



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:26 PM UTC

PDB ID : 7NYW / pdb_00007nyw
EMDB ID : EMD-12656
Title : Cryo-EM structure of the MukBEF-MatP-DNA head module
Authors : Buermann, F.; Lowe, J.
Deposited on : 2021-03-23
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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

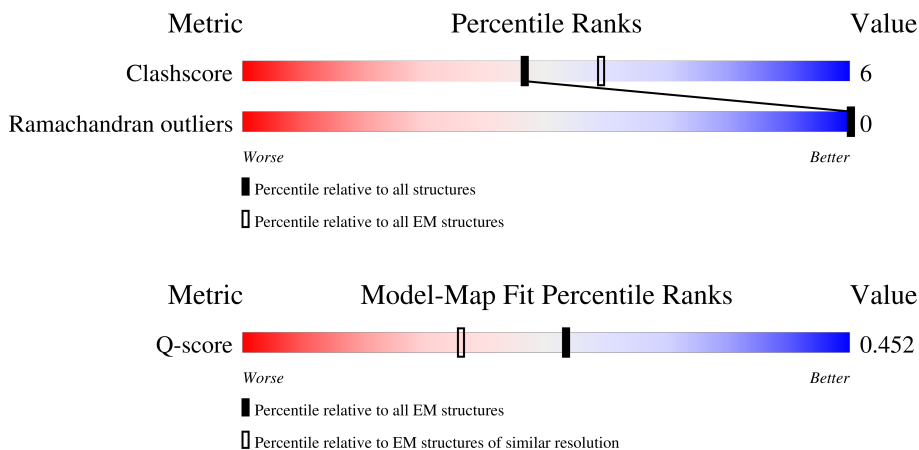
1 Overall quality at a glance

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.



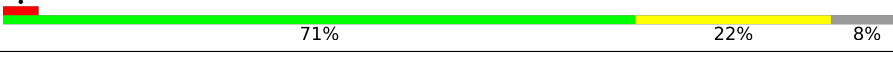
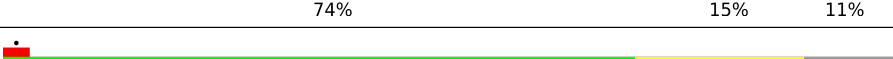
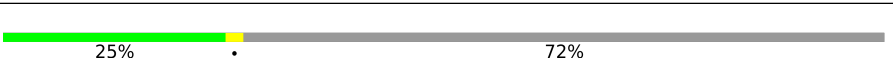
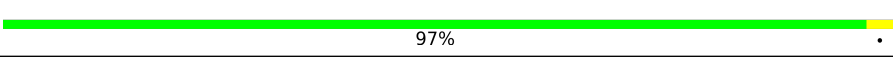
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1482	
1	B	1482	
2	C	440	
2	D	440	
3	E	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	240	
4	G	78	
4	H	78	
5	I	151	
5	J	151	
6	K	80	
7	L	80	
8	M	30	
8	N	30	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 48634 atoms, of which 23846 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	685	Total	C	H	N	O	S	0	0
			11041	3411	5563	1025	1020	22		
1	B	858	Total	C	H	N	O	S	0	0
			13847	4273	6953	1289	1306	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	335	Total	C	H	N	O	S	0	0
			5330	1702	2626	470	524	8		
2	D	94	Total	C	H	N	O	S	0	0
			1469	461	736	125	143	4		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	72	Total	C	H	N	O	S	0	0
			1105	349	543	85	127	1		

- Molecule 5 is a protein called Macrodmain Ter protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	134	Total	C	H	N	O	S	0	0
			2272	714	1137	215	202	4		
5	J	135	Total	C	H	N	O	S	0	0
			2288	719	1144	217	204	4		

- Molecule 6 is a DNA chain called matS2 DNA 80 b, oligo FBA769.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	22	Total	C	H	N	O	P	0	0
			694	214	249	80	130	21		

- Molecule 7 is a DNA chain called matS2 DNA 80 b, oligo FBA770.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	22	Total	C	H	N	O	P	0	0
			702	216	248	84	132	22		

- Molecule 8 is a DNA chain called DNA 80 b.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	30	Total	C	H	N	O	P	0	0
			961	300	346	105	180	30		
8	N	30	Total	C	H	N	O	P	0	0
			961	300	346	105	180	30		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

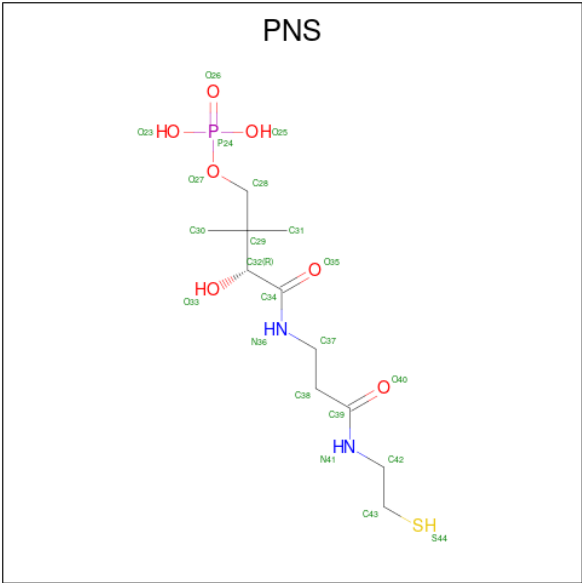
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	
9	B	1	Total	Mg	0
			1	1	

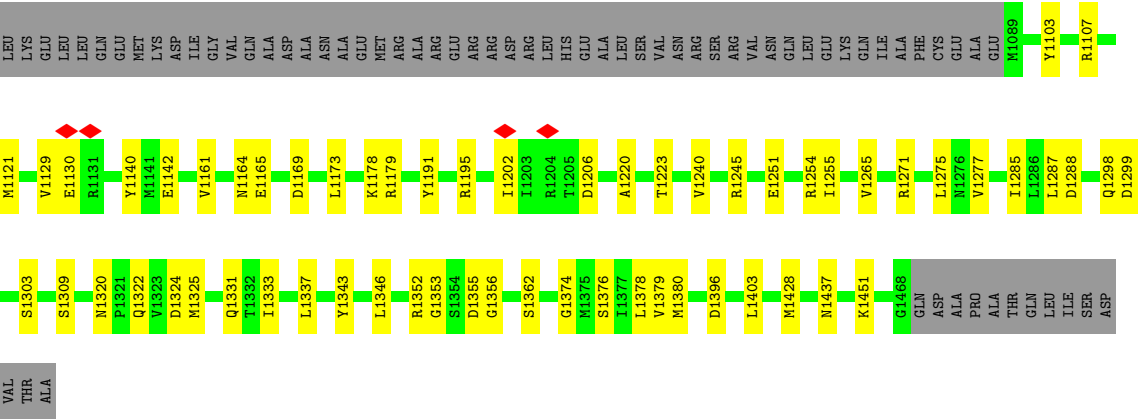
- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



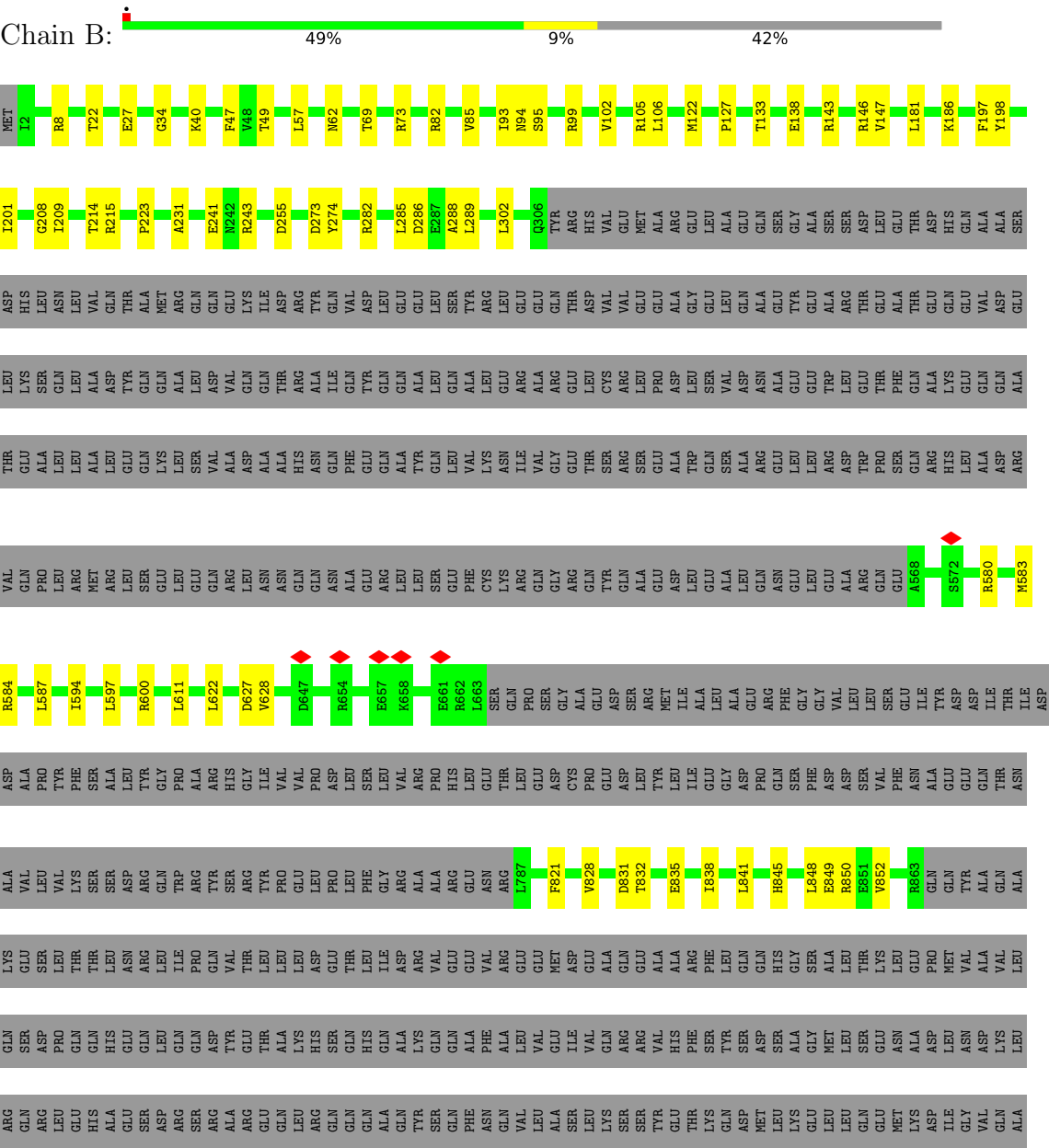
Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
10	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

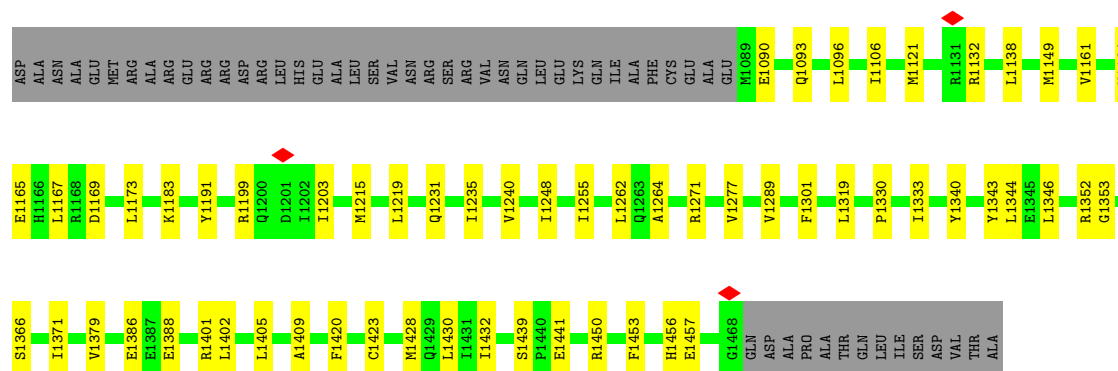
- Molecule 11 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



