7	PRO	-	expression tag	UNP Q8THG8
X	-6	GLN	-	expression tag	UNP Q8THG8
X	-5	PHE	-	expression tag	UNP Q8THG8
X	-4	GLU	-	expression tag	UNP Q8THG8
X	-3	LYS	-	expression tag	UNP Q8THG8
X	-2	GLY	-	expression tag	UNP Q8THG8
X	-1	GLY	-	expression tag	UNP Q8THG8
X	0	GLY	-	expression tag	UNP Q8THG8



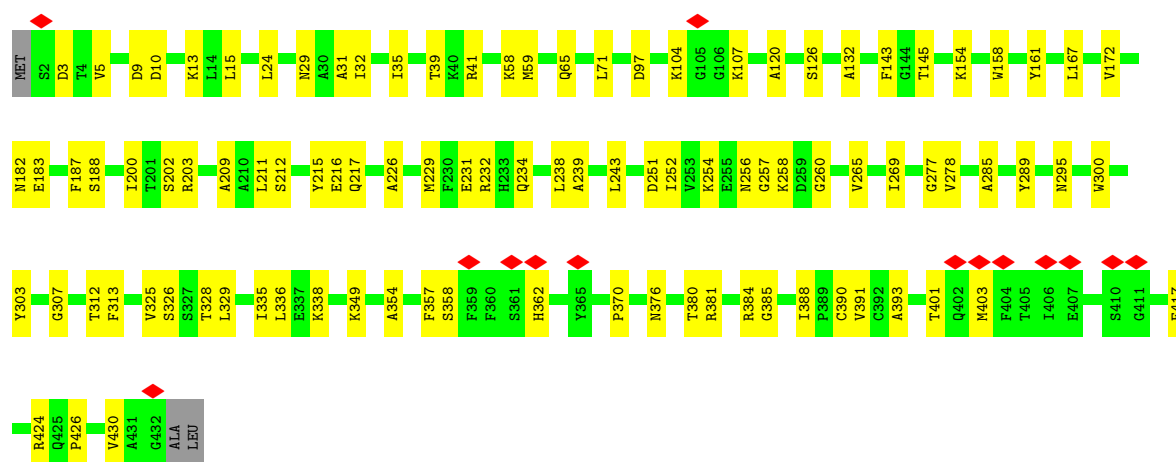
• Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain C: 78% 21%



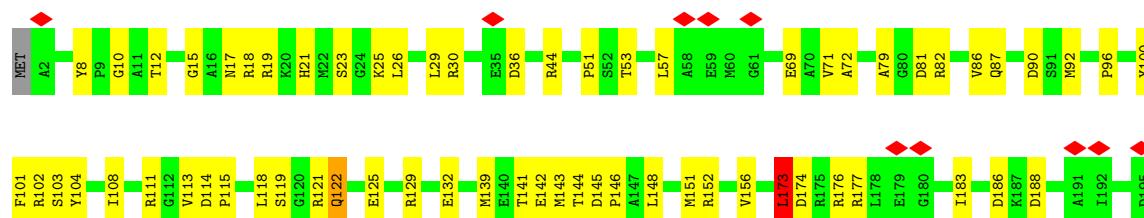
• Molecule 2: Methyl-coenzyme M reductase subunit beta

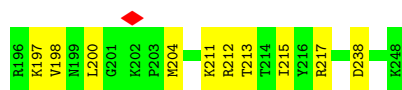
Chain D: 77% 23%



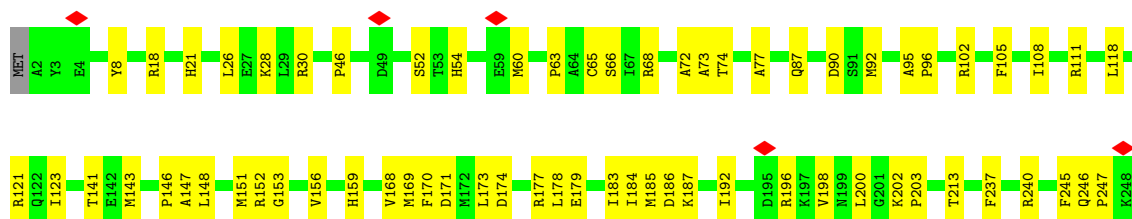
• Molecule 3: Methyl-coenzyme M reductase subunit gamma

Chain E: 70% 29%

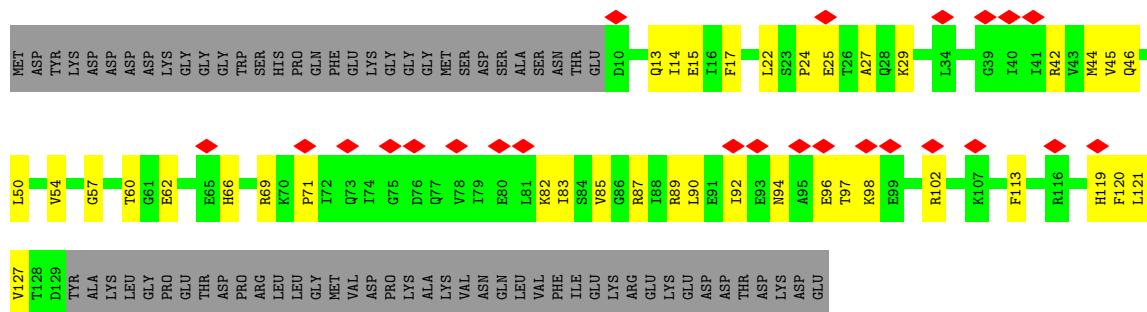




- Molecule 3: Methyl-coenzyme M reductase subunit gamma



- Molecule 4: Methyl coenzyme M reductase, subunit D



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.710	Depositor
Minimum map value	-0.639	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	249.76001, 249.76001, 249.76001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.115, 1.115, 1.115	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MHS, AGM, SMC

