



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:00 PM UTC

PDB ID : 9GM5 / pdb_00009gm5
EMDB ID : EMD-51441
Title : OCCM maturation intermediate stalled with an Arginine Finger mutation in Mcm5: Conformer 1
Authors : Butryn, A.; Costa, A.
Deposited on : 2024-08-28
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

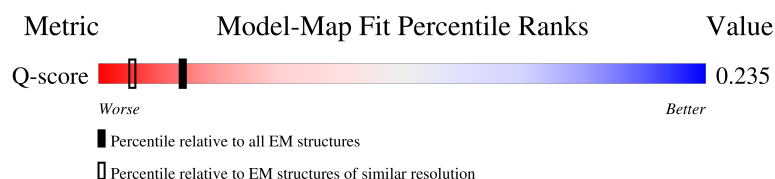
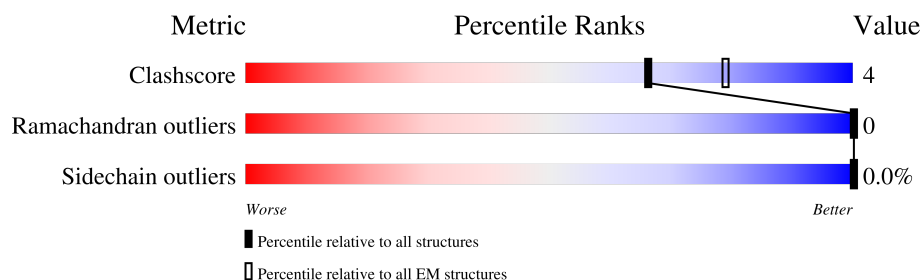
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



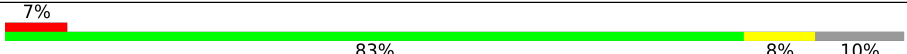
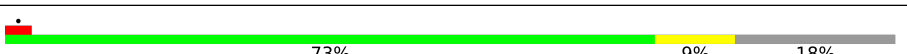
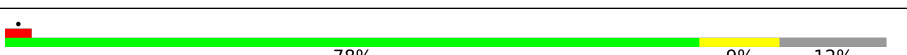
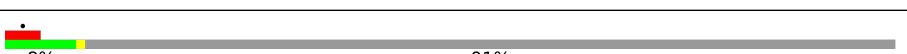
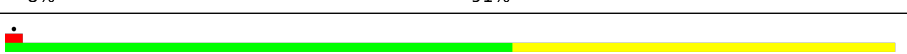
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	2	868	
2	3	1006	
3	4	933	
4	5	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	 55% 11% 33%
6	7	845	 16% 64% 5% 32%
7	8	604	 19% 76% 7% 16%
8	A	949	 13% 40% 56%
9	B	560	 36% 60%
10	C	616	 7% 83% 8% 10%
11	D	529	 73% 9% 18%
12	E	479	 78% 9% 12%
13	F	435	 8% 91%
14	X	42	 57% 43%
14	Y	42	 64% 36%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52641 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	637	Total	C	N	O	S	0	0
			5059	3180	909	951	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	585	Total	C	N	O	S	0	0
			4583	2889	814	868	12		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	626	Total	C	N	O	S	0	0
			4964	3117	848	968	31		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	638	Total	C	N	O	S	0	0
			5059	3188	881	967	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	549	ALA	ARG	engineered mutation	UNP P29496

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	677	Total	C	N	O	S	0	0
			5408	3428	936	1015	29		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	577	Total	C	N	O	S	0	0
			4541	2864	788	863	26		

- Molecule 7 is a protein called Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	505	Total	C	N	O	S	0	0
			4047	2583	688	757	19		

- Molecule 8 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	415	Total	C	N	O	S	0	0
			3310	2112	565	615	18		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P54784
A	-33	LYS	-	expression tag	UNP P54784
A	-32	ARG	-	expression tag	UNP P54784
A	-31	ARG	-	expression tag	UNP P54784
A	-30	TRP	-	expression tag	UNP P54784
A	-29	LYS	-	expression tag	UNP P54784
A	-28	LYS	-	expression tag	UNP P54784
A	-27	ASN	-	expression tag	UNP P54784
A	-26	PHE	-	expression tag	UNP P54784
A	-25	ILE	-	expression tag	UNP P54784
A	-24	ALA	-	expression tag	UNP P54784
A	-23	VAL	-	expression tag	UNP P54784
A	-22	SER	-	expression tag	UNP P54784
A	-21	ALA	-	expression tag	UNP P54784
A	-20	ALA	-	expression tag	UNP P54784
A	-19	ASN	-	expression tag	UNP P54784
A	-18	ARG	-	expression tag	UNP P54784
A	-17	PHE	-	expression tag	UNP P54784
A	-16	LYS	-	expression tag	UNP P54784
A	-15	LYS	-	expression tag	UNP P54784
A	-14	ILE	-	expression tag	UNP P54784
A	-13	SER	-	expression tag	UNP P54784
A	-12	SER	-	expression tag	UNP P54784
A	-11	SER	-	expression tag	UNP P54784
A	-10	GLY	-	expression tag	UNP P54784

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P54784
A	-8	LEU	-	expression tag	UNP P54784
A	-7	GLU	-	expression tag	UNP P54784
A	-6	ASN	-	expression tag	UNP P54784
A	-5	LEU	-	expression tag	UNP P54784
A	-4	TYR	-	expression tag	UNP P54784
A	-3	PHE	-	expression tag	UNP P54784
A	-2	GLN	-	expression tag	UNP P54784
A	-1	GLY	-	expression tag	UNP P54784
A	0	GLU	-	expression tag	UNP P54784

- Molecule 9 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	222	Total	C	N	O	S	0	0
			1845	1204	299	332	10		

- Molecule 10 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	557	Total	C	N	O	S	0	0
			4618	2985	760	857	16		

- Molecule 11 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	434	Total	C	N	O	S	0	0
			3542	2274	601	654	13		

- Molecule 12 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	420	Total	C	N	O	S	0	0
			3444	2247	546	637	14		

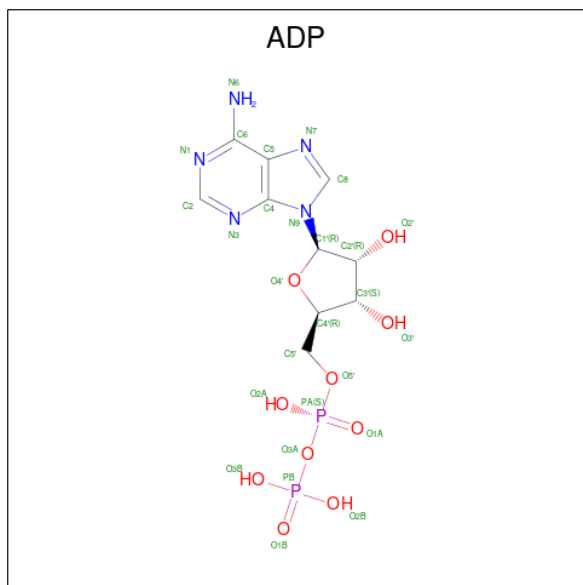
- Molecule 13 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	38	Total	C	N	O	S	0	0
			324	207	55	60	2		

- Molecule 14 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	42	Total	C	N	O	P	0	0
			861	409	158	252	42		
14	Y	42	Total	C	N	O	P	0	0
			861	409	158	252	42		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

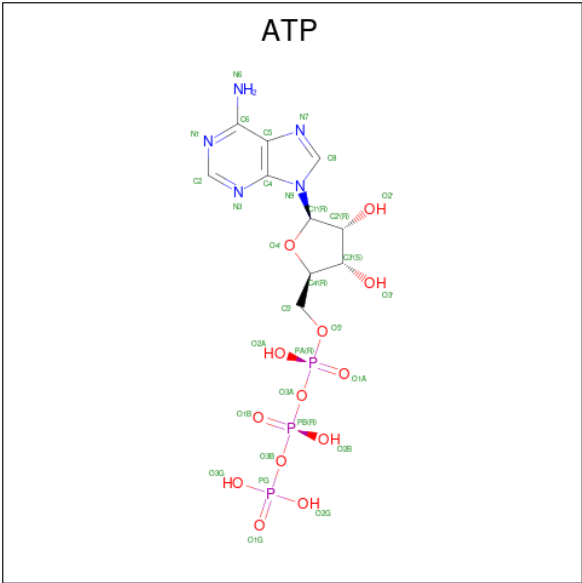
Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Zn	0
			1	1	
16	4	1	Total	Zn	0
			1	1	
16	5	1	Total	Zn	0
			1	1	
16	6	1	Total	Zn	0
			1	1	

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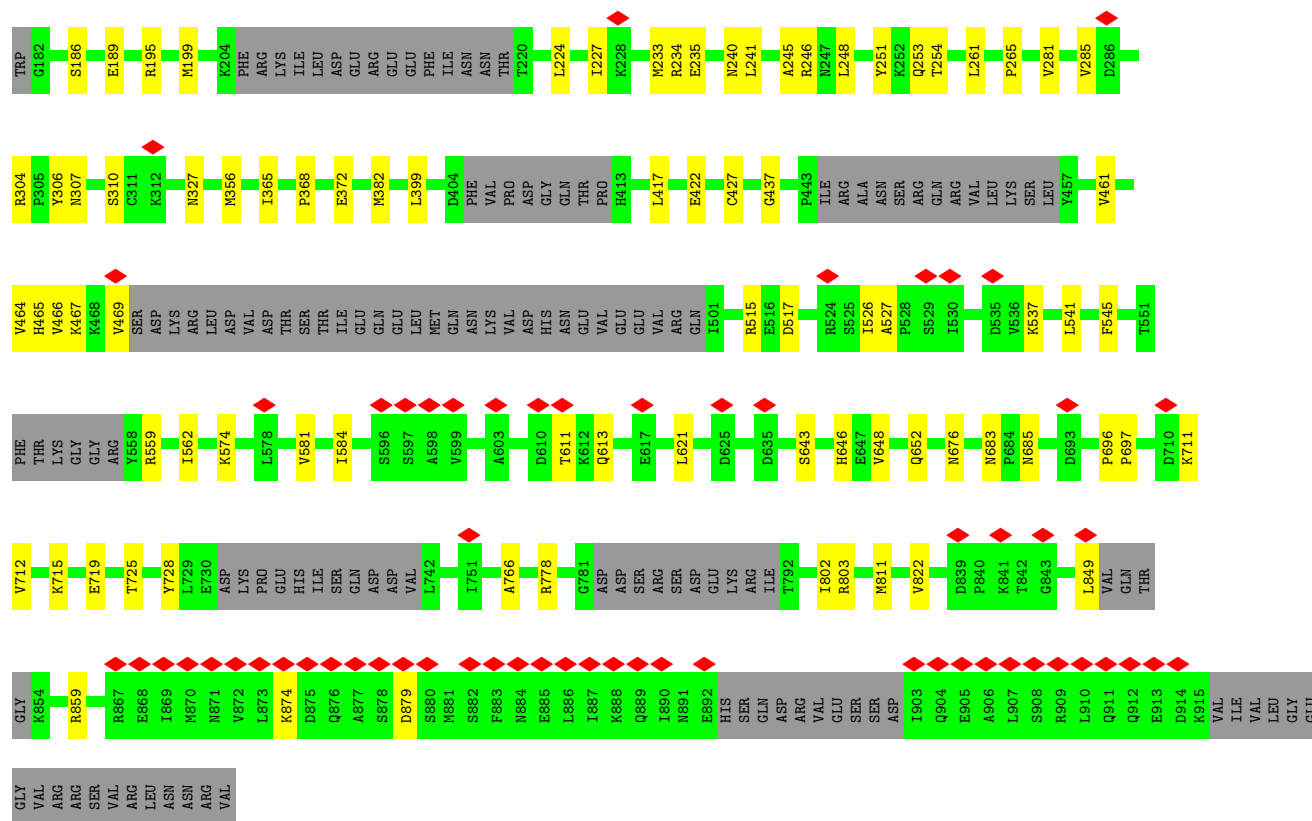
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Mol	Chain	Residues	Atoms		AltConf
16	7	1	Total	Zn	0
			1	1	

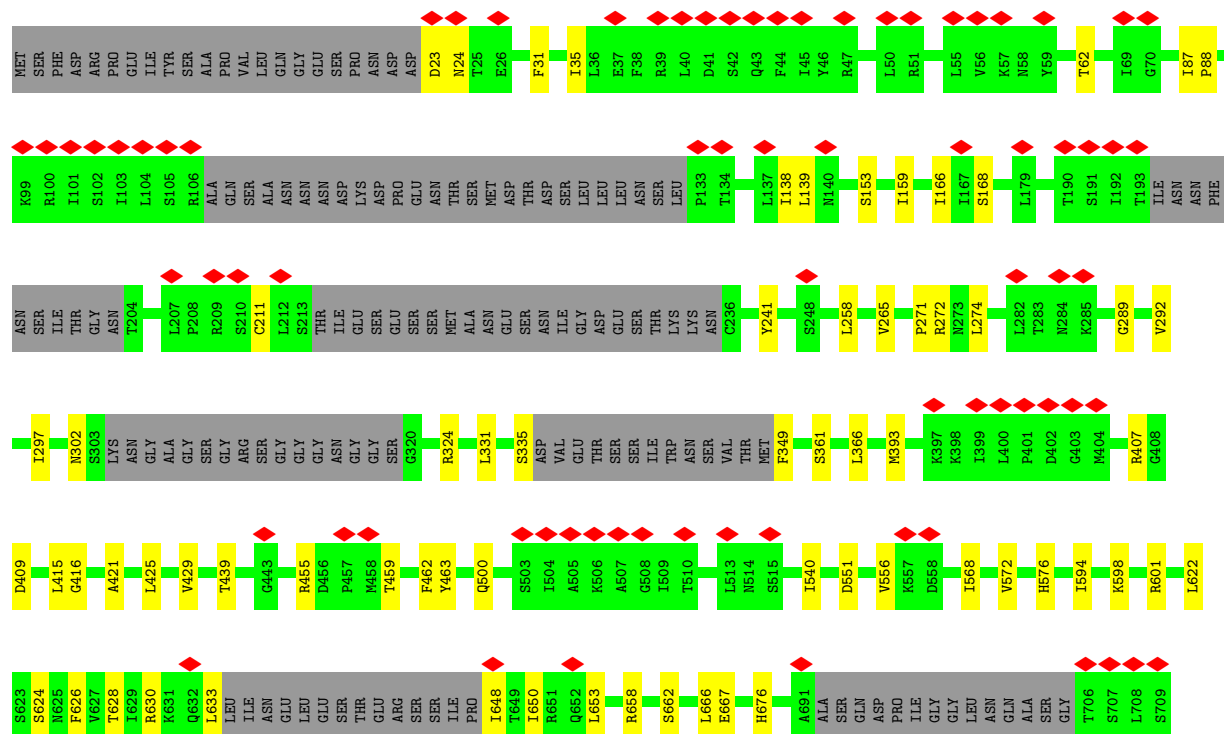
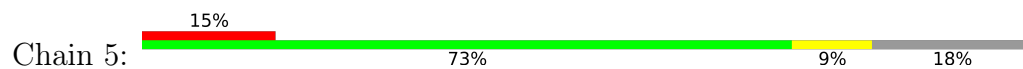
- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

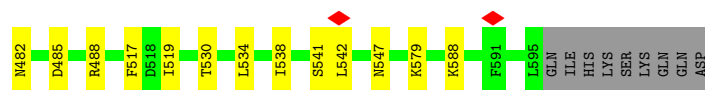


Mol	Chain	Residues	Atoms					AltConf
17	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