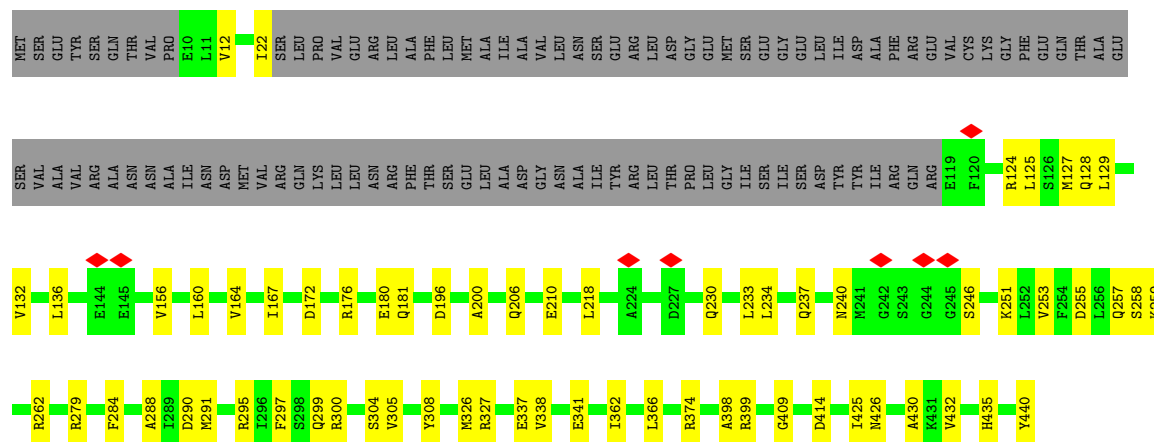


● Molecule 1: Chromosome partition protein MukB

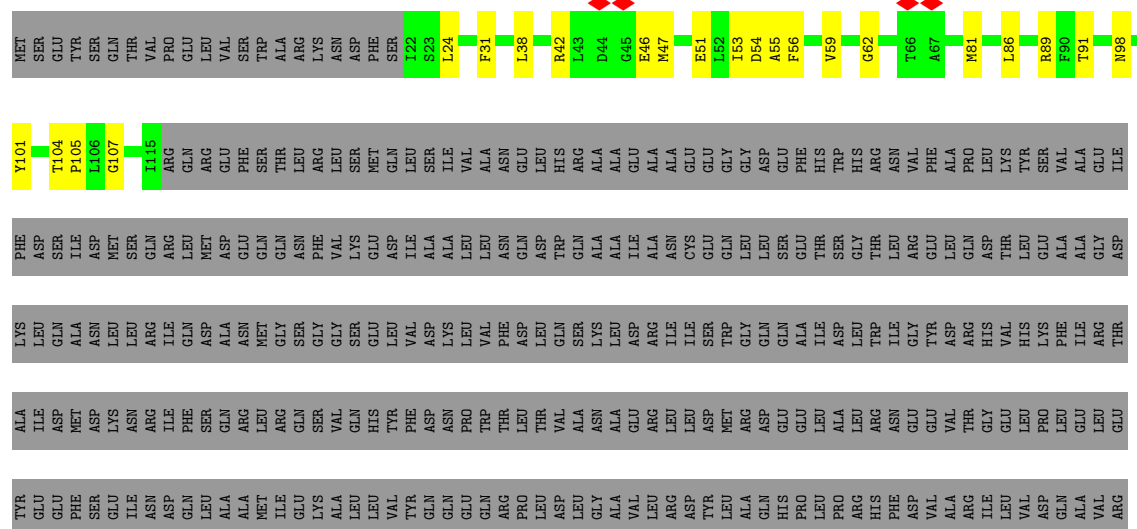




● Molecule 2: Chromosome partition protein MukF



● Molecule 2: Chromosome partition protein MukF



LEU GLY VAL ALA GLU ASP PHE SER LEU PRO ALA GLU TRP LEU ALA ASN ASP TYR GLY ALA LYS VAL GLN ALA HIS VAL ILE ASP THR TYR

• Molecule 3: Chromosome partition protein MukE

Chain E:



MET S2 E7 D39 E52 Q53 I66 E70 R76 L82 L91 D92 M93 M94 L99 L102 Q112 E123 V137 R140 S141 S142 G143 S144 D147 K150 K154 T158 R161 L171 K177 T180 T181 V184 V191

D207 A210 M211 P212 V213 GLU GLY SER LEU SER LEU ASP ASP SER GLU ASN ASP THR PRO ASN SER ALA GLU GLY ALA GLY ASP GLN PRO

• Molecule 3: Chromosome partition protein MukE

Chain F:



MET SER SER THR ILE GLU F9 E25 D42 N43 E52 Q53 V63 R78 I83 L104 S105 P106 E107 R108 L109 G113 Y121 I125 D129 K132 L133 M134 V137 N138 Q139 R140 S141 S142 G143 S144 D145 L146 L151 V155 N174 N175

I180 T181 A183 V184 F187 G188 A189 D190 V191 R192 S193 G194 D195 D196 P197 R198 E199 R203 M204 I205 R206 ASP GLY ALA MET PRO VAL GLU SER LEU SER LEU ASP SER ASN ASP THR PRO ASP ASN SER ALA GLY GLN PRO

• Molecule 4: Acyl carrier protein

Chain G:



MET SER T2 I3 V7 I11 G12 E20 T23 N24 N25 F28 M44 A45 L46 E47 E57 I62 T63 T64 V65 Q66 A67 I72 N73 G74 HIS GLN ALA

• Molecule 4: Acyl carrier protein

Chain H:



MET SER T2 L15 G16 E20 N24 V29 E30 A34 B35 S36 V40 V43 T64 V65 Q66 N73 G74 HIS GLN ALA

• Molecule 5: Macrodomain Ter protein

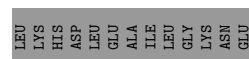
Chain I:

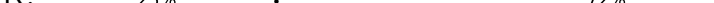


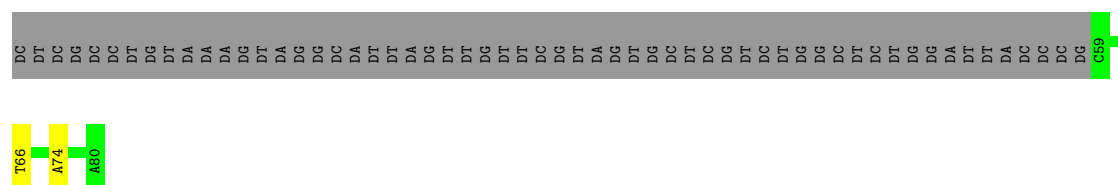
V1 E10 T29 I32 A40 L47 P51 V52 R53 V54 I58 M62 L66 M70 K71 Q72 R78 N83 A84 T89 R90 V100 V120 K129 Y132 A133 M134 GLN MET SER SER LEU LYS HIS ASP LEU ALA ALA ILE LEU LYS ASN

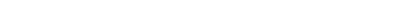
GLU

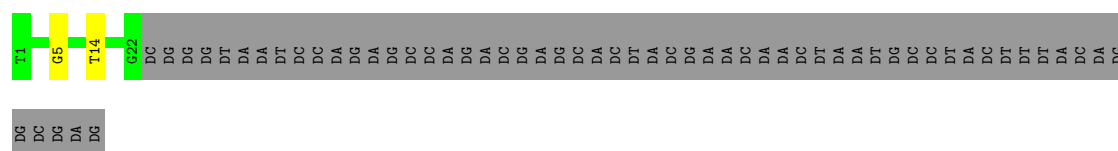
• Molecule 5: Macrodomain Ter protein



- Chain K:  25% . 72%

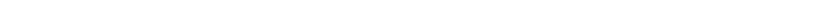


- Chain L:  25% . 72%



- Chain M: 97% .



- Chain N:  73% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200438	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	462.23843, 462.23843, 462.23843	wwPDB
Map dimensions	318, 318, 318	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45358, 1.45358, 1.45358	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: PNS, MG, ATP

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	0/5553	0.27	0/7469
1	B	0.13	0/6981	0.26	0/9385
2	C	0.12	0/2753	0.27	0/3727
2	D	0.09	0/741	0.23	0/1000
3	E	0.12	0/1753	0.25	0/2361
3	F	0.12	0/1648	0.28	0/2218
4	G	0.11	0/565	0.24	0/765
4	H	0.11	0/565	0.25	0/765
5	I	0.12	0/1160	0.25	0/1560
5	J	0.13	0/1169	0.26	0/1572
6	K	0.21	0/498	0.42	0/766
7	L	0.21	0/509	0.40	0/784
8	M	0.22	0/689	0.49	0/1061
8	N	0.18	0/689	0.43	0/1061
All	All	0.14	0/25273	0.29	0/34494

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	5478	5563	5559	59	0
1	B	6894	6953	6947	90	0
2	C	2704	2626	2623	47	0
2	D	733	736	735	20	0
3	E	1722	1719	1718	30	0
3	F	1619	1627	1626	20	0
4	G	562	543	542	12	0
4	H	562	543	542	6	0
5	I	1135	1137	1136	18	0
5	J	1144	1144	1144	18	0
6	K	445	249	250	2	0
7	L	454	248	249	2	0
8	M	615	346	346	1	0
8	N	615	346	346	5	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	31	12	12	3	0
10	B	31	12	12	1	0
11	G	21	21	21	1	0
11	H	21	21	21	0	0
All	All	24788	23846	23829	295	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 6.

