



Full wwPDB EM Validation Report ⓘ

Feb 27, 2025 – 06:27 pm GMT

PDB ID : 9GJP
EMDB ID : EMD-51401
Title : OCCM maturation intermediate stalled with an Arginine Finger mutation in Mcm5: Conformer 2
Authors : Butryn, A.; Costa, A.
Deposited on : 2024-08-22
Resolution : 3.40 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.dev117
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) : 2.41

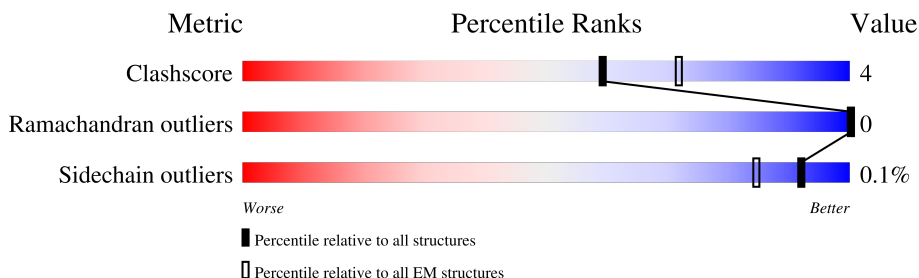
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	2	868	
2	3	1006	
3	4	933	
4	5	775	
5	6	1017	
6	7	845	
7	8	604	
8	A	949	

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Mol	Chain	Length	Quality of chain
9	B	620	
10	C	616	
11	D	529	
12	E	479	
13	F	435	
14	X	42	
14	Y	42	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50292 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	120	Total	C	N	O	S	0	0
			961	613	161	180	7		

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		

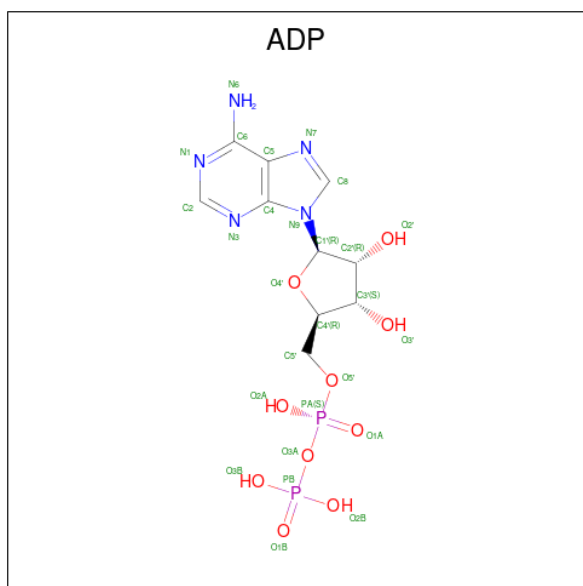
- Molecule 13 is a protein called Origin recognition complex subunit 6.

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 (42-MER).

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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

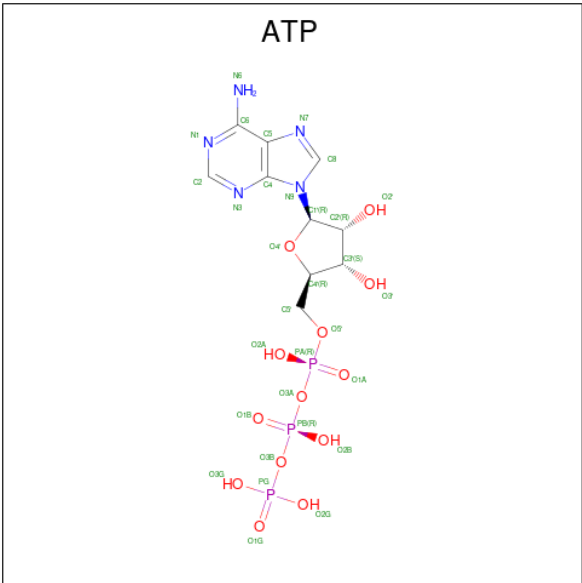
Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Zn	0
			1	1	
16	4	1	Total	Zn	0
			1	1	

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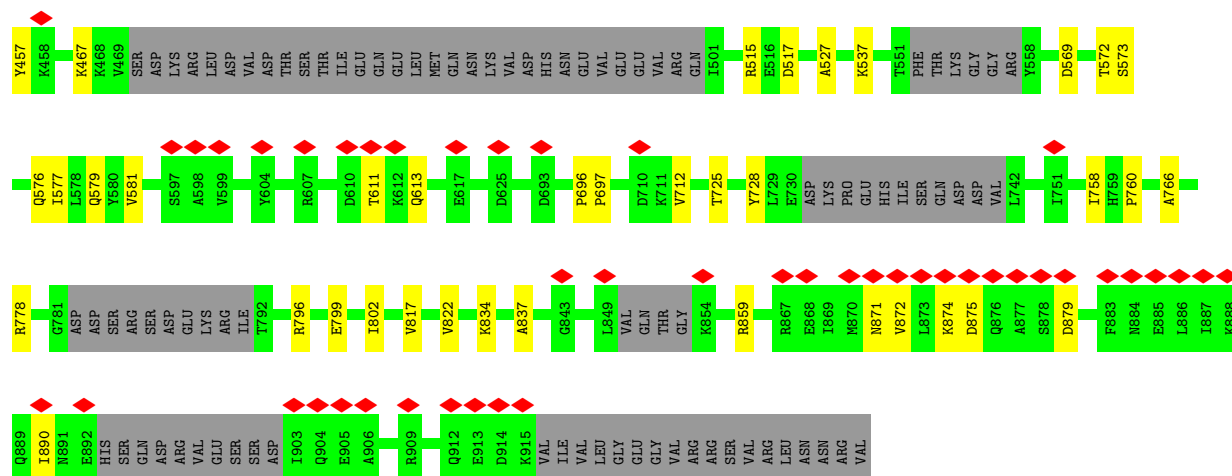
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Mol	Chain	Residues	Atoms		AltConf
16	5	1	Total	Zn	0
			1	1	
16	6	1	Total	Zn	0
			1	1	
16	7	1	Total	Zn	0
			1	1	

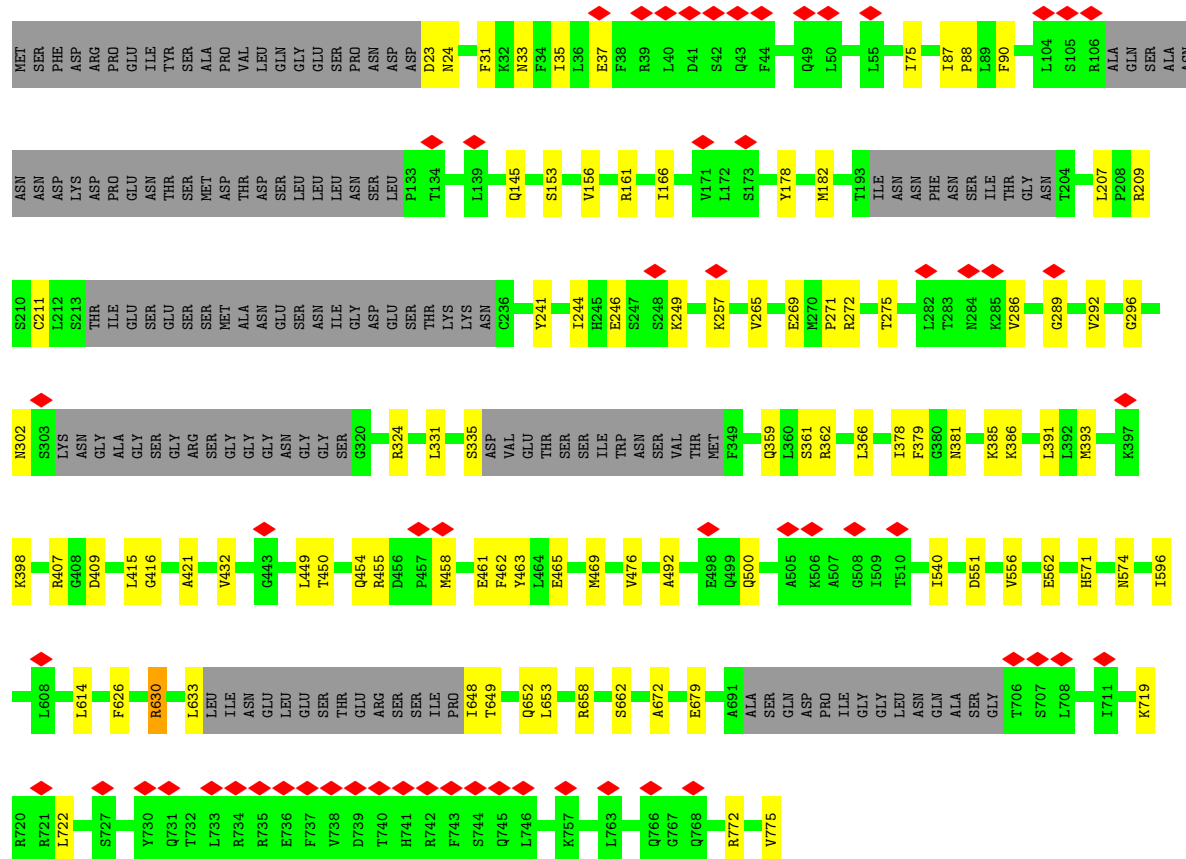
- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



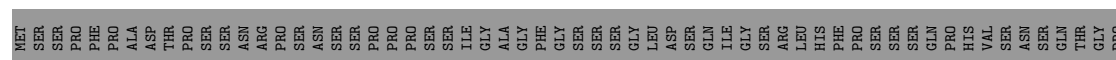
Mol	Chain	Residues	Atoms					AltConf
17	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	E	1	Total	C	N	O	P	0
			31	10	5	13	3	



