



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 08:42 PM EST

PDB ID : 8SY7
EMDB ID : EMD-40864
Title : E. coli DNA-directed RNA polymerase transcription elongation complex
bound the unnatural dB-STP base pair in the active site
Authors : Shan, Z.; Lyumkis, D.; Oh, J.; Wang, D.
Deposited on : 2023-05-24
Resolution : 2.65 Å(reported)
Based on initial model : 6ALH

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.39

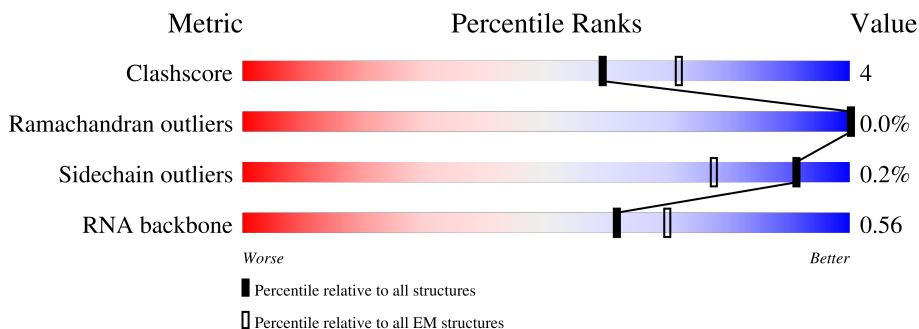
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	329	<div> <div>60%</div> <div>7%</div> <div>33%</div> </div>
1	G	329	<div> <div>59%</div> <div>8%</div> <div>33%</div> </div>
2	I	1342	<div> <div>80%</div> <div>8%</div> <div>13%</div> </div>
3	J	1430	<div> <div>65%</div> <div>8%</div> <div>26%</div> </div>
4	K	91	<div> <div>73%</div> <div>9%</div> <div>19%</div> </div>
5	N	18	<div> <div>56%</div> <div>6%</div> <div>39%</div> </div>
6	R	9	<div> <div>56%</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
7	T	29	<div><div></div><div>48%</div><div>24%</div><div>•</div><div>24%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21159 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	1	0
			1571	989	284	292	6		
1	G	221	Total	C	N	O	S	0	0
			1654	1038	289	321	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1170	Total	C	N	O	S	0	0
			8526	5366	1515	1609	36		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1052	Total	C	N	O	S	0	0
			7552	4764	1382	1366	40		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	74	Total	C	N	O	S	0	0
			545	338	104	102	1		

- Molecule 5 is a DNA chain called Non-template single stranded DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	11	Total	C	N	O	P	0	0
			227	108	48	61	10		

- Molecule 6 is a RNA chain called RNA oligomer.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	9	Total	C	N	O	P	0	0
			194	88	40	58	8		

- Molecule 7 is a DNA chain called Template single stranded DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	22	Total	C	N	O	P	0	0
			444	212	73	137	22		

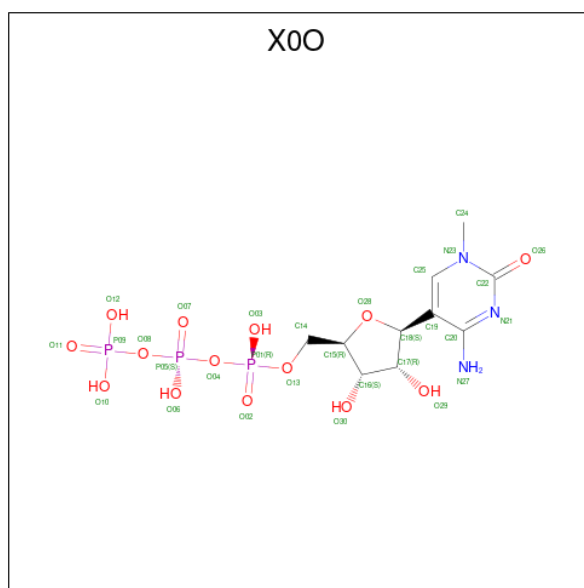
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	J	2	Total	Zn	0
			2	2	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

- Molecule 10 is [[(2 {R},3 {S},4 {R},5 {S})-5-(4-azanyl-1-methyl-2-oxidanylidene-pyrimidin-5-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: X0O) (formula: C₁₀H₁₈N₃O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	J	1	Total	C	N	O	P	0
			30	10	3	14	3	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	25	Total	O	0
			25	25	
11	G	32	Total	O	0
			32	32	
11	I	205	Total	O	0
			205	205	
11	J	136	Total	O	0
			136	136	
11	K	4	Total	O	0
			4	4	

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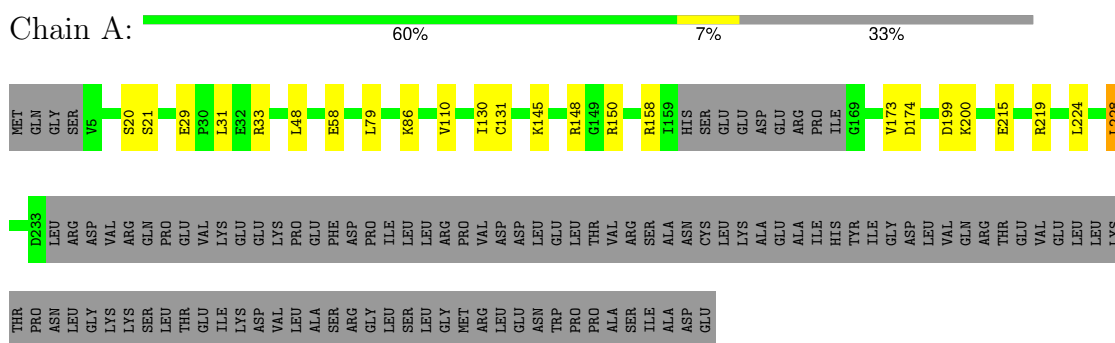
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Mol	Chain	Residues	Atoms		AltConf
11	R	4	Total 4	O 4	0
11	T	7	Total 7	O 7	0

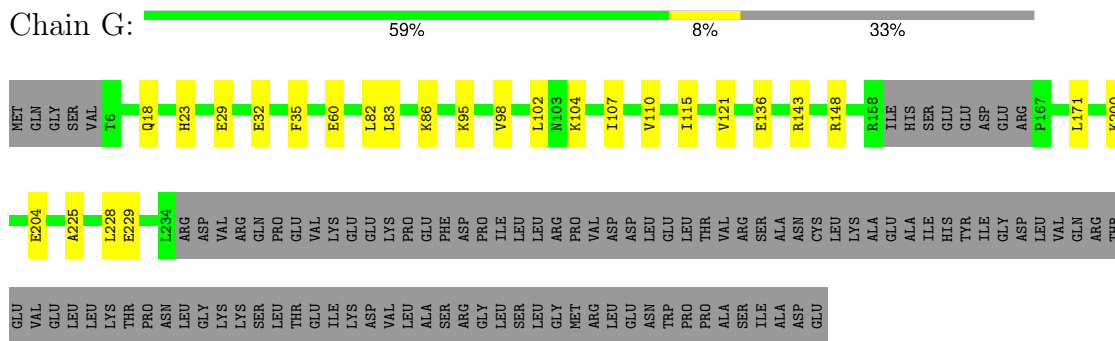
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

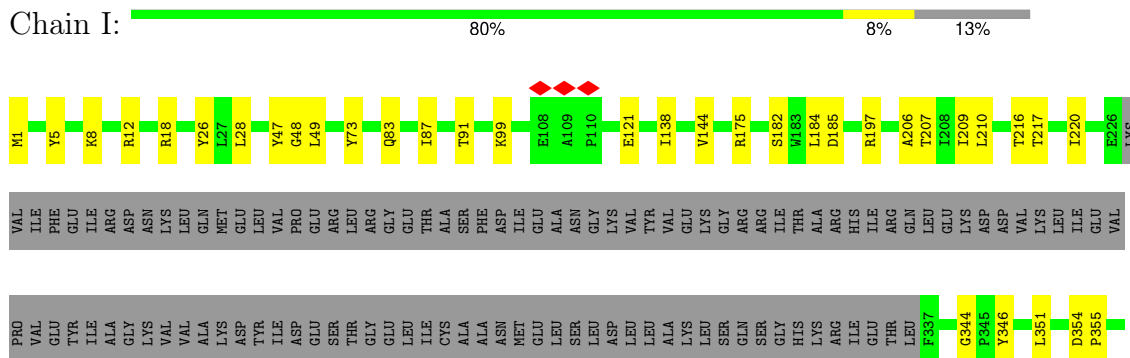
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



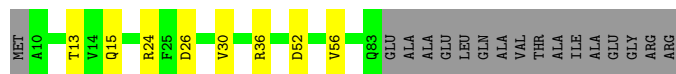
- Molecule 2: DNA-directed RNA polymerase subunit beta





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:  73% 9% 19%



- Molecule 5: Non-template single stranded DNA

Chain N:  56% 6% 39%



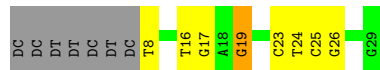
- Molecule 6: RNA oligomer

Chain R:  56% 44%



- Molecule 7: Template single stranded DNA

Chain T:  48% 24% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1326857	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	58140	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.521	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	275.2, 275.2, 275.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: IGU, ZN, X0O, MG

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	0.24	0/1591	0.53	1/2166 (0.0%)
1	G	0.24	0/1674	0.53	0/2274
2	I	0.25	0/8667	0.50	0/11769
3	J	0.24	0/7671	0.51	1/10426 (0.0%)
4	K	0.24	0/547	0.49	0/741
5	N	0.48	0/256	0.73	0/394
6	R	0.18	0/218	0.64	0/339
7	T	0.51	0/468	0.93	0/716
All	All	0.26	0/21092	0.53	2/28825 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	LEU	CA-CB-CG	5.72	128.47	115.30
3	J	1261	LEU	CA-CB-CG	5.49	127.93	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	47	TYR	Peptide
3	J	77	ARG	Peptide

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	1571	0	1540	17	0
1	G	1654	0	1655	15	0
2	I	8526	0	7930	63	0
3	J	7552	0	7187	79	0
4	K	545	0	541	5	0
5	N	227	0	124	1	0
6	R	194	0	98	1	0
7	T	444	0	250	6	0
8	J	2	0	0	0	0
9	J	1	0	0	0	0
10	J	30	0	0	1	0
11	A	25	0	0	1	0
11	G	32	0	0	1	0
11	I	205	0	0	1	0
11	J	136	0	0	4	0
11	K	4	0	0	0	0
11	R	4	0	0	0	0
11	T	7	0	0	0	0
All	All	21159	0	19325	174	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 4.

