



Full wwPDB EM Validation Report ⓘ

Mar 2, 2025 – 04:37 PM EST

PDB ID : 8UB9
EMDB ID : EMD-42079
Title : Diversity-generating retroelement (DGR) ribonucleoprotein reverse transcriptase- Active state (N-empty) 1a
Authors : Biswas, T.; Handa, S.; Ghosh, P.
Deposited on : 2023-09-22
Resolution : 3.07 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

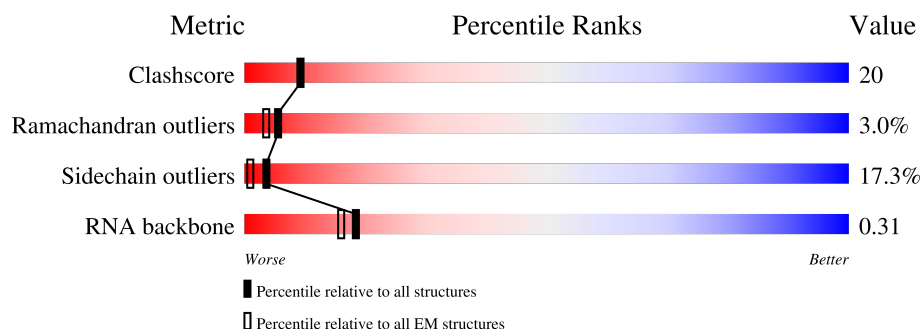
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	328	
2	B	290	
2	C	290	
2	D	290	
2	E	290	
2	F	290	
3	G	19	

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Mol	Chain	Length	Quality of chain
4	H	36	<div><div></div><div>6%</div><div>17%</div><div>14%</div><div>6%</div><div>64%</div></div>
5	I	140	<div><div></div><div>8%</div><div>26%</div><div>39%</div><div>22%</div><div>•</div><div>13%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10370 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2690	1723	495	463	9		

- Molecule 2 is a protein called Avd.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	122	Total	C	N	O	S	0	0
			976	631	172	166	7		
2	C	111	Total	C	N	O	S	0	0
			888	578	157	148	5		
2	D	111	Total	C	N	O	S	0	0
			888	577	161	145	5		
2	E	110	Total	C	N	O	S	0	0
			876	569	156	146	5		
2	F	111	Total	C	N	O	S	0	0
			888	577	161	145	5		

- Molecule 3 is a RNA chain called Diversity-generating retroelement (DGR) RNA avd.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	13	Total	C	N	O	P	0	0
			289	127	58	91	13		

- Molecule 4 is a RNA chain called Diversity-generating retroelement (DGR) RNA TR.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	13	Total	C	N	O	P	0	0
			270	121	44	92	13		

- Molecule 5 is a RNA chain called Diversity-generating retroelement (DGR) RNA Sp.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	122	2605	1161	464	858	122	0	0

LYS
ALA
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VAL
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THR
GLU
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LYS
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HIS
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PHE
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ALA
ASN
ALA

• Molecule 2: Avd

Chain C: 20% 15% 62%

MET
GLU
PRO
ILE
GLU
GLU
ALA
THR
LYS
CYS
Y11
D12
I16
V17
E21
I24
S25
Y26
I30
A31
I34
P35
R36
K37
H38
G39
V40
A41
R42
E43
M44
F45
L46
V53
F56
I57
V58
A59
R63
Q64
K67
L68
Y69
A70
A71
D72
A73
R79
F80
S81

L82
R83
F84
L85
A86
G87
I88
Q89
R90
P91
H92
A93
R94
T95
V99
E100
V104
L105
I106
I112
I117
V120
ARG
LYS
GLU
THR
LYS
VAL
GLN
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• Molecule 2: Avd

Chain D: 19% 18% 62%

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GLU
GLU
ALA
THR
LYS
CYS
ASP
Q13
M14
L15
I16
V17
E18
E21
I24
L27
Y28
P29
I30
A31
R36
K37
H38
R42
E43
M44
F45
L50
G51
Q52
V53
E54
L55
S62
N63
Q64
V65
L68
L75
A76
F80
W81
L82
L85

A86
G87
I88
Q89
K90
P91
H92
A93
N94
Q98
V99
E100
T101
A102
Q103
V104
L105
I106
V109
L113
W116
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A118
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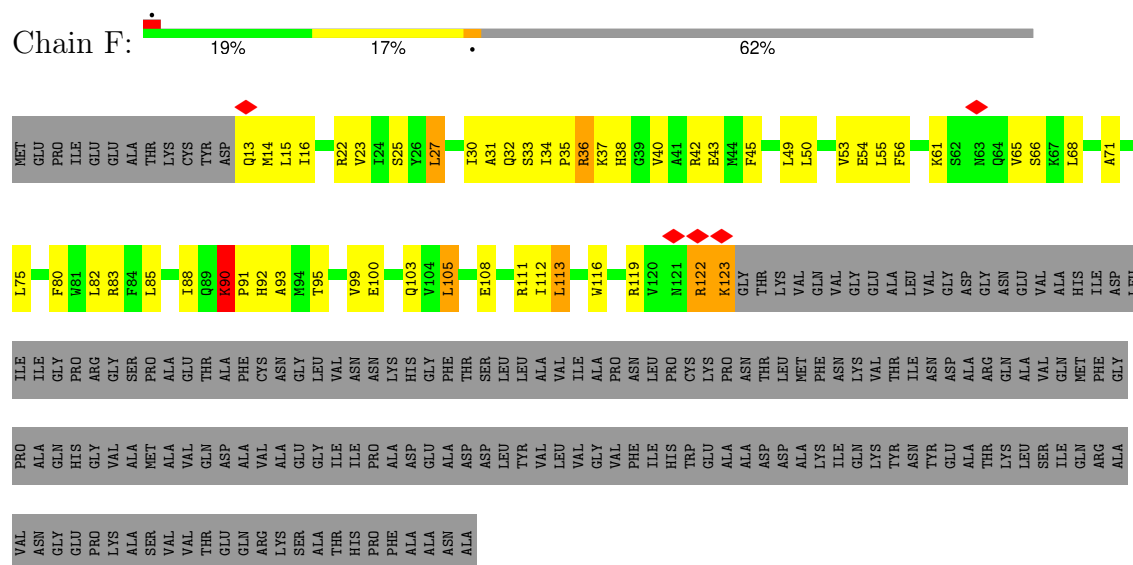
• Molecule 2: Avd

Chain E: 19% 17% 62%

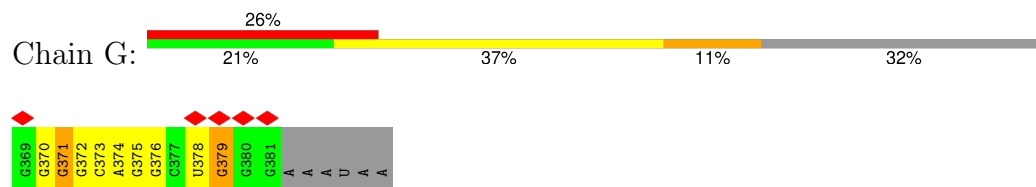
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Y20
E21
I24
S25
Y26
A31
I34
P35
R36
K37
V40
A41
R42
E43
M44
F45
L46
L50
G51
Q52
V53
E54
L55
G60
K61
S62
N63
Q64
V65
S66
K67
L68
L75
A76
M77

F80
W81
L82
R83
F84
L85
A86
G87
I88
Q89
K90
P91
H92
A93
M94
T95
P96
H97
Q98
V99
E100
T101
V104
L105
I106
V109
G110
R111
I112
L113
W116
R119
V120
N121
ARG
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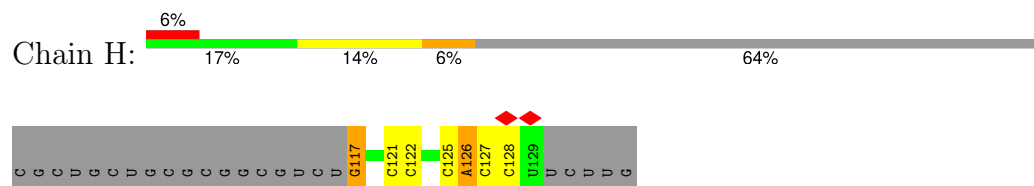
- Molecule 2: Avd



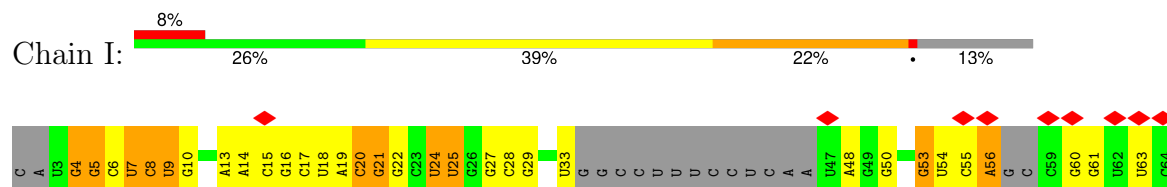
- Molecule 3: Diversity-generating retroelement (DGR) RNA and

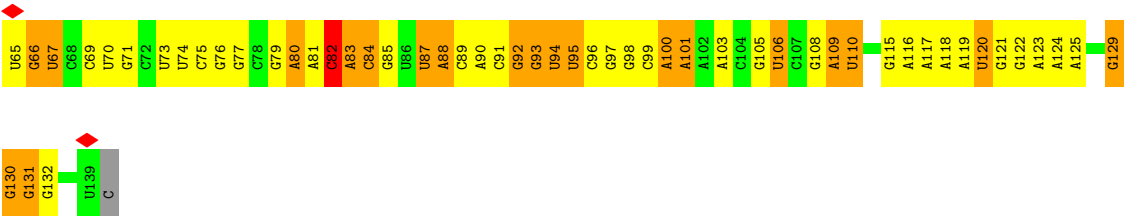


- Molecule 4: Diversity-generating retroelement (DGR) RNA TR



- Molecule 5: Diversity-generating retroelement (DGR) RNA Sp





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.605	Depositor
Minimum map value	-0.927	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.52	0/2761	0.72	0/3731
2	B	0.54	0/996	0.63	0/1345
2	C	0.54	0/907	0.74	1/1226 (0.1%)
2	D	0.53	0/906	0.64	0/1222
2	E	0.53	0/894	0.63	0/1208
2	F	0.54	0/906	0.64	0/1222
3	G	0.94	2/324 (0.6%)	0.81	0/506
4	H	0.62	0/299	0.97	1/462 (0.2%)
5	I	0.69	0/2909	1.08	4/4529 (0.1%)
All	All	0.59	2/10902 (0.0%)	0.83	6/15451 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	378	U	O3'-P	-12.73	1.45	1.61
3	G	371	G	O3'-P	6.35	1.68	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	67	U	P-O3'-C3'	-10.14	107.53	119.70
5	I	24	U	P-O3'-C3'	-10.02	107.68	119.70
2	C	91	PRO	N-CA-CB	-7.74	94.01	103.30
5	I	82	C	P-O3'-C3'	-6.00	112.50	119.70
4	H	117	G	P-O3'-C3'	-5.50	113.10	119.70
5	I	25	U	P-O3'-C3'	-5.31	113.33	119.70