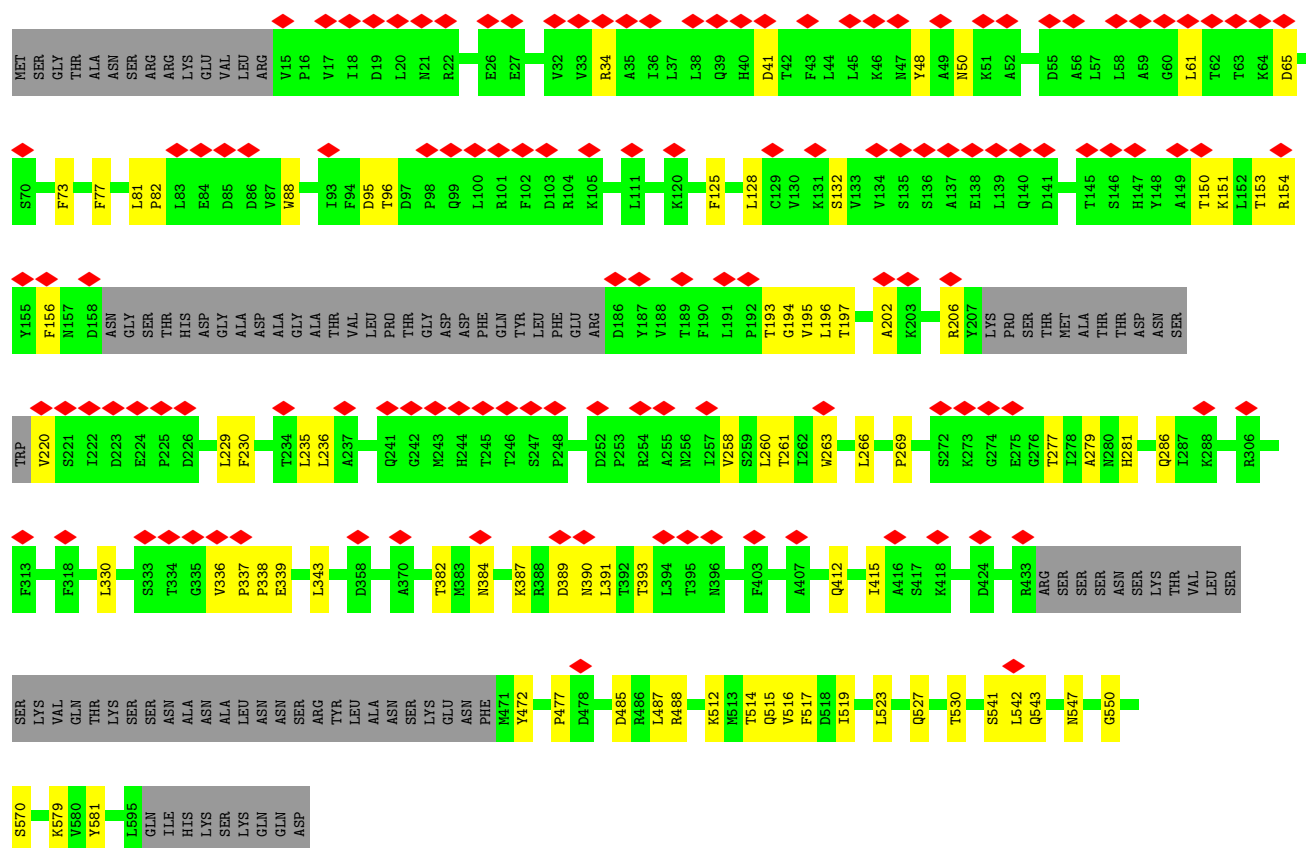
• Molecule 4: Minichromosome maintenance protein 5



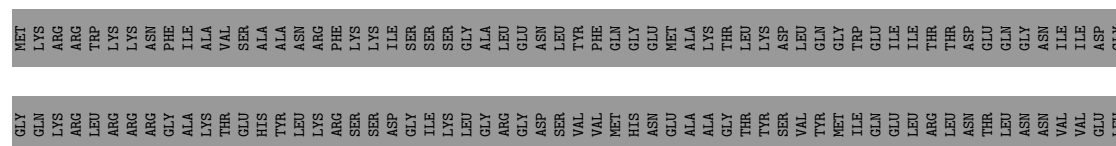
• Molecule 5: DNA replication licensing factor MCM6



- Molecule 7: Cell division cycle protein CDT1



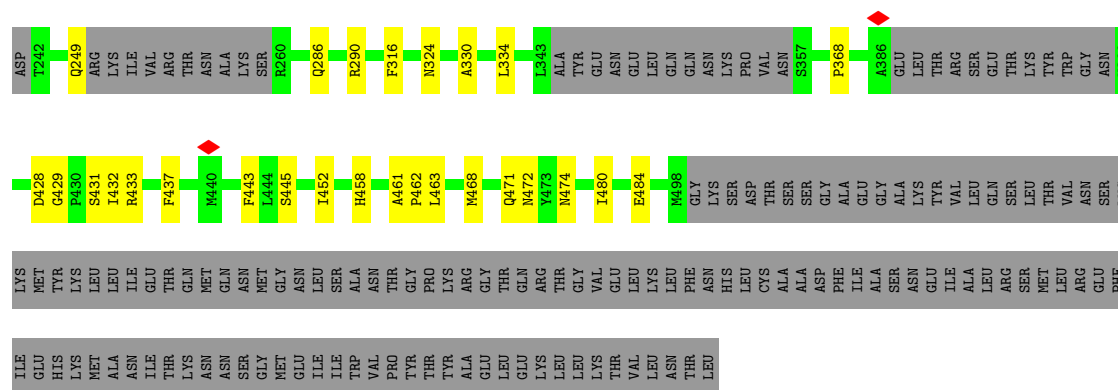
- Molecule 8: Origin recognition complex subunit 1



Residue Class	Number of amino acids
G853	1
N856	2
R888	1
E900	1
M905	1
N906	2
E907	2
ASP	0
GLU	0
THR	0
LEU	0
ARG	0
ASN	0
LEU	0

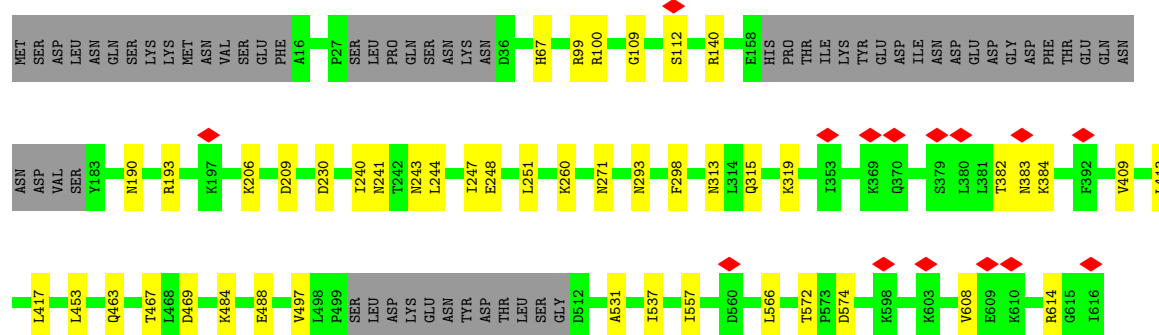
Chain B: 31% 1% 64%

[illegible]



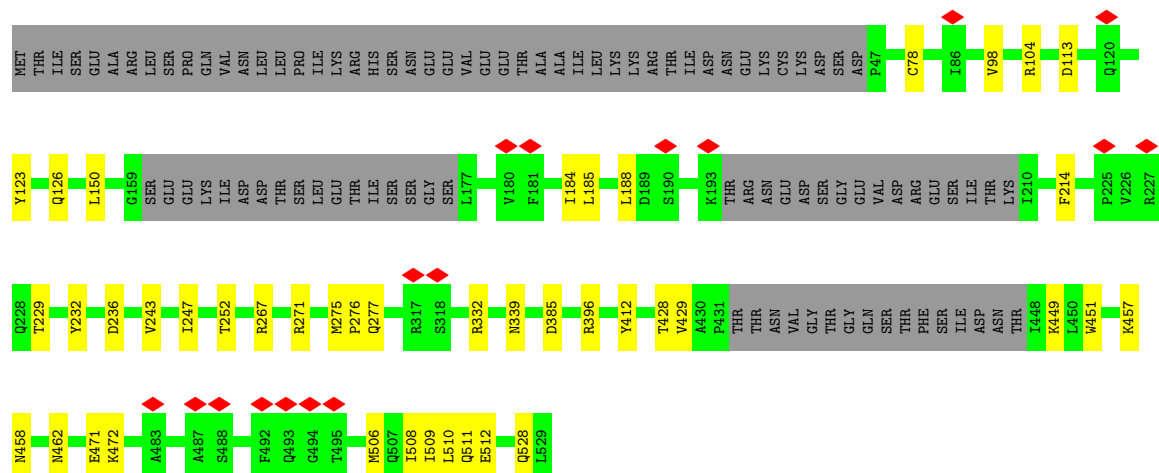
• Molecule 10: Origin recognition complex subunit 3

Chain C: 83% 7% 10%



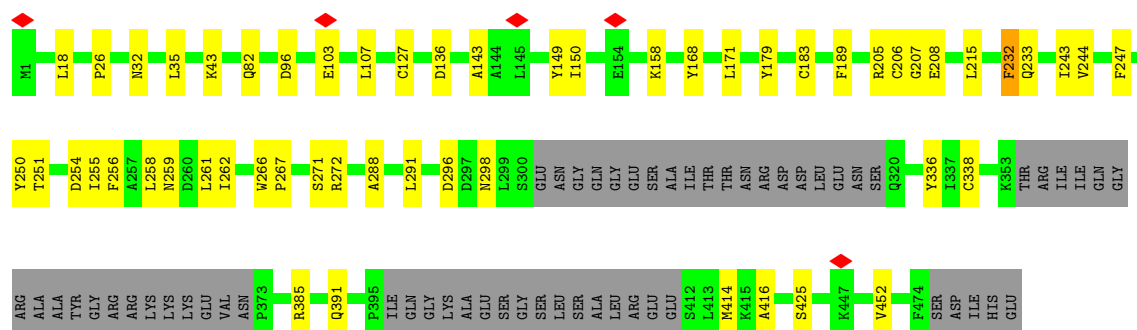
• Molecule 11: Origin recognition complex subunit 4

Chain D: 74% 8% 18%



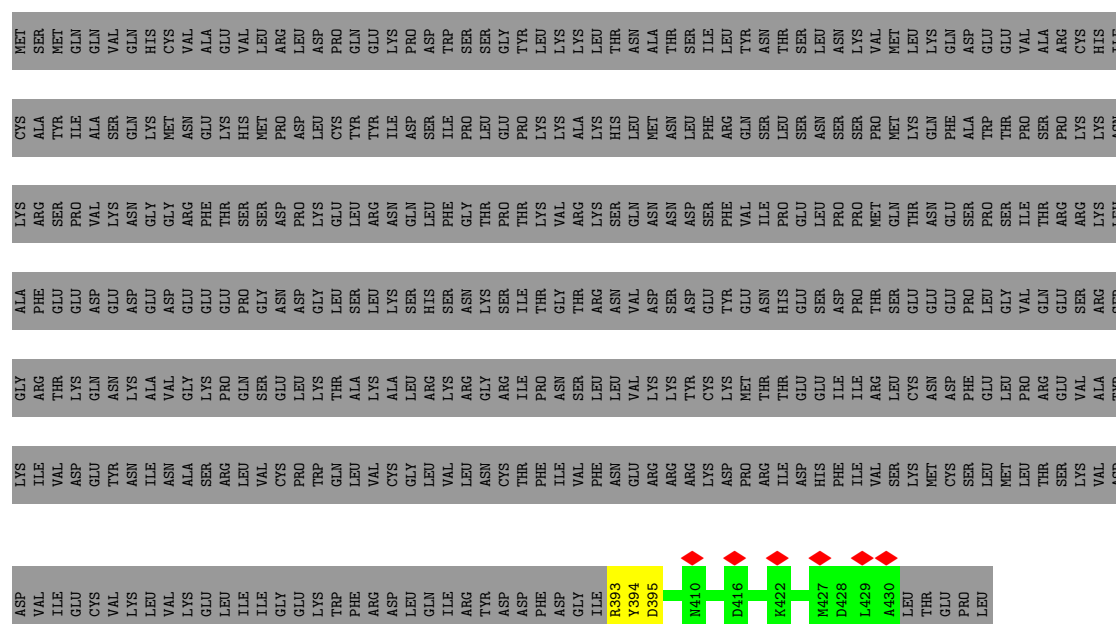
• Molecule 12: Origin recognition complex subunit 5