All (174) 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)
7:T:19:IGU:O4'	7:T:19:IGU:C1'	1.66	1.21
1:G:82:LEU:HD11	1:G:171:LEU:HD23	1.71	0.72
3:J:789:LYS:HE3	3:J:931:THR:HA	1.72	0.71
1:A:58:GLU:HB3	1:A:145:LYS:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:182:SER:HB2	2:I:389:PHE:HE1	1.55	0.69
2:I:435:ILE:HG12	2:I:440:GLY:HA3	1.74	0.69
3:J:482:ALA:O	4:K:24:ARG:NH1	2.28	0.67
2:I:550:VAL:HG23	3:J:780:ARG:HD2	1.76	0.67
2:I:802:VAL:HG12	2:I:1096:ILE:HB	1.77	0.67
3:J:77:ARG:HH22	3:J:79:LYS:HG2	1.58	0.67
3:J:538:ARG:NH2	11:J:1602:HOH:O	2.27	0.67
3:J:45:ASN:ND2	3:J:50:LYS:O	2.27	0.66
1:A:29:GLU:HB2	1:A:200:LYS:HG3	1.76	0.65
3:J:77:ARG:HG2	3:J:78:LEU:H	1.61	0.65
2:I:619:ALA:HB2	2:I:654:ASP:HB2	1.81	0.62
1:A:79:LEU:HD21	3:J:526:VAL:HG11	1.82	0.61
2:I:12:ARG:HG3	2:I:1181:PRO:HB2	1.83	0.61
3:J:245:LEU:HD21	3:J:249:LEU:HB2	1.83	0.61
2:I:18:ARG:O	2:I:1156:ARG:NH1	2.33	0.61
3:J:77:ARG:HH12	3:J:79:LYS:HG2	1.66	0.61
3:J:557:LYS:HD3	3:J:561:GLY:HA2	1.82	0.61
3:J:644:MET:O	3:J:764:ARG:NH1	2.34	0.61
3:J:60:ARG:NH1	3:J:89:GLY:O	2.35	0.60
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.35	0.59
2:I:841:ARG:HG2	2:I:1046:VAL:HG12	1.85	0.59
3:J:781:LYS:NZ	11:J:1610:HOH:O	2.35	0.58
3:J:430:HIS:CE1	3:J:432:LEU:HB2	2.38	0.58
2:I:99:LYS:HA	2:I:121:GLU:HA	1.87	0.57
2:I:1117:LEU:HD13	2:I:1195:ILE:HG12	1.85	0.57
3:J:842:ARG:NH1	11:J:1608:HOH:O	2.32	0.57
3:J:77:ARG:HH12	3:J:79:LYS:H	1.52	0.56
3:J:519:ASN:ND2	3:J:709:ARG:O	2.39	0.56
2:I:5:TYR:HA	2:I:8:LYS:HE2	1.87	0.56
1:A:215:GLU:OE2	1:A:219:ARG:HD3	2.06	0.56
3:J:115:TRP:HE1	3:J:308:ASP:HB2	1.72	0.55
3:J:1330:ARG:O	3:J:1334:GLU:HG3	2.07	0.55
3:J:77:ARG:NH1	3:J:79:LYS:H	2.05	0.54
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.89	0.54
3:J:85:CYS:SG	3:J:90:VAL:N	2.78	0.54
1:G:86:LYS:NZ	11:G:403:HOH:O	2.40	0.54
2:I:812:PHE:CD2	2:I:813:GLU:HG2	2.43	0.54
3:J:20:ILE:HD12	3:J:1344:LEU:HD21	1.90	0.54
3:J:384:LYS:HD2	3:J:415:VAL:HG22	1.90	0.53
2:I:1:MET:HA	2:I:1159:VAL:HG22	1.90	0.53
3:J:1259:GLN:O	3:J:1262:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:O	1:A:219:ARG:HG2	2.09	0.53
2:I:411:ARG:NH2	2:I:427:ASP:OD1	2.41	0.53
3:J:282:LEU:HD21	3:J:292:VAL:HG22	1.90	0.52
3:J:674:THR:HG22	3:J:676:GLY:H	1.75	0.52
3:J:1224:ARG:HB2	3:J:1228:ALA:HB2	1.91	0.52
2:I:422:LYS:O	2:I:426:ILE:HG12	2.10	0.52
2:I:175:ARG:HG3	2:I:185:ASP:HB3	1.91	0.52
2:I:934:PHE:O	2:I:1048:LYS:HA	2.10	0.52
1:A:33:ARG:HH11	2:I:1081:PRO:HG3	1.74	0.52
1:A:199:ASP:OD2	11:A:401:HOH:O	2.19	0.51
3:J:44:ILE:HG13	3:J:57:PHE:HB2	1.92	0.51
4:K:13:THR:HG22	4:K:15:GLN:H	1.75	0.51
1:A:48:LEU:HD11	3:J:535:ARG:HG3	1.93	0.51
1:A:31:LEU:HB2	1:A:199:ASP:HB2	1.92	0.51
3:J:703:THR:O	3:J:703:THR:HG22	2.10	0.51
2:I:184:LEU:HB2	2:I:389:PHE:CE2	2.46	0.50
4:K:26:ASP:O	4:K:30:VAL:HG23	2.11	0.50
3:J:1314:LEU:HD13	3:J:1330:ARG:HH22	1.77	0.50
3:J:128:LEU:HD13	3:J:188:LEU:HD23	1.93	0.50
3:J:43:THR:HG22	3:J:45:ASN:H	1.77	0.49
3:J:77:ARG:NH2	3:J:79:LYS:HG2	2.26	0.49
3:J:909:ILE:HD11	3:J:913:GLU:HG3	1.94	0.49
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.77	0.49
3:J:411:ILE:O	3:J:415:VAL:HG23	2.12	0.49
3:J:807:LEU:HD11	3:J:894:VAL:HG13	1.93	0.49
3:J:1261:LEU:HD12	3:J:1261:LEU:O	2.12	0.49
3:J:518:VAL:HB	3:J:707:ILE:HD12	1.94	0.49
1:G:102:LEU:HD12	1:G:115:ILE:HG12	1.94	0.49
3:J:464:ASP:OD1	6:R:9:G:O2'	2.20	0.49
1:G:95:LYS:O	1:G:148:ARG:NH1	2.42	0.49
3:J:309:ASN:OD1	3:J:310:GLY:N	2.46	0.49
3:J:77:ARG:HG2	3:J:78:LEU:N	2.25	0.49
3:J:274:ASN:OD1	3:J:275:ARG:N	2.45	0.49
3:J:694:SER:HB2	3:J:738:ARG:HD2	1.94	0.49
2:I:565:GLU:OE2	3:J:783:LEU:HD13	2.12	0.49
2:I:1314:GLN:HB2	4:K:36:ARG:HH21	1.77	0.48
3:J:123:ARG:HH11	3:J:1337:VAL:HG21	1.78	0.48
3:J:720:ASN:O	3:J:724:MET:HG3	2.14	0.48
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.45	0.48
4:K:52:ASP:HB3	4:K:56:VAL:HG23	1.96	0.48
2:I:185:ASP:OD1	2:I:197:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:THR:OG1	2:I:138:ILE:O	2.18	0.47
1:A:228:LEU:HD12	1:A:228:LEU:O	2.14	0.47
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.46	0.47
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.95	0.47
1:G:23:HIS:NE2	1:G:204:GLU:OE2	2.45	0.47
1:G:225:ALA:O	1:G:229:GLU:HG3	2.15	0.47
2:I:1296:ASP:OD1	2:I:1296:ASP:N	2.46	0.47
2:I:1106:ARG:NH2	10:J:1504:XOO:O12	2.45	0.47
3:J:734:ALA:O	3:J:738:ARG:HG2	2.15	0.47
1:A:86:LYS:HE3	1:A:174:ASP:HB2	1.96	0.47
2:I:402:ARG:HD3	2:I:416:GLY:HA3	1.97	0.47
2:I:448:LEU:HD11	2:I:554:HIS:HD2	1.80	0.47
1:G:107:ILE:HD12	1:G:136:GLU:HG2	1.96	0.46
5:N:10:DG:H22	7:T:8:DT:H3	1.63	0.46
2:I:210:LEU:HD13	2:I:220:ILE:HD12	1.97	0.46
2:I:1257:GLN:HG2	2:I:1296:ASP:HB3	1.98	0.46
3:J:45:ASN:ND2	3:J:48:THR:O	2.48	0.46
2:I:8:LYS:HE3	2:I:1171:ARG:HH22	1.81	0.46
1:A:20:SER:OG	1:A:21:SER:N	2.49	0.46
3:J:823:THR:O	3:J:838:ARG:NH1	2.48	0.46
2:I:5:TYR:HD1	2:I:8:LYS:HZ3	1.64	0.46
2:I:742:TYR:HB2	2:I:745:GLU:HG2	1.99	0.46
3:J:538:ARG:HA	3:J:538:ARG:HD2	1.70	0.45
3:J:926:PRO:HG2	3:J:1248:ILE:HD11	1.98	0.45
2:I:598:VAL:HG23	2:I:627:GLY:HA3	1.98	0.45
3:J:96:LYS:O	3:J:99:ARG:HG2	2.16	0.45
3:J:233:LYS:HB2	3:J:236:TRP:CZ2	2.51	0.45
2:I:206:ALA:O	2:I:209:ILE:HG22	2.17	0.45
2:I:727:VAL:HG12	2:I:773:LEU:HD13	1.97	0.45
3:J:1362:GLY:O	3:J:1365:TYR:HB3	2.16	0.45
2:I:882:ILE:HD11	2:I:885:GLY:HA2	1.98	0.45
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.99	0.45
3:J:566:LYS:HE2	3:J:566:LYS:HB3	1.82	0.44
2:I:49:LEU:HD23	2:I:73:TYR:CZ	2.52	0.44
1:A:224:LEU:HG	1:G:228:LEU:HD11	1.99	0.44
3:J:64:PRO:HG3	3:J:91:GLU:O	2.18	0.44
2:I:83:GLN:O	2:I:87:ILE:HG12	2.17	0.44
2:I:144:VAL:HG23	2:I:515:MET:HG3	2.00	0.43
3:J:233:LYS:HB2	3:J:236:TRP:CE2	2.53	0.43
3:J:370:LYS:HE2	3:J:409:TRP:CZ3	2.53	0.43
3:J:77:ARG:NH1	3:J:79:LYS:HG2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:24:DT:H2'	7:T:25:DC:C6	2.53	0.43
2:I:811:ASN:HA	2:I:815:SER:HB2	1.99	0.43
3:J:430:HIS:HD2	3:J:925:GLU:HG3	1.83	0.43
3:J:662:ALA:O	3:J:665:GLN:HB2	2.18	0.43
1:A:130:ILE:HG22	1:A:131:CYS:SG	2.59	0.43
2:I:217:THR:HG23	2:I:351:LEU:HD11	1.99	0.43
1:G:60:GLU:HG3	1:G:143:ARG:HH21	1.84	0.43
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.54	0.43
2:I:719:LYS:HE3	2:I:719:LYS:HB2	1.80	0.42
2:I:344:GLY:HA3	2:I:346:TYR:CE2	2.53	0.42
2:I:464:PHE:HA	2:I:498:ILE:HD11	2.02	0.42
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.88	0.42
2:I:559:CYS:HB2	2:I:662:SER:HB3	2.01	0.42
3:J:245:LEU:O	3:J:250:ARG:NH2	2.52	0.42
2:I:49:LEU:HD23	2:I:73:TYR:CE1	2.54	0.42
3:J:381:ILE:HD11	3:J:412:LEU:HD13	2.02	0.42
7:T:23:DC:H2'	7:T:24:DT:C6	2.54	0.42
2:I:549:ASP:OD1	2:I:550:VAL:N	2.50	0.42
1:G:83:LEU:HB3	2:I:694:ARG:HH21	1.83	0.42
2:I:636:CYS:HB2	2:I:645:PHE:CD1	2.55	0.41
2:I:1244:HIS:CG	2:I:1262:LYS:HG3	2.55	0.41
1:A:158:ARG:NH2	1:A:173:VAL:O	2.48	0.41
2:I:48:GLY:HA2	2:I:461:GLU:OE1	2.20	0.41
3:J:41:PRO:HD2	3:J:54:ASP:O	2.19	0.41
3:J:99:ARG:HB3	3:J:248:ASP:HB2	2.02	0.41
3:J:817:HIS:HA	11:J:1626:HOH:O	2.20	0.41
3:J:1221:LEU:HB2	3:J:1229:VAL:HG11	2.02	0.41
1:G:29:GLU:OE2	1:G:200:LYS:HB2	2.21	0.41
2:I:354:ASP:HA	2:I:355:PRO:HD3	1.94	0.41
2:I:26:TYR:OH	11:I:1401:HOH:O	2.21	0.41
3:J:1349:GLU:OE1	3:J:1349:GLU:N	2.47	0.41
3:J:425:ARG:HG2	3:J:427:PRO:HD2	2.02	0.41
7:T:16:DT:H2'	7:T:17:DG:C8	2.55	0.41
1:G:143:ARG:HE	1:G:143:ARG:HB2	1.72	0.41
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.55	0.41
2:I:207:THR:HG21	2:I:351:LEU:HB3	2.02	0.41
2:I:813:GLU:OE2	3:J:460:ASP:HA	2.21	0.41
2:I:832:HIS:CD2	2:I:1058:ARG:HG3	2.56	0.41
3:J:70:CYS:SG	3:J:74:LYS:N	2.94	0.41
3:J:490:ILE:HD11	3:J:609:TYR:CE1	2.56	0.41
1:G:98:VAL:HG21	1:G:121:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:216:THR:O	2:I:220:ILE:HG12	2.21	0.41
2:I:583:GLU:HG2	2:I:584:TYR:N	2.36	0.41
3:J:78:LEU:O	3:J:81:ARG:HB3	2.21	0.40
2:I:1151:LEU:HD12	2:I:1201:LEU:HD22	2.02	0.40
7:T:25:DC:H2'	7:T:26:DG:C8	2.56	0.40
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.56	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	217/329 (66%)	215 (99%)	2 (1%)	0	100	100
1	G	217/329 (66%)	214 (99%)	3 (1%)	0	100	100
2	I	1162/1342 (87%)	1115 (96%)	47 (4%)	0	100	100
3	J	1044/1430 (73%)	1006 (96%)	37 (4%)	1 (0%)	48	67
4	K	72/91 (79%)	70 (97%)	2 (3%)	0	100	100
All	All	2712/3521 (77%)	2620 (97%)	91 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	45	ASN