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	2690	0	2686	147	0
2	B	976	0	1014	58	0
2	C	888	0	923	55	0
2	D	888	0	936	40	0
2	E	876	0	914	42	0
2	F	888	0	936	38	0
3	G	289	0	143	7	0
4	H	270	0	141	7	0
5	I	2605	0	1317	85	0
All	All	10370	0	9010	379	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 20.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:LYS:HE2	2:C:90:LYS:H	1.30	0.96
2:E:86:ALA:HB2	2:E:99:VAL:HG21	1.57	0.83
5:I:92:G:H3'	5:I:93:G:H4'	1.61	0.83
1:A:168:LEU:HD22	1:A:189:PHE:HZ	1.46	0.80
5:I:82:C:H1'	5:I:84:C:C4	2.17	0.80
1:A:4:ARG:O	1:A:160:HIS:HB2	1.82	0.79
5:I:80:A:N7	5:I:81:A:N6	2.30	0.79
1:A:6:ARG:NH1	5:I:122:G:N7	2.32	0.78
1:A:147:ASP:HB2	1:A:193:TYR:OH	1.83	0.78
2:D:75:LEU:HD22	2:D:106:ILE:HG23	1.64	0.77
2:C:38:HIS:CE1	2:C:90:LYS:HB2	2.21	0.76
1:A:163:ALA:HB2	5:I:120:U:O4	1.85	0.76
2:C:25:SER:HA	2:D:88:ILE:HG23	1.68	0.76
2:C:35:PRO:HG2	2:C:91:PRO:HB3	1.67	0.75
2:F:23:VAL:HG22	2:F:105:LEU:HB3	1.69	0.74
1:A:279:ARG:HH12	5:I:54:U:H5'	1.53	0.73
2:D:16:ILE:HG12	2:D:109:VAL:HG23	1.69	0.73
1:A:315:LEU:HD12	5:I:83:A:C4	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:75:LEU:HD21	2:E:109:VAL:HG23	1.70	0.72
1:A:36:LEU:HB3	2:B:14:MET:HB3	1.72	0.71
1:A:159:ILE:O	1:A:161:CYS:N	2.25	0.70
1:A:302:SER:CB	5:I:53:G:H1'	2.21	0.70
2:E:53:VAL:HG21	2:F:80:PHE:CZ	2.26	0.69
2:F:32:GLN:O	5:I:4:G:N2	2.24	0.69
4:H:126:A:H61	5:I:48:A:H61	1.40	0.69
2:B:53:VAL:HG21	2:C:80:PHE:CZ	2.27	0.69
1:A:11:GLN:HB2	1:A:93:ILE:HG12	1.72	0.68
2:B:43:GLU:HA	2:C:40:VAL:HG21	1.74	0.68
2:B:86:ALA:HB2	2:B:99:VAL:HG21	1.75	0.68
2:E:13:GLN:HB3	2:E:60:GLY:HA3	1.74	0.68
2:E:98:GLN:NE2	5:I:17:C:O3'	2.27	0.67
5:I:108:G:H3'	5:I:109:A:H5''	1.75	0.67
1:A:213:TYR:CD1	1:A:261:LEU:HD21	2.29	0.67
2:C:90:LYS:O	2:C:91:PRO:C	2.34	0.66
1:A:146:ILE:HG12	1:A:193:TYR:CD2	2.30	0.66
2:C:82:LEU:HD22	2:C:94:MET:SD	2.36	0.66
1:A:140:SER:HA	1:A:247:SER:HB3	1.77	0.66
1:A:262:GLY:HA2	1:A:273:ARG:HE	1.61	0.66
1:A:264:ARG:N	1:A:271:LEU:O	2.25	0.66
1:A:205:LEU:HD21	1:A:233:ARG:HG2	1.77	0.65
5:I:82:C:H4'	5:I:83:A:OP1	1.96	0.65
3:G:373:C:H1'	5:I:82:C:OP1	1.97	0.65
1:A:115:THR:HG23	1:A:261:LEU:HD22	1.79	0.64
2:F:75:LEU:HD12	2:F:113:LEU:HD12	1.79	0.64
1:A:274:LYS:HE2	5:I:81:A:C2	2.32	0.64
1:A:313:HIS:HB3	5:I:88:A:H5'	1.79	0.63
4:H:126:A:H61	5:I:48:A:N6	1.95	0.63
1:A:258:ILE:HG22	1:A:260:PHE:HB2	1.81	0.62
2:E:53:VAL:HG11	2:F:80:PHE:CG	2.35	0.62
2:B:34:ILE:O	2:B:42:ARG:NH1	2.33	0.61
1:A:124:ALA:HB1	1:A:128:ARG:HH11	1.64	0.61
1:A:200:LEU:HD13	1:A:237:PHE:CD1	2.36	0.61
5:I:70:U:H4'	5:I:71:G:C8	2.35	0.61
1:A:104:PRO:HG3	5:I:130:G:H4'	1.83	0.61
2:E:53:VAL:HG11	2:F:80:PHE:CD1	2.35	0.61
2:C:93:ALA:O	2:C:94:MET:C	2.38	0.61
2:B:50:LEU:HD21	2:C:84:PHE:CE1	2.36	0.61
1:A:213:TYR:CG	1:A:261:LEU:HD21	2.36	0.60
5:I:80:A:C4	5:I:81:A:N7	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:O	5:I:105:G:H4'	2.02	0.60
1:A:279:ARG:NH1	5:I:54:U:H5'	2.17	0.60
1:A:168:LEU:HD22	1:A:189:PHE:CZ	2.32	0.60
1:A:18:LEU:HD13	1:A:50:GLN:HB2	1.83	0.60
2:B:40:VAL:HG23	5:I:4:G:N7	2.17	0.59
2:C:17:VAL:O	2:C:21:GLU:HG2	2.02	0.59
1:A:53:LEU:HD23	1:A:58:TYR:HB2	1.85	0.59
1:A:179:ILE:HG23	1:A:186:SER:HB3	1.83	0.59
2:C:91:PRO:O	2:C:92:HIS:HB2	2.01	0.59
2:D:27:LEU:HD23	2:D:30:ILE:HD12	1.85	0.59
2:F:35:PRO:HG3	2:F:92:HIS:CG	2.38	0.59
1:A:79:LEU:HB3	1:A:83:ASP:HB2	1.84	0.58
2:F:36:ARG:HB2	5:I:5:G:OP1	2.04	0.58
1:A:115:THR:HA	1:A:261:LEU:HD13	1.85	0.58
2:B:53:VAL:HG11	2:C:80:PHE:CG	2.38	0.58
2:B:31:ALA:HB2	2:B:45:PHE:CE2	2.38	0.58
1:A:196:ALA:HB3	1:A:242:LEU:HD11	1.86	0.57
1:A:277:VAL:HG13	1:A:315:LEU:HD11	1.84	0.57
5:I:100:A:O2'	5:I:101:A:OP2	2.19	0.57
1:A:128:ARG:NH1	5:I:95:U:OP1	2.36	0.57
2:B:28:TYR:CE1	2:B:50:LEU:HD11	2.40	0.57
1:A:265:ILE:HG12	1:A:270:LYS:HG3	1.86	0.57
2:C:87:GLY:O	2:C:88:ILE:C	2.42	0.57
2:B:53:VAL:HG11	2:C:80:PHE:CD1	2.40	0.57
1:A:41:TYR:CZ	2:C:79:ARG:HD3	2.41	0.56
2:C:90:LYS:HB3	2:C:91:PRO:HD2	1.86	0.56
2:F:27:LEU:HG	2:F:45:PHE:HZ	1.71	0.56
1:A:36:LEU:HD12	2:B:11:TYR:CE1	2.40	0.56
1:A:106:THR:OG1	1:A:198:ASP:OD2	2.22	0.56
1:A:155:ILE:HG22	1:A:155:ILE:O	2.06	0.56
1:A:273:ARG:NH2	5:I:56:A:OP1	2.38	0.56
2:F:68:LEU:HD21	2:F:116:TRP:CD2	2.40	0.56
1:A:126:LEU:HD13	1:A:220:LEU:HD22	1.87	0.56
5:I:80:A:C5	5:I:81:A:N6	2.74	0.56
1:A:58:TYR:CE2	1:A:86:VAL:HG11	2.40	0.56
2:C:90:LYS:O	2:C:92:HIS:N	2.38	0.56
1:A:148:ARG:HG2	1:A:173:PRO:O	2.07	0.55
2:B:89:GLN:HG2	2:B:93:ALA:HB2	1.88	0.55
3:G:372:G:N2	5:I:81:A:O2'	2.39	0.55
1:A:124:ALA:HB2	5:I:94:U:H1'	1.87	0.55
2:D:17:VAL:O	2:D:21:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:GLU:HG2	2:E:40:VAL:HG22	1.88	0.55
1:A:103:LEU:HD23	1:A:104:PRO:HD2	1.88	0.55
2:D:31:ALA:HB2	2:D:45:PHE:CE2	2.42	0.55
1:A:58:TYR:CE1	1:A:86:VAL:HG21	2.41	0.55
2:B:27:LEU:HD23	2:B:30:ILE:HD11	1.88	0.55
1:A:31:ARG:O	2:B:11:TYR:OH	2.24	0.55
1:A:122:VAL:HG21	1:A:260:PHE:CD2	2.42	0.55
2:B:84:PHE:CE1	2:F:50:LEU:HD21	2.41	0.55
1:A:41:TYR:CE2	2:C:79:ARG:HD3	2.42	0.54
1:A:302:SER:HB2	5:I:53:G:H1'	1.89	0.54
2:F:34:ILE:O	2:F:42:ARG:NH1	2.39	0.54
1:A:208:ARG:HG2	5:I:130:G:OP1	2.07	0.54
2:C:86:ALA:HB2	2:C:99:VAL:HG21	1.89	0.54
1:A:158:LYS:NZ	5:I:106:U:OP1	2.34	0.54
2:C:88:ILE:HG13	2:C:88:ILE:O	2.08	0.54
1:A:313:HIS:ND1	5:I:88:A:O4'	2.41	0.53
2:C:31:ALA:HB2	2:C:45:PHE:CE2	2.43	0.53
1:A:159:ILE:C	1:A:161:CYS:H	2.12	0.53
1:A:274:LYS:HE2	5:I:81:A:N1	2.24	0.53
2:C:68:LEU:HD11	2:C:120:VAL:HG21	1.90	0.53
1:A:263:TYR:HA	1:A:272:LEU:HA	1.91	0.53
2:D:113:LEU:O	2:D:117:ILE:HG12	2.09	0.53
2:E:82:LEU:HB3	2:E:99:VAL:HG13	1.89	0.53
1:A:202:HIS:HD1	1:A:210:TRP:HE1	1.56	0.53
2:D:82:LEU:HD11	2:D:106:ILE:HD12	1.90	0.53
1:A:3:LYS:HD3	5:I:109:A:C2	2.44	0.52
1:A:151:LEU:HD21	1:A:189:PHE:HB3	1.91	0.52
1:A:33:TRP:HH2	2:B:9:LYS:HB2	1.74	0.52
1:A:133:HIS:CD2	1:A:224:PRO:HB3	2.43	0.52
1:A:53:LEU:HD21	1:A:86:VAL:HG22	1.91	0.52
1:A:134:PHE:CE2	1:A:252:ALA:HB3	2.45	0.52
2:B:88:ILE:HG23	2:F:25:SER:HA	1.91	0.52
2:B:101:THR:HG21	4:H:126:A:H4'	1.92	0.52
2:E:94:MET:HE2	2:E:99:VAL:HG22	1.90	0.52
2:F:31:ALA:HB2	2:F:45:PHE:CE2	2.45	0.52
1:A:108:ALA:HB2	1:A:214:MET:H	1.73	0.52
5:I:121:G:H2'	5:I:122:G:O4'	2.10	0.52
1:A:8:LEU:HB3	1:A:93:ILE:HG21	1.93	0.51
1:A:231:PHE:HE1	1:A:246:ILE:HG21	1.76	0.51
2:C:43:GLU:HG3	2:C:44:MET:N	2.25	0.51
4:H:126:A:N1	5:I:48:A:N1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:HB3	1:A:265:ILE:HD12	1.92	0.51
2:D:28:TYR:CZ	2:E:88:ILE:HD11	2.46	0.51
1:A:98:PHE:CZ	1:A:155:ILE:HA	2.45	0.51
2:E:34:ILE:HG12	2:E:93:ALA:HB1	1.92	0.51
1:A:5:HIS:HB3	1:A:8:LEU:HD21	1.93	0.51
1:A:172:LEU:HD11	1:A:179:ILE:HG12	1.92	0.51
1:A:152:TYR:CE2	1:A:172:LEU:HD23	2.46	0.51
1:A:160:HIS:CD2	5:I:110:U:C2	2.99	0.51
2:C:59:ALA:HB1	2:C:68:LEU:HD23	1.91	0.51
1:A:63:TYR:HB3	1:A:77:SER:HB2	1.93	0.51
1:A:122:VAL:O	1:A:126:LEU:HB2	2.11	0.51
2:B:45:PHE:CD2	2:B:85:LEU:HD11	2.46	0.51
2:B:61:LYS:HG3	2:C:73:ALA:HA	1.93	0.51
1:A:231:PHE:CE1	1:A:246:ILE:HG21	2.46	0.50
1:A:65:GLU:HA	1:A:77:SER:HA	1.94	0.50
1:A:33:TRP:HH2	2:B:9:LYS:CB	2.24	0.50
1:A:94:VAL:O	1:A:97:ILE:HG12	2.12	0.50
1:A:8:LEU:HB2	1:A:164:THR:OG1	2.11	0.50
1:A:108:ALA:O	1:A:110:ARG:N	2.44	0.50
2:B:68:LEU:HD21	2:B:116:TRP:CD2	2.47	0.50
2:E:92:HIS:CD2	5:I:19:A:C6	2.99	0.50
3:G:372:G:H2'	3:G:373:C:C6	2.47	0.50
2:B:7:ALA:O	2:B:61:LYS:HE3	2.12	0.49
1:A:76:ILE:HG21	4:H:117:G:C4	2.47	0.49
1:A:198:ASP:CG	1:A:212:ARG:HE	2.16	0.49
2:F:82:LEU:HB3	2:F:99:VAL:HG13	1.94	0.49
2:B:68:LEU:HD21	2:B:116:TRP:CE2	2.47	0.49
1:A:147:ASP:HB3	1:A:150:ALA:H	1.76	0.49
1:A:308:GLN:HE22	4:H:122:C:H5''	1.77	0.49
2:C:64:GLN:HB3	2:C:67:LYS:HG2	1.95	0.49
5:I:83:A:H2'	5:I:84:C:C5	2.48	0.49
1:A:172:LEU:HD22	1:A:189:PHE:HD2	1.77	0.48
2:B:16:ILE:HD11	2:B:113:LEU:HB2	1.93	0.48
2:C:82:LEU:HD11	2:C:106:ILE:HD12	1.95	0.48
3:G:379:G:C6	5:I:60:G:C6	3.01	0.48
2:E:37:LYS:HA	5:I:7:U:O4'	2.12	0.48
1:A:139:PHE:HB2	1:A:215:ASP:HB2	1.94	0.48
2:E:52:GLN:OE1	2:E:75:LEU:HD13	2.12	0.48
2:E:31:ALA:HB2	2:E:45:PHE:CE2	2.48	0.48
5:I:69:C:O2'	5:I:70:U:H5'	2.14	0.48
2:C:85:LEU:O	2:C:88:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:LEU:HD21	2:E:84:PHE:CZ	2.49	0.48
1:A:25:THR:OG1	1:A:85:LEU:HA	2.13	0.48
2:F:90:LYS:HD2	2:F:91:PRO:HD2	1.94	0.48
1:A:304:SER:HA	1:A:316:PHE:HZ	1.79	0.48
2:C:35:PRO:O	2:C:38:HIS:N	2.47	0.48
2:D:31:ALA:O	2:D:42:ARG:HG3	2.14	0.48
5:I:124:A:H2'	5:I:125:A:C8	2.49	0.47
1:A:101:GLY:HA2	5:I:105:G:O3'	2.14	0.47