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	0.43	0/3560	0.65	0/4830
1	B	0.44	0/3738	0.71	10/5074 (0.2%)
2	C	0.41	0/3195	0.61	0/4324
2	D	0.39	0/3190	0.62	0/4317
3	E	0.39	0/1965	0.65	1/2653 (0.0%)
3	F	0.45	0/1965	0.68	0/2653
4	X	0.28	0/976	0.66	0/1314
All	All	0.41	0/18589	0.65	11/25165 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	GLN	N-CA-C	7.94	122.02	109.39
1	B	419	SER	N-CA-C	-7.92	97.25	109.52
1	B	162	GLU	N-CA-C	-7.87	97.12	109.72
1	B	100	LEU	N-CA-C	-7.82	103.05	112.59
1	B	420	GLN	N-CA-C	-6.36	104.09	112.24
1	B	354	ASP	N-CA-C	6.10	122.04	113.56
1	B	421	ARG	N-CA-C	-5.76	98.53	110.80
3	E	173	LEU	N-CA-C	-5.48	98.70	108.13
1	B	407	LYS	N-CA-C	5.22	117.05	111.36
1	B	408	PHE	CA-C-N	-5.12	113.74	120.96
1	B	408	PHE	C-N-CA	-5.12	113.74	120.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3519	0	3375	77	0
1	B	3693	0	3558	129	0
2	C	3148	0	3129	71	0
2	D	3143	0	3124	67	0
3	E	1926	0	1871	53	0
3	F	1926	0	1871	46	0
4	X	960	0	998	29	0
All	All	18315	0	17926	414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (414) 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:B:132:LYS:CE	2:C:403:MET:SD	2.24	1.26
1:B:147:LEU:HD11	1:B:179:ILE:HD11	1.29	1.15
1:B:132:LYS:HE2	2:C:403:MET:SD	1.88	1.11
1:B:419:SER:O	1:B:420:GLN:CD	2.01	1.04
1:A:476:ASN:HD22	1:A:497:ASN:HD21	1.09	0.99
1:B:145:HIS:O	1:B:149:THR:HG23	1.69	0.93
1:B:132:LYS:HE3	2:C:403:MET:SD	2.08	0.93
1:B:419:SER:C	1:B:420:GLN:OE1	2.17	0.87
1:B:147:LEU:HD11	1:B:179:ILE:CD1	2.04	0.87
1:B:416:PHE:HZ	1:B:463:PHE:HB2	1.43	0.83
3:E:121:ARG:HD2	3:E:156:VAL:HG21	1.58	0.83
1:B:414:ASP:OD1	1:B:417:GLY:CA	2.26	0.83
1:B:451:MET:HE1	1:B:466:PHE:HE2	1.42	0.83
1:A:423:THR:HG1	1:A:466:PHE:HZ	1.24	0.83
1:B:355:ILE:HD12	1:B:355:ILE:H	1.47	0.79
3:E:118:LEU:HG	3:E:121:ARG:HE	1.50	0.77
1:B:416:PHE:HZ	1:B:463:PHE:CB	1.98	0.76
1:B:414:ASP:OD1	1:B:417:GLY:HA2	1.86	0.76
1:B:346:TYR:HD2	1:B:420:GLN:HB3	1.51	0.75
3:E:103:SER:OG	3:E:122:GLN:NE2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASN:HD22	1:B:497:ASN:HD21	1.35	0.73
1:A:151:ASN:OD1	1:A:176:TYR:HA	1.88	0.73
1:B:132:LYS:NZ	2:C:403:MET:SD	2.62	0.72
1:B:147:LEU:HD21	1:B:179:ILE:CD1	2.20	0.72
1:A:467:ASP:OD1	1:A:470:ASP:HB2	1.88	0.72
1:B:476:ASN:ND2	1:B:497:ASN:HD21	1.88	0.71
1:B:419:SER:O	1:B:420:GLN:OE1	2.07	0.70
1:B:149:THR:HG21	1:B:252:ALA:HB2	1.75	0.69
1:B:197:ASN:H	1:B:200:LYS:HE3	1.55	0.69
1:B:416:PHE:CZ	1:B:463:PHE:CB	2.76	0.68
1:A:403:GLU:O	1:A:407:LYS:HB2	1.94	0.67
3:F:146:PRO:HB2	3:F:183:ILE:HG12	1.77	0.67
1:A:464:PHE:HB3	2:C:359:PHE:HD2	1.61	0.66
1:B:147:LEU:HD21	1:B:179:ILE:HD12	1.77	0.66
1:B:318:LEU:HD13	1:B:357:ASP:OD1	1.94	0.66
1:B:460:ARG:NH1	3:F:92:MET:SD	2.69	0.66
1:A:100:LEU:HD23	1:A:100:LEU:O	1.96	0.66
1:A:476:ASN:HD22	1:A:497:ASN:ND2	1.89	0.65
1:B:476:ASN:HD22	1:B:497:ASN:ND2	1.95	0.65
2:C:360:PHE:HB3	2:C:367:GLY:HA3	1.78	0.65
3:E:102:ARG:HB2	3:E:122:GLN:HG2	1.79	0.65
4:X:42:ARG:HD2	4:X:121:LEU:HD21	1.78	0.64
3:E:72:ALA:O	3:E:111:ARG:NH1	2.30	0.64
1:B:115:ILE:HD12	1:B:303:ILE:HD13	1.80	0.64
1:B:277:MET:SD	1:B:277:MET:N	2.68	0.64
3:F:26:LEU:HD11	3:F:143:MET:HE3	1.79	0.64
2:D:209:ALA:HB2	2:D:393:ALA:HB2	1.78	0.63
1:B:268:ALA:HA	1:B:272:ALA:HB3	1.80	0.63
4:X:50:LEU:O	4:X:69:ARG:NH2	2.32	0.63
2:D:257:GLY:O	3:F:111:ARG:NH1	2.32	0.63
1:B:478:LEU:HD23	2:C:147:MET:HG2	1.79	0.63
2:C:11:ARG:NH1	3:E:69:GLU:OE1	2.31	0.62
1:A:476:ASN:ND2	1:A:497:ASN:HD21	1.88	0.62
2:C:247:ASN:O	2:C:251:ASP:HB2	1.99	0.62
4:X:24:PRO:HB3	4:X:71:PRO:HA	1.82	0.62
2:C:263:GLY:HA3	3:E:108:ILE:HG23	1.81	0.61
3:F:178:LEU:HD21	3:F:203:PRO:HG3	1.82	0.61
3:F:21:HIS:NE2	3:F:96:PRO:O	2.33	0.61
1:B:250:ILE:HD13	1:B:257:ALA:HA	1.82	0.61
1:B:224:ILE:HD13	1:B:237:THR:HA	1.83	0.61
1:B:113:ASP:OD2	1:B:230:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HH22	2:D:376:ASN:ND2	1.97	0.61
2:C:45:VAL:HG22	2:C:172:VAL:HG22	1.83	0.61
1:A:172:VAL:HG13	1:A:225:PRO:HG3	1.83	0.61
2:D:211:LEU:HG	2:D:426:PRO:HG3	1.82	0.60
3:E:21:HIS:NE2	3:E:96:PRO:O	2.34	0.60
2:D:5:VAL:HG11	2:D:239:ALA:HB1	1.84	0.60
1:B:178:LYS:HD3	1:B:196:ILE:HG23	1.83	0.60
1:A:245:ILE:HD11	1:A:270:LYS:HB3	1.83	0.60
1:B:180:PHE:HB3	1:B:196:ILE:HG13	1.82	0.60
1:B:324:GLY:O	1:B:328:TYR:HB2	2.02	0.60
2:D:229:MET:HE3	3:F:247:PRO:HD2	1.84	0.59
1:A:423:THR:OG1	1:A:466:PHE:HZ	1.85	0.59
2:C:58:LYS:HA	2:C:65:GLN:HA	1.85	0.59
1:A:133:ARG:HE	2:D:403:MET:HB3	1.67	0.59
3:F:52:SER:OG	3:F:54:HIS:O	2.21	0.58
1:A:120:ILE:HB	1:A:275:VAL:HB	1.85	0.58
1:A:418:GLY:HA2	1:A:421:ARG:HE	1.68	0.58
1:B:516:HIS:HB3	1:B:521:ASP:HB2	1.86	0.58
2:C:326:SER:O	2:C:358:SER:OG	2.21	0.58
1:B:155:PRO:HG3	1:B:175:CYS:HB2	1.86	0.58
1:B:346:TYR:CD2	1:B:420:GLN:HB3	2.36	0.58
2:C:326:SER:HB3	2:C:358:SER:HA	1.86	0.58
1:B:284:ARG:NH2	2:D:376:ASN:ND2	2.52	0.57
3:E:177:ARG:NH2	3:E:186:ASP:OD1	2.34	0.57
1:A:484:GLU:O	1:A:495:TYR:OH	2.22	0.57
3:E:113:VAL:HG23	3:E:115:PRO:HD3	1.85	0.57
3:F:72:ALA:HB3	3:F:111:ARG:HH22	1.67	0.57
3:E:96:PRO:HA	3:E:213:THR:HA	1.85	0.57
2:C:217:GLN:HG3	2:C:238:LEU:HD13	1.85	0.57
2:C:156:ALA:O	2:C:171:ASN:ND2	2.37	0.57
3:E:81:ASP:OD2	3:E:129:ARG:NH1	2.37	0.57
3:F:192:ILE:HA	4:X:62:GLU:HG3	1.87	0.57
1:A:500:MET:N	1:A:500:MET:SD	2.77	0.57
1:B:132:LYS:HZ1	2:C:403:MET:HB2	1.70	0.57
3:F:90:ASP:OD1	3:F:102:ARG:NH2	2.34	0.56
1:B:416:PHE:CZ	1:B:463:PHE:HB3	2.39	0.56
2:D:380:THR:HB	2:D:388:ILE:HD11	1.88	0.56
2:D:258:LYS:O	3:F:111:ARG:NH2	2.39	0.56
3:F:87:GLN:NE2	3:F:123:ILE:HD13	2.21	0.56
1:A:464:PHE:HB3	2:C:359:PHE:CD2	2.41	0.56
1:B:136:LYS:NZ	1:B:253:TYR:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:HE1	1:B:241:ALA:HA	1.88	0.56
1:A:108:MET:HE1	1:A:326:MET:HB2	1.88	0.56
1:B:419:SER:O	1:B:420:GLN:CG	2.53	0.56
4:X:14:ILE:HD12	4:X:98:LYS:HD2	1.87	0.55
4:X:14:ILE:HG23	4:X:90:LEU:HB2	1.87	0.55
1:B:489:GLU:OE2	1:B:516:HIS:NE2	2.39	0.55
3:E:102:ARG:NH2	3:E:144:THR:OG1	2.36	0.55
1:B:285:AGM:NH2	2:D:183:GLU:OE2	2.39	0.55
1:B:456:GLU:OE2	2:D:338:LYS:NZ	2.40	0.55
2:D:234:GLN:OE1	2:D:384:ARG:NH2	2.39	0.55
2:C:60:GLY:O	2:C:64:ARG:NH1	2.39	0.55
3:F:151:MET:HE2	3:F:185:MET:HE1	1.89	0.55
1:A:230:ARG:HE	1:B:230:ARG:HG3	1.72	0.55
2:D:58:LYS:HG2	2:D:65:GLN:HG3	1.88	0.54
3:E:188:ASP:OD1	3:E:188:ASP:N	2.36	0.54
2:D:39:THR:HG1	2:D:215:TYR:HH	1.49	0.54
3:E:12:THR:HG23	3:E:15:GLY:H	1.72	0.54
2:C:44:ALA:HB2	2:C:416:VAL:HG21	1.89	0.54
1:B:326:MET:SD	1:B:326:MET:C	2.91	0.54
1:B:416:PHE:CZ	1:B:463:PHE:HB2	2.32	0.54
1:B:500:MET:SD	1:B:500:MET:N	2.81	0.54
1:B:486:LEU:HD22	2:C:162:PRO:HD2	1.89	0.54
1:A:133:ARG:NH1	2:D:401:THR:O	2.41	0.54
1:A:491:ARG:NH2	1:A:498:TYR:OH	2.41	0.54
2:D:202:SER:OG	2:D:424:ARG:NH2	2.41	0.54
1:B:419:SER:HB2	1:B:420:GLN:OE1	2.08	0.54
2:D:29:ASN:HB3	2:D:32:ILE:HG22	1.90	0.54
2:D:183:GLU:HB3	2:D:187:PHE:HD2	1.72	0.54
1:B:117:ARG:NH1	1:B:174:ASP:OD2	2.41	0.53
3:F:185:MET:HB3	3:F:198:VAL:HB	1.90	0.53
1:A:422:ALA:HB3	1:A:466:PHE:HE2	1.74	0.53
1:B:349:ALA:HA	1:B:352:THR:OG1	2.07	0.53
1:B:554:ILE:HA	4:X:126:THR:HA	1.90	0.53
3:F:202:LYS:HD3	3:F:203:PRO:HD2	1.90	0.53
2:D:277:GLY:O	2:D:295:ASN:ND2	2.41	0.53
1:B:132:LYS:NZ	2:C:403:MET:HB2	2.24	0.53
3:E:142:GLU:OE1	3:E:212:ARG:NH1	2.41	0.53
2:C:73:TYR:HH	2:C:145:THR:HG1	1.54	0.53
1:A:292:PRO:HB2	1:A:332:TRP:HB2	1.90	0.53
1:B:195:VAL:CG1	1:B:197:ASN:OD1	2.56	0.53
2:C:69:ARG:NH2	2:C:148:TYR:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:ALA:HB3	2:D:289:TYR:HB3	1.91	0.53
1:A:110:GLN:HB2	1:A:559:PRO:HB3	1.90	0.52
1:A:463:PHE:O	1:A:465:GLY:N	2.42	0.52
2:D:216:GLU:HG2	2:D:385:GLY:HA2	1.91	0.52
2:D:182:ASN:HD21	2:D:188:SER:HB3	1.73	0.52
4:X:57:GLY:O	4:X:60:THR:OG1	2.23	0.52
2:C:56:SER:O	2:C:65:GLN:NE2	2.35	0.52
3:E:146:PRO:O	3:E:176:ARG:NH1	2.42	0.52
3:F:179:GLU:HB2	3:F:184:ILE:HG13	1.92	0.52
1:B:80:GLN:HB2	4:X:82:LYS:HD3	1.91	0.52
1:B:470:ASP:OD2	1:B:504:HIS:NE2	2.41	0.52
1:A:464:PHE:CB	2:C:359:PHE:HD2	2.23	0.52
1:B:318:LEU:CD1	1:B:357:ASP:OD1	2.58	0.52
1:B:451:MET:CE	1:B:466:PHE:HE2	2.19	0.52
2:C:421:GLU:OE1	2:C:424:ARG:NH1	2.42	0.52
2:D:41:ARG:NH1	2:D:97:ASP:O	2.42	0.52
2:D:269:ILE:HD13	2:D:307:GLY:HA3	1.92	0.52
1:B:356:LEU:O	1:B:356:LEU:HD12	2.10	0.52
2:D:24:LEU:HD13	2:D:243:LEU:HD12	1.92	0.52
3:E:174:ASP:O	3:E:177:ARG:NH1	2.43	0.52
1:B:410:THR:O	4:X:87:ARG:NH2	2.39	0.51
2:C:45:VAL:HB	2:C:109:LEU:HB2	1.90	0.51
2:C:90:VAL:HG23	2:C:130:VAL:HG12	1.92	0.51
1:B:419:SER:C	1:B:420:GLN:CD	2.70	0.51
3:E:183:ILE:HG23	3:E:200:LEU:HB2	1.92	0.51
1:A:258:GLY:HA2	2:D:362:HIS:HB3	1.90	0.51
2:D:357:PHE:HE2	2:D:380:THR:HG22	1.76	0.51
1:A:327:LEU:HA	1:A:331:ILE:HD12	1.91	0.51
2:C:3:ASP:OD2	2:C:232:ARG:NE	2.40	0.51
3:E:29:LEU:HD21	3:E:204:MET:HE3	1.93	0.51
1:A:472:SMC:HB2	2:C:349:LYS:HA	1.92	0.51
2:C:182:ASN:HA	2:C:376:ASN:HD21	1.75	0.51
1:A:422:ALA:HB3	1:A:466:PHE:CE2	2.46	0.51
2:D:29:ASN:HD21	2:D:430:VAL:HG13	1.76	0.51
1:B:87:THR:HG22	1:B:94:VAL:HB	1.93	0.51
1:B:321:VAL:HG23	1:B:510:GLY:HA3	1.92	0.51
1:A:315:LYS:NZ	1:A:361:TYR:OH	2.43	0.50
1:B:416:PHE:CD2	1:B:416:PHE:O	2.65	0.50
2:C:329:LEU:HB2	2:C:354:ALA:HB2	1.92	0.50
3:F:46:PRO:HG2	3:F:196:ARG:HH22	1.76	0.50
4:X:50:LEU:HD12	4:X:83:ILE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LYS:HZ1	2:C:403:MET:CB	2.25	0.50
3:F:147:ALA:HB1	3:F:168:VAL:HA	1.94	0.50
2:D:104:LYS:O	2:D:107:LYS:NZ	2.36	0.50
2:D:226:ALA:HB1	2:D:231:GLU:HA	1.93	0.50
1:B:87:THR:HG21	4:X:119:HIS:HB3	1.93	0.50
1:A:233:ASP:OD1	1:A:233:ASP:N	2.44	0.49
1:B:398:THR:HG21	1:B:450:SER:HA	1.92	0.49
1:B:484:GLU:O	1:B:495:TYR:OH	2.24	0.49
1:A:285:AGM:NH1	2:C:183:GLU:OE1	2.44	0.49
2:D:200:ILE:O	2:D:424:ARG:NH2	2.45	0.49
2:D:325:VAL:HG21	2:D:391:VAL:HG22	1.93	0.49
3:E:146:PRO:HB2	3:E:183:ILE:HG21	1.93	0.49
3:F:174:ASP:HB3	3:F:177:ARG:HH21	1.77	0.49
1:B:179:ILE:HG23	1:B:219:TRP:O	2.13	0.49
4:X:13:GLN:OE1	4:X:121:LEU:N	2.42	0.49
1:A:326:MET:SD	1:A:327:LEU:N	2.86	0.49
1:A:297:PHE:HB3	1:A:509:ALA:HA	1.94	0.49
2:C:350:VAL:HG23	2:C:387:ALA:HB2	1.95	0.49
2:D:312:THR:HA	2:D:328:THR:HG21	1.95	0.49
1:B:277:MET:HB3	1:B:529:LEU:HD21	1.95	0.48
4:X:94:ASN:HB3	4:X:96:GLU:HG3	1.95	0.48