All (295) 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:223:PRO:O	1:B:1340:TYR:OH	1.89	0.90
1:B:186:LYS:NZ	1:B:1388:GLU:OE2	2.11	0.83
1:A:1251:GLU:OE1	1:A:1254:ARG:NH1	2.12	0.82
1:B:255:ASP:OD2	1:B:1199:ARG:NH2	2.13	0.81
2:C:262:ARG:NH2	2:D:42:ARG:O	2.15	0.79
1:B:8:ARG:NH2	1:B:27:GLU:OE2	2.18	0.77
1:A:292:ARG:NH1	1:A:1103:TYR:OH	2.18	0.77
3:F:52:GLU:OE1	3:F:53:GLN:NE2	2.18	0.76
1:A:152:GLU:OE1	1:A:152:GLU:N	2.19	0.74
1:A:1245:ARG:NH2	1:A:1288:ASP:OD1	2.21	0.73
4:G:23:THR:OG1	4:G:25:ASN:OD1	2.04	0.72
1:A:1142:GLU:N	1:A:1142:GLU:OE1	2.22	0.72
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.23	0.70
1:B:143:ARG:NH2	2:C:341:GLU:OE2	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:7:GLU:N	3:E:7:GLU:OE1	2.25	0.69
2:C:240:ASN:OD1	2:C:246:SER:OG	2.03	0.69
1:B:622:LEU:HD12	1:B:628:VAL:HG22	1.74	0.69
5:J:71:LYS:O	5:J:75:ARG:NH1	2.26	0.68
1:A:1352:ARG:NH1	10:B:1502:ATP:O3'	2.27	0.68
5:J:84:ALA:O	5:J:90:ARG:NH1	2.26	0.68
1:B:273:ASP:OD1	1:B:274:TYR:N	2.25	0.68
1:A:1299:ASP:O	1:A:1303:SER:OG	2.12	0.67
1:B:241:GLU:OE2	2:C:279:ARG:NH1	2.27	0.67
2:D:51:GLU:OE1	2:D:51:GLU:N	2.27	0.67
1:A:221:LEU:HD13	1:A:1275:LEU:HD22	1.77	0.67
1:A:1437:ASN:ND2	1:B:1409:ALA:O	2.29	0.66
3:E:144:SER:OG	3:E:147:ASP:OD1	2.13	0.66
3:F:42:ASP:OD1	3:F:43:ASN:N	2.27	0.66
1:B:1248:ILE:HG23	1:B:1344:LEU:HD21	1.78	0.66
3:E:82:LEU:HD11	3:F:25:GLU:OE1	1.97	0.65
1:B:1132:ARG:NH1	1:B:1191:TYR:OH	2.30	0.65
1:B:849:GLU:OE1	1:B:850:ARG:NH2	2.29	0.64
4:G:46:LEU:HD21	4:G:72:ILE:HD11	1.78	0.64
1:B:49:THR:HG21	1:B:106:LEU:HD21	1.79	0.64
1:B:197:PHE:O	1:B:201:ILE:HD12	1.98	0.64
5:I:47:LEU:HD11	5:I:53:ARG:HB2	1.80	0.63
1:A:69:THR:OG1	1:B:215:ARG:NH2	2.29	0.63
1:A:1271:ARG:NH2	1:A:1353:GLY:O	2.31	0.63
1:B:85:VAL:HG23	1:B:105:ARG:HD3	1.81	0.63
1:B:99:ARG:NH1	1:B:127:PRO:O	2.31	0.63
1:A:1161:VAL:HG12	1:A:1161:VAL:O	1.99	0.63
2:C:12:VAL:HG11	2:D:62:GLY:HA3	1.81	0.63
2:D:38:LEU:HD22	2:D:47:MET:CE	2.29	0.63
5:J:21:LYS:NZ	7:L:14:DT:OP1	2.30	0.62
3:E:70:GLU:N	3:E:70:GLU:OE1	2.31	0.62
1:A:1362:SER:O	1:B:62:ASN:ND2	2.32	0.62
3:F:137:VAL:HG23	3:F:138:ASN:H	1.63	0.62
1:B:1405:LEU:HB3	1:B:1432:ILE:HG22	1.81	0.61
1:B:622:LEU:HD13	1:B:627:ASP:OD2	2.00	0.61
1:A:174:TYR:CE2	1:A:178:MET:HE2	2.36	0.61
1:B:34:GLY:O	1:B:40:LYS:NZ	2.34	0.60
3:F:107:GLU:OE2	3:F:113:GLY:N	2.34	0.60
1:B:209:ILE:HG23	1:B:214:THR:HG21	1.82	0.60
2:C:160:LEU:O	2:C:164:VAL:HG22	2.02	0.60
4:H:24:ASN:O	4:H:66:GLN:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD23	1:B:198:TYR:HB2	1.82	0.59
1:B:273:ASP:OD2	1:B:1183:LYS:NZ	2.25	0.59
1:A:1275:LEU:HB2	1:A:1380:MET:HE1	1.84	0.59
1:B:69:THR:HG21	8:N:16:DT:OP2	2.03	0.58
2:C:290:ASP:OD1	2:C:291:MET:N	2.36	0.58
3:E:92:ASP:OD2	3:E:161:ARG:NE	2.37	0.58
1:B:583:MET:HE1	1:B:852:VAL:HG23	1.85	0.58
1:B:1231:GLN:O	1:B:1235:ILE:HD12	2.04	0.57
3:F:63:VAL:HG21	3:F:83:ILE:HD12	1.86	0.57
5:I:129:LYS:NZ	5:J:125:ASP:OD2	2.37	0.57
1:B:828:VAL:HG12	1:B:828:VAL:O	2.03	0.57
2:C:22:ILE:O	2:D:24:LEU:N	2.37	0.57
10:A:1502:ATP:O1G	1:B:1366:SER:OG	2.22	0.57
1:A:94:ASN:ND2	1:A:181:LEU:O	2.38	0.56
1:B:1453:PHE:O	1:B:1456:HIS:ND1	2.39	0.56
5:I:29:THR:HG21	5:I:40:ALA:HB3	1.87	0.56
2:C:362:ILE:HG22	2:C:366:LEU:HD12	1.88	0.56
5:J:91:LYS:NZ	6:K:66:DT:OP2	2.32	0.56
3:E:137:VAL:HG13	3:E:154:LYS:HD2	1.88	0.56
1:A:1277:VAL:HG22	1:A:1346:LEU:CD2	2.35	0.56
3:E:154:LYS:O	3:E:158:THR:HG23	2.06	0.56
1:B:102:VAL:HG12	1:B:122:MET:HE2	1.88	0.55
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.89	0.55
1:A:53:PRO:HB3	1:A:104:VAL:HG11	1.87	0.55
1:B:302:LEU:HD12	1:B:1096:LEU:HD13	1.87	0.55
2:D:38:LEU:O	2:D:42:ARG:N	2.40	0.55
8:N:5:DA:H2'	8:N:6:DT:H71	1.88	0.55
2:C:300:ARG:NE	3:E:191:VAL:O	2.37	0.55
2:D:98:ASN:CG	3:E:171:LEU:HD13	2.31	0.55
1:A:1107:ARG:NH1	4:G:47:GLU:OE2	2.39	0.55
3:E:66:ILE:HD13	3:E:76:ARG:NH2	2.22	0.55
10:A:1502:ATP:O3'	1:B:1352:ARG:NH1	2.40	0.55
2:C:305:VAL:HG13	3:E:94:MET:HE1	1.90	0.54
5:I:84:ALA:O	5:I:90:ARG:NH1	2.40	0.54
3:F:129:ASP:OD2	3:F:132:LYS:NZ	2.40	0.54
1:A:292:ARG:NH2	4:G:47:GLU:OE1	2.40	0.54
1:A:1277:VAL:HG22	1:A:1346:LEU:HD23	1.90	0.54
1:A:221:LEU:HD13	1:A:1275:LEU:CD2	2.38	0.54
2:C:124:ARG:O	2:C:128:GLN:OE1	2.26	0.53
2:C:124:ARG:O	2:C:127:MET:HG3	2.08	0.53
2:C:206:GLN:O	2:C:210:GLU:OE1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:GLU:N	2:D:46:GLU:OE1	2.41	0.53
5:I:62:MET:HE1	5:I:66:LEU:HD23	1.89	0.53
1:A:1322:GLN:OE1	1:A:1322:GLN:N	2.39	0.53
3:E:210:ALA:C	3:E:211:MET:HE2	2.34	0.53
1:A:1107:ARG:HA	4:G:44:MET:HE2	1.91	0.52
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.09	0.52
5:I:47:LEU:HD21	5:I:54:VAL:HA	1.90	0.52
1:B:94:ASN:OD1	1:B:95:SER:N	2.40	0.52
1:B:22:THR:OG1	1:B:133:THR:OG1	2.26	0.52
2:C:196:ASP:HB2	2:C:200:ALA:HB2	1.90	0.52
2:C:300:ARG:NH2	3:E:191:VAL:O	2.43	0.52
4:G:62:ILE:HG22	4:G:62:ILE:O	2.10	0.52
5:I:120:VAL:CG2	5:J:100:VAL:HG22	2.40	0.51
5:J:14:LYS:O	5:J:18:LEU:HD23	2.09	0.51
1:B:1203:ILE:O	1:B:1203:ILE:HG22	2.10	0.51
1:B:1248:ILE:HD11	1:B:1343:TYR:HB2	1.92	0.51
3:E:211:MET:HE2	3:E:211:MET:N	2.26	0.51
3:F:134:MET:O	3:F:138:ASN:N	2.42	0.51
1:A:217:LEU:HG	1:A:221:LEU:HD12	1.93	0.51
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.46	0.51
3:F:121:TYR:CE2	3:F:125:ILE:HD11	2.46	0.51
1:B:285:LEU:O	1:B:289:LEU:HD23	2.11	0.51
2:D:38:LEU:HD22	2:D:47:MET:HE2	1.93	0.51
1:A:1451:LYS:NZ	2:C:409:GLY:O	2.44	0.51
1:B:243:ARG:NH2	1:B:1301:PHE:O	2.40	0.50
4:H:36:SER:O	4:H:40:VAL:HG23	2.12	0.50
1:A:96:ARG:NH1	1:A:1396:ASP:OD1	2.44	0.50
1:A:1309:SER:OG	1:A:1331:GLN:NE2	2.45	0.50
1:A:1333:ILE:O	1:A:1337:LEU:HD23	2.10	0.50
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.12	0.50
2:D:31:PHE:HE1	2:D:55:ALA:HB3	1.76	0.50
1:A:1140:TYR:OH	1:B:835:GLU:OE1	2.28	0.50
2:C:284:PHE:O	2:C:288:ALA:N	2.38	0.50
3:F:121:TYR:CZ	3:F:125:ILE:HD11	2.47	0.50
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	1.93	0.50
5:J:58:ILE:HG23	5:J:62:MET:SD	2.52	0.50
3:F:182:GLU:OE1	3:F:182:GLU:N	2.37	0.49
4:G:57:GLU:OE1	4:G:57:GLU:N	2.45	0.49
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.12	0.49
1:B:57:LEU:HD23	1:B:198:TYR:CB	2.42	0.49
3:E:66:ILE:HD12	3:E:76:ARG:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:58:ILE:HD13	5:I:70:MET:HE1	1.94	0.49
1:A:263:ILE:HD11	1:A:1191:TYR:CE1	2.47	0.49
1:A:1169:ASP:O	1:A:1173:LEU:HG	2.12	0.49
3:F:137:VAL:HG23	3:F:138:ASN:N	2.26	0.49
5:I:62:MET:CE	5:I:66:LEU:HD23	2.42	0.49
1:A:1285:ILE:HD11	1:A:1320:ASN:OD1	2.12	0.49
1:B:274:TYR:HE2	1:B:1121:MET:HE1	1.77	0.49
1:B:1277:VAL:HG12	1:B:1346:LEU:HD13	1.94	0.49
1:B:82:ARG:NH2	1:B:1457:GLU:O	2.45	0.49
3:F:134:MET:HA	3:F:134:MET:HE2	1.95	0.49
5:J:65:ASP:OD2	5:J:69:ARG:NH1	2.41	0.49
1:A:289:LEU:O	11:G:101:PNS:S44	2.58	0.49
3:F:151:LEU:O	3:F:155:VAL:HG23	2.13	0.48
1:B:1289:VAL:HG21	1:B:1319:LEU:HD22	1.95	0.48
3:E:171:LEU:HD12	3:E:177:LYS:HB2	1.95	0.48
1:B:1262:LEU:HD23	1:B:1264:ALA:H	1.79	0.48
1:B:1289:VAL:HG21	1:B:1319:LEU:CD2	2.43	0.48