Chain E: 76% 11% 12%



• Molecule 13: Origin recognition complex subunit 6

Chain F: 8% 91%



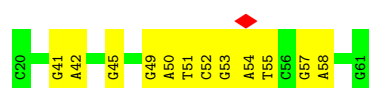
• Molecule 14: DNA (42-MER)

Chain X: 31% 69%



• Molecule 14: DNA (42-MER)

Chain Y: 71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS 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	0.892	Depositor
Minimum map value	-0.216	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.14	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

5.1 Standard geometry

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	0.24	0/5145	0.50	0/6945
2	3	0.23	0/4661	0.48	0/6323
3	4	0.24	0/5024	0.47	0/6775
4	5	0.24	0/5131	0.48	0/6921
5	6	0.24	0/5495	0.49	0/7406
6	7	0.24	0/4609	0.48	0/6222
7	8	0.24	0/4123	0.47	0/5588
8	A	0.25	0/971	0.45	0/1302
9	B	0.25	0/1892	0.42	0/2556
10	C	0.24	0/4717	0.42	0/6364
11	D	0.24	0/3606	0.44	0/4873
12	E	0.24	0/3526	0.43	0/4791
13	F	0.22	0/328	0.45	0/440
14	X	0.51	0/965	0.98	0/1487
14	Y	0.50	0/965	0.98	0/1487
All	All	0.26	0/51158	0.50	0/69480

