



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:13 AM UTC

PDB ID : 8ZP9 / pdb_00008zp9
EMDB ID : EMD-60330
Title : Cryo-EM structure of Cas5-HNH Cascade bound with sDNA, Conf2
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on : 2024-05-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

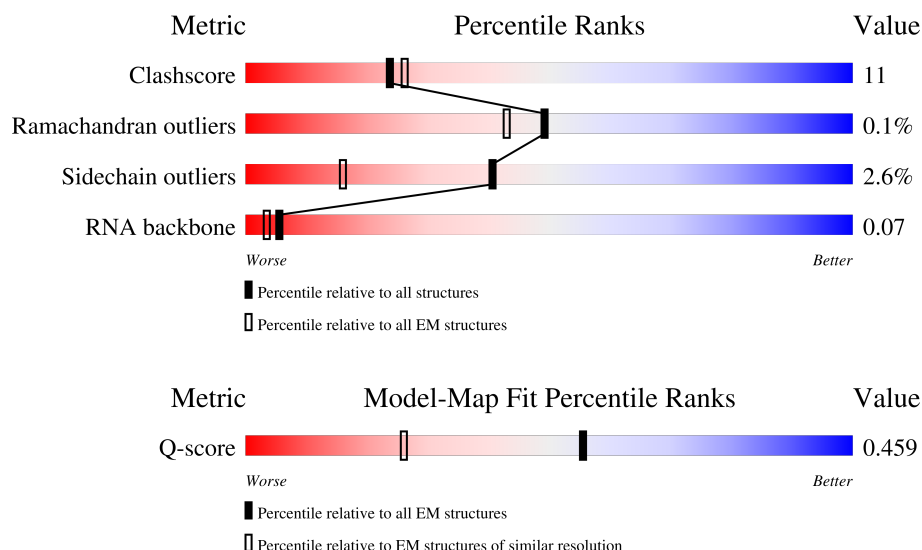
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	61	
2	F	378	
2	G	378	

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Mol	Chain	Length	Quality of chain
2	H	378	77%21%..
2	I	378	5% 72%26%..
2	J	378	8% 71%26%..
2	K	378	13% 66%25%9%
3	B	388	23% 44%15%41%
4	M	60	17% 47%8%45%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19297 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	P	0	0
			879	393	162	284	40		

- Molecule 2 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	368	Total	C	N	O	S	0	0
			2819	1782	489	536	12		
2	H	375	Total	C	N	O	S	0	0
			2878	1812	503	551	12		
2	I	373	Total	C	N	O	S	0	0
			2854	1800	498	544	12		
2	J	374	Total	C	N	O	S	0	0
			2845	1794	496	543	12		
2	K	344	Total	C	N	O	S	0	0
			2646	1670	468	497	11		
2	G	255	Total	C	N	O	S	0	0
			1927	1220	336	363	8		

- Molecule 3 is a protein called CRISPR system Cascade subunit CasD.

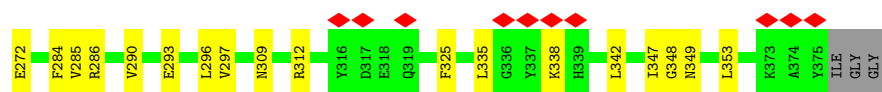
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	228	Total	C	N	O	S	0	0
			1780	1139	321	313	7		

There is a discrepancy between the modelled and reference sequences:

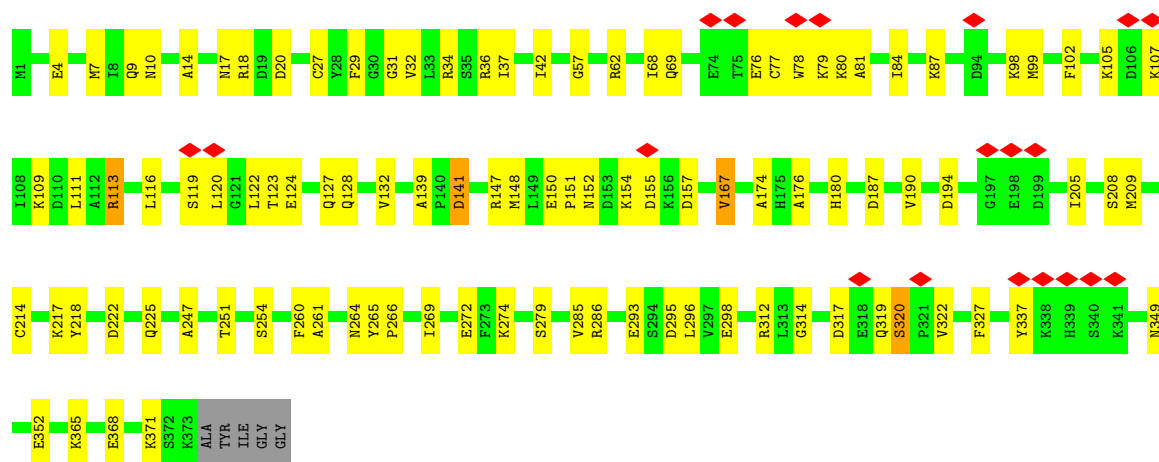
Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	ALA	conflict	UNP A0A1V6F8C5

- Molecule 4 is a DNA chain called DNA (60-MER).

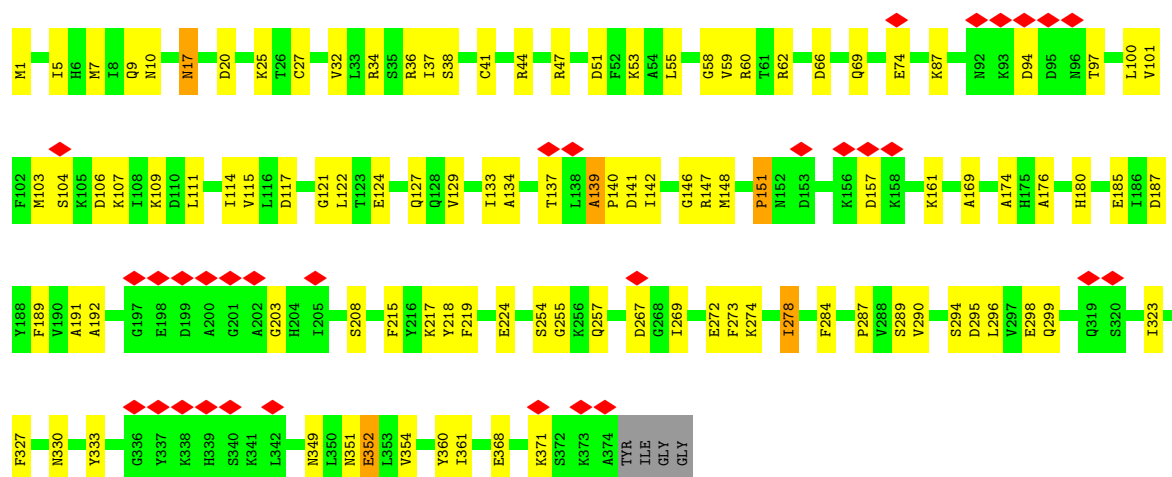
Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	33	Total 669	C 319	N 119	O 198	P 33	0	0



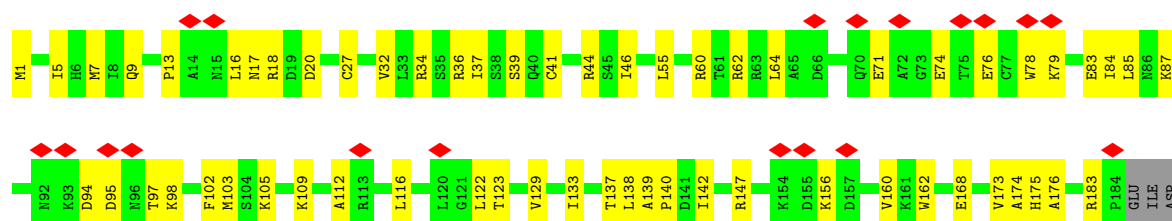
• Molecule 2: CRISPR system Cascade subunit CasC