1:B:147:LEU:HD21	1:B:179:ILE:HG13	1.95	0.48
1:B:414:ASP:OD1	1:B:414:ASP:O	2.30	0.48
3:E:51:PRO:HG2	3:E:82:ARG:HH11	1.77	0.48
2:C:37:LEU:HD23	2:C:41:ARG:HD3	1.95	0.48
1:B:147:LEU:HD21	1:B:179:ILE:CG1	2.43	0.48
1:B:292:PRO:HB2	1:B:332:TRP:HB2	1.94	0.48
2:D:10:ASP:OD1	3:F:66:SER:OG	2.27	0.48
1:A:391:LYS:NZ	3:E:238:ASP:OD2	2.38	0.48
2:C:320:ARG:HG3	3:E:57:LEU:HD21	1.96	0.48
2:D:132:ALA:HA	2:D:172:VAL:HG21	1.95	0.48
3:E:10:GLY:O	3:E:19:ARG:NH1	2.43	0.48
3:F:174:ASP:HB2	3:F:187:LYS:HZ2	1.77	0.48
4:X:102:ARG:HG3	4:X:113:PHE:HZ	1.78	0.48
2:C:11:ARG:O	2:C:13:LYS:NZ	2.47	0.48
2:C:193:MET:HA	2:C:374:ASN:HB3	1.95	0.48
3:E:17:ASN:ND2	3:E:211:LYS:O	2.44	0.48
3:F:183:ILE:HG23	3:F:200:LEU:HB3	1.96	0.48
1:B:445:SER:HB2	3:F:237:PHE:HZ	1.78	0.48
2:D:143:PHE:HD2	2:D:145:THR:HB	1.79	0.48
4:X:92:ILE:HD12	4:X:97:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PRO:HD2	1:B:494:ASN:HD21	1.78	0.47
3:E:44:ARG:NH2	3:E:132:GLU:OE2	2.41	0.47
1:B:197:ASN:HB2	1:B:200:LYS:HG2	1.96	0.47
4:X:89:ARG:HD3	4:X:120:PHE:HB3	1.96	0.47
1:A:489:GLU:OE1	1:A:516:HIS:NE2	2.48	0.47
1:B:355:ILE:HD12	1:B:355:ILE:N	2.21	0.47
2:C:103:ILE:HG13	2:C:104:LYS:HG2	1.96	0.47
3:F:96:PRO:HA	3:F:213:THR:HA	1.95	0.47
2:C:211:LEU:HB2	2:C:426:PRO:HG3	1.96	0.47
2:D:313:PHE:HE1	2:D:393:ALA:HB1	1.80	0.47
1:B:195:VAL:HG11	1:B:197:ASN:OD1	2.14	0.47
2:C:181:ASN:O	2:C:376:ASN:ND2	2.47	0.47
3:E:26:LEU:HD13	3:E:143:MET:HB2	1.97	0.47
3:F:87:GLN:HG3	3:F:153:GLY:HA2	1.97	0.47
3:F:171:ASP:O	4:X:66:HIS:NE2	2.39	0.47
2:D:183:GLU:HG2	2:D:381:ARG:HD2	1.97	0.47
1:A:92:ASP:N	1:A:92:ASP:OD1	2.45	0.47
1:B:548:GLU:OE1	1:B:551:ARG:NH1	2.48	0.47
3:E:30:ARG:NH1	3:E:141:THR:O	2.48	0.47
1:A:172:VAL:CG1	1:A:225:PRO:HG3	2.45	0.47
1:A:236:GLN:HB3	1:B:287:ARG:HH11	1.80	0.47
1:A:173:ASP:N	1:A:173:ASP:OD1	2.49	0.46
1:B:414:ASP:OD1	1:B:417:GLY:N	2.47	0.46
2:C:154:LYS:HE2	2:C:158:TRP:CG	2.50	0.46
2:C:209:ALA:HB2	2:C:393:ALA:HB2	1.97	0.46
1:A:326:MET:HE3	1:A:549:PHE:CE1	2.51	0.46
1:A:373:GLY:O	1:A:381:ASN:ND2	2.44	0.46
3:E:51:PRO:HB2	3:E:82:ARG:HE	1.80	0.46
3:F:30:ARG:NH1	3:F:200:LEU:O	2.43	0.46
2:C:7:ILE:HG21	2:C:431:ALA:HB2	1.97	0.46
3:E:101:PHE:HA	3:E:104:TYR:HD2	1.80	0.46
3:F:95:ALA:HA	3:F:148:LEU:HD13	1.97	0.46
3:E:8:TYR:OH	3:E:18:ARG:NH2	2.48	0.46
1:A:394:ALA:HB3	1:A:449:LEU:HD23	1.96	0.46
1:B:160:VAL:O	1:B:160:VAL:HG23	2.16	0.46
2:D:203:ARG:HH11	3:F:63:PRO:HG3	1.81	0.46
3:F:118:LEU:HD13	3:F:121:ARG:HE	1.79	0.46
3:F:152:ARG:NH1	3:F:170:PHE:O	2.39	0.46
1:B:304:VAL:HG11	1:B:320:VAL:HG22	1.97	0.46
1:B:409:PRO:HD2	4:X:17:PHE:CE1	2.50	0.46
3:F:65:CYS:HB3	3:F:68:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:O	1:A:167:THR:N	2.49	0.46
2:C:304:ALA:O	2:C:308:THR:OG1	2.28	0.46
3:F:8:TYR:OH	3:F:18:ARG:NH2	2.49	0.46
3:F:73:ALA:O	3:F:74:THR:OG1	2.31	0.46
1:A:242:ALA:HB1	1:A:270:LYS:HD3	1.97	0.45
1:B:555:ARG:HB2	4:X:127:VAL:HG12	1.99	0.45
1:A:285:AGM:HE22	1:A:285:AGM:HB2	1.86	0.45
1:A:491:ARG:HD3	1:A:498:TYR:HE2	1.79	0.45
2:D:9:ASP:OD1	2:D:13:LYS:N	2.49	0.45
3:E:173:LEU:HG	3:E:173:LEU:O	2.16	0.45
2:D:256:ASN:HB3	2:D:260:GLY:HA3	1.98	0.45
3:E:36:ASP:HB2	3:E:198:VAL:HG22	1.99	0.45
1:B:123:LEU:HB3	1:B:127:HIS:CD2	2.51	0.45
1:B:299:HIS:HD1	1:B:529:LEU:HD22	1.82	0.45
2:D:329:LEU:HB2	2:D:354:ALA:HB2	1.99	0.45
3:F:105:PHE:CG	3:F:143:MET:HE1	2.52	0.45
1:B:121:VAL:HG23	1:B:220:GLN:HE21	1.82	0.45
2:D:312:THR:HG21	2:D:390:CYS:HB3	1.99	0.45
1:A:168:HIS:HB2	1:B:104:ASN:OD1	2.17	0.45
2:C:220:ILE:HA	2:C:223:MET:HG3	1.99	0.45
3:E:174:ASP:OD1	3:E:174:ASP:N	2.49	0.45
1:A:154:MET:HB3	1:A:175:CYS:SG	2.57	0.44
1:A:460:ARG:NH1	3:E:92:MET:HG2	2.32	0.44
2:C:36:ILE:HD11	2:D:120:ALA:HA	1.99	0.44
2:C:54:LEU:O	2:C:71:LEU:N	2.43	0.44
2:C:256:ASN:HB3	2:C:260:GLY:HA3	1.98	0.44
2:D:349:LYS:HZ2	2:D:384:ARG:HE	1.64	0.44
2:D:9:ASP:HB3	2:D:15:LEU:HD21	1.98	0.44
3:F:121:ARG:HB3	3:F:156:VAL:HG21	1.99	0.44
1:A:325:CYS:O	1:A:329:ASP:HB2	2.17	0.44
1:B:295:LEU:O	1:B:328:TYR:OH	2.31	0.44
1:B:179:ILE:HG22	1:B:180:PHE:N	2.32	0.44
3:F:73:ALA:O	3:F:77:ALA:HB3	2.17	0.44
4:X:15:GLU:HA	4:X:89:ARG:HA	2.00	0.44
1:B:243:MET:HE2	1:B:243:MET:HB3	1.90	0.44
2:D:278:VAL:HG21	2:D:303:TYR:CE2	2.53	0.44
1:A:154:MET:HG2	1:A:175:CYS:HB2	1.99	0.44
1:A:333:LEU:HA	1:B:239:ARG:HH22	1.82	0.44
1:B:278:GLY:HA3	1:B:290:ASN:HA	2.00	0.44
1:B:477:VAL:HA	1:B:491:ARG:HH12	1.83	0.44
1:A:463:PHE:HE1	3:E:119:SER:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:NZ	1:B:319:GLU:OE1	2.42	0.44
1:B:414:ASP:OD1	1:B:414:ASP:C	2.60	0.44
3:E:53:THR:HB	3:E:82:ARG:HG2	2.00	0.44
4:X:24:PRO:HA	4:X:27:ALA:HB3	2.00	0.44
2:C:320:ARG:NH1	3:E:71:VAL:O	2.51	0.43
2:C:39:THR:OG1	2:C:215:TYR:OH	2.24	0.43
3:F:173:LEU:HD22	4:X:54:VAL:HG22	1.99	0.43
2:D:39:THR:OG1	2:D:215:TYR:OH	2.21	0.43
2:D:200:ILE:HG12	2:D:417:PHE:HB2	2.00	0.43
3:E:104:TYR:O	3:E:108:ILE:HG13	2.18	0.43
1:A:321:VAL:HG23	1:A:510:GLY:HA3	2.01	0.43
1:B:147:LEU:CD1	1:B:179:ILE:CD1	2.87	0.43
1:B:444:LEU:HB3	1:B:477:VAL:HG11	2.01	0.43
2:D:278:VAL:HG21	2:D:303:TYR:HE2	1.83	0.43
3:E:23:SER:OG	3:E:25:LYS:NZ	2.38	0.43
3:E:197:LYS:HE3	3:E:197:LYS:HB3	1.86	0.43
3:E:215:ILE:HG22	3:E:217:ARG:HG3	2.00	0.43
1:A:168:HIS:CE1	1:A:170:ALA:HB3	2.54	0.43
1:A:326:MET:HG2	1:A:549:PHE:CE2	2.53	0.43
1:B:200:LYS:HG3	1:B:201:MET:HG2	2.00	0.43
1:B:202:PHE:HB3	1:B:206:GLN:HB2	1.99	0.43
1:B:146:TYR:O	1:B:149:THR:OG1	2.33	0.43
2:D:154:LYS:HE2	2:D:158:TRP:CG	2.53	0.43
2:D:251:ASP:OD2	2:D:254:LYS:NZ	2.52	0.43
3:E:79:ALA:HB3	3:E:129:ARG:HH12	1.83	0.43
3:E:114:ASP:HB3	3:E:125:GLU:HB2	2.01	0.43
3:F:159:HIS:HA	3:F:169:MET:HE3	2.00	0.43
4:X:22:LEU:HB2	4:X:85:VAL:HG23	2.01	0.43
1:B:355:ILE:H	1:B:355:ILE:CD1	2.24	0.42
1:A:468:LEU:HD12	2:C:352:GLY:O	2.19	0.42
2:C:226:ALA:HB1	2:C:231:GLU:HA	2.00	0.42
2:C:346:ASP:HB3	2:C:349:LYS:HB2	2.01	0.42
2:D:300:TRP:CZ2	2:D:336:LEU:HD21	2.54	0.42
3:E:118:LEU:HD23	3:E:121:ARG:HB2	2.01	0.42
1:B:163:MET:H	1:B:163:MET:HE2	1.84	0.42
1:B:293:GLY:HA2	1:B:493:PRO:HB2	2.00	0.42
1:B:452:TYR:OH	3:F:240:ARG:NH2	2.53	0.42
2:C:38:ASP:HA	2:C:41:ARG:HG2	2.01	0.42
2:C:124:TYR:OH	2:C:177:SER:O	2.36	0.42
2:D:252:ILE:HG21	2:D:265:VAL:HG13	2.01	0.42
2:D:349:LYS:NZ	2:D:384:ARG:HE	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HB	1:A:253:TYR:CE2	2.55	0.42
1:B:154:MET:C	1:B:156:GLY:H	2.28	0.42
1:B:174:ASP:OD2	1:B:226:THR:OG1	2.26	0.42
1:B:198:VAL:HG12	1:B:207:ALA:CB	2.50	0.42
1:B:206:GLN:HA	1:B:522:ALA:HB2	2.01	0.42
3:E:90:ASP:OD1	3:E:102:ARG:NH1	2.53	0.42
1:B:140:PRO:O	1:B:144:ASN:ND2	2.53	0.42
2:C:222:GLU:HG3	2:D:126:SER:HB3	2.02	0.42
2:D:212:SER:O	2:D:216:GLU:HB2	2.20	0.42
2:C:313:PHE:HE1	2:C:393:ALA:HB1	1.85	0.42
2:D:326:SER:HB2	2:D:358:SER:HB3	2.01	0.42
3:F:28:LYS:HA	3:F:141:THR:HA	2.01	0.42
1:B:179:ILE:CG2	1:B:180:PHE:N	2.82	0.42
2:C:301:ASN:OD1	2:C:346:ASP:N	2.50	0.42
2:D:161:TYR:HB2	2:D:167:LEU:HA	2.02	0.42
1:A:472:SMC:HB2	2:C:349:LYS:HG2	2.02	0.42
1:A:313:PRO:HB2	1:A:435:LEU:HD22	2.02	0.42
3:E:100:TYR:HB3	3:E:104:TYR:CE2	2.55	0.42
1:B:455:LYS:HB2	1:B:461:LEU:HD22	2.02	0.42
1:A:102:TYR:HA	1:A:108:MET:HG3	2.01	0.41
1:B:181:THR:HG22	1:B:218:THR:HG23	2.02	0.41
2:D:31:ALA:O	2:D:35:ILE:HD12	2.20	0.41
4:X:25:GLU:O	4:X:29:LYS:NZ	2.45	0.41
1:A:167:THR:OG1	1:A:168:HIS:N	2.50	0.41
1:A:464:PHE:CE2	2:C:362:HIS:HB2	2.55	0.41
1:B:87:THR:HA	1:B:94:VAL:HA	2.02	0.41
2:C:296:ASP:HB3	2:C:299:MET:HB2	2.03	0.41
2:D:370:PRO:HB2	2:D:391:VAL:HG13	2.02	0.41
2:C:110:LEU:HD13	2:C:416:VAL:HB	2.01	0.41
2:D:59:MET:HE2	2:D:59:MET:HB3	1.86	0.41
3:E:100:TYR:HB3	3:E:104:TYR:HE2	1.85	0.41
1:A:402:ILE:HD11	1:A:454:HIS:HA	2.02	0.41
1:A:468:LEU:HD13	2:C:356:GLY:HA3	2.02	0.41
1:B:361:TYR:HA	1:B:364:VAL:HG12	2.03	0.41
3:E:139:MET:HE3	3:E:139:MET:HB3	1.82	0.41
1:A:117:ARG:NH1	1:A:174:ASP:O	2.43	0.41
1:A:513:GLN:O	1:A:517:SER:HB3	2.21	0.41
1:B:195:VAL:HG12	1:B:197:ASN:OD1	2.21	0.41
1:B:357:ASP:O	1:B:358:ASN:C	2.63	0.41
2:D:217:GLN:HG3	2:D:238:LEU:HB2	2.02	0.41
1:A:440:ALA:HB1	1:A:488:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:GLY:O	2:C:160:SER:OG	2.38	0.41
4:X:44:MET:O	4:X:89:ARG:N	2.48	0.41
1:A:431:VAL:O	1:A:435:LEU:HG	2.20	0.41
2:D:3:ASP:OD1	2:D:232:ARG:NH1	2.46	0.41
2:D:335:ILE:HG21	3:F:108:ILE:HD11	2.02	0.41
3:E:87:GLN:HG3	3:E:152:ARG:O	2.21	0.41
3:F:60:MET:HE2	3:F:60:MET:HB3	1.74	0.41
1:B:80:GLN:HG2	4:X:45:VAL:HG13	2.02	0.41
2:D:71:LEU:HD23	2:D:143:PHE:CE2	2.55	0.41
1:A:530:LYS:HE2	1:A:530:LYS:HB2	1.93	0.40
4:X:87:ARG:HH22	4:X:89:ARG:HH21	1.69	0.40
1:A:172:VAL:HG12	1:A:175:CYS:SG	2.61	0.40
1:A:328:TYR:O	1:A:332:TRP:HB3	2.21	0.40
1:B:147:LEU:CD2	1:B:179:ILE:HD12	2.48	0.40
3:E:86:VAL:HG23	3:E:151:MET:HE3	2.03	0.40
3:F:245:PHE:CD2	3:F:246:GLN:HG2	2.56	0.40
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.87	0.40
2:C:75:LEU:HD23	2:C:143:PHE:HE2	1.87	0.40
2:C:210:ALA:O	2:C:214:ILE:HG12	2.21	0.40
4:X:17:PHE:CD2	4:X:87:ARG:HG2	2.56	0.40
1:B:439:ASN:ND2	2:C:148:TYR:HB3	2.35	0.40
3:E:145:ASP:HB3	3:E:148:LEU:HB2	2.03	0.40
3:F:186:ASP:OD1	3:F:186:ASP:N	2.54	0.40
1:A:116:ARG:O	1:A:290:ASN:ND2	2.55	0.40
2:C:32:ILE:HG23	2:C:214:ILE:HG23	2.03	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	452/570 (79%)	427 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	477/570 (84%)	449 (94%)	28 (6%)	0	100	100
2	C	430/434 (99%)	411 (96%)	19 (4%)	0	100	100
2	D	429/434 (99%)	411 (96%)	18 (4%)	0	100	100
3	E	245/248 (99%)	234 (96%)	11 (4%)	0	100	100
3	F	245/248 (99%)	232 (95%)	13 (5%)	0	100	100
4	X	118/193 (61%)	110 (93%)	8 (7%)	0	100	100
All	All	2396/2697 (89%)	2274 (95%)	122 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	356/442 (80%)	355 (100%)	1 (0%)	86	87
1	B	376/442 (85%)	374 (100%)	2 (0%)	81	85
2	C	325/327 (99%)	325 (100%)	0	100	100
2	D	325/327 (99%)	325 (100%)	0	100	100
3	E	199/200 (100%)	197 (99%)	2 (1%)	68	79
3	F	199/200 (100%)	199 (100%)	0	100	100
4	X	109/171 (64%)	108 (99%)	1 (1%)	70	80
All	All	1889/2109 (90%)	1883 (100%)	6 (0%)	84	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	PHE
1	B	162	GLU
1	B	408	PHE
3	E	122	GLN
3	E	173	LEU