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

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	34	0
3	4	4964	0	5031	49	0
4	5	5059	0	5144	57	0
5	6	5408	0	5458	76	0
6	7	4541	0	4583	25	0
7	8	4047	0	4117	52	0
8	A	961	0	993	8	0
9	B	1845	0	1815	15	0
10	C	4618	0	4589	29	0
11	D	3542	0	3610	31	0
12	E	3444	0	3463	39	0
13	F	324	0	330	2	0
14	X	861	0	473	21	0
14	Y	861	0	473	9	0
15	2	27	0	12	0	0
15	4	27	0	12	2	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	0	0
17	E	31	0	12	1	0
All	All	50292	0	49914	437	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 (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:553:ILE:HG13	4:5:630:ARG:HE	1.48	0.78
3:4:245:ALA:HB3	3:4:307:ASN:H	1.49	0.77
7:8:269:PRO:HA	7:8:277:THR:HA	1.68	0.76
7:8:337:PRO:HB3	7:8:384:ASN:HB2	1.71	0.71
3:4:527:ALA:HB3	3:4:537:LYS:HE3	1.73	0.71
5:6:523:GLU:OE1	5:6:946:ASN:ND2	2.22	0.70
2:3:210:HIS:ND1	2:3:235:ASP:OD2	2.24	0.70
3:4:310:SER:HA	3:4:327:ASN:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:260:LYS:NZ	12:E:298:ASN:O	2.24	0.70
2:3:307:ASN:ND2	2:3:308:GLN:OE1	2.25	0.69
7:8:485:ASP:OD1	7:8:488:ARG:NH1	2.25	0.69
10:C:382:THR:OG1	10:C:384:LYS:NZ	2.26	0.69
3:4:304:ARG:NH2	3:4:422:GLU:OE2	2.26	0.68
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.74	0.68
10:C:140:ARG:NH2	14:X:12:DC:OP2	2.27	0.67
1:2:416:ASP:OD2	4:5:272:ARG:NH2	2.27	0.67
4:5:455:ARG:HA	4:5:462:PHE:HA	1.75	0.67
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.77	0.66
5:6:972:ARG:HH22	11:D:385:ASP:HB2	1.60	0.65
5:6:942:LEU:HD13	7:8:477:PRO:HG2	1.77	0.65
2:3:307:ASN:O	2:3:310:ASN:ND2	2.27	0.65
4:5:386:LYS:NZ	4:5:679:GLU:OE2	2.28	0.65
10:C:293:ASN:HB2	10:C:467:THR:HG22	1.81	0.62
4:5:257:LYS:NZ	4:5:458:MET:SD	2.73	0.62
5:6:144:LYS:HD3	5:6:193:ALA:HB1	1.81	0.62
4:5:33:ASN:ND2	4:5:37:GLU:OE1	2.33	0.62
5:6:552:LEU:HD21	5:6:755:ILE:HG12	1.82	0.62
2:3:393:LEU:HD12	2:3:397:SER:HB2	1.82	0.62
2:3:716:ARG:NH2	2:3:722:ASN:OD1	2.32	0.62
3:4:365:ILE:HB	5:6:419:SER:HA	1.82	0.62
2:3:449:ASP:HA	2:3:455:ARG:HA	1.82	0.61
1:2:613:ASN:ND2	1:2:616:ASP:OD2	2.33	0.61
3:4:186:SER:HB3	3:4:189:GLU:HB3	1.82	0.61
3:4:195:ARG:NH2	3:4:199:MET:SD	2.72	0.61
9:B:468:MET:O	9:B:472:ASN:ND2	2.33	0.61
5:6:568:ASP:OD2	5:6:659:GLN:NE2	2.25	0.61
5:6:120:GLU:OE1	5:6:134:LYS:NZ	2.29	0.61
10:C:248:GLU:O	11:D:457:LYS:NZ	2.33	0.60
13:F:393:ARG:NH2	13:F:395:ASP:OD1	2.34	0.60
5:6:364:ASN:ND2	5:6:367:GLU:OE2	2.31	0.60
1:2:536:ASP:HB3	1:2:645:SER:HB3	1.83	0.60
10:C:260:LYS:NZ	12:E:296:ASP:O	2.28	0.60
4:5:178:TYR:HB3	4:5:249:LYS:HB2	1.82	0.60
5:6:553:GLY:O	5:6:812:ARG:NH1	2.34	0.60
5:6:592:ALA:HB3	5:6:595:SER:HB2	1.82	0.60
10:C:190:ASN:OD1	10:C:193:ARG:NH2	2.33	0.60
1:2:356:ASN:HA	1:2:433:ASN:HB2	1.83	0.59
1:2:655:GLY:HA3	5:6:704:PRO:HD3	1.85	0.59
5:6:172:GLU:HG3	5:6:173:GLN:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:417:PRO:HB2	5:6:448:LEU:HD21	1.85	0.59
3:4:872:VAL:HG21	3:4:890:ILE:HD11	1.83	0.59
4:5:649:THR:H	4:5:652:GLN:HG2	1.68	0.59
5:6:557:LYS:HB2	5:6:565:LEU:HD12	1.84	0.59
10:C:99:ARG:NH1	12:E:208:GLU:OE2	2.36	0.59
5:6:273:VAL:HB	7:8:541:SER:HA	1.84	0.58
4:5:719:LYS:NZ	4:5:775:VAL:OXT	2.34	0.58
15:4:1001:ADP:O1B	6:7:593:ARG:NH1	2.32	0.58
1:2:382:TYR:HB2	4:5:153:SER:HB2	1.86	0.58
6:7:453:ASP:OD2	6:7:544:GLN:NE2	2.36	0.58
4:5:409:ASP:OD1	4:5:500:GLN:NE2	2.31	0.58
6:7:441:ASP:OD1	6:7:449:LYS:NZ	2.33	0.58
12:E:103:GLU:H	12:E:107:LEU:HD12	1.69	0.57
4:5:626:PHE:HB2	4:5:653:LEU:HD13	1.87	0.57
11:D:113:ASP:OD2	12:E:158:LYS:NZ	2.37	0.57
10:C:100:ARG:NH2	10:C:230:ASP:OD1	2.37	0.57
8:A:797:LEU:O	11:D:332:ARG:NH2	2.36	0.57
14:X:35:DT:H2"	14:X:36:DC:C5	2.39	0.57
5:6:347:ASN:OD1	5:6:350:ARG:N	2.38	0.57
5:6:522:ASP:HB3	5:6:525:ILE:HG23	1.87	0.57
5:6:303:GLU:N	5:6:354:LEU:O	2.28	0.57
2:3:40:ASP:OD1	2:3:41:SER:N	2.38	0.56
7:8:195:VAL:HG13	7:8:236:LEU:HD13	1.87	0.56
4:5:391:LEU:HD21	4:5:476:VAL:HG11	1.87	0.56
10:C:298:PHE:HB2	10:C:469:ASP:HA	1.87	0.56
3:4:802:ILE:HD11	5:6:732:VAL:HG22	1.88	0.56
11:D:188:LEU:HD13	11:D:243:VAL:HG11	1.87	0.56
5:6:554:GLY:N	5:6:567:GLY:O	2.38	0.56
5:6:652:ILE:O	5:6:656:MET:HG3	2.06	0.56
4:5:722:LEU:O	4:5:772:ARG:NH1	2.38	0.56
2:3:223:THR:OG1	4:5:246:GLU:OE1	2.22	0.55
3:4:579:GLN:OE1	6:7:543:GLN:NE2	2.38	0.55
14:X:43:DT:H2"	14:X:44:DC:C6	2.41	0.55
12:E:243:ILE:HG13	12:E:247:PHE:HD2	1.70	0.55
5:6:589:VAL:HG11	5:6:597:TYR:HB2	1.87	0.55
11:D:275:MET:O	11:D:277:GLN:NE2	2.40	0.55
1:2:813:ILE:HG12	1:2:841:VAL:HG11	1.88	0.55
5:6:594:ARG:HB3	5:6:631:ALA:HA	1.89	0.55
10:C:209:ASP:OD2	10:C:241:ASN:ND2	2.32	0.54
12:E:143:ALA:O	12:E:179:TYR:OH	2.24	0.54
3:4:425:ASP:OD2	5:6:280:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:387:LYS:NZ	7:8:389:ASP:HB3	2.22	0.54
10:C:109:GLY:N	10:C:240:ILE:O	2.41	0.54
12:E:205:ARG:NH2	12:E:259:ASN:O	2.40	0.54
7:8:202:ALA:HB2	7:8:229:LEU:HB2	1.90	0.54
3:4:246:ARG:NH2	3:4:307:ASN:OD1	2.38	0.54
5:6:747:SER:HB3	5:6:750:GLN:HG3	1.90	0.54
7:8:338:PRO:HG2	7:8:343:LEU:HD11	1.89	0.54
7:8:390:ASN:OD1	7:8:391:LEU:N	2.39	0.54
11:D:396:ARG:NH2	11:D:528:GLN:O	2.41	0.53
3:4:874:LYS:NZ	3:4:879:ASP:OD1	2.40	0.53
5:6:608:LEU:HA	5:6:627:ALA:HB3	1.90	0.53
5:6:918:ARG:HD2	11:D:429:VAL:HG22	1.90	0.53
1:2:689:GLU:OE2	5:6:782:LYS:NZ	2.38	0.53
1:2:494:ILE:HD12	1:2:494:ILE:H	1.72	0.53
3:4:284:ILE:HG23	3:4:290:ASP:HB3	1.91	0.53
7:8:61:LEU:HA	7:8:65:ASP:HB2	1.91	0.53
7:8:197:THR:HG22	7:8:261:THR:HG23	1.89	0.53
14:X:33:DG:H2"	14:X:34:DA:C8	2.44	0.53
10:C:383:ASN:ND2	10:C:383:ASN:O	2.42	0.53
11:D:98:VAL:HG22	11:D:271:ARG:HB2	1.91	0.53
5:6:271:PRO:HA	7:8:542:LEU:HD22	1.91	0.53
6:7:236:GLY:N	6:7:355:PHE:O	2.36	0.53
8:A:847:LYS:HG2	8:A:853:GLY:HA2	1.89	0.52
4:5:275:THR:OG1	4:5:458:MET:SD	2.65	0.52
4:5:421:ALA:HA	15:5:901:ADP:H5'2	1.92	0.52
2:3:668:ILE:O	2:3:670:GLN:NE2	2.42	0.52
7:8:339:GLU:HA	7:8:382:THR:HG22	1.90	0.52
1:2:294:HIS:CD2	1:2:412:ALA:HB1	2.44	0.52
8:A:791:ILE:HD11	8:A:900:GLU:HB2	1.92	0.52
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.92	0.52
10:C:247:ILE:HG23	10:C:251:LEU:HD12	1.91	0.52
11:D:412:TYR:OH	11:D:451:TRP:O	2.17	0.52
12:E:205:ARG:NE	12:E:259:ASN:OD1	2.41	0.52
3:4:259:HIS:HA	3:4:262:LEU:HD12	1.92	0.52
3:4:397:ILE:HG23	3:4:417:LEU:HB2	1.92	0.52
9:B:330:ALA:HA	9:B:334:LEU:HB3	1.92	0.52
5:6:118:PHE:HD2	5:6:161:ARG:HD2	1.74	0.51
6:7:318:LEU:HD22	6:7:320:GLN:HE22	1.75	0.51
6:7:520:ILE:HG12	6:7:562:SER:HB2	1.91	0.51
4:5:416:GLY:HA3	4:5:556:VAL:HG22	1.92	0.51
3:4:766:ALA:HB1	3:4:822:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:41:DG:C8	14:X:41:DG:H5'	2.46	0.51
4:5:415:LEU:HD21	4:5:540:ILE:HD11	1.93	0.51
1:2:501:MET:HG3	1:2:516:ALA:HB2	1.93	0.51
5:6:197:LEU:HD22	5:6:261:ARG:HG2	1.93	0.51
2:3:564:HIS:HA	2:3:567:ARG:HD3	1.93	0.51
1:2:631:ILE:HD11	1:2:633:LYS:HD3	1.92	0.51
8:A:888:ARG:HH12	11:D:512:GLU:CD	2.13	0.51
14:Y:53:DG:H2''	14:Y:54:DA:C8	2.45	0.51
3:4:796:ARG:NE	3:4:799:GLU:OE2	2.44	0.50
4:5:361:SER:HA	4:5:366:LEU:HD22	1.91	0.50
3:4:374:ILE:O	3:4:377:ASN:ND2	2.44	0.50
7:8:125:PHE:HA	7:8:128:LEU:HD12	1.93	0.50
2:3:169:ARG:NH1	2:3:269:GLN:OE1	2.45	0.50
14:Y:57:DG:H2''	14:Y:58:DA:C8	2.47	0.50
14:X:45:DG:H2'	14:X:46:DA:C8	2.46	0.50
11:D:229:THR:HA	11:D:232:TYR:HB3	1.94	0.50
12:E:18:LEU:HD21	12:E:35:LEU:HD21	1.94	0.50
4:5:87:ILE:HA	4:5:90:PHE:HB2	1.94	0.50
7:8:570:SER:H	7:8:581:TYR:HE1	1.59	0.50
12:E:35:LEU:HB3	12:E:189:PHE:CE2	2.46	0.50
12:E:336:TYR:HA	12:E:452:VAL:HG21	1.93	0.50
4:5:630:ARG:NH1	4:5:648:ILE:O	2.45	0.50
3:4:871:ASN:O	3:4:875:ASP:N	2.42	0.49
1:2:183:LEU:O	1:2:209:ARG:NH2	2.38	0.49
1:2:625:GLU:HB3	1:2:808:ARG:HH22	1.76	0.49
2:3:23:ASP:OD1	2:3:26:ARG:NH2	2.44	0.49
9:B:445:SER:HB3	9:B:452:ILE:HD12	1.94	0.49
5:6:137:ARG:HA	5:6:140:ILE:HD12	1.94	0.49
11:D:510:LEU:HD12	11:D:510:LEU:H	1.78	0.49
2:3:356:LYS:HG2	2:3:359:ILE:HB	1.95	0.49
7:8:387:LYS:HZ2	7:8:389:ASP:HB3	1.76	0.49
7:8:412:GLN:HA	7:8:415:ILE:HG12	1.95	0.49
8:A:806:TYR:O	8:A:810:ASN:ND2	2.45	0.49
2:3:296:GLY:HA3	2:3:323:GLY:HA2	1.93	0.49
3:4:443:PRO:HB3	3:4:457:TYR:CZ	2.48	0.49
4:5:292:VAL:HG12	4:5:335:SER:HB2	1.93	0.49
5:6:145:ILE:HG23	7:8:336:VAL:HG21	1.94	0.49
2:3:391:LYS:HB2	2:3:399:LEU:HD12	1.95	0.49
11:D:339:ASN:ND2	12:E:183:CYS:O	2.33	0.49
6:7:81:ASP:HA	6:7:205:LYS:HG2	1.95	0.48
10:C:112:SER:HB2	10:C:206:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:202:TYR:HA	2:3:209:PHE:HA	1.95	0.48
14:X:20:DC:H2"	14:X:21:DG:C8	2.48	0.48
4:5:265:VAL:HG21	4:5:271:PRO:HG3	1.96	0.48
5:6:559:THR:HG22	5:6:561:GLU:H	1.78	0.48
6:7:409:ASP:OD1	6:7:412:ASN:ND2	2.32	0.48
14:X:29:DG:H2"	14:X:30:DA:C8	2.48	0.48
1:2:417:VAL:HG21	1:2:456:ILE:HG21	1.95	0.48
2:3:119:ALA:HA	2:3:221:LEU:HB3	1.96	0.48
2:3:201:HIS:ND1	2:3:241:LEU:HD13	2.28	0.48
5:6:816:VAL:HG12	5:6:818:GLU:H	1.78	0.48
11:D:123:TYR:HB3	11:D:126:GLN:HB2	1.94	0.48
14:X:16:DC:H2"	14:X:17:DG:C8	2.49	0.48
1:2:610:ASP:O	1:2:617:ARG:NH1	2.45	0.48
7:8:61:LEU:O	7:8:154:ARG:NH2	2.47	0.48
7:8:512:LYS:NZ	7:8:543:GLN:OE1	2.29	0.48
14:X:22:DA:H2"	14:X:23:DT:H72	1.94	0.48
7:8:515:GLN:OE1	7:8:543:GLN:NE2	2.40	0.48
9:B:432:ILE:HG13	9:B:437:PHE:CE1	2.48	0.48
12:E:391:GLN:HE22	12:E:414:MET:H	1.61	0.48
1:2:231:ILE:HG23	1:2:279:THR:HG22	1.94	0.48
5:6:330:PRO:HD2	5:6:344:TRP:CD1	2.49	0.48
7:8:81:LEU:HD12	7:8:82:PRO:HD2	1.96	0.48
8:A:790:VAL:O	8:A:794:MET:HG2	2.14	0.48
4:5:449:LEU:HB3	4:5:469:MET:HG3	1.95	0.47
5:6:516:LEU:HD21	5:6:757:TYR:HB2	1.96	0.47
10:C:484:LYS:HD3	12:E:416:ALA:HB3	1.96	0.47
11:D:185:LEU:HD22	11:D:243:VAL:HB	1.95	0.47
5:6:772:TYR:OH	11:D:429:VAL:O	2.28	0.47
2:3:164:HIS:HB3	2:3:180:VAL:HA	1.96	0.47
3:4:290:ASP:OD1	3:4:291:TYR:N	2.41	0.47
7:8:527:GLN:HB2	7:8:581:TYR:HA	1.95	0.47
11:D:509:ILE:HG22	11:D:511:GLN:H	1.79	0.47
2:3:145:SER:O	2:3:149:SER:OG	2.33	0.47
3:4:728:TYR:HE1	6:7:652:MET:HG3	1.78	0.47
6:7:30:GLN:HA	6:7:62:LYS:HB2	1.95	0.47
3:4:859:ARG:NH2	8:A:905:MET:O	2.47	0.47
6:7:526:PHE:HZ	6:7:537:ILE:HG21	1.78	0.47
3:4:395:GLN:NE2	3:4:425:ASP:OD1	2.48	0.47
3:4:696:PRO:N	3:4:697:PRO:HD2	2.29	0.47
5:6:520:VAL:HG22	5:6:754:TYR:CE1	2.50	0.47
11:D:471:GLU:OE1	11:D:472:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:206:CYS:HB2	12:E:233:GLN:HG3	1.95	0.47
12:E:338:CYS:O	12:E:385:ARG:NH1	2.47	0.47
1:2:774:ILE:HG13	1:2:825:LEU:HD22	1.97	0.47
6:7:29:LYS:HA	6:7:61:PRO:HA	1.97	0.47
9:B:429:GLY:O	9:B:433:ARG:HG3	2.14	0.47
4:5:450:THR:HG21	4:5:492:ALA:HB1	1.97	0.47
5:6:406:ASP:OD1	5:6:407:VAL:N	2.47	0.47
10:C:243:ASN:OD1	10:C:244:LEU:N	2.42	0.47
1:2:439:ASN:HA	1:2:445:PRO:HA	1.97	0.46
5:6:158:LEU:HD22	5:6:267:PHE:CE2	2.50	0.46
7:8:195:VAL:HG23	7:8:235:LEU:HD23	1.96	0.46
10:C:537:ILE:HD11	10:C:608:VAL:HB	1.97	0.46
12:E:215:LEU:HD11	12:E:266:TRP:NE1	2.31	0.46
4:5:145:GLN:HG3	4:5:161:ARG:HB3	1.97	0.46