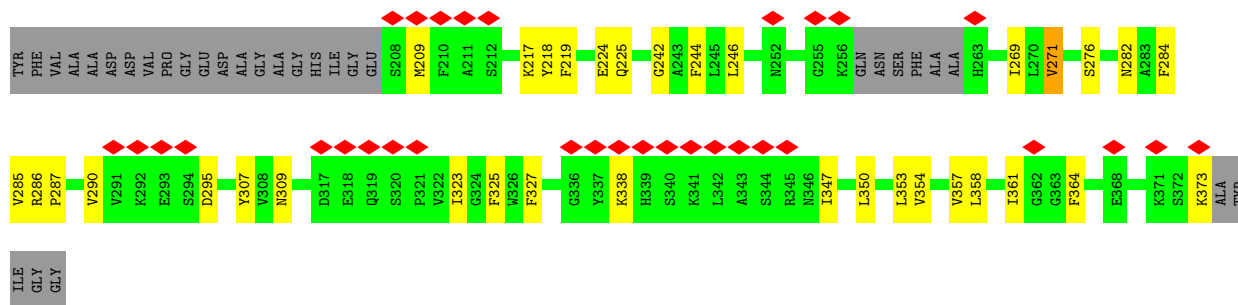


• Molecule 2: CRISPR system Cascade subunit CasC

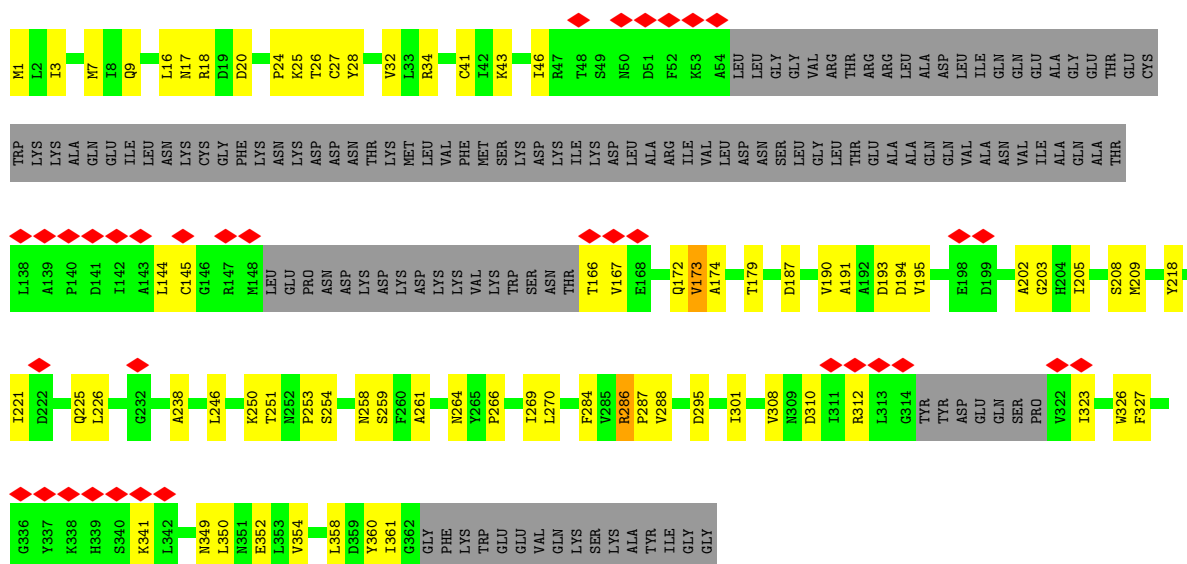


• Molecule 2: CRISPR system Cascade subunit CasC

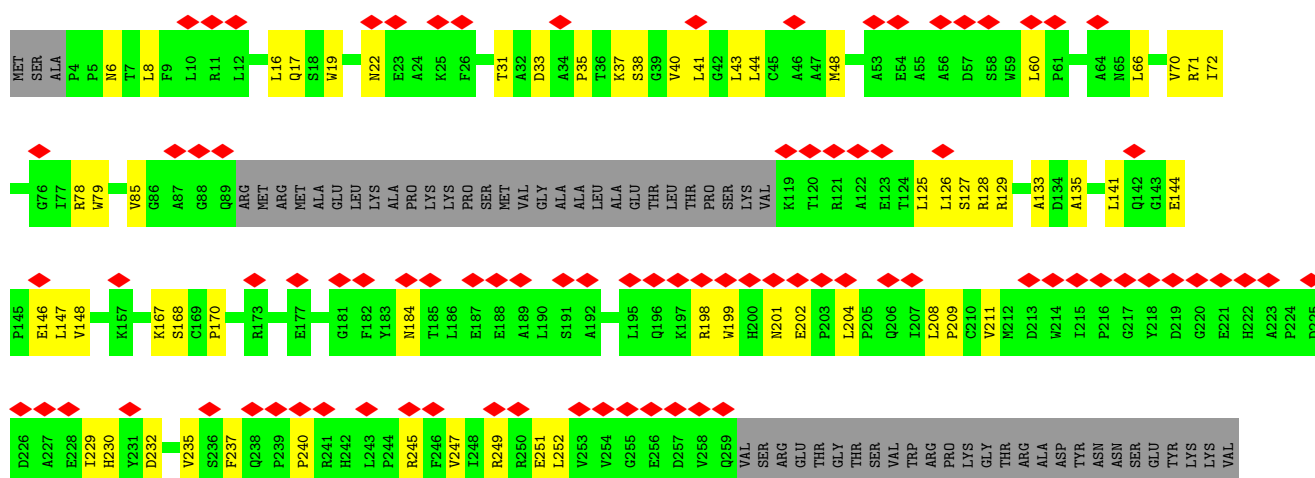
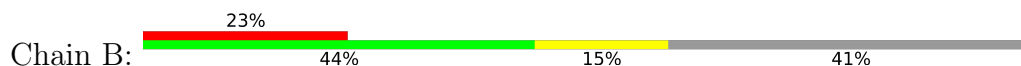




• Molecule 2: CRISPR system Cascade subunit CasC



• Molecule 3: CRISPR system Cascade subunit CasD



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

THR
ASN
ARG
ILE
ASP
PRO
CYS
ASP
PRO
ILE
TRP
ARG
GLU
ARG
ILE
LEU
ALA
LYS
ARG
LYS
GLU
ILE
VAL
GLU
PHE
ARG
SER
ARG
GLY
GLN
R377
PHE
ARG
LYS
MET
LYS
PRO
GLU
GLU
ASN
GLY

● Molecule 4: DNA (60-MER)



DC
DG
DA
DG
DA
DG
DC
DT
DT
DG
DA
DC
DA
DT
DT
DG
DT
DT
G20
G21
A24
A29
A33
A34
T35
T36
T37
C43
G44
A48
T49
C50
C51
T52
DT
DA
DC
DC
DA
DG
DC
DT

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.205	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.124	Depositor
Map size ($\text{\AA}$)	290.88, 290.88, 290.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	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	0.14	0/984	0.35	0/1534
2	F	0.13	0/2875	0.32	0/3900
2	G	0.13	0/1967	0.34	0/2670
2	H	0.13	0/2934	0.28	0/3977
2	I	0.14	0/2911	0.33	0/3949
2	J	0.15	0/2901	0.35	0/3937
2	K	0.15	0/2695	0.37	0/3648
3	B	0.15	0/1829	0.37	0/2491
4	M	0.19	0/748	0.37	0/1150
All	All	0.14	0/19844	0.34	0/27256

