



Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 09:53 am GMT

PDB ID : 8S0B
EMDB ID : EMD-19620
Title : H. sapiens MCM bound to double stranded DNA and ORC6 as part of the MCM-ORC complex
Authors : Greiwe, J.F.; Weissmann, F.; Diffley, J.F.X.; Costa, A.
Deposited on : 2024-02-13
Resolution : 3.60 Å(reported)
Based on initial model : .

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 : 1.8.4, CSD as541be (2020)
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) : 2.40

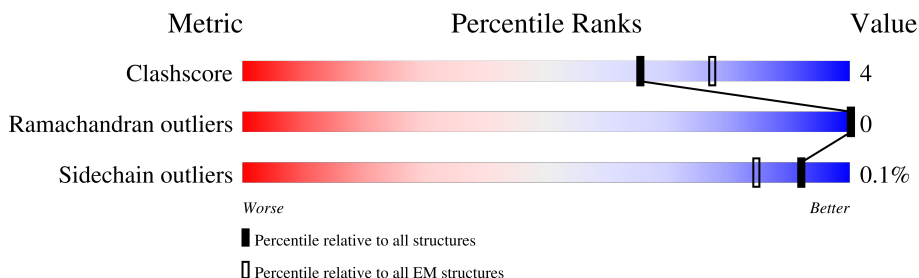
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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

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	F	251	<div> <div>10%</div> <div>65%</div> <div>5%</div> <div>30%</div> </div>
2	2	904	<div> <div>63%</div> <div>8%</div> <div>29%</div> </div>
3	3	810	<div> <div>66%</div> <div>8%</div> <div>26%</div> </div>
4	4	863	<div> <div>66%</div> <div>6%</div> <div>28%</div> </div>
5	5	734	<div> <div>75%</div> <div>7%</div> <div>19%</div> </div>
6	6	821	<div> <div>73%</div> <div>6%</div> <div>21%</div> </div>
7	7	719	<div> <div>68%</div> <div>8%</div> <div>24%</div> </div>
8	X	45	<div> <div>16%</div> <div>24%</div> <div>76%</div> </div>

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Mol	Chain	Length	Quality of chain
9	Y	45	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 32424 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 Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	175	Total	C	N	O	S	0	0
			1341	846	232	250	13		

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	643	Total	C	N	O	S	0	0
			5093	3206	909	948	30		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	598	Total	C	N	O	S	0	0
			4715	2954	837	898	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-1	GLY	-	expression tag	UNP P25205
3	0	GLU	-	expression tag	UNP P25205

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	623	Total	C	N	O	S	0	0
			4969	3130	880	932	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	650	MET	LEU	variant	UNP P33991

- Molecule 5 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	595	Total	C	N	O	S	0	0
			4679	2936	834	874	35		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	652	Total	C	N	O	S	0	0
			5259	3322	930	980	27		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	548	Total	C	N	O	S	0	0
			4338	2737	760	811	30		

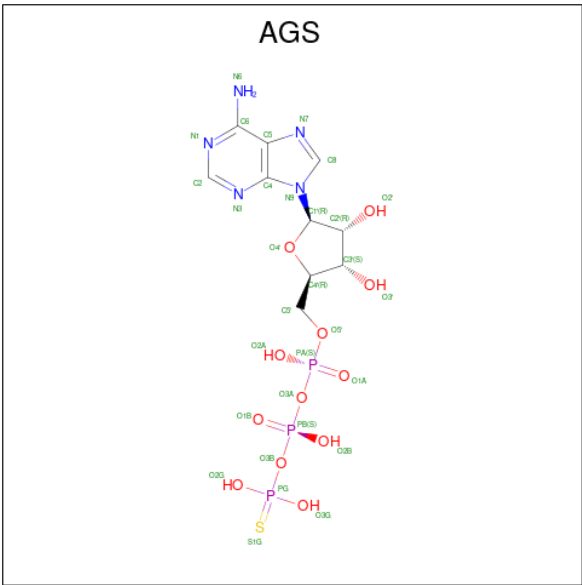
- Molecule 8 is a DNA chain called DNA (45-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	45	Total	C	N	O	P	0	0
			921	438	168	270	45		

- Molecule 9 is a DNA chain called DNA (45-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	45	Total	C	N	O	P	0	0
			924	439	170	270	45		

- Molecule 10 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	2	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	6	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	7	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

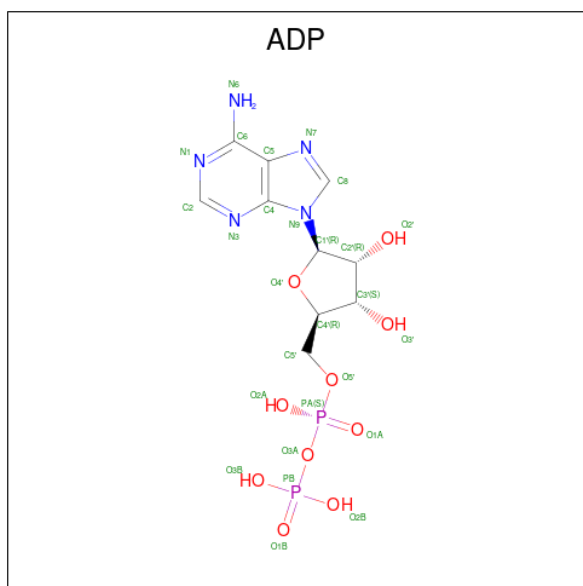
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	2	1	Total	Mg	0
			1	1	
11	3	1	Total	Mg	0
			1	1	
11	5	1	Total	Mg	0
			1	1	
11	6	1	Total	Mg	0
			1	1	
11	7	2	Total	Mg	0
			2	2	

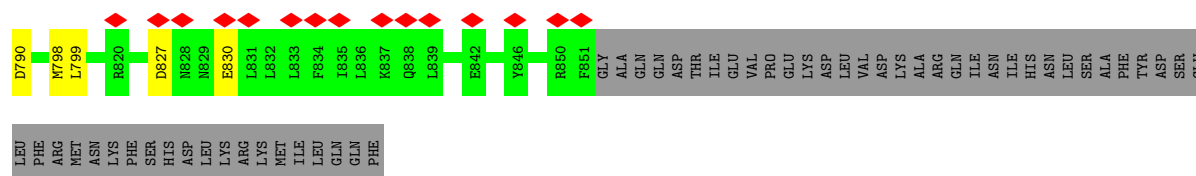
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	2	1	Total	Zn	0
			1	1	
12	4	1	Total	Zn	0
			1	1	
12	5	1	Total	Zn	0
			1	1	
12	6	1	Total	Zn	0
			1	1	
12	7	1	Total	Zn	0
			1	1	

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

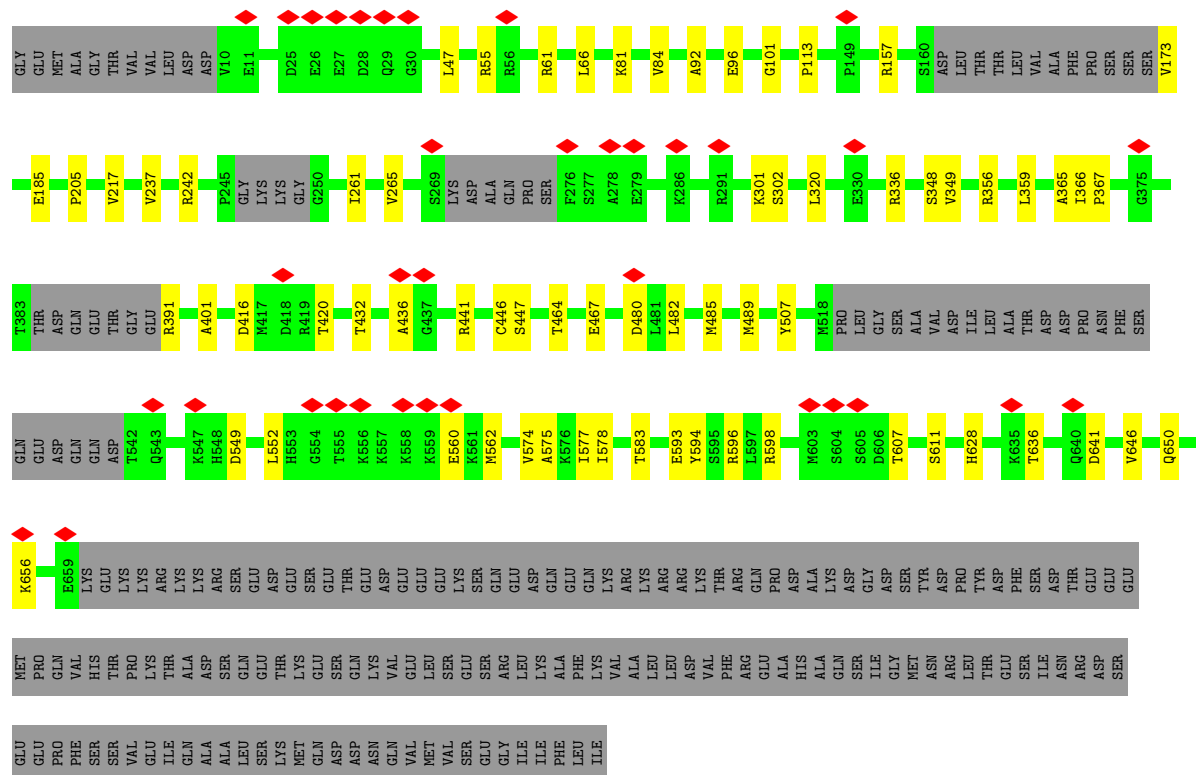


Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	5	1	Total	C	N	O	P	0
			27	10	5	10	2	



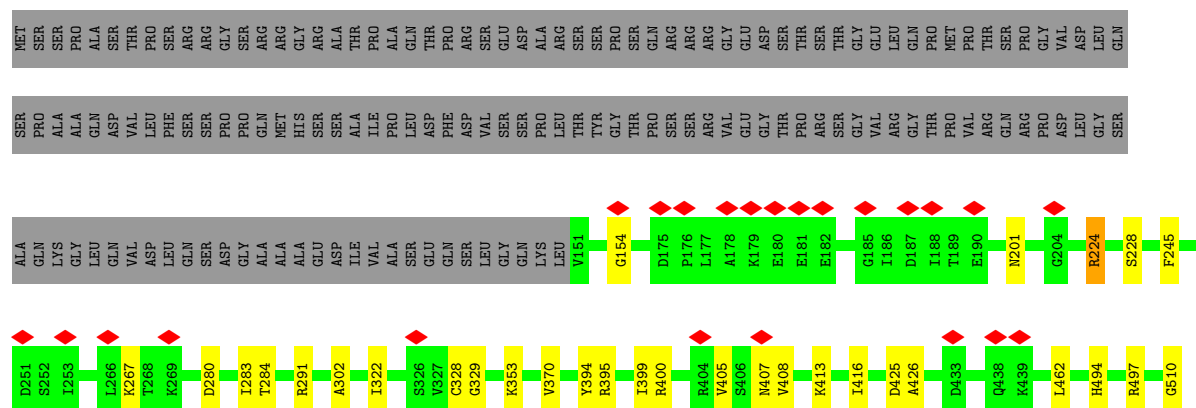
• Molecule 3: DNA replication licensing factor MCM3