4:5:379:PHE:HB2	4:5:571:HIS:ND1	2.31	0.46
9:B:428:ASP:OD2	9:B:458:HIS:N	2.44	0.46
5:6:948:LEU:HD13	7:8:487:LEU:HD11	1.97	0.46
6:7:545:THR:HA	6:7:559:ALA:H	1.80	0.46
1:2:262:LYS:HE3	7:8:330:LEU:HB3	1.98	0.46
8:A:847:LYS:O	8:A:853:GLY:N	2.48	0.46
3:4:573:SER:HB2	3:4:576:GLN:HB2	1.98	0.46
4:5:630:ARG:HH22	4:5:633:LEU:HD23	1.81	0.46
9:B:368:PRO:O	9:B:431:SER:OG	2.31	0.46
12:E:35:LEU:HB3	12:E:189:PHE:CZ	2.51	0.46
14:X:44:DC:H2"	14:X:45:DG:C8	2.51	0.46
4:5:211:CYS:HA	4:5:241:TYR:CE2	2.51	0.46
1:2:183:LEU:HB3	1:2:186:LEU:HD12	1.98	0.45
1:2:187:SER:HA	1:2:197:TRP:HE1	1.81	0.45
3:4:434:GLU:HB3	3:4:467:LYS:HB3	1.98	0.45
5:6:598:THR:OG1	5:6:603:SER:OG	2.23	0.45
14:X:42:DA:H2"	14:X:43:DT:C6	2.51	0.45
4:5:454:GLN:NE2	4:5:465:GLU:OE1	2.47	0.45
1:2:327:ARG:NH2	4:5:269:GLU:OE1	2.49	0.45
12:E:288:ALA:HB1	12:E:291:LEU:HD12	1.99	0.45
7:8:154:ARG:HG3	7:8:258:VAL:HG22	1.98	0.45
1:2:234:LEU:HD22	1:2:242:LEU:HG	1.99	0.45
5:6:312:ASP:O	5:6:315:ARG:NH1	2.45	0.45
3:4:611:THR:HG22	3:4:613:GLN:HG2	1.99	0.45
5:6:828:TYR:CE1	11:D:428:THR:HG21	2.51	0.45
12:E:266:TRP:HB3	12:E:267:PRO:HD3	1.99	0.45
5:6:580:SER:HB3	15:6:1101:ADP:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:61:PRO:HB2	6:7:64:MET:HB2	1.99	0.45
6:7:103:VAL:HG11	6:7:207:LEU:HD11	1.98	0.45
6:7:518:ASN:N	6:7:560:ARG:O	2.49	0.45
7:8:34:ARG:HA	7:8:132:SER:HB3	1.98	0.45
7:8:193:THR:HB	7:8:281:HIS:CD2	2.52	0.45
5:6:519:MET:SD	5:6:750:GLN:HB3	2.56	0.44
6:7:470:LEU:HD12	6:7:522:CYS:HB3	1.98	0.44
7:8:48:TYR:CE2	7:8:50:ASN:HB2	2.51	0.44
9:B:474:ASN:OD1	10:C:319:LYS:HE2	2.17	0.44
14:X:19:DT:H2"	14:X:20:DC:C5	2.52	0.44
1:2:625:GLU:HG3	1:2:626:GLN:NE2	2.31	0.44
4:5:182:MET:HB2	4:5:244:ILE:HD11	1.98	0.44
10:C:271:ASN:HD21	10:C:313:ASN:CG	2.21	0.44
12:E:136:ASP:CG	12:E:171:LEU:H	2.21	0.44
1:2:670:THR:HG23	1:2:672:PRO:HD2	1.99	0.44
2:3:413:THR:OG1	2:3:415:LYS:NZ	2.50	0.44
5:6:134:LYS:HE2	5:6:137:ARG:HD3	1.98	0.44
6:7:233:ASP:O	6:7:237:GLN:NE2	2.42	0.44
10:C:409:VAL:HG22	10:C:453:LEU:HD22	2.00	0.44
10:C:497:VAL:O	13:F:394:TYR:OH	2.31	0.44
12:E:32:ASN:ND2	12:E:150:ILE:O	2.43	0.44
1:2:780:GLN:OE1	4:5:574:ASN:ND2	2.50	0.44
3:4:760:PRO:HB2	3:4:817:VAL:HG23	2.00	0.44
5:6:321:VAL:HG12	5:6:323:GLN:NE2	2.32	0.44
7:8:194:GLY:HA2	7:8:263:TRP:CD1	2.53	0.44
12:E:262:ILE:O	12:E:266:TRP:HB2	2.18	0.44
2:3:110:PHE:CE1	2:3:114:ILE:HD11	2.52	0.44
14:Y:41:DG:H2"	14:Y:42:DA:C8	2.53	0.44
14:Y:51:DT:H2"	14:Y:52:DC:C6	2.52	0.44
1:2:243:GLU:OE1	1:2:243:GLU:N	2.50	0.44
1:2:444:PHE:N	1:2:444:PHE:CD1	2.84	0.44
1:2:792:ASP:HB3	1:2:861:PHE:CE1	2.53	0.44
3:4:245:ALA:HB3	3:4:307:ASN:N	2.25	0.44
4:5:166:ILE:O	4:5:289:GLY:N	2.34	0.44
4:5:296:GLY:HA2	4:5:331:LEU:HG	1.98	0.44
5:6:272:THR:HB	7:8:519:ILE:HG23	2.00	0.44
5:6:929:GLU:OE1	5:6:996:LYS:NZ	2.49	0.44
5:6:1002:HIS:O	5:6:1004:ASN:N	2.41	0.44
9:B:286:GLN:O	9:B:290:ARG:NE	2.46	0.44
11:D:214:PHE:HB2	11:D:247:ILE:HA	1.99	0.44
12:E:26:PRO:HB3	12:E:127:CYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:12:DC:H1'	14:X:13:DG:C8	2.53	0.44
4:5:432:VAL:HG22	4:5:596:ILE:HG13	1.99	0.44
5:6:347:ASN:OD1	5:6:349:THR:N	2.50	0.44
11:D:236:ASP:OD2	11:D:267:ARG:NE	2.48	0.44
12:E:243:ILE:HD11	12:E:261:LEU:HB3	1.99	0.44
14:Y:53:DG:H2''	14:Y:54:DA:H8	1.81	0.44
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.99	0.44
5:6:749:GLU:HG2	7:8:550:GLY:HA3	2.00	0.44
11:D:462:ASN:ND2	12:E:251:THR:O	2.45	0.44
12:E:82:GLN:NE2	12:E:96:ASP:OD1	2.49	0.44
5:6:293:THR:O	5:6:362:GLN:N	2.45	0.44
5:6:304:LEU:HD11	5:6:307:ALA:HB2	1.99	0.44
6:7:443:ARG:HE	6:7:445:GLY:HA2	1.83	0.44
7:8:514:THR:HA	7:8:517:PHE:CE2	2.53	0.44
12:E:149:TYR:HB3	12:E:168:TYR:OH	2.18	0.44
1:2:382:TYR:CD2	4:5:156:VAL:HG21	2.53	0.43
5:6:1004:ASN:HB3	11:D:449:LYS:HB3	1.98	0.43
3:4:243:LEU:N	3:4:304:ARG:O	2.50	0.43
7:8:88:TRP:O	7:8:156:PHE:N	2.50	0.43
14:X:25:DG:C2	14:Y:45:DG:C2	3.06	0.43
1:2:705:ARG:NH2	1:2:755:ILE:HD12	2.33	0.43
1:2:790:TYR:CG	1:2:810:LEU:HD12	2.54	0.43
3:4:569:ASP:O	3:4:572:THR:HG22	2.18	0.43
4:5:381:ASN:O	4:5:385:LYS:HG3	2.18	0.43
5:6:340:ASN:ND2	5:6:343:PHE:O	2.37	0.43
14:X:26:DA:C8	14:X:27:DT:H72	2.53	0.43
3:4:349:CYS:SG	3:4:381:SER:OG	2.77	0.43
4:5:407:ARG:HD3	4:5:409:ASP:HB2	2.00	0.43
5:6:566:ARG:NH1	5:6:568:ASP:O	2.51	0.43
12:E:43:LYS:NZ	17:E:501:ATP:O1B	2.50	0.43
12:E:254:ASP:OD1	12:E:255:ILE:N	2.51	0.43
12:E:271:SER:OG	12:E:272:ARG:NH1	2.48	0.43
14:Y:54:DA:H2'	14:Y:55:DT:H71	1.99	0.43
1:2:543:GLY:HA3	1:2:683:VAL:HB	1.99	0.43
3:4:234:ARG:NH2	3:4:235:GLU:OE2	2.45	0.43
5:6:795:ILE:HG23	5:6:799:GLN:HB2	2.01	0.43
14:X:37:DG:H2''	14:X:38:DA:C8	2.53	0.43
1:2:221:GLU:HG3	1:2:222:THR:H	1.84	0.43
3:4:725:THR:HA	3:4:728:TYR:CE2	2.54	0.43
4:5:31:PHE:HE1	4:5:75:ILE:HD12	1.84	0.43
10:C:488:GLU:OE1	10:C:614:ARG:NH1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:215:LEU:HD22	12:E:232:PHE:CE1	2.54	0.43
3:4:573:SER:HB3	15:4:1001:ADP:C4	2.54	0.43
4:5:378:ILE:HD11	4:5:385:LYS:HE2	2.01	0.43
1:2:627:GLN:HB3	1:2:643:ARG:HA	2.01	0.43
3:4:318:ASN:OD1	6:7:341:ARG:NH1	2.42	0.43
3:4:834:LYS:HG2	3:4:837:ALA:HB3	2.01	0.43
5:6:657:GLU:OE2	5:6:658:GLN:NE2	2.43	0.43
9:B:463:LEU:HD12	12:E:425:SER:HB3	2.01	0.43
11:D:104:ARG:HG2	11:D:252:THR:HG21	2.01	0.43
12:E:254:ASP:OD1	12:E:256:PHE:N	2.52	0.43
2:3:276:VAL:HG11	2:3:294:VAL:HG21	2.01	0.43
2:3:478:MET:O	2:3:483:ARG:NH1	2.52	0.43
4:5:614:LEU:HA	4:5:672:ALA:HB3	2.00	0.43
7:8:151:LYS:NZ	7:8:153:THR:OG1	2.45	0.43
10:C:572:THR:HG22	10:C:574:ASP:H	1.84	0.43
14:X:21:DG:H2"	14:X:22:DA:C8	2.54	0.43
2:3:698:THR:O	2:3:701:THR:OG1	2.30	0.42
3:4:257:LEU:O	3:4:261:LEU:N	2.41	0.42
4:5:23:ASP:OD1	4:5:24:ASN:N	2.48	0.42
5:6:918:ARG:NH2	7:8:472:TYR:OH	2.41	0.42
7:8:206:ARG:HH21	7:8:220:VAL:N	2.15	0.42
11:D:506:MET:HG3	11:D:508:ILE:H	1.83	0.42
1:2:319:ARG:NH2	1:2:425:GLU:OE1	2.44	0.42
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.42	0.42
3:4:778:ARG:HE	5:6:724:ASP:CG	2.23	0.42
4:5:87:ILE:HG23	4:5:88:PRO:HD3	2.01	0.42
4:5:286:VAL:HG11	4:5:292:VAL:HG11	2.01	0.42
4:5:359:GLN:OE1	4:5:362:ARG:NH2	2.41	0.42
2:3:489:VAL:HG13	2:3:508:ALA:HB1	2.01	0.42
3:4:515:ARG:NE	3:4:517:ASP:OD1	2.35	0.42
4:5:87:ILE:CG2	4:5:88:PRO:HD3	2.49	0.42
9:B:324:ASN:ND2	9:B:484:GLU:OE2	2.29	0.42
10:C:413:LEU:HA	10:C:417:LEU:HB2	2.01	0.42
11:D:150:LEU:HD22	11:D:184:ILE:HG12	2.01	0.42
14:X:29:DG:H2"	14:X:30:DA:H8	1.83	0.42
1:2:253:LYS:HB3	1:2:256:LEU:HB3	2.00	0.42
1:2:255:ILE:HG23	7:8:393:THR:HB	2.01	0.42
2:3:533:ILE:HG22	2:3:535:LEU:HG	2.01	0.42
3:4:244:ASP:HA	3:4:306:TYR:CE2	2.55	0.42
5:6:357:GLN:N	5:6:381:LEU:O	2.50	0.42
7:8:530:THR:HA	7:8:579:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:52:DC:H2"	14:Y:53:DG:C8	2.54	0.42
1:2:795:ARG:NE	4:5:562:GLU:OE2	2.53	0.42
5:6:609:THR:HG22	5:6:628:LEU:HD12	2.02	0.42
12:E:206:CYS:SG	12:E:207:GLY:N	2.93	0.42
14:Y:49:DG:H2"	14:Y:50:DA:C8	2.54	0.42
2:3:114:ILE:HG22	2:3:179:LEU:HD22	2.01	0.42
1:2:434:TYR:CD1	1:2:448:ALA:HB3	2.54	0.42
5:6:274:HIS:NE2	7:8:523:LEU:HD23	2.34	0.42
5:6:354:LEU:HD23	5:6:382:ARG:HD3	2.02	0.42
5:6:1004:ASN:HA	11:D:449:LYS:HD3	2.02	0.42
1:2:300:PHE:CE2	1:2:302:THR:HB	2.55	0.41
1:2:300:PHE:HE2	1:2:302:THR:HB	1.85	0.41
1:2:599:ALA:O	1:2:644:CYS:HB3	2.20	0.41
3:4:442:ILE:O	3:4:457:TYR:N	2.53	0.41
7:8:41:ASP:OD1	7:8:41:ASP:N	2.51	0.41
7:8:77:PHE:CD2	7:8:286:GLN:HB3	2.55	0.41
3:4:319:PRO:HG2	6:7:309:ALA:HA	2.01	0.41
4:5:393:MET:HB2	4:5:662:SER:OG	2.20	0.41
5:6:918:ARG:NE	11:D:429:VAL:HG13	2.35	0.41
3:4:712:VAL:HG11	6:7:672:LYS:HD3	2.02	0.41
4:5:398:LYS:HB2	4:5:398:LYS:HE2	1.85	0.41
6:7:289:CYS:HB3	6:7:295:LYS:HG2	2.03	0.41
7:8:73:PHE:CE2	7:8:77:PHE:HA	2.55	0.41
4:5:461:GLU:HB2	4:5:463:TYR:HE1	1.85	0.41
7:8:512:LYS:O	7:8:516:VAL:HG23	2.20	0.41
10:C:557:ILE:HG23	10:C:566:LEU:HG	2.02	0.41
14:X:8:DC:H2"	14:X:9:DG:C8	2.56	0.41
14:X:17:DG:H2"	14:X:18:DA:C8	2.55	0.41
2:3:402:ASP:OD1	2:3:493:GLN:NE2	2.31	0.41
9:B:471:GLN:NE2	10:C:315:GLN:HG3	2.36	0.41
12:E:136:ASP:N	12:E:136:ASP:OD1	2.53	0.41
3:4:332:VAL:HG23	3:4:433:ILE:HG13	2.03	0.41
5:6:512:GLU:OE2	7:8:547:ASN:ND2	2.54	0.41
7:8:150:THR:HB	7:8:260:LEU:HD11	2.02	0.41
4:5:302:ASN:OD1	4:5:324:ARG:NH1	2.54	0.41
7:8:73:PHE:CD1	7:8:81:LEU:HB2	2.55	0.41
9:B:316:PHE:HB3	9:B:480:ILE:HG21	2.03	0.41
2:3:118:PRO:HB2	2:3:221:LEU:HD23	2.01	0.41
4:5:207:LEU:O	4:5:209:ARG:NH1	2.50	0.41
4:5:551:ASP:OD2	4:5:658:ARG:NH1	2.54	0.41
5:6:120:GLU:OE2	5:6:192:TYR:OH	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:463:GLN:O	10:C:467:THR:HG23	2.21	0.41
12:E:244:VAL:HG22	12:E:258:LEU:HD13	2.03	0.41
7:8:266:LEU:HB3	7:8:279:ALA:HB2	2.03	0.41
4:5:421:ALA:HB2	15:5:901:ADP:C8	2.55	0.40
7:8:196:LEU:HD21	7:8:230:PHE:HD2	1.85	0.40
9:B:461:ALA:N	9:B:462:PRO:HD2	2.35	0.40
11:D:458:ASN:HB2	12:E:250:TYR:CE1	2.56	0.40
6:7:193:PRO:HD2	6:7:196:LEU:HD12	2.03	0.40
1:2:335:LYS:HE3	1:2:336:TYR:CE2	2.56	0.40
1:2:336:TYR:O	1:2:380:THR:HG23	2.21	0.40
2:3:667:VAL:HG21	2:3:717:LEU:HA	2.03	0.40
3:4:577:ILE:O	3:4:581:VAL:HG23	2.21	0.40
4:5:31:PHE:O	4:5:35:ILE:HG12	2.22	0.40
9:B:249:GLN:NE2	10:C:531:ALA:O	2.39	0.40
1:2:700:VAL:HG21	5:6:770:ARG:HA	2.04	0.40
5:6:657:GLU:OE1	5:6:798:ARG:NH1	2.47	0.40
7:8:95:ASP:OD1	7:8:96:THR:N	2.55	0.40
5:6:923:VAL:HA	5:6:926:GLU:HB2	2.03	0.40
11:D:78:CYS:SG	11:D:276:PRO:HD3	2.62	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%)	609 (96%)	22 (4%)	0	100	100
2	3	575/1006 (57%)	565 (98%)	10 (2%)	0	100	100
3	4	606/933 (65%)	583 (96%)	23 (4%)	0	100	100
4	5	622/775 (80%)	608 (98%)	14 (2%)	0	100	100
5	6	659/1017 (65%)	644 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	7	561/845 (66%)	549 (98%)	12 (2%)	0	100	100
7	8	497/604 (82%)	482 (97%)	15 (3%)	0	100	100
8	A	118/949 (12%)	113 (96%)	5 (4%)	0	100	100
9	B	214/620 (34%)	209 (98%)	5 (2%)	0	100	100
10	C	549/616 (89%)	540 (98%)	9 (2%)	0	100	100
11	D	426/529 (80%)	417 (98%)	9 (2%)	0	100	100
12	E	412/479 (86%)	405 (98%)	7 (2%)	0	100	100
13	F	36/435 (8%)	36 (100%)	0	0	100	100
All	All	5906/9676 (61%)	5760 (98%)	146 (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%)	559 (100%)	1 (0%)	92	96
2	3	509/864 (59%)	509 (100%)	0	100	100
3	4	567/848 (67%)	566 (100%)	1 (0%)	92	96
4	5	571/687 (83%)	570 (100%)	1 (0%)	92	96
5	6	596/886 (67%)	596 (100%)	0	100	100
6	7	507/753 (67%)	507 (100%)	0	100	100
7	8	459/545 (84%)	459 (100%)	0	100	100
8	A	109/842 (13%)	109 (100%)	0	100	100
9	B	208/573 (36%)	207 (100%)	1 (0%)	86	91
10	C	519/576 (90%)	518 (100%)	1 (0%)	92	96
11	D	400/488 (82%)	400 (100%)	0	100	100
12	E	392/440 (89%)	391 (100%)	1 (0%)	91	95
13	F	36/406 (9%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5433/8678 (63%)	5427 (100%)	6 (0%)	92 97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	676	ARG
3	4	352	CYS
4	5	630	ARG
9	B	443	PHE
10	C	67	HIS
12	E	232	PHE