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	879	0	444	29	0
2	F	2819	0	2745	61	0
2	G	1927	0	1854	52	0
2	H	2878	0	2805	61	0
2	I	2854	0	2766	69	0
2	J	2845	0	2746	79	0
2	K	2646	0	2603	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1780	0	1762	40	0
4	M	669	0	372	4	0
All	All	19297	0	18097	407	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 (407) 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:J:272:GLU:OE2	2:J:274:LYS:NZ	2.10	0.84
1:A:6:C:N4	1:A:8:G:N7	2.29	0.81
2:F:44:ARG:HH22	2:G:194:ASP:HB3	1.44	0.81
2:F:295:ASP:HB3	2:H:286:ARG:HG2	1.62	0.81
2:J:55:LEU:HB3	2:J:140:PRO:HG2	1.64	0.80
1:A:7:C:O2'	2:F:18:ARG:NH1	2.16	0.79
2:F:49:SER:HB2	2:F:251:THR:HG21	1.65	0.78
2:J:187:ASP:OD1	2:K:36:ARG:NH1	2.16	0.77
2:I:349:ASN:HB3	2:I:352:GLU:HG3	1.68	0.76
2:F:68:ILE:HG21	2:F:116:LEU:HD21	1.69	0.74
2:F:103:MET:HE3	2:F:133:ILE:HD13	1.69	0.74
2:H:9:GLN:HE22	2:H:252:ASN:HD21	1.36	0.73
2:H:114:ILE:HD13	2:H:128:GLN:HB3	1.71	0.73
2:J:295:ASP:HB3	2:K:286:ARG:HG2	1.70	0.72
2:J:103:MET:HG3	2:J:104:SER:H	1.55	0.72
2:K:168:GLU:OE2	2:K:225:GLN:NE2	2.22	0.71
2:I:9:GLN:NE2	2:I:264:ASN:O	2.23	0.70
2:I:84:ILE:HD12	2:I:116:LEU:HD12	1.72	0.70
2:K:7:MET:HG3	2:K:217:LYS:HB2	1.72	0.69
1:A:21:G:OP2	2:I:18:ARG:NH2	2.27	0.68
2:J:139:ALA:HB3	2:J:142:ILE:HD12	1.75	0.68
3:B:72:ILE:HD12	3:B:209:PRO:HB2	1.74	0.67
1:A:1:G:OP1	2:G:25:LYS:NZ	2.27	0.67
2:I:102:PHE:O	2:I:147:ARG:NH1	2.27	0.67
2:J:59:VAL:H	2:J:104:SER:HB2	1.59	0.66
2:J:111:LEU:O	2:J:115:VAL:HG23	1.95	0.66
2:F:1:MET:HE1	2:F:361:ILE:HG23	1.78	0.66
2:F:127:GLN:HE21	2:F:161:LYS:H	1.44	0.65
2:K:37:ILE:HB	2:K:176:ALA:HB3	1.77	0.65
2:F:174:ALA:HB2	2:G:261:ALA:HB3	1.77	0.65
3:B:249:ARG:NH1	3:B:251:GLU:OE2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:ARG:NH1	2:F:165:THR:O	2.30	0.64
2:F:24:PRO:HD3	2:F:209:MET:HB3	1.79	0.64
2:H:261:ALA:HB3	2:I:174:ALA:HB2	1.79	0.64
2:F:103:MET:HE1	2:F:108:ILE:HB	1.81	0.63
2:F:172:GLN:HG2	2:G:258:ASN:HA	1.80	0.63
2:J:134:ALA:HA	2:J:147:ARG:HH22	1.63	0.63
2:K:32:VAL:HG21	2:K:287:PRO:HG3	1.80	0.63
2:I:286:ARG:HG3	2:I:286:ARG:HH11	1.64	0.63
2:H:7:MET:HG3	2:H:269:ILE:HG12	1.82	0.62
2:I:7:MET:HE3	2:I:266:PRO:HG3	1.81	0.62
2:G:9:GLN:NE2	2:G:264:ASN:O	2.31	0.62
3:B:85:VAL:HB	3:B:125:LEU:HB2	1.82	0.61
2:F:9:GLN:NE2	2:F:264:ASN:O	2.32	0.61
2:F:195:VAL:O	2:H:63:ARG:NH1	2.33	0.61
2:F:102:PHE:HB3	2:F:147:ARG:HD3	1.82	0.61
2:K:269:ILE:HB	2:K:327:PHE:HD2	1.66	0.61
2:F:338:LYS:HD2	2:F:339:HIS:N	2.16	0.60
2:K:16:LEU:HD22	2:K:37:ILE:HD11	1.83	0.60
2:I:4:GLU:OE1	2:I:218:TYR:OH	2.16	0.60
2:G:323:ILE:HD11	2:G:360:TYR:HE2	1.66	0.60
2:I:76:GLU:OE1	2:I:76:GLU:N	2.34	0.60
3:B:127:SER:HB2	3:B:129:ARG:HE	1.65	0.60
3:B:17:GLN:NE2	3:B:135:ALA:O	2.35	0.60
2:F:180:HIS:HD2	2:F:183:ARG:HH22	1.50	0.60
2:H:9:GLN:NE2	2:H:264:ASN:O	2.35	0.60
2:F:358:LEU:HA	2:F:361:ILE:HD12	1.83	0.59
2:I:368:GLU:HA	2:I:371:LYS:HZ3	1.67	0.59
2:G:221:ILE:HD11	2:G:226:LEU:HD12	1.84	0.59
2:J:59:VAL:N	2:J:104:SER:HB2	2.17	0.59
2:J:60:ARG:HG2	2:J:100:LEU:HD22	1.84	0.59
2:F:261:ALA:HB3	2:H:174:ALA:HB2	1.85	0.59
2:K:156:LYS:HZ1	2:K:162:TRP:CD1	2.21	0.58
2:J:191:ALA:HB3	2:J:203:GLY:HA3	1.86	0.58
2:G:269:ILE:HD12	2:G:327:PHE:CD2	2.38	0.58
3:B:31:THR:O	3:B:78:ARG:NH2	2.36	0.58
2:J:94:ASP:OD1	2:J:94:ASP:N	2.37	0.58
2:J:323:ILE:HD11	2:J:360:TYR:HE2	1.67	0.58
2:H:9:GLN:HE22	2:H:252:ASN:ND2	2.02	0.58
1:A:9:U:OP2	2:F:18:ARG:NH2	2.37	0.58
2:K:64:LEU:HD12	2:K:85:LEU:HD21	1.84	0.58
2:I:7:MET:HG2	2:I:269:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:G:OP2	2:I:190:VAL:N	2.35	0.57
2:J:38:SER:OG	2:J:41:CYS:SG	2.56	0.57
2:J:69:GLN:O	2:J:69:GLN:NE2	2.33	0.57
2:J:323:ILE:HD11	2:J:360:TYR:CE2	2.39	0.57
3:B:144:GLU:OE1	3:B:146:GLU:N	2.37	0.57
3:B:71:ARG:HE	3:B:208:LEU:HD11	1.69	0.57
2:I:20:ASP:N	2:I:20:ASP:OD1	2.34	0.57
2:J:294:SER:OG	2:J:298:GLU:OE1	2.20	0.57
2:H:247:ALA:O	2:H:251:THR:HG22	2.05	0.57
2:G:26:THR:O	3:B:79:TRP:NE1	2.32	0.57
1:A:13:G:H22	2:F:205:ILE:HD11	1.69	0.57
2:G:27:CYS:SG	2:G:28:TYR:N	2.78	0.57
1:A:30:G:O2'	2:K:41:CYS:SG	2.63	0.57
2:I:7:MET:HB2	2:I:217:LYS:HB2	1.87	0.56
3:B:70:VAL:HB	3:B:211:VAL:HB	1.87	0.56
2:I:265:TYR:CE2	2:J:278:ILE:HD11	2.40	0.56
2:K:112:ALA:O	2:K:116:LEU:HG	2.05	0.56
2:G:17:ASN:HB3	2:G:25:LYS:HG3	1.86	0.56
1:A:7:C:H4'	1:A:8:G:OP1	2.05	0.56
2:H:103:MET:HE2	2:H:133:ILE:HG12	1.88	0.56
1:A:-6:U:O2'	3:B:38:SER:OG	2.17	0.56
2:F:62:ARG:HD2	2:G:202:ALA:HB1	1.86	0.56
2:G:350:LEU:O	2:G:354:VAL:HG23	2.05	0.55
3:B:229:ILE:O	3:B:230:HIS:ND1	2.38	0.55
2:I:222:ASP:HB3	2:I:225:GLN:HB3	1.87	0.55
2:I:261:ALA:HB3	2:J:174:ALA:HB2	1.86	0.55
2:J:1:MET:HE1	2:J:273:PHE:HB3	1.88	0.55
2:H:64:LEU:HD21	2:H:103:MET:HE1	1.89	0.55
1:A:-7:G:H22	2:G:225:GLN:HG3	1.72	0.55
3:B:40:VAL:O	3:B:44:LEU:HD22	2.05	0.55
2:K:102:PHE:HB3	2:K:147:ARG:HD3	1.88	0.55
3:B:48:MET:N	3:B:48:MET:HE2	2.21	0.55
2:I:174:ALA:HB3	2:I:218:TYR:HB3	1.88	0.55
2:J:157:ASP:OD1	2:J:157:ASP:N	2.40	0.54
2:K:78:TRP:HE3	2:K:79:LYS:HD2	1.72	0.54
2:H:46:ILE:O	2:H:49:SER:OG	2.22	0.54
2:H:325:PHE:HD2	2:H:347:ILE:HD11	1.72	0.54
2:J:32:VAL:HG21	2:J:287:PRO:HG3	1.89	0.54
2:H:41:CYS:SG	2:H:253:PRO:HB3	2.48	0.54
2:I:99:MET:HB3	4:M:34:DA:H4'	1.88	0.54
2:H:272:GLU:OE2	2:H:312:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:A:H2'	2:I:148:MET:HG3	1.90	0.54
2:H:34:ARG:NH2	2:H:284:PHE:O	2.39	0.54
2:J:121:GLY:N	2:J:124:GLU:OE2	2.32	0.54
2:G:269:ILE:HD12	2:G:327:PHE:HD2	1.72	0.53
2:H:254:SER:HA	2:H:257:GLN:HG3	1.90	0.53
2:H:17:ASN:HB3	2:H:25:LYS:HG3	1.90	0.53
2:G:187:ASP:HB3	2:G:208:SER:HB2	1.91	0.53
3:B:199:TRP:NE1	3:B:201:ASN:O	2.41	0.53
2:I:190:VAL:HG12	2:I:205:ILE:HG12	1.91	0.53
3:B:6:ASN:OD1	3:B:6:ASN:N	2.41	0.53
2:F:37:ILE:HB	2:F:176:ALA:HB3	1.90	0.53
2:J:87:LYS:NZ	2:J:122:LEU:HB3	2.23	0.53
2:K:358:LEU:HD22	2:K:364:PHE:HB3	1.91	0.53
2:G:32:VAL:HG21	2:G:287:PRO:HG3	1.91	0.53
2:J:10:ASN:ND2	2:K:282:ASN:OD1	2.35	0.52
2:G:7:MET:HG2	2:G:269:ILE:HG23	1.91	0.52
2:G:43:LYS:HG3	2:G:173:VAL:HG11	1.91	0.52
2:I:62:ARG:NH2	2:I:98:LYS:O	2.38	0.52
2:H:24:PRO:HD3	2:H:209:MET:HB3	1.90	0.52
2:H:156:LYS:NZ	2:H:157:ASP:O	2.43	0.52
2:I:87:LYS:NZ	2:I:123:THR:HA	2.25	0.52
3:B:66:LEU:HD12	3:B:141:LEU:HB3	1.90	0.52
2:K:5:ILE:HG13	2:K:271:VAL:HG13	1.92	0.52
2:J:47:ARG:NH1	2:J:141:ASP:OD2	2.43	0.52
2:K:271:VAL:HG21	2:K:353:LEU:HD11	1.91	0.51
2:H:55:LEU:HD13	2:H:240:THR:HA	1.92	0.51
2:F:20:ASP:OD1	2:F:20:ASP:N	2.42	0.51
2:G:254:SER:O	2:G:254:SER:OG	2.29	0.51
2:G:270:LEU:HB2	2:G:326:TRP:HE3	1.76	0.51
2:J:103:MET:HG3	2:J:104:SER:N	2.23	0.51
4:M:24:DA:C8	4:M:24:DA:H5'	2.45	0.51
1:A:6:C:HO2'	2:F:41:CYS:HG	1.58	0.51
2:H:37:ILE:HB	2:H:176:ALA:HB3	1.93	0.51
1:A:-4:A:H2'	1:A:-3:A:H5''	1.92	0.50
2:H:57:GLY:O	2:H:105:LYS:N	2.39	0.50
2:H:94:ASP:OD1	2:H:94:ASP:N	2.44	0.50
2:K:64:LEU:HB2	2:K:85:LEU:HD11	1.91	0.50
2:F:84:ILE:HD12	2:F:87:LYS:HZ1	1.76	0.50
2:H:180:HIS:HD2	2:H:296:LEU:HD11	1.76	0.50
2:K:1:MET:SD	2:K:1:MET:N	2.74	0.50
2:F:273:PHE:HZ	2:F:357:VAL:HG13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:ASP:OD1	2:H:141:ASP:N	2.38	0.50
2:H:17:ASN:HD22	2:H:37:ILE:HG23	1.76	0.50
2:I:157:ASP:OD1	2:I:157:ASP:N	2.42	0.50
2:J:187:ASP:HB3	2:J:208:SER:HB3	1.93	0.50
3:B:204:LEU:HD12	3:B:204:LEU:H	1.77	0.50
2:F:180:HIS:HD2	2:F:183:ARG:NH2	2.10	0.50
2:I:107:LYS:O	2:I:111:LEU:HD23	2.11	0.50
2:J:17:ASN:HB3	2:J:25:LYS:HG3	1.91	0.50
2:K:55:LEU:HD22	2:K:140:PRO:HG3	1.93	0.50
2:I:99:MET:HE1	2:I:151:PRO:HA	1.93	0.49
2:J:20:ASP:OD1	2:J:20:ASP:N	2.41	0.49
1:A:13:G:N7	2:H:20:ASP:HA	2.27	0.49
2:F:58:GLY:HA2	2:F:104:SER:HA	1.94	0.49
1:A:13:G:N1	2:F:188:TYR:OH	2.44	0.49
1:A:29:A:C5	2:J:189:PHE:HE2	2.30	0.49
2:F:305:SER:HB3	2:F:335:LEU:HG	1.94	0.49
2:I:194:ASP:HB2	2:J:59:VAL:HG23	1.93	0.49
3:B:129:ARG:HD3	3:B:129:ARG:N	2.26	0.49
2:K:174:ALA:HB3	2:K:218:TYR:HB3	1.93	0.49
2:H:347:ILE:HG22	2:H:349:ASN:H	1.78	0.49
2:I:32:VAL:HG23	2:I:34:ARG:HE	1.77	0.49
2:K:20:ASP:N	2:K:20:ASP:OD1	2.46	0.49
2:I:247:ALA:O	2:I:251:THR:HG22	2.13	0.48
2:G:310:ASP:O	2:G:312:ARG:N	2.44	0.48
2:F:325:PHE:HB3	2:F:347:ILE:HD11	1.94	0.48
2:K:87:LYS:NZ	2:K:123:THR:OG1	2.42	0.48
2:J:254:SER:HA	2:J:257:GLN:HG3	1.96	0.48
2:K:83:GLU:HB3	2:K:122:LEU:HD11	1.96	0.48
2:H:297:VAL:HG23	2:I:285:VAL:HG21	1.96	0.48
2:F:32:VAL:HG21	2:F:287:PRO:HG3	1.96	0.48
2:H:32:VAL:HG23	2:H:34:ARG:HE	1.78	0.48
2:J:180:HIS:CD2	2:J:296:LEU:HD21	2.49	0.48
2:K:60:ARG:HG3	2:K:102:PHE:CD1	2.49	0.48
2:G:166:THR:OG1	2:G:167:VAL:N	2.45	0.48
2:I:27:CYS:HB3	2:I:36:ARG:HD3	1.96	0.48
2:G:144:LEU:HD12	2:G:145:CYS:H	1.78	0.48
1:A:12:G:N2	2:F:190:VAL:HG21	2.28	0.48
2:H:60:ARG:HG2	2:H:100:LEU:HD22	1.95	0.48
2:G:28:TYR:O	3:B:133:ALA:HB1	2.13	0.48
2:G:41:CYS:SG	2:G:253:PRO:HB3	2.54	0.48
2:J:127:GLN:OE1	2:J:161:LYS:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:237:PHE:HA	3:B:240:PRO:HA	1.95	0.47
3:B:230:HIS:HB3	3:B:232:ASP:OD1	2.13	0.47
2:F:180:HIS:CD2	2:F:183:ARG:HH22	2.30	0.47
2:H:55:LEU:HD21	2:H:239:HIS:ND1	2.29	0.47
2:I:141:ASP:OD1	2:I:141:ASP:N	2.36	0.47
2:G:190:VAL:HG12	2:G:205:ILE:HG23	1.97	0.47
3:B:198:ARG:N	3:B:202:GLU:OE2	2.46	0.47
2:I:80:LYS:O	2:I:84:ILE:HG13	2.15	0.47
2:J:58:GLY:HA3	2:J:141:ASP:OD2	2.15	0.47
2:K:13:PRO:HA	2:K:16:LEU:HG	1.97	0.47