5.3.2 Protein sidechains [i](#)

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	153/286 (54%)	151 (99%)	2 (1%)	65	80
1	G	176/286 (62%)	175 (99%)	1 (1%)	84	92
2	I	807/1157 (70%)	807 (100%)	0	100	100
3	J	691/1189 (58%)	690 (100%)	1 (0%)	92	97
4	K	53/75 (71%)	53 (100%)	0	100	100
All	All	1880/2993 (63%)	1876 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148[A]	ARG
1	A	148[B]	ARG
1	G	18	GLN
3	J	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	45	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	7/9 (77%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	2	U
6	R	4	G
6	R	6	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	IGU	T	19	7	21,24,25	4.92	13 (61%)	29,35,38	1.62	4 (13%)

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
7	IGU	T	19	7	-	2/7/21/22	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	19	IGU	O4'-C1'	10.79	1.66	1.42
7	T	19	IGU	C4-N3	9.16	1.51	1.33
7	T	19	IGU	C5-C6	8.44	1.58	1.40
7	T	19	IGU	O4'-C4'	-7.59	1.28	1.45
7	T	19	IGU	C2'-C1'	-6.68	1.34	1.52
7	T	19	IGU	C2-N1	5.12	1.50	1.39
7	T	19	IGU	C6-N6	5.05	1.44	1.34
7	T	19	IGU	C2-N3	4.60	1.47	1.36
7	T	19	IGU	O3'-C3'	-4.29	1.34	1.43
7	T	19	IGU	C3'-C4'	3.97	1.63	1.53
7	T	19	IGU	C6-N1	2.34	1.41	1.37
7	T	19	IGU	C8-N7	2.30	1.39	1.32
7	T	19	IGU	C5-N7	-2.29	1.34	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	19	IGU	C5-C6-N6	-3.57	120.12	124.66
7	T	19	IGU	C5-C4-N3	-3.46	120.49	127.60
7	T	19	IGU	N9-C8-N7	-3.10	107.66	113.40
7	T	19	IGU	C8-N7-C5	2.18	108.15	104.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	19	IGU	O4'-C4'-C5'-O5'
7	T	19	IGU	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	19	IGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
10	X0O	J	1504	-	29,31,31	5.70	18 (62%)	39,49,49	1.88	10 (25%)

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
10	X0O	J	1504	-	-	3/22/38/38	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1504	X0O	C22-N23	15.29	1.63	1.39
10	J	1504	X0O	O28-C18	-11.37	1.28	1.43
10	J	1504	X0O	C17-C16	-10.80	1.24	1.53
10	J	1504	X0O	C25-C19	10.38	1.49	1.35
10	J	1504	X0O	C17-C18	9.98	1.67	1.53
10	J	1504	X0O	C20-N21	7.84	1.46	1.34
10	J	1504	X0O	P01-O04	5.50	1.65	1.59
10	J	1504	X0O	P05-O04	5.45	1.65	1.59
10	J	1504	X0O	P05-O08	5.45	1.65	1.59
10	J	1504	X0O	C20-N27	4.44	1.45	1.34
10	J	1504	X0O	C14-C15	-4.03	1.39	1.51
10	J	1504	X0O	C22-N21	-3.63	1.29	1.36
10	J	1504	X0O	O30-C16	3.51	1.51	1.43
10	J	1504	X0O	O28-C15	3.07	1.51	1.45
10	J	1504	X0O	O26-C22	-2.69	1.18	1.23
10	J	1504	X0O	C16-C15	2.60	1.59	1.53
10	J	1504	X0O	C25-N23	-2.52	1.30	1.36
10	J	1504	X0O	O29-C17	2.24	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1504	X0O	C16-C17-C18	5.48	108.16	101.69
10	J	1504	X0O	O26-C22-N21	-5.14	114.23	122.33
10	J	1504	X0O	C24-N23-C22	3.80	122.09	118.56
10	J	1504	X0O	N23-C22-N21	3.24	123.59	119.16
10	J	1504	X0O	C24-N23-C25	-3.17	114.43	120.58
10	J	1504	X0O	O26-C22-N23	2.82	122.17	118.76
10	J	1504	X0O	C25-N23-C22	2.56	123.48	120.44
10	J	1504	X0O	C19-C20-N21	-2.34	119.36	121.75
10	J	1504	X0O	O28-C18-C17	2.30	108.34	105.15
10	J	1504	X0O	C20-N21-C22	-2.09	117.90	120.81

There are no chirality outliers.