2:D:45:PHE:CD2	2:D:85:LEU:HD11	2.49	0.47
2:E:89:GLN:HB3	2:E:91:PRO:HD2	1.96	0.47
2:E:52:GLN:HG2	2:E:55:LEU:HD12	1.97	0.47
1:A:8:LEU:HD12	1:A:159:ILE:HG23	1.95	0.47
2:B:13:GLN:HE21	2:B:61:LYS:HD3	1.79	0.47
2:B:28:TYR:HB3	2:B:29:PRO:HD3	1.95	0.47
2:F:37:LYS:HE3	2:F:38:HIS:NE2	2.29	0.47
2:F:68:LEU:HD21	2:F:116:TRP:CE2	2.50	0.47
2:B:46:LEU:HD23	2:B:46:LEU:HA	1.64	0.47
2:C:35:PRO:O	2:C:36:ARG:C	2.52	0.47
2:F:27:LEU:HD12	2:F:30:ILE:HD11	1.95	0.47
2:B:13:GLN:NE2	2:B:61:LYS:HD3	2.30	0.47
2:D:53:VAL:HG11	2:E:80:PHE:CG	2.49	0.47
2:D:68:LEU:HD13	2:D:68:LEU:HA	1.78	0.47
5:I:90:A:H2'	5:I:91:C:O4'	2.15	0.47
5:I:91:C:H2'	5:I:92:G:C8	2.50	0.47
5:I:95:U:H2'	5:I:96:C:C6	2.50	0.47
2:D:53:VAL:HG21	2:E:80:PHE:CZ	2.50	0.47
2:E:26:TYR:CE2	2:E:101:THR:HB	2.50	0.47
2:B:13:GLN:HG3	2:B:14:MET:N	2.30	0.47
1:A:57:ASN:HD22	1:A:57:ASN:HA	1.48	0.46
2:D:54:GLU:OE1	2:E:77:MET:HB2	2.16	0.46
1:A:296:LEU:HD21	1:A:325:ILE:HG21	1.95	0.46
1:A:103:LEU:HD12	1:A:199:ARG:HG2	1.97	0.46
2:C:16:ILE:HD13	2:C:112:ILE:HB	1.97	0.46
2:D:82:LEU:HB3	2:D:99:VAL:HG13	1.98	0.46
2:E:24:ILE:HD11	2:E:53:VAL:CG2	2.46	0.46
5:I:80:A:C5	5:I:81:A:N7	2.84	0.46
1:A:90:LEU:HD13	1:A:168:LEU:HD23	1.97	0.46
1:A:315:LEU:HA	5:I:83:A:H4'	1.97	0.46
1:A:318:TRP:CD2	5:I:83:A:H5'	2.51	0.46
2:B:81:TRP:HH2	2:F:50:LEU:HD13	1.81	0.46
5:I:80:A:N7	5:I:81:A:C6	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ALA:HB2	2:B:45:PHE:HE2	1.77	0.46
2:E:20:TYR:HA	2:E:109:VAL:HG11	1.98	0.46
1:A:108:ALA:HB3	1:A:191:ASN:OD1	2.16	0.46
2:B:16:ILE:HG12	2:B:109:VAL:HG13	1.98	0.46
2:F:85:LEU:HD23	2:F:88:ILE:HD12	1.97	0.46
2:B:82:LEU:HD11	2:B:106:ILE:HD12	1.97	0.46
1:A:259:ASN:ND2	5:I:79:G:OP1	2.48	0.45
2:B:50:LEU:HD21	2:C:84:PHE:CZ	2.51	0.45
2:C:90:LYS:HE2	2:C:90:LYS:N	2.13	0.45
2:E:13:GLN:HG3	2:E:14:MET:N	2.32	0.45
2:C:40:VAL:HA	2:C:43:GLU:HG2	1.97	0.45
2:F:27:LEU:HD12	2:F:27:LEU:HA	1.77	0.45
5:I:70:U:H5''	5:I:71:G:O4'	2.17	0.45
1:A:134:PHE:CD1	1:A:258:ILE:HG12	2.52	0.45
2:B:80:PHE:CE1	2:F:53:VAL:HG21	2.52	0.45
2:E:67:LYS:HZ3	2:E:67:LYS:HG3	1.71	0.45
2:D:38:HIS:NE2	2:D:91:PRO:HD2	2.32	0.45
2:E:12:ASP:O	2:E:16:ILE:HG13	2.16	0.45
2:F:27:LEU:HB3	2:F:49:LEU:HD22	1.99	0.45
3:G:370:G:N2	5:I:70:U:H1'	2.31	0.45
1:A:142:PHE:CD2	1:A:215:ASP:HB3	2.52	0.45
1:A:4:ARG:NH2	5:I:123:A:O5'	2.50	0.45
1:A:30:ARG:HA	1:A:35:TYR:CD2	2.52	0.45
1:A:202:HIS:NE2	5:I:129:G:O3'	2.50	0.45
2:D:24:ILE:HD11	2:D:53:VAL:CG2	2.47	0.45
1:A:82:LYS:HE2	1:A:82:LYS:HB2	1.52	0.44
2:C:68:LEU:HD12	2:C:117:ILE:HA	2.00	0.44
1:A:60:ARG:HD2	1:A:79:LEU:HD11	1.99	0.44
2:D:68:LEU:HB3	2:D:117:ILE:CD1	2.46	0.44
1:A:171:VAL:HG13	1:A:185:THR:HG21	1.99	0.44
1:A:213:TYR:CD2	1:A:261:LEU:HD11	2.52	0.44
2:B:20:TYR:CE2	2:B:52:GLN:HB3	2.53	0.44
2:E:17:VAL:HG12	2:E:21:GLU:OE2	2.17	0.44
5:I:20:C:H4'	5:I:21:G:O5'	2.17	0.44
2:F:56:PHE:CE1	2:F:71:ALA:HB1	2.52	0.44
2:E:67:LYS:H	2:E:67:LYS:HG2	1.65	0.44
2:B:8:THR:HG23	2:C:69:TYR:CE1	2.53	0.44
2:C:34:ILE:HG22	2:C:38:HIS:HB2	1.98	0.44
2:E:31:ALA:O	2:E:42:ARG:HG3	2.18	0.44
2:C:53:VAL:HG11	2:D:80:PHE:CG	2.53	0.44
2:F:122:ARG:HD2	2:F:122:ARG:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:HB	2:C:42:ARG:HB2	2.00	0.44
2:D:28:TYR:CD2	2:E:84:PHE:HZ	2.35	0.44
2:E:106:ILE:HA	2:E:109:VAL:HG22	1.98	0.44
2:F:32:GLN:HG2	5:I:4:G:N1	2.33	0.44
2:F:68:LEU:HD23	2:F:68:LEU:HA	1.76	0.44
1:A:140:SER:HA	1:A:247:SER:CB	2.46	0.43
1:A:143:PHE:HB2	1:A:144:PRO:HD3	1.99	0.43
2:B:21:GLU:OE2	2:C:83:ARG:HD2	2.18	0.43
2:E:16:ILE:HG13	2:E:16:ILE:H	1.48	0.43
2:B:84:PHE:HA	2:B:88:ILE:HD12	2.00	0.43
2:F:108:GLU:O	2:F:112:ILE:HG13	2.19	0.43
1:A:311:ASP:O	5:I:87:U:H4'	2.18	0.43
2:B:28:TYR:CE1	2:C:84:PHE:HZ	2.37	0.43
3:G:371:G:C2	5:I:69:C:C2	3.06	0.43
5:I:80:A:H2'	5:I:81:A:C4	2.54	0.43
1:A:152:TYR:OH	1:A:168:LEU:O	2.36	0.43
1:A:169:ARG:HG2	1:A:174:ASP:HB2	2.01	0.43
1:A:254:VAL:HG12	1:A:267:PRO:HD3	2.00	0.43
2:E:46:LEU:HD23	2:E:46:LEU:HA	1.80	0.43
2:E:68:LEU:HD21	2:E:116:TRP:CE2	2.54	0.43
2:B:85:LEU:O	2:B:93:ALA:HB3	2.19	0.43
5:I:110:U:H2'	5:I:122:G:O6	2.18	0.43
2:C:94:MET:HG2	2:C:99:VAL:HG22	2.00	0.43
3:G:371:G:H21	5:I:81:A:H8	1.67	0.43
1:A:94:VAL:HG13	1:A:98:PHE:CE2	2.53	0.42
2:D:81:TRP:O	2:D:85:LEU:HG	2.18	0.42
2:F:123:LYS:H	2:F:123:LYS:HG2	1.35	0.42
1:A:132:THR:OG1	1:A:133:HIS:ND1	2.40	0.42
2:B:57:ILE:O	2:B:61:LYS:HG2	2.19	0.42
2:F:88:ILE:HG22	2:F:93:ALA:HA	2.01	0.42
5:I:115:G:N2	5:I:117:A:H3'	2.33	0.42
2:B:21:GLU:CD	2:C:83:ARG:HH11	2.22	0.42
1:A:179:ILE:HG23	1:A:186:SER:CB	2.49	0.42
2:B:82:LEU:HB3	2:B:99:VAL:HG13	2.00	0.42
2:C:16:ILE:HD13	2:C:16:ILE:HA	1.80	0.42
5:I:69:C:C2'	5:I:70:U:H5'	2.50	0.42
5:I:130:G:H8	5:I:130:G:OP2	2.02	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.84	0.42
1:A:105:TYR:HB2	1:A:210:TRP:CH2	2.54	0.42
1:A:108:ALA:HB2	1:A:214:MET:N	2.33	0.42
5:I:16:G:N2	5:I:24:U:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HB2	1:A:82:LYS:HG3	2.01	0.42
1:A:75:LEU:HD22	1:A:75:LEU:HA	1.72	0.42
1:A:272:LEU:HD12	5:I:83:A:N1	2.35	0.42
2:D:90:LYS:HD3	2:D:90:LYS:HA	1.79	0.42
2:D:106:ILE:HA	2:D:109:VAL:HG12	2.00	0.42
2:E:46:LEU:HB3	2:F:40:VAL:HG11	2.01	0.42
1:A:81:PHE:CE1	1:A:85:LEU:HD12	2.55	0.42
1:A:99:GLU:O	1:A:110:ARG:NH1	2.53	0.42
1:A:261:LEU:HA	1:A:261:LEU:HD23	1.72	0.42
1:A:263:TYR:CD1	1:A:263:TYR:N	2.87	0.42
2:B:24:ILE:HD11	2:B:53:VAL:CG2	2.49	0.42
2:B:80:PHE:CZ	2:F:53:VAL:HG21	2.55	0.42
2:F:37:LYS:HD2	5:I:25:U:O2'	2.19	0.42
1:A:52:GLU:OE1	2:B:1:MET:HB2	2.20	0.41
1:A:273:ARG:NH2	5:I:55:C:O3'	2.53	0.41
5:I:103:A:H61	5:I:130:G:H1	1.68	0.41
1:A:296:LEU:O	1:A:300:LEU:HB2	2.20	0.41
2:B:100:GLU:O	2:B:104:VAL:HG23	2.20	0.41
2:C:35:PRO:HG2	2:C:91:PRO:CB	2.45	0.41
2:C:100:GLU:O	2:C:104:VAL:HG23	2.20	0.41
2:D:94:MET:HG2	2:D:98:GLN:HB2	2.01	0.41
1:A:270:LYS:HE2	1:A:270:LYS:HB3	1.62	0.41
2:E:100:GLU:O	2:E:104:VAL:HG23	2.20	0.41
2:F:34:ILE:HG22	2:F:38:HIS:HB2	2.00	0.41
1:A:24:LYS:HD2	1:A:92:ASN:HD21	1.84	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.89	0.41
1:A:155:ILE:HG22	1:A:168:LEU:HD13	2.02	0.41
1:A:155:ILE:CG2	1:A:168:LEU:HD13	2.50	0.41
2:B:80:PHE:CG	2:F:53:VAL:HG11	2.55	0.41
2:D:36:ARG:HB3	5:I:8:C:OP1	2.21	0.41
2:B:61:LYS:HG3	2:C:73:ALA:CA	2.50	0.41
2:D:68:LEU:HD11	2:D:116:TRP:CD2	2.55	0.41
2:D:91:PRO:O	2:D:93:ALA:N	2.53	0.41
2:F:80:PHE:O	2:F:83:ARG:HG2	2.20	0.41
1:A:159:ILE:HG13	1:A:168:LEU:HD11	2.01	0.41
2:B:81:TRP:O	2:B:85:LEU:HG	2.20	0.41
2:C:46:LEU:HA	2:C:46:LEU:HD23	1.78	0.41
2:D:68:LEU:HD11	2:D:116:TRP:CE3	2.56	0.41
5:I:66:G:C5	5:I:67:U:C4	3.09	0.41
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.88	0.41
1:A:134:PHE:CE1	1:A:258:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:HE2	5:I:81:A:H2	1.83	0.41
2:B:27:LEU:O	2:B:31:ALA:N	2.51	0.41
2:D:30:ILE:HG21	2:D:94:MET:HG3	2.03	0.41
1:A:108:ALA:HA	1:A:213:TYR:CE2	2.55	0.41
2:B:27:LEU:HD11	2:B:82:LEU:HD21	2.02	0.41
2:C:26:TYR:O	2:C:30:ILE:HG12	2.21	0.41
2:C:35:PRO:O	2:C:37:LYS:N	2.54	0.41
2:D:52:GLN:HG2	2:D:55:LEU:HD12	2.03	0.41
2:D:102:ALA:HA	2:D:105:LEU:HD12	2.02	0.41
5:I:116:A:H2'	5:I:117:A:O4'	2.21	0.41
1:A:315:LEU:HG	5:I:83:A:O4'	2.20	0.41
2:E:96:PRO:O	2:E:100:GLU:HG3	2.21	0.41
1:A:119:VAL:HG11	1:A:263:TYR:CD1	2.56	0.40
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.76	0.40
2:D:100:GLU:O	2:D:104:VAL:HG23	2.21	0.40
5:I:80:A:C2	5:I:81:A:N7	2.90	0.40
1:A:49:LEU:HD13	2:B:1:MET:HE3	2.03	0.40
2:C:56:PHE:CE1	2:C:71:ALA:HB1	2.57	0.40
2:C:89:GLN:H	2:C:89:GLN:HG3	1.50	0.40
2:D:87:GLY:HA2	2:D:92:HIS:ND1	2.36	0.40
4:H:125:C:O2	5:I:50:G:C2	2.75	0.40
2:C:24:ILE:HG22	2:D:88:ILE:HG21	2.02	0.40
2:C:57:ILE:HG21	2:D:76:ALA:HB3	2.03	0.40
2:E:35:PRO:HA	5:I:24:U:H5'	2.04	0.40
5:I:9:U:H2'	5:I:10:G:C8	2.56	0.40
1:A:8:LEU:HB3	1:A:93:ILE:CG2	2.51	0.40
1:A:104:PRO:HD3	5:I:131:G:C5	2.57	0.40
1:A:128:ARG:CZ	5:I:95:U:OP1	2.69	0.40
2:D:28:TYR:CE2	2:D:50:LEU:HD11	2.56	0.40
2:E:21:GLU:OE2	2:F:83:ARG:HD2	2.22	0.40
2:E:95:THR:HG21	5:I:18:U:H4'	2.04	0.40
1:A:262:GLY:HA2	1:A:273:ARG:NE	2.31	0.40
2:B:28:TYR:HE1	2:B:50:LEU:HD11	1.86	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	326/328 (99%)	272 (83%)	40 (12%)	14 (4%)	2	11
2	B	120/290 (41%)	108 (90%)	7 (6%)	5 (4%)	2	12
2	C	109/290 (38%)	94 (86%)	10 (9%)	5 (5%)	2	10
2	D	109/290 (38%)	99 (91%)	9 (8%)	1 (1%)	14	43
2	E	108/290 (37%)	99 (92%)	9 (8%)	0	100	100
2	F	109/290 (38%)	101 (93%)	7 (6%)	1 (1%)	14	43
All	All	881/1778 (50%)	773 (88%)	82 (9%)	26 (3%)	5	17