2:K:242:GLY:O	2:K:246:LEU:HD23	2.14	0.47
2:G:179:THR:O	2:G:288:VAL:HG23	2.15	0.47
2:I:68:ILE:HG23	2:I:113:ARG:HG3	1.97	0.47
2:I:272:GLU:OE1	2:I:274:LYS:NZ	2.40	0.47
2:J:289:SER:O	2:J:299:GLN:NE2	2.45	0.47
2:G:16:LEU:HD22	2:G:253:PRO:HB2	1.94	0.47
2:K:209:MET:HA	2:K:209:MET:HE3	1.96	0.47
2:G:34:ARG:NH2	2:G:284:PHE:O	2.40	0.47
2:G:349:ASN:HB3	2:G:352:GLU:HG2	1.97	0.47
4:M:43:DC:H2'	4:M:44:DG:C4	2.50	0.47
2:F:315:TYR:OH	2:G:266:PRO:O	2.32	0.47
2:I:180:HIS:CD2	2:I:296:LEU:HD21	2.49	0.47
2:H:107:LYS:HG3	2:H:136:ALA:HB2	1.96	0.47
2:K:246:LEU:HA	2:K:350:LEU:HD21	1.97	0.47
2:I:295:ASP:OD1	2:I:298:GLU:HB3	2.16	0.46
2:J:330:ASN:CG	2:J:330:ASN:O	2.58	0.46
2:K:17:ASN:O	2:K:18:ARG:HD2	2.14	0.46
2:K:98:LYS:HB2	2:K:98:LYS:NZ	2.30	0.46
2:G:24:PRO:HD3	2:G:209:MET:HB3	1.98	0.46
2:F:46:ILE:HG23	2:F:247:ALA:HB3	1.96	0.46
2:H:147:ARG:HB3	2:H:167:VAL:HG12	1.97	0.46
2:K:325:PHE:HD2	2:K:357:VAL:HG12	1.81	0.46
2:F:53:LYS:HB2	2:F:53:LYS:NZ	2.31	0.46
2:I:187:ASP:HB3	2:I:208:SER:HB3	1.98	0.46
2:I:218:TYR:CE2	2:I:279:SER:HB2	2.50	0.46
2:J:27:CYS:HB3	2:J:36:ARG:HD3	1.97	0.46
2:J:146:GLY:H	2:J:169:ALA:HB2	1.80	0.46
2:G:191:ALA:HB3	2:G:203:GLY:HA3	1.98	0.46
2:G:286:ARG:HD2	2:G:286:ARG:HA	1.58	0.46
2:F:33:LEU:HD23	2:F:33:LEU:HA	1.80	0.46
2:H:69:GLN:OE1	2:H:69:GLN:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:103:MET:HE1	2:J:111:LEU:CD1	2.46	0.46
1:A:29:A:C6	2:J:189:PHE:HE2	2.34	0.46
2:H:309:ASN:HA	2:H:342:LEU:HD21	1.98	0.46
2:H:338:LYS:HE2	2:H:338:LYS:HB2	1.83	0.46
2:F:342:LEU:HD23	2:F:343:ALA:H	1.81	0.45
2:H:103:MET:HG2	2:H:104:SER:N	2.31	0.45
2:I:254:SER:O	2:I:254:SER:OG	2.33	0.45
2:H:347:ILE:HD13	2:H:353:LEU:HA	1.99	0.45
2:J:103:MET:HE3	2:J:133:ILE:HD13	1.98	0.45
2:J:62:ARG:NH1	2:J:97:THR:O	2.49	0.45
2:I:42:ILE:H	2:I:42:ILE:HG13	1.62	0.45
2:K:34:ARG:NH1	2:K:284:PHE:O	2.49	0.45
2:G:26:THR:HB	3:B:79:TRP:HZ2	1.82	0.45
1:A:8:G:H1'	1:A:9:U:H2'	1.97	0.45
2:I:78:TRP:CD1	2:I:79:LYS:HG3	2.52	0.45
2:G:193:ASP:O	2:G:195:VAL:HG13	2.17	0.45
2:I:14:ALA:HA	2:I:260:PHE:HB3	1.99	0.45
2:K:156:LYS:HE3	2:K:160:VAL:HG23	1.98	0.45
2:F:327:PHE:HB2	2:F:353:LEU:HD22	1.98	0.45
2:J:129:VAL:O	2:J:133:ILE:HG12	2.17	0.45
2:J:185:GLU:OE1	2:K:27:CYS:HA	2.17	0.45
2:H:144:LEU:HD22	2:H:171:LEU:HB2	1.99	0.45
2:J:51:ASP:OD1	2:J:51:ASP:N	2.50	0.45
2:J:111:LEU:HA	2:J:114:ILE:HD12	1.98	0.45
2:H:20:ASP:OD1	2:H:20:ASP:N	2.48	0.44
2:H:187:ASP:HB3	2:H:208:SER:HB2	2.00	0.44
2:I:81:ALA:HA	2:I:116:LEU:HD11	1.98	0.44
2:K:74:GLU:OE1	2:K:76:GLU:N	2.50	0.44
3:B:33:ASP:OD1	3:B:33:ASP:N	2.48	0.44
2:H:47:ARG:NH1	2:H:141:ASP:OD2	2.51	0.44
2:J:368:GLU:HA	2:J:371:LYS:HE3	1.98	0.44
2:K:183:ARG:HD2	2:K:183:ARG:N	2.33	0.44
3:B:8:LEU:HB2	3:B:148:VAL:HG13	1.99	0.44
2:H:293:GLU:CD	2:H:293:GLU:H	2.25	0.44
2:J:295:ASP:HB2	2:K:285:VAL:HG12	1.99	0.44
2:G:174:ALA:HB3	2:G:218:TYR:HB3	1.99	0.44
2:G:238:ALA:HB1	2:G:358:LEU:HD22	2.00	0.44
2:H:55:LEU:HD21	2:H:239:HIS:CE1	2.52	0.44
2:J:58:GLY:HA2	2:J:104:SER:O	2.17	0.44
3:B:37:LYS:HG3	3:B:41:LEU:HD13	1.99	0.44
2:G:174:ALA:HB2	3:B:170:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:211:VAL:HG13	3:B:247:VAL:HG13	1.99	0.44
2:F:149:LEU:O	2:F:165:THR:HG21	2.17	0.44
2:J:87:LYS:HZ3	2:J:122:LEU:HB3	1.82	0.44
2:J:224:GLU:OE1	2:J:224:GLU:HA	2.18	0.44
2:K:71:GLU:N	2:K:71:GLU:OE1	2.50	0.44
2:G:1:MET:HE1	2:G:361:ILE:HG12	1.98	0.44
2:G:246:LEU:O	2:G:250:LYS:HG2	2.17	0.44
2:K:102:PHE:CD2	2:K:142:ILE:HD13	2.53	0.43
2:K:224:GLU:N	2:K:224:GLU:OE1	2.51	0.43
2:I:37:ILE:HB	2:I:176:ALA:HB3	2.01	0.43
1:A:24:C:OP2	2:J:44:ARG:HG3	2.18	0.43
2:F:59:VAL:HB	2:F:105:LYS:HG3	2.00	0.43
2:I:319:GLN:HB3	2:I:320:SER:H	1.54	0.43
2:J:7:MET:HE2	2:J:217:LYS:HD2	2.00	0.43
2:F:78:TRP:NE1	2:F:82:GLN:HE21	2.16	0.43
2:I:119:SER:OG	2:I:120:LEU:N	2.51	0.43
2:I:152:ASN:OD1	2:I:154:LYS:N	2.47	0.43
1:A:1:G:N7	2:G:20:ASP:HA	2.34	0.43
2:H:309:ASN:HB2	2:H:342:LEU:HD11	2.00	0.43
2:I:29:PHE:HB3	2:I:34:ARG:HG3	2.01	0.43
2:I:319:GLN:OE1	2:I:320:SER:N	2.52	0.43
2:J:37:ILE:HB	2:J:176:ALA:HB3	2.01	0.43
2:J:66:ASP:OD1	2:J:66:ASP:N	2.51	0.43
2:K:103:MET:HE1	2:K:133:ILE:HD12	1.99	0.43
2:K:286:ARG:HB3	2:K:286:ARG:NH1	2.34	0.43
1:A:30:G:OP1	2:J:192:ALA:HB3	2.19	0.43
2:K:138:LEU:HD23	2:K:138:LEU:HA	1.79	0.43
2:H:156:LYS:HE3	2:H:156:LYS:HB3	1.83	0.43
2:I:298:GLU:OE2	2:I:337:TYR:OH	2.24	0.43
2:I:312:ARG:NH1	2:I:312:ARG:HG3	2.34	0.43
2:J:174:ALA:HB3	2:J:218:TYR:HB3	2.01	0.43
2:K:156:LYS:HZ1	2:K:162:TRP:HD1	1.63	0.43
2:G:295:ASP:OD1	2:G:295:ASP:N	2.51	0.43
2:F:113:ARG:HA	2:F:113:ARG:HD2	1.73	0.42
2:J:361:ILE:HD12	2:J:361:ILE:HA	1.81	0.42
2:K:137:THR:O	2:K:139:ALA:N	2.51	0.42
2:H:152:ASN:O	2:H:156:LYS:HB2	2.19	0.42
2:I:4:GLU:OE2	2:I:274:LYS:HD2	2.19	0.42
2:J:69:GLN:HE21	2:J:69:GLN:C	2.25	0.42
2:F:127:GLN:NE2	2:F:161:LYS:O	2.52	0.42
2:H:191:ALA:O	2:H:203:GLY:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:155:ASP:OD1	2:I:155:ASP:N	2.52	0.42
2:K:102:PHE:HD1	2:K:102:PHE:HA	1.79	0.42
2:J:269:ILE:HB	2:J:327:PHE:HD2	1.83	0.42
2:K:87:LYS:HZ1	2:K:123:THR:HG1	1.64	0.42
2:K:290:VAL:HG11	2:K:295:ASP:HB3	2.01	0.42
3:B:230:HIS:O	3:B:245:ARG:N	2.50	0.42
2:I:128:GLN:O	2:I:132:VAL:HG13	2.20	0.42
2:K:62:ARG:O	2:K:97:THR:OG1	2.32	0.42
2:F:180:HIS:HE1	2:F:214:CYS:H	1.66	0.42
2:F:325:PHE:CD1	2:F:345:ARG:HG2	2.54	0.42
2:F:357:VAL:HG12	2:F:361:ILE:HD11	2.01	0.42
2:H:51:ASP:OD1	2:H:51:ASP:N	2.53	0.42
2:H:193:ASP:OD2	2:I:62:ARG:HG2	2.20	0.42
2:J:106:ASP:O	2:J:109:LYS:NZ	2.51	0.42
2:I:57:GLY:O	2:I:139:ALA:HB1	2.20	0.42
2:K:105:LYS:HD2	2:K:105:LYS:HA	1.62	0.42
2:F:233:ASP:OD2	2:F:236:LEU:HB2	2.20	0.42
2:J:117:ASP:OD1	2:J:117:ASP:C	2.63	0.42
2:K:282:ASN:HB2	2:K:307:TYR:CZ	2.55	0.42
3:B:184:ASN:OD1	3:B:184:ASN:N	2.53	0.42
3:B:208:LEU:HD22	3:B:252:LEU:HB3	2.01	0.42
2:F:325:PHE:HD1	2:F:345:ARG:HG2	1.85	0.41
2:K:84:ILE:HG21	2:K:129:VAL:HG21	2.01	0.41
3:B:128:ARG:C	3:B:129:ARG:HD3	2.45	0.41
1:A:13:G:C4	1:A:14:A:N6	2.88	0.41
2:F:347:ILE:HG22	2:F:349:ASN:H	1.85	0.41
2:K:109:LYS:HD3	2:K:109:LYS:HA	1.83	0.41
2:K:129:VAL:O	2:K:133:ILE:HG12	2.21	0.41
2:K:373:LYS:HA	2:K:373:LYS:HD2	1.82	0.41
2:H:17:ASN:HD21	2:H:41:CYS:CB	2.32	0.41
2:H:290:VAL:HG21	2:I:31:GLY:HA3	2.02	0.41
2:J:351:ASN:O	2:J:354:VAL:HG12	2.19	0.41
2:J:368:GLU:OE1	2:J:368:GLU:N	2.48	0.41
2:K:9:GLN:OE1	2:K:217:LYS:NZ	2.53	0.41
1:A:7:C:OP2	2:G:190:VAL:HG22	2.20	0.41
2:F:120:LEU:HD12	2:F:121:GLY:H	1.85	0.41
2:I:365:LYS:HB2	2:I:368:GLU:OE1	2.20	0.41
2:G:270:LEU:HB2	2:G:326:TRP:CE3	2.55	0.41
2:G:341:LYS:HA	2:G:341:LYS:HD2	1.73	0.41
3:B:144:GLU:CD	3:B:147:LEU:H	2.28	0.41
1:A:3:U:OP2	2:G:18:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:GLY:O	2:I:314:GLY:HA2	2.20	0.41
2:I:10:ASN:HA	2:I:214:CYS:HA	2.02	0.41
2:I:105:LYS:O	2:I:109:LYS:HB2	2.21	0.41
2:I:122:LEU:C	2:I:124:GLU:H	2.29	0.41
2:J:349:ASN:O	2:J:352:GLU:HG2	2.21	0.41
2:K:94:ASP:OD1	2:K:95:ASP:N	2.44	0.41
2:K:246:LEU:CD2	2:K:354:VAL:HG21	2.50	0.41
3:B:19:TRP:CG	3:B:35:PRO:HA	2.55	0.41
3:B:60:LEU:HG	3:B:235:VAL:HG23	2.01	0.41
1:A:27:U:OP2	2:J:255:GLY:HA2	2.20	0.41
2:I:293:GLU:N	2:I:293:GLU:OE1	2.53	0.41
2:J:59:VAL:H	2:J:104:SER:CB	2.29	0.41
2:G:360:TYR:CD1	2:G:360:TYR:C	2.99	0.41
3:B:144:GLU:OE1	3:B:144:GLU:C	2.63	0.41
1:A:10:C:C4	2:H:148:MET:HE3	2.56	0.41
2:F:78:TRP:CE2	2:F:82:GLN:NE2	2.89	0.41
2:H:19:ASP:OD1	2:H:19:ASP:N	2.38	0.41
2:H:149:LEU:HD12	2:H:149:LEU:HA	1.96	0.41
2:I:69:GLN:HB2	2:I:77:CYS:HB2	2.01	0.41
2:I:209:MET:HE2	2:I:209:MET:HB2	2.01	0.41
2:J:5:ILE:HB	2:J:219:PHE:HB2	2.02	0.41
2:K:39:SER:HB2	2:K:175:HIS:CD2	2.56	0.41
2:G:144:LEU:HD12	2:G:145:CYS:N	2.35	0.41
3:B:35:PRO:HD2	3:B:70:VAL:HG11	2.02	0.41
2:F:274:LYS:HE3	2:F:278:ILE:HB	2.03	0.41
2:J:9:GLN:O	2:J:215:PHE:N	2.45	0.41
2:J:103:MET:HE1	2:J:111:LEU:HD13	2.02	0.41
2:J:107:LYS:NZ	2:J:107:LYS:HB3	2.35	0.41
2:J:267:ASP:HB2	2:J:333:TYR:CE1	2.56	0.41
2:K:173:VAL:HG22	2:K:219:PHE:HD1	1.85	0.41
2:J:34:ARG:NH1	2:J:284:PHE:O	2.52	0.40
2:J:349:ASN:HB3	2:J:352:GLU:CD	2.45	0.40
2:K:46:ILE:HD13	2:K:244:PHE:CE1	2.56	0.40
2:G:3:ILE:HB	2:G:221:ILE:HG23	2.02	0.40
3:B:167:LYS:HB2	3:B:167:LYS:HE3	1.90	0.40
2:F:150:GLU:O	2:F:150:GLU:HG3	2.21	0.40
2:F:280:TYR:CZ	2:F:308:VAL:HG22	2.56	0.40
2:G:27:CYS:SG	3:B:16:LEU:HD21	2.62	0.40
1:A:30:G:O4'	2:K:44:ARG:HD3	2.21	0.40
2:F:297:VAL:HG23	2:H:285:VAL:HG11	2.03	0.40
2:F:310:ASP:OD1	2:F:310:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:335:LEU:HD23	2:H:335:LEU:HA	1.92	0.40
2:J:151:PRO:O	4:M:29:DA:H2''	2.22	0.40
2:F:144:LEU:HD22	2:F:171:LEU:HB2	2.03	0.40
2:K:7:MET:HB3	2:K:269:ILE:HG12	2.03	0.40
2:I:147:ARG:N	2:I:167:VAL:HG22	2.36	0.40
2:I:269:ILE:HB	2:I:327:PHE:HD2	1.86	0.40
2:J:295:ASP:C	2:J:295:ASP:OD1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	364/378 (96%)	350 (96%)	14 (4%)	0	100	100
2	G	247/378 (65%)	235 (95%)	12 (5%)	0	100	100
2	H	373/378 (99%)	349 (94%)	24 (6%)	0	100	100
2	I	371/378 (98%)	339 (91%)	31 (8%)	1 (0%)	36	66
2	J	372/378 (98%)	343 (92%)	27 (7%)	2 (0%)	24	55
2	K	338/378 (89%)	317 (94%)	21 (6%)	0	100	100
3	B	223/388 (58%)	214 (96%)	9 (4%)	0	100	100
All	All	2288/2656 (86%)	2147 (94%)	138 (6%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	151	PRO
2	J	139	ALA
2	I	322	VAL