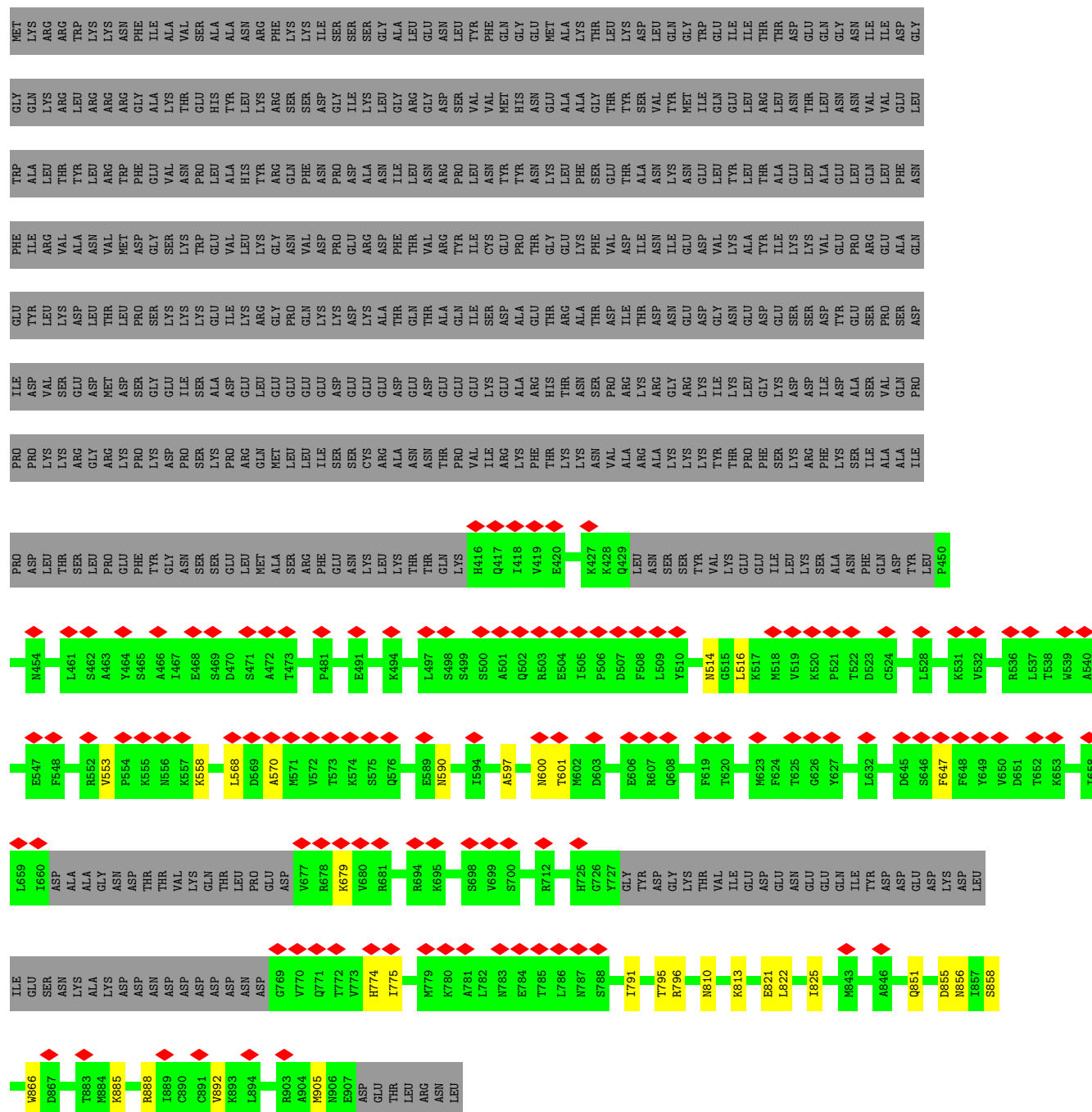


• Molecule 4: Minichromosome maintenance protein 5



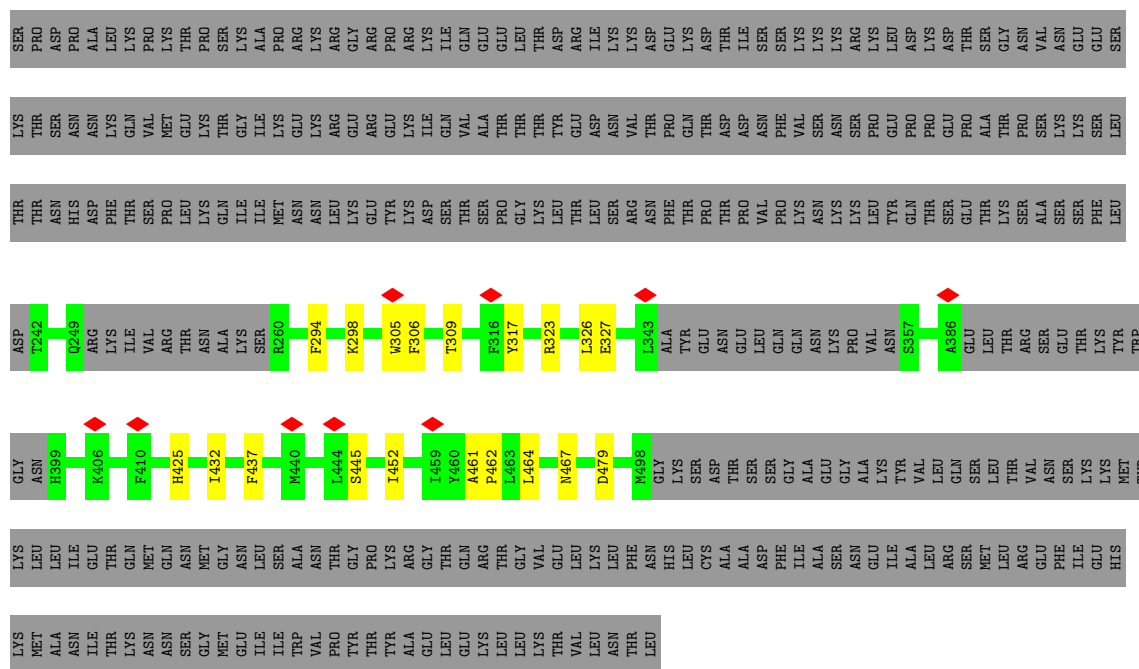


• Molecule 8: Origin recognition complex subunit 1

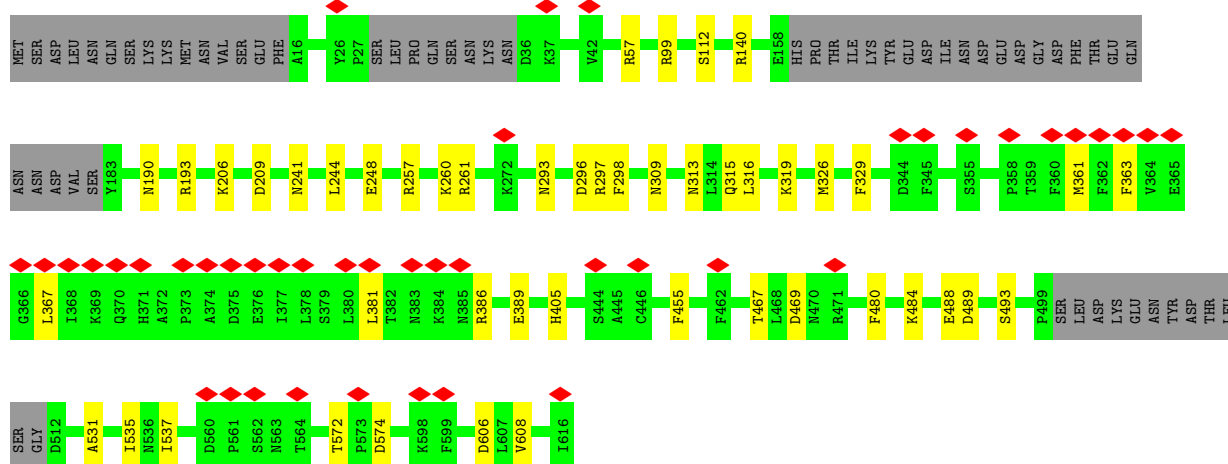
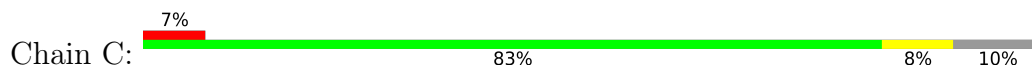


• Molecule 9: Origin recognition complex subunit 2

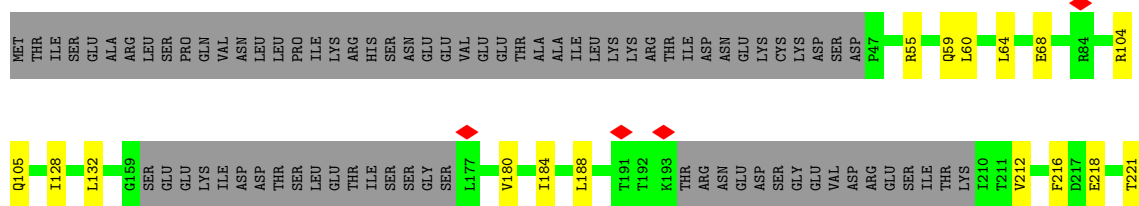


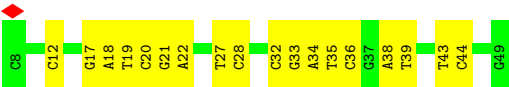


• Molecule 10: Origin recognition complex subunit 3

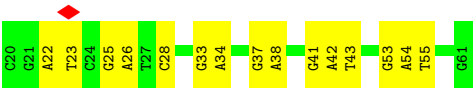


• Molecule 11: Origin recognition complex subunit 4





• Molecule 14: DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49788	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 ($e^-/\text{\AA}^2$)	30.34	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.674	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	418.0, 418.0, 418.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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: ADP, ATP, 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	2	0.12	0/5145	0.34	0/6945
2	3	0.11	0/4661	0.31	0/6323
3	4	0.12	0/5024	0.34	0/6775
4	5	0.11	0/5131	0.31	0/6921
5	6	0.12	0/5495	0.34	0/7406
6	7	0.11	0/4609	0.30	0/6222
7	8	0.12	0/4123	0.35	0/5588
8	A	0.10	0/3358	0.27	0/4519
9	B	0.12	0/1892	0.31	0/2556
10	C	0.11	0/4717	0.31	0/6364
11	D	0.12	0/3606	0.32	0/4873
12	E	0.12	0/3526	0.32	0/4791
13	F	0.09	0/328	0.27	0/440
14	X	0.19	0/965	0.42	0/1487
14	Y	0.20	0/965	0.44	0/1487
All	All	0.12	0/53545	0.32	0/72697