All (3) torsion outliers are listed below:

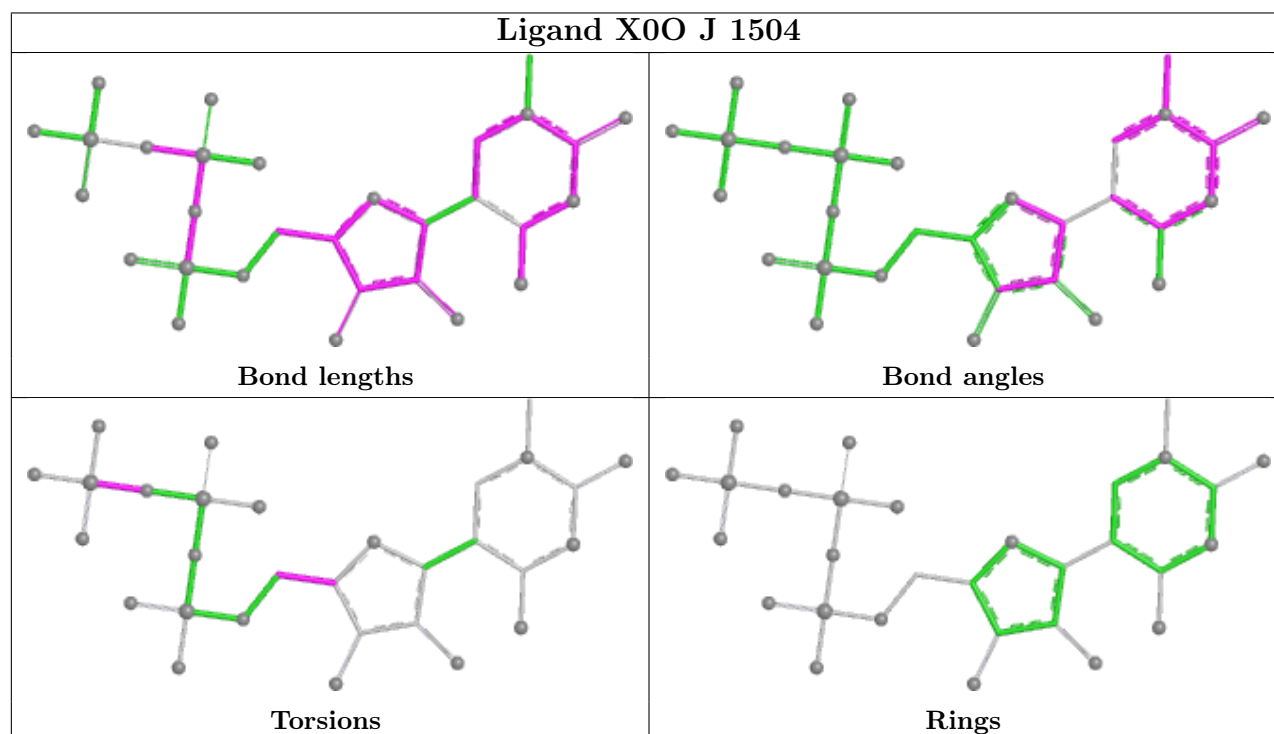
Mol	Chain	Res	Type	Atoms
10	J	1504	X0O	O13-C14-C15-C16
10	J	1504	X0O	O13-C14-C15-O28
10	J	1504	X0O	P05-O08-P09-O12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1504	X0O	1	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.

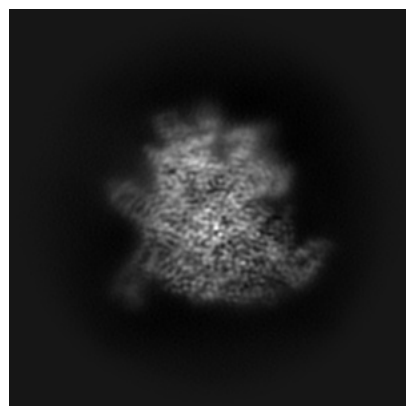
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40864. These allow visual inspection of the internal detail of the map and identification of artifacts.

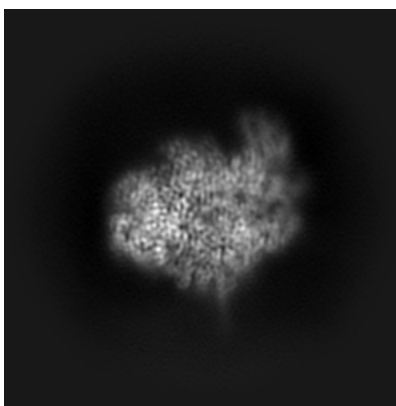
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

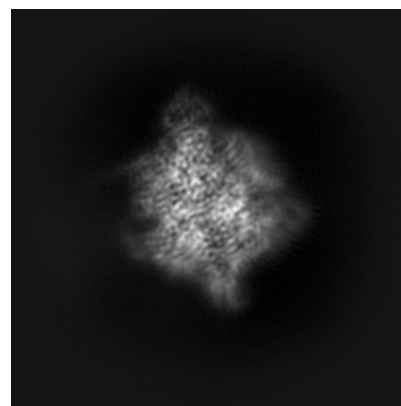
6.1.1 Primary map



X

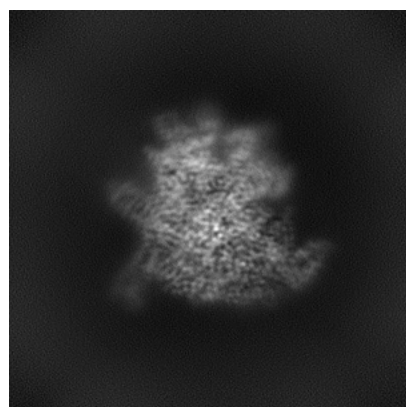


Y

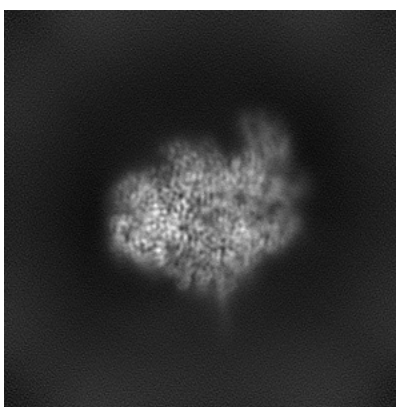


Z

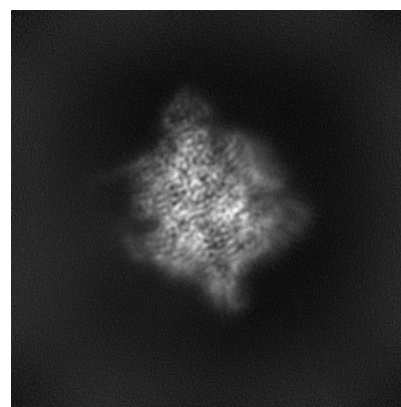
6.1.2 Raw map



X



Y

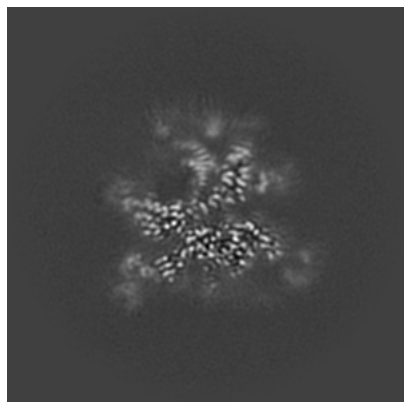


Z

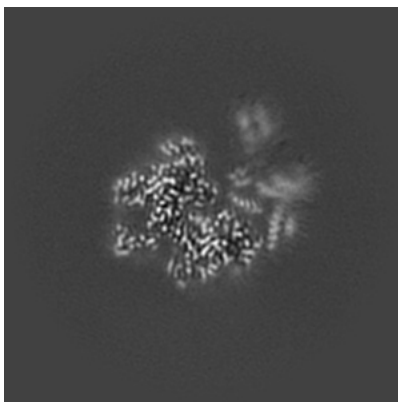
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