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	
2	F	295/313 (94%)	290 (98%)	5 (2%)	53	83
2	G	199/313 (64%)	191 (96%)	8 (4%)	28	63
2	H	302/313 (96%)	295 (98%)	7 (2%)	44	78
2	I	297/313 (95%)	289 (97%)	8 (3%)	39	74
2	J	293/313 (94%)	284 (97%)	9 (3%)	35	70
2	K	279/313 (89%)	272 (98%)	7 (2%)	42	76
3	B	183/323 (57%)	179 (98%)	4 (2%)	45	78
All	All	1848/2201 (84%)	1800 (97%)	48 (3%)	41	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	1	MET
2	F	12	SER
2	F	17	ASN
2	F	32	VAL
2	F	259	SER
2	H	7	MET
2	H	64	LEU
2	H	102	PHE
2	H	122	LEU
2	H	124	GLU
2	H	138	LEU
2	H	141	ASP
2	I	17	ASN
2	I	113	ARG
2	I	127	GLN
2	I	141	ASP
2	I	150	GLU
2	I	167	VAL
2	I	317	ASP
2	I	320	SER

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Mol	Chain	Res	Type
2	J	17	ASN
2	J	53	LYS
2	J	74	GLU
2	J	101	VAL
2	J	137	THR
2	J	148	MET
2	J	278	ILE
2	J	290	VAL
2	J	352	GLU
2	K	271	VAL
2	K	276	SER
2	K	309	ASN
2	K	323	ILE
2	K	338	LYS
2	K	347	ILE
2	K	361	ILE
2	G	46	ILE
2	G	172	GLN
2	G	173	VAL
2	G	251	THR
2	G	259	SER
2	G	286	ARG
2	G	301	ILE
2	G	308	VAL
3	B	22	ASN
3	B	43	LEU
3	B	126	LEU
3	B	168	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	82	GLN
2	F	180	HIS
2	F	306	ASN
2	F	339	HIS
2	F	351	ASN
2	H	9	GLN
2	H	17	ASN
2	H	82	GLN
2	H	96	ASN
2	H	118	ASN

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Mol	Chain	Res	Type
2	H	204	HIS
2	H	252	ASN
2	I	82	GLN
2	I	128	GLN
2	I	204	HIS
2	I	225	GLN
2	I	275	ASN
2	J	6	HIS
2	J	82	GLN
2	J	92	ASN
2	J	172	GLN
2	J	309	ASN
2	J	331	ASN
2	K	92	ASN
2	K	96	ASN
2	K	131	ASN
2	K	306	ASN
2	G	346	ASN
3	B	17	GLN
3	B	22	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	40/61 (65%)	23 (57%)	2 (5%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-6	U
1	A	-5	G
1	A	-3	A
1	A	1	G
1	A	2	A
1	A	8	G
1	A	9	U
1	A	10	C
1	A	11	A
1	A	12	G
1	A	13	G
1	A	14	A

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Mol	Chain	Res	Type
1	A	16	A
1	A	19	A
1	A	23	G
1	A	25	G
1	A	26	C
1	A	27	U
1	A	28	U
1	A	29	A
1	A	31	C
1	A	32	A
1	A	33	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	C
1	A	9	U

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-60330. These allow visual inspection of the internal detail of the map and identification of artifacts.

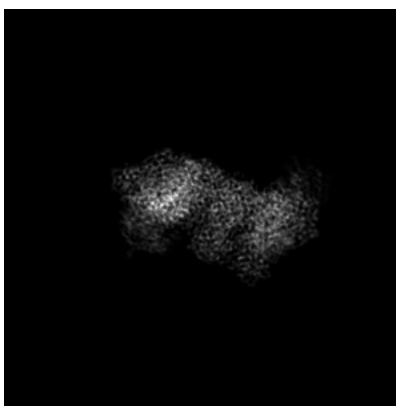
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