Chain 3: 66% 8% 26%

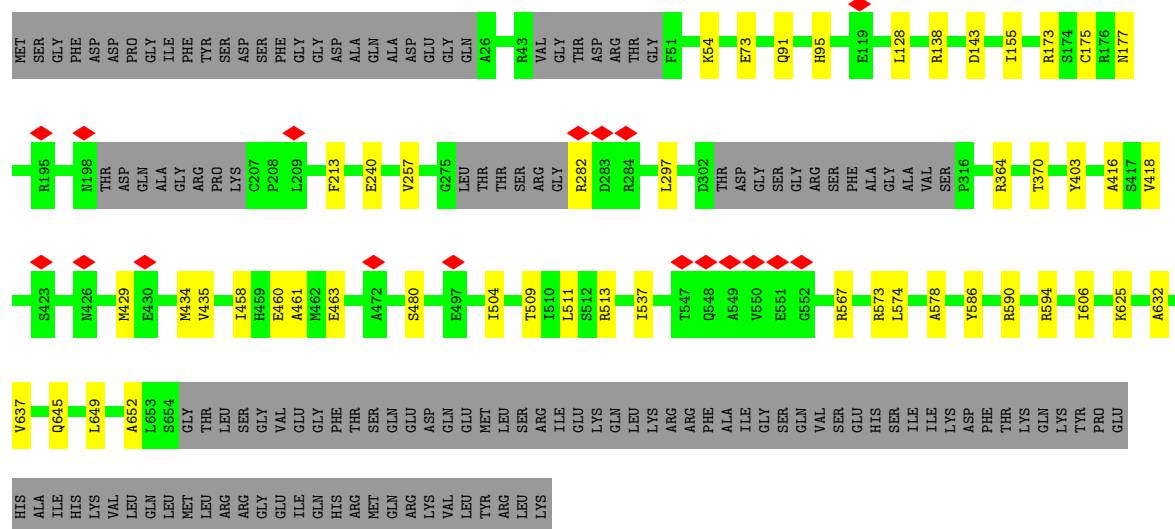


• Molecule 4: DNA replication licensing factor MCM4

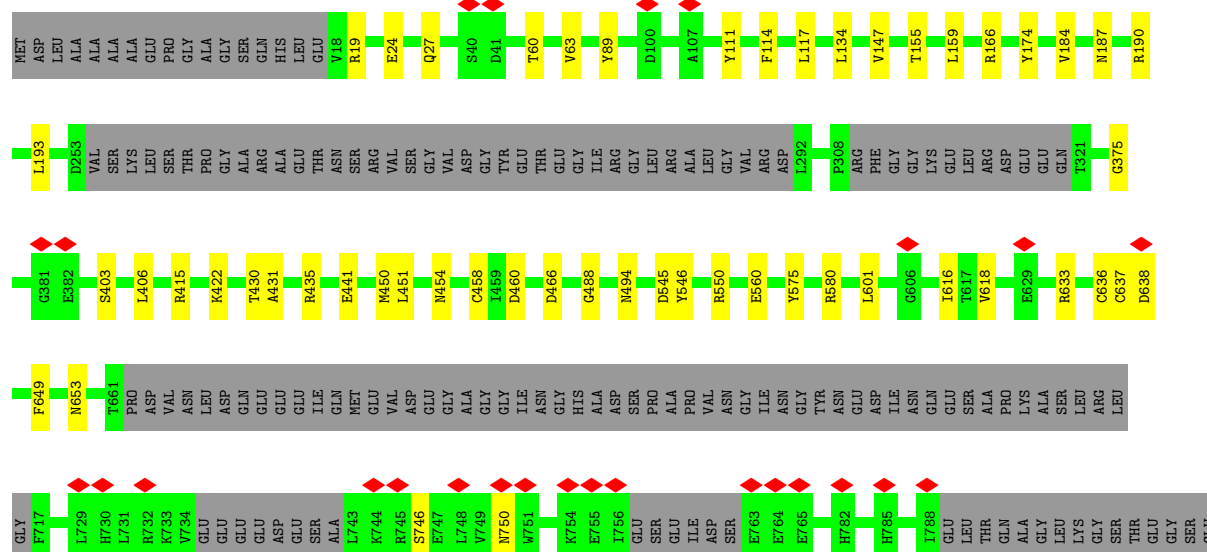
Chain 4: 66% 6% 28%



- Molecule 5: DNA replication licensing factor MCM5

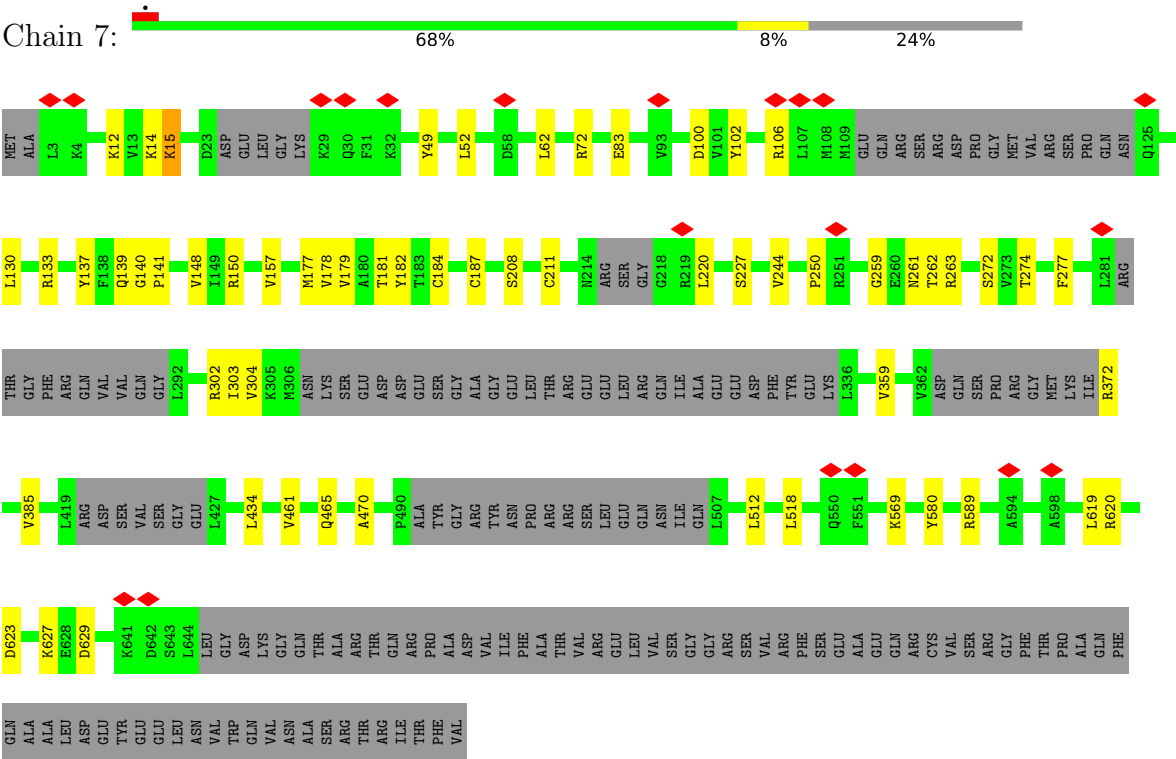


- Molecule 6: DNA replication licensing factor MCM6

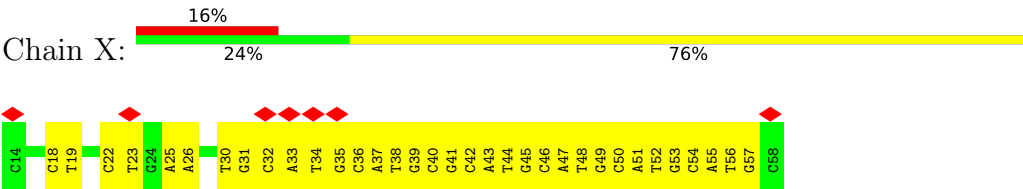


SER
TYR
GLU
GLU
ASP
PRO
TYR
LEU
VAL
VAL
ASN
PRO
ASN
TYR
LEU
LEU
GLU
ASP

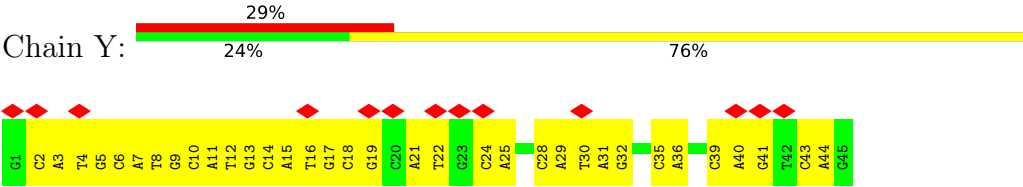
● Molecule 7: DNA replication licensing factor MCM7



● Molecule 8: DNA (45-mer)



● Molecule 9: DNA (45-mer)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182341	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 ($e^-/\text{\AA}^2$)	49.28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.304	Depositor
Minimum map value	-0.892	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: AGS, ADP, MG, ZN

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	F	0.25	0/1354	0.46	0/1817
2	2	0.26	0/5190	0.48	0/7015
3	3	0.25	0/4784	0.49	0/6447
4	4	0.25	0/5059	0.48	0/6841
5	5	0.25	0/4750	0.49	0/6386
6	6	0.26	0/5345	0.49	0/7207
7	7	0.25	0/4402	0.49	0/5942
8	X	0.51	0/1032	0.95	0/1590
9	Y	0.50	0/1036	0.91	0/1597
All	All	0.28	0/32952	0.53	0/44842