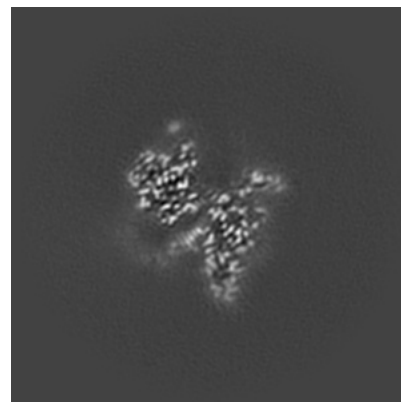
6.2.1 Primary map



X Index: 160

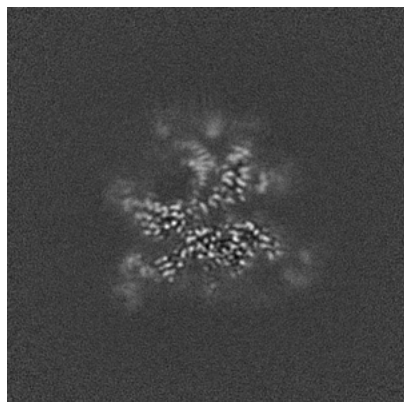


Y Index: 160

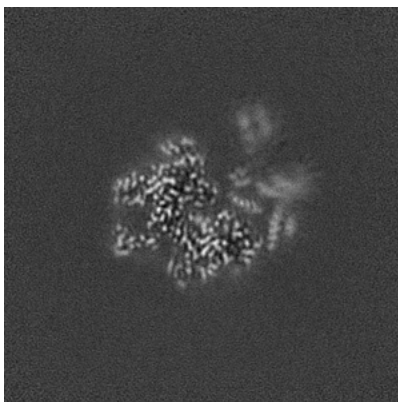


Z Index: 160

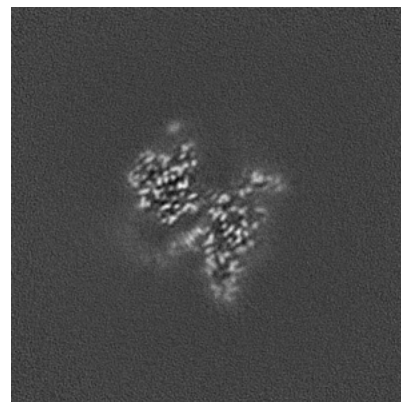
6.2.2 Raw map



X Index: 160



Y Index: 160

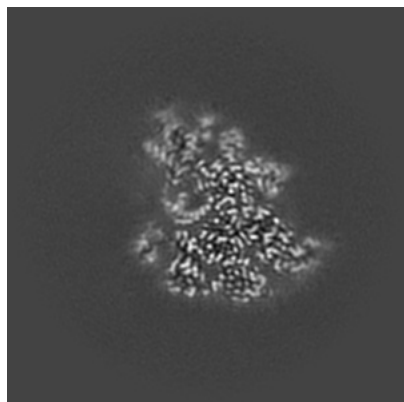


Z Index: 160

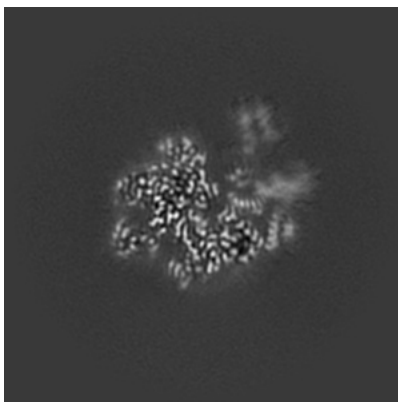
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

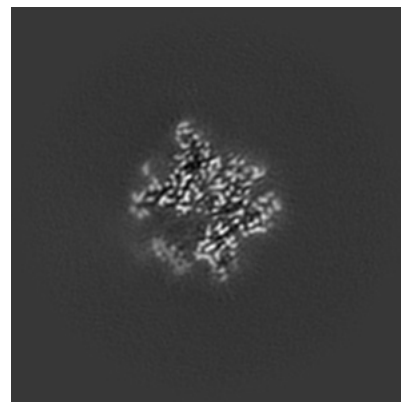
6.3.1 Primary map



X Index: 144

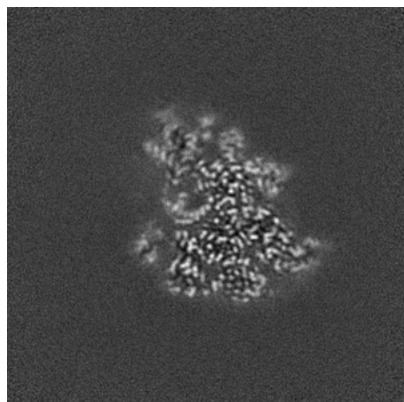


Y Index: 158

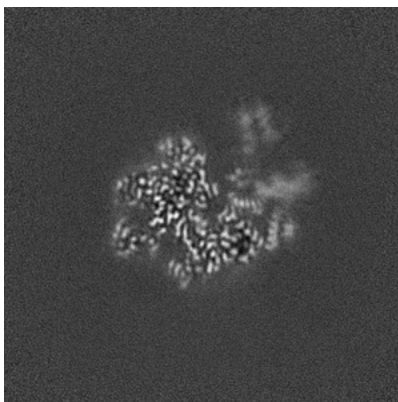


Z Index: 144

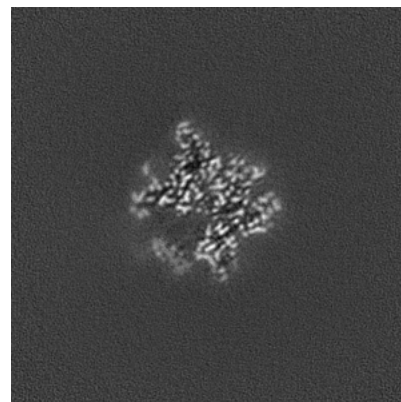
6.3.2 Raw map



X Index: 144



Y Index: 158

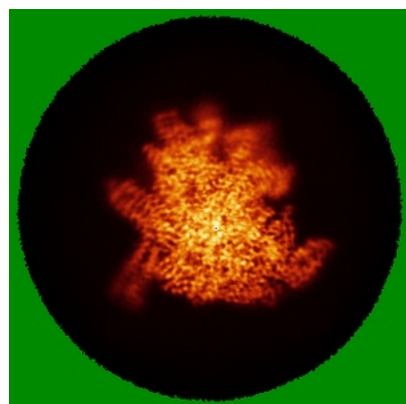


Z Index: 144

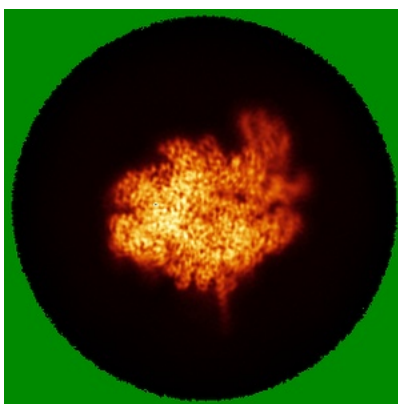
The images above show the largest variance slices of the map in three orthogonal directions.

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

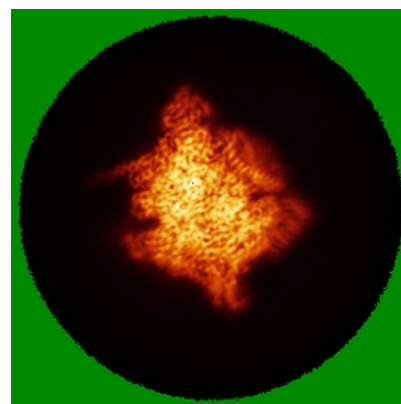
6.4.1 Primary map



X

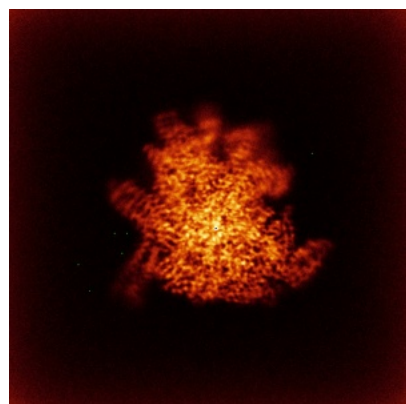


Y

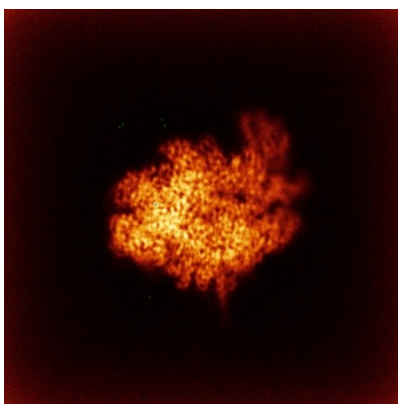


Z

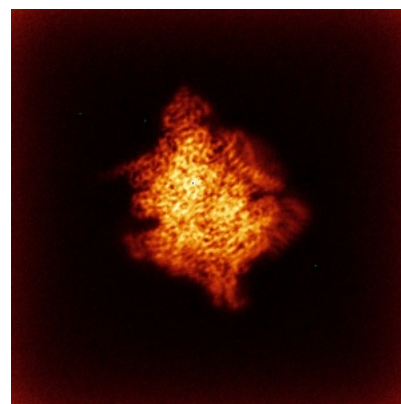
6.4.2 Raw map



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.