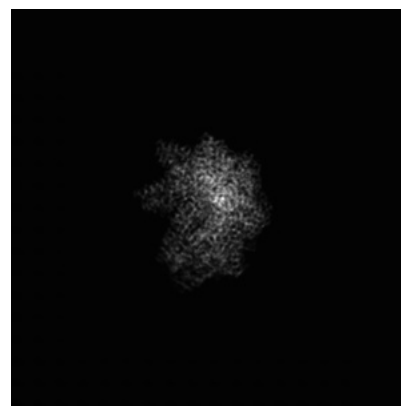
6.1.1 Primary map



X

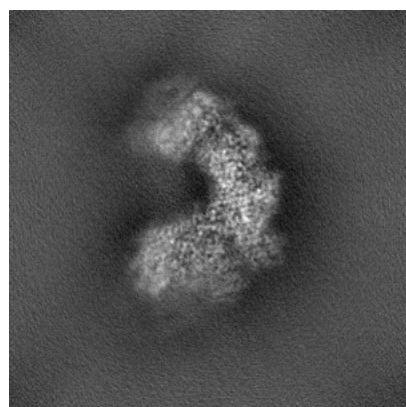


Y

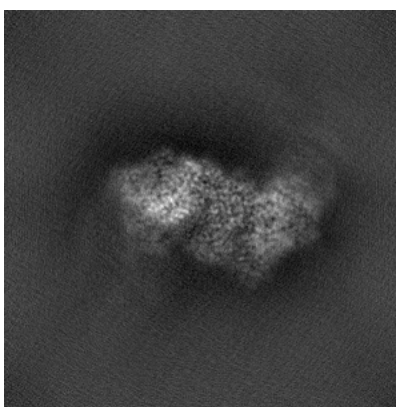


Z

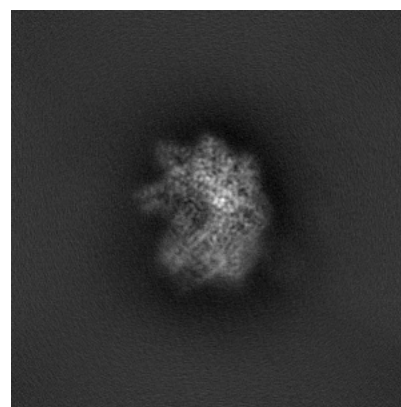
6.1.2 Raw map



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: 180

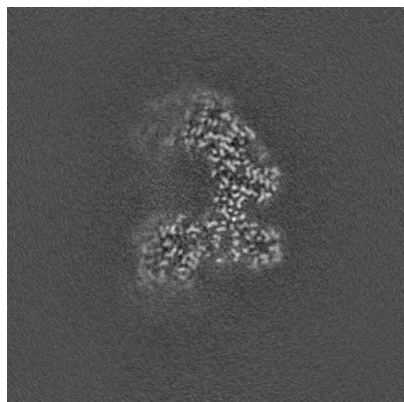


Y Index: 180

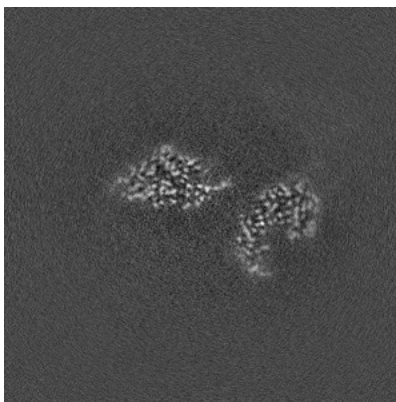


Z Index: 180

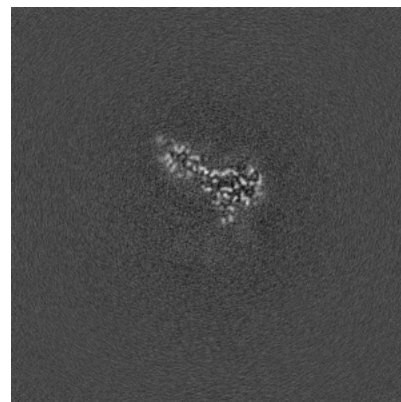
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 191

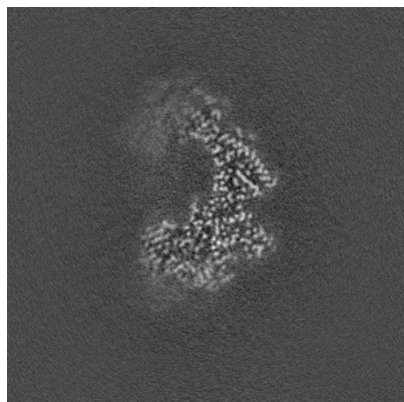


Y Index: 189

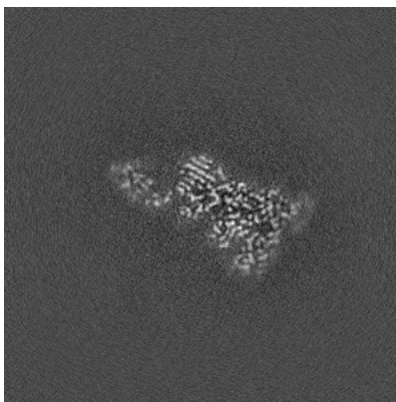


Z Index: 150

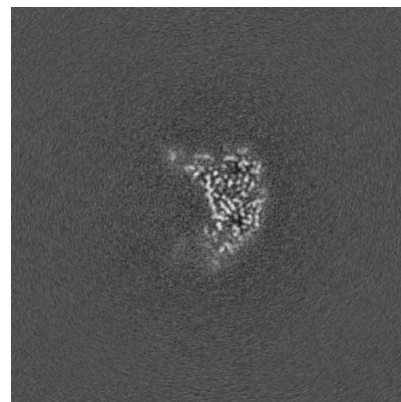
6.3.2 Raw map



X Index: 190



Y Index: 200



Z Index: 165

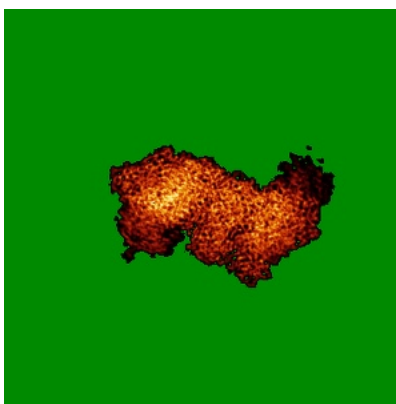
The images above show the largest variance slices of the map in three orthogonal directions.

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

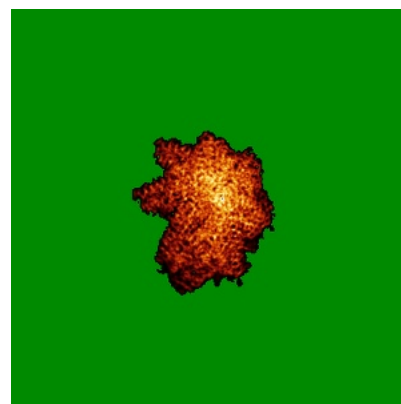
6.4.1 Primary map



X

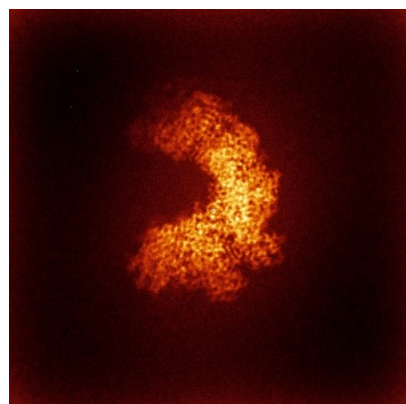


Y

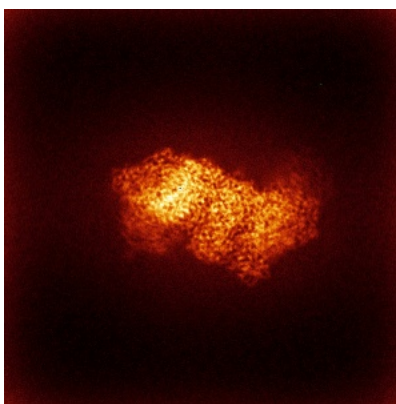


Z

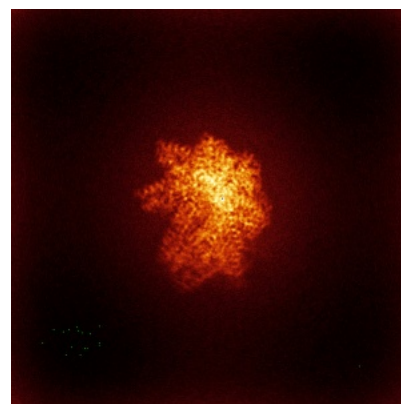
6.4.2 Raw map



X



Y

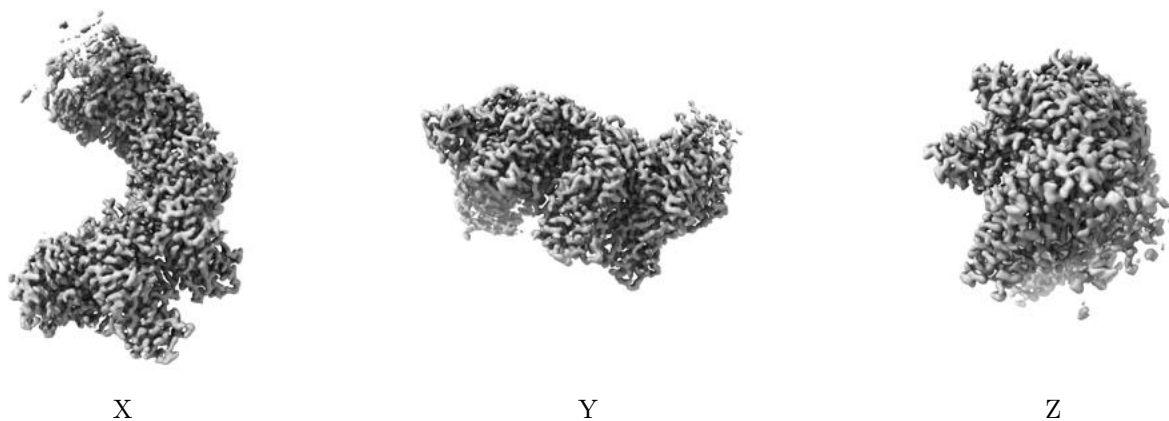


Z

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.

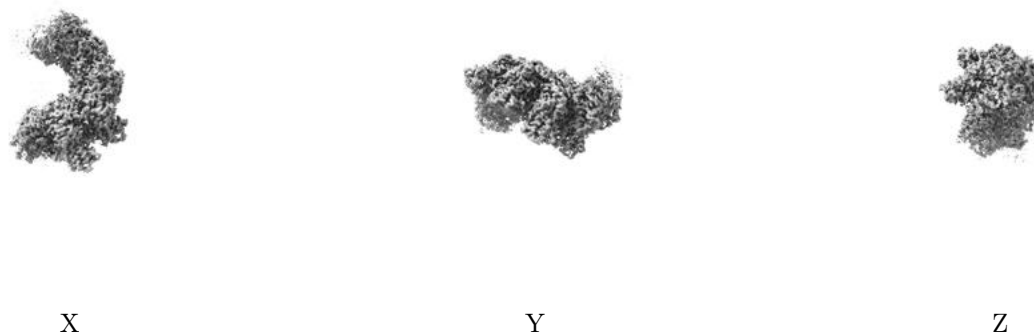
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.124. 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.

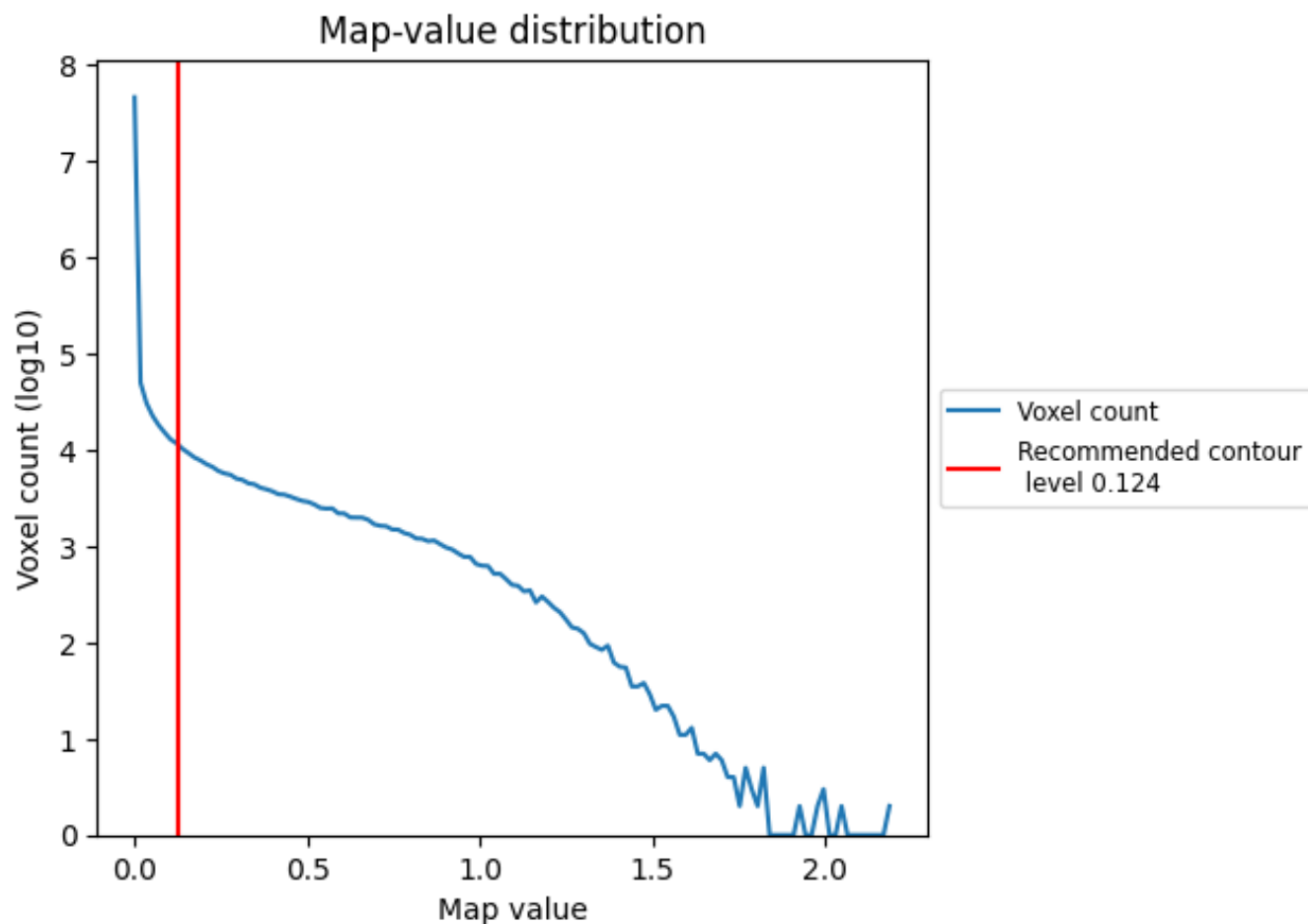
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