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	F	1341	0	1418	8	0
2	2	5093	0	5097	47	0
3	3	4715	0	4760	40	0
4	4	4969	0	5002	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	4679	0	4755	29	0
6	6	5259	0	5313	34	0
7	7	4338	0	4403	35	0
8	X	921	0	507	19	0
9	Y	924	0	507	20	0
10	2	31	0	12	0	0
10	6	31	0	12	1	0
10	7	31	0	12	1	0
11	2	1	0	0	0	0
11	3	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	2	0	0	0	0
12	2	1	0	0	0	0
12	4	1	0	0	0	0
12	5	1	0	0	0	0
12	6	1	0	0	0	0
12	7	1	0	0	0	0
13	3	27	0	12	1	0
13	4	27	0	12	0	0
13	5	27	0	12	1	0
All	All	32424	0	31834	242	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 (242) 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)
6:6:60:THR:HG22	6:6:111:TYR:HB2	1.68	0.74
4:4:224:ARG:NH1	4:4:228:SER:OG	2.22	0.72
1:F:2:GLY:N	2:2:340:CYS:HG	1.88	0.70
7:7:620:ARG:NH2	7:7:629:ASP:OD1	2.24	0.70
2:2:325:VAL:HA	2:2:368:THR:HG23	1.74	0.69
4:4:328:CYS:SG	4:4:329:GLY:N	2.65	0.69
5:5:578:ALA:HB1	5:5:637:VAL:HG21	1.73	0.69
4:4:302:ALA:HB2	4:4:322:ILE:HD13	1.75	0.68
9:Y:21:DA:H2''	9:Y:22:DT:H5''	1.73	0.68
7:7:184:CYS:HB3	7:7:187:CYS:SG	2.34	0.67
2:2:488:HIS:HB3	2:2:491:ILE:HD12	1.76	0.67
2:2:777:HIS:ND1	2:2:790:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:130:LEU:HB2	7:7:179:VAL:HG11	1.76	0.66
5:5:586:TYR:OH	5:5:590:ARG:NH2	2.29	0.65
3:3:391:ARG:NH1	3:3:436:ALA:O	2.30	0.65
4:4:659:ASP:OD1	7:7:589:ARG:NH1	2.29	0.65
3:3:628:HIS:HB3	3:3:641:ASP:OD1	1.97	0.64
7:7:14:LYS:NZ	7:7:83:GLU:OE1	2.29	0.64
2:2:565:VAL:HA	6:6:488:GLY:HA2	1.79	0.64
4:4:400:ARG:HA	4:4:408:VAL:HG12	1.79	0.64
6:6:575:TYR:OH	6:6:636:CYS:SG	2.56	0.64
4:4:494:HIS:ND1	6:6:560:GLU:OE1	2.31	0.64
5:5:54:LYS:NZ	5:5:73:GLU:OE1	2.30	0.63
1:F:6:ILE:HG23	1:F:52:LEU:HD21	1.79	0.63
4:4:283:ILE:HD12	4:4:394:TYR:HB2	1.80	0.63
5:5:138:ARG:NH1	5:5:240:GLU:OE2	2.33	0.62
8:X:22:DC:H2'	8:X:23:DT:H71	1.82	0.62
7:7:262:THR:HG22	7:7:263:ARG:HG3	1.82	0.62
4:4:201:ASN:HB2	4:4:245:PHE:HE1	1.65	0.62
4:4:280:ASP:OD1	4:4:395:ARG:NH1	2.33	0.61
3:3:489:MET:O	5:5:594:ARG:NH1	2.33	0.61
5:5:91:GLN:O	5:5:95:HIS:ND1	2.34	0.61
6:6:27:GLN:HG3	6:6:89:TYR:HB3	1.81	0.61
5:5:509:THR:O	5:5:513:ARG:NH1	2.35	0.60
3:3:237:VAL:HG22	3:3:265:VAL:HG12	1.83	0.60
4:4:405:VAL:HG12	4:4:407:ASN:H	1.67	0.59
7:7:100:ASP:OD1	7:7:133:ARG:NH1	2.35	0.59
8:X:42:DC:H2''	8:X:43:DA:C8	2.38	0.59
7:7:208:SER:HB2	7:7:211:CYS:SG	2.42	0.59
9:Y:14:DC:H2''	9:Y:15:DA:C8	2.38	0.58
2:2:605:GLU:OE2	5:5:403:TYR:OH	2.20	0.58
3:3:574:VAL:HA	3:3:577:ILE:HD12	1.84	0.58
3:3:336:ARG:NH2	3:3:480:ASP:OD2	2.37	0.58
3:3:359:LEU:HD23	3:3:365:ALA:HB1	1.86	0.58
4:4:497:ARG:NH2	10:6:901:AGS:O3'	2.36	0.57
7:7:148:VAL:HG12	7:7:150:ARG:H	1.70	0.57
9:Y:28:DC:H2''	9:Y:29:DA:C8	2.39	0.57
1:F:165:SER:HB3	1:F:172:PHE:HZ	1.69	0.57
4:4:748:ARG:NH2	4:4:754:GLU:OE2	2.36	0.57
2:2:385:VAL:HG21	2:2:391:PRO:HG3	1.86	0.56
5:5:416:ALA:HB2	5:5:435:VAL:HG21	1.87	0.56
7:7:12:LYS:HE2	7:7:62:LEU:HD11	1.88	0.56
7:7:244:VAL:HG21	7:7:250:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:46:DC:H2''	8:X:47:DA:C8	2.40	0.56
3:3:47:LEU:O	3:3:101:GLY:N	2.36	0.56
6:6:415:ARG:NH1	6:6:451:LEU:O	2.39	0.56
5:5:175:CYS:SG	5:5:177:ASN:ND2	2.64	0.55
8:X:38:DT:H2''	8:X:39:DG:C8	2.42	0.55
9:Y:24:DC:H2''	9:Y:25:DA:C8	2.41	0.55
4:4:267:LYS:HA	4:4:284:THR:OG1	2.06	0.55
9:Y:30:DT:H2''	9:Y:31:DA:C8	2.42	0.55
9:Y:39:DC:H2''	9:Y:40:DA:C8	2.42	0.54
3:3:157:ARG:NH1	3:3:173:VAL:O	2.39	0.54
6:6:649:PHE:O	6:6:653:ASN:ND2	2.41	0.54
4:4:291:ARG:HD2	4:4:353:LYS:HD2	1.90	0.54
8:X:54:DC:H2''	8:X:55:DA:C8	2.43	0.54
5:5:504:ILE:HG21	5:5:511:LEU:HD11	1.88	0.54
10:7:802:AGS:O1B	10:7:802:AGS:O3G	2.26	0.54
5:5:364:ARG:HG2	5:5:370:THR:HG22	1.90	0.54
3:3:302:SER:OG	3:3:562:MET:SD	2.55	0.53
3:3:593:GLU:OE1	3:3:646:VAL:HG21	2.07	0.53
6:6:430:THR:OG1	6:6:431:ALA:N	2.40	0.53
8:X:30:DT:H2''	8:X:31:DG:C8	2.43	0.53
3:3:607:THR:HG22	3:3:656:LYS:HG2	1.91	0.53
2:2:293:GLU:OE1	2:2:295:ARG:NH2	2.42	0.53
9:Y:10:DC:H2''	9:Y:11:DA:C8	2.44	0.53
4:4:510:GLY:O	4:4:516:LYS:NZ	2.41	0.53
9:Y:12:DT:H2''	9:Y:13:DG:C8	2.44	0.53
6:6:575:TYR:HH	6:6:636:CYS:HG	1.55	0.53
7:7:372:ARG:HD2	7:7:465:GLN:HG3	1.89	0.53
2:2:502:GLY:O	2:2:779:ARG:NH1	2.40	0.53
9:Y:2:DC:H2''	9:Y:3:DA:C8	2.44	0.53
2:2:589:PHE:HE1	2:2:600:ILE:HD13	1.74	0.52
7:7:261:ASN:HB3	7:7:303:ILE:HD12	1.91	0.52
5:5:143:ASP:OD1	5:5:143:ASP:N	2.42	0.52
4:4:549:LYS:NZ	4:4:553:THR:O	2.43	0.52
8:X:52:DT:H2''	8:X:53:DG:C8	2.45	0.52
5:5:173:ARG:HD2	5:5:213:PHE:HE1	1.75	0.52
6:6:746:SER:O	6:6:750:ASN:ND2	2.43	0.52
3:3:366:ILE:HD12	3:3:401:ALA:HB2	1.91	0.51
5:5:155:ILE:HG13	5:5:257:VAL:HG11	1.92	0.51
2:2:382:PRO:O	6:6:494:ASN:ND2	2.43	0.51
2:2:827:ASP:HB3	2:2:830:GLU:HG3	1.93	0.51
3:3:242:ARG:HD3	3:3:261:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:4:DT:H2''	9:Y:5:DG:C8	2.46	0.51
2:2:687:HIS:CD2	2:2:689:SER:H	2.29	0.51
8:X:48:DT:H2''	8:X:49:DG:C8	2.46	0.51
8:X:50:DC:H2''	8:X:51:DA:C8	2.45	0.51
3:3:594:TYR:CZ	3:3:598:ARG:HD2	2.46	0.51
5:5:418:VAL:HG22	5:5:429:MET:HG2	1.91	0.51
6:6:159:LEU:HD12	6:6:190:ARG:HB3	1.92	0.51
6:6:454:ASN:OD1	6:6:580:ARG:NH1	2.44	0.50
8:X:25:DA:H2''	8:X:26:DA:C8	2.46	0.50
2:2:542:ARG:NH1	2:2:580:ASP:O	2.44	0.50
6:6:117:LEU:HD21	6:6:134:LEU:HG	1.92	0.50
3:3:55:ARG:HH21	3:3:66:LEU:HD11	1.77	0.50
3:3:185:GLU:OE1	7:7:72:ARG:NH1	2.38	0.50
3:3:507:TYR:O	5:5:573:ARG:NH1	2.45	0.50
3:3:81:LYS:NZ	3:3:96:GLU:O	2.34	0.49
4:4:154:GLY:HA3	7:7:102:TYR:CE1	2.47	0.49
4:4:511:ASP:N	4:4:511:ASP:OD1	2.41	0.49
4:4:718:ARG:HD2	4:4:729:ALA:HB3	1.92	0.49
9:Y:6:DC:H2''	9:Y:7:DA:C8	2.47	0.49
5:5:434:MET:O	5:5:480:SER:OG	2.26	0.49
2:2:783:ARG:NH1	2:2:790:ASP:OD1	2.45	0.49
2:2:247:PHE:HB3	2:2:255:LEU:HD11	1.94	0.49
7:7:569:LYS:NZ	7:7:623:ASP:OD1	2.39	0.49
4:4:399:ILE:HD11	4:4:413:LYS:HB2	1.95	0.49
7:7:359:VAL:HG21	7:7:619:LEU:HD21	1.95	0.49
2:2:222:MET:HG2	2:2:227:ARG:HB2	1.94	0.48
2:2:776:ALA:O	2:2:780:ILE:HG13	2.14	0.48
1:F:76:LYS:HE2	1:F:163:ALA:HB1	1.95	0.48
6:6:187:ASN:ND2	6:6:190:ARG:O	2.46	0.48
9:Y:8:DT:H2''	9:Y:9:DG:C8	2.48	0.48
2:2:766:HIS:HB3	2:2:798:MET:SD	2.52	0.48
2:2:768:GLU:OE2	13:5:801:ADP:O2'	2.30	0.48
7:7:140:GLY:H	7:7:274:THR:HG21	1.78	0.48
9:Y:43:DC:H2''	9:Y:44:DA:C8	2.48	0.48
7:7:580:TYR:CE2	7:7:627:LYS:HE3	2.49	0.48
2:2:747:TYR:CD1	2:2:767:ILE:HD11	2.48	0.48
7:7:140:GLY:N	7:7:274:THR:HG21	2.29	0.48
5:5:574:LEU:HD23	5:5:632:ALA:HB3	1.96	0.48
6:6:375:GLY:O	6:6:633:ARG:NH1	2.47	0.48
3:3:205:PRO:HB3	5:5:429:MET:SD	2.54	0.48
3:3:575:ALA:HA	3:3:578:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:36:DC:H2''	8:X:37:DA:H8	1.79	0.48
9:Y:16:DT:H2''	9:Y:17:DG:C8	2.49	0.48
7:7:52:LEU:HB2	7:7:141:PRO:HG3	1.94	0.47
9:Y:18:DC:H2''	9:Y:19:DG:H8	1.78	0.47
6:6:406:LEU:HG	6:6:458:CYS:HB3	1.96	0.47
6:6:422:LYS:NZ	6:6:466:ASP:OD1	2.47	0.47
8:X:56:DT:H2''	8:X:57:DG:C8	2.49	0.47
2:2:420:ASN:HD21	2:2:437:THR:HG22	1.78	0.47
4:4:718:ARG:NH1	6:6:545:ASP:OD1	2.48	0.47
3:3:356:ARG:NH2	5:5:460:GLU:OE2	2.47	0.47
3:3:446:CYS:SG	3:3:447:SER:N	2.88	0.47
5:5:463:GLU:OE2	5:5:513:ARG:NH2	2.48	0.46
2:2:223:CYS:HA	2:2:274:TYR:OH	2.15	0.46
5:5:458:ILE:HA	5:5:461:ALA:HB3	1.97	0.46
6:6:174:TYR:HE1	6:6:193:LEU:HD11	1.79	0.46
7:7:385:VAL:HG12	7:7:385:VAL:O	2.15	0.46
9:Y:18:DC:H2''	9:Y:19:DG:C8	2.50	0.46
2:2:612:SER:HA	2:2:616:ILE:O	2.16	0.45
8:X:36:DC:H2''	8:X:37:DA:C8	2.50	0.45
3:3:113:PRO:HB3	3:3:217:VAL:HG23	1.99	0.45
2:2:208:ASP:OD1	2:2:212:HIS:N	2.49	0.45
3:3:482:LEU:HD12	3:3:611:SER:HB2	1.97	0.45
5:5:282:ARG:NH2	6:6:441:GLU:O	2.50	0.45
1:F:171:ILE:HG23	6:6:184:VAL:HG12	1.99	0.45
2:2:302:LEU:HD22	2:2:420:ASN:OD1	2.17	0.45
7:7:137:TYR:OH	7:7:259:GLY:HA3	2.17	0.45
5:5:606:ILE:HD12	5:5:652:ALA:HA	1.98	0.44
6:6:601:LEU:HG	6:6:616:ILE:HD13	1.99	0.44
2:2:490:ASP:OD1	2:2:490:ASP:N	2.49	0.44
2:2:687:HIS:HD2	2:2:689:SER:H	1.64	0.44
7:7:12:LYS:O	7:7:15:LYS:HG3	2.17	0.44
8:X:40:DC:H2''	8:X:41:DG:C8	2.53	0.44
6:6:155:THR:HG22	6:6:166:ARG:O	2.18	0.44
2:2:426:LEU:HB2	2:2:435:PHE:CE1	2.53	0.44
4:4:592:GLU:OE1	4:4:643:ARG:NH2	2.49	0.44
2:2:750:LEU:HD11	2:2:799:LEU:HD21	2.00	0.44
3:3:301:LYS:NZ	3:3:560:GLU:OE1	2.51	0.43
2:2:544:ILE:HG21	2:2:575:ALA:HB1	1.99	0.43
2:2:322:LEU:HB3	2:2:325:VAL:HG22	2.00	0.43
5:5:128:LEU:HD12	5:5:297:LEU:HD13	2.00	0.43
8:X:19:DT:O2	9:Y:41:DG:N2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:44:DT:H2''	8:X:45:DG:C8	2.54	0.43
3:3:349:VAL:HG12	3:3:349:VAL:O	2.18	0.43
8:X:32:DC:H2''	8:X:33:DA:C8	2.53	0.43
2:2:318:VAL:HG13	2:2:403:VAL:HG11	1.99	0.43
1:F:169:LYS:HA	1:F:172:PHE:HD2	1.84	0.43
6:6:19:ARG:HD3	6:6:24:GLU:OE1	2.18	0.43
6:6:27:GLN:CG	6:6:89:TYR:HB3	2.47	0.43
7:7:157:VAL:HA	7:7:277:PHE:HD2	1.84	0.43
9:Y:35:DC:H2''	9:Y:36:DA:C8	2.54	0.43
7:7:512:LEU:HA	7:7:518:LEU:HD11	2.01	0.43
2:2:352:CYS:HB3	2:2:355:CYS:SG	2.58	0.43
4:4:425:ASP:OD1	4:4:426:ALA:N	2.51	0.43
2:2:413:GLU:HB2	2:2:445:ALA:HB3	2.01	0.42
2:2:420:ASN:ND2	2:2:437:THR:HG22	2.34	0.42
2:2:489:GLU:OE1	2:2:710:TYR:OH	2.24	0.42
6:6:403:SER:OG	6:6:460:ASP:OD2	2.37	0.42
7:7:182:TYR:HB3	7:7:220:LEU:HB3	2.01	0.42
3:3:348:SER:HA	13:3:901:ADP:H5'2	2.00	0.42
6:6:431:ALA:HB2	6:6:450:MET:SD	2.60	0.42
4:4:744:HIS:CD2	4:4:760:GLU:HG2	2.55	0.42
7:7:434:LEU:HD13	7:7:461:VAL:HG21	2.01	0.42
2:2:377:ARG:NH1	2:2:393:SER:OG	2.53	0.42
2:2:558:ALA:HA	2:2:572:GLU:O	2.20	0.42
3:3:583:THR:CG2	3:3:636:THR:HB	2.50	0.42
2:2:799:LEU:HD23	2:2:799:LEU:HA	1.85	0.42
3:3:549:ASP:HB3	3:3:552:LEU:HB2	2.01	0.42
5:5:645:GLN:HG2	5:5:649:LEU:HD12	2.01	0.42
7:7:177:MET:SD	7:7:227:SER:HB3	2.60	0.42
2:2:687:HIS:CG	2:2:688:PRO:HD2	2.55	0.41
2:2:740:GLN:HG2	5:5:537:ILE:HG21	2.02	0.41
6:6:435:ARG:HE	9:Y:22:DT:P	2.43	0.41
7:7:49:TYR:HB3	7:7:139:GLN:HE21	1.85	0.41
8:X:34:DT:H2''	8:X:35:DG:C8	2.54	0.41
3:3:349:VAL:HG12	3:3:485:MET:HE2	2.02	0.41
3:3:464:THR:N	3:3:467:GLU:OE1	2.44	0.41
4:4:370:VAL:HG11	4:4:416:ILE:HD12	2.01	0.41
6:6:637:CYS:SG	6:6:638:ASP:N	2.93	0.41
3:3:596:ARG:NH2	3:3:650:GLN:OE1	2.44	0.41
4:4:587:LEU:HB3	4:4:591:MET:SD	2.59	0.41
3:3:359:LEU:HD11	3:3:367:PRO:HB3	2.02	0.41
7:7:178:VAL:HG12	7:7:179:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:218:ARG:NH1	2:2:231:VAL:O	2.54	0.41
2:2:675:LEU:HD21	6:6:618:VAL:HG21	2.03	0.41
3:3:432:THR:HG22	3:3:441:ARG:HG2	2.03	0.41
3:3:574:VAL:O	3:3:578:ILE:HG13	2.21	0.41
4:4:462:LEU:HD22	4:4:687:LEU:HD13	2.02	0.41
4:4:698:ILE:HD13	4:4:749:LEU:HA	2.03	0.41
5:5:567:ARG:HA	5:5:625:LYS:HE2	2.02	0.41
7:7:106:ARG:HH22	7:7:181:THR:HG21	1.86	0.41
7:7:272:SER:HB3	7:7:304:VAL:HG23	2.02	0.41
4:4:592:GLU:OE2	4:4:732:ARG:NH1	2.54	0.41
9:Y:31:DA:H2"	9:Y:32:DG:C8	2.56	0.41
2:2:203:LEU:HD23	2:2:203:LEU:HA	1.91	0.40
3:3:416:ASP:O	3:3:420:THR:HG23	2.21	0.40
1:F:118:LEU:HD23	1:F:118:LEU:HA	1.90	0.40
3:3:61:ARG:HD3	3:3:61:ARG:HA	1.91	0.40
8:X:18:DC:H2"	8:X:19:DT:C6	2.56	0.40
2:2:298:ARG:HG2	6:6:147:VAL:HG11	2.02	0.40
2:2:763:THR:OG1	2:2:764:VAL:N	2.55	0.40
3:3:84:VAL:HG12	3:3:92:ALA:HB2	2.03	0.40
6:6:63:VAL:O	6:6:114:PHE:HA	2.22	0.40
1:F:108:ILE:O	1:F:111:VAL:HB	2.22	0.40
3:3:320:LEU:HD23	3:3:320:LEU:HA	1.91	0.40
4:4:538:SER:HA	7:7:470:ALA:O	2.21	0.40
6:6:546:TYR:O	6:6:550:ARG:HG2	2.22	0.40
7:7:274:THR:HB	7:7:302:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	171/251 (68%)	169 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	637/904 (70%)	616 (97%)	21 (3%)	0	100	100
3	3	586/810 (72%)	573 (98%)	13 (2%)	0	100	100
4	4	619/863 (72%)	603 (97%)	16 (3%)	0	100	100
5	5	585/734 (80%)	565 (97%)	20 (3%)	0	100	100
6	6	640/821 (78%)	625 (98%)	15 (2%)	0	100	100
7	7	530/719 (74%)	517 (98%)	13 (2%)	0	100	100
All	All	3768/5102 (74%)	3668 (97%)	100 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	151/217 (70%)	151 (100%)	0	100	100
2	2	563/781 (72%)	563 (100%)	0	100	100
3	3	516/708 (73%)	516 (100%)	0	100	100
4	4	551/753 (73%)	550 (100%)	1 (0%)	92	96
5	5	510/625 (82%)	510 (100%)	0	100	100
6	6	590/724 (82%)	590 (100%)	0	100	100
7	7	475/619 (77%)	474 (100%)	1 (0%)	92	96
All	All	3356/4427 (76%)	3354 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	224	ARG
7	7	15	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	687	HIS
3	3	310	HIS