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	2	5059	0	5120	49	0
2	3	4583	0	4643	32	0
3	4	4964	0	5031	48	0
4	5	5059	0	5144	45	0
5	6	5408	0	5458	74	0
6	7	4541	0	4583	23	0
7	8	4047	0	4117	27	0
8	A	3310	0	3406	20	0
9	B	1845	0	1815	11	0
10	C	4618	0	4589	30	0
11	D	3542	0	3610	35	0
12	E	3444	0	3463	31	0
13	F	324	0	330	4	0
14	X	861	0	473	13	0
14	Y	861	0	473	11	0
15	2	27	0	12	2	0
15	4	27	0	12	1	0
15	5	27	0	12	2	0
15	6	27	0	12	1	0
16	2	1	0	0	0	0
16	4	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
17	D	31	0	12	1	0
17	E	31	0	12	0	0
All	All	52641	0	52327	406	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 (406) 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)
10:C:112:SER:HB2	10:C:206:LYS:HE2	1.66	0.77
11:D:339:ASN:ND2	12:E:183:CYS:O	2.19	0.76
2:3:553:ILE:HG13	4:5:630:ARG:HE	1.48	0.76
7:8:269:PRO:HA	7:8:277:THR:HA	1.69	0.74
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.70	0.72
10:C:257:ARG:NH2	11:D:458:ASN:OD1	2.24	0.70
5:6:592:ALA:HB3	5:6:595:SER:HB2	1.73	0.70
6:7:584:ILE:HG23	6:7:586:LEU:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:233:MET:HE3	3:4:241:LEU:HD13	1.73	0.69
3:4:399:LEU:HD12	3:4:417:LEU:HD11	1.74	0.69
11:D:59:GLN:HG2	11:D:64:LEU:HD11	1.75	0.69
5:6:568:ASP:OD2	5:6:659:GLN:NE2	2.26	0.67
7:8:337:PRO:HB3	7:8:384:ASN:HB2	1.76	0.67
8:A:558:LYS:NZ	8:A:590:ASN:O	2.27	0.66
3:4:711:LYS:NZ	3:4:849:LEU:O	2.29	0.66
6:7:331:LEU:HD21	6:7:376:LEU:HB2	1.78	0.66
4:5:87:ILE:HG23	4:5:88:PRO:HD3	1.79	0.65
3:4:859:ARG:NH2	8:A:905:MET:O	2.29	0.65
12:E:74:LEU:HD22	12:E:108:LEU:HD22	1.78	0.64
5:6:311:CYS:SG	5:6:340:ASN:ND2	2.66	0.64
5:6:559:THR:HG22	5:6:561:GLU:H	1.62	0.64
6:7:236:GLY:N	6:7:355:PHE:O	2.27	0.64
4:5:722:LEU:O	4:5:772:ARG:NH1	2.28	0.63
10:C:190:ASN:OD1	10:C:193:ARG:NH2	2.31	0.63
10:C:293:ASN:HB2	10:C:467:THR:HG22	1.80	0.63
5:6:589:VAL:HG11	5:6:597:TYR:HB2	1.80	0.63
2:3:307:ASN:ND2	2:3:308:GLN:OE1	2.27	0.62
5:6:313:MET:H	5:6:340:ASN:ND2	1.97	0.62
15:4:1001:ADP:O1B	6:7:593:ARG:NH1	2.32	0.61
12:E:143:ALA:O	12:E:179:TYR:OH	2.18	0.61
2:3:307:ASN:O	2:3:310:ASN:ND2	2.29	0.61
3:4:245:ALA:HB3	3:4:307:ASN:H	1.66	0.60
2:3:40:ASP:OD1	2:3:41:SER:N	2.33	0.60
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.84	0.60
5:6:303:GLU:N	5:6:354:LEU:O	2.27	0.60
5:6:347:ASN:OD1	5:6:350:ARG:N	2.33	0.60
3:4:527:ALA:HB3	3:4:537:LYS:HE3	1.83	0.59
5:6:312:ASP:O	5:6:315:ARG:NH1	2.34	0.59
5:6:639:ASP:OD1	5:6:640:GLU:N	2.35	0.59
11:D:387:GLU:HG2	11:D:459:VAL:HG13	1.85	0.58
5:6:625:ALA:HA	5:6:629:MET:HE3	1.85	0.58
8:A:796:ARG:O	11:D:332:ARG:NH2	2.32	0.58
1:2:382:TYR:HB2	4:5:153:SER:HB2	1.85	0.58
5:6:557:LYS:HB2	5:6:565:LEU:HD12	1.85	0.58
1:2:613:ASN:ND2	1:2:616:ASP:OD2	2.34	0.58
14:X:35:DT:H2"	14:X:36:DC:C5	2.39	0.58
7:8:364:LEU:HD11	7:8:373:VAL:HG11	1.86	0.58
8:A:822:LEU:HD21	8:A:866:TRP:HH2	1.67	0.58
12:E:35:LEU:HD23	12:E:189:PHE:HZ	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:258:LEU:O	4:5:274:LEU:N	2.36	0.58
4:5:361:SER:HA	4:5:366:LEU:HD22	1.85	0.58
10:C:57:ARG:NH1	10:C:329:PHE:O	2.36	0.58
3:4:683:ASN:OD1	3:4:685:ASN:ND2	2.32	0.57
12:E:205:ARG:NE	12:E:259:ASN:OD1	2.37	0.57
12:E:239:PHE:HE2	12:E:262:ILE:HG23	1.69	0.57
9:B:467:ASN:OD1	12:E:422:GLN:NE2	2.26	0.57
1:2:333:GLN:O	1:2:383:ARG:N	2.37	0.57
3:4:240:ASN:OD1	3:4:241:LEU:N	2.37	0.57
3:4:195:ARG:NH2	3:4:199:MET:SD	2.78	0.57
3:4:874:LYS:NZ	3:4:879:ASP:OD1	2.36	0.56
4:5:630:ARG:NH1	4:5:648:ILE:O	2.38	0.56
5:6:516:LEU:HD21	5:6:757:TYR:HB2	1.86	0.56
10:C:248:GLU:O	11:D:457:LYS:NZ	2.38	0.56
1:2:416:ASP:OD2	4:5:272:ARG:NH2	2.39	0.56
4:5:455:ARG:HA	4:5:462:PHE:HA	1.87	0.56
5:6:512:GLU:OE2	7:8:547:ASN:ND2	2.29	0.56
4:5:393:MET:HG3	4:5:666:LEU:HB2	1.87	0.55
1:2:536:ASP:HB3	1:2:645:SER:HB3	1.89	0.55
3:4:261:LEU:HD11	3:4:265:PRO:HA	1.89	0.55
5:6:144:LYS:HD3	5:6:193:ALA:HB1	1.88	0.55
6:7:30:GLN:HA	6:7:62:LYS:HB2	1.89	0.54
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.31	0.54
1:2:260:LEU:HD12	1:2:264:PRO:HA	1.89	0.54
1:2:808:ARG:NH1	15:5:901:ADP:O3A	2.38	0.54
2:3:410:ASP:O	2:3:415:LYS:NZ	2.35	0.54
1:2:759:PRO:HB2	1:2:762:LEU:HD13	1.89	0.54
4:5:159:ILE:HG12	4:5:297:ILE:HG12	1.90	0.54
11:D:105:GLN:NE2	12:E:182:HIS:O	2.32	0.54
6:7:29:LYS:HA	6:7:61:PRO:HA	1.90	0.53
4:5:630:ARG:HH22	4:5:633:LEU:HD23	1.71	0.53
14:X:43:DT:H2"	14:X:44:DC:C6	2.43	0.53
10:C:209:ASP:OD2	10:C:241:ASN:ND2	2.32	0.53
4:5:626:PHE:HB2	4:5:653:LEU:HD13	1.89	0.53
3:4:802:ILE:HD11	5:6:732:VAL:HG22	1.90	0.53
14:X:21:DG:H2"	14:X:22:DA:C8	2.44	0.53
1:2:526:ASN:ND2	1:2:531:HIS:O	2.40	0.53
4:5:622:LEU:HB3	4:5:653:LEU:HD11	1.90	0.53
7:8:390:ASN:OD1	7:8:391:LEU:N	2.42	0.53
12:E:36:GLN:NE2	12:E:172:GLU:O	2.38	0.53
3:4:574:LYS:NZ	3:4:676:ASN:OD1	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:600:ASN:OD1	8:A:601:THR:N	2.43	0.52
2:3:449:ASP:HA	2:3:455:ARG:HA	1.91	0.52
3:4:310:SER:HA	3:4:327:ASN:HB3	1.90	0.52
3:4:224:LEU:HD13	3:4:227:ILE:HG13	1.90	0.52
4:5:719:LYS:NZ	4:5:775:VAL:OXT	2.35	0.52
1:2:183:LEU:HB3	1:2:186:LEU:HD12	1.92	0.52
5:6:816:VAL:HG12	5:6:818:GLU:H	1.74	0.52
1:2:778:LEU:HD22	4:5:576:HIS:HB3	1.92	0.52
7:8:325:LEU:HD11	7:8:383:MET:HE2	1.92	0.52
4:5:753:TYR:CE2	4:5:757:LYS:HE3	2.45	0.51
14:X:33:DG:H2''	14:X:34:DA:C8	2.44	0.51
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.75	0.51
5:6:144:LYS:HA	5:6:196:LEU:HD21	1.93	0.51
7:8:294:ALA:O	7:8:298:TYR:N	2.37	0.51
3:4:581:VAL:HA	3:4:584:ILE:HG22	1.93	0.51
4:5:166:ILE:O	4:5:289:GLY:N	2.30	0.51
3:4:246:ARG:NH2	3:4:307:ASN:OD1	2.42	0.51
3:4:621:LEU:HD21	3:4:648:VAL:HG21	1.93	0.51
14:X:38:DA:H2'	14:X:39:DT:H71	1.93	0.51
14:Y:42:DA:H2'	14:Y:43:DT:H71	1.93	0.50
5:6:502:GLU:O	5:6:506:ASN:ND2	2.40	0.50
10:C:572:THR:HG22	10:C:574:ASP:H	1.75	0.50
5:6:272:THR:HB	7:8:519:ILE:HG23	1.94	0.50
8:A:570:ALA:O	11:D:227:ARG:NH1	2.45	0.50
9:B:445:SER:HB3	9:B:452:ILE:HD12	1.92	0.50
11:D:412:TYR:OH	11:D:451:TRP:O	2.26	0.50
14:Y:53:DG:H2''	14:Y:54:DA:H8	1.77	0.50
2:3:716:ARG:NH2	2:3:722:ASN:OD1	2.38	0.50
2:3:235:ASP:HB2	2:3:241:LEU:HD21	1.94	0.50
1:2:434:TYR:HB2	1:2:448:ALA:H	1.77	0.49
8:A:568:LEU:HD22	8:A:597:ALA:HB1	1.93	0.49
10:C:261:ARG:NH2	12:E:260:ASP:OD1	2.44	0.49
11:D:230:LEU:O	11:D:234:LEU:HG	2.12	0.49
5:6:580:SER:HB3	15:6:1101:ADP:C8	2.47	0.49
5:6:763:PRO:HA	5:6:817:ASP:HB3	1.93	0.49
8:A:553:VAL:HB	8:A:558:LYS:HE3	1.94	0.49
10:C:489:ASP:O	10:C:493:SER:N	2.42	0.49
3:4:725:THR:HA	3:4:728:TYR:CE2	2.48	0.49
11:D:188:LEU:HD13	11:D:243:VAL:HG11	1.93	0.49
12:E:82:GLN:NE2	12:E:96:ASP:OD1	2.45	0.49
11:D:230:LEU:HD12	11:D:231:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:19:DT:H2"	14:X:20:DC:C5	2.47	0.49
3:4:437:GLY:HA2	3:4:464:VAL:HG23	1.94	0.49
4:5:349:PHE:HE1	4:5:601:ARG:HG3	1.77	0.49
4:5:753:TYR:CZ	4:5:757:LYS:HE3	2.48	0.49
11:D:320:LEU:O	11:D:324:ILE:HG13	2.12	0.49
6:7:456:VAL:HG22	6:7:596:ILE:HB	1.93	0.48
3:4:712:VAL:HA	6:7:668:ARG:HH21	1.78	0.48
4:5:551:ASP:OD1	4:5:658:ARG:NH1	2.45	0.48
4:5:594:ILE:HG23	4:5:598:LYS:HE3	1.95	0.48
5:6:569:ILE:HG23	5:6:710:ASP:HB2	1.94	0.48
5:6:653:HIS:HB3	5:6:708:ARG:NH1	2.28	0.48
1:2:221:GLU:HG3	1:2:222:THR:H	1.77	0.48
1:2:231:ILE:HG23	1:2:279:THR:HG22	1.95	0.48
3:4:526:ILE:HD11	3:4:541:LEU:HD22	1.95	0.48
5:6:364:ASN:ND2	5:6:367:GLU:OE2	2.44	0.48
6:7:529:MET:HE1	6:7:537:ILE:HG13	1.95	0.48
11:D:230:LEU:HD12	11:D:231:LEU:HG	1.95	0.48
4:5:407:ARG:HD3	4:5:409:ASP:HB2	1.94	0.48
3:4:304:ARG:NH2	3:4:422:GLU:OE2	2.39	0.48
5:6:301:ARG:O	5:6:356:TRP:N	2.47	0.48
8:A:851:GLN:OE1	8:A:858:SER:OG	2.26	0.48
1:2:271:PHE:HE2	1:2:295:VAL:HG11	1.79	0.47
3:4:251:TYR:CE2	3:4:253:GLN:HB2	2.49	0.47
7:8:73:PHE:CD1	7:8:81:LEU:HB2	2.49	0.47
8:A:647:PHE:CD1	8:A:679:LYS:HE3	2.49	0.47
1:2:277:GLU:O	1:2:281:LEU:HG	2.13	0.47
3:4:234:ARG:NH2	3:4:235:GLU:OE2	2.38	0.47
4:5:425:LEU:O	4:5:429:VAL:HG23	2.14	0.47
4:5:568:ILE:O	4:5:572:VAL:HG23	2.14	0.47
12:E:35:LEU:HB3	12:E:189:PHE:CE2	2.50	0.47
3:4:365:ILE:HB	5:6:419:SER:HA	1.95	0.47
2:3:393:LEU:HD12	2:3:397:SER:HB2	1.96	0.47
5:6:918:ARG:HD2	11:D:429:VAL:HG22	1.95	0.47
8:A:855:ASP:OD1	8:A:856:ASN:N	2.47	0.47
10:C:484:LYS:NZ	10:C:488:GLU:OE2	2.39	0.47
12:E:262:ILE:O	12:E:266:TRP:HB2	2.14	0.47
3:4:715:LYS:O	3:4:719:GLU:HG2	2.14	0.47
4:5:87:ILE:CG2	4:5:88:PRO:HD3	2.44	0.47
7:8:338:PRO:HG2	7:8:343:LEU:HD11	1.96	0.47
8:A:888:ARG:HH12	11:D:512:GLU:CD	2.22	0.47
14:X:33:DG:H2"	14:X:34:DA:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.96	0.47
1:2:519:LEU:O	1:2:771:ARG:NH1	2.45	0.47
14:Y:37:DG:H2"	14:Y:38:DA:C8	2.50	0.47
4:5:416:GLY:HA3	4:5:556:VAL:HG22	1.95	0.47
9:B:323:ARG:NE	9:B:327:GLU:OE2	2.40	0.47
1:2:294:HIS:CD2	1:2:412:ALA:HB1	2.50	0.47
2:3:195:LYS:N	2:3:251:ILE:O	2.48	0.47
6:7:66:MET:O	6:7:70:VAL:HG23	2.14	0.47
9:B:461:ALA:N	9:B:462:PRO:HD2	2.30	0.46
3:4:368:PRO:HB2	3:4:382:MET:HG3	1.98	0.46
5:6:292:GLY:HA3	5:6:361:ILE:HD12	1.98	0.46
1:2:700:VAL:HG11	5:6:770:ARG:HB3	1.97	0.46
4:5:393:MET:HB2	4:5:662:SER:OG	2.15	0.46
2:3:533:ILE:HG22	2:3:535:LEU:HG	1.98	0.46
3:4:248:LEU:HA	3:4:254:THR:HB	1.97	0.46
5:6:939:TRP:O	5:6:943:GLN:HG2	2.16	0.46
8:A:885:LYS:HB3	11:D:476:GLY:HA3	1.98	0.46
10:C:361:MET:HG2	13:F:418:TYR:CE1	2.50	0.46
10:C:606:ASP:OD1	10:C:606:ASP:N	2.48	0.46
4:5:409:ASP:OD2	4:5:500:GLN:NE2	2.42	0.46
1:2:624:MET:HG2	1:2:646:ILE:HD12	1.98	0.46
5:6:795:ILE:HG23	5:6:799:GLN:HB2	1.98	0.46
5:6:912:MET:HE1	5:6:961:ALA:HA	1.96	0.46
11:D:510:LEU:HD12	11:D:510:LEU:H	1.80	0.46
6:7:350:ASP:OD1	6:7:384:HIS:NE2	2.36	0.46
7:8:485:ASP:OD1	7:8:488:ARG:NH1	2.44	0.46
1:2:511:ILE:O	1:2:515:VAL:HG23	2.16	0.46
5:6:145:ILE:HG23	7:8:336:VAL:HG21	1.96	0.46
5:6:164:GLY:O	5:6:168:MET:HG2	2.16	0.46
12:E:338:CYS:SG	12:E:389:ILE:HD12	2.56	0.46
1:2:536:ASP:OD1	1:2:627:GLN:NE2	2.43	0.45
2:3:244:GLU:OE2	6:7:14:TYR:OH	2.21	0.45
2:3:352:LYS:HG2	2:3:356:LYS:NZ	2.31	0.45
5:6:368:ILE:HD13	5:6:374:PRO:HB3	1.99	0.45
6:7:675:MET:HE3	6:7:683:GLN:HB2	1.98	0.45
6:7:684:ALA:HA	6:7:688:THR:HG21	1.98	0.45
2:3:23:ASP:OD1	2:3:26:ARG:NH2	2.45	0.45
11:D:400:ARG:HH12	11:D:414:GLU:CD	2.23	0.45
12:E:215:LEU:HD22	12:E:232:PHE:CE1	2.51	0.45
1:2:655:GLY:HA3	5:6:704:PRO:HD3	1.99	0.45
1:2:813:ILE:HG12	1:2:841:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:24:ARG:HH12	2:3:120:TYR:HB3	1.82	0.45