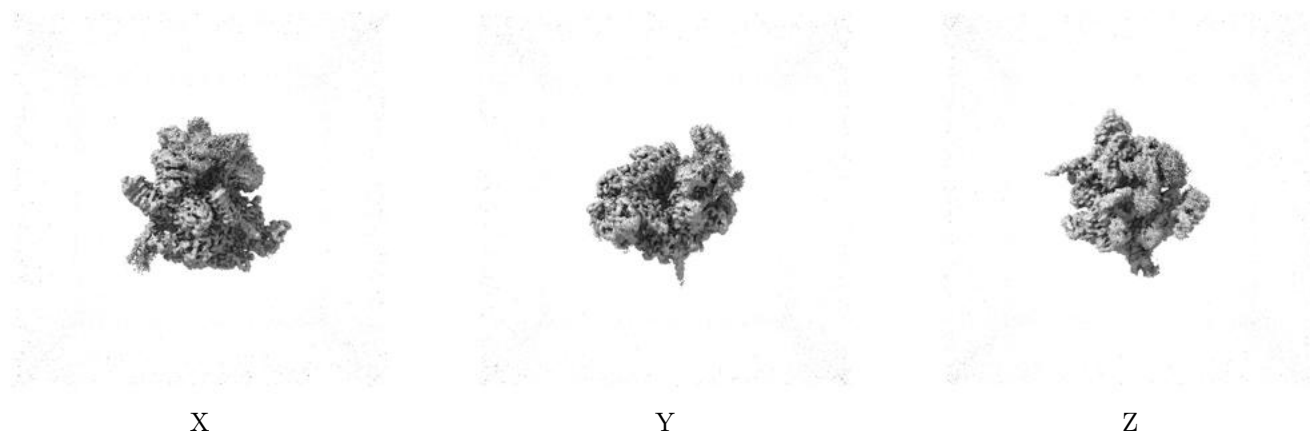
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

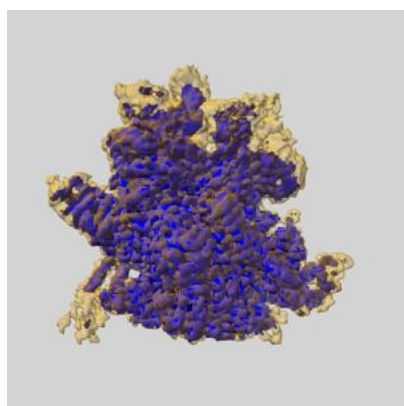
6.6 Mask visualisation [i](#)

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

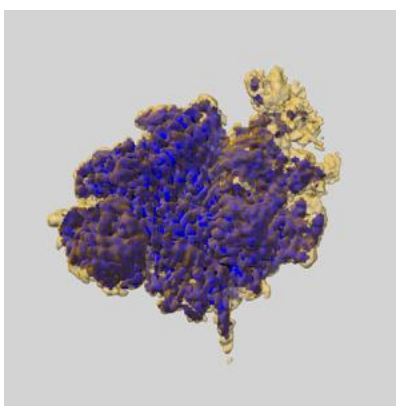
A mask typically either:

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

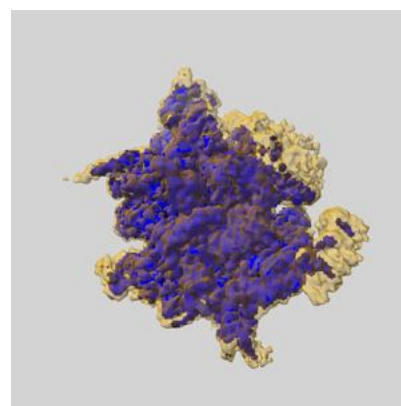
6.6.1 emd_40864_msk_1.map [i](#)



X



Y

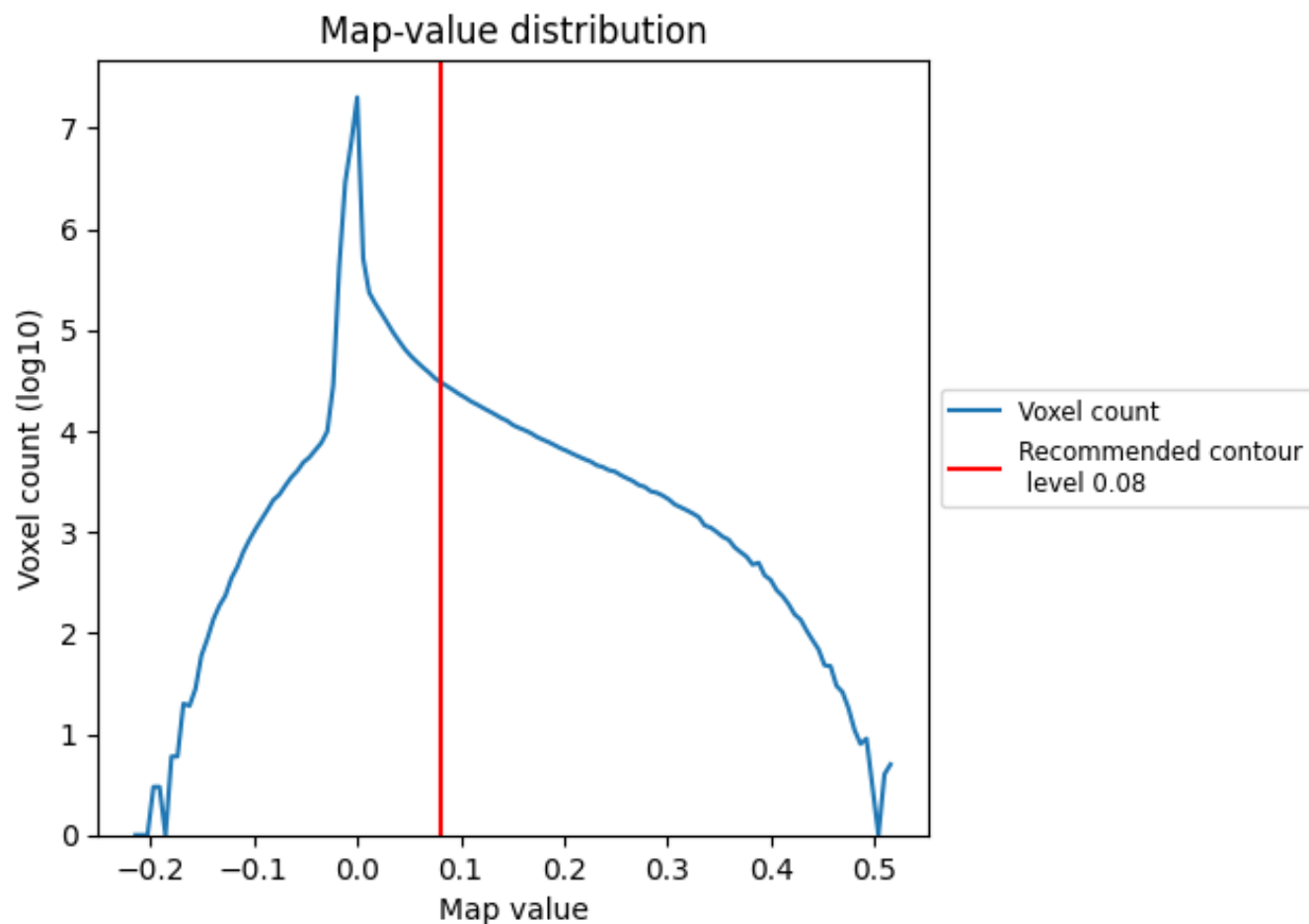


Z

7 Map analysis [i](#)

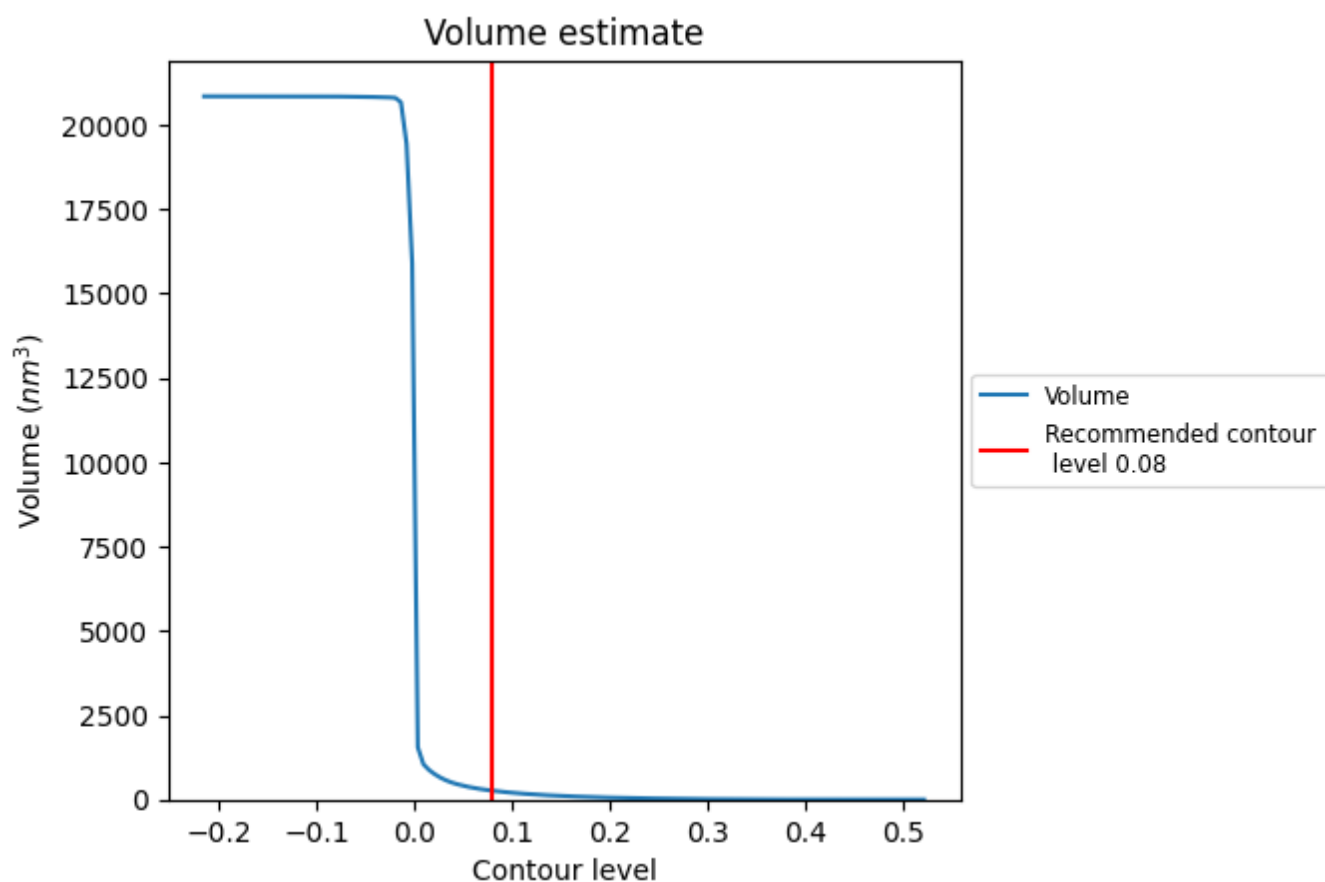
This section contains the results of statistical analysis of the map.