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Mol	Chain	Res	Type
4	X	46	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	220	GLN
1	A	330	GLN
1	A	372	ASN
1	A	476	ASN
1	A	526	ASN
1	B	109	GLN
1	B	161	GLN
1	B	220	GLN
1	B	345	GLN
1	B	476	ASN
1	B	481	GLN
2	C	180	GLN
2	C	295	ASN
2	C	315	ASN
2	C	324	ASN
2	D	29	ASN
2	D	137	GLN
2	D	173	GLN
2	D	182	ASN
2	D	246	ASN
2	D	315	ASN
3	E	122	GLN
3	F	54	HIS
3	F	87	GLN
3	F	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MHS	B	271	1	10,11,12	1.66	2 (20%)	5,14,16	1.04	1 (20%)
1	SMC	B	472	1	5,6,7	1.14	1 (20%)	3,6,8	1.65	1 (33%)
1	AGM	A	285	1	10,11,12	1.28	1 (10%)	7,13,15	1.27	0
1	SMC	A	472	1	5,6,7	1.26	1 (20%)	3,6,8	1.83	1 (33%)
1	AGM	B	285	1	10,11,12	1.44	1 (10%)	7,13,15	2.69	3 (42%)
1	MHS	A	271	1	10,11,12	1.79	2 (20%)	5,14,16	2.01	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	B	271	1	-	0/5/6/8	0/1/1/1
1	SMC	B	472	1	-	1/3/5/7	-
1	AGM	A	285	1	-	4/10/11/13	-
1	SMC	A	472	1	-	3/3/5/7	-
1	AGM	B	285	1	-	6/10/11/13	-
1	MHS	A	271	1	-	2/5/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	MHS	CD2-CG	3.51	1.41	1.36
1	B	271	MHS	CD2-CG	3.48	1.41	1.36
1	B	285	AGM	CZ-NE1	3.28	1.38	1.33
1	A	285	AGM	CZ-NE1	2.97	1.38	1.33
1	A	271	MHS	CG-ND1	2.64	1.42	1.38
1	A	472	SMC	CB-SG	-2.30	1.75	1.81
1	B	472	SMC	CB-SG	-2.08	1.76	1.81
1	B	271	MHS	CM-ND1	-2.02	1.42	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	AGM	CD-NE1-CZ	5.14	133.16	123.59
1	B	285	AGM	NE1-CZ-NH2	3.58	126.72	120.58
1	A	271	MHS	CM-ND1-CG	3.42	130.34	126.69
1	B	285	AGM	CG-CD-NE1	2.73	115.10	110.42
1	B	472	SMC	CB-CA-C	-2.55	103.87	110.80
1	A	472	SMC	CA-CB-SG	-2.45	110.07	114.04
1	A	271	MHS	ND1-CE1-NE2	-2.31	111.57	112.94
1	B	271	MHS	ND1-CE1-NE2	-2.12	111.68	112.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	271	MHS	N-CA-CB-CG
1	A	285	AGM	CE2-CD-CG-CB
1	A	472	SMC	N-CA-CB-SG
1	A	472	SMC	C-CA-CB-SG
1	B	285	AGM	N-CA-CB-CG
1	B	285	AGM	C-CA-CB-CG
1	B	285	AGM	CE2-CD-CG-CB
1	B	285	AGM	NE1-CD-CG-CB
1	B	285	AGM	CG-CD-NE1-CZ
1	B	285	AGM	CE2-CD-NE1-CZ
1	A	285	AGM	NE1-CD-CG-CB
1	A	271	MHS	C-CA-CB-CG
1	A	285	AGM	CA-CB-CG-CD
1	A	472	SMC	CA-CB-SG-CS
1	B	472	SMC	CA-CB-SG-CS
1	A	285	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	AGM	2	0
1	A	472	SMC	2	0
1	B	285	AGM	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