5:I:83:ASN:O	5:I:89:THR:OG1	2.28	0.48
2:C:181:GLN:O	2:C:181:GLN:NE2	2.47	0.48
2:D:104:THR:HG23	2:D:107:GLY:H	1.79	0.48
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.48
1:B:288:ALA:HB2	1:B:1106:ILE:CG2	2.44	0.47
1:B:282:ARG:NH2	1:B:286:ASP:OD1	2.48	0.47
2:D:91:THR:HG21	3:E:112:GLN:HB3	1.96	0.47
1:B:587:LEU:HD13	1:B:848:LEU:HD22	1.95	0.47
4:G:2:THR:OG1	4:G:3:ILE:N	2.46	0.47
5:I:47:LEU:HD12	5:I:47:LEU:O	2.15	0.47
1:B:1271:ARG:NH1	1:B:1353:GLY:O	2.46	0.47
2:D:104:THR:OG1	2:D:105:PRO:HD2	2.15	0.47
1:A:70:SER:OG	1:A:72:SER:O	2.20	0.46
2:C:251:LYS:O	2:C:255:ASP:N	2.46	0.46
3:E:141:SER:OG	3:E:147:ASP:OD2	2.31	0.46
5:I:100:VAL:HG22	5:J:120:VAL:CG2	2.46	0.46
1:A:1121:MET:HA	1:A:1121:MET:HE2	1.98	0.46
2:D:56:PHE:HA	2:D:59:VAL:HG12	1.97	0.46
4:G:28:PHE:CE1	4:G:65:VAL:HG22	2.51	0.46
1:B:1255:ILE:HG21	1:B:1277:VAL:HG11	1.97	0.46
3:E:91:LEU:HG	3:E:158:THR:HG21	1.98	0.46
1:A:1206:ASP:OD1	1:A:1206:ASP:N	2.49	0.46
1:B:273:ASP:OD1	1:B:273:ASP:C	2.58	0.46
1:B:302:LEU:HD12	1:B:1096:LEU:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:52:GLU:OE2	3:E:53:GLN:NE2	2.49	0.46
1:B:94:ASN:ND2	1:B:181:LEU:O	2.49	0.46
3:E:102:LEU:HD21	3:E:123:GLU:HG3	1.96	0.46
5:J:18:LEU:HD22	5:J:70:MET:HE1	1.98	0.46
5:J:51:PRO:HA	5:J:54:VAL:HG23	1.98	0.46
2:C:233:LEU:HB3	2:C:257:GLN:NE2	2.31	0.46
8:N:23:DA:C8	8:N:24:DT:H72	2.51	0.46
1:B:1420:PHE:HE2	1:B:1439:SER:HG	1.63	0.45
1:A:78:HIS:NE2	1:A:108:GLN:OE1	2.49	0.45
1:B:1330:PRO:HA	1:B:1333:ILE:HG22	1.98	0.45
3:E:76:ARG:NH1	3:E:207:ASP:O	2.49	0.45
1:B:1169:ASP:O	1:B:1173:LEU:HG	2.16	0.45
2:C:237:GLN:HB2	2:C:253:VAL:HG11	1.97	0.45
2:C:374:ARG:O	2:C:440:TYR:OH	2.24	0.45
5:I:72:GLN:NE2	6:K:74:DA:OP2	2.47	0.45
1:B:1441:GLU:N	1:B:1441:GLU:OE1	2.50	0.45
2:C:125:LEU:O	2:C:129:LEU:HD23	2.16	0.45
5:J:79:LYS:NZ	5:J:83:ASN:OD1	2.49	0.45
1:B:1164:ASN:OD1	1:B:1165:GLU:N	2.50	0.45
1:B:1215:MET:O	1:B:1219:LEU:HD13	2.16	0.45
3:E:52:GLU:OE1	3:E:52:GLU:N	2.36	0.45
2:C:297:PHE:HE1	3:E:191:VAL:HG23	1.81	0.45
1:A:72:SER:OG	1:A:73:ARG:N	2.50	0.45
3:E:158:THR:HG22	3:E:161:ARG:NH2	2.32	0.45
10:A:1502:ATP:PG	1:B:1366:SER:HG	2.40	0.44
5:I:51:PRO:HA	5:I:54:VAL:HG12	2.00	0.44
1:B:583:MET:HE2	1:B:848:LEU:HG	1.98	0.44
1:B:594:ILE:HD11	1:B:841:LEU:HB3	1.99	0.44
2:C:326:MET:HE1	3:F:187:PHE:CE1	2.52	0.44
2:C:218:LEU:HD23	2:C:218:LEU:O	2.17	0.44
2:C:414:ASP:OD1	2:C:435:HIS:ND1	2.51	0.44
5:I:32:ILE:HD12	5:I:32:ILE:H	1.83	0.44
1:A:1355:ASP:OD1	1:A:1356:GLY:N	2.47	0.44
1:B:1138:LEU:HD22	1:B:1149:MET:HE1	2.00	0.44
1:B:208:GLY:HA2	1:B:1371:ILE:HA	2.00	0.44
2:C:156:VAL:HG12	2:C:156:VAL:O	2.18	0.44
3:E:181:THR:O	3:E:184:VAL:HG22	2.18	0.44
5:I:52:VAL:HG13	5:I:53:ARG:HG2	2.00	0.44
5:J:42:ASP:O	5:J:46:LYS:HG2	2.18	0.44
2:C:253:VAL:O	2:C:257:GLN:HG2	2.18	0.44
1:A:263:ILE:HG23	1:A:264:THR:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:107:LEU:HD11	5:J:111:ARG:HE	1.83	0.43
1:B:597:LEU:C	1:B:838:ILE:HD11	2.44	0.43
2:D:89:ARG:NH1	2:D:101:TYR:OH	2.42	0.43
8:N:12:DT:H2''	8:N:13:DA:C8	2.53	0.43
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.19	0.43
5:J:15:TRP:HB2	5:J:54:VAL:HG21	1.99	0.43
1:A:1403:LEU:HD12	1:A:1428:MET:SD	2.58	0.43
4:H:64:THR:HG22	4:H:65:VAL:N	2.33	0.43
5:I:78:ARG:NH1	7:L:5:DG:OP2	2.50	0.43
1:A:231:ALA:HB1	1:A:1240:VAL:HG22	2.00	0.43
3:E:39:ASP:OD2	3:E:181:THR:HG22	2.19	0.43
3:E:99:LEU:HD22	3:E:180:ILE:HG12	2.01	0.43
1:B:47:PHE:CZ	1:B:1402:LEU:HD13	2.54	0.43
1:A:1324:ASP:OD1	1:A:1325:MET:N	2.51	0.43
1:B:73:ARG:HG3	1:B:73:ARG:O	2.18	0.43
1:B:622:LEU:HD12	1:B:628:VAL:CG2	2.46	0.43
2:D:86:LEU:C	2:D:104:THR:HG22	2.44	0.43
1:B:1090:GLU:OE2	1:B:1093:GLN:NE2	2.52	0.43
1:B:1231:GLN:NE2	1:B:1235:ILE:HD13	2.34	0.43
1:B:147:VAL:CG2	2:C:338:VAL:HG23	2.49	0.42
1:B:600:ARG:NH2	1:B:832:THR:O	2.52	0.42
1:B:1386:GLU:OE1	1:B:1401:ARG:NH2	2.52	0.42
2:C:230:GLN:O	2:C:234:LEU:HD13	2.19	0.42
2:C:304:SER:O	2:C:308:TYR:N	2.53	0.42
2:C:258:SER:O	2:C:259:LYS:C	2.62	0.42
2:D:31:PHE:CD2	2:D:81:MET:HE1	2.54	0.42
1:B:1161:VAL:HG13	1:B:1167:LEU:HD22	2.01	0.42
2:C:136:LEU:HD21	2:C:233:LEU:HG	2.02	0.42
2:C:297:PHE:CE1	3:E:191:VAL:HG23	2.55	0.42
3:F:78:ARG:NH1	8:M:19:DA:OP1	2.53	0.42
1:A:1255:ILE:CD1	1:A:1277:VAL:HG21	2.50	0.42
2:C:124:ARG:C	2:C:128:GLN:OE1	2.63	0.42
1:A:1374:GLY:O	1:A:1378:LEU:HG	2.20	0.42
1:B:138:GLU:O	1:B:146:ARG:N	2.47	0.42
2:C:124:ARG:O	2:C:125:LEU:C	2.63	0.42
2:C:327:ARG:NH2	8:N:7:DA:OP1	2.47	0.42
3:F:104:LEU:HD21	3:F:198:ARG:HD3	2.00	0.42
1:B:146:ARG:NH1	2:C:337:GLU:OE1	2.52	0.42
2:C:295:ARG:O	2:C:299:GLN:OE1	2.38	0.42
4:H:40:VAL:O	4:H:43:VAL:HG12	2.19	0.42
1:B:611:LEU:HD13	1:B:821:PHE:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1423:CYS:SG	1:B:1430:LEU:HD11	2.60	0.42
1:B:1450:ARG:NH1	1:B:1457:GLU:OE1	2.49	0.42
2:C:132:VAL:HG23	2:C:167:ILE:HG21	2.02	0.42
1:B:8:ARG:HG3	1:B:93:ILE:HG12	2.02	0.41
2:C:425:ILE:HD13	2:C:432:VAL:CG2	2.50	0.41
2:D:53:ILE:HG13	2:D:54:ASP:N	2.35	0.41
3:F:174:ASN:OD1	3:F:175:ASN:N	2.53	0.41
1:A:1191:TYR:O	1:A:1195:ARG:N	2.53	0.41
1:B:1248:ILE:HD11	1:B:1343:TYR:CB	2.50	0.41
1:A:1287:LEU:HD21	1:A:1343:TYR:CE2	2.56	0.41
2:C:172:ASP:O	2:C:176:ARG:HG3	2.20	0.41
5:J:18:LEU:HB3	5:J:44:LEU:HD21	2.01	0.41
1:A:1129:VAL:O	1:A:1130:GLU:C	2.64	0.41
1:A:1178:LYS:C	1:A:1179:ARG:HD2	2.45	0.41
2:C:180:GLU:OE2	2:D:104:THR:OG1	2.32	0.41
1:B:1379:VAL:HG12	1:B:1428:MET:SD	2.61	0.41
4:G:64:THR:HG23	4:G:67:ALA:H	1.85	0.41
1:A:1161:VAL:O	1:A:1161:VAL:CG1	2.68	0.41
1:A:1164:ASN:OD1	1:A:1165:GLU:N	2.53	0.41
2:D:86:LEU:O	2:D:104:THR:HG22	2.21	0.41
1:A:54:ASP:OD1	1:A:56:THR:N	2.47	0.41
3:E:137:VAL:HG12	3:E:150:LYS:HD2	2.03	0.41
1:B:831:ASP:OD1	1:B:832:THR:N	2.47	0.41
4:H:29:VAL:HG13	4:H:30:GLU:N	2.36	0.41
1:A:1287:LEU:HD21	1:A:1343:TYR:HE2	1.86	0.40
1:B:231:ALA:HB1	1:B:1240:VAL:HG22	2.01	0.40
1:B:580:ARG:O	1:B:584:ARG:HG2	2.20	0.40
3:F:139:GLN:HG2	3:F:140:ARG:N	2.36	0.40
4:G:7:VAL:O	4:G:11:ILE:HG22	2.21	0.40
4:H:15:LEU:HD22	4:H:34:ALA:HB2	2.03	0.40
5:I:10:GLU:OE2	5:I:78:ARG:NE	2.49	0.40
5:J:22:HIS:HB2	5:J:28:ILE:HD13	2.03	0.40
1:A:1220:ALA:O	1:A:1223:THR:OG1	2.34	0.40
1:A:1265:VAL:O	1:A:1265:VAL:HG23	2.20	0.40
2:C:398:ALA:O	2:C:399:ARG:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	681/1482 (46%)	651 (96%)	30 (4%)	0	100	100
1	B	836/1482 (56%)	806 (96%)	30 (4%)	0	100	100
2	C	331/440 (75%)	316 (96%)	15 (4%)	0	100	100
2	D	92/440 (21%)	89 (97%)	3 (3%)	0	100	100
3	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
4	G	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	H	70/78 (90%)	67 (96%)	3 (4%)	0	100	100
5	I	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	J	133/151 (88%)	131 (98%)	2 (2%)	0	100	100
All	All	2751/4782 (58%)	2650 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
11	PNS	H	101	4	14,20,21	0.23	0	18,26,29	0.47	0
10	ATP	B	1502	9	32,33,33	0.51	0	48,52,52	0.72	2 (4%)
11	PNS	G	101	4	14,20,21	0.23	0	18,26,29	0.36	0
10	ATP	A	1502	9	32,33,33	0.55	0	48,52,52	0.72	2 (4%)