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.

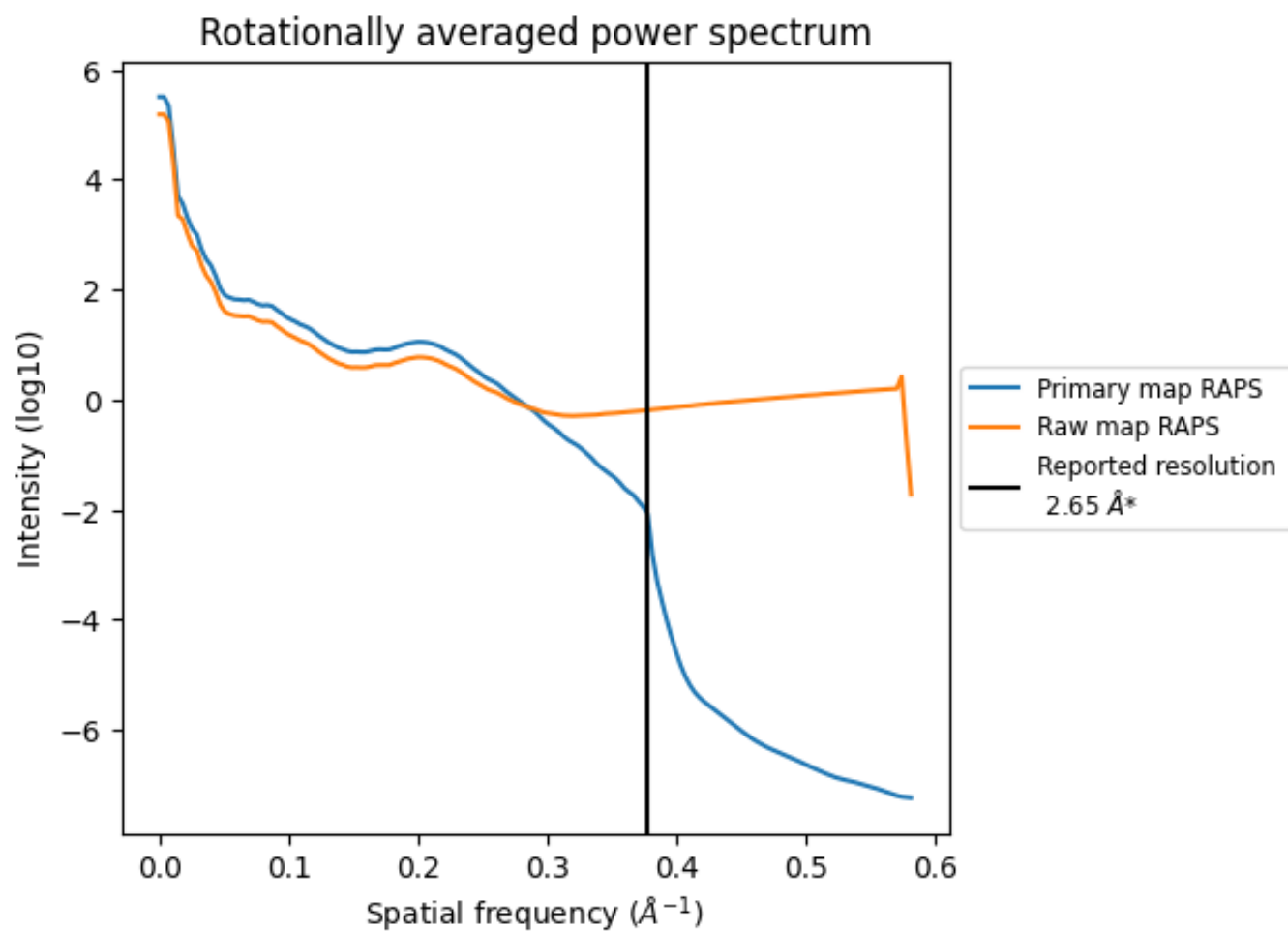
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm^3 ; this corresponds to an approximate mass of 238 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 ⓘ

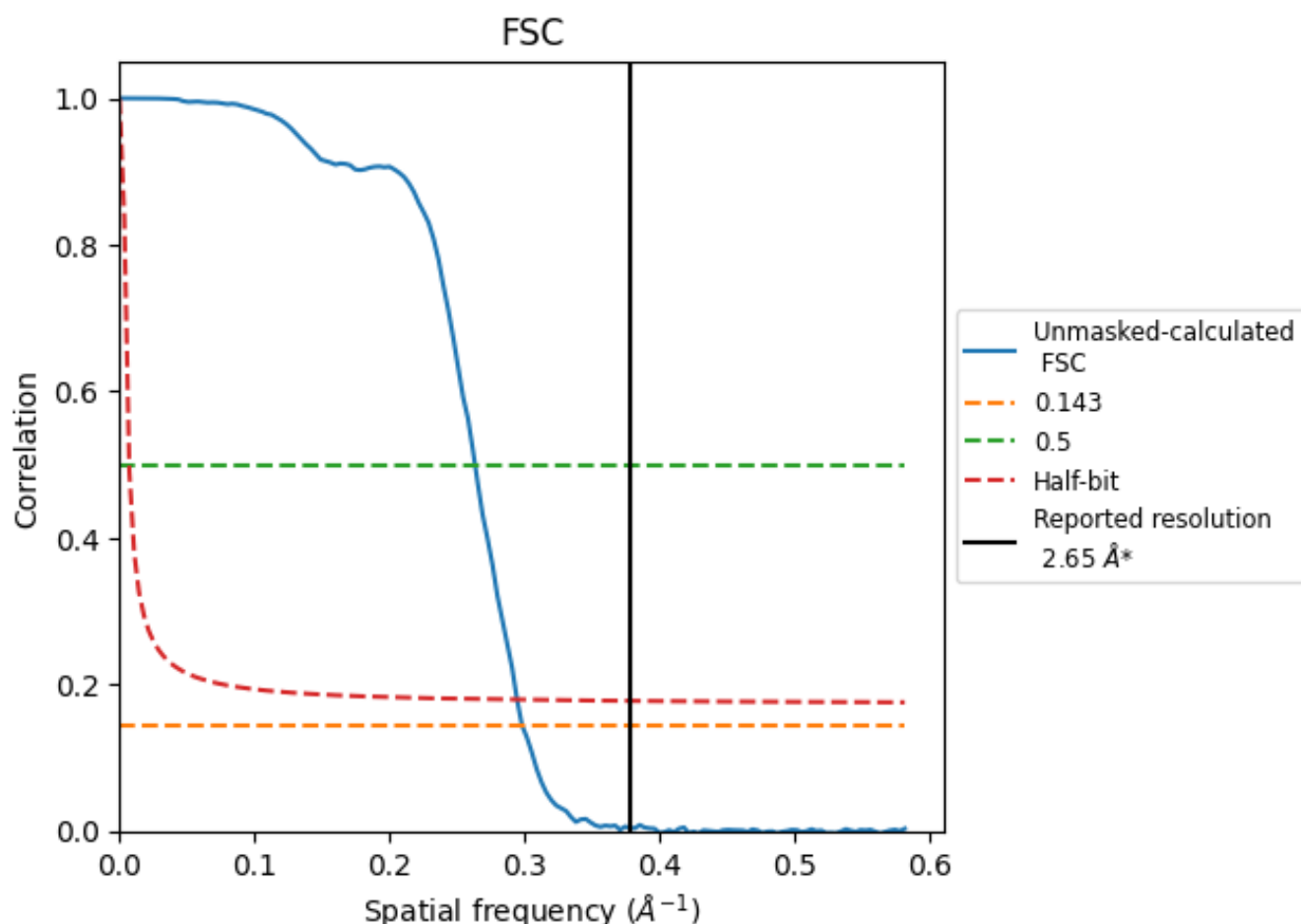


*Reported resolution corresponds to spatial frequency of 0.377 \AA^{-1}

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 0.377 \AA^{-1}

8.2 Resolution estimates [i](#)

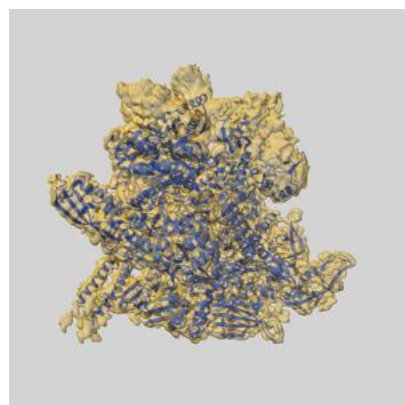
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.35	3.80	3.40