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 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	$\# Z > 2$
13	ADP	5	801	11	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
10	AGS	2	1001	11	26,33,33	0.72	1 (3%)	26,52,52	1.04	2 (7%)
10	AGS	6	901	11	26,33,33	0.73	1 (3%)	26,52,52	1.10	2 (7%)
10	AGS	7	802	11	26,33,33	0.72	1 (3%)	26,52,52	1.05	2 (7%)
13	ADP	3	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
13	ADP	4	902	11	24,29,29	0.94	1 (4%)	29,45,45	1.49	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
13	ADP	5	801	11	-	6/12/32/32	0/3/3/3
10	AGS	2	1001	11	-	5/17/38/38	0/3/3/3
10	AGS	6	901	11	-	0/17/38/38	0/3/3/3
10	AGS	7	802	11	-	3/17/38/38	0/3/3/3
13	ADP	3	901	-	-	1/12/32/32	0/3/3/3
13	ADP	4	902	11	-	5/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	801	ADP	C5-C4	2.48	1.47	1.40
13	3	901	ADP	C5-C4	2.46	1.47	1.40
13	4	902	ADP	C5-C4	2.45	1.47	1.40
10	2	1001	AGS	PG-S1G	2.17	1.95	1.90
10	6	901	AGS	PG-S1G	2.12	1.95	1.90
10	7	802	AGS	PG-S1G	2.09	1.95	1.90

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	901	AGS	PA-O3A-PB	-3.97	119.21	132.83
13	5	801	ADP	C3'-C2'-C1'	3.77	106.65	100.98
13	4	902	ADP	C3'-C2'-C1'	3.70	106.56	100.98
13	3	901	ADP	PA-O3A-PB	-3.67	120.25	132.83
13	3	901	ADP	C3'-C2'-C1'	3.60	106.39	100.98
10	2	1001	AGS	PA-O3A-PB	-3.52	120.73	132.83
13	5	801	ADP	PA-O3A-PB	-3.52	120.76	132.83
10	7	802	AGS	PA-O3A-PB	-3.47	120.91	132.83
13	4	902	ADP	PA-O3A-PB	-3.44	121.02	132.83
13	3	901	ADP	N3-C2-N1	-3.16	123.74	128.68
13	5	801	ADP	N3-C2-N1	-3.07	123.88	128.68
13	4	902	ADP	N3-C2-N1	-3.06	123.90	128.68
13	4	902	ADP	C4-C5-N7	-2.70	106.59	109.40
13	3	901	ADP	C4-C5-N7	-2.64	106.65	109.40
13	5	801	ADP	C4-C5-N7	-2.59	106.70	109.40
10	6	901	AGS	C5-C6-N6	2.30	123.84	120.35
10	2	1001	AGS	C5-C6-N6	2.25	123.78	120.35
10	7	802	AGS	C5-C6-N6	2.23	123.74	120.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	2	1001	AGS	C5'-O5'-PA-O1A
10	2	1001	AGS	C5'-O5'-PA-O2A
10	7	802	AGS	C5'-O5'-PA-O2A
13	4	902	ADP	C5'-O5'-PA-O1A
13	5	801	ADP	C5'-O5'-PA-O1A
13	4	902	ADP	O4'-C4'-C5'-O5'
13	4	902	ADP	C3'-C4'-C5'-O5'
13	5	801	ADP	O4'-C4'-C5'-O5'
13	5	801	ADP	C3'-C4'-C5'-O5'
10	7	802	AGS	C5'-O5'-PA-O3A
13	4	902	ADP	C5'-O5'-PA-O3A
10	2	1001	AGS	PA-O3A-PB-O1B
10	7	802	AGS	C5'-O5'-PA-O1A
13	4	902	ADP	C5'-O5'-PA-O2A
13	5	801	ADP	C5'-O5'-PA-O2A
13	5	801	ADP	PA-O3A-PB-O2B
10	2	1001	AGS	PG-O3B-PB-O2B
10	2	1001	AGS	C5'-O5'-PA-O3A
13	5	801	ADP	C5'-O5'-PA-O3A
13	3	901	ADP	O4'-C4'-C5'-O5'

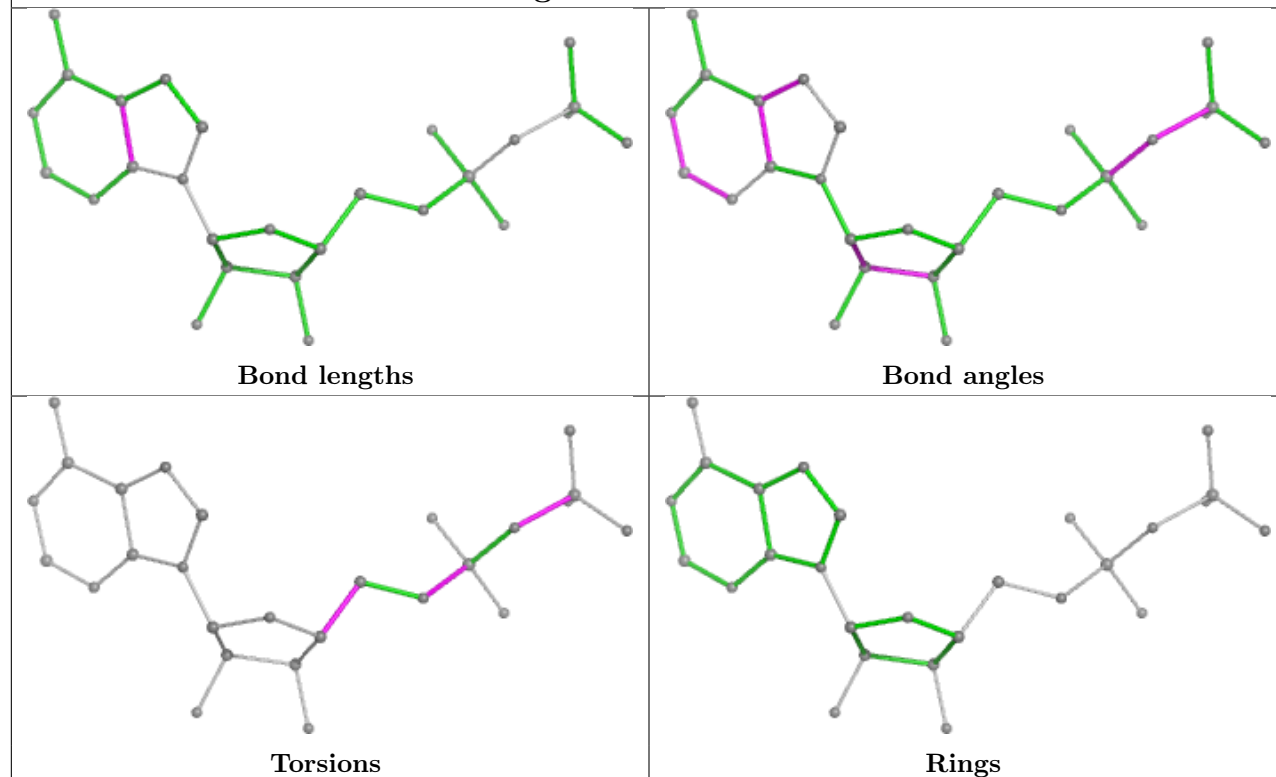
There are no ring outliers.

4 monomers are involved in 4 short contacts:

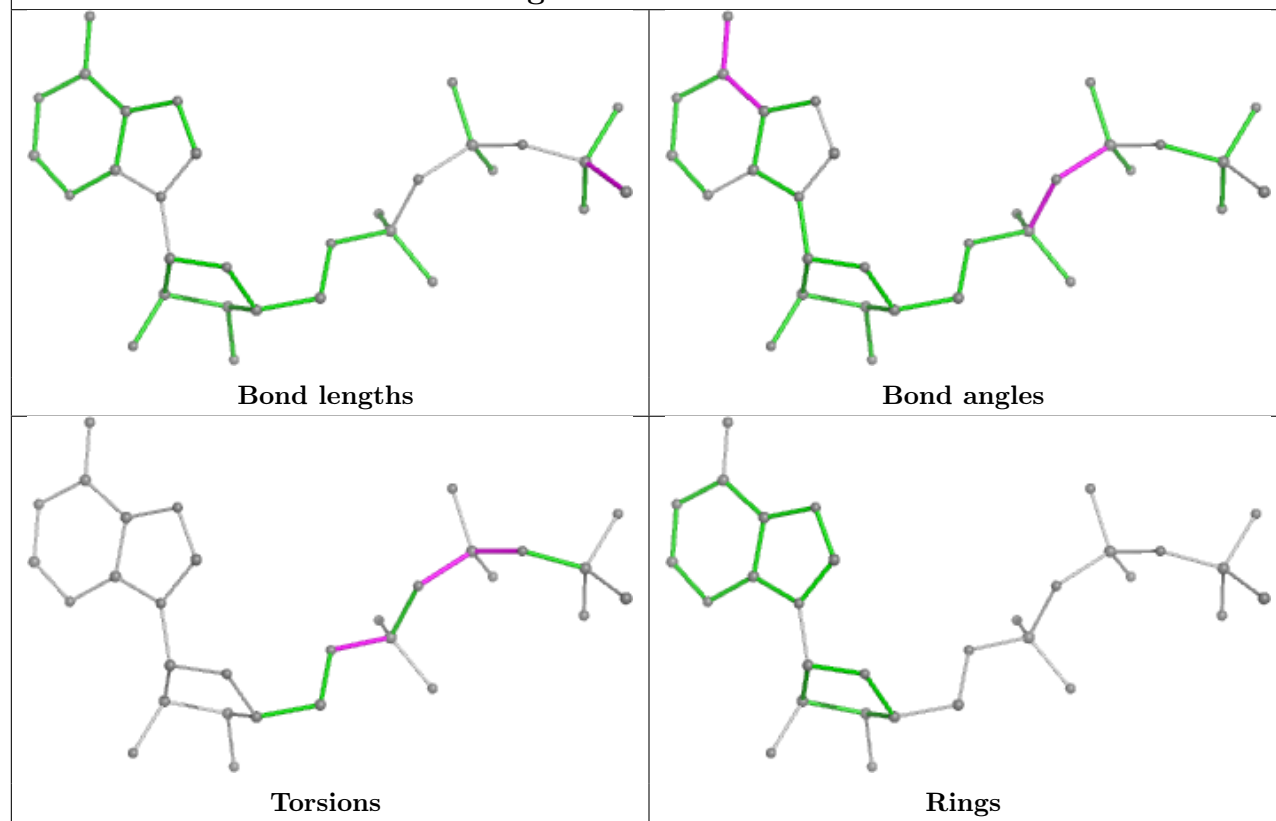
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	801	ADP	1	0
10	6	901	AGS	1	0
10	7	802	AGS	1	0
13	3	901	ADP	1	0