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	109	CYS
1	A	140	SER
2	C	88	ILE
2	C	91	PRO
2	C	92	HIS
1	A	149	ALA
1	A	160	HIS
1	A	163	ALA
1	A	222	ASP
1	A	255	SER
2	B	92	HIS
2	C	12	ASP
2	C	94	MET
2	D	92	HIS
1	A	40	GLU
1	A	177	VAL
1	A	214	MET
2	B	93	ALA
2	B	2	GLU

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Mol	Chain	Res	Type
2	B	63	ASN
1	A	193	TYR
2	B	4	ILE
1	A	178	GLY
1	A	71	PRO
2	F	90	LYS

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	278/278 (100%)	234 (84%)	44 (16%)	2	8
2	B	102/232 (44%)	87 (85%)	15 (15%)	2	10
2	C	92/232 (40%)	80 (87%)	12 (13%)	3	13
2	D	92/232 (40%)	76 (83%)	16 (17%)	1	6
2	E	91/232 (39%)	73 (80%)	18 (20%)	1	4
2	F	92/232 (40%)	68 (74%)	24 (26%)	0	1
All	All	747/1438 (52%)	618 (83%)	129 (17%)	3	6

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	23	ARG
1	A	37	GLU
1	A	42	ASP
1	A	57	ASN
1	A	65	GLU
1	A	67	LEU
1	A	68	VAL
1	A	75	LEU
1	A	82	LYS
1	A	94	VAL
1	A	97	ILE

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Mol	Chain	Res	Type
1	A	103	LEU
1	A	110	ARG
1	A	126	LEU
1	A	128	ARG
1	A	129	THR
1	A	137	SER
1	A	147	ASP
1	A	156	ASP
1	A	158	LYS
1	A	161	CYS
1	A	171	VAL
1	A	177	VAL
1	A	179	ILE
1	A	185	THR
1	A	197	VAL
1	A	200	LEU
1	A	204	GLU
1	A	208	ARG
1	A	216	ASP
1	A	227	LEU
1	A	256	ARG
1	A	272	LEU
1	A	274	LYS
1	A	275	SER
1	A	276	SER
1	A	279	ARG
1	A	283	LYS
1	A	290	HIS
1	A	293	ASP
1	A	296	LEU
1	A	298	ARG
1	A	302	SER
2	B	8	THR
2	B	13	GLN
2	B	19	ARG
2	B	37	LYS
2	B	54	GLU
2	B	62	SER
2	B	64	GLN
2	B	65	VAL
2	B	66	SER
2	B	89	GLN

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Mol	Chain	Res	Type
2	B	90	LYS
2	B	95	THR
2	B	100	GLU
2	B	115	SER
2	B	119	ARG
2	C	11	TYR
2	C	16	ILE
2	C	36	ARG
2	C	43	GLU
2	C	64	GLN
2	C	68	LEU
2	C	89	GLN
2	C	90	LYS
2	C	91	PRO
2	C	92	HIS
2	C	94	MET
2	C	95	THR
2	D	14	MET
2	D	15	LEU
2	D	18	GLU
2	D	36	ARG
2	D	52	GLN
2	D	62	SER
2	D	63	ASN
2	D	64	GLN
2	D	65	VAL
2	D	68	LEU
2	D	89	GLN
2	D	101	THR
2	D	103	GLN
2	D	119	ARG
2	D	122	ARG
2	D	123	LYS
2	E	13	GLN
2	E	16	ILE
2	E	36	ARG
2	E	43	GLU
2	E	50	LEU
2	E	52	GLN
2	E	62	SER
2	E	63	ASN
2	E	65	VAL