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

Mol	Chain	Res	Type
4	5	574	ASN
9	B	472	ASN

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	$\# Z > 2$
15	ADP	5	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
15	ADP	4	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)
15	ADP	6	1101	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
17	ATP	D	601	-	26,33,33	0.60	0	31,52,52	0.80	1 (3%)
15	ADP	2	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
17	ATP	E	501	-	26,33,33	0.61	0	31,52,52	0.79	1 (3%)

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
15	ADP	5	901	-	-	2/12/32/32	0/3/3/3
15	ADP	4	1001	-	-	5/12/32/32	0/3/3/3
15	ADP	6	1101	-	-	3/12/32/32	0/3/3/3
17	ATP	D	601	-	-	5/18/38/38	0/3/3/3
15	ADP	2	901	-	-	6/12/32/32	0/3/3/3
17	ATP	E	501	-	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	1001	ADP	C5-C4	2.51	1.47	1.40
15	5	901	ADP	C5-C4	2.51	1.47	1.40
15	6	1101	ADP	C5-C4	2.49	1.47	1.40
15	2	901	ADP	C5-C4	2.43	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	901	ADP	PA-O3A-PB	-3.69	120.16	132.83
15	2	901	ADP	PA-O3A-PB	-3.68	120.19	132.83
15	6	1101	ADP	C3'-C2'-C1'	3.65	106.47	100.98
15	6	1101	ADP	PA-O3A-PB	-3.47	120.92	132.83
15	2	901	ADP	C3'-C2'-C1'	3.45	106.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	1001	ADP	N3-C2-N1	-3.16	123.74	128.68
15	2	901	ADP	N3-C2-N1	-3.14	123.77	128.68
15	6	1101	ADP	N3-C2-N1	-3.14	123.77	128.68
15	5	901	ADP	N3-C2-N1	-3.13	123.78	128.68
15	4	1001	ADP	C3'-C2'-C1'	3.02	105.52	100.98
15	5	901	ADP	C3'-C2'-C1'	2.90	105.34	100.98
15	4	1001	ADP	PA-O3A-PB	-2.83	123.10	132.83
15	6	1101	ADP	C4-C5-N7	-2.69	106.59	109.40
15	4	1001	ADP	C4-C5-N7	-2.55	106.74	109.40
15	5	901	ADP	C4-C5-N7	-2.48	106.81	109.40
15	2	901	ADP	C4-C5-N7	-2.43	106.87	109.40
17	D	601	ATP	C5-C6-N6	2.30	123.84	120.35
17	E	501	ATP	C5-C6-N6	2.26	123.78	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	2	901	ADP	C5'-O5'-PA-O3A
15	4	1001	ADP	C5'-O5'-PA-O2A
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	PB-O3B-PG-O3G
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
15	4	1001	ADP	O4'-C4'-C5'-O5'
15	4	1001	ADP	C3'-C4'-C5'-O5'
17	D	601	ATP	C4'-C5'-O5'-PA
15	4	1001	ADP	C5'-O5'-PA-O3A
17	E	501	ATP	C4'-C5'-O5'-PA
15	2	901	ADP	PA-O3A-PB-O1B
15	6	1101	ADP	O4'-C4'-C5'-O5'
15	2	901	ADP	O4'-C4'-C5'-O5'
15	2	901	ADP	PA-O3A-PB-O2B
15	2	901	ADP	PA-O3A-PB-O3B
15	5	901	ADP	C5'-O5'-PA-O3A
17	E	501	ATP	C5'-O5'-PA-O3A
17	E	501	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	E	501	ATP	PB-O3A-PA-O2A
15	2	901	ADP	C5'-O5'-PA-O1A
15	4	1001	ADP	C5'-O5'-PA-O1A