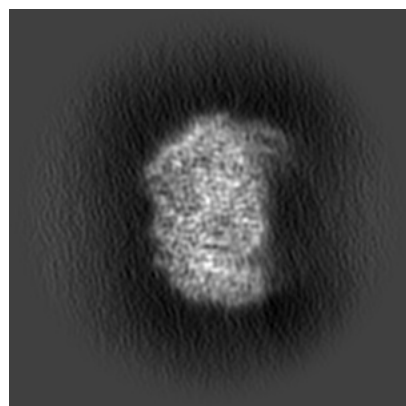
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29979. These allow visual inspection of the internal detail of the map and identification of artifacts.

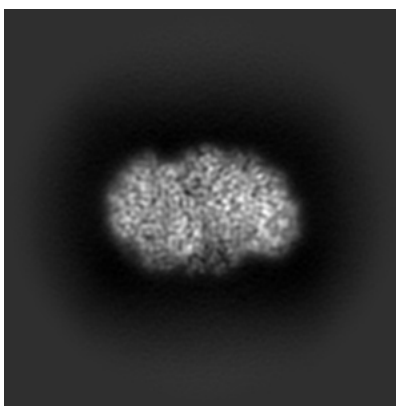
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

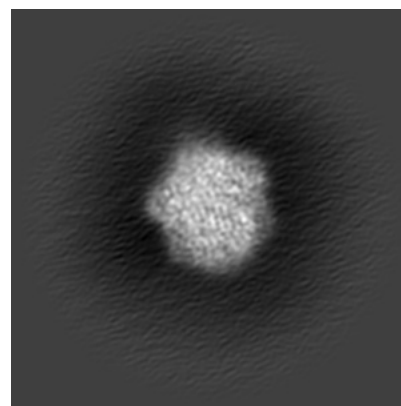
6.1.1 Primary map



X

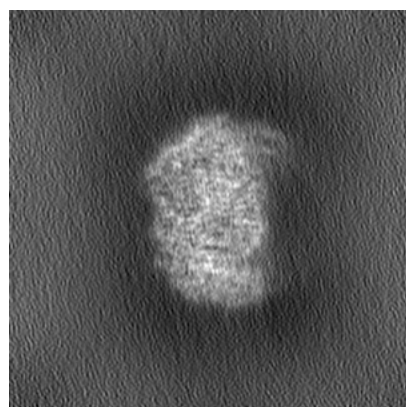


Y

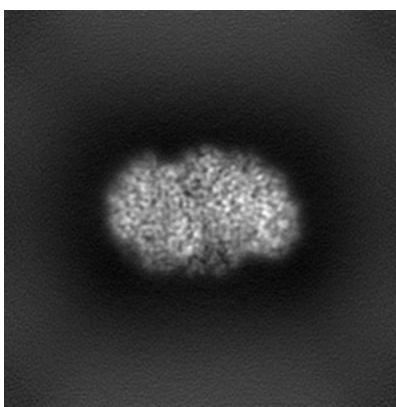


Z

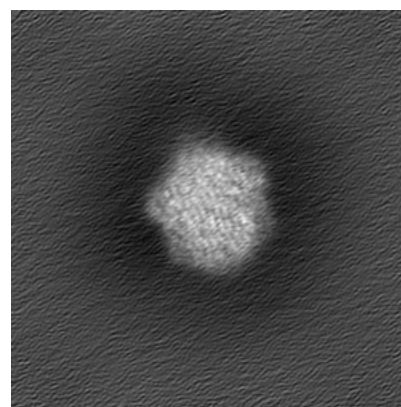
6.1.2 Raw map



X



Y

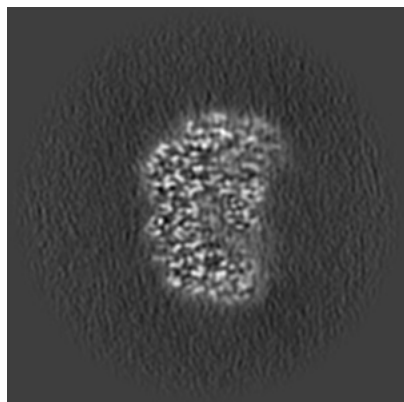


Z

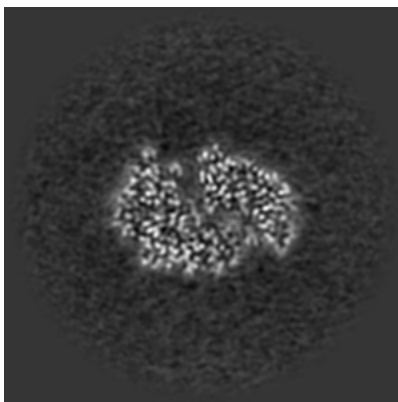
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

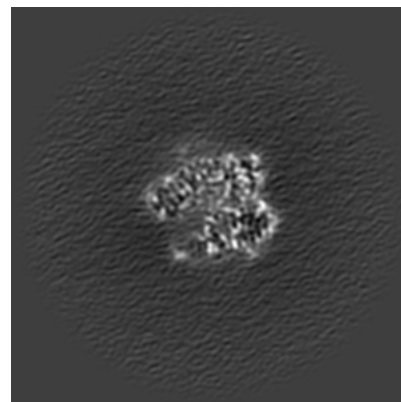
6.2.1 Primary map



X Index: 112

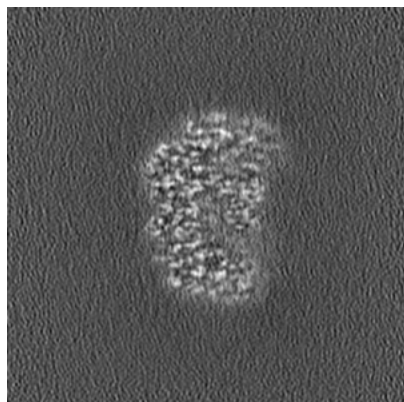


Y Index: 112

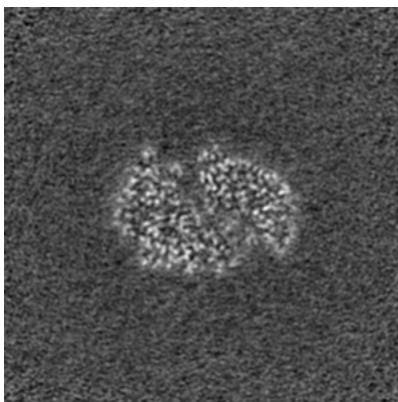


Z Index: 112

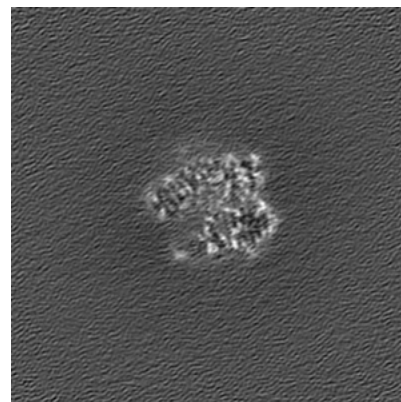
6.2.2 Raw map



X Index: 112



Y Index: 112

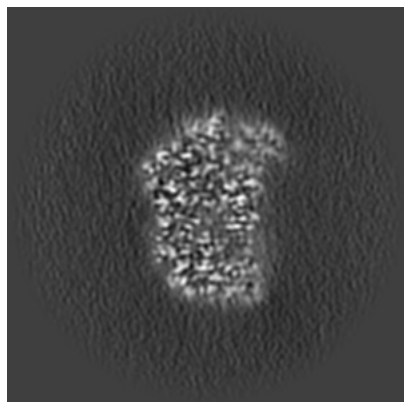


Z Index: 112

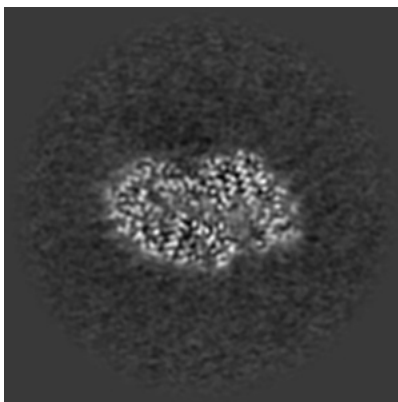
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