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
11	PNS	H	101	4	-	4/24/26/27	-
10	ATP	B	1502	9	-	3/22/38/38	0/3/3/3
11	PNS	G	101	4	-	3/24/26/27	-
10	ATP	A	1502	9	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1502	ATP	O2'-C2'-C3'	-2.10	105.09	111.82
10	A	1502	ATP	O3'-C3'-C2'	-2.05	105.23	111.82
10	B	1502	ATP	O3'-C3'-C2'	-2.05	105.24	111.82
10	B	1502	ATP	O2'-C2'-C3'	-2.00	105.40	111.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

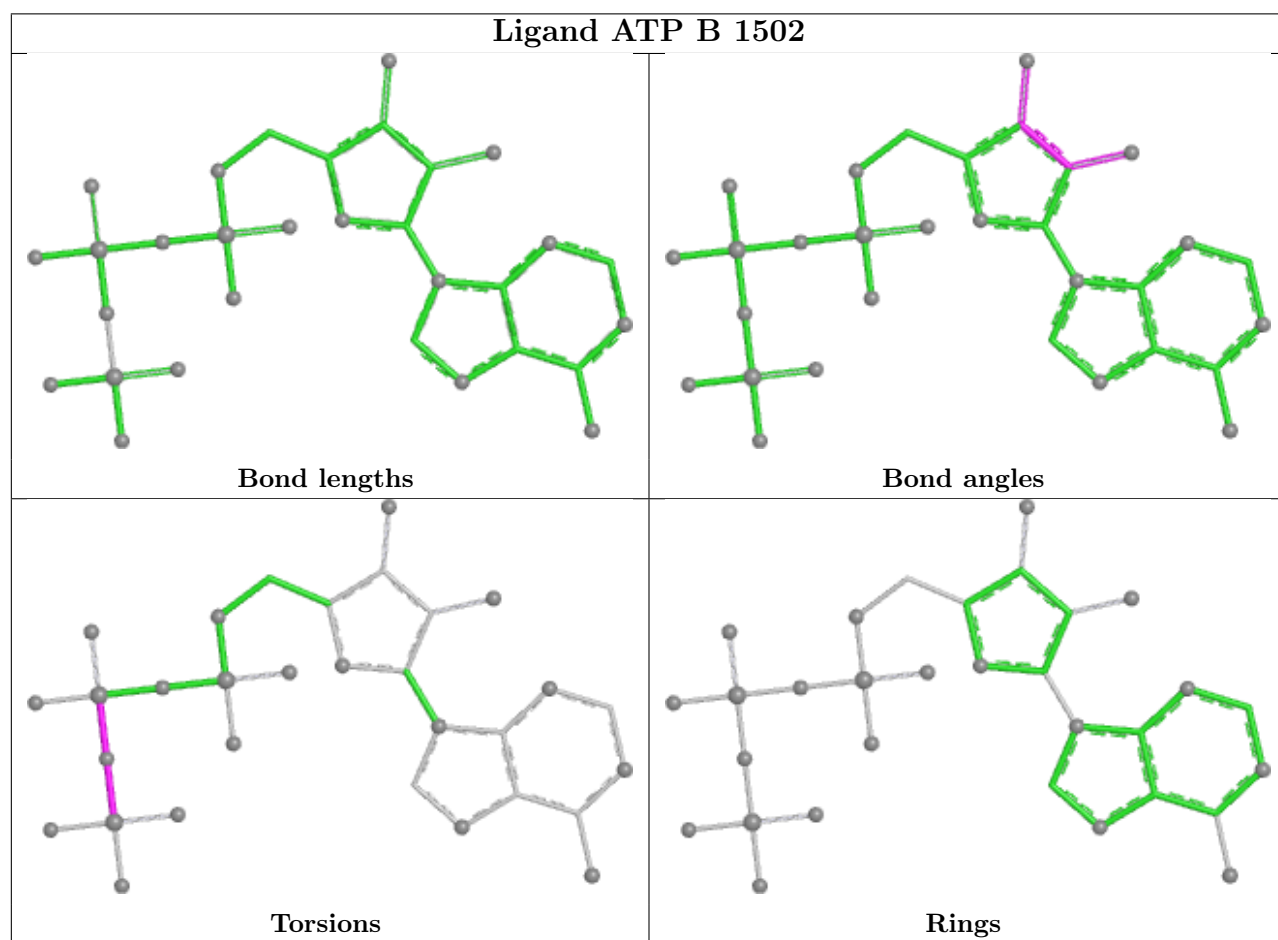
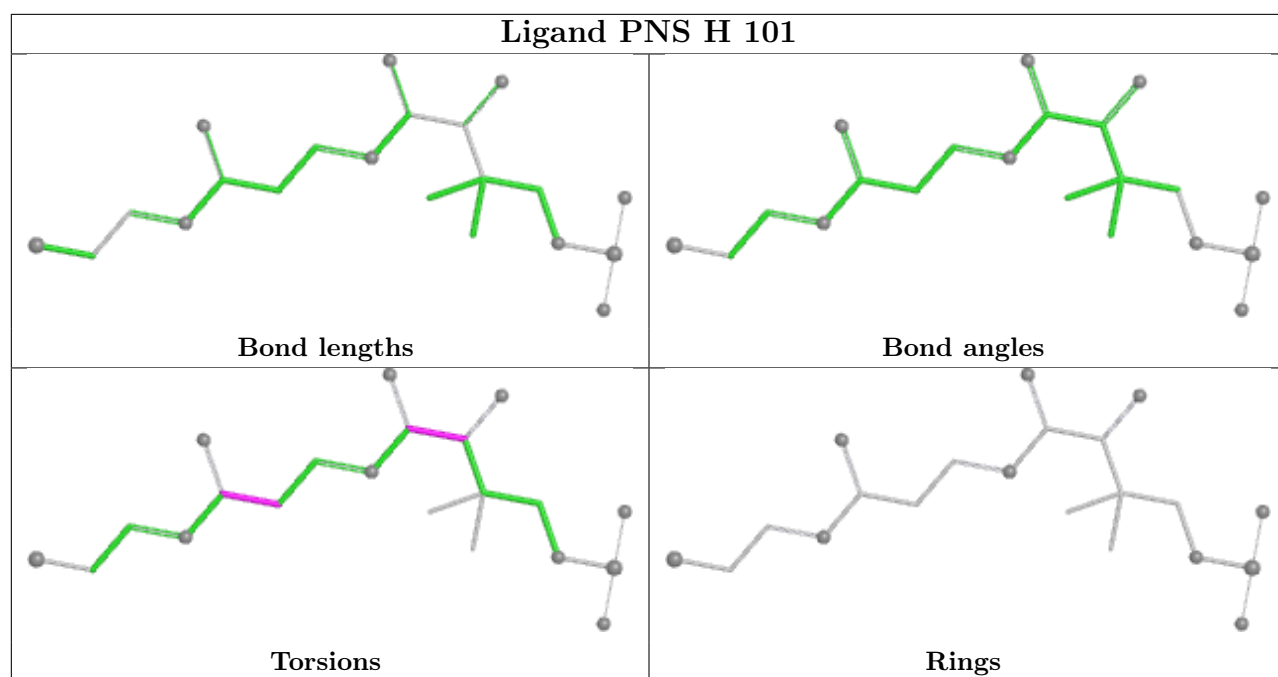
Mol	Chain	Res	Type	Atoms
11	H	101	PNS	C37-C38-C39-N41
11	G	101	PNS	O33-C32-C34-O35
11	H	101	PNS	O33-C32-C34-O35
11	H	101	PNS	C37-C38-C39-O40
10	B	1502	ATP	PB-O3B-PG-O1G
11	G	101	PNS	C43-C42-N41-C39
10	A	1502	ATP	PA-O3A-PB-O2B
10	B	1502	ATP	PG-O3B-PB-O1B
10	B	1502	ATP	PG-O3B-PB-O2B
11	G	101	PNS	O33-C32-C34-N36
11	H	101	PNS	O33-C32-C34-N36
10	A	1502	ATP	PA-O3A-PB-O1B

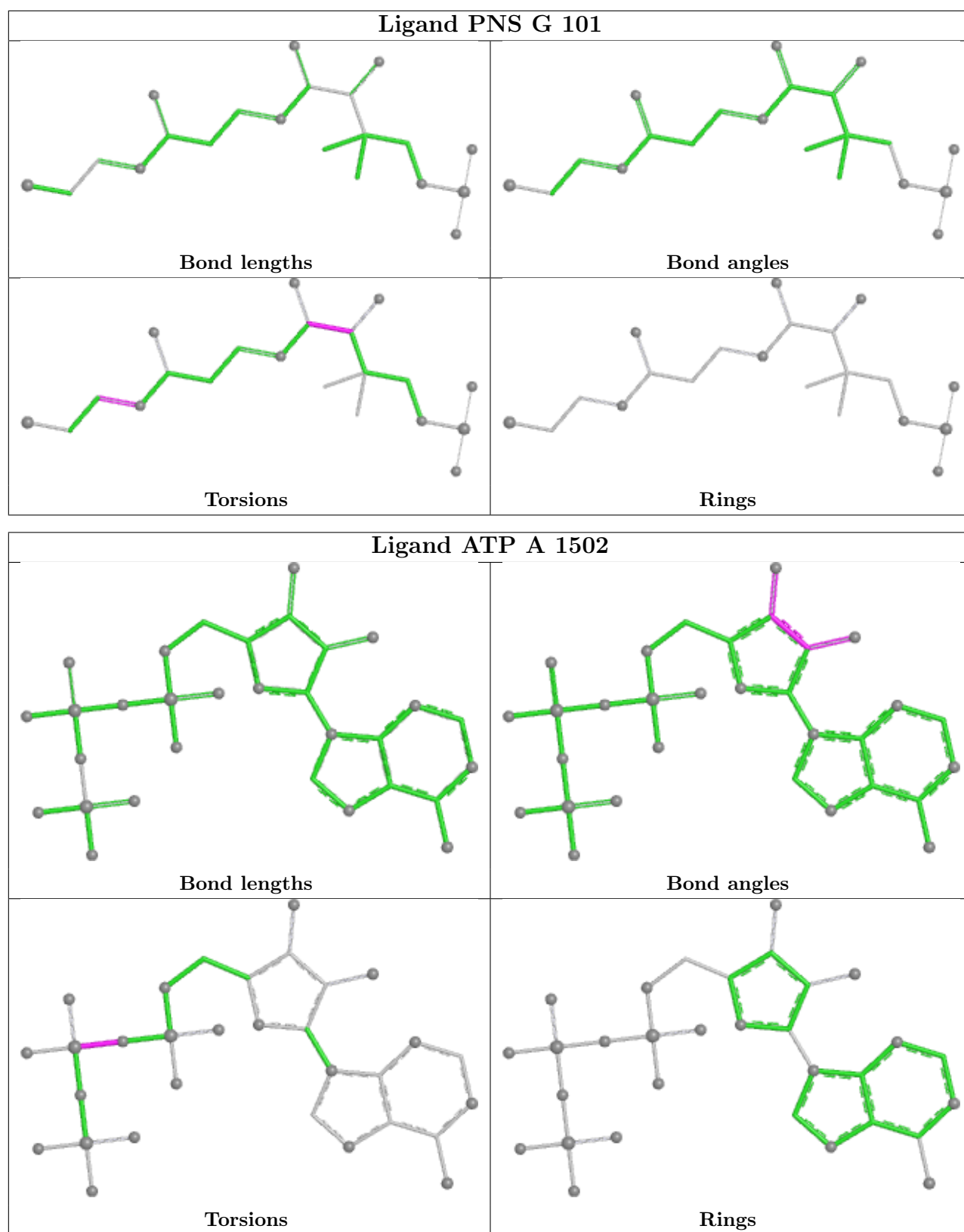
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1502	ATP	1	0
11	G	101	PNS	1	0
10	A	1502	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

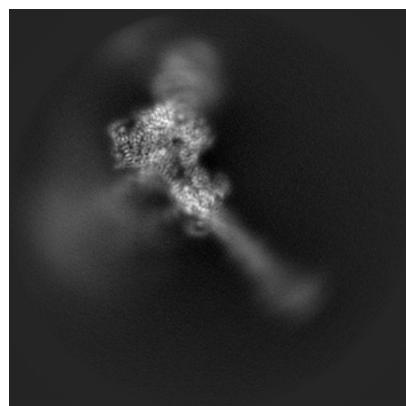
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12656. These allow visual inspection of the internal detail of the map and identification of artifacts.