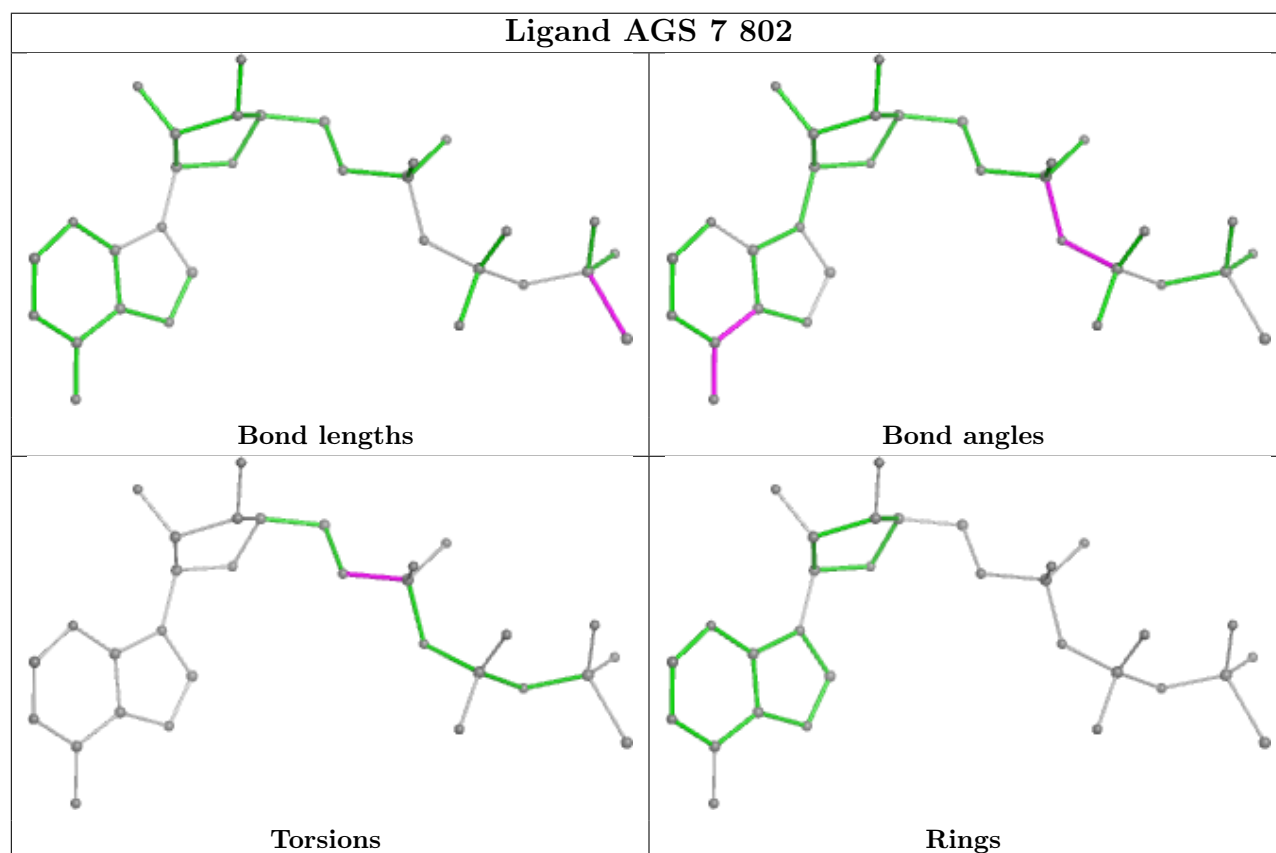
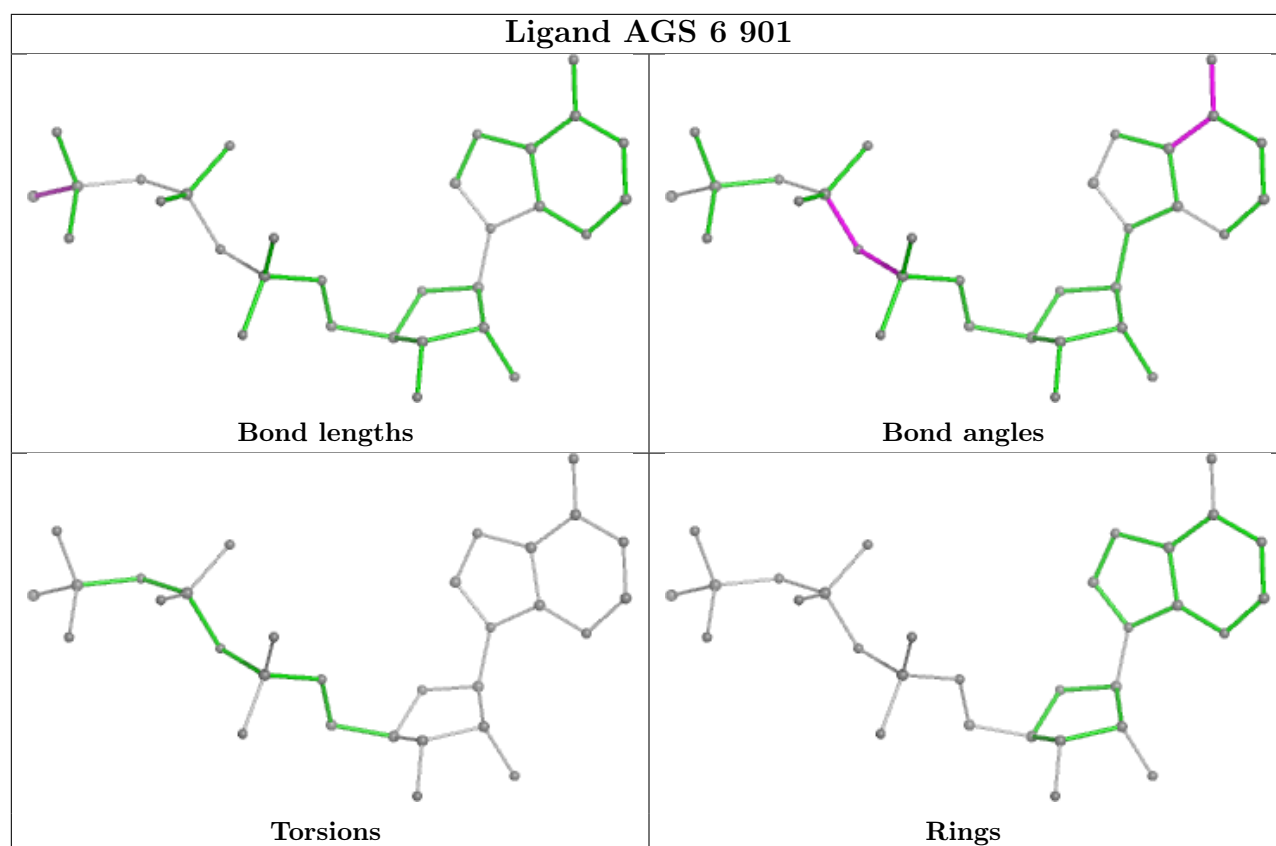
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand ADP 5 801

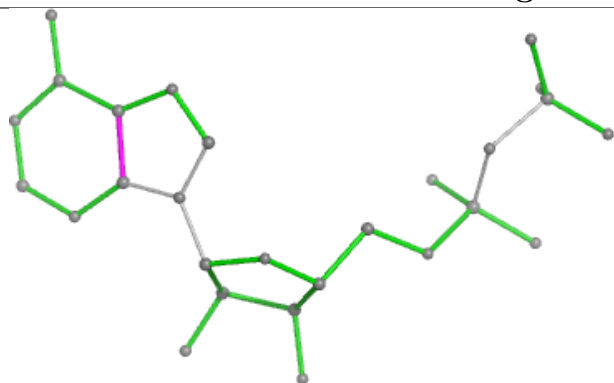


Ligand AGS 2 1001

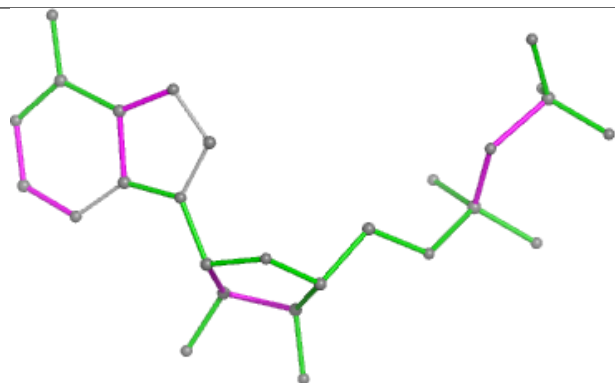




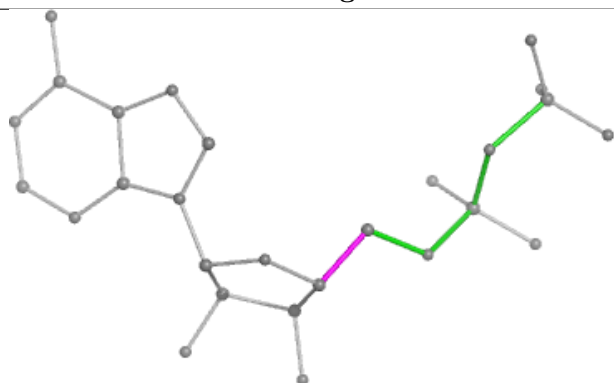
Ligand ADP 3 901



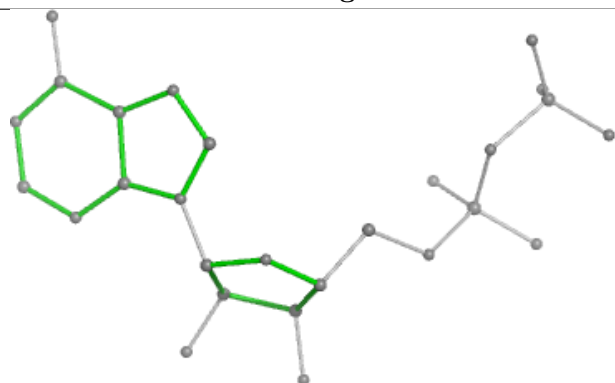
Bond lengths



Bond angles

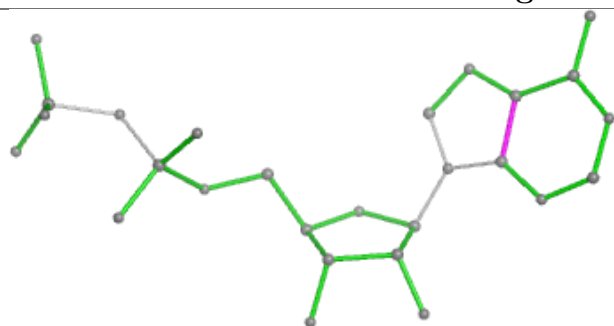


Torsions

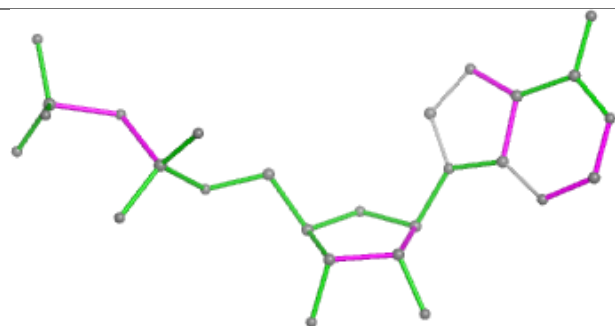


Rings

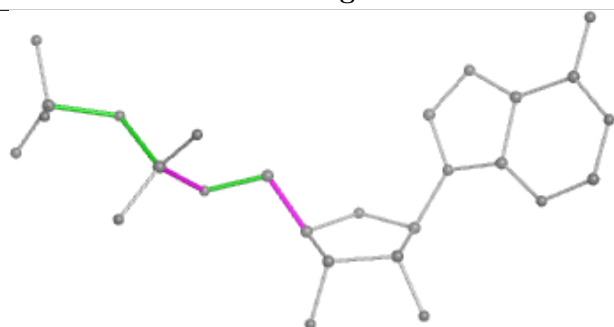
Ligand ADP 4 902



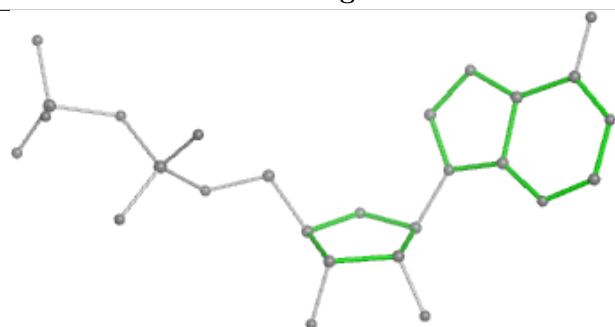
Bond lengths



Bond angles



Torsions



Rings

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.

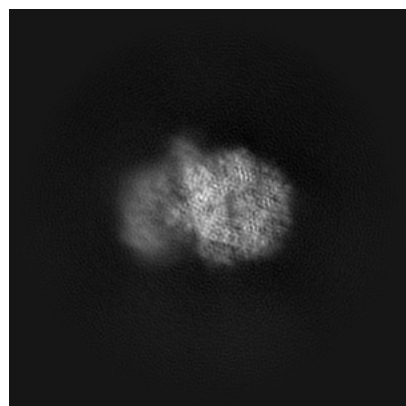
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19620. These allow visual inspection of the internal detail of the map and identification of artifacts.