4:5:624:SER:O	4:5:628:THR:HG23	2.17	0.45
6:7:206:PRO:HB3	6:7:352:THR:HG21	1.98	0.45
2:3:711:ALA:O	2:3:715:VAL:HG23	2.16	0.45
4:5:31:PHE:O	4:5:35:ILE:HG12	2.17	0.45
5:6:273:VAL:HB	7:8:541:SER:HA	1.98	0.45
5:6:772:TYR:CZ	5:6:776:LYS:HE2	2.52	0.45
5:6:186:ARG:HA	5:6:189:VAL:HG12	1.98	0.45
6:7:643:ALA:O	6:7:647:THR:HG23	2.16	0.45
7:8:48:TYR:CE2	7:8:50:ASN:HB2	2.52	0.45
9:B:464:LEU:HD21	12:E:444:LEU:HG	1.97	0.45
1:2:271:PHE:CE2	1:2:295:VAL:HG11	2.52	0.45
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.39	0.45
5:6:520:VAL:HG22	5:6:754:TYR:CE1	2.51	0.45
5:6:972:ARG:NH1	11:D:385:ASP:OD1	2.40	0.45
10:C:99:ARG:NH1	12:E:208:GLU:OE2	2.46	0.45
5:6:268:PHE:HB3	5:6:458:HIS:CD2	2.51	0.45
11:D:55:ARG:HH22	11:D:68:GLU:CD	2.25	0.45
11:D:393:SER:O	11:D:397:VAL:HG23	2.16	0.45
5:6:522:ASP:HB3	5:6:525:ILE:HG23	1.98	0.44
1:2:242:LEU:HD12	1:2:275:ALA:HB1	1.99	0.44
1:2:255:ILE:HG23	7:8:393:THR:HB	1.98	0.44
3:4:611:THR:HG22	3:4:613:GLN:HG2	1.98	0.44
3:4:766:ALA:HB1	3:4:822:VAL:HG21	1.99	0.44
12:E:218:ARG:NH1	12:E:221:GLU:OE1	2.48	0.44
5:6:553:GLY:O	5:6:812:ARG:NH1	2.50	0.44
11:D:104:ARG:NH1	17:D:601:ATP:O3G	2.44	0.44
12:E:266:TRP:HB3	12:E:267:PRO:HD3	2.00	0.44
5:6:197:LEU:HD22	5:6:261:ARG:HG2	1.99	0.44
4:5:459:THR:OG1	4:5:463:TYR:OH	2.30	0.44
7:8:534:LEU:O	7:8:538:ILE:HG12	2.18	0.44
8:A:822:LEU:HD13	8:A:892:VAL:HG21	1.99	0.44
14:Y:25:DG:H2"	14:Y:26:DA:C8	2.53	0.44
1:2:633:LYS:NZ	14:Y:28:DC:OP2	2.48	0.44
3:4:559:ARG:HD3	3:4:652:GLN:HG2	1.99	0.44
11:D:506:MET:HG3	11:D:508:ILE:H	1.82	0.44
14:X:17:DG:H2"	14:X:18:DA:C8	2.53	0.44
14:X:32:DC:H2"	14:X:33:DG:C8	2.52	0.44
7:8:154:ARG:HG3	7:8:258:VAL:HG22	1.99	0.44
8:A:514:ASN:OD1	8:A:516:LEU:N	2.50	0.44
13:F:393:ARG:HE	13:F:396:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:41:DG:H2"	14:Y:42:DA:C8	2.53	0.43
1:2:294:HIS:CG	1:2:412:ALA:HB1	2.53	0.43
2:3:211:TYR:CE1	6:7:6:PRO:HB2	2.53	0.43
9:B:326:LEU:HB2	9:B:425:HIS:HE1	1.83	0.43
10:C:381:LEU:HD22	13:F:422:LYS:HE3	2.00	0.43
4:5:415:LEU:HD21	4:5:540:ILE:HD11	2.01	0.43
3:4:696:PRO:N	3:4:697:PRO:HD2	2.34	0.43
8:A:810:ASN:HA	8:A:813:LYS:HG2	2.00	0.43
10:C:386:ARG:HD3	10:C:389:GLU:OE2	2.19	0.43
4:5:211:CYS:HA	4:5:241:TYR:CE2	2.54	0.43
4:5:265:VAL:HG21	4:5:271:PRO:HG3	2.00	0.43
1:2:336:TYR:O	1:2:380:THR:HG23	2.18	0.43
3:4:240:ASN:HD21	3:4:304:ARG:HG3	1.83	0.43
7:8:530:THR:HA	7:8:579:LYS:HA	2.00	0.43
1:2:663:LEU:HD13	1:2:803:PHE:HE1	1.82	0.43
2:3:164:HIS:HB3	2:3:180:VAL:HA	1.99	0.43
4:5:62:THR:HA	4:5:138:ILE:HB	2.00	0.43
7:8:61:LEU:HA	7:8:65:ASP:HB2	2.01	0.43
1:2:327:ARG:NH1	1:2:418:SER:O	2.51	0.43
15:2:901:ADP:O2B	5:6:798:ARG:NH2	2.37	0.43
5:6:186:ARG:O	5:6:189:VAL:HG12	2.19	0.43
5:6:718:ASP:OD1	5:6:719:CYS:N	2.51	0.43
3:4:515:ARG:NH2	3:4:517:ASP:OD2	2.38	0.43
4:5:421:ALA:HB2	15:5:901:ADP:C8	2.54	0.43
11:D:180:VAL:O	11:D:184:ILE:HG13	2.17	0.43
11:D:519:LYS:HG2	11:D:524:TYR:CE2	2.54	0.43
12:E:18:LEU:HD21	12:E:35:LEU:HD21	2.00	0.43
14:X:27:DT:H2"	14:X:28:DC:C6	2.54	0.43
1:2:774:ILE:HG13	1:2:825:LEU:HD22	2.00	0.43
3:4:562:ILE:HG13	3:4:803:ARG:HD2	2.00	0.43
5:6:109:GLU:OE1	5:6:112:ARG:NH2	2.37	0.43
5:6:172:GLU:HG3	5:6:173:GLN:HG3	1.99	0.43
5:6:330:PRO:HD2	5:6:344:TRP:CD1	2.54	0.43
6:7:469:LEU:O	6:7:473:ILE:HG12	2.18	0.43
9:B:432:ILE:HG13	9:B:437:PHE:CE1	2.54	0.43
10:C:140:ARG:NH2	14:X:12:DC:OP2	2.52	0.43
7:8:480:GLN:C	7:8:482:ASN:H	2.26	0.42
9:B:305:TRP:CZ3	9:B:309:THR:HG21	2.54	0.42
1:2:676:ARG:HG3	1:2:808:ARG:NH2	2.35	0.42
2:3:687:ARG:HH12	6:7:602:ASP:CG	2.26	0.42
4:5:626:PHE:CZ	4:5:650:ILE:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:233:ASP:O	6:7:237:GLN:NE2	2.52	0.42
10:C:309:ASN:O	10:C:313:ASN:ND2	2.52	0.42
8:A:821:GLU:O	8:A:825:ILE:HG13	2.19	0.42
11:D:128:ILE:HG22	11:D:212:VAL:HG13	2.01	0.42
4:5:667:GLU:OE1	4:5:676:HIS:NE2	2.43	0.42
14:Y:54:DA:H2'	14:Y:55:DT:H71	2.01	0.42
3:4:467:LYS:HE2	3:4:469:VAL:HB	2.02	0.42
4:5:168:SER:OG	4:5:463:TYR:HB3	2.18	0.42
9:B:317:TYR:CZ	9:B:479:ASP:HB2	2.55	0.42
11:D:132:LEU:HD12	11:D:216:PHE:CZ	2.54	0.42
14:Y:22:DA:C2'	14:Y:23:DT:H71	2.49	0.42
5:6:174:TYR:HB3	5:6:400:VAL:HG11	2.00	0.42
2:3:94:HIS:HB3	2:3:153:TRP:CD2	2.55	0.42
4:5:302:ASN:OD1	4:5:324:ARG:NH1	2.52	0.42
5:6:645:ASP:HB2	5:6:648:ASP:OD2	2.20	0.42
11:D:458:ASN:ND2	12:E:250:TYR:OH	2.52	0.42
1:2:447:PHE:O	5:6:302:PRO:HD2	2.19	0.42
2:3:353:LEU:HD23	2:3:356:LYS:HE2	2.00	0.42
10:C:298:PHE:HB2	10:C:469:ASP:HA	2.00	0.42
11:D:218:GLU:O	11:D:221:THR:OG1	2.28	0.42
12:E:136:ASP:OD1	12:E:136:ASP:N	2.53	0.42
1:2:540:LEU:HB2	1:2:677:PHE:CE2	2.55	0.42
1:2:565:PHE:HA	1:2:605:LEU:HB2	2.02	0.42
3:4:427:CYS:SG	3:4:466:VAL:HG21	2.60	0.42
5:6:134:LYS:HE2	5:6:137:ARG:HD3	2.01	0.42
5:6:303:GLU:HB2	5:6:356:TRP:HB2	2.01	0.42
5:6:695:LEU:HD11	5:6:714:VAL:HG21	2.02	0.42
6:7:455:ASN:ND2	6:7:541:MET:SD	2.93	0.42
7:8:339:GLU:OE2	7:8:378:ARG:NH1	2.50	0.42
7:8:517:PHE:HE1	7:8:588:LYS:HB3	1.85	0.42
10:C:296:ASP:OD1	10:C:297:ARG:N	2.53	0.42
1:2:211:LEU:HD23	1:2:256:LEU:HD21	2.01	0.42
7:8:412:GLN:HA	7:8:415:ILE:HG12	2.02	0.42
12:E:329:LYS:O	12:E:333:ILE:HG12	2.20	0.42
1:2:573:ALA:N	1:2:616:ASP:OD1	2.53	0.41
5:6:585:LEU:HD12	5:6:639:ASP:HB2	2.02	0.41
8:A:774:HIS:CE1	8:A:775:ILE:HG22	2.55	0.41
10:C:315:GLN:O	10:C:319:LYS:HG3	2.20	0.41
12:E:280:GLU:HG2	12:E:283:ALA:H	1.83	0.41
14:Y:22:DA:H2''	14:Y:23:DT:H71	2.01	0.41
14:Y:53:DG:H2''	14:Y:54:DA:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:748:GLN:O	1:2:752:GLU:HG3	2.21	0.41
2:3:558:ASP:HA	2:3:561:ILE:HG22	2.01	0.41
5:6:354:LEU:HD23	5:6:382:ARG:HD3	2.01	0.41
7:8:480:GLN:C	7:8:482:ASN:N	2.78	0.41
12:E:36:GLN:NE2	12:E:173:THR:HA	2.34	0.41
12:E:192:TYR:O	12:E:253:ASN:ND2	2.53	0.41
12:E:271:SER:OG	12:E:272:ARG:NH1	2.53	0.41
4:5:23:ASP:OD1	4:5:24:ASN:N	2.49	0.41
5:6:937:VAL:HG11	5:6:958:ARG:HG3	2.01	0.41
10:C:537:ILE:HD11	10:C:608:VAL:HB	2.02	0.41
1:2:434:TYR:CD1	1:2:448:ALA:HB3	2.55	0.41
4:5:292:VAL:HG12	4:5:335:SER:HB2	2.02	0.41
5:6:271:PRO:HA	7:8:542:LEU:HD22	2.03	0.41
5:6:657:GLU:HG3	5:6:658:GLN:OE1	2.20	0.41
10:C:244:LEU:HD13	12:E:299:LEU:HG	2.01	0.41
10:C:316:LEU:HD11	10:C:480:PHE:CZ	2.55	0.41
12:E:64:PRO:HD2	12:E:133:ASP:O	2.20	0.41
14:X:17:DG:H2"	14:X:18:DA:H8	1.84	0.41
3:4:356:MET:HE2	3:4:372:GLU:HG2	2.02	0.41
13:F:393:ARG:NH2	13:F:395:ASP:OD1	2.51	0.41
3:4:417:LEU:HD22	3:4:461:VAL:HB	2.01	0.41
8:A:791:ILE:O	8:A:795:THR:HG23	2.20	0.41
14:X:32:DC:H2"	14:X:33:DG:H8	1.85	0.41
7:8:111:LEU:HD23	7:8:111:LEU:HA	1.95	0.41
10:C:363:PHE:CZ	10:C:367:LEU:HD11	2.55	0.41
14:Y:33:DG:H2"	14:Y:34:DA:C8	2.56	0.41
1:2:215:LEU:HD11	1:2:271:PHE:CE1	2.55	0.41
15:2:901:ADP:C8	5:6:797:VAL:HG11	2.56	0.41
3:4:186:SER:HB3	3:4:189:GLU:HB3	2.02	0.41
3:4:643:SER:HA	3:4:646:HIS:CE1	2.56	0.41
5:6:972:ARG:HH22	11:D:385:ASP:HB2	1.85	0.41
10:C:484:LYS:HD3	12:E:416:ALA:HB3	2.01	0.41
1:2:678:ASP:OD2	1:2:815:ARG:NH2	2.36	0.41
2:3:24:ARG:NH1	2:3:120:TYR:O	2.52	0.41
2:3:194:PRO:HA	2:3:252:ASP:HA	2.02	0.41
2:3:350:ILE:HG23	2:3:659:TYR:CD2	2.56	0.41
3:4:545:PHE:CE1	3:4:811:MET:HA	2.56	0.41
5:6:312:ASP:H	5:6:340:ASN:ND2	2.19	0.41
5:6:770:ARG:O	5:6:774:VAL:HG12	2.20	0.41
6:7:107:GLN:NE2	6:7:237:GLN:HB3	2.36	0.41
7:8:30:LEU:HB3	7:8:31:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:405:HIS:CD2	10:C:455:PHE:HB2	2.56	0.41
11:D:60:LEU:O	11:D:338:LYS:HD2	2.21	0.41
11:D:423:ASN:HA	11:D:426:ILE:HD12	2.03	0.41
9:B:294:PHE:O	9:B:298:LYS:HG3	2.20	0.41
11:D:396:ARG:NH2	11:D:528:GLN:O	2.53	0.41
5:6:1002:HIS:ND1	5:6:1003:PRO:HD2	2.35	0.40
8:A:822:LEU:HD11	8:A:866:TRP:CZ2	2.56	0.40
9:B:306:PHE:CD2	10:C:326:MET:HE3	2.56	0.40
10:C:260:LYS:HB3	12:E:264:PHE:CZ	2.56	0.40
10:C:531:ALA:HB1	10:C:535:ILE:HD11	2.03	0.40
1:2:506:TYR:HB2	1:2:698:PHE:CD1	2.55	0.40
3:4:422:GLU:H	3:4:422:GLU:CD	2.29	0.40
4:5:139:LEU:HD12	4:5:331:LEU:HD13	2.04	0.40
5:6:170:ILE:HD13	5:6:181:LEU:HD21	2.02	0.40
1:2:630:SER:HB3	4:5:439:THR:HA	2.04	0.40
2:3:368:ALA:HB3	2:3:378:LYS:HE2	2.02	0.40
3:4:778:ARG:HH22	5:6:717:ASP:CG	2.28	0.40
5:6:143:MET:HG2	5:6:148:LEU:HB2	2.03	0.40
2:3:169:ARG:NH2	2:3:266:PRO:HD2	2.37	0.40
3:4:281:VAL:O	3:4:285:VAL:HG12	2.21	0.40
3:4:306:TYR:HB3	3:4:465:HIS:CD2	2.57	0.40
5:6:525:ILE:HD12	5:6:526:TYR:N	2.36	0.40
6:7:88:TYR:CE2	6:7:92:LYS:HE3	2.56	0.40
11:D:519:LYS:HG2	11:D:524:TYR:CZ	2.57	0.40
1:2:275:ALA:O	1:2:279:THR:HG23	2.22	0.40
2:3:201:HIS:ND1	2:3:241:LEU:HD13	2.36	0.40
2:3:713:ALA:O	2:3:717:LEU:N	2.54	0.40
3:4:246:ARG:HB2	3:4:307:ASN:ND2	2.36	0.40
5:6:176:ARG:O	5:6:179:PRO:HD2	2.21	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	2	631/868 (73%)	618 (98%)	13 (2%)	0	100	100
2	3	575/1006 (57%)	563 (98%)	12 (2%)	0	100	100
3	4	606/933 (65%)	583 (96%)	23 (4%)	0	100	100
4	5	622/775 (80%)	615 (99%)	7 (1%)	0	100	100
5	6	659/1017 (65%)	645 (98%)	14 (2%)	0	100	100
6	7	561/845 (66%)	549 (98%)	12 (2%)	0	100	100
7	8	497/604 (82%)	480 (97%)	17 (3%)	0	100	100
8	A	407/949 (43%)	401 (98%)	6 (2%)	0	100	100
9	B	214/560 (38%)	210 (98%)	4 (2%)	0	100	100
10	C	549/616 (89%)	538 (98%)	11 (2%)	0	100	100
11	D	426/529 (80%)	419 (98%)	7 (2%)	0	100	100
12	E	412/479 (86%)	406 (98%)	6 (2%)	0	100	100
13	F	36/435 (8%)	36 (100%)	0	0	100	100
All	All	6195/9616 (64%)	6063 (98%)	132 (2%)	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	2	560/770 (73%)	560 (100%)	0	100	100
2	3	509/864 (59%)	509 (100%)	0	100	100
3	4	567/848 (67%)	567 (100%)	0	100	100
4	5	571/687 (83%)	571 (100%)	0	100	100
5	6	596/886 (67%)	595 (100%)	1 (0%)	87	86
6	7	507/753 (67%)	507 (100%)	0	100	100
7	8	459/545 (84%)	459 (100%)	0	100	100
8	A	366/842 (44%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B	208/517 (40%)	208 (100%)	0	100	100
10	C	519/576 (90%)	519 (100%)	0	100	100
11	D	400/488 (82%)	400 (100%)	0	100	100
12	E	392/440 (89%)	392 (100%)	0	100	100
13	F	36/406 (9%)	36 (100%)	0	100	100
All	All	5690/8622 (66%)	5689 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	658	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	294	HIS
1	2	780	GLN
2	3	239	ASN
2	3	670	GLN
2	3	673	GLN
2	3	677	ASN
3	4	242	ASN
3	4	259	HIS
3	4	263	ASN
3	4	274	GLN
3	4	912	GLN
4	5	96	GLN
4	5	185	ASN
4	5	587	GLN
4	5	758	HIS
5	6	340	ASN
5	6	458	HIS
5	6	633	ASN
5	6	669	HIS
6	7	107	GLN
6	7	336	ASN
7	8	50	ASN
7	8	281	HIS
8	A	815	ASN