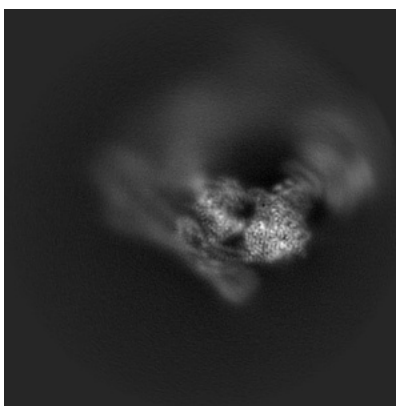
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

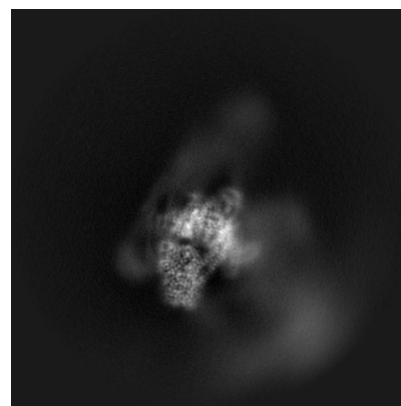
6.1.1 Primary map



X

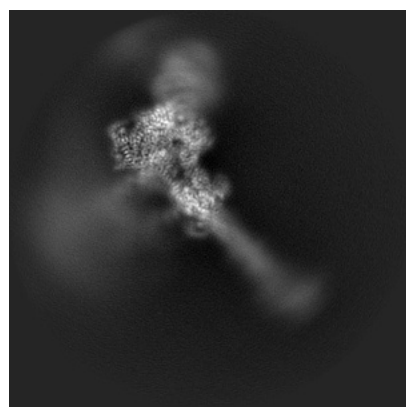


Y

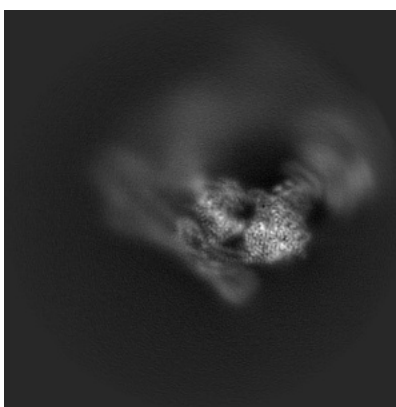


Z

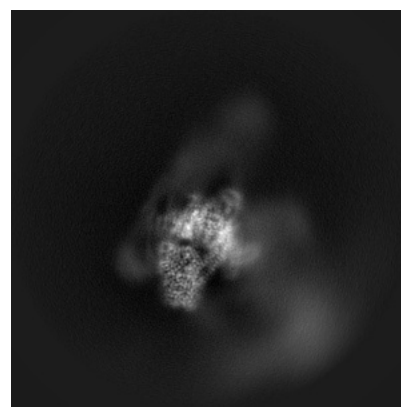
6.1.2 Raw map



X



Y

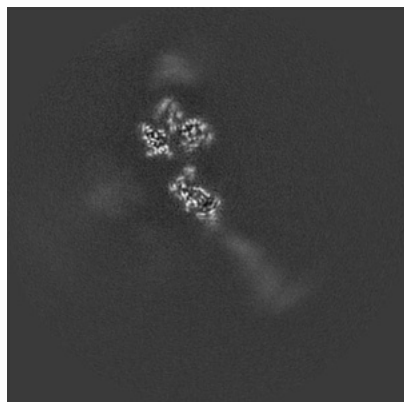


Z

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

6.2 Central slices [i](#)

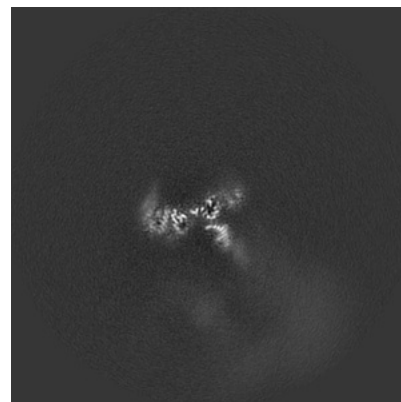
6.2.1 Primary map



X Index: 159

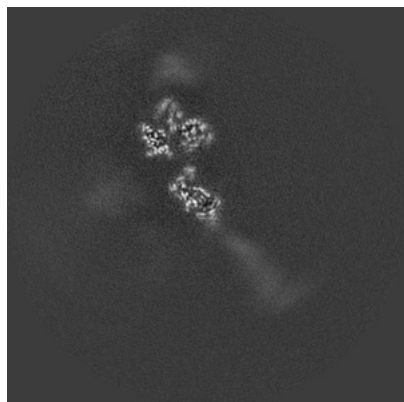


Y Index: 159



Z Index: 159

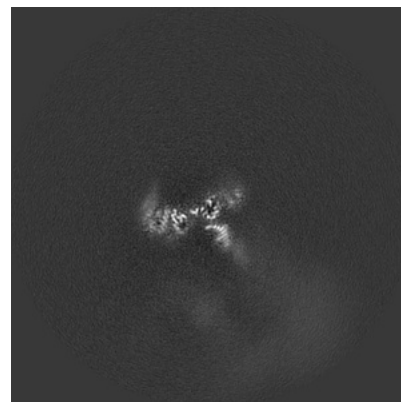
6.2.2 Raw map



X Index: 159



Y Index: 159

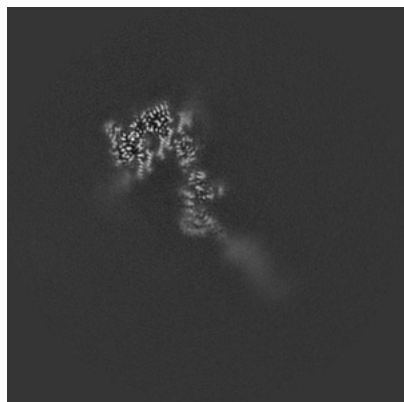


Z Index: 159

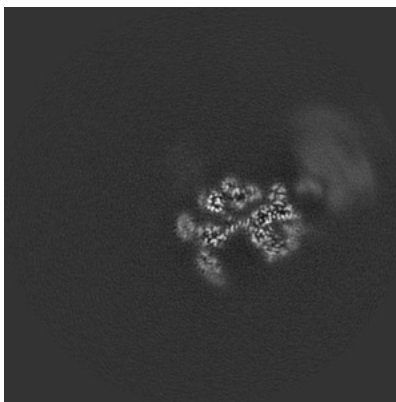
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

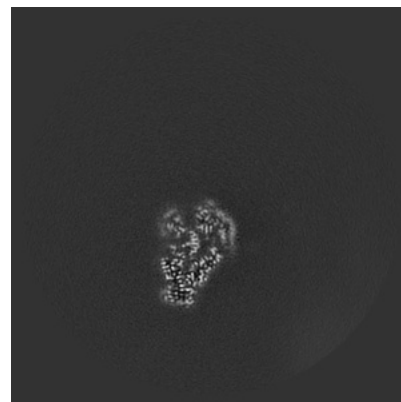
6.3.1 Primary map



X Index: 141



Y Index: 145

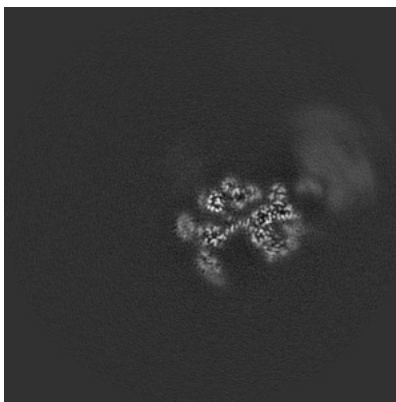


Z Index: 216

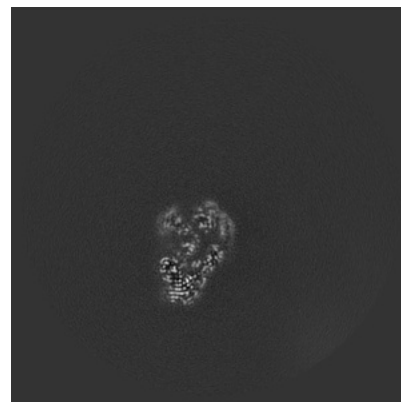
6.3.2 Raw map



X Index: 141



Y Index: 145



Z Index: 214

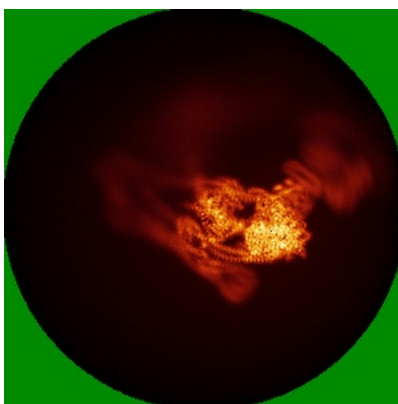
The images above show the largest variance slices of the map in three orthogonal directions.

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

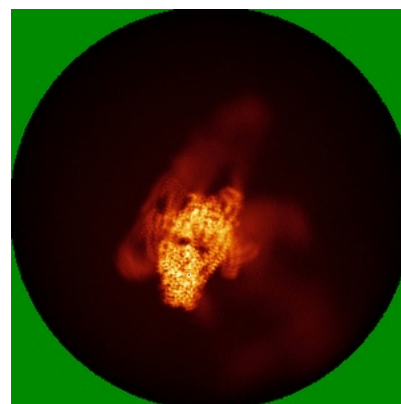
6.4.1 Primary map



X



Y

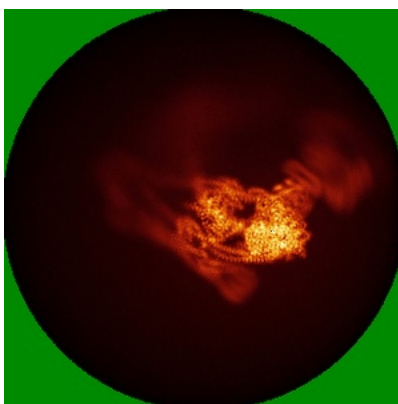


Z

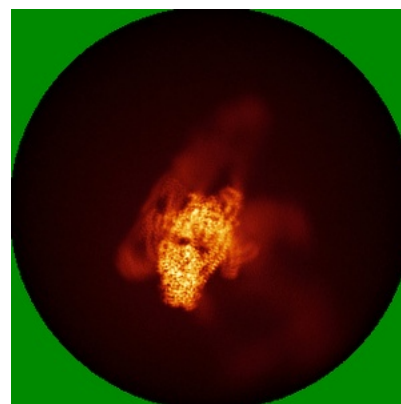
6.4.2 Raw map



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](#)

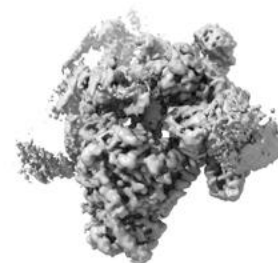
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

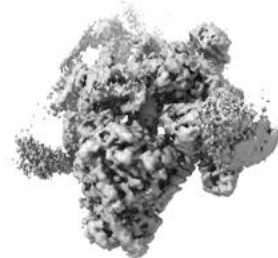
6.5.2 Raw map



X



Y



Z

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.

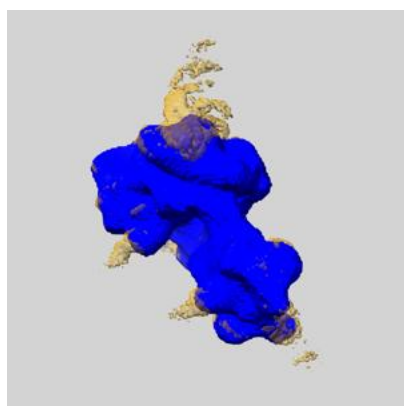
6.6 Mask visualisation [i](#)

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

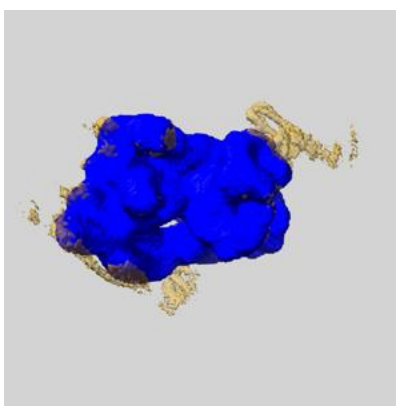
A mask typically either:

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

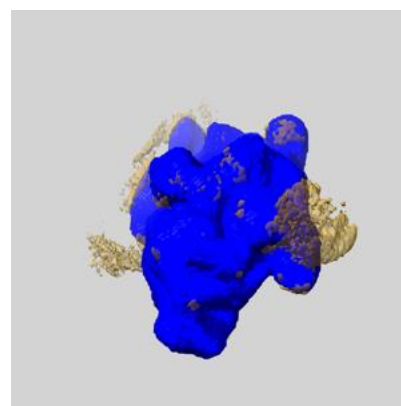
6.6.1 emd_12656_msk_1.map [i](#)