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Mol	Chain	Res	Type
2	E	66	SER
2	E	67	LYS
2	E	75	LEU
2	E	83	ARG
2	E	85	LEU
2	E	89	GLN
2	E	90	LYS
2	E	95	THR
2	E	113	LEU
2	F	13	GLN
2	F	14	MET
2	F	15	LEU
2	F	16	ILE
2	F	22	ARG
2	F	27	LEU
2	F	33	SER
2	F	36	ARG
2	F	43	GLU
2	F	54	GLU
2	F	55	LEU
2	F	61	LYS
2	F	65	VAL
2	F	66	SER
2	F	90	LYS
2	F	95	THR
2	F	100	GLU
2	F	103	GLN
2	F	105	LEU
2	F	111	ARG
2	F	113	LEU
2	F	119	ARG
2	F	122	ARG
2	F	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	308	GLN
2	C	13	GLN
2	C	121	ASN
2	D	13	GLN

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Mol	Chain	Res	Type
2	D	32	GLN
2	E	52	GLN
2	E	98	GLN
2	F	13	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	12/19 (63%)	4 (33%)	0
4	H	12/36 (33%)	4 (33%)	0
5	I	119/140 (85%)	53 (44%)	4 (3%)
All	All	143/195 (73%)	61 (42%)	4 (2%)

All (61) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	374	A
3	G	375	G
3	G	376	G
3	G	379	G
4	H	121	C
4	H	126	A
4	H	127	C
4	H	128	C
5	I	4	G
5	I	5	G
5	I	6	C
5	I	7	U
5	I	8	C
5	I	9	U
5	I	13	A
5	I	14	A
5	I	15	C
5	I	20	C
5	I	21	G
5	I	22	G
5	I	27	G
5	I	28	C
5	I	29	G
5	I	33	U
5	I	53	G

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Mol	Chain	Res	Type
5	I	56	A
5	I	61	G
5	I	63	U
5	I	65	U
5	I	66	G
5	I	73	U
5	I	74	U
5	I	75	C
5	I	76	G
5	I	77	G
5	I	80	A
5	I	82	C
5	I	83	A
5	I	84	C
5	I	85	G
5	I	87	U
5	I	88	A
5	I	89	C
5	I	92	G
5	I	93	G
5	I	94	U
5	I	95	U
5	I	97	G
5	I	98	G
5	I	99	C
5	I	101	A
5	I	106	U
5	I	109	A
5	I	110	U
5	I	118	A
5	I	119	A
5	I	120	U
5	I	129	G
5	I	130	G
5	I	131	G
5	I	132	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	I	20	C
5	I	83	A

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Mol	Chain	Res	Type
5	I	94	U
5	I	100	A

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.

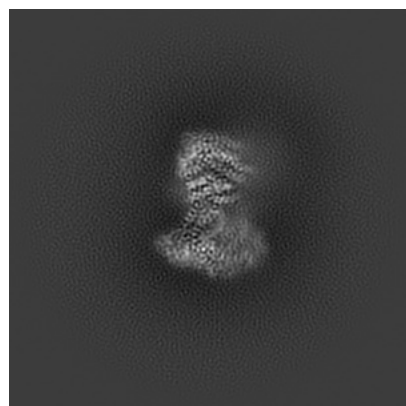
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42079. These allow visual inspection of the internal detail of the map and identification of artifacts.

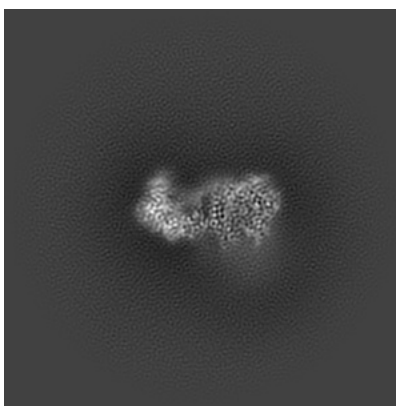
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

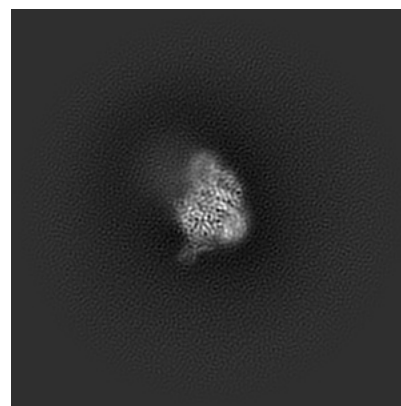
6.1.1 Primary map



X

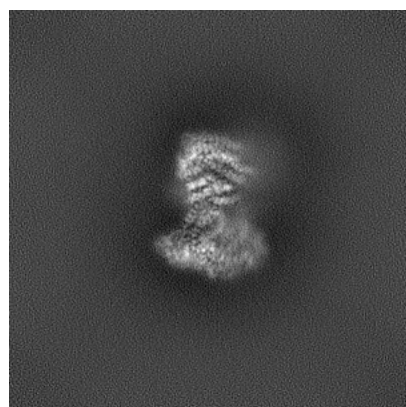


Y

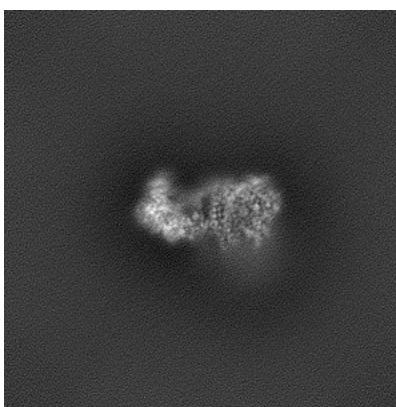


Z

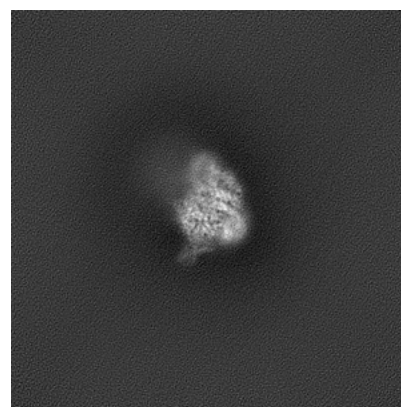
6.1.2 Raw map



X



Y

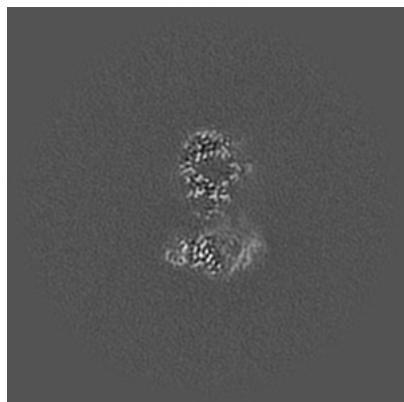


Z

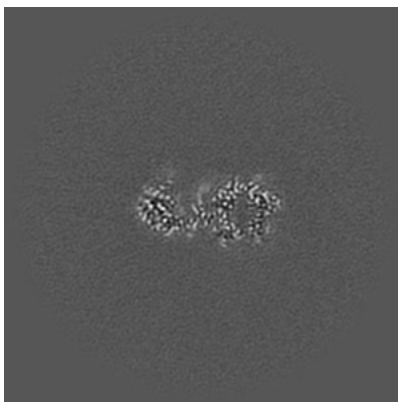
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

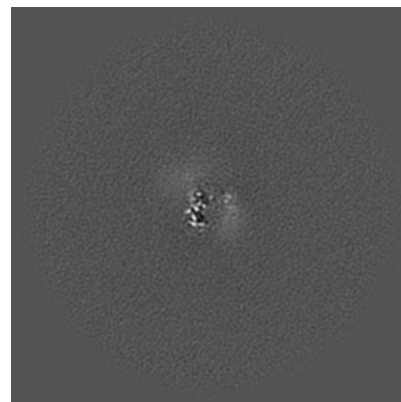
6.2.1 Primary map



X Index: 160

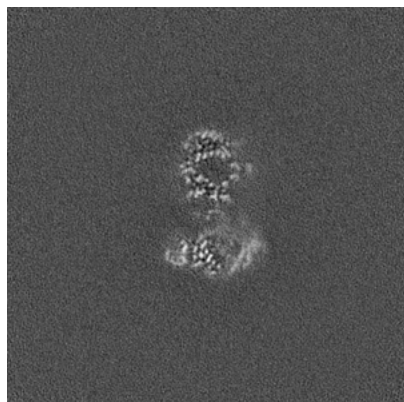


Y Index: 160

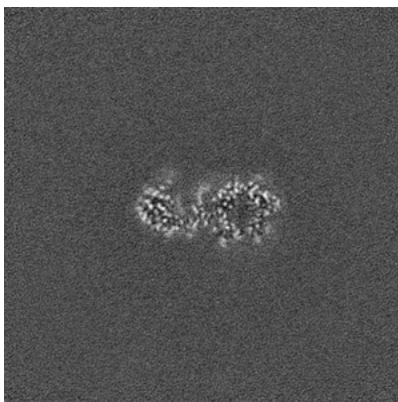


Z Index: 160

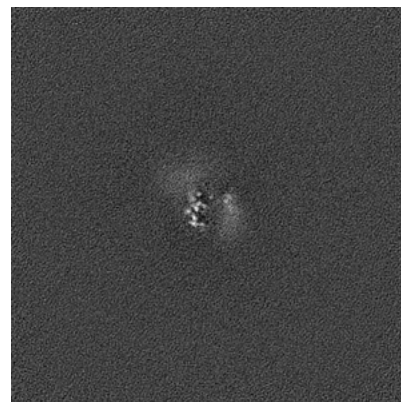
6.2.2 Raw map



X Index: 160



Y Index: 160

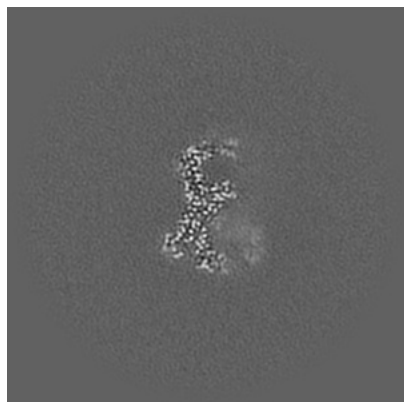


Z Index: 160

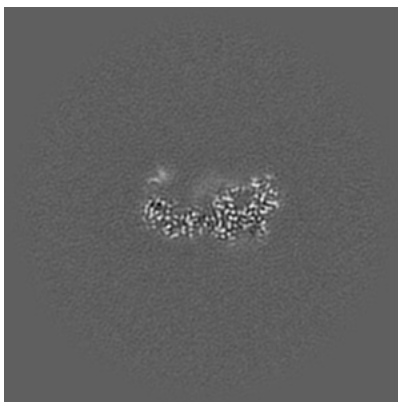
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