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Mol	Chain	Res	Type
9	B	425	HIS
9	B	426	ASN
9	B	435	ASN
10	C	22	HIS
10	C	38	HIS
10	C	71	GLN
10	C	271	ASN
10	C	312	HIS
11	D	277	GLN
11	D	304	GLN
11	D	491	GLN
12	E	248	HIS
13	F	407	GLN

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 11 ligands modelled in this entry, 5 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	$\# Z > 2$
17	ATP	D	601	-	32,33,33	0.32	0	48,52,52	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	ADP	6	1101	-	28,29,29	1.41	4 (14%)	43,45,45	1.88	9 (20%)
17	ATP	E	501	-	32,33,33	0.41	0	48,52,52	0.34	0
15	ADP	5	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
15	ADP	2	901	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	8 (18%)
15	ADP	4	1001	-	28,29,29	1.43	5 (17%)	43,45,45	1.81	9 (20%)

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
17	ATP	D	601	-	-	5/22/38/38	0/3/3/3
15	ADP	6	1101	-	-	2/16/32/32	0/3/3/3
17	ATP	E	501	-	-	5/22/38/38	0/3/3/3
15	ADP	5	901	-	-	1/16/32/32	0/3/3/3
15	ADP	2	901	-	-	4/16/32/32	0/3/3/3
15	ADP	4	1001	-	-	2/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5	901	ADP	C5-C4	4.72	1.47	1.39
15	6	1101	ADP	C5-C4	4.70	1.47	1.39
15	4	1001	ADP	C5-C4	4.70	1.47	1.39
15	2	901	ADP	C5-C4	4.65	1.47	1.39
15	4	1001	ADP	C5-C6	2.76	1.48	1.41
15	5	901	ADP	C5-C6	2.74	1.48	1.41
15	6	1101	ADP	C5-C6	2.74	1.48	1.41
15	2	901	ADP	C5-C6	2.61	1.48	1.41
15	2	901	ADP	C5-N7	-2.37	1.34	1.39
15	5	901	ADP	C8-N7	2.33	1.36	1.31
15	4	1001	ADP	C8-N7	2.31	1.36	1.31
15	5	901	ADP	C5-N7	-2.31	1.34	1.39
15	6	1101	ADP	C8-N7	2.29	1.36	1.31
15	4	1001	ADP	C5-N7	-2.27	1.34	1.39
15	6	1101	ADP	C5-N7	-2.27	1.34	1.39
15	2	901	ADP	C8-N7	2.25	1.36	1.31
15	4	1001	ADP	PA-O3A	2.15	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	901	ADP	C5-C4-N3	-6.23	118.14	126.72
15	6	1101	ADP	C5-C4-N3	-6.03	118.41	126.72
15	4	1001	ADP	C5-C4-N3	-5.92	118.57	126.72
15	2	901	ADP	C5-C4-N3	-5.86	118.65	126.72
15	5	901	ADP	N3-C4-N9	4.88	135.46	127.17
15	2	901	ADP	N3-C4-N9	4.82	135.37	127.17
15	6	1101	ADP	N3-C4-N9	4.72	135.19	127.17
15	4	1001	ADP	N3-C4-N9	4.66	135.09	127.17
15	5	901	ADP	C2-N3-C4	3.84	121.21	111.83
15	6	1101	ADP	C2-N3-C4	3.73	120.95	111.83
15	4	1001	ADP	C2-N3-C4	3.71	120.90	111.83
15	2	901	ADP	C2-N3-C4	3.61	120.65	111.83
15	6	1101	ADP	C4-C5-N7	-3.56	106.52	110.58
15	5	901	ADP	C4-C5-N7	-3.53	106.55	110.58
15	4	1001	ADP	C4-C5-N7	-3.46	106.63	110.58
15	5	901	ADP	N3-C2-N1	-3.19	123.75	128.58
15	4	1001	ADP	N3-C2-N1	-3.15	123.81	128.58
15	6	1101	ADP	N3-C2-N1	-3.12	123.86	128.58
15	2	901	ADP	C4-C5-N7	-3.08	107.06	110.58
15	2	901	ADP	N3-C2-N1	-3.06	123.95	128.58
15	6	1101	ADP	C3'-C2'-C1'	2.73	106.62	101.46
15	2	901	ADP	C4-N9-C8	2.67	108.54	105.74
15	6	1101	ADP	C5-N7-C8	2.62	107.56	103.45
15	2	901	ADP	C3'-C2'-C1'	2.58	106.34	101.46
15	4	1001	ADP	C4-N9-C8	2.55	108.42	105.74
15	5	901	ADP	C5-N7-C8	2.55	107.46	103.45
15	4	1001	ADP	C5-N7-C8	2.50	107.38	103.45
15	6	1101	ADP	C4-N9-C8	2.45	108.31	105.74
15	5	901	ADP	C4-N9-C8	2.40	108.26	105.74
15	2	901	ADP	C5-N7-C8	2.32	107.10	103.45
15	5	901	ADP	C3'-C2'-C1'	2.24	105.71	101.46
15	4	1001	ADP	C3'-C2'-C1'	2.10	105.44	101.46
15	6	1101	ADP	C6-C5-N7	2.02	135.98	132.09
15	4	1001	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	2	901	ADP	C5'-O5'-PA-O2A
15	2	901	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	5	901	ADP	C5'-O5'-PA-O1A
15	6	1101	ADP	C5'-O5'-PA-O2A
15	6	1101	ADP	C5'-O5'-PA-O3A
17	D	601	ATP	PB-O3B-PG-O2G
17	D	601	ATP	C5'-O5'-PA-O2A
17	D	601	ATP	C5'-O5'-PA-O3A
17	E	501	ATP	C5'-O5'-PA-O1A
17	E	501	ATP	C5'-O5'-PA-O2A
17	E	501	ATP	C5'-O5'-PA-O3A
17	D	601	ATP	C4'-C5'-O5'-PA
15	4	1001	ADP	C3'-C4'-C5'-O5'
15	4	1001	ADP	O4'-C4'-C5'-O5'
15	2	901	ADP	C5'-O5'-PA-O1A
17	E	501	ATP	O4'-C4'-C5'-O5'
17	E	501	ATP	C4'-C5'-O5'-PA
15	2	901	ADP	PA-O3A-PB-O3B
17	D	601	ATP	PB-O3B-PG-O3G

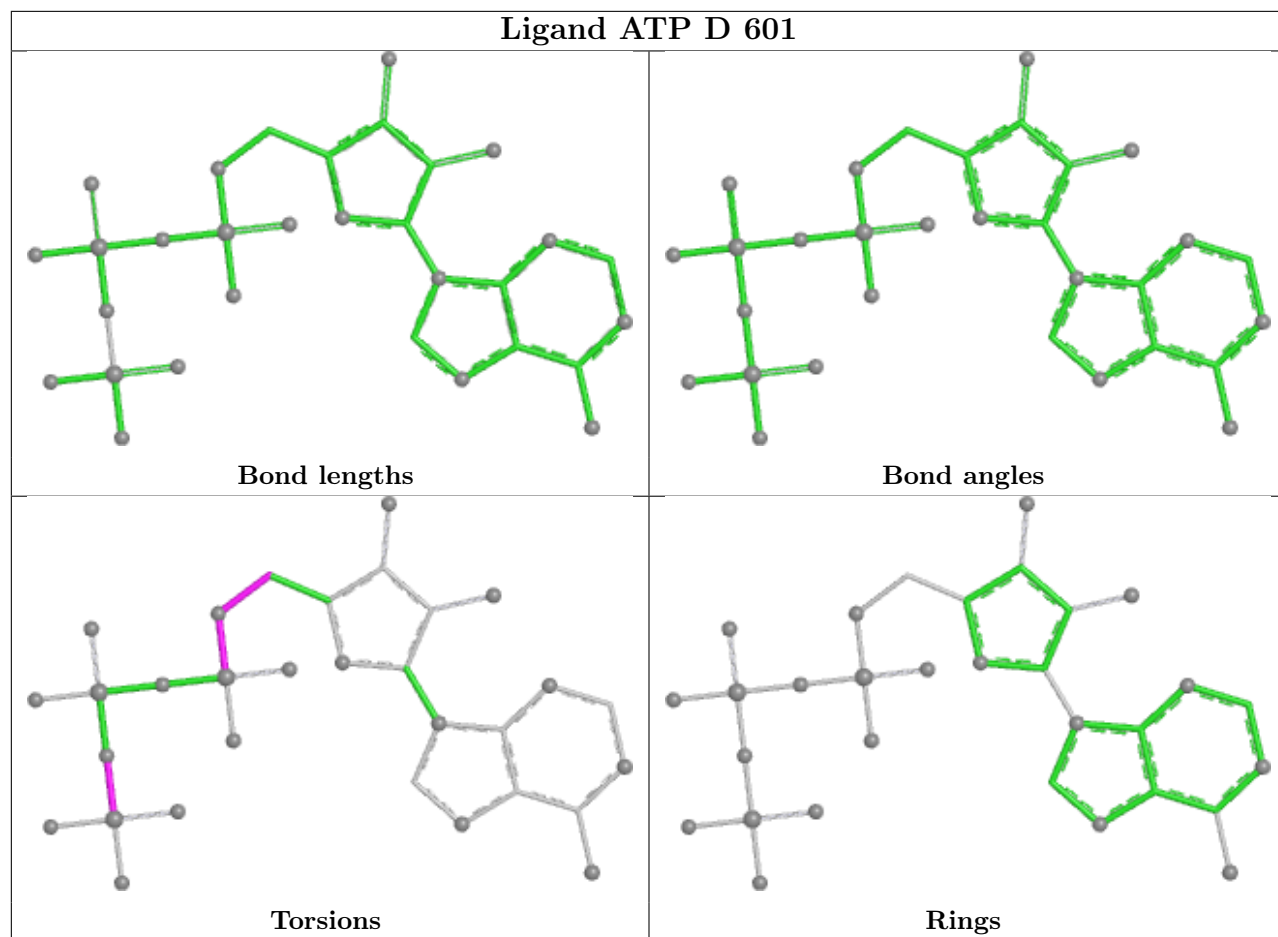
There are no ring outliers.

5 monomers are involved in 7 short contacts:

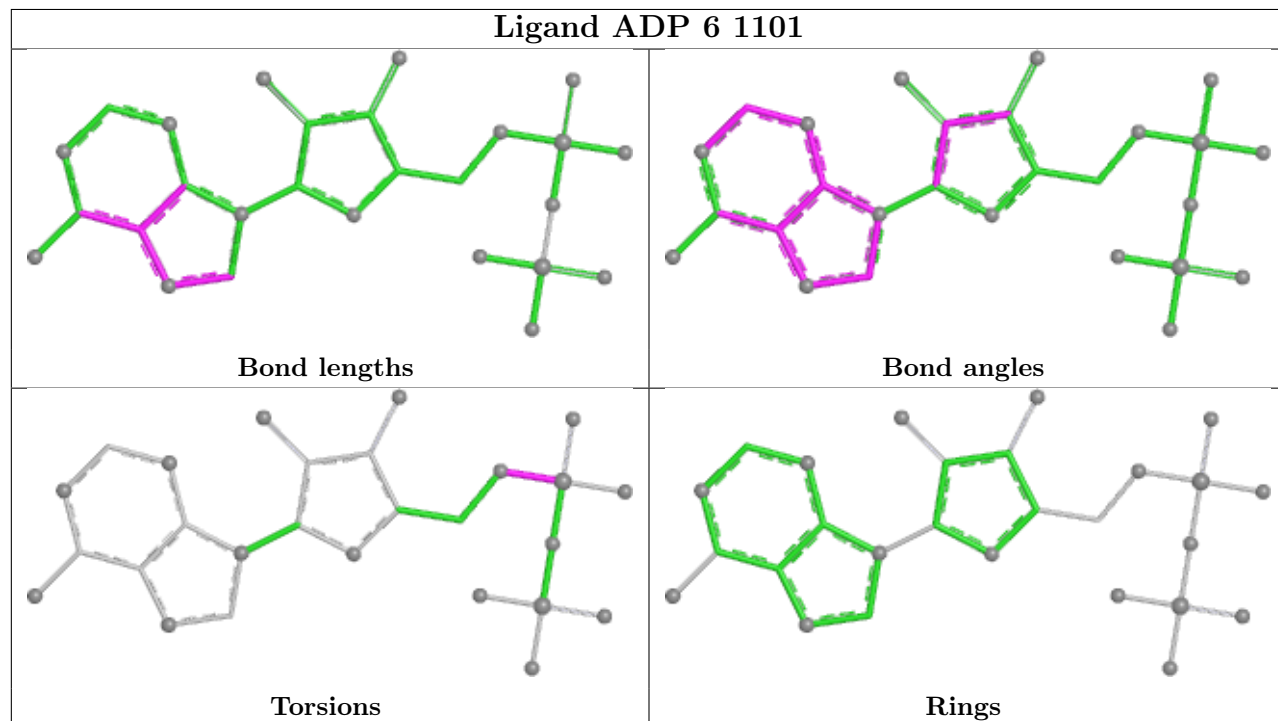
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	601	ATP	1	0
15	6	1101	ADP	1	0
15	5	901	ADP	2	0
15	2	901	ADP	2	0
15	4	1001	ADP	1	0

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.