X



Y

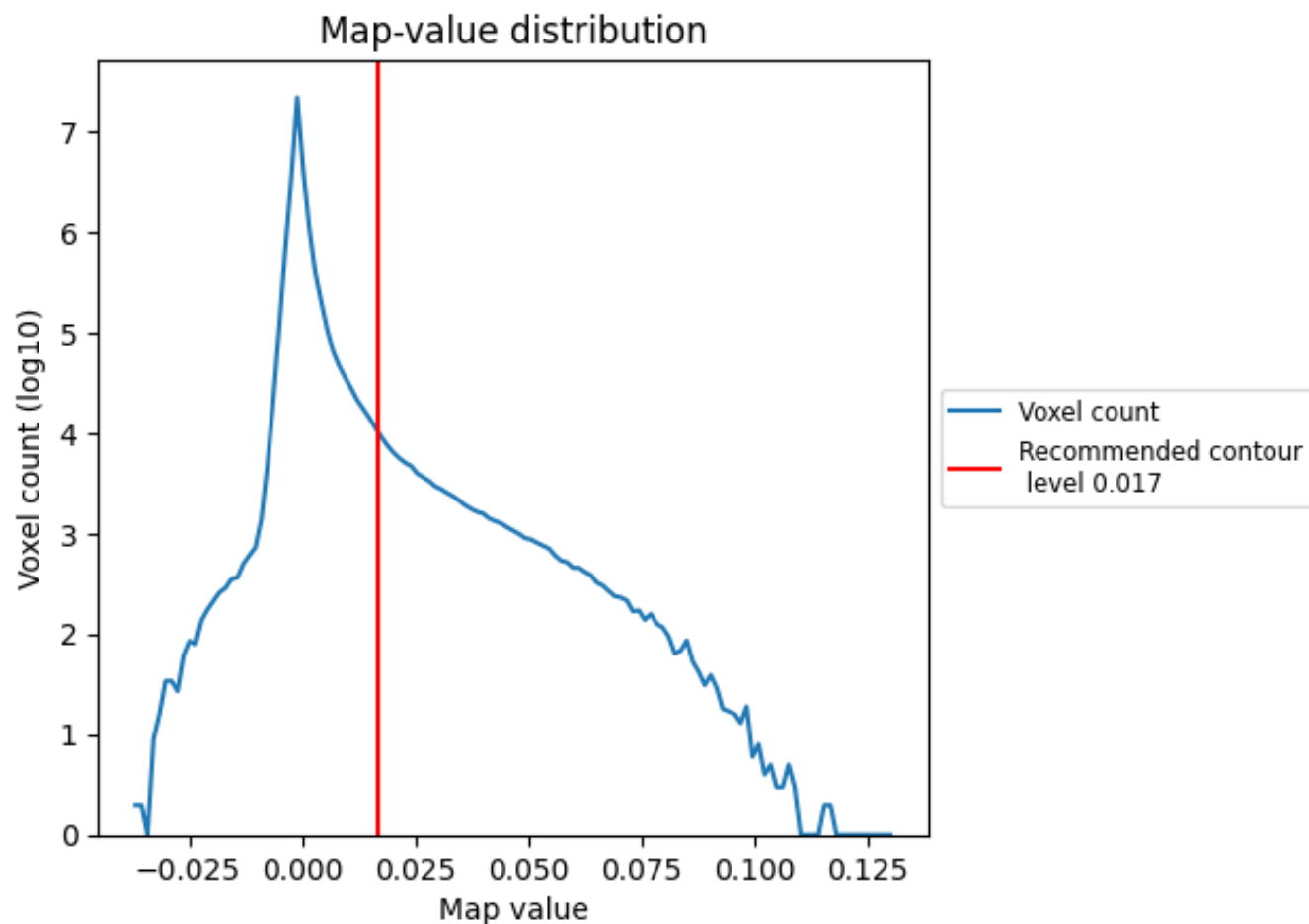


Z

7 Map analysis [i](#)

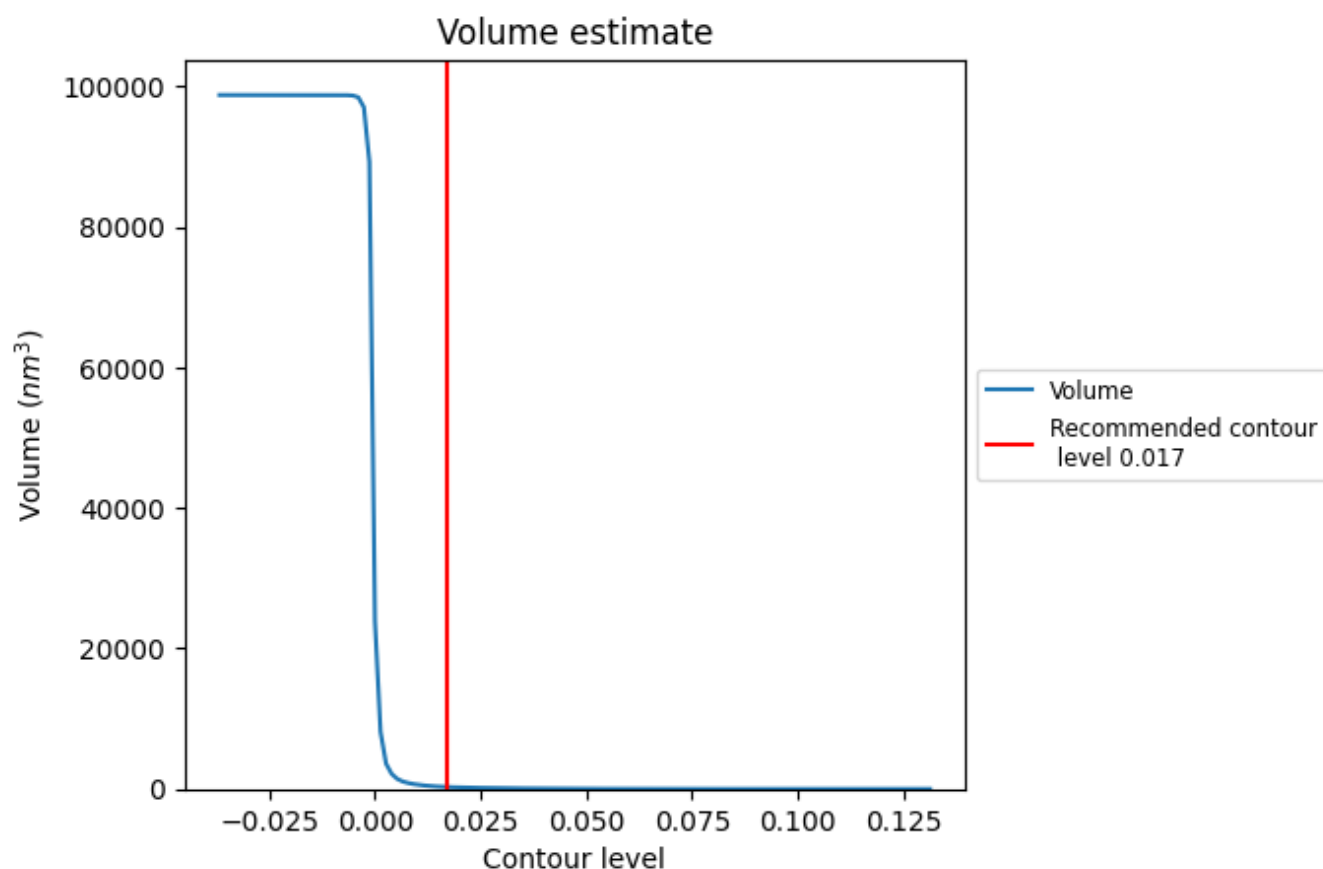
This section contains the results of statistical analysis of the map.

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.

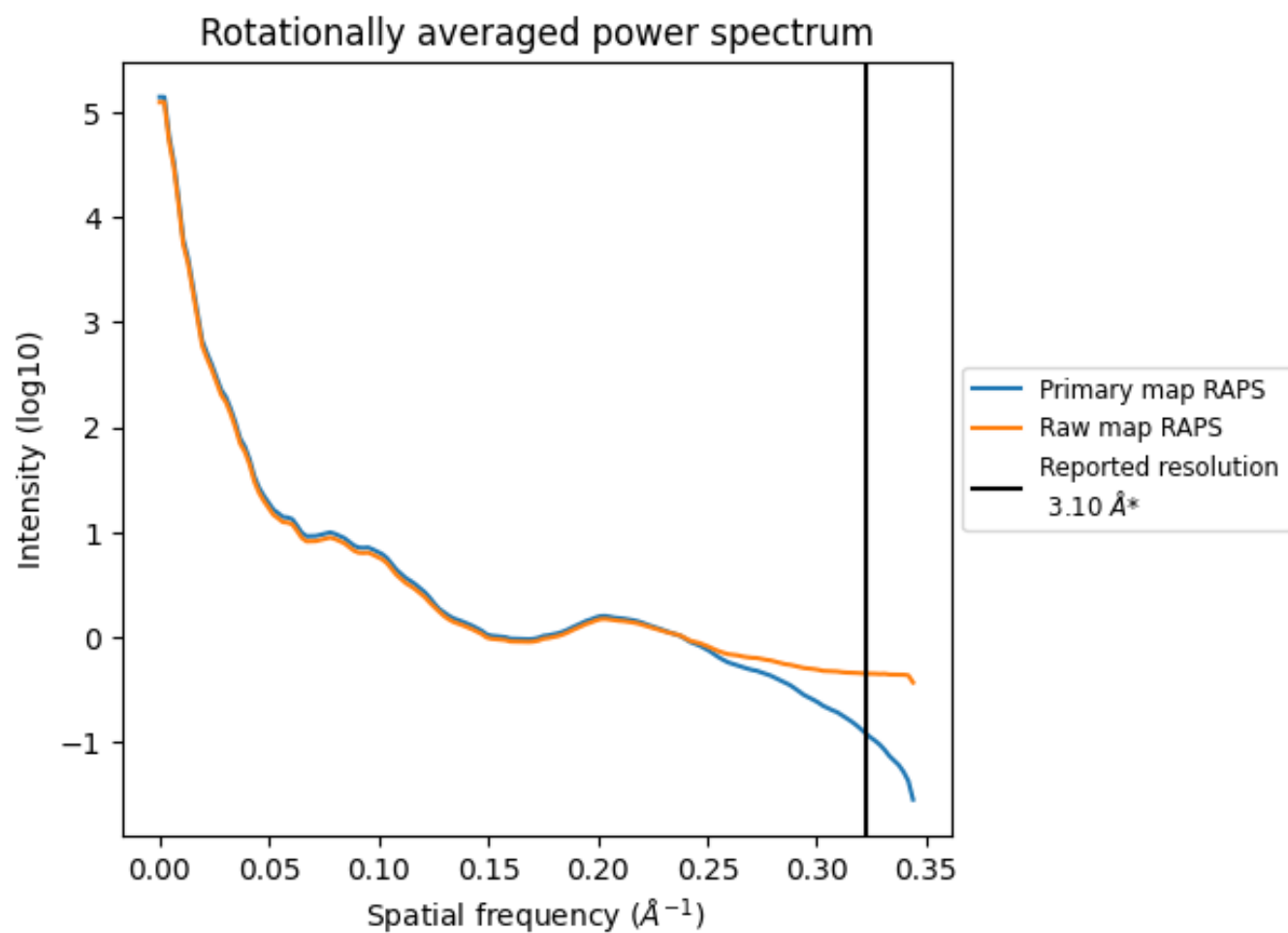
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm^3 ; this corresponds to an approximate mass of 252 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 ⓘ

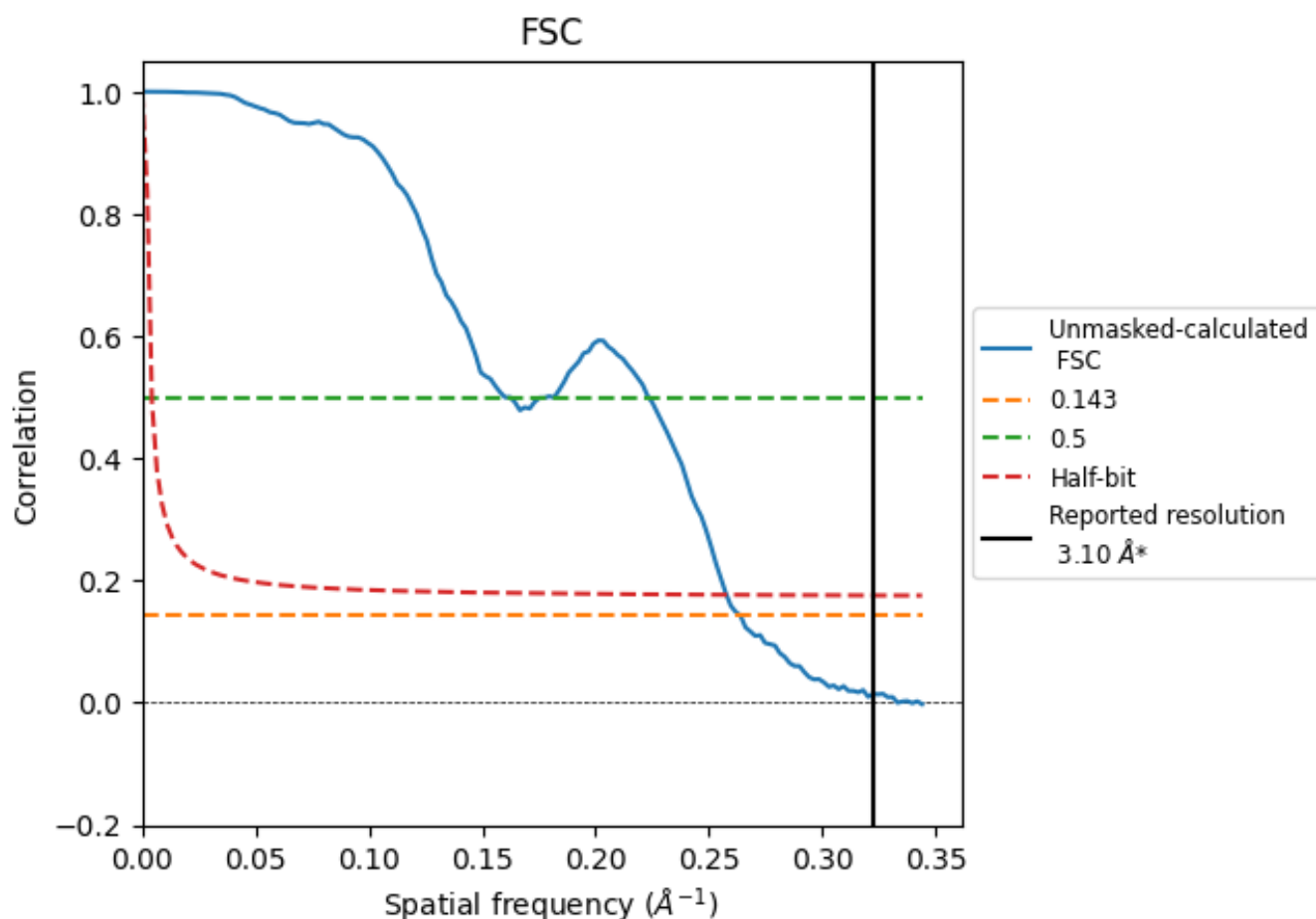


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

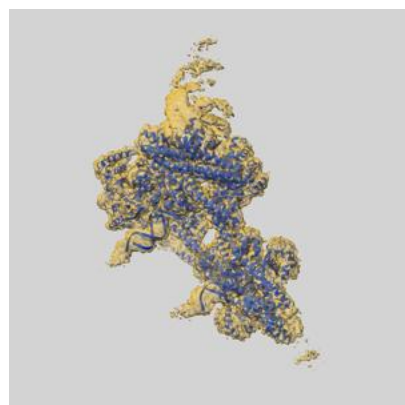
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	6.25	3.88

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

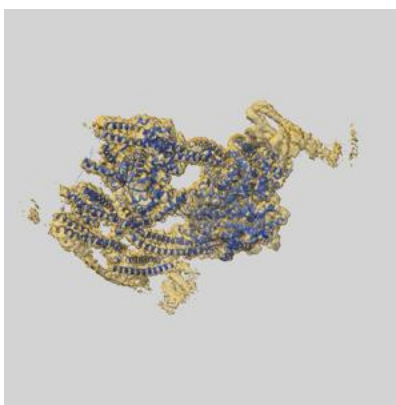
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12656 and PDB model 7NYW. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

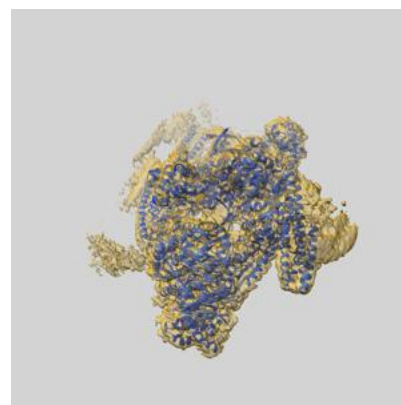
9.1 Map-model overlay [i](#)



X



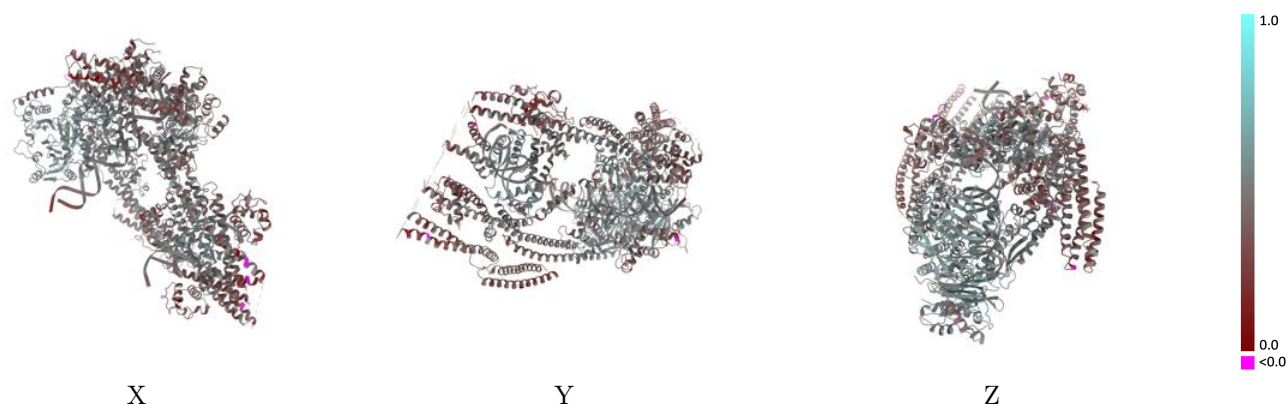
Y



Z

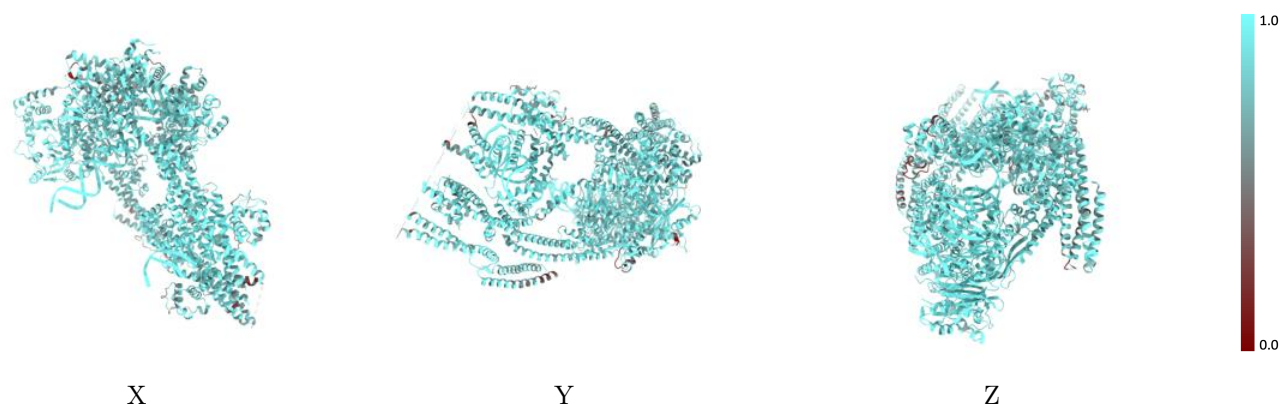
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



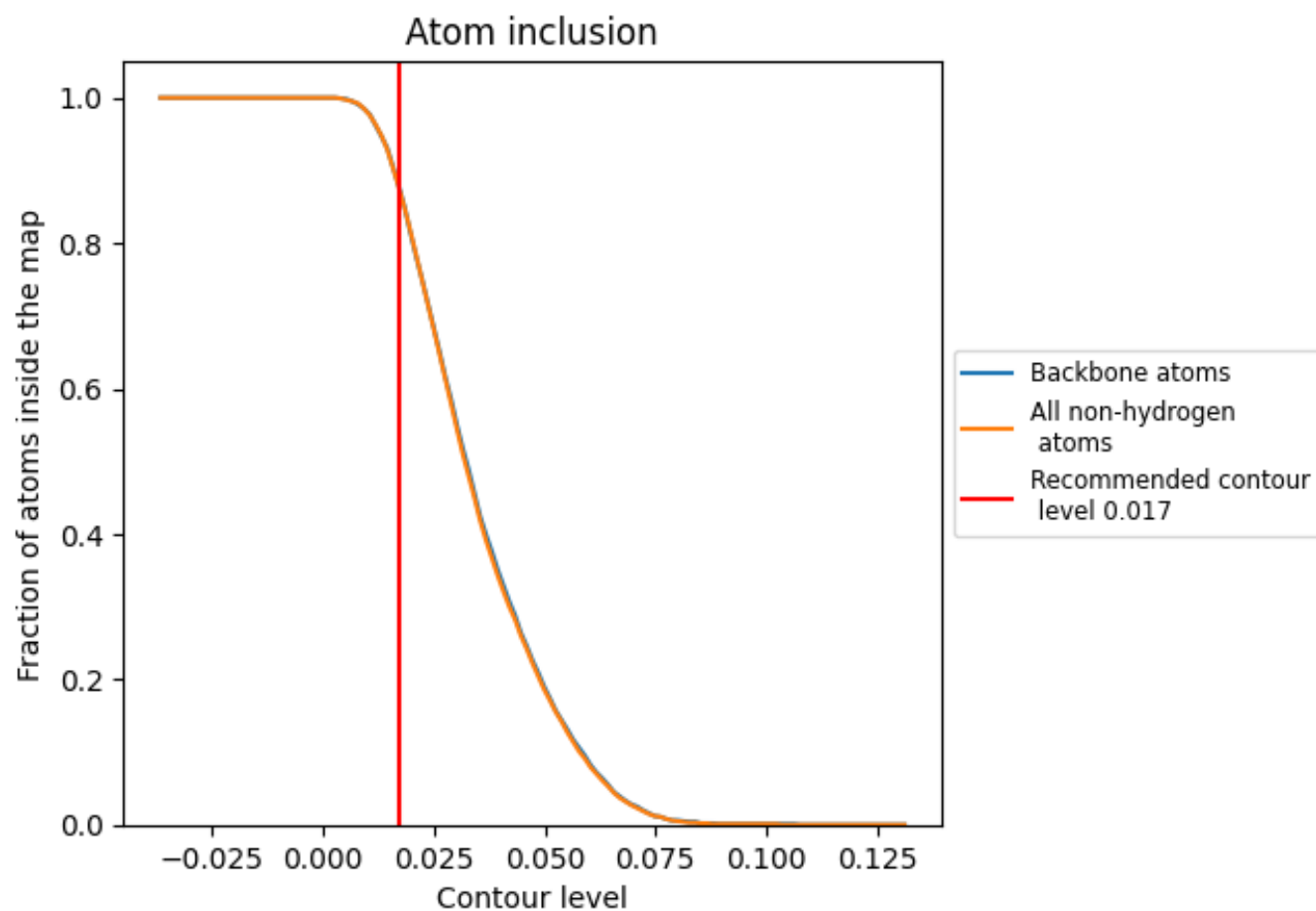
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.4520
A	 0.9150	 0.4850
B	 0.8890	 0.4640
C	 0.8360	 0.4130
D	 0.8030	 0.3790
E	 0.8980	 0.4680
F	 0.8360	 0.4260
G	 0.7980	 0.3330
H	 0.8020	 0.3290
I	 0.9170	 0.4930
J	 0.8920	 0.4410
K	 0.9870	 0.4900
L	 0.9800	 0.4890
M	 0.9840	 0.4390
N	 0.9810	 0.4470