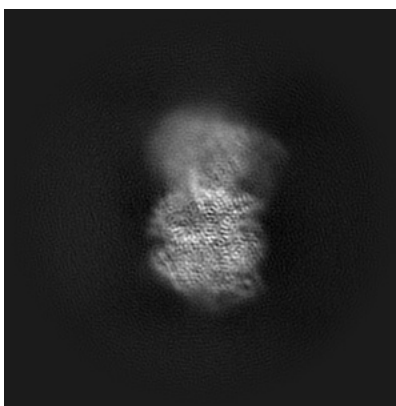
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

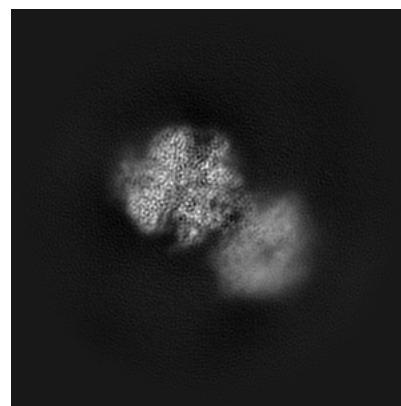
6.1.1 Primary map



X

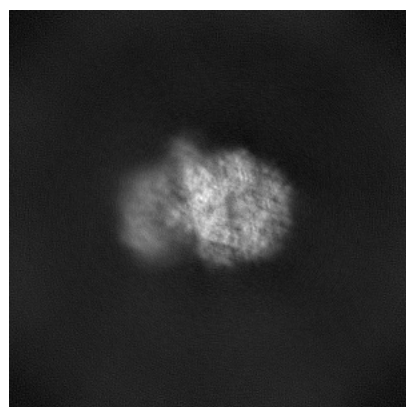


Y

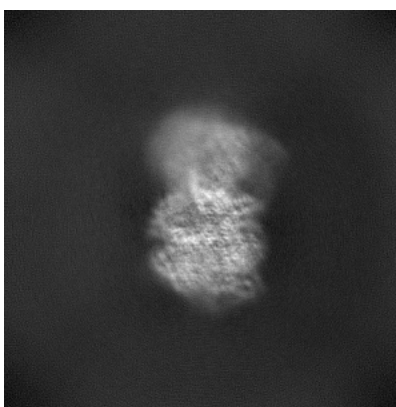


Z

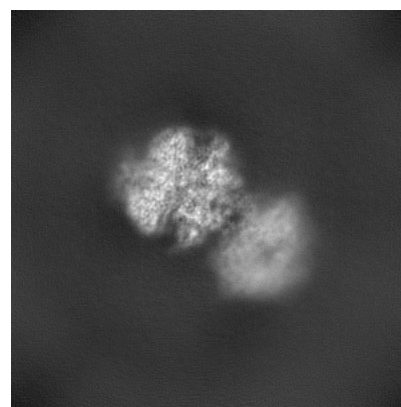
6.1.2 Raw map



X



Y

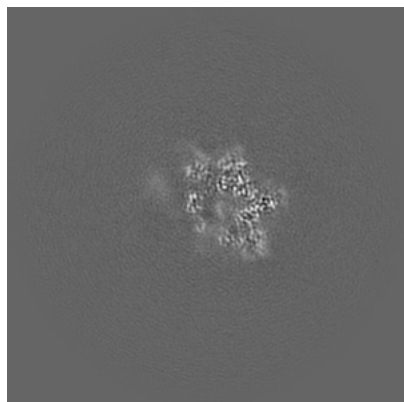


Z

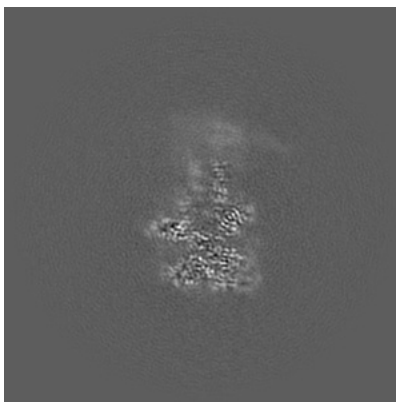
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

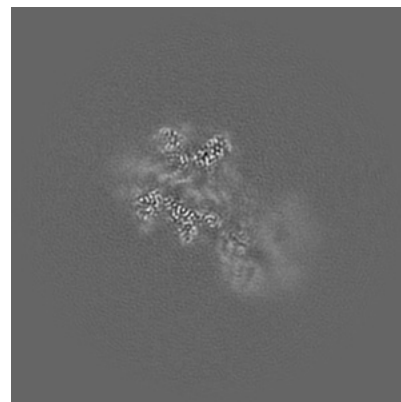
6.2.1 Primary map



X Index: 200

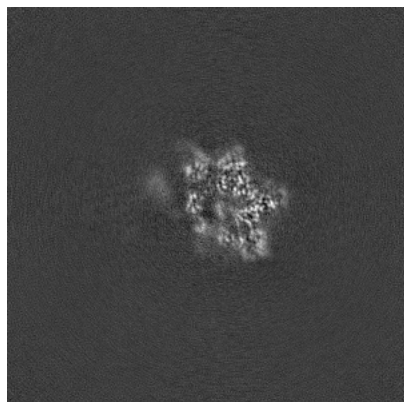


Y Index: 200

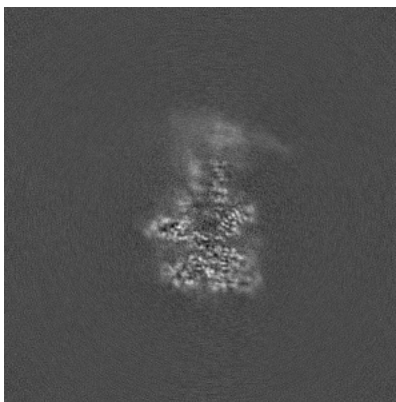


Z Index: 200

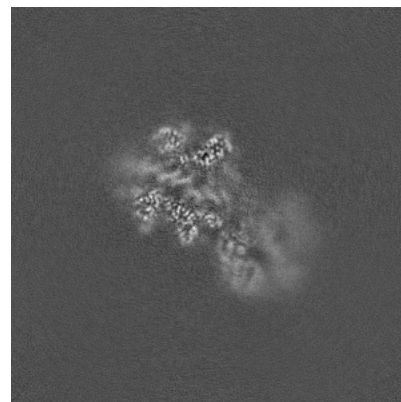
6.2.2 Raw map



X Index: 200



Y Index: 200

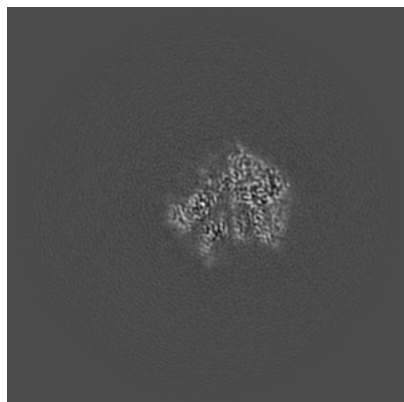


Z Index: 200

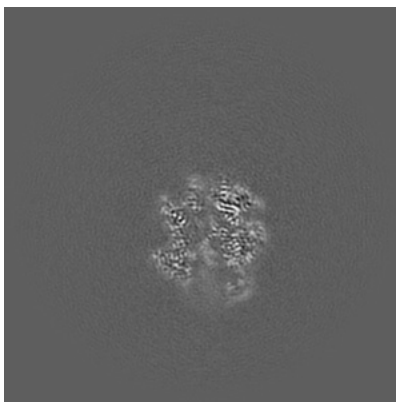
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

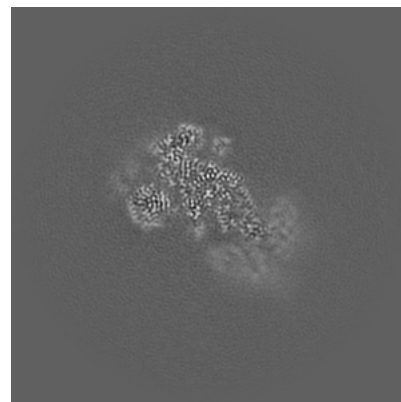
6.3.1 Primary map



X Index: 171

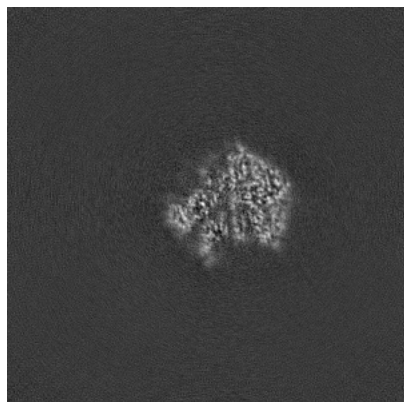


Y Index: 232

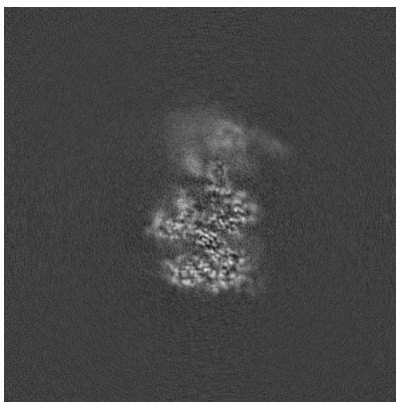


Z Index: 221

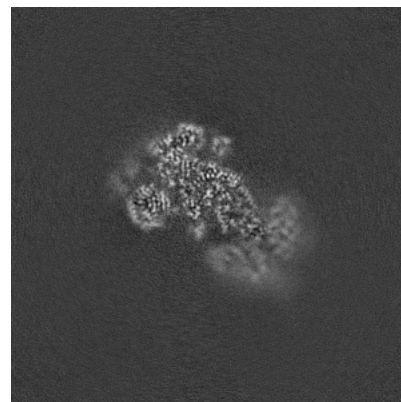
6.3.2 Raw map



X Index: 171



Y Index: 196

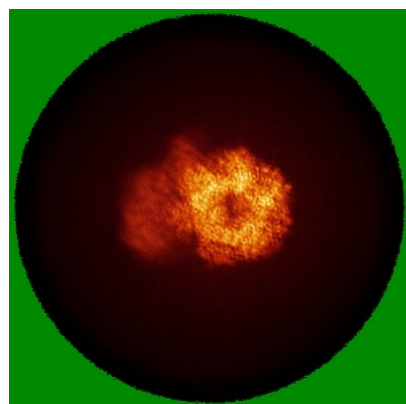


Z Index: 221

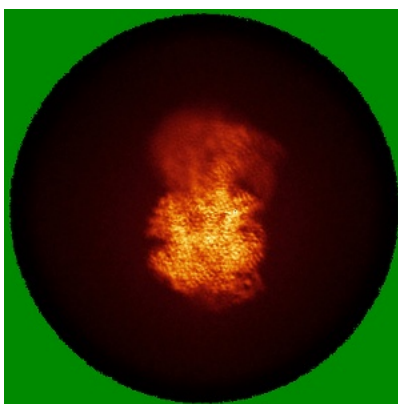
The images above show the largest variance slices of the map in three orthogonal directions.

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

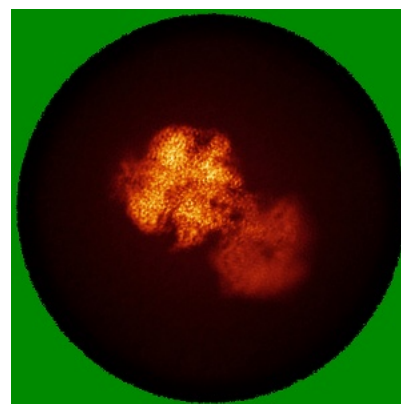
6.4.1 Primary map



X

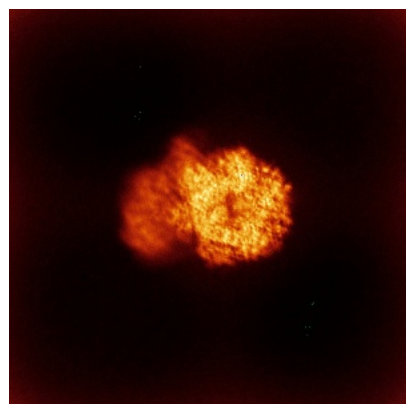


Y

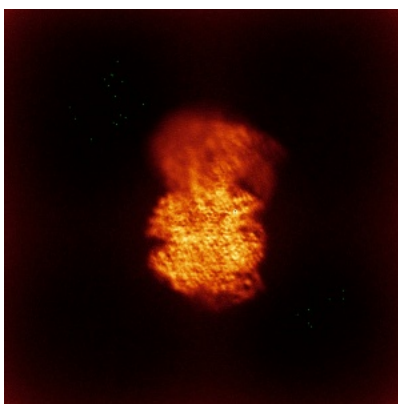


Z

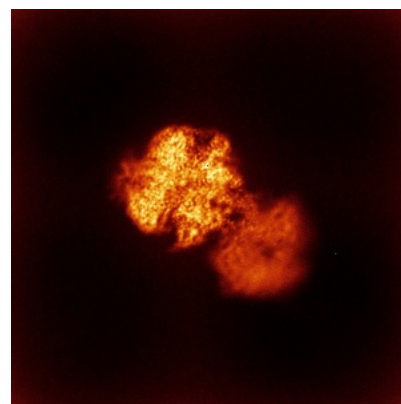
6.4.2 Raw map



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 0.17. 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.