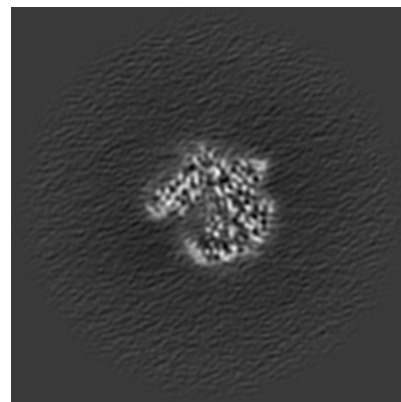
6.3.1 Primary map



X Index: 115

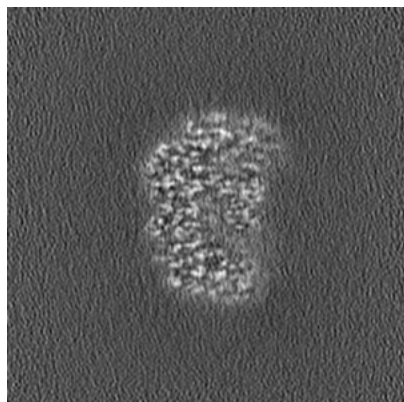


Y Index: 122

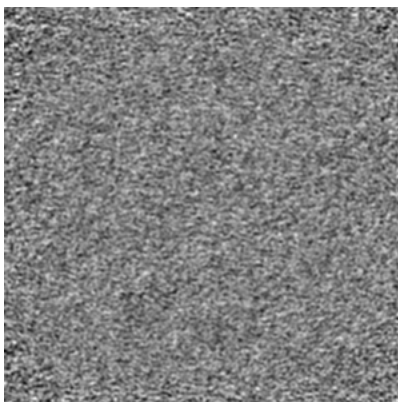


Z Index: 117

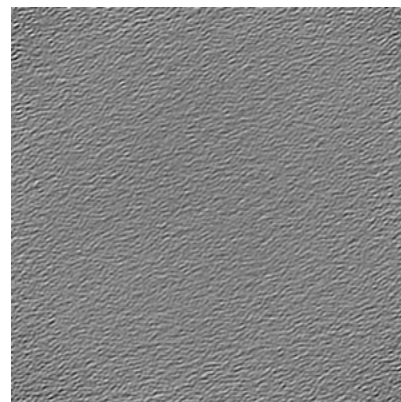
6.3.2 Raw map



X Index: 112



Y Index: 0

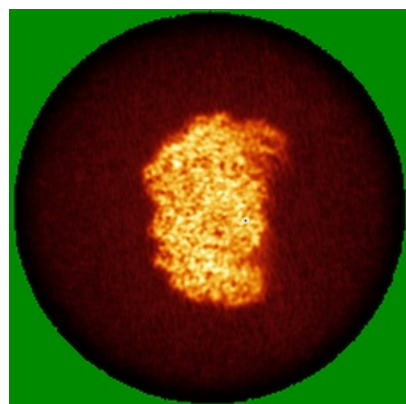


Z Index: 0

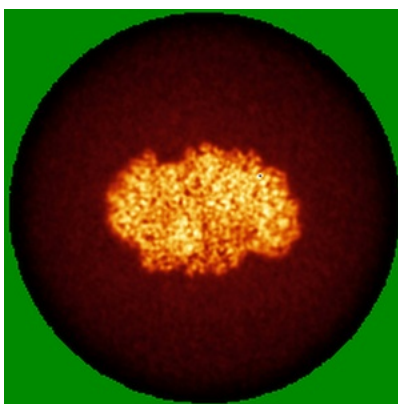
The images above show the largest variance slices of the map in three orthogonal directions.

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

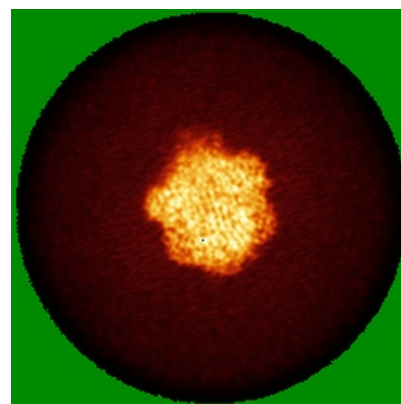
6.4.1 Primary map



X

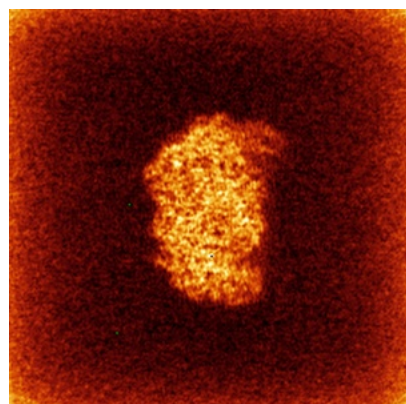


Y

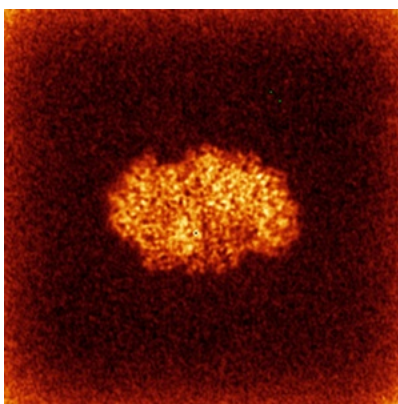


Z

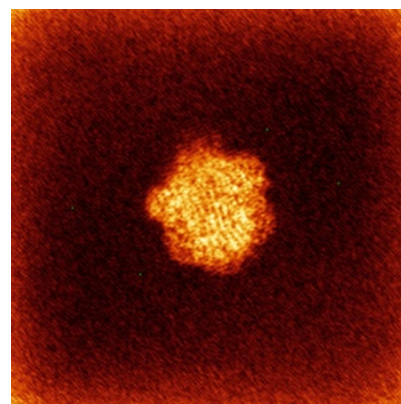
6.4.2 Raw map



X



Y

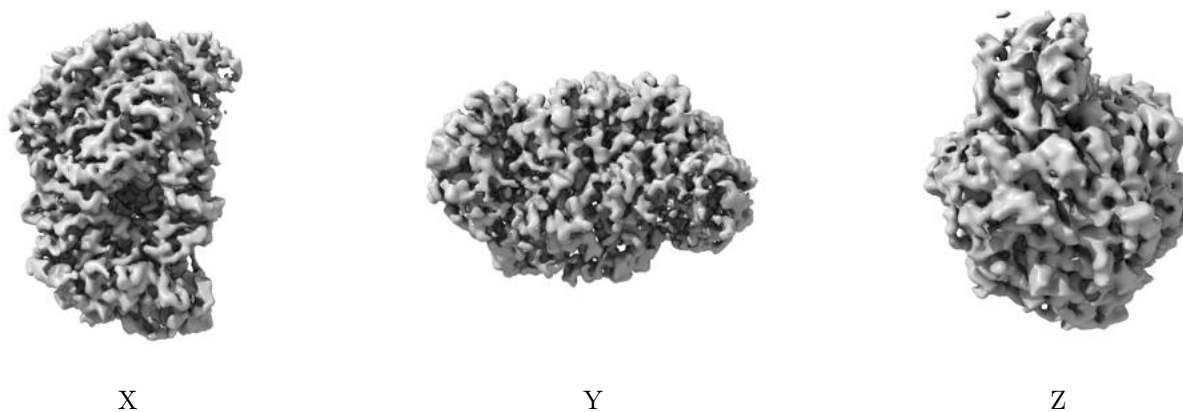


Z

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

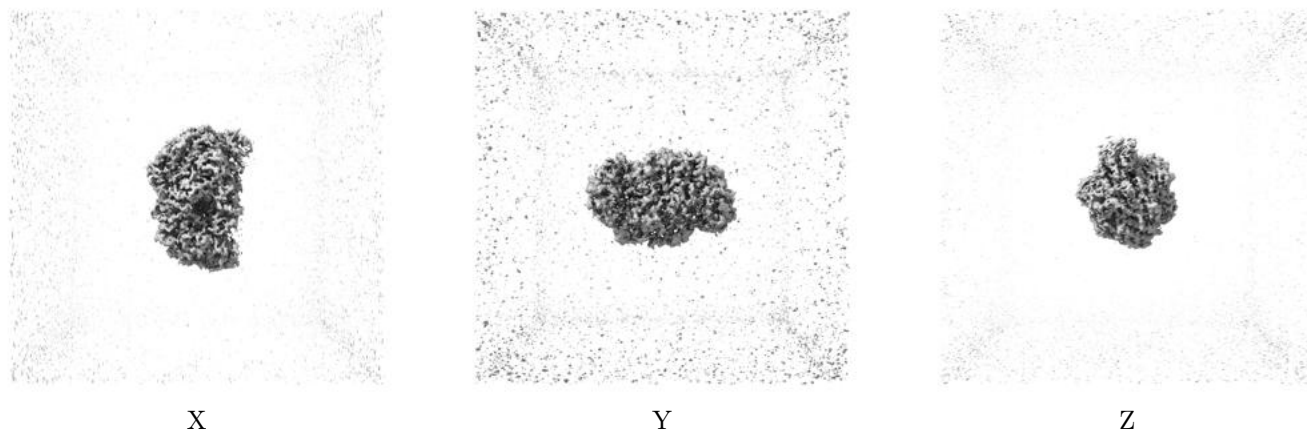
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

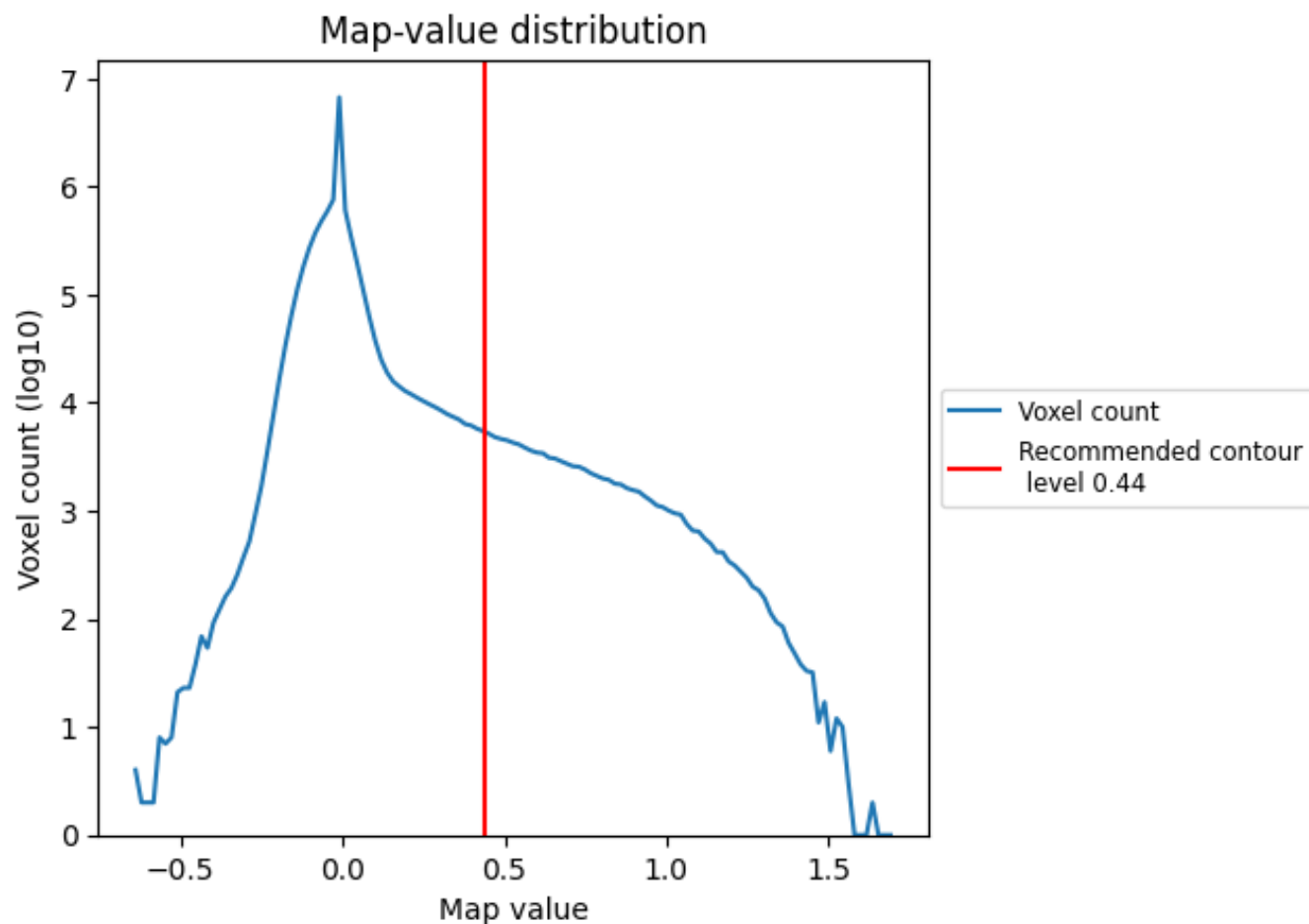
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