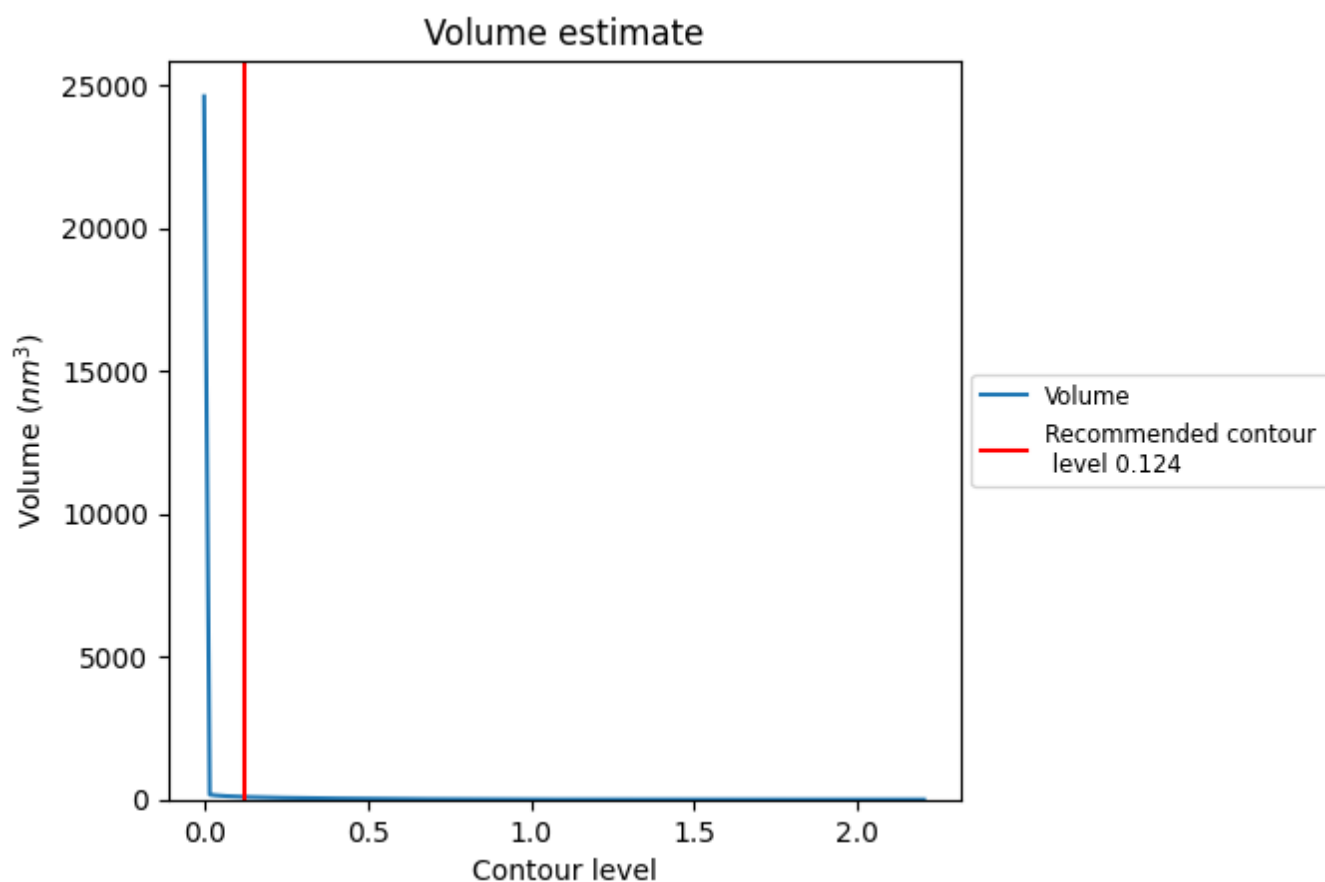
This section contains the results of statistical analysis of the map.

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.

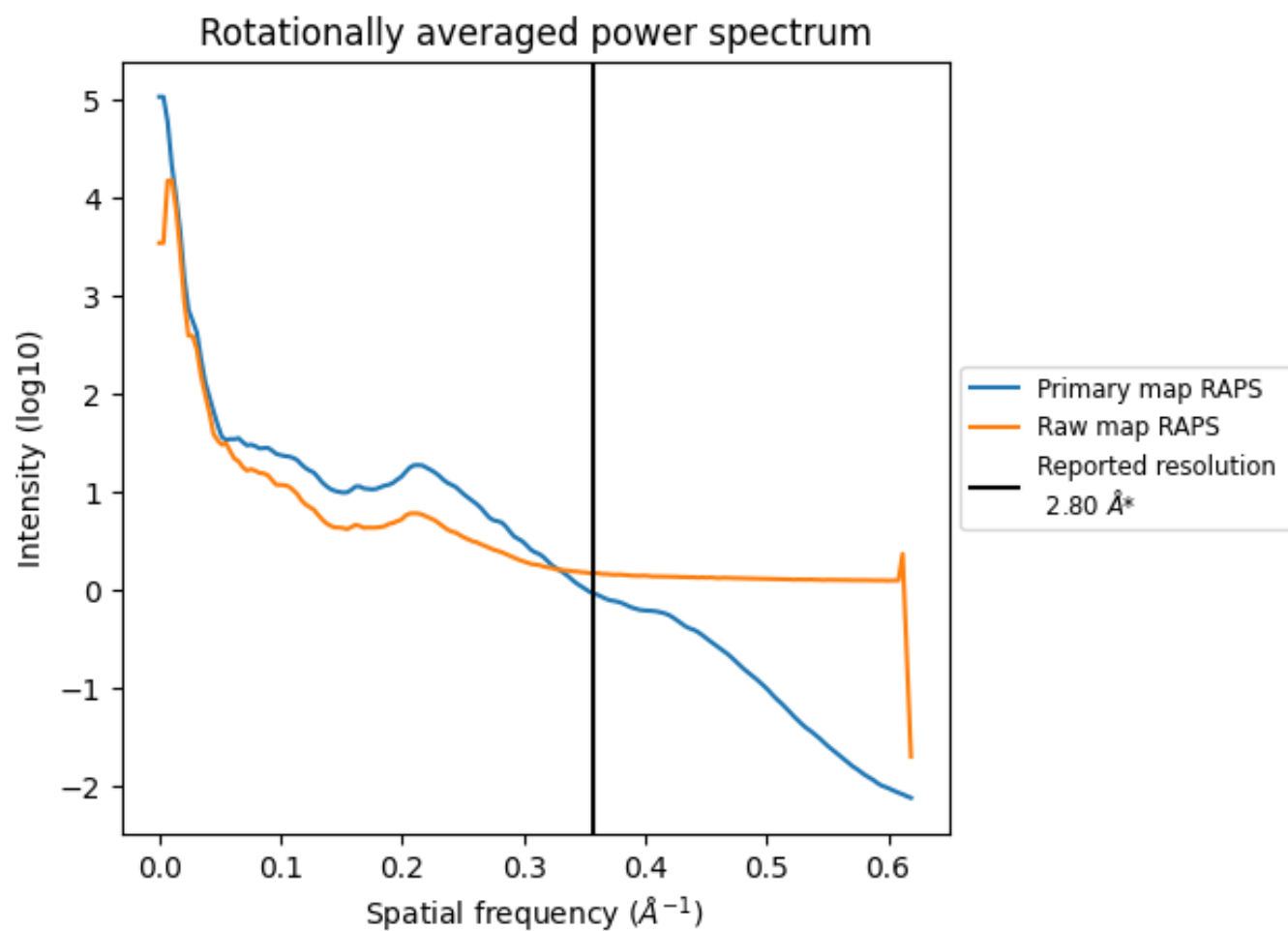
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