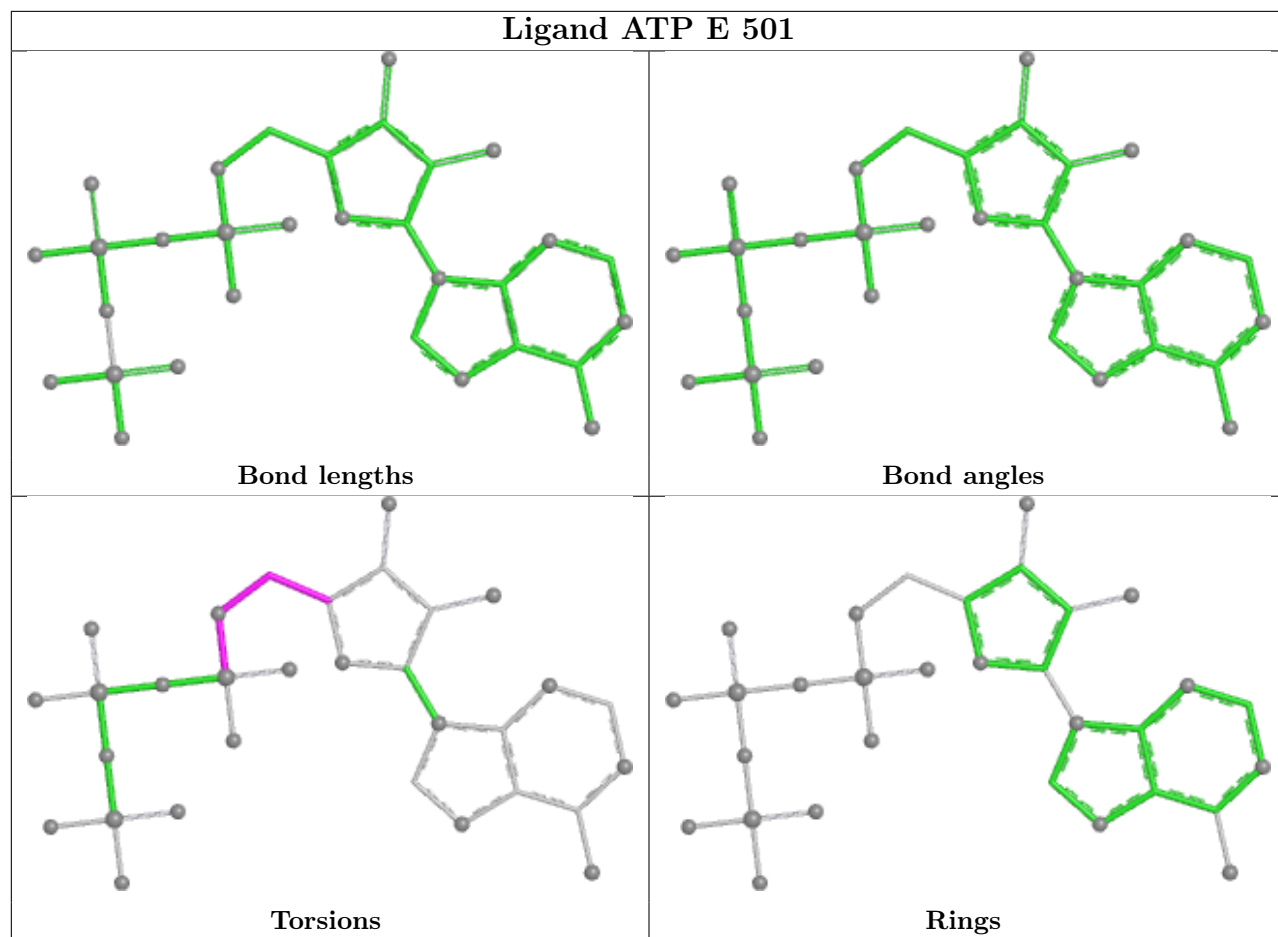
Ligand ATP D 601



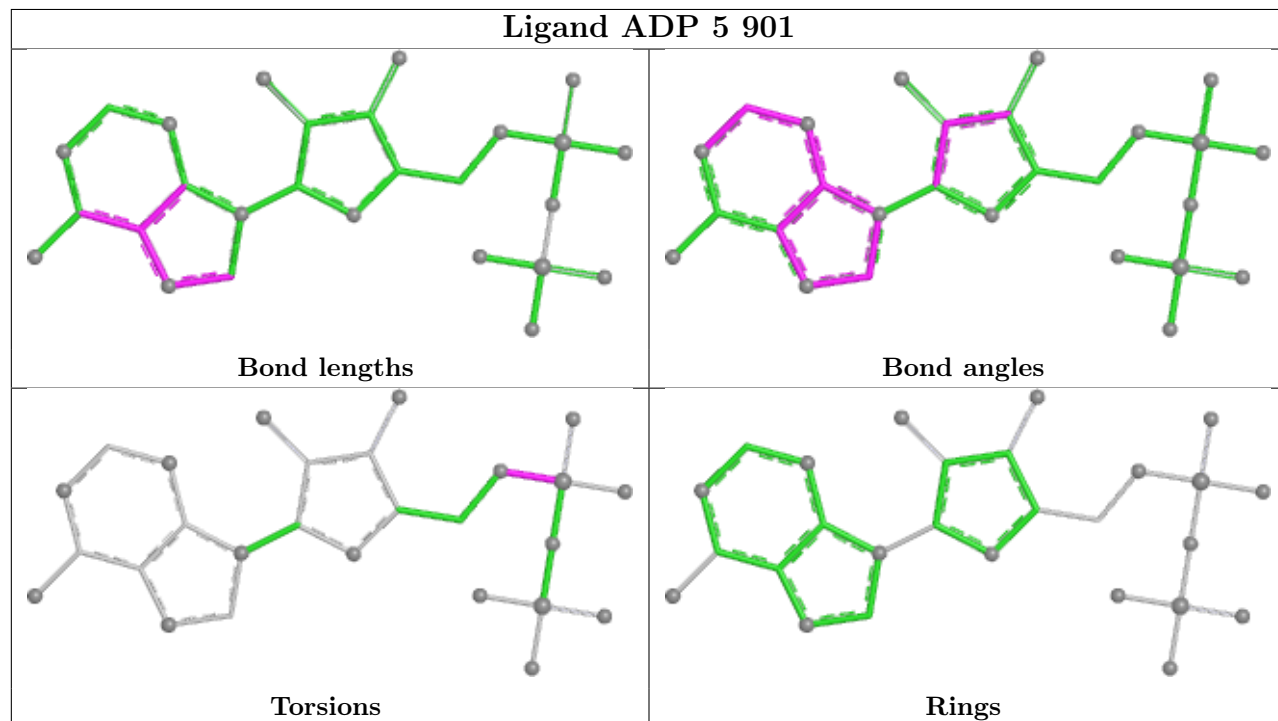
Ligand ADP 6 1101

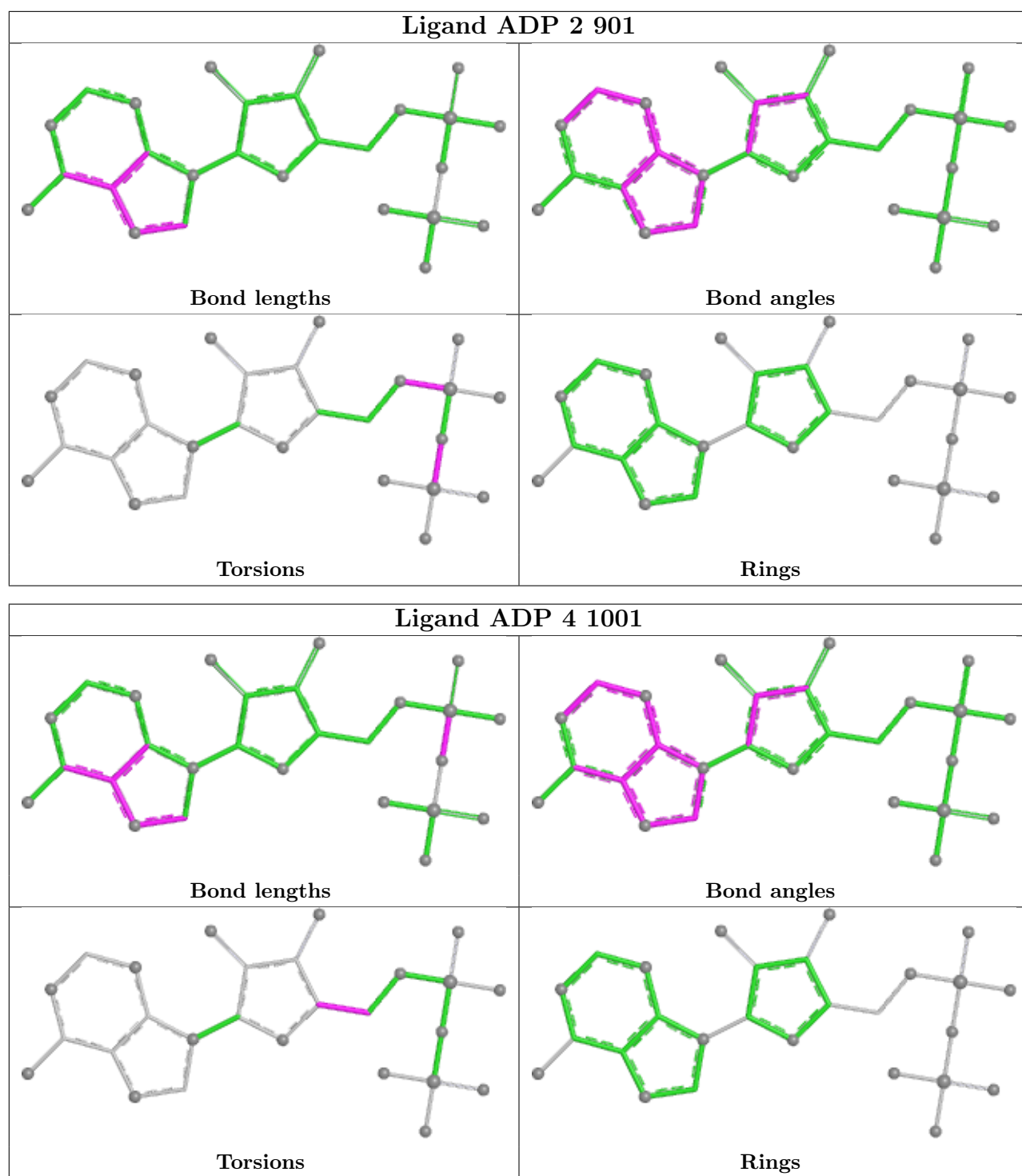


Ligand ATP E 501



Ligand ADP 5 901





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.

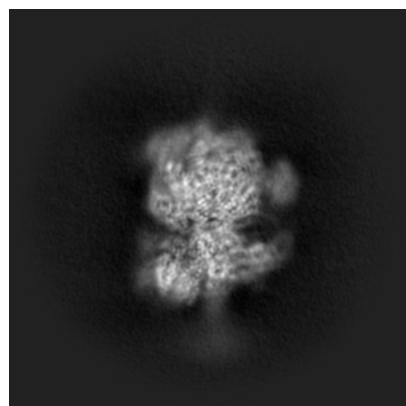
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51441. These allow visual inspection of the internal detail of the map and identification of artifacts.

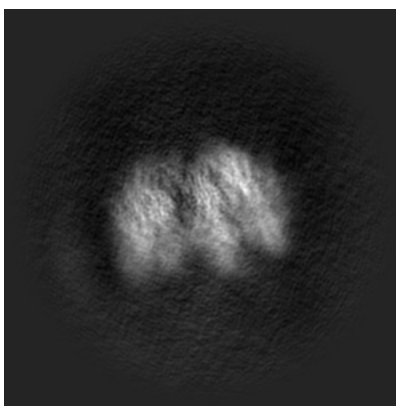
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

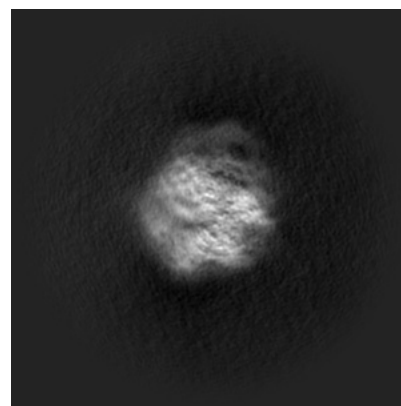
6.1.1 Primary map



X

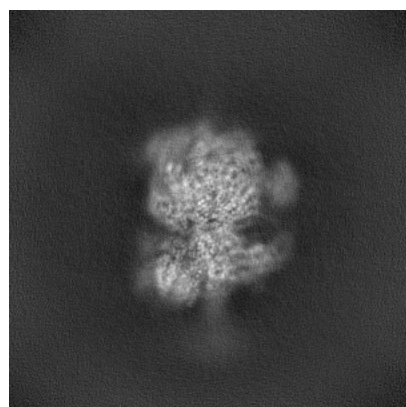


Y

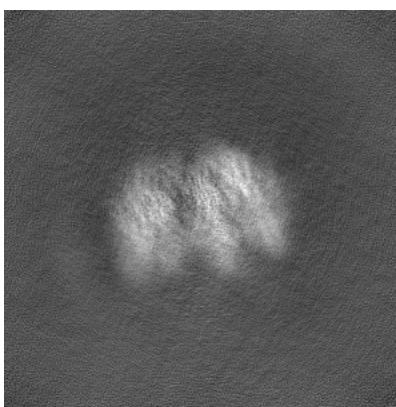


Z

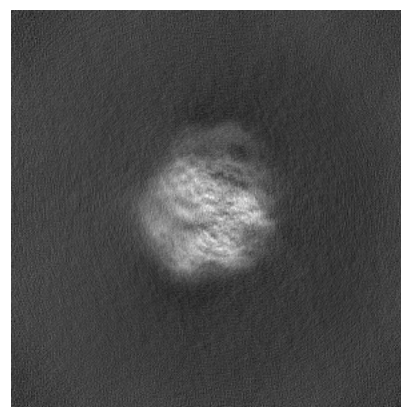
6.1.2 Raw map



X



Y

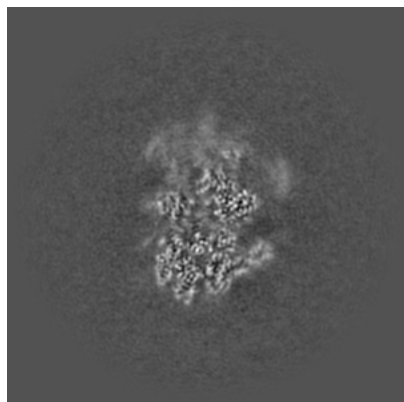


Z

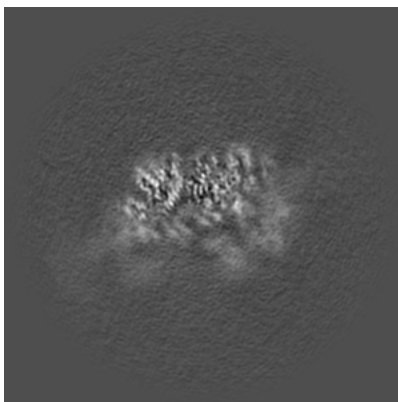
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

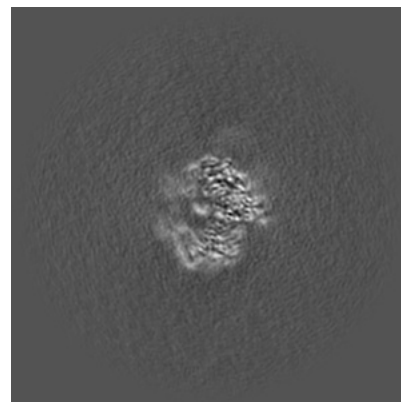
6.2.1 Primary map



X Index: 220

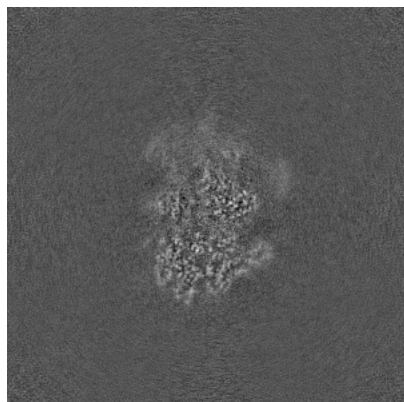


Y Index: 220

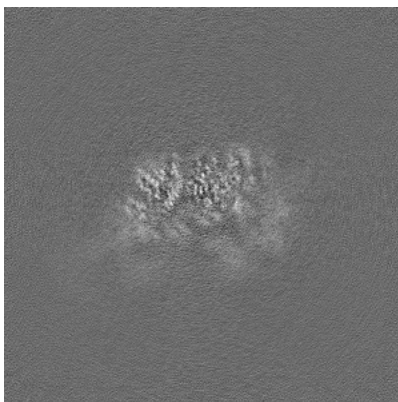


Z Index: 220

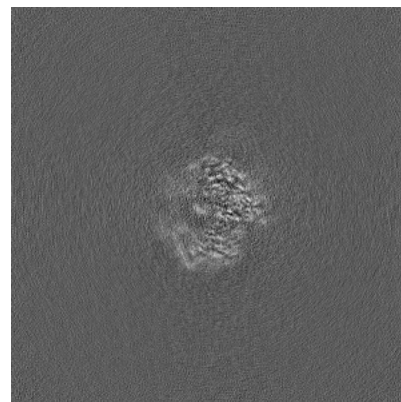
6.2.2 Raw map



X Index: 220



Y Index: 220

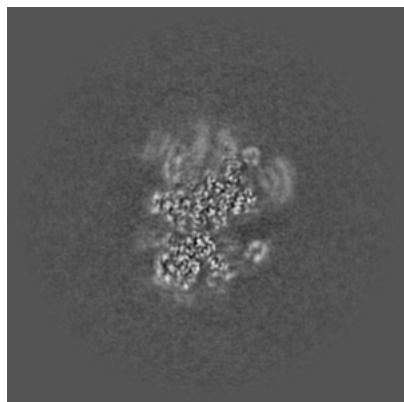


Z Index: 220

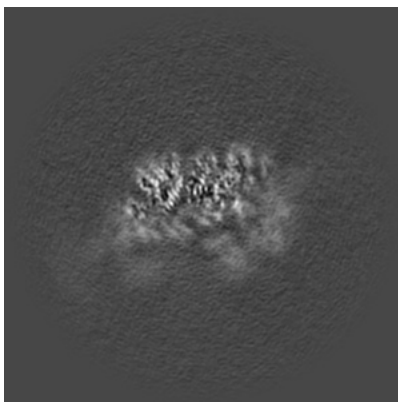
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

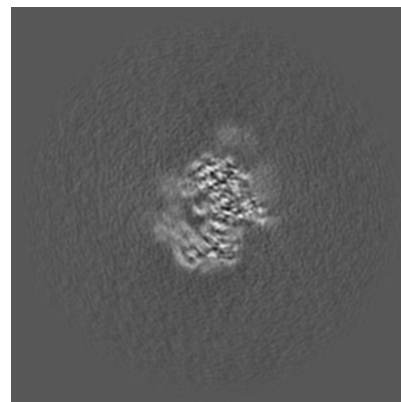
6.3.1 Primary map



X Index: 230

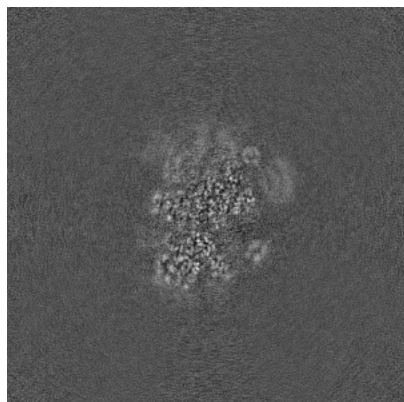


Y Index: 219

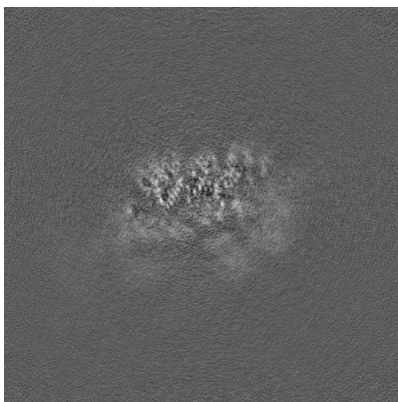


Z Index: 224

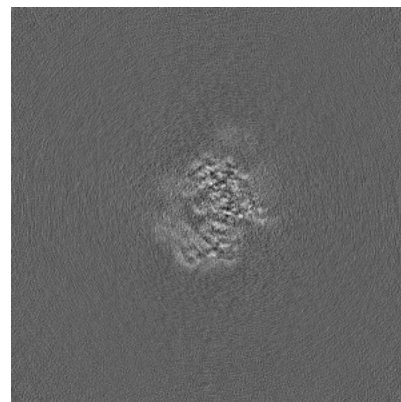
6.3.2 Raw map



X Index: 231



Y Index: 218

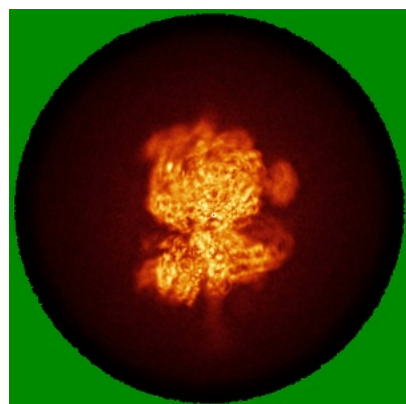


Z Index: 224

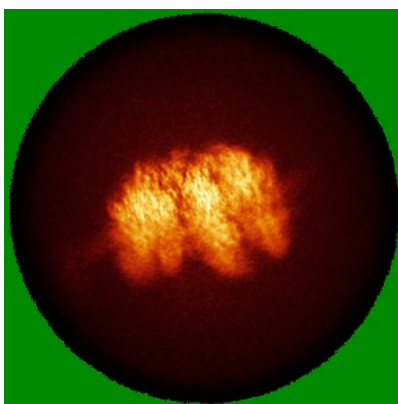
The images above show the largest variance slices of the map in three orthogonal directions.