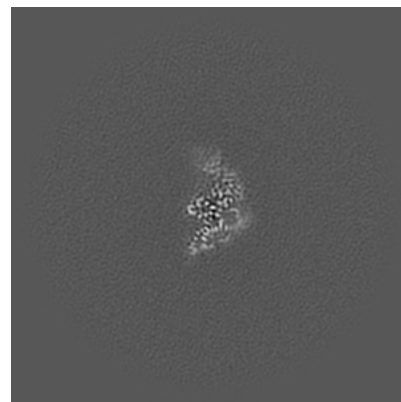
6.3.1 Primary map



X Index: 150

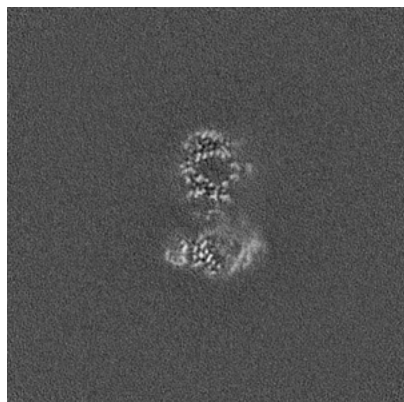


Y Index: 152

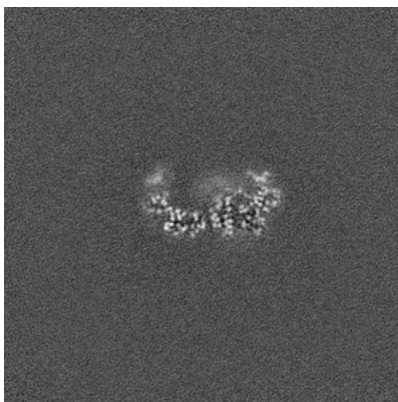


Z Index: 123

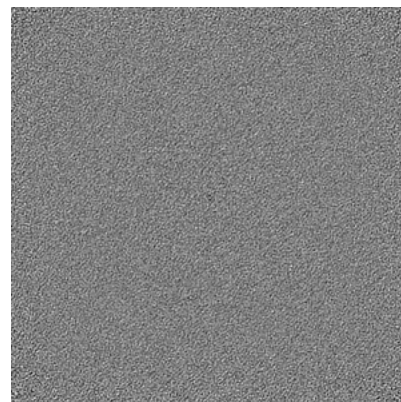
6.3.2 Raw map



X Index: 160



Y Index: 147

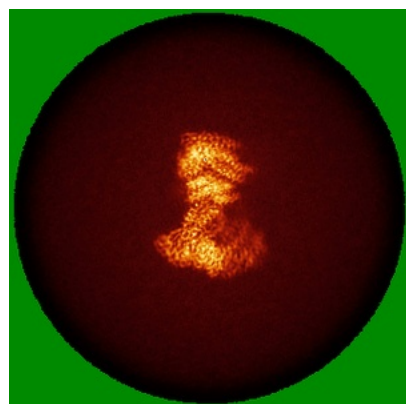


Z Index: 0

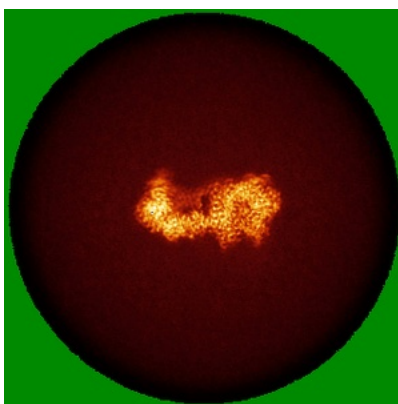
The images above show the largest variance slices of the map in three orthogonal directions.

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

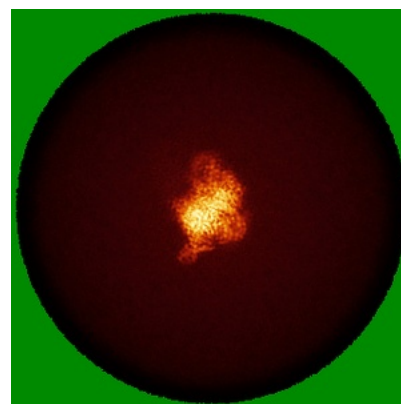
6.4.1 Primary map



X

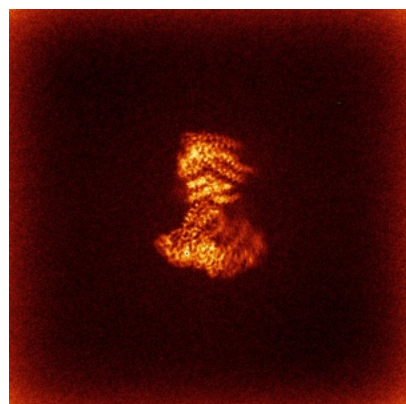


Y

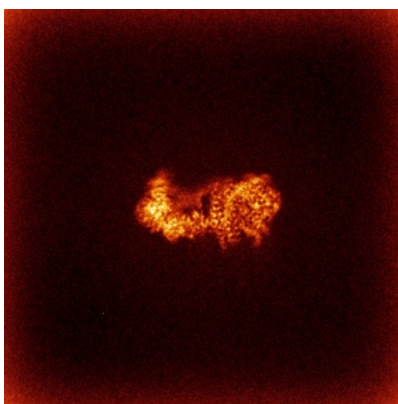


Z

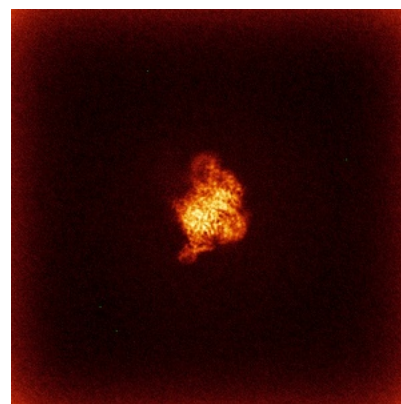
6.4.2 Raw map



X



Y

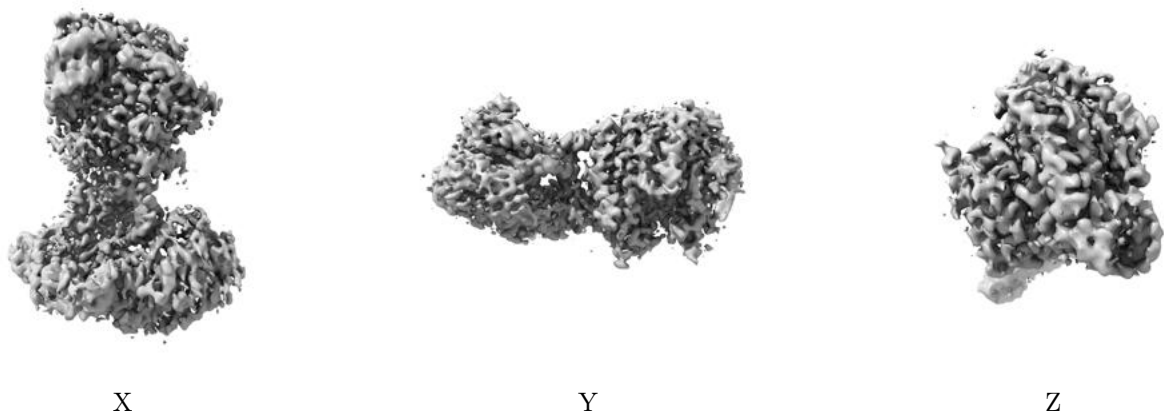


Z

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.

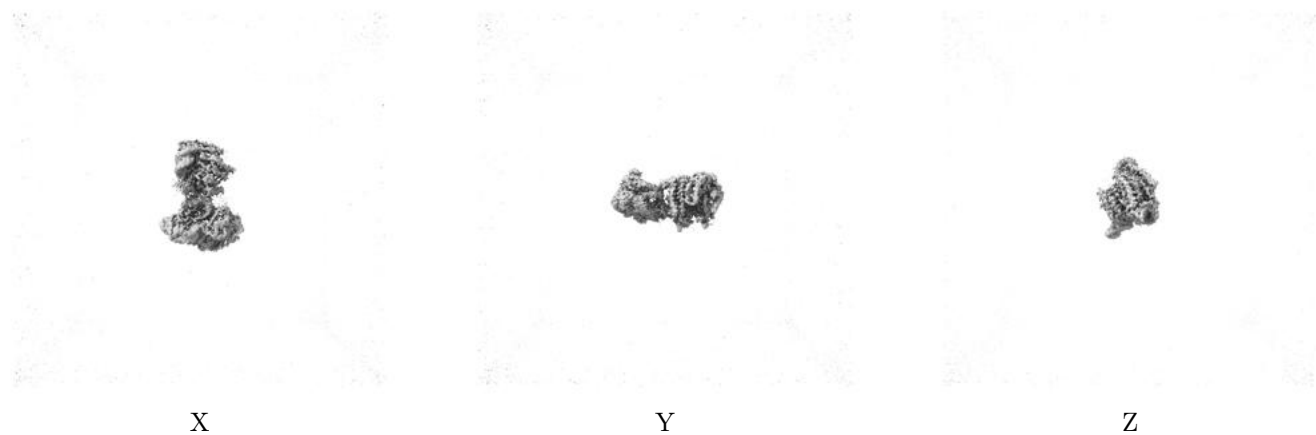
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

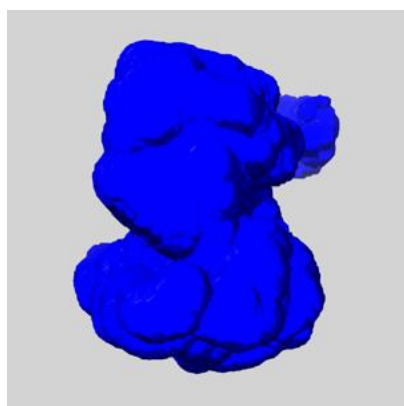
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

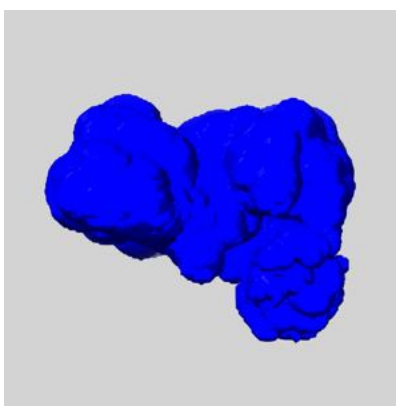
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

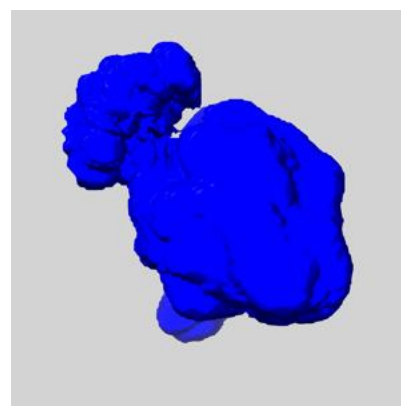
6.6.1 emd_42079_msk_1.map [i](#)