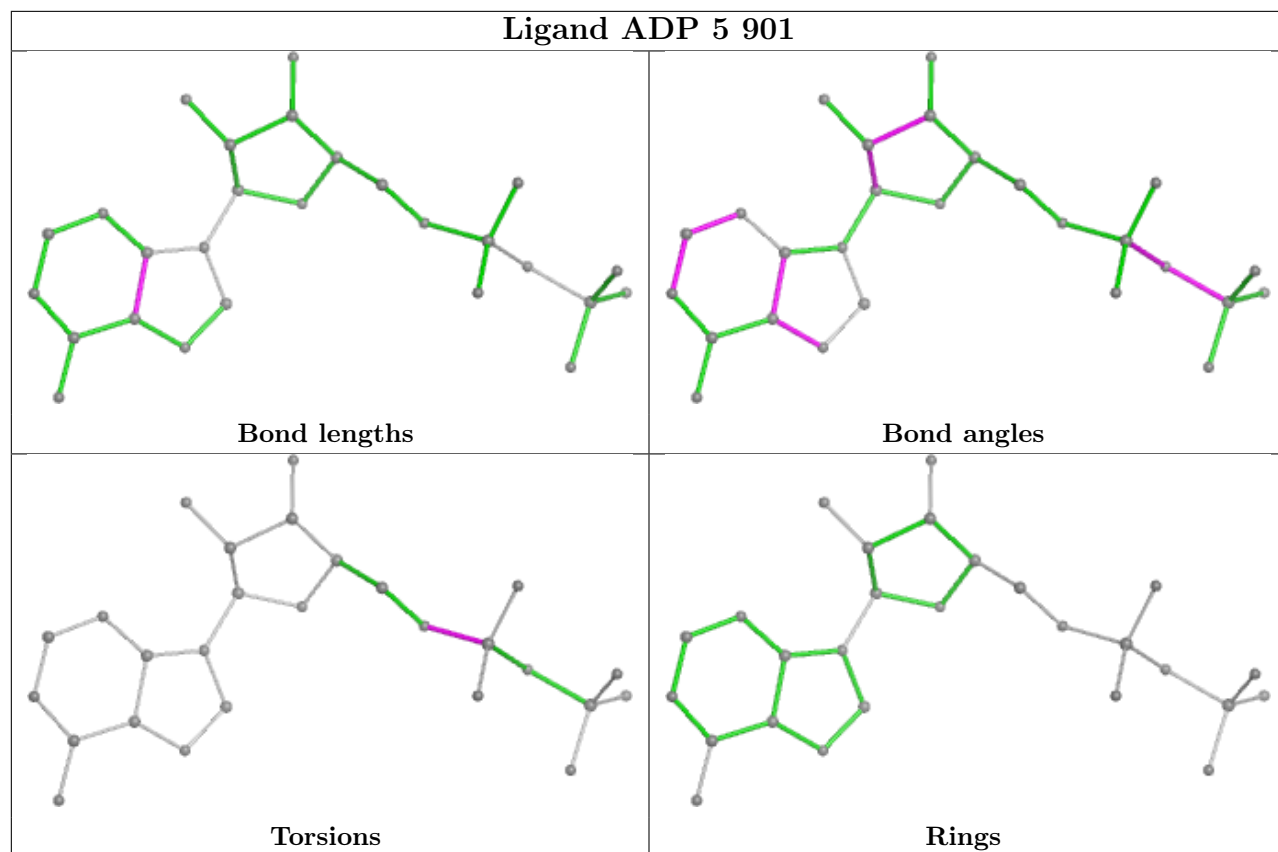
There are no ring outliers.

4 monomers are involved in 6 short contacts:

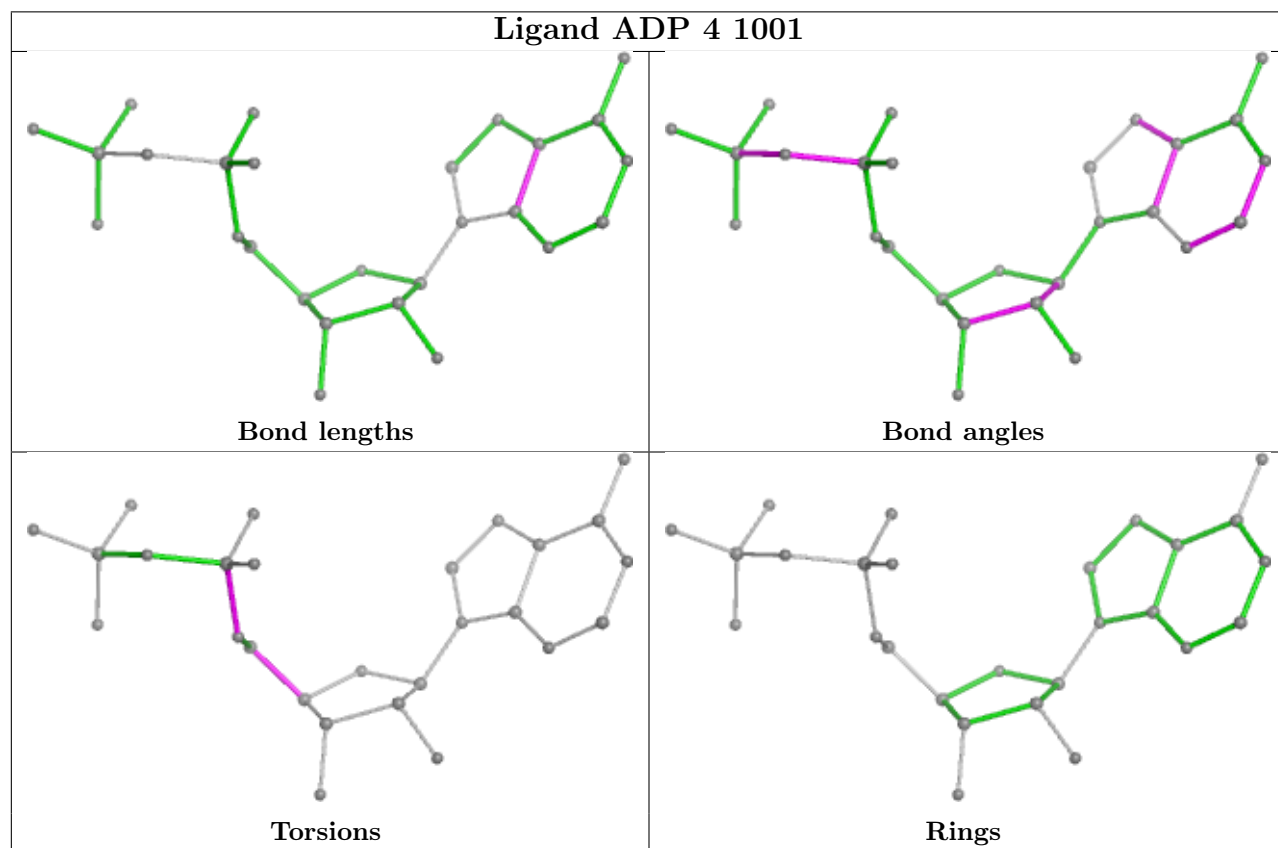
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	5	901	ADP	2	0
15	4	1001	ADP	2	0
15	6	1101	ADP	1	0
17	E	501	ATP	1	0

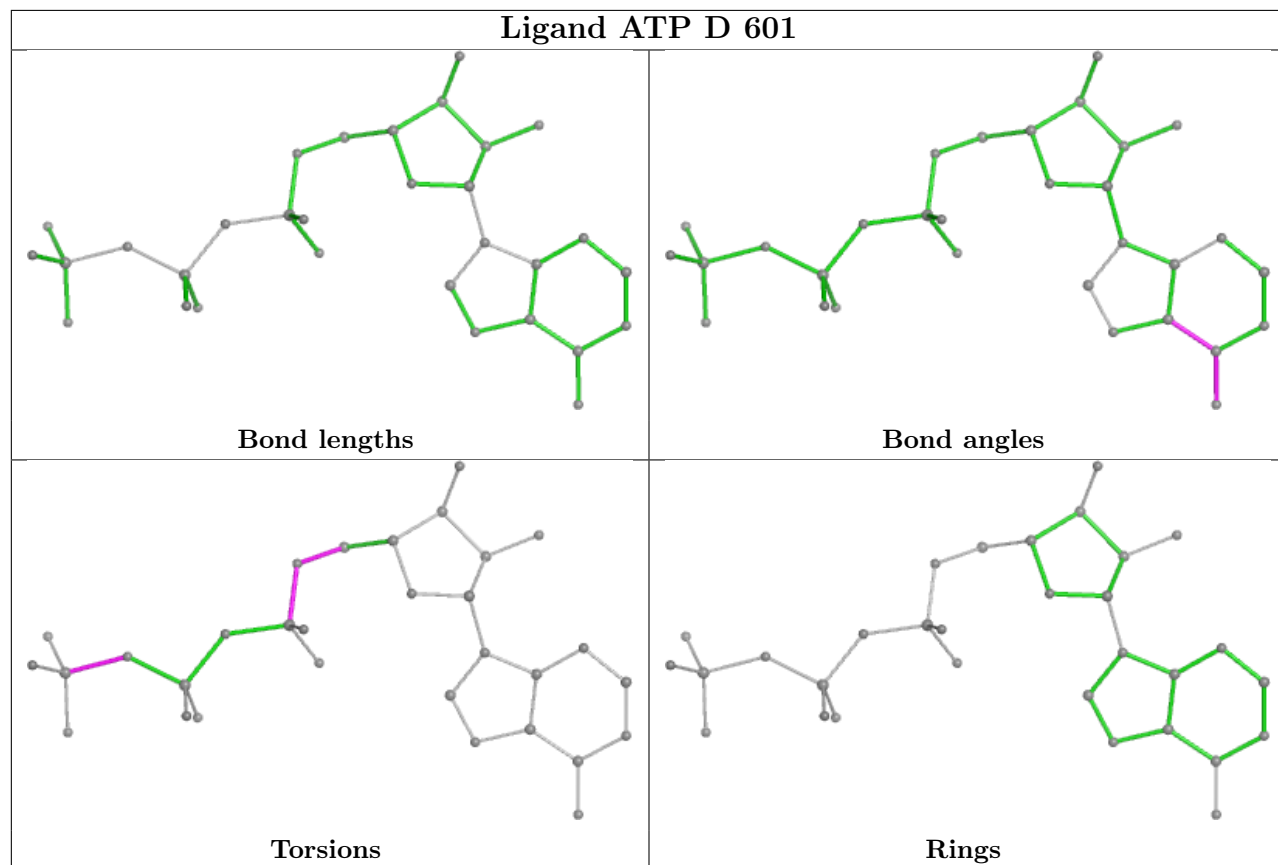
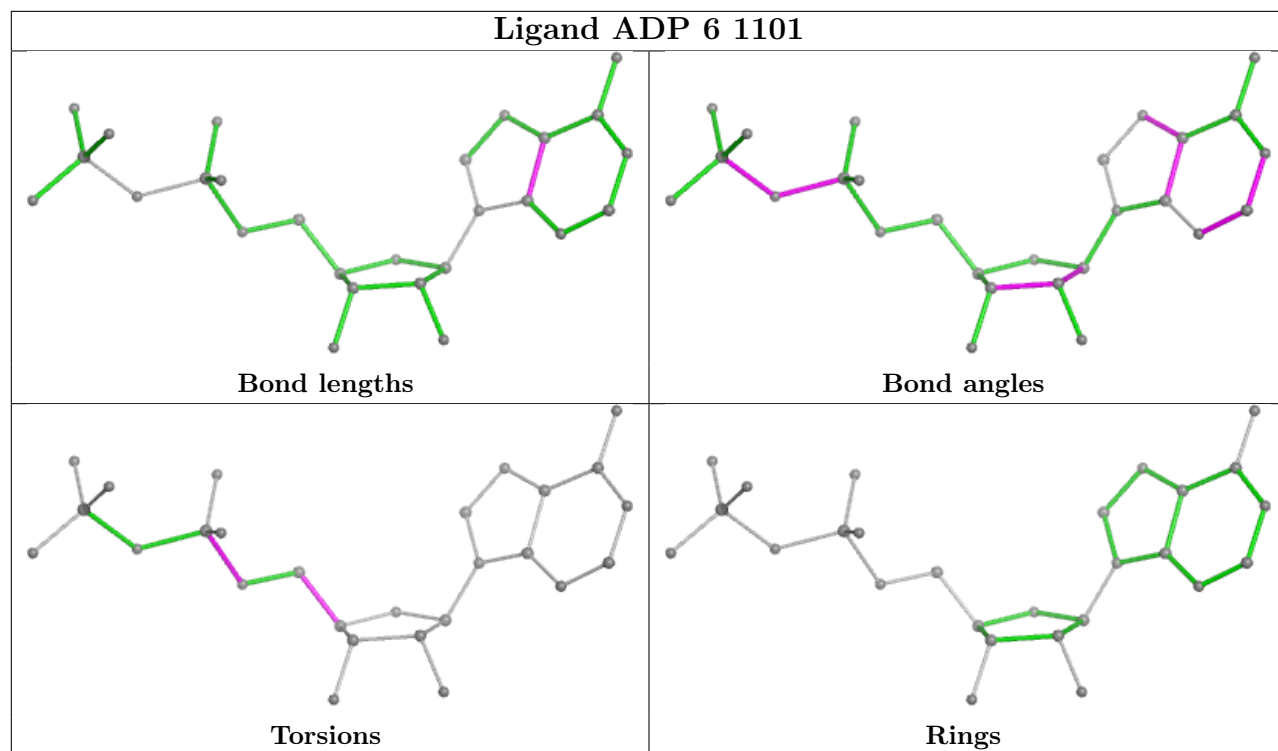
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5 901