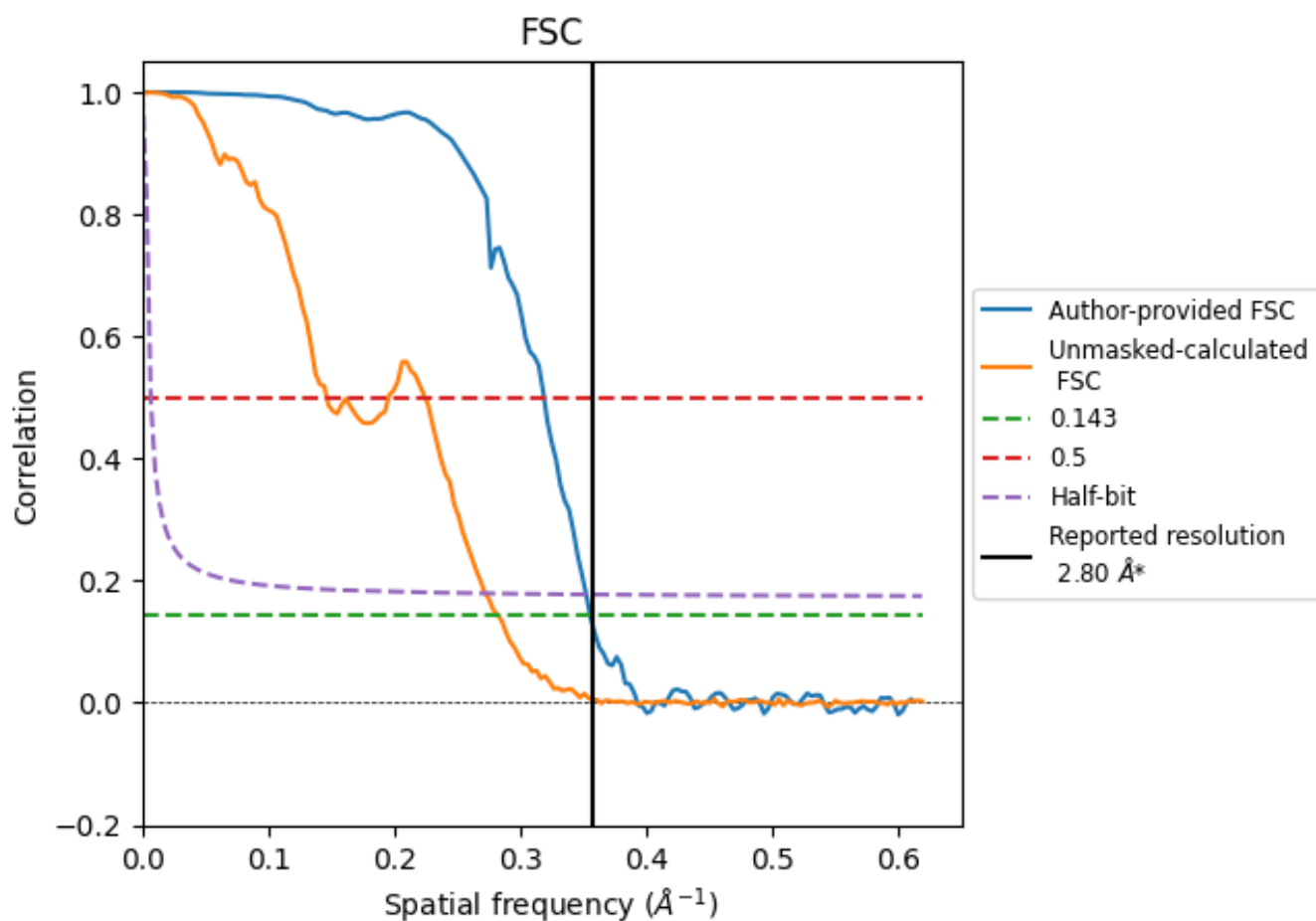


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

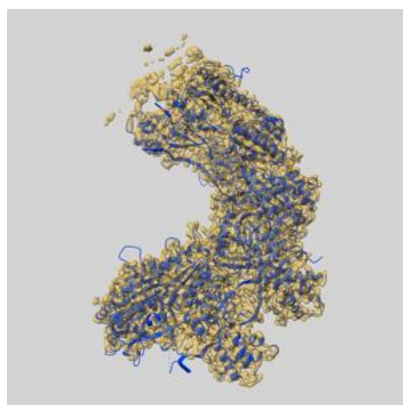
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.14	2.84
Unmasked-calculated*	3.54	6.83	3.67

*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 3.54 differs from the reported value 2.8 by more than 10 %

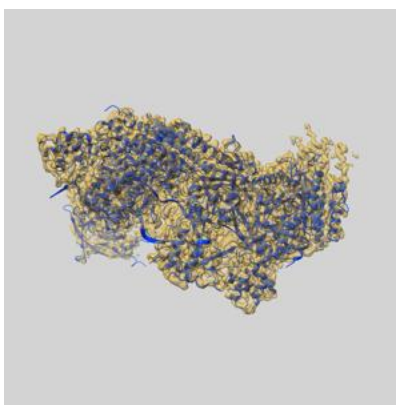
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60330 and PDB model 8ZP9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

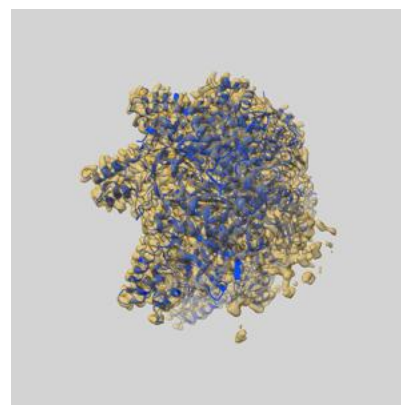
9.1 Map-model overlay [i](#)



X



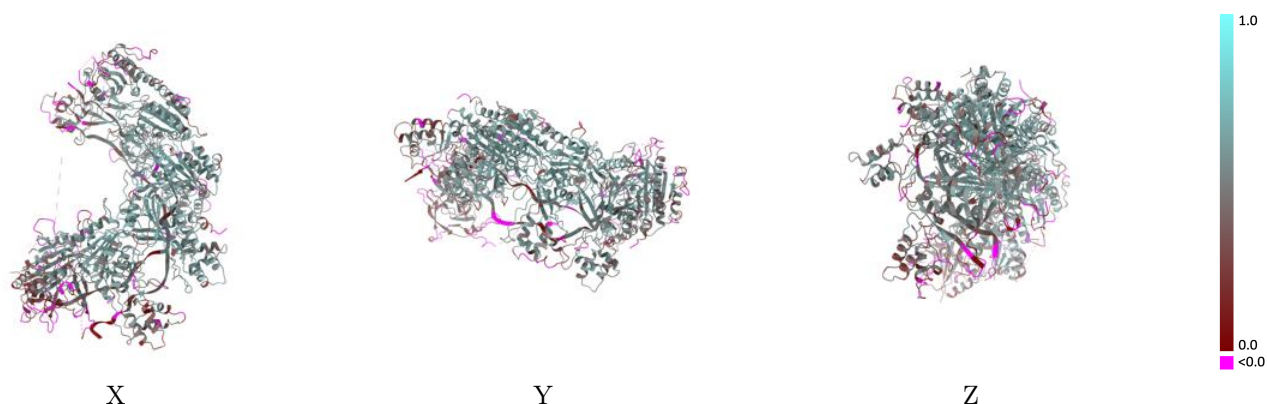
Y



Z

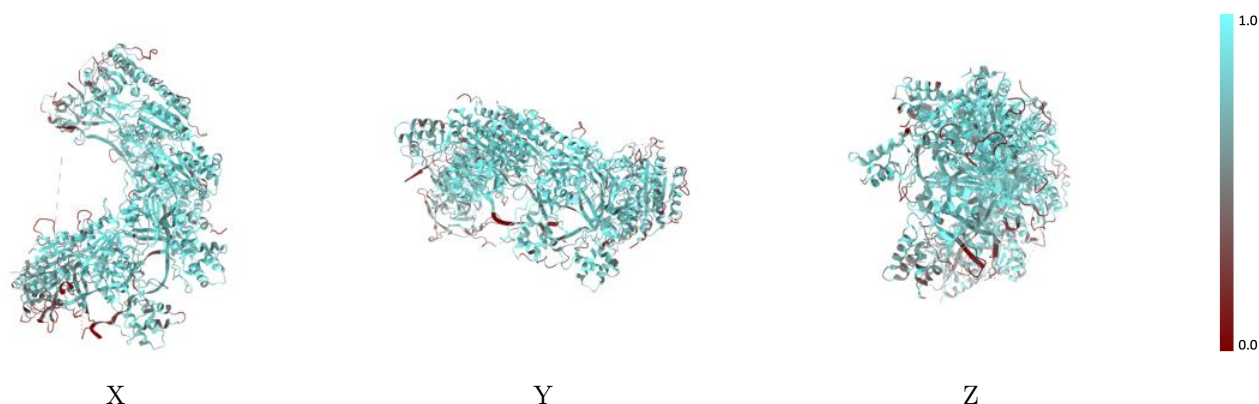
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



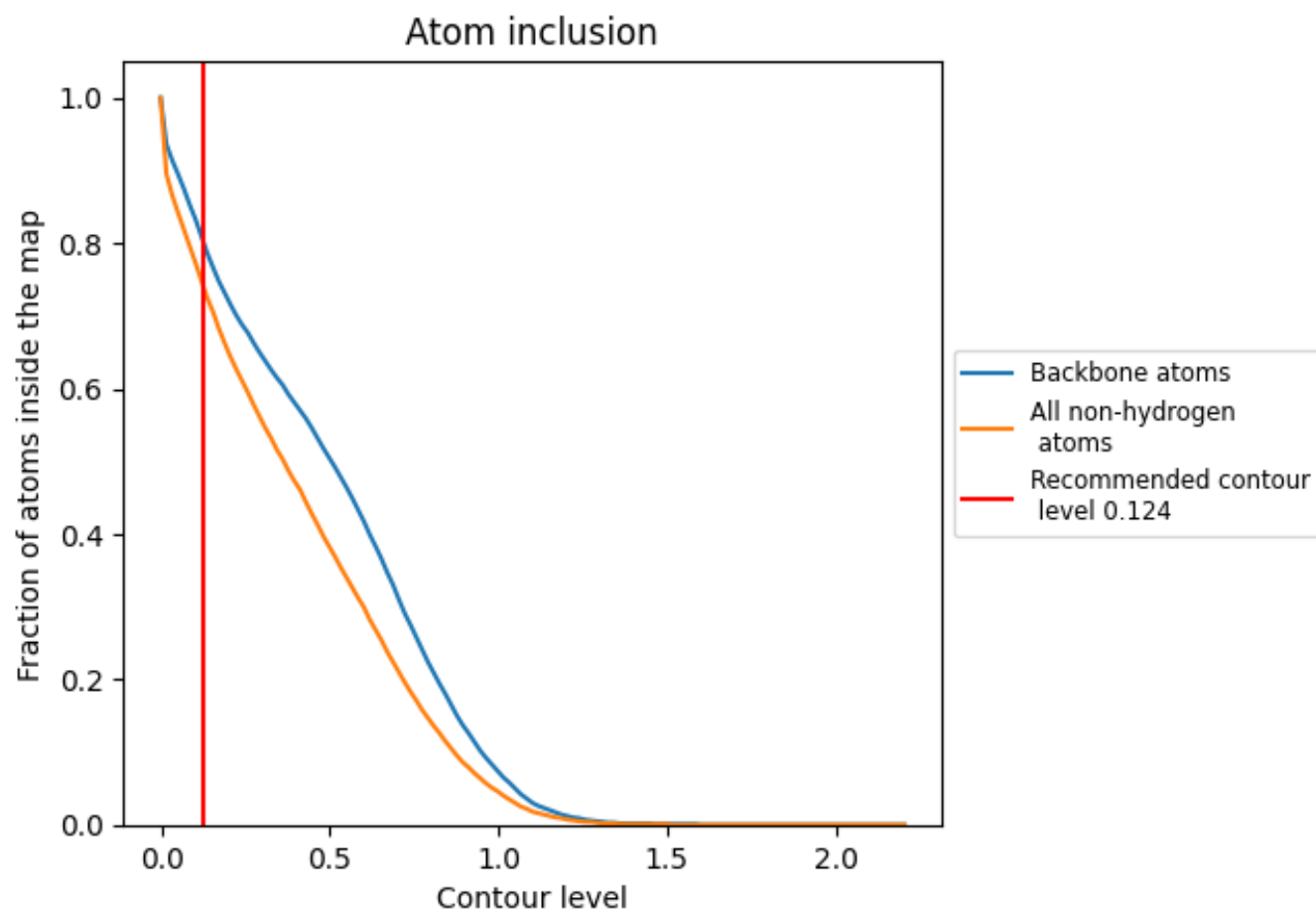
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.124).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.4590
A	0.7040	0.3480
B	0.5020	0.2570
F	0.7990	0.5070
G	0.7290	0.4470
H	0.8360	0.5550
I	0.8260	0.5370
J	0.7780	0.4900
K	0.6780	0.4130
M	0.5680	0.2860

1.0

0.0

<0.0