*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 3.35 differs from the reported value 2.65 by more than 10 %

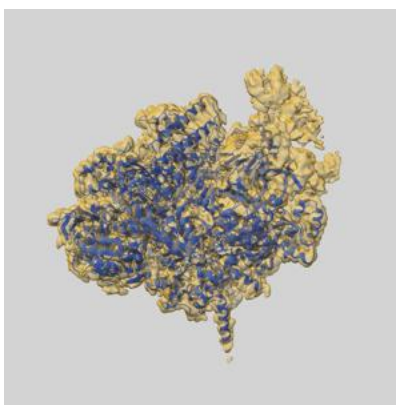
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40864 and PDB model 8SY7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

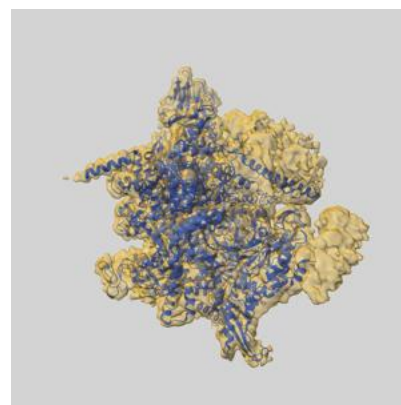
9.1 Map-model overlay [i](#)



X



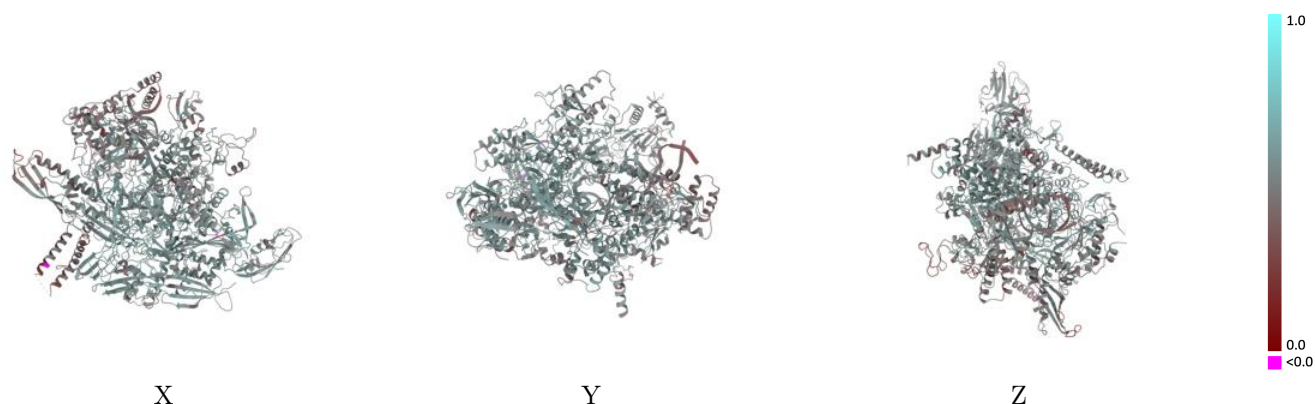
Y



Z

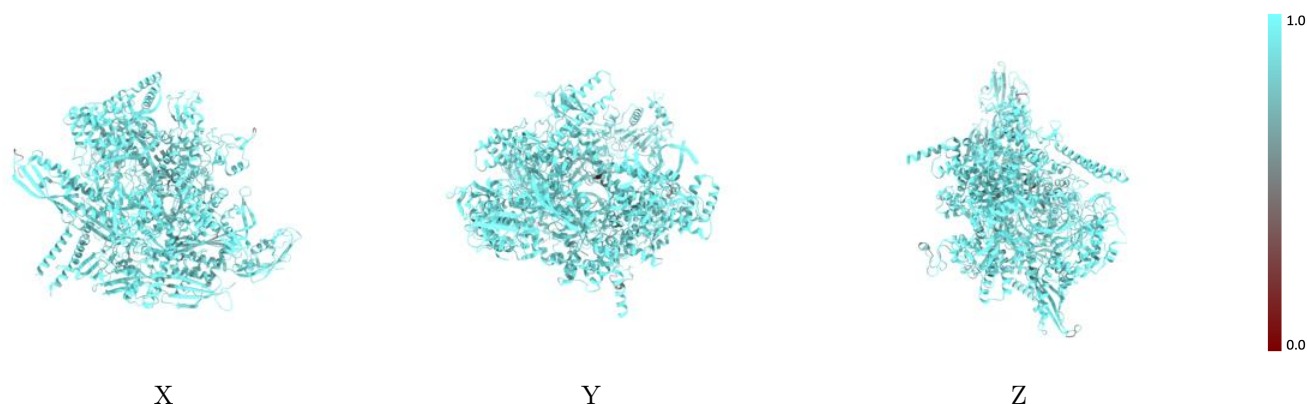
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



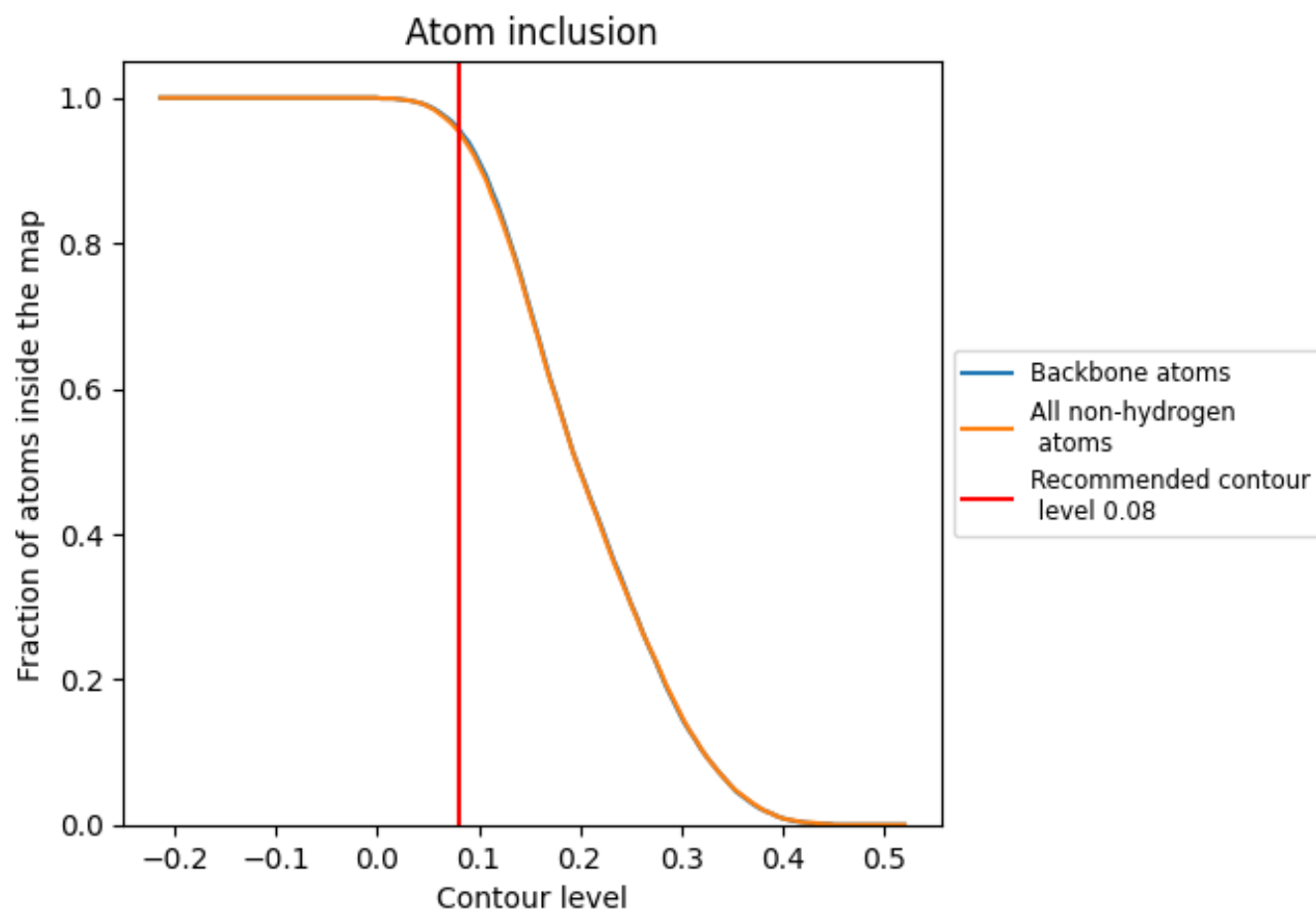
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9540	<div><div></div></div> 0.5220
A	<div><div></div></div> 0.9260	<div><div></div></div> 0.5270
G	<div><div></div></div> 0.9490	<div><div></div></div> 0.5460
I	<div><div></div></div> 0.9620	<div><div></div></div> 0.5320
J	<div><div></div></div> 0.9530	<div><div></div></div> 0.5100
K	<div><div></div></div> 0.9380	<div><div></div></div> 0.5270
N	<div><div></div></div> 0.9780	<div><div></div></div> 0.4520
R	<div><div></div></div> 0.9900	<div><div></div></div> 0.5090
T	<div><div></div></div> 0.9820	<div><div></div></div> 0.4760

1.0

0.0

<0.0