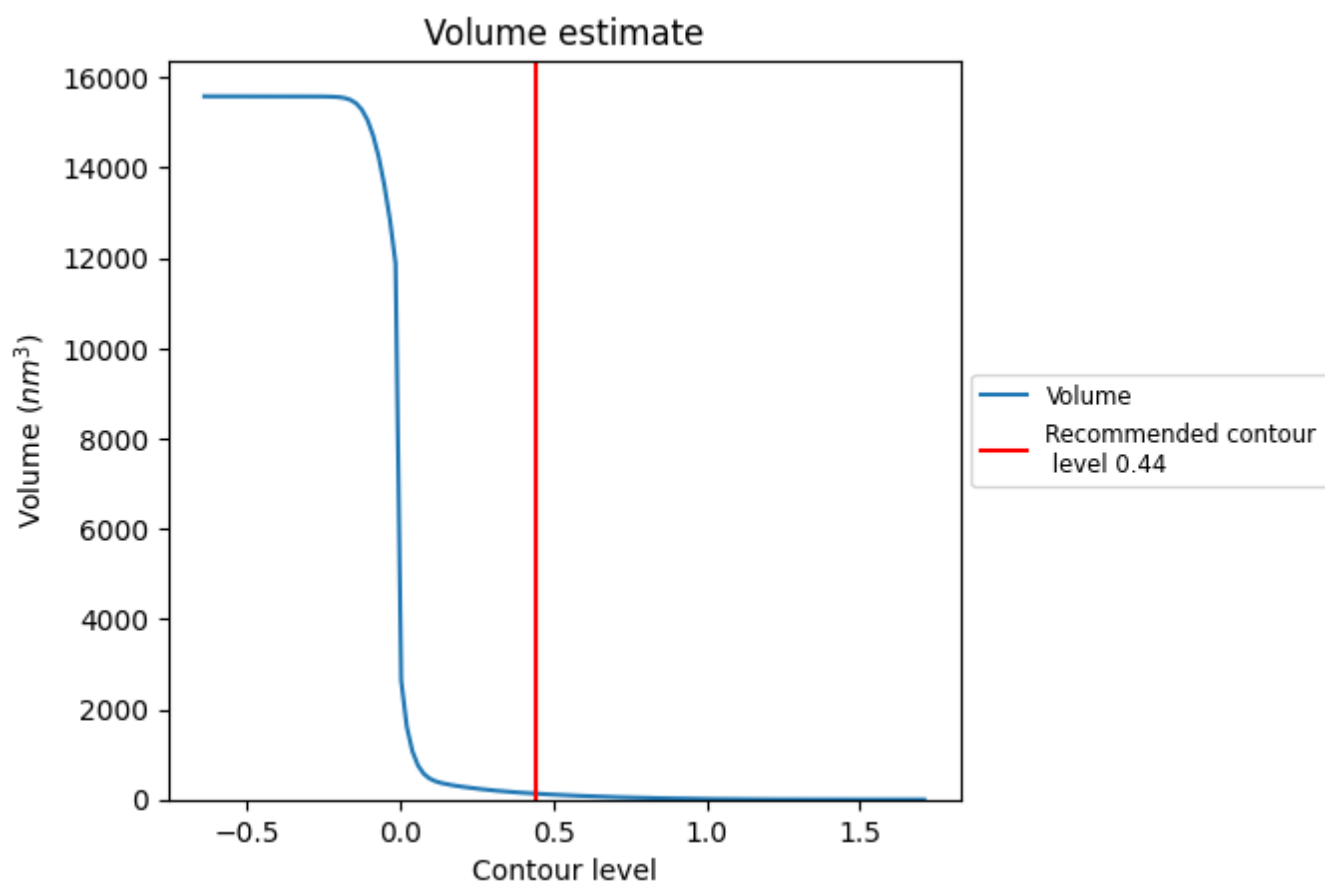
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

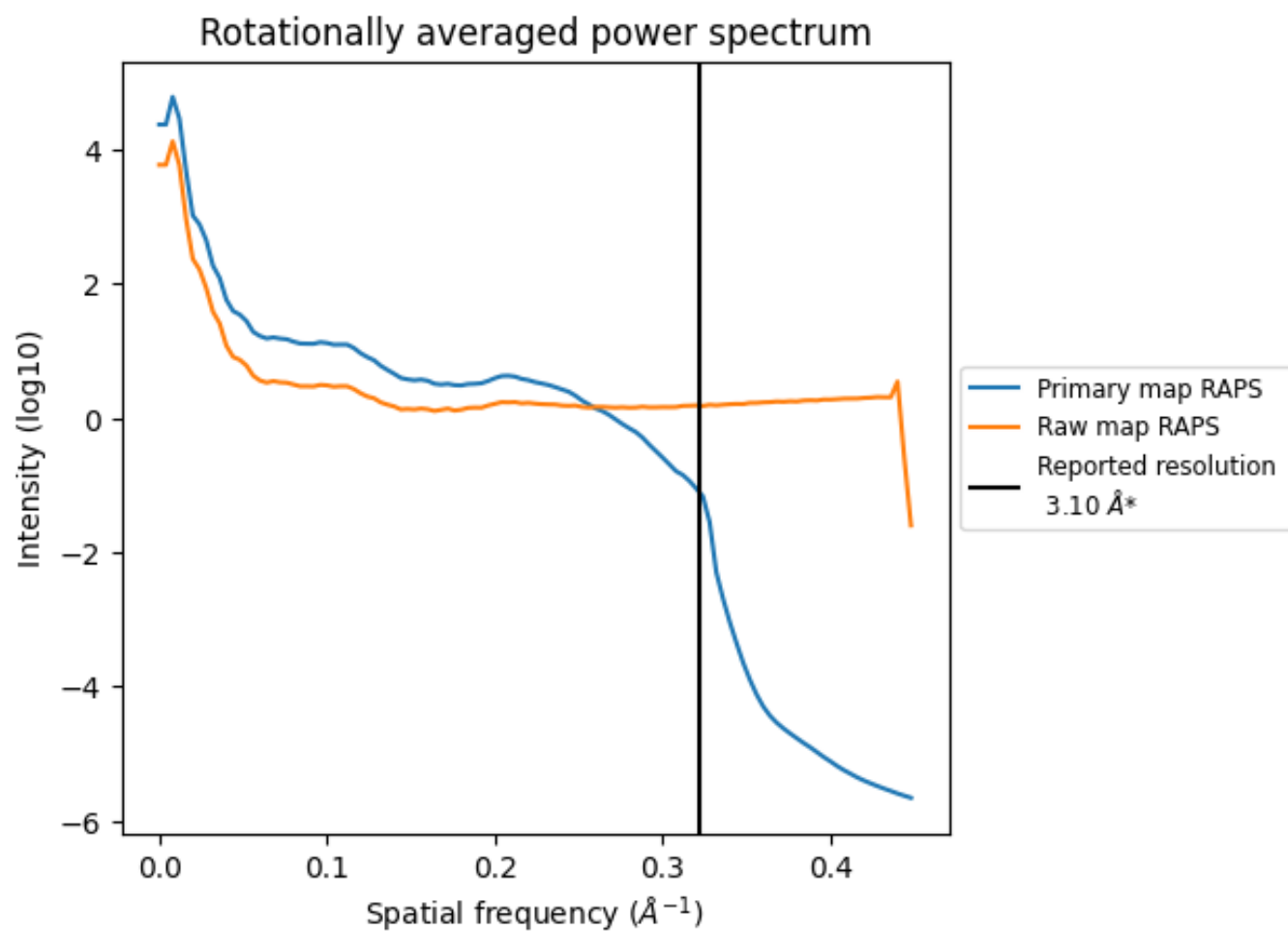
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 ⓘ