X



Y

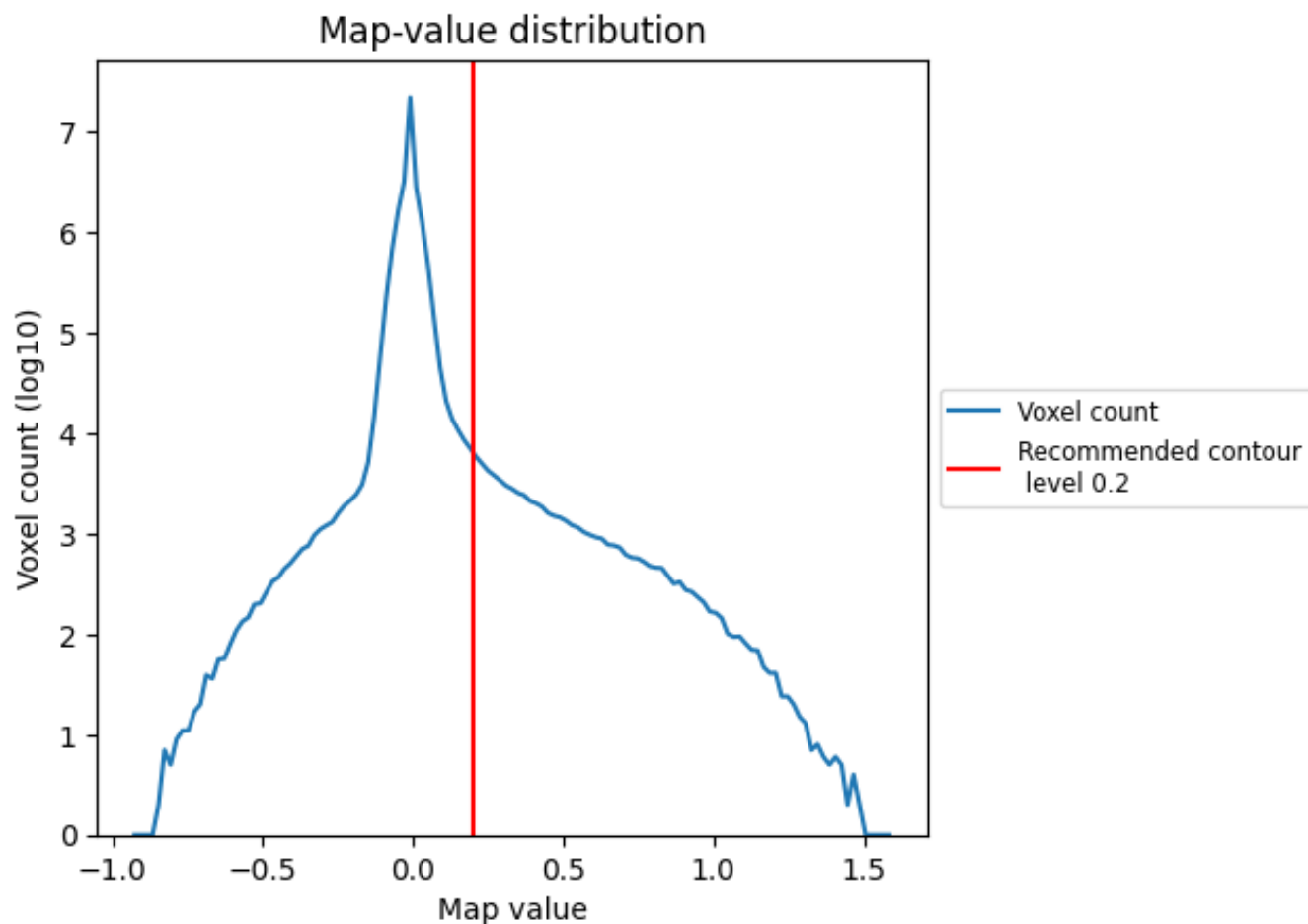


Z

7 Map analysis [i](#)

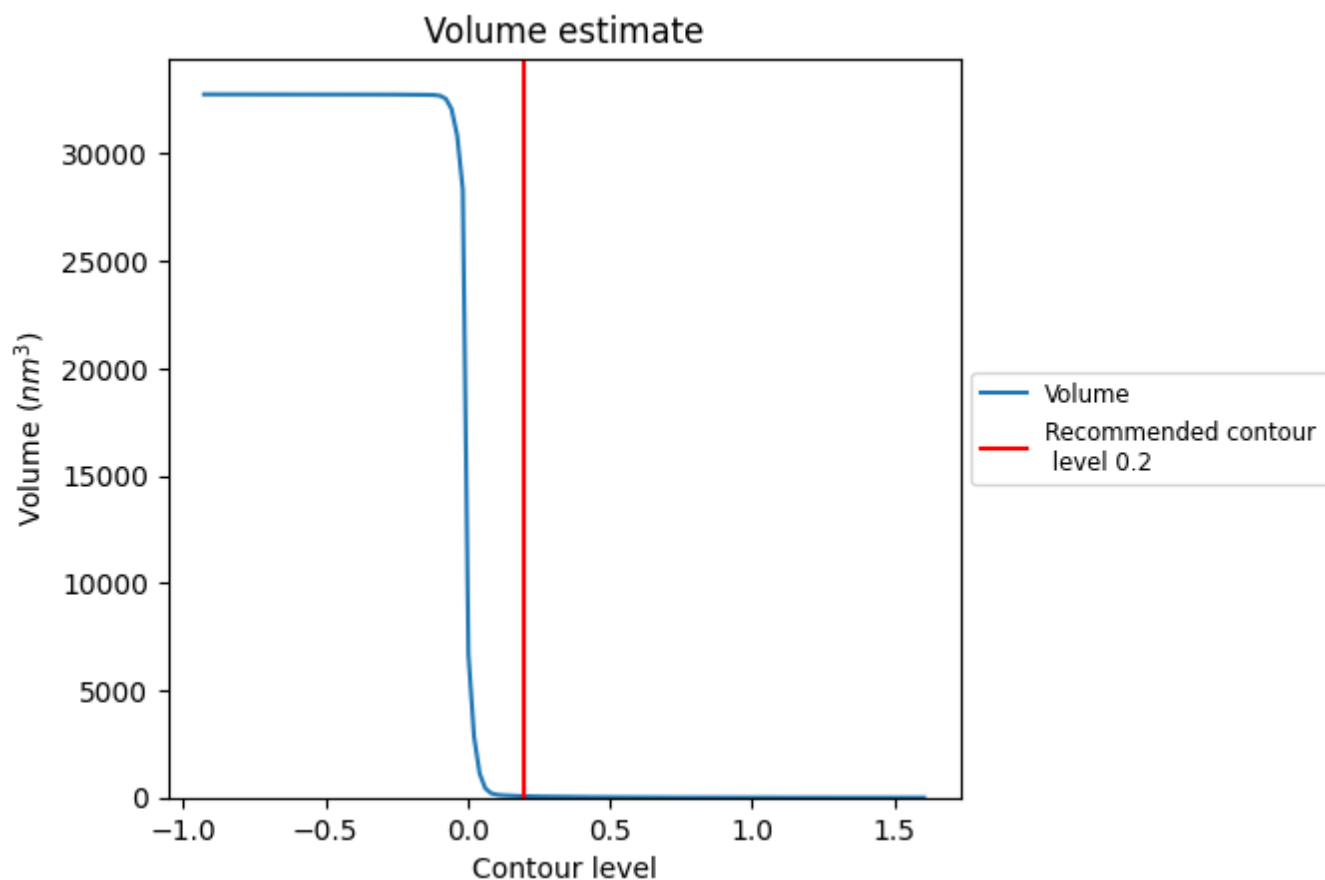
This section contains the results of statistical analysis of the map.

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.

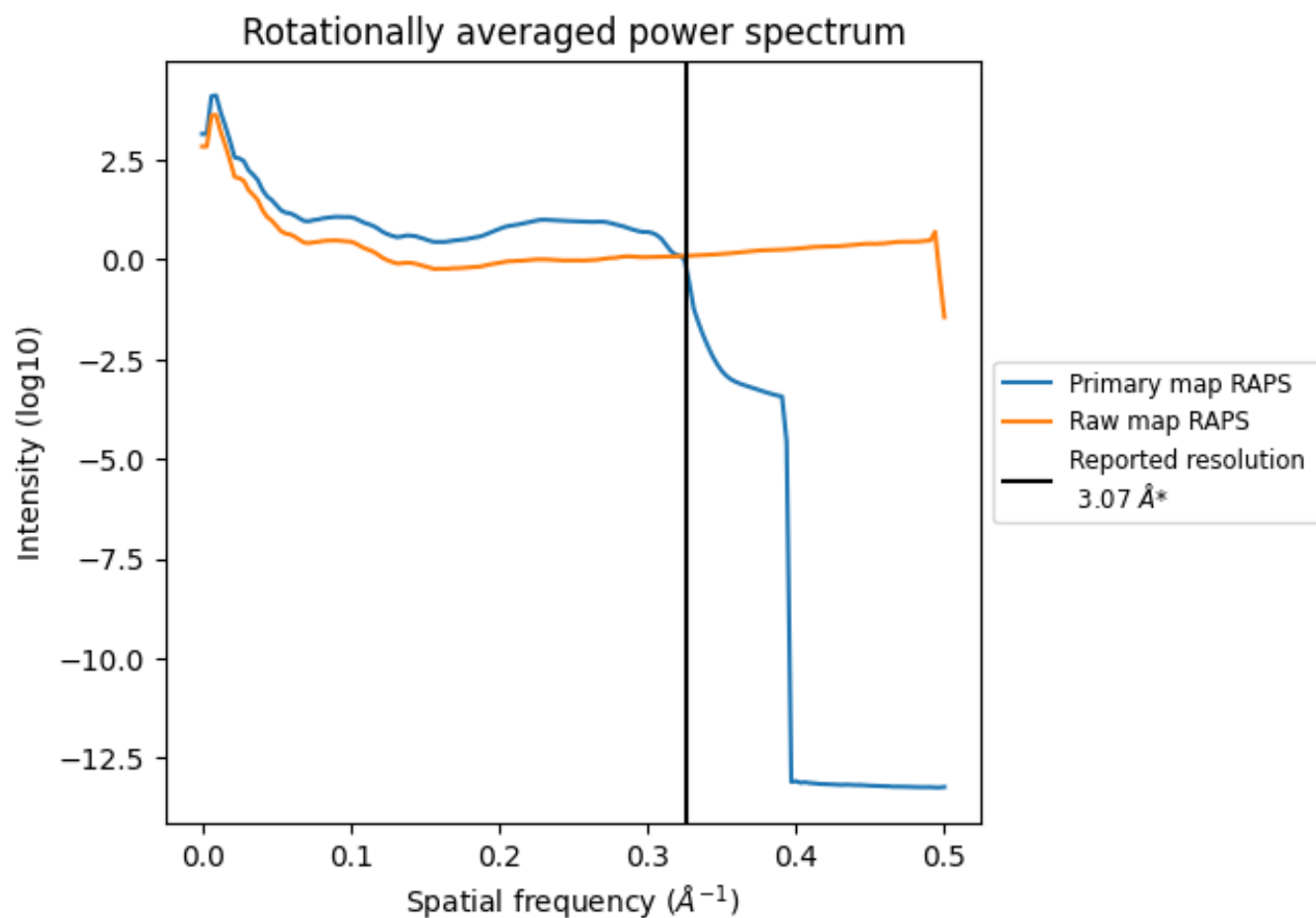
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 57 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 ⓘ