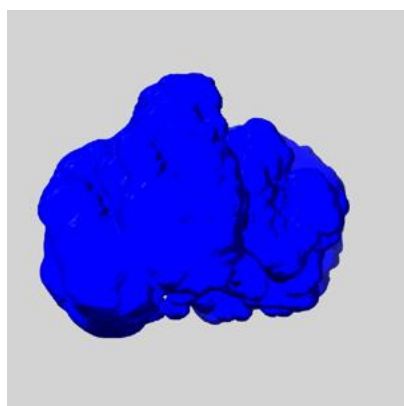
6.6 Mask visualisation [i](#)

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

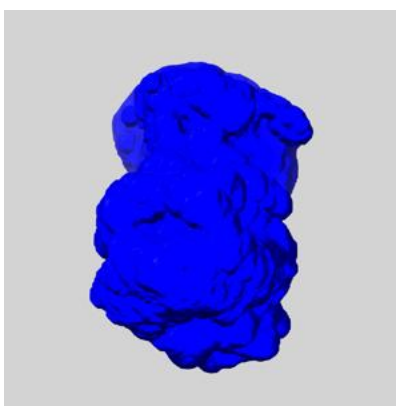
A mask typically either:

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

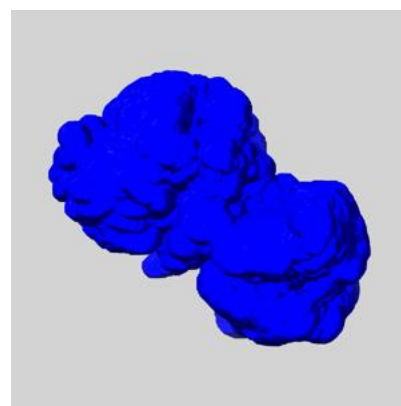
6.6.1 emd_19620_msk_1.map [i](#)



X



Y

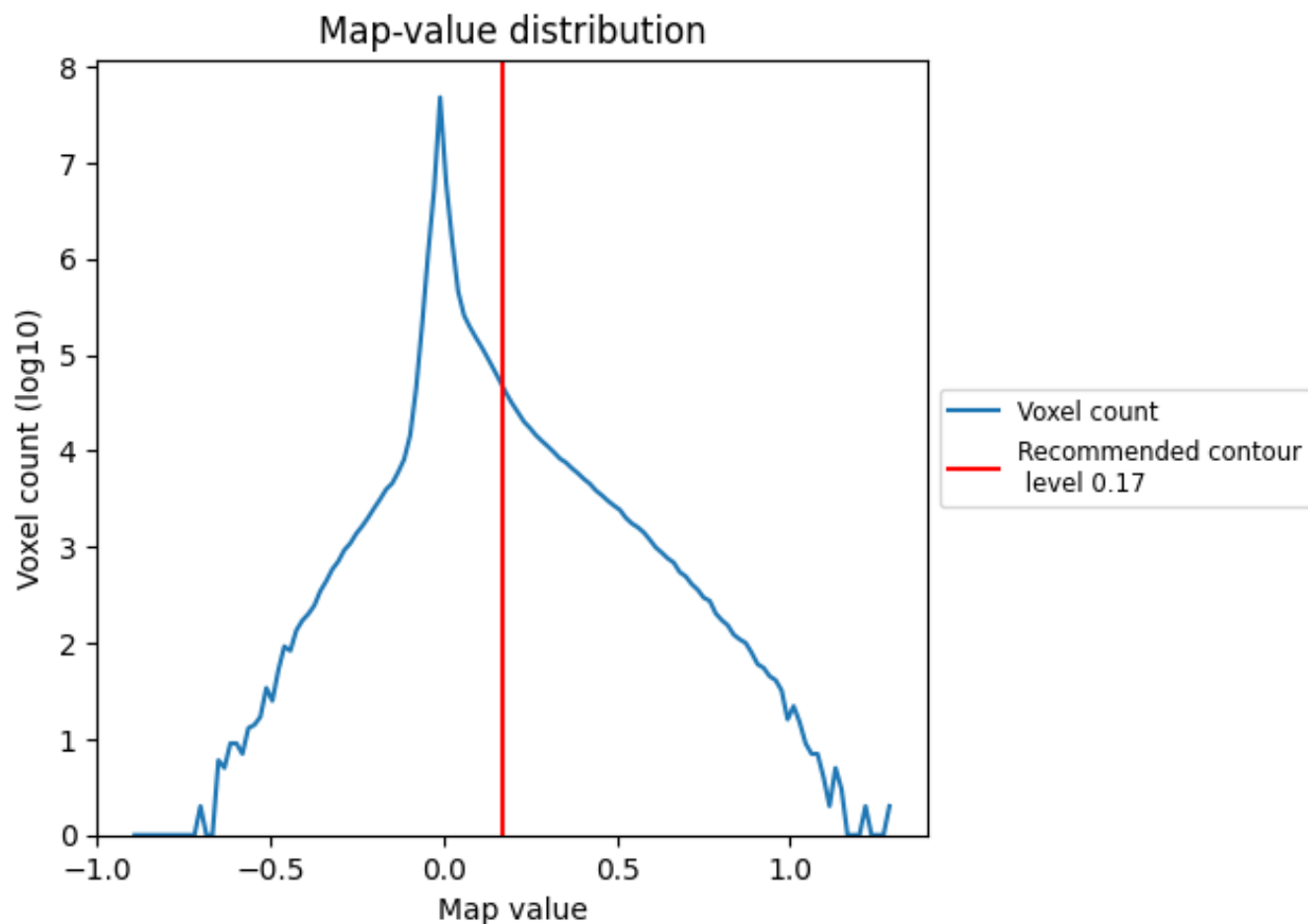


Z

7 Map analysis [i](#)

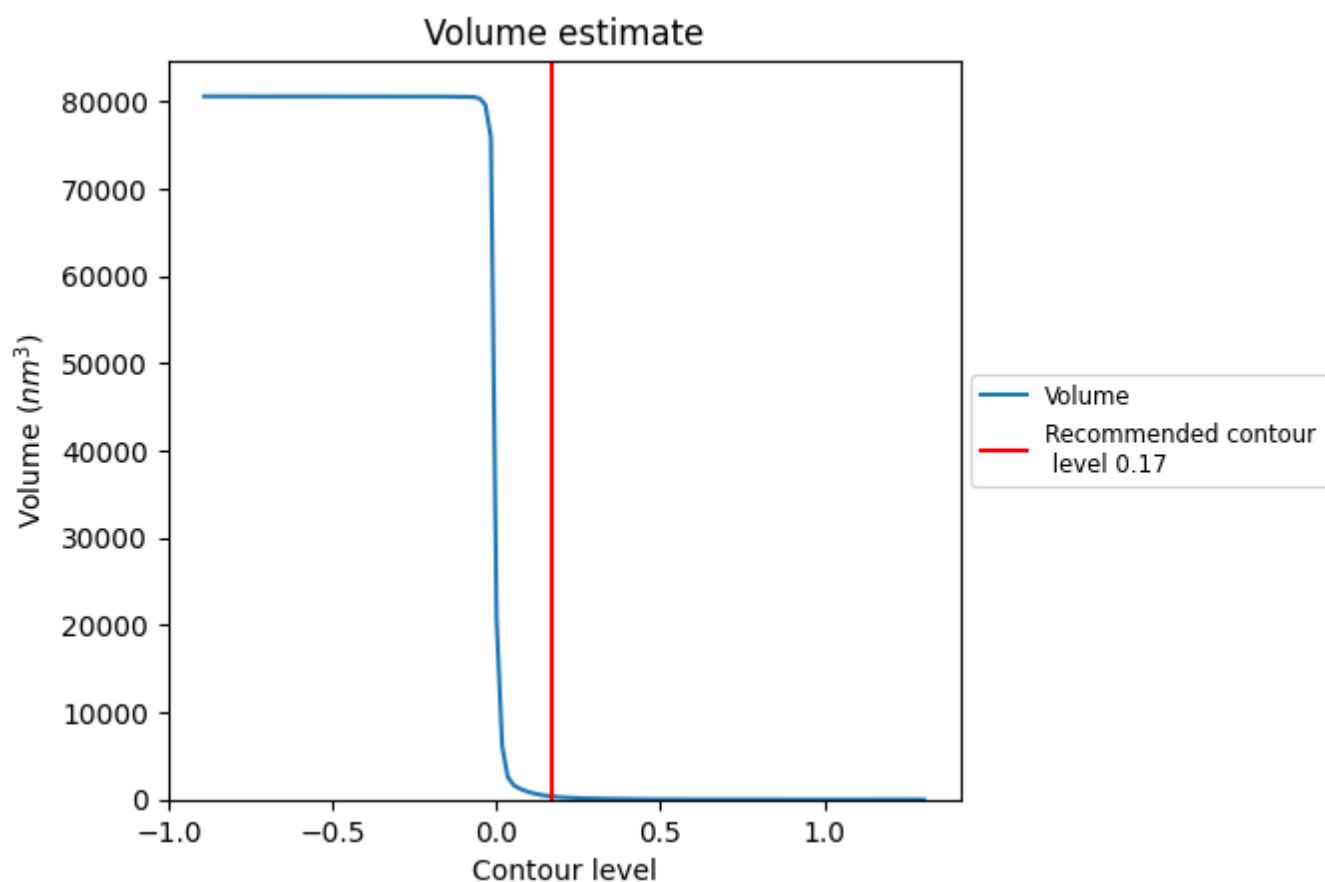
This section contains the results of statistical analysis of the map.

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.

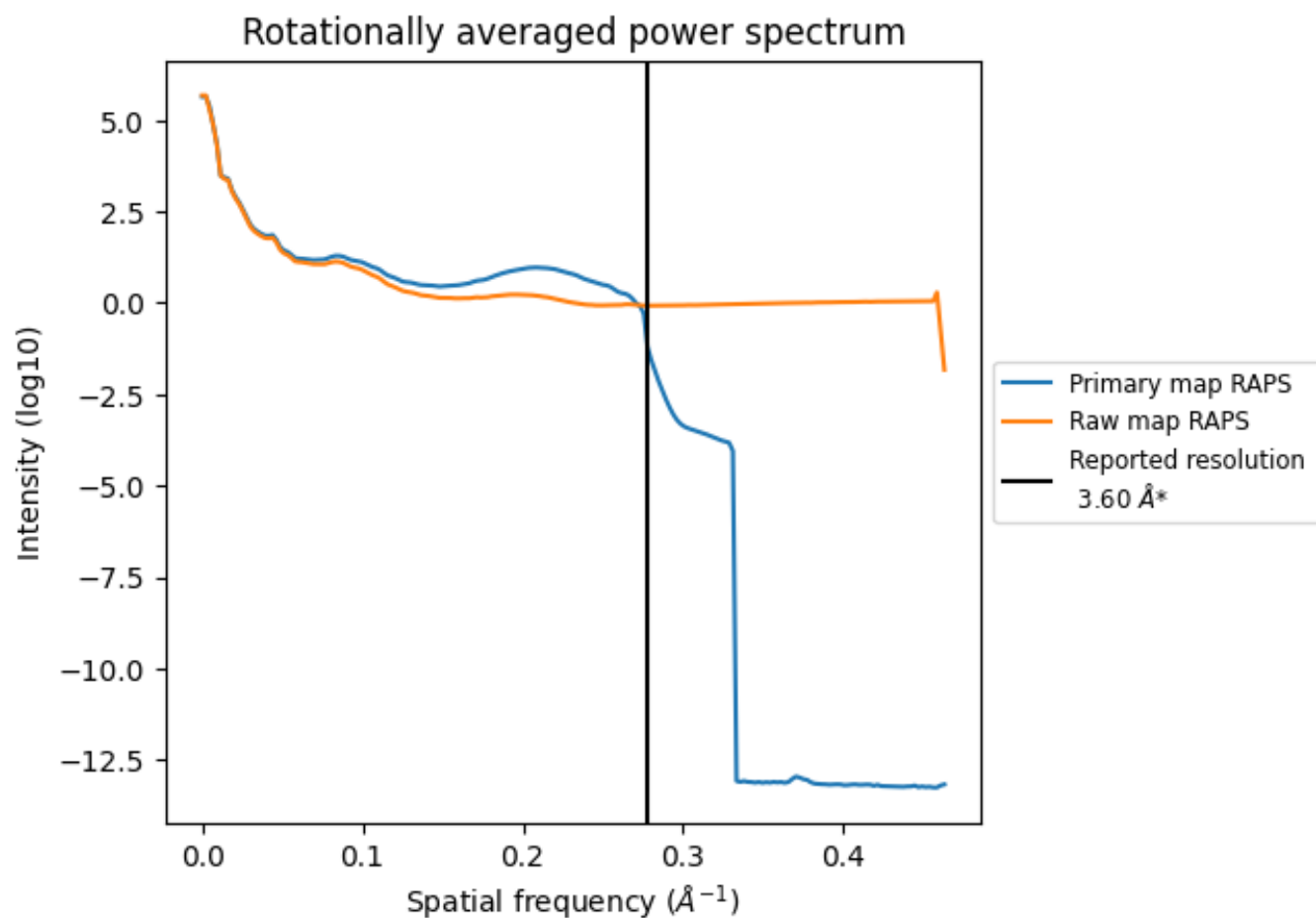
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 353 nm³; this corresponds to an approximate mass of 318 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 ⓘ