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

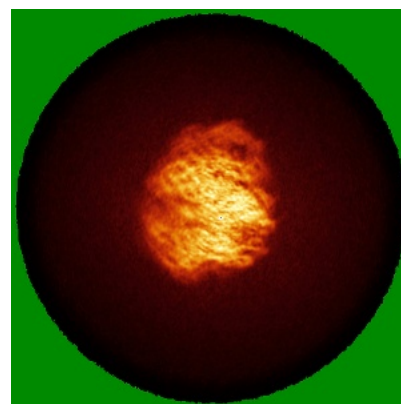
6.4.1 Primary map



X

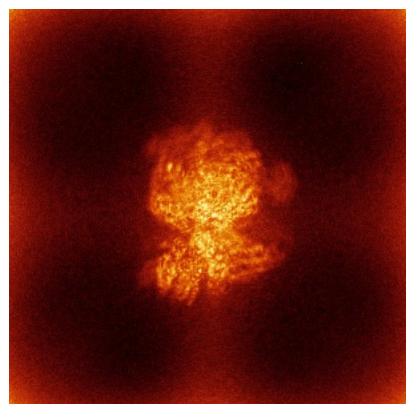


Y

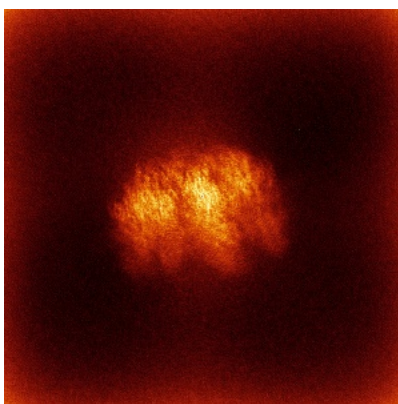


Z

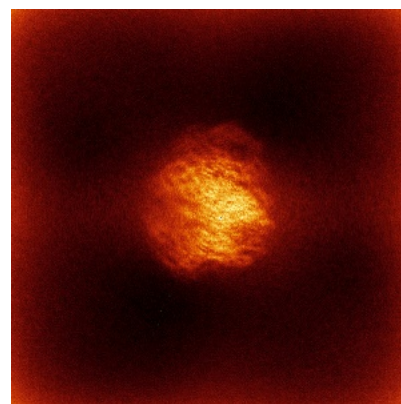
6.4.2 Raw map



X



Y

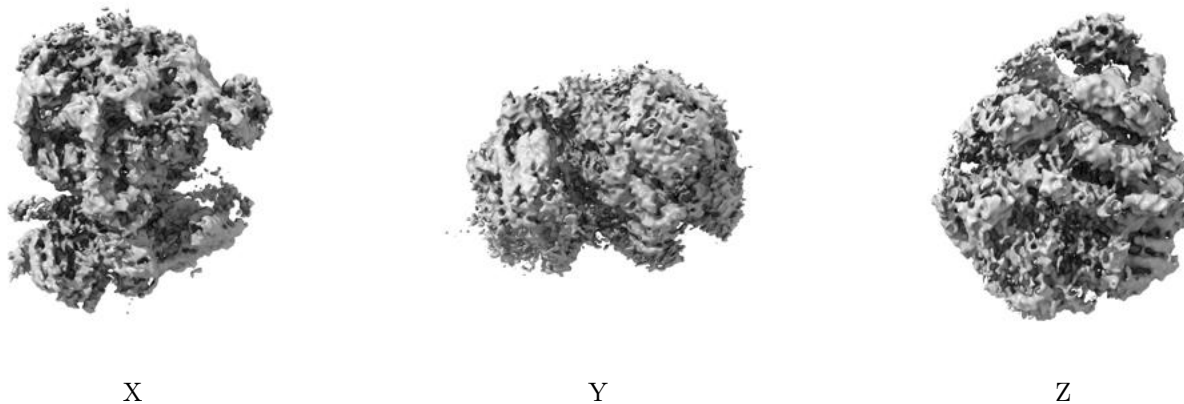


Z

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.

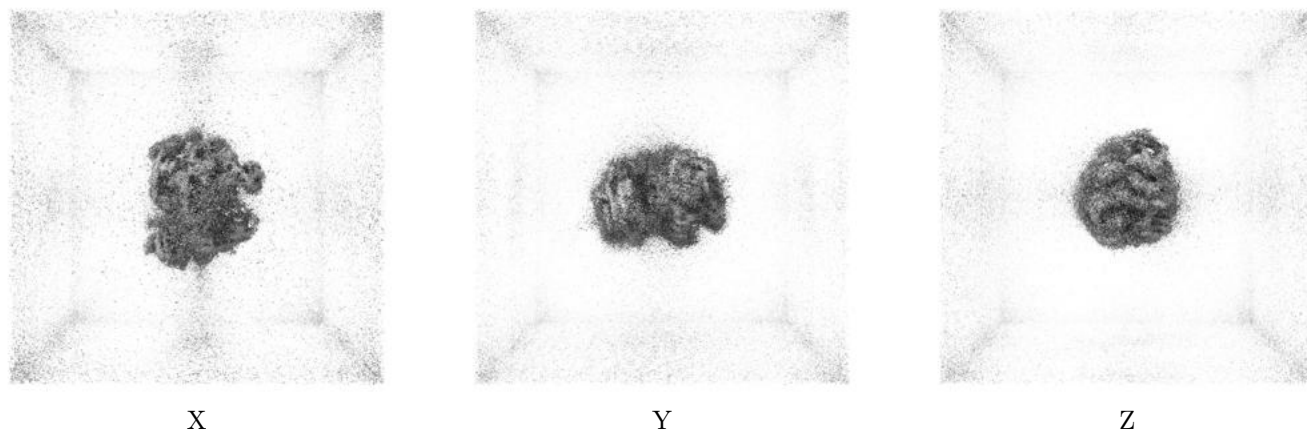
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

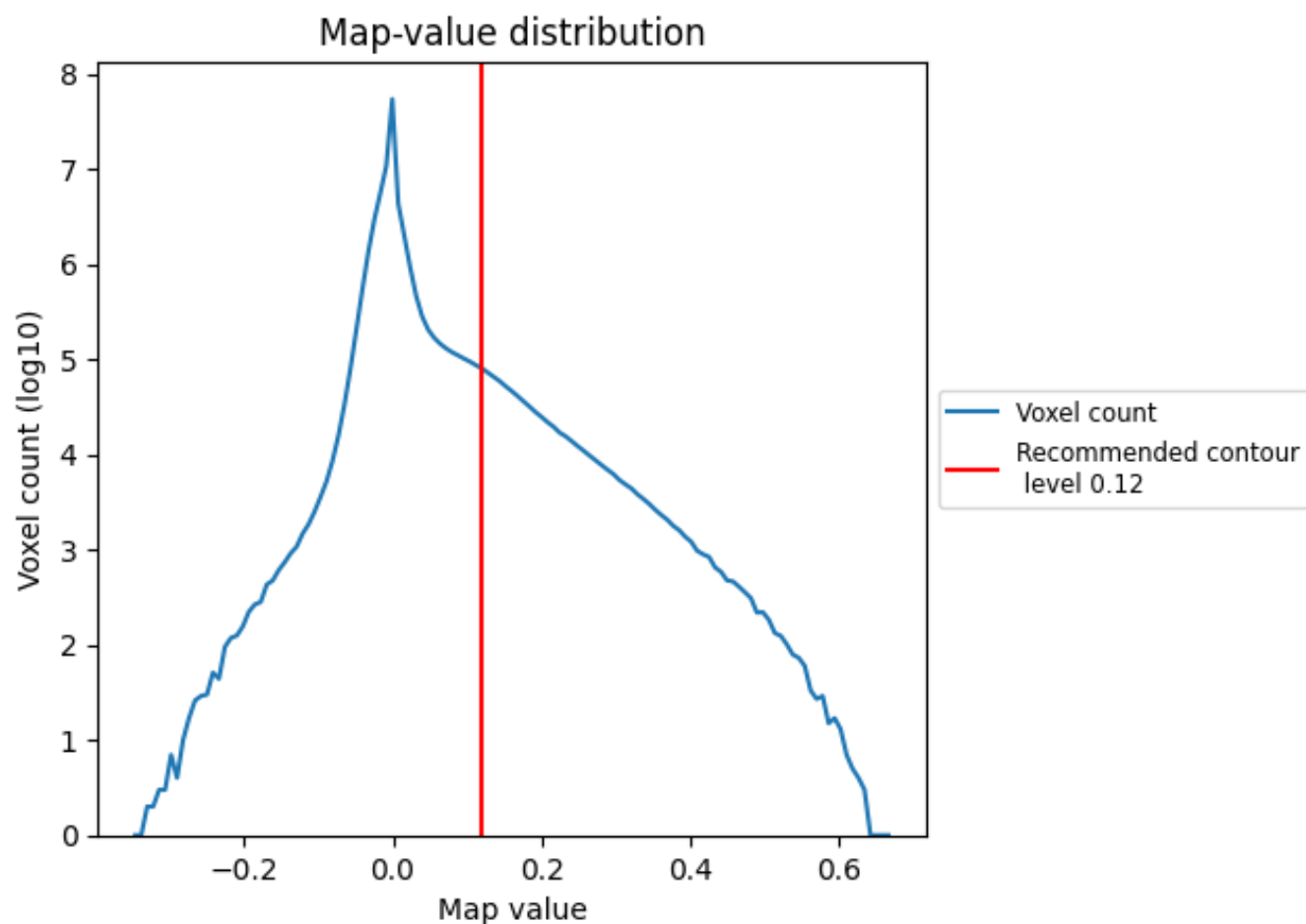
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

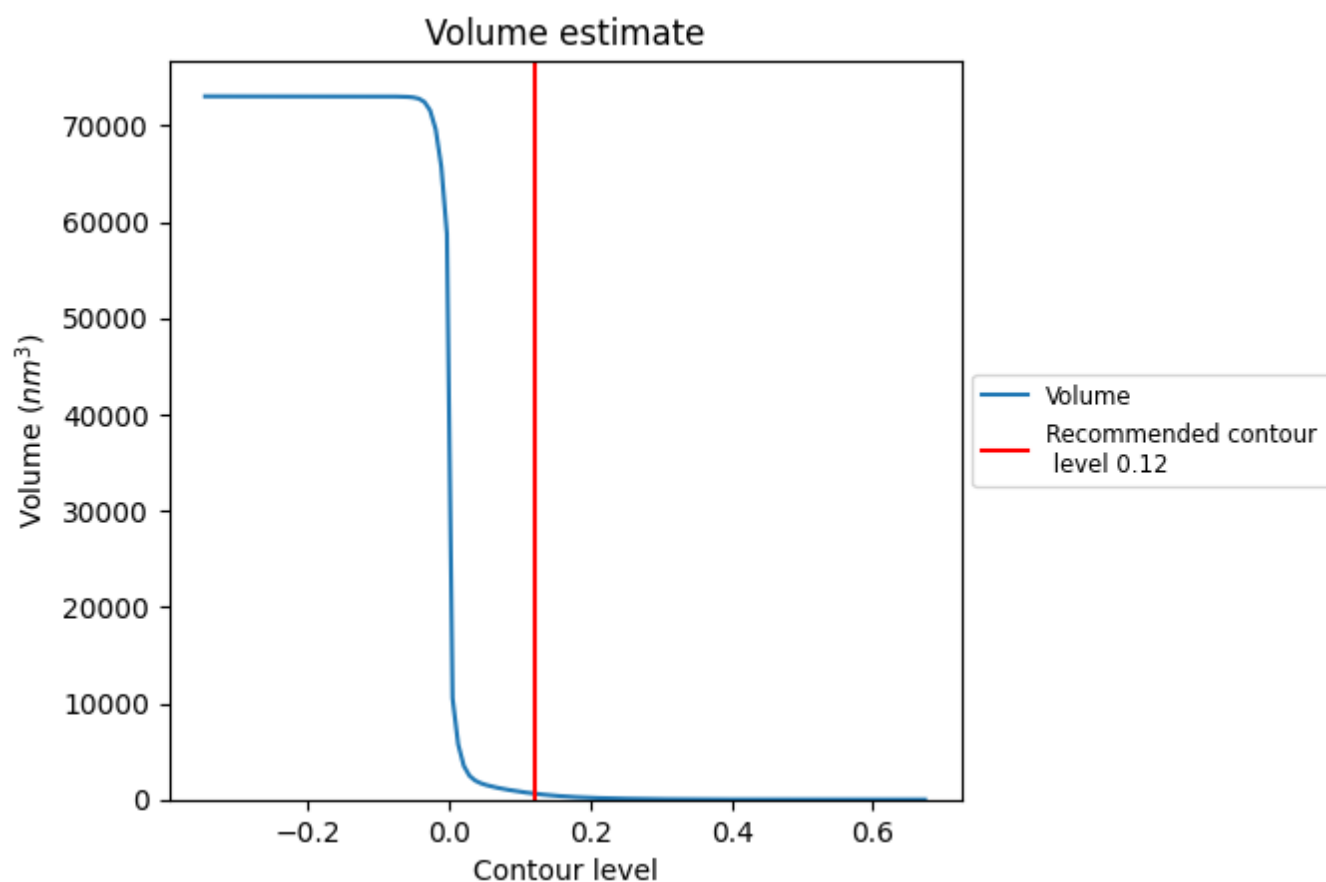
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