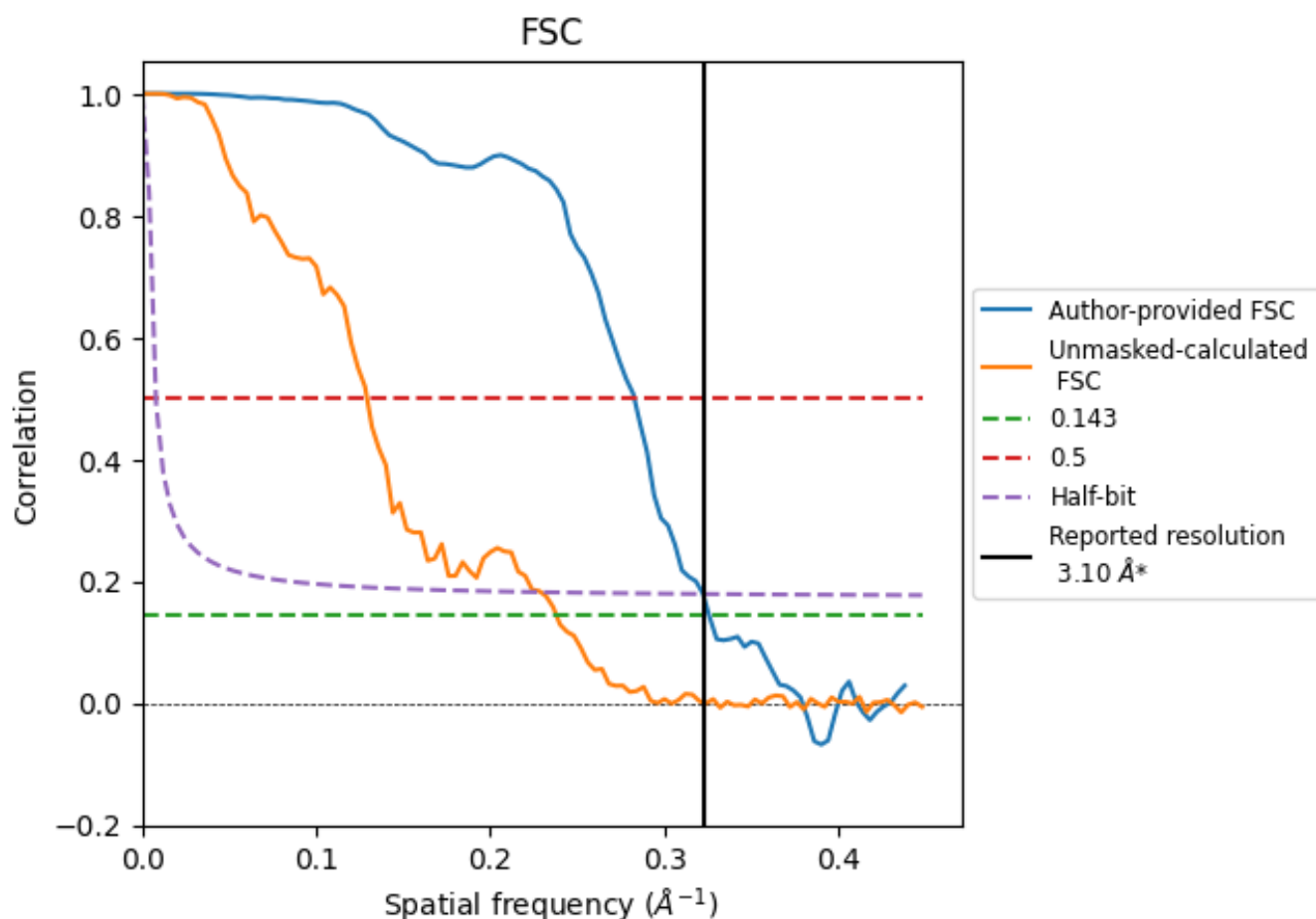


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

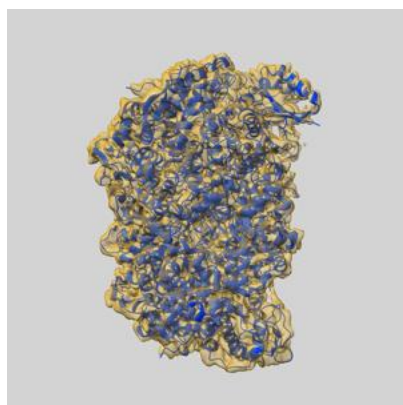
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.53	3.10
Unmasked-calculated*	4.20	7.73	4.36

*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 4.20 differs from the reported value 3.1 by more than 10 %

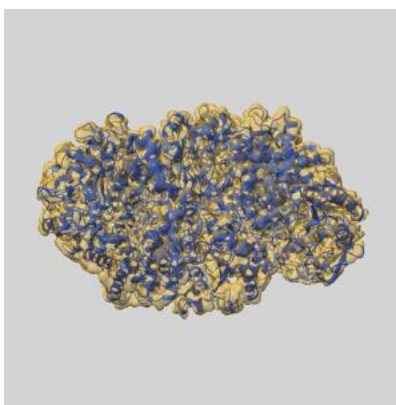
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29979 and PDB model 8GF6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

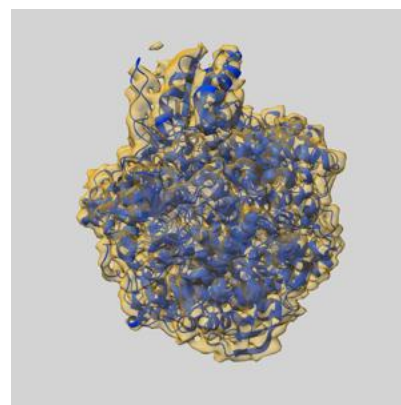
9.1 Map-model overlay [i](#)



X



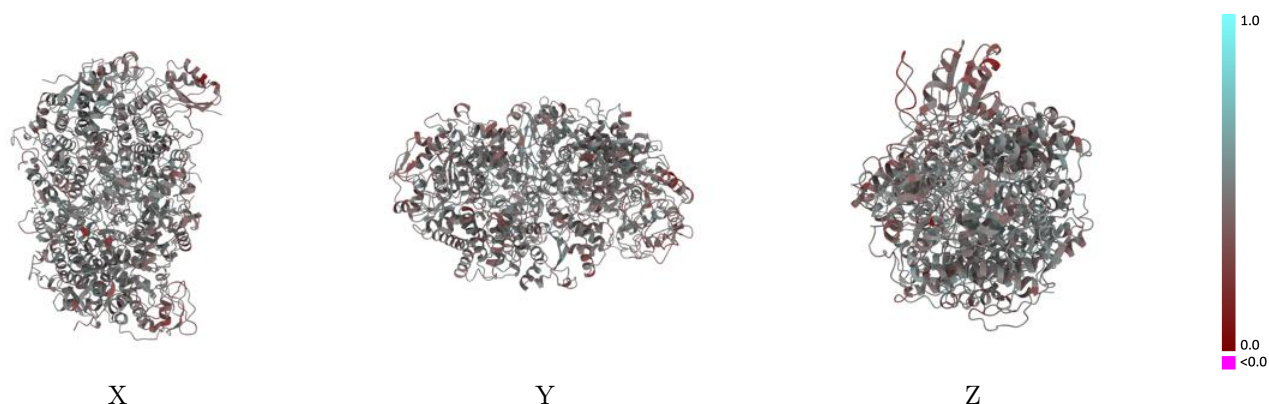
Y



Z

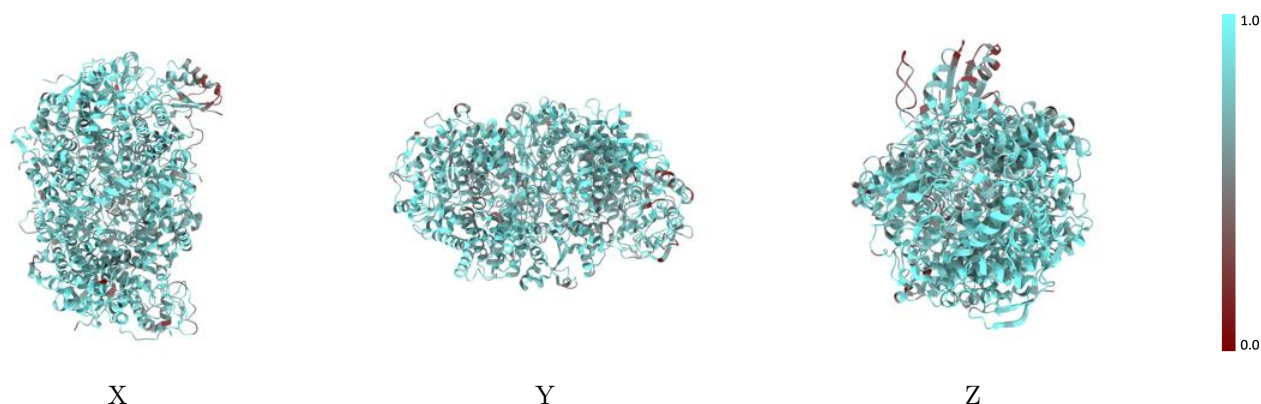
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



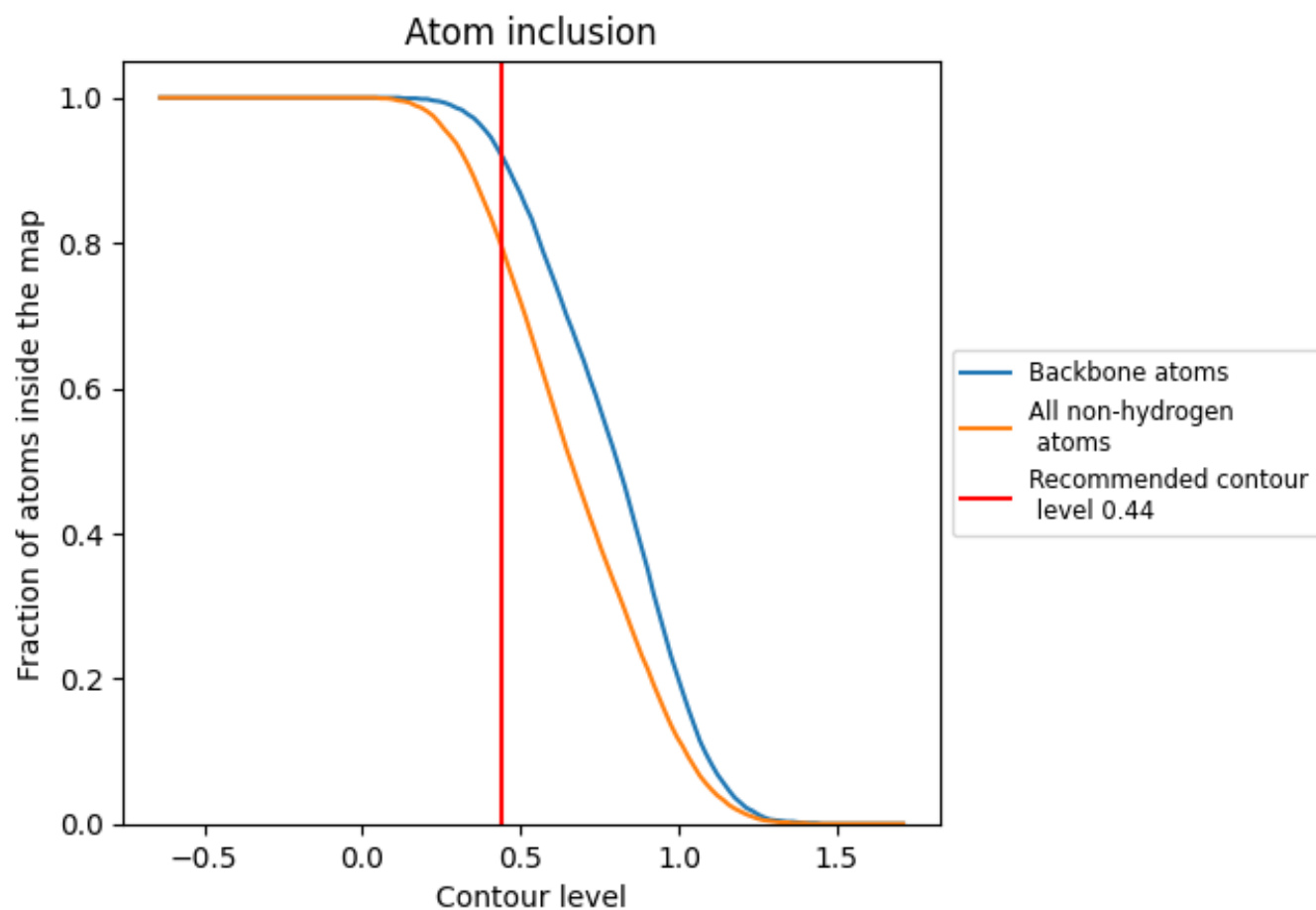
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.44).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 80% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.4550
A	0.7780	0.4460
B	0.7940	0.4610
C	0.8200	0.4760
D	0.8120	0.4700
E	0.8000	0.4370
F	0.8500	0.4570
X	0.6060	0.3800

1.0

0.0

<0.0