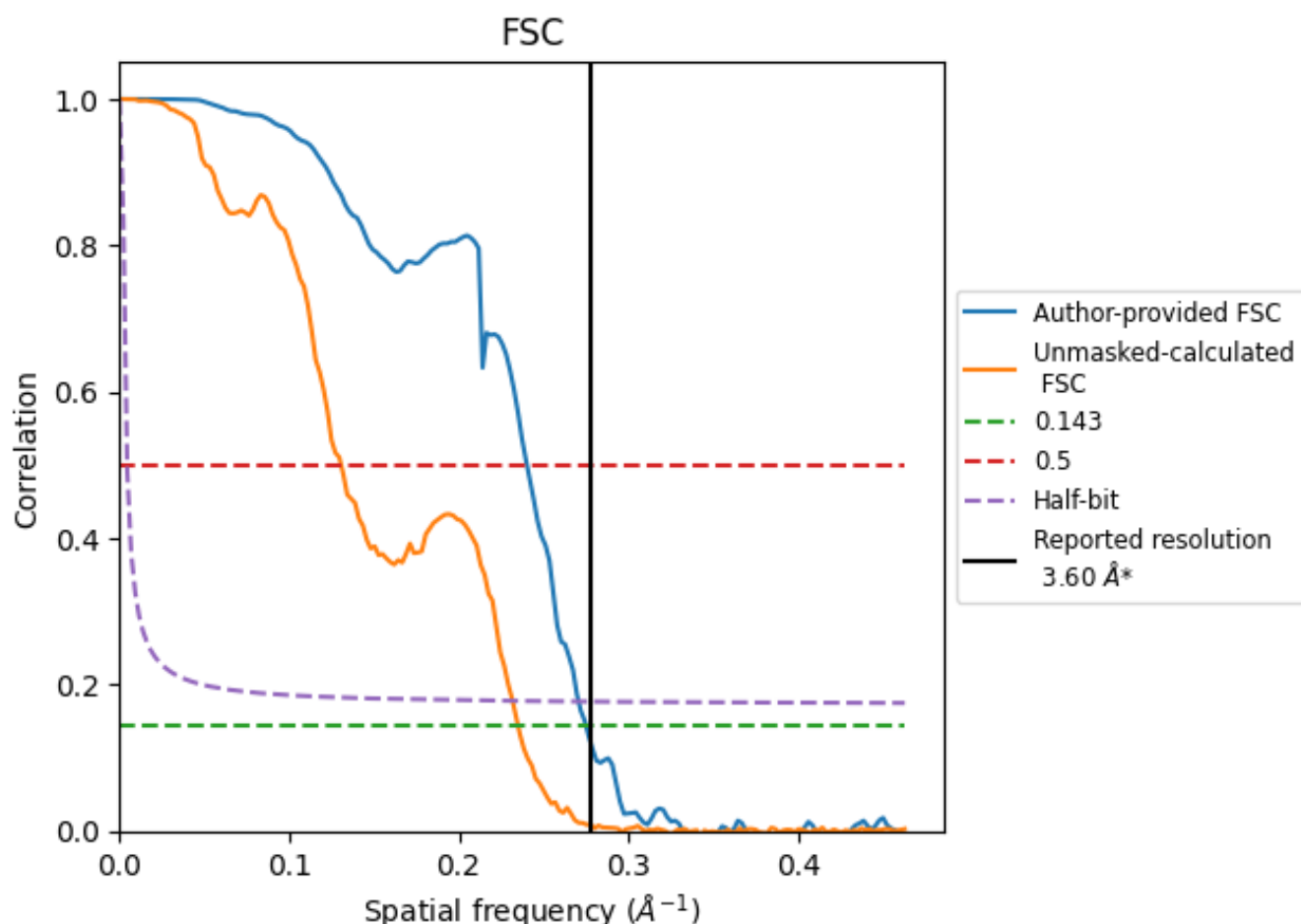


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

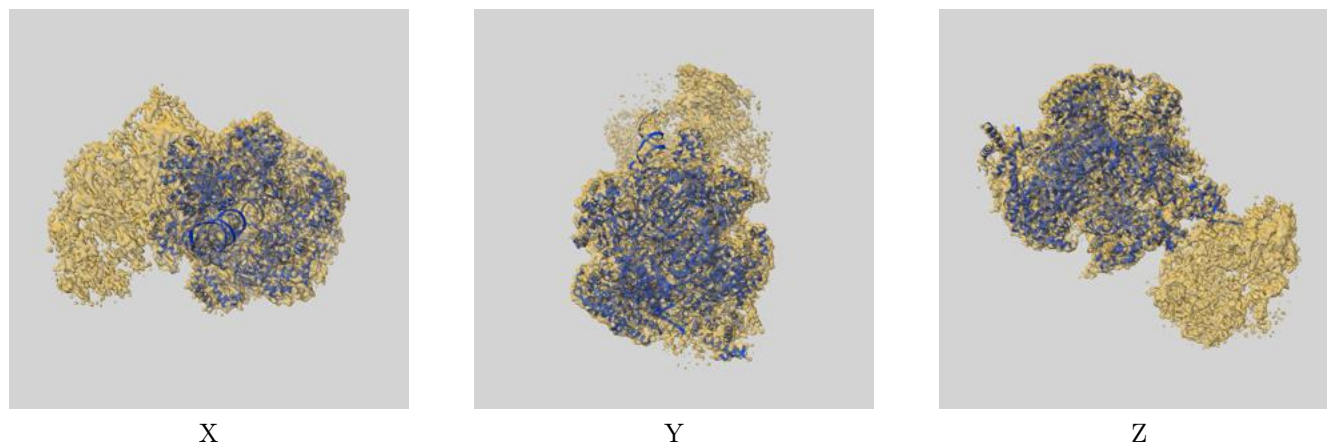
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.16	3.69
Unmasked-calculated*	4.26	7.65	4.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

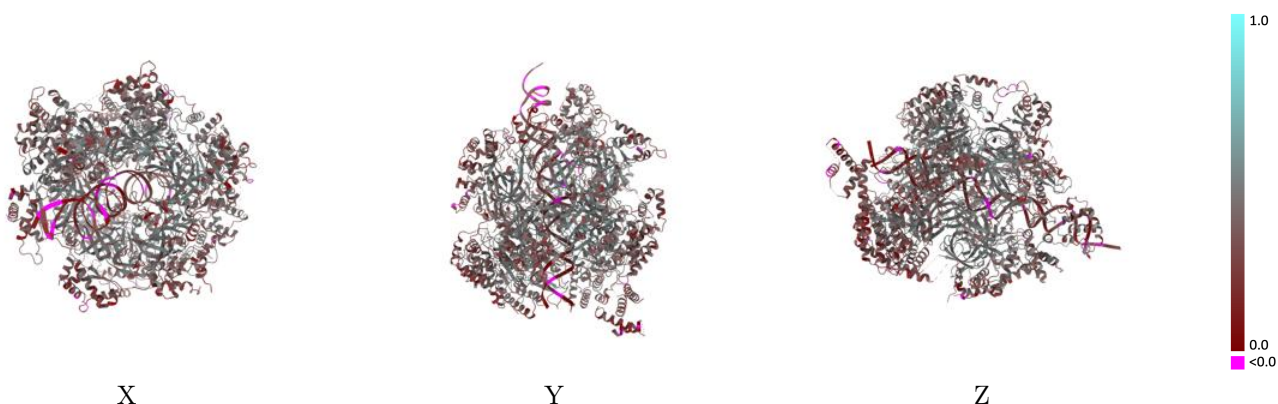
This section contains information regarding the fit between EMDB map EMD-19620 and PDB model 8S0B. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



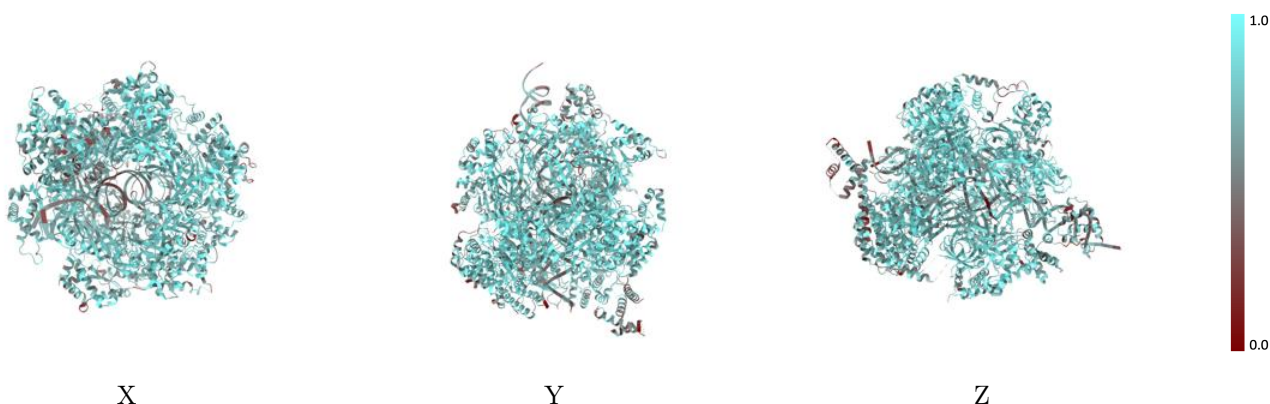
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



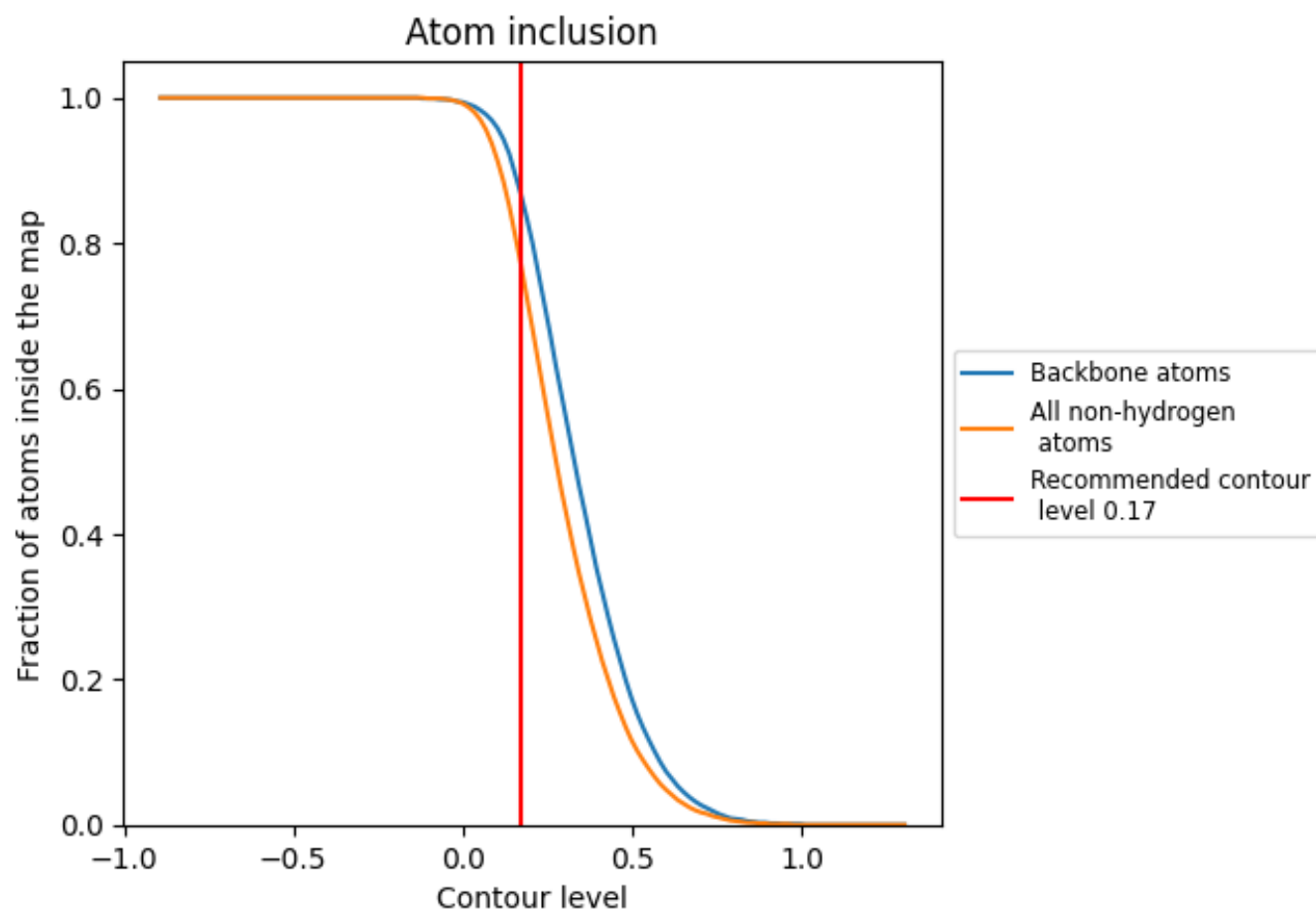
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7750</div>	<div><div></div>0.3770</div>
2	<div><div></div>0.7860</div>	<div><div></div>0.3860</div>
3	<div><div></div>0.7770</div>	<div><div></div>0.3780</div>
4	<div><div></div>0.8180</div>	<div><div></div>0.4180</div>
5	<div><div></div>0.7980</div>	<div><div></div>0.3940</div>
6	<div><div></div>0.7980</div>	<div><div></div>0.3970</div>
7	<div><div></div>0.7950</div>	<div><div></div>0.3770</div>
F	<div><div></div>0.6280</div>	<div><div></div>0.3850</div>
X	<div><div></div>0.5850</div>	<div><div></div>0.1460</div>
Y	<div><div></div>0.5400</div>	<div><div></div>0.1260</div>

1.0

0.0

<0.0