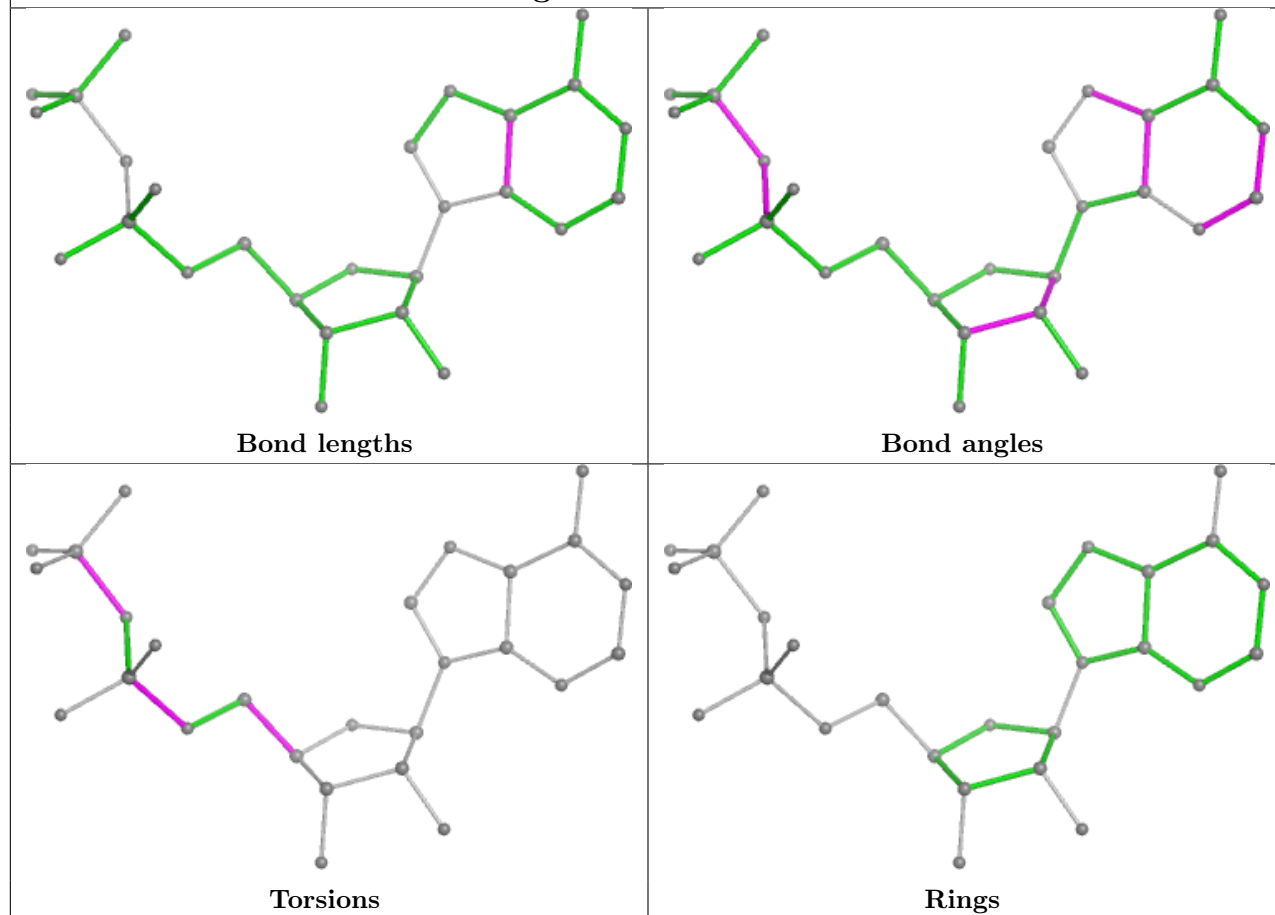


Ligand ADP 4 1001

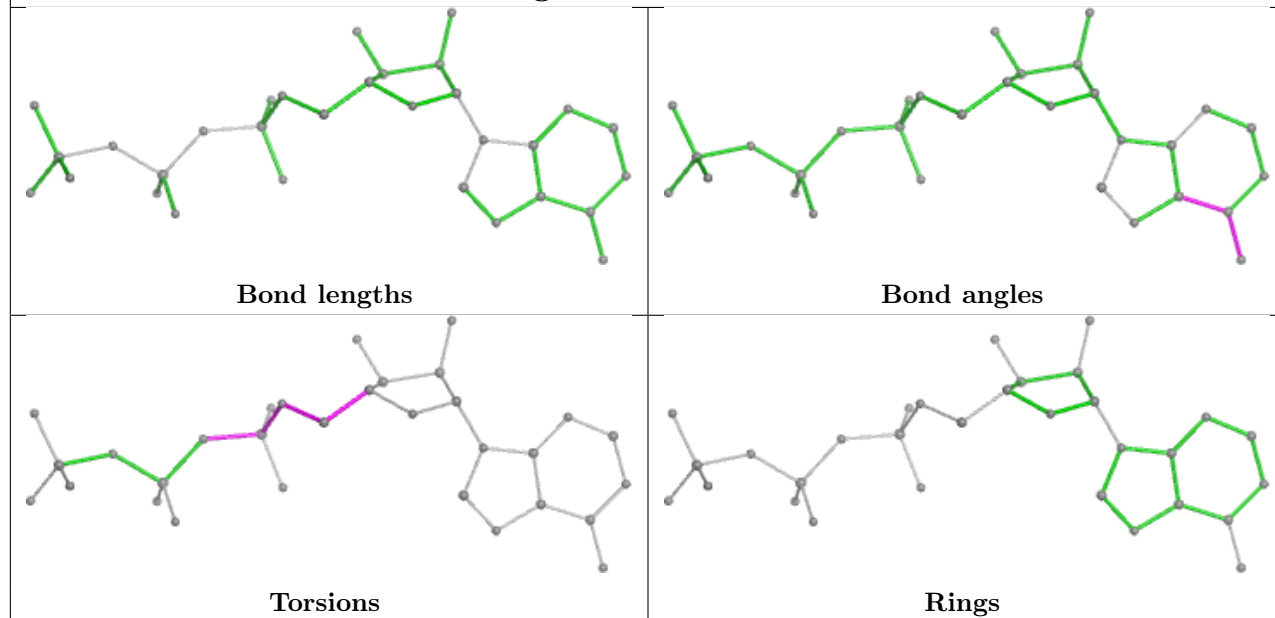




Ligand ADP 2 901



Ligand ATP E 501



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.

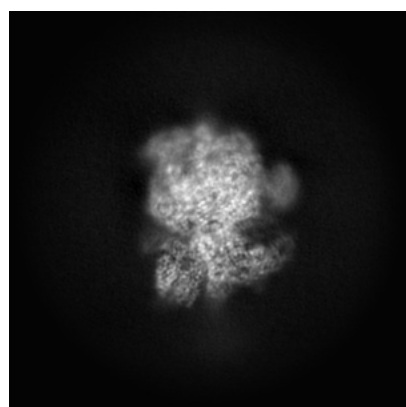
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51401. These allow visual inspection of the internal detail of the map and identification of artifacts.

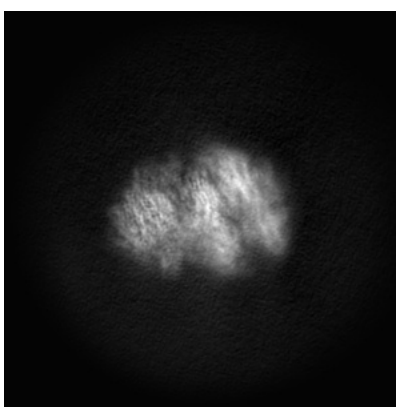
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

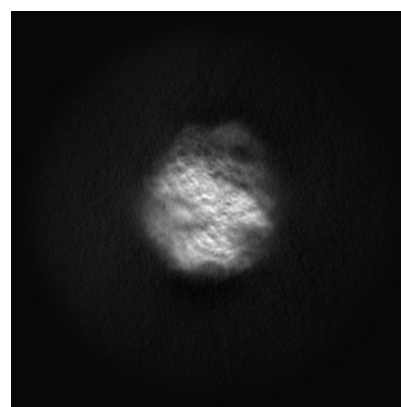
6.1.1 Primary map



X



Y

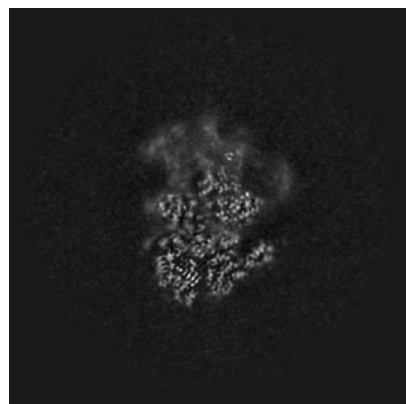


Z

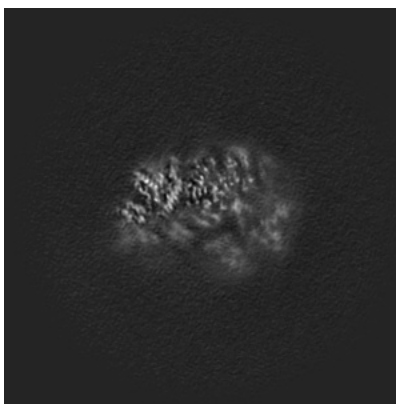
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