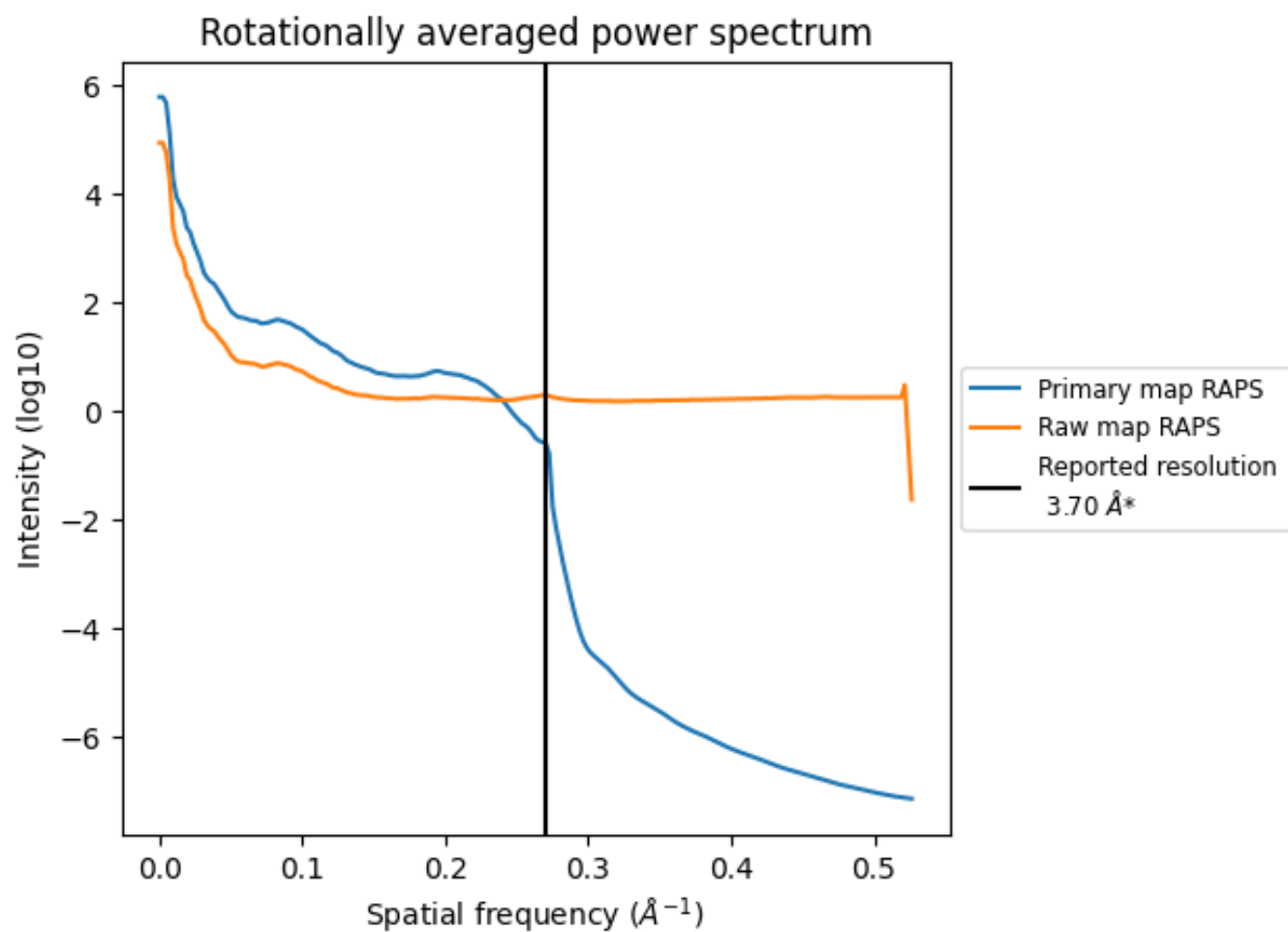
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 624 nm^3 ; this corresponds to an approximate mass of 564 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 ⓘ

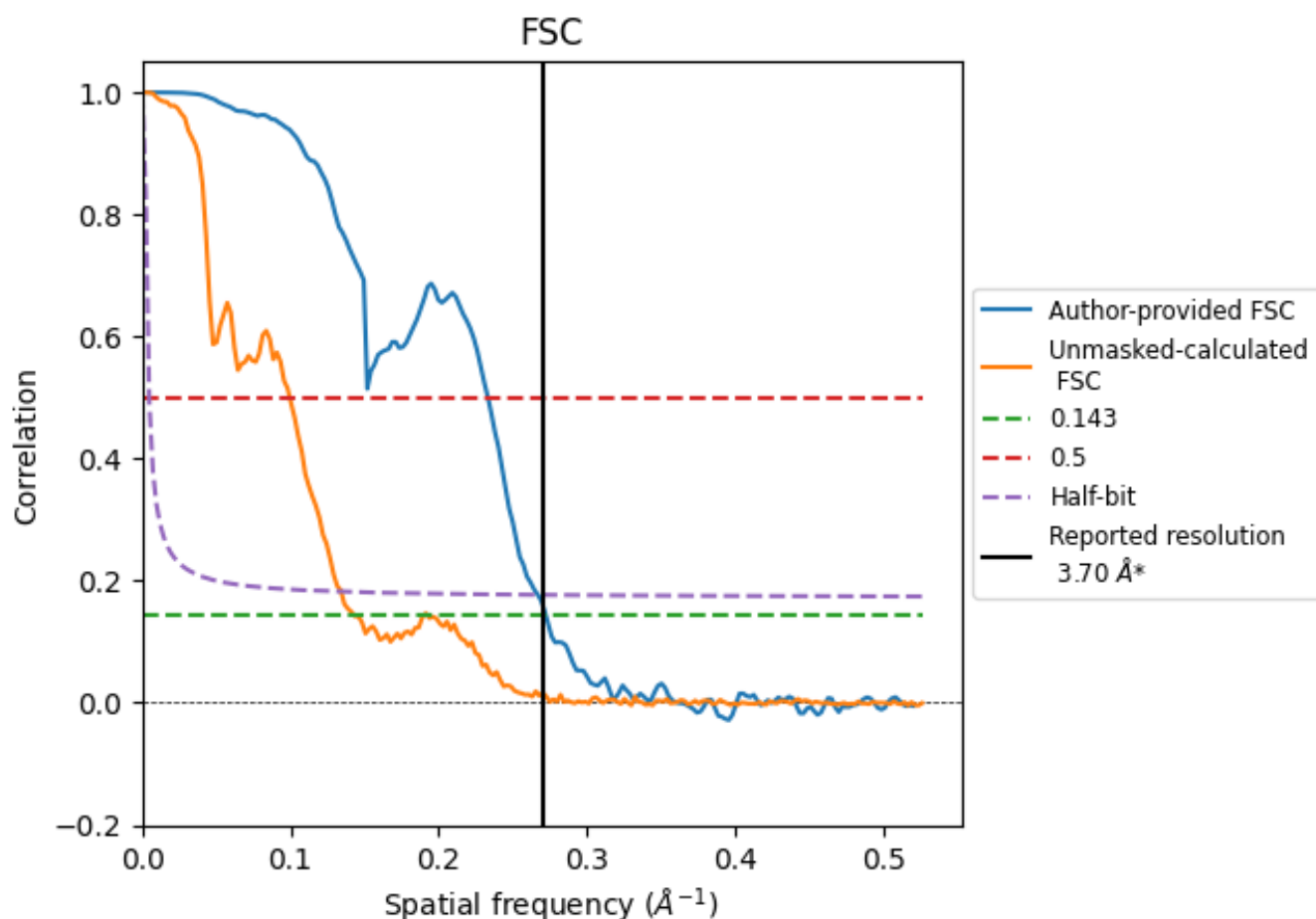


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

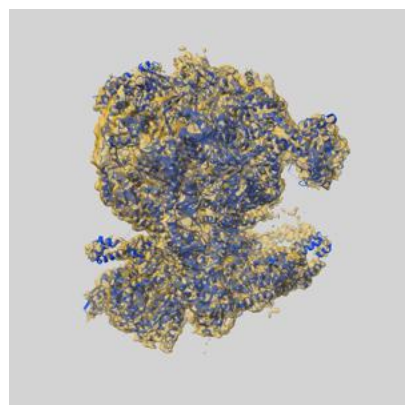
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.29	3.75
Unmasked-calculated*	6.99	10.05	7.45

*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 6.99 differs from the reported value 3.7 by more than 10 %

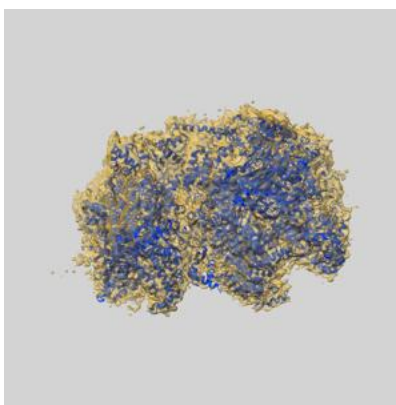
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51441 and PDB model 9GM5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

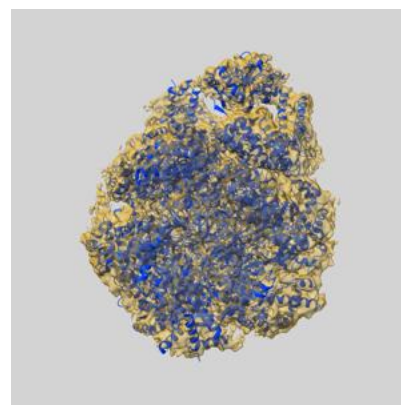
9.1 Map-model overlay [i](#)



X



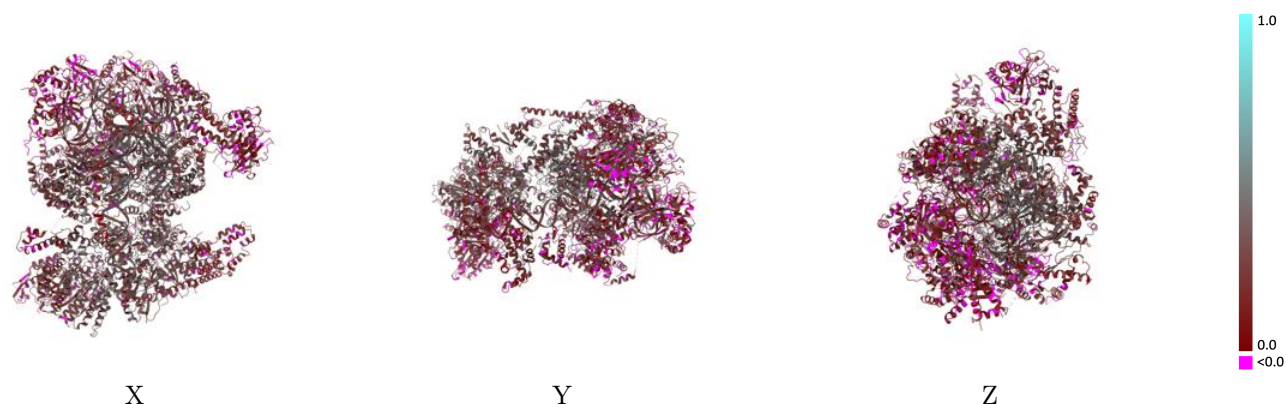
Y



Z

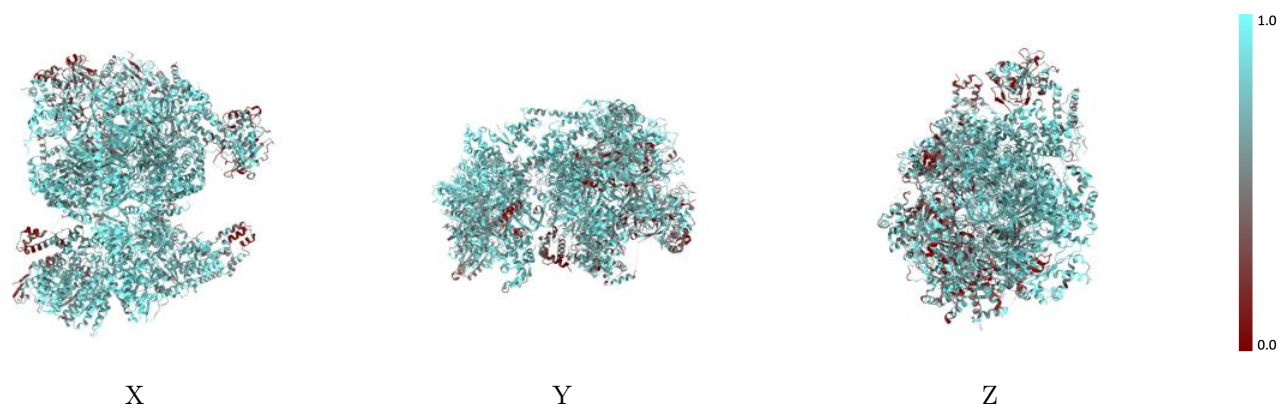
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



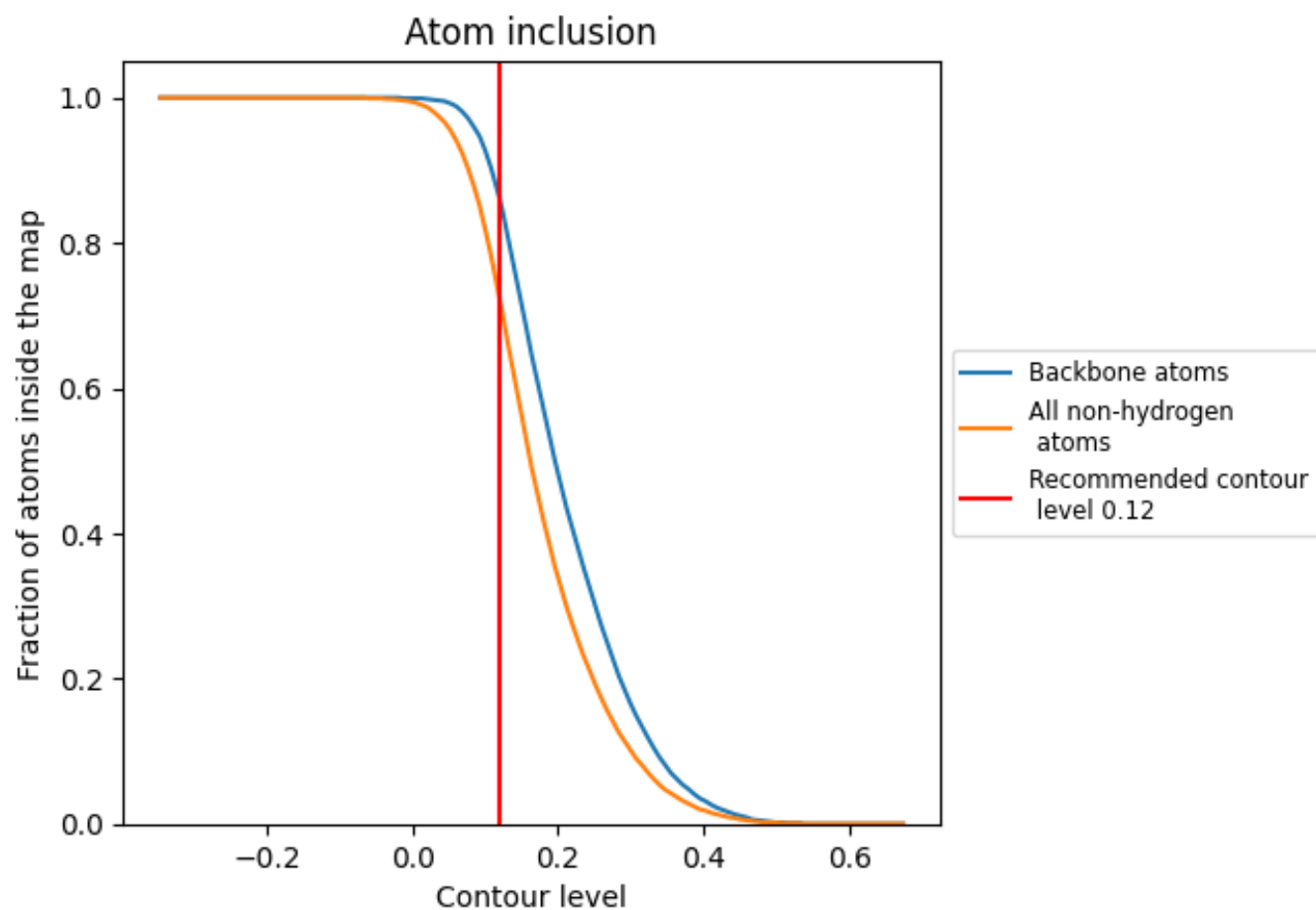
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.2350
2	0.8080	0.3360
3	0.5370	0.1140
4	0.7560	0.2500
5	0.6780	0.1960
6	0.8340	0.3300
7	0.6390	0.1400
8	0.6300	0.1750
A	0.5940	0.1630
B	0.7810	0.2170
C	0.7510	0.2400
D	0.7920	0.2900
E	0.8370	0.3410
F	0.4790	0.1200
X	0.8790	0.2520
Y	0.8910	0.2670

1.0

0.0

<0.0