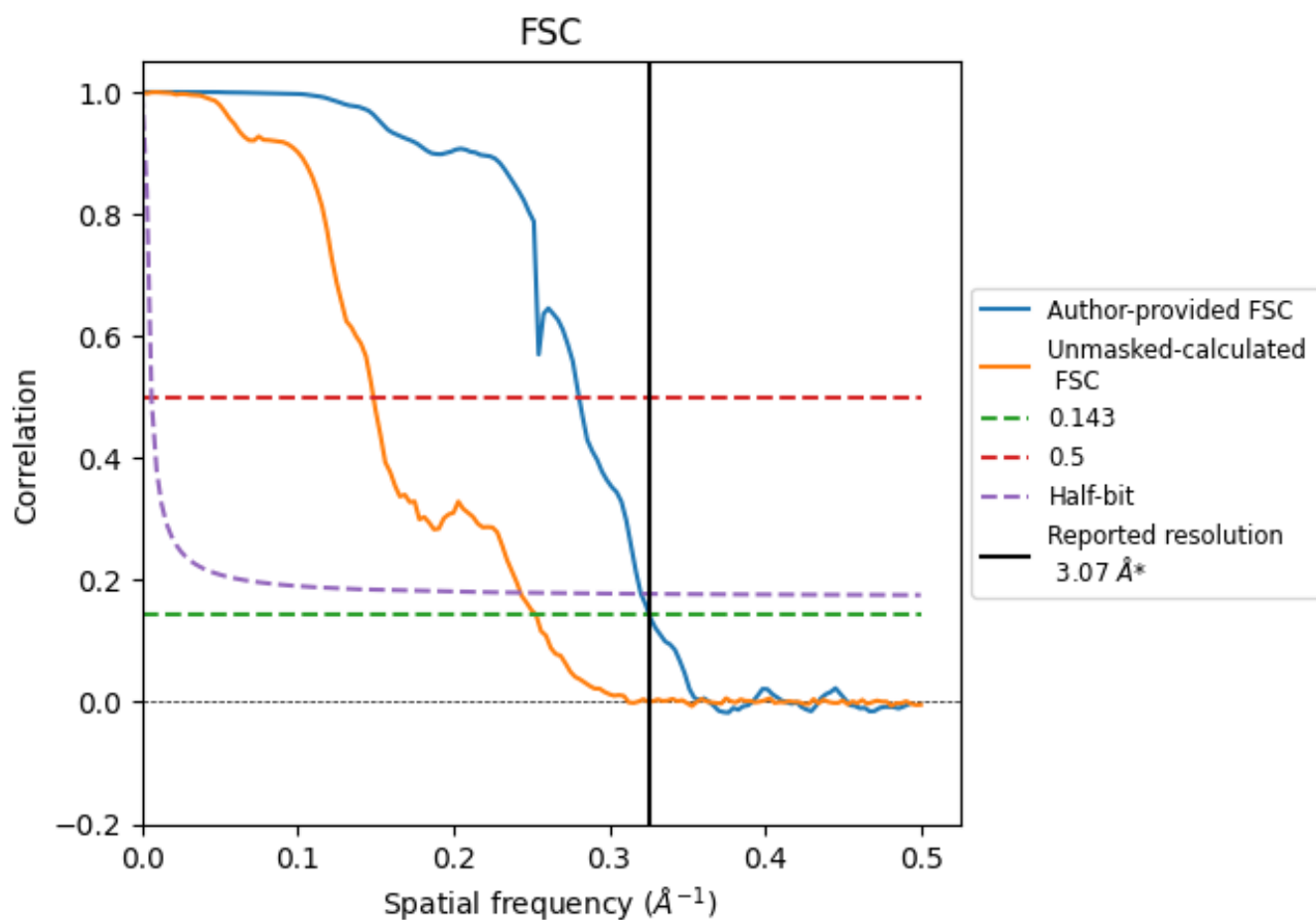


*Reported resolution corresponds to spatial frequency of 0.326 \AA^{-1}

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 0.326 \AA^{-1}

8.2 Resolution estimates [i](#)

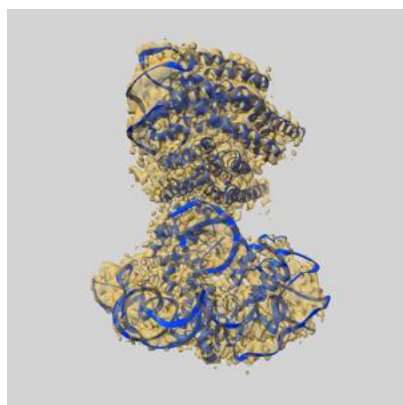
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.56	3.12
Unmasked-calculated*	3.95	6.73	4.12

*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 3.95 differs from the reported value 3.07 by more than 10 %

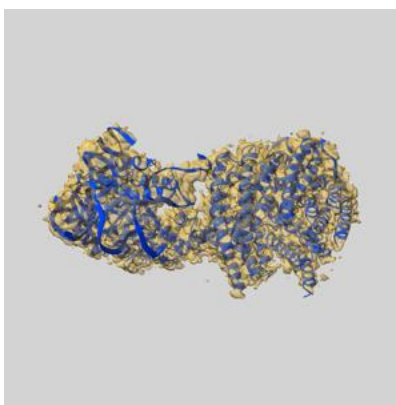
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42079 and PDB model 8UB9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

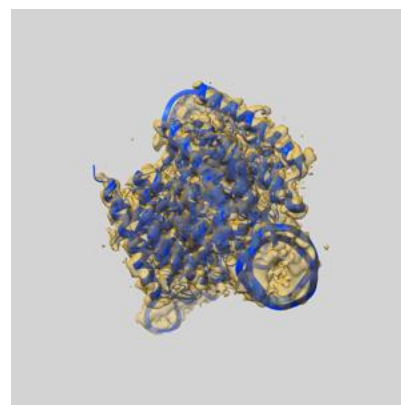
9.1 Map-model overlay [i](#)



X



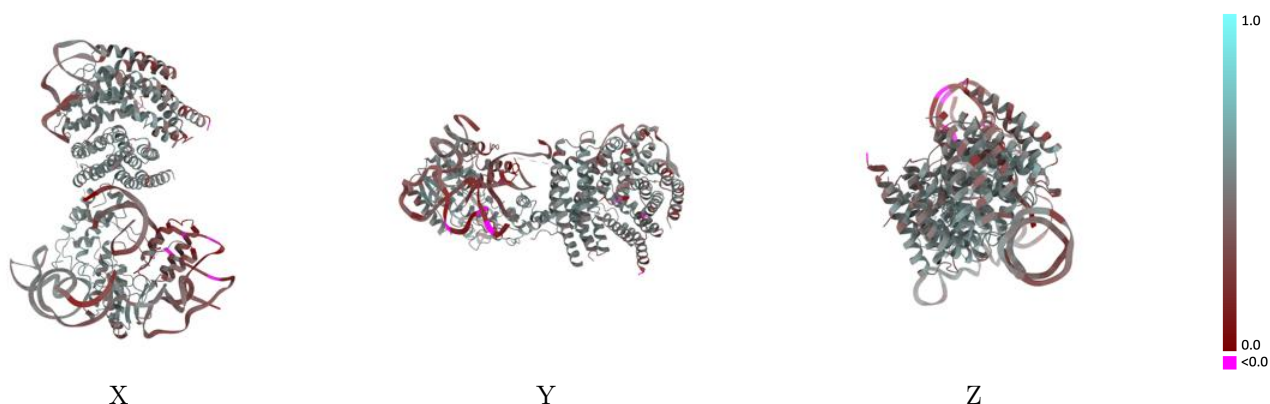
Y



Z

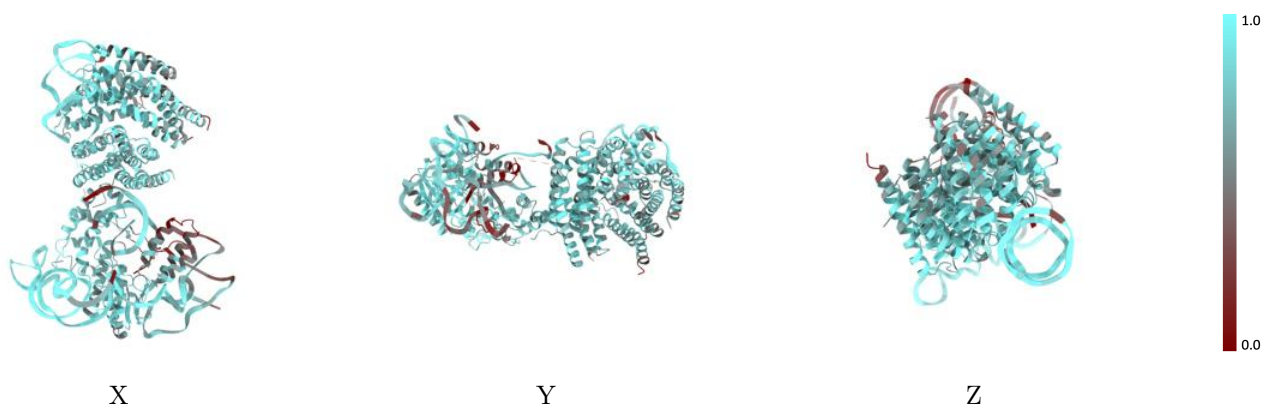
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



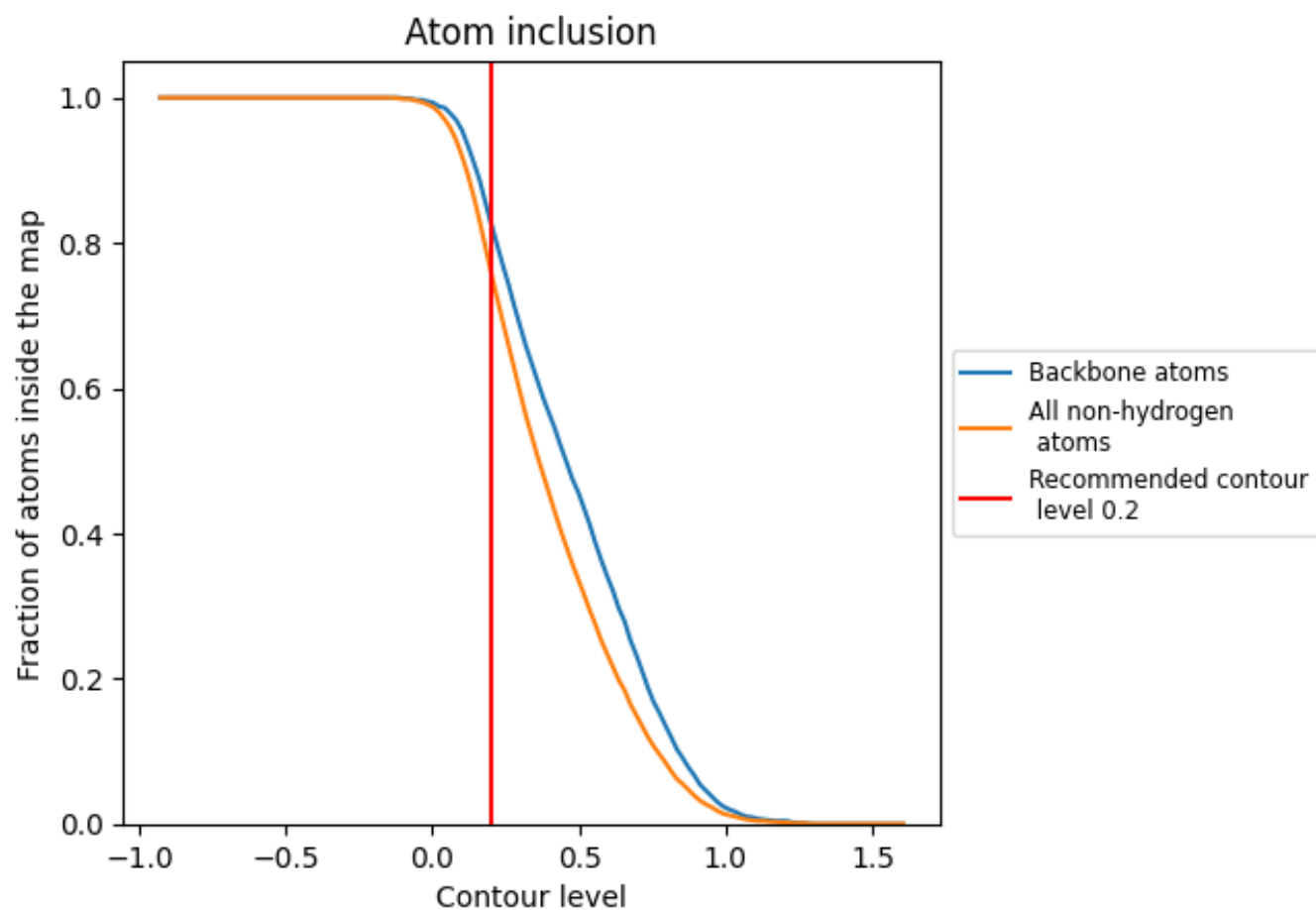
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7600	<div></div> 0.4420
A	<div></div> 0.7460	<div></div> 0.4730
B	<div></div> 0.8100	<div></div> 0.5100
C	<div></div> 0.8210	<div></div> 0.5190
D	<div></div> 0.7650	<div></div> 0.4730
E	<div></div> 0.7680	<div></div> 0.4640
F	<div></div> 0.7510	<div></div> 0.4510
G	<div></div> 0.5260	<div></div> 0.1750
H	<div></div> 0.6150	<div></div> 0.3030
I	<div></div> 0.7750	<div></div> 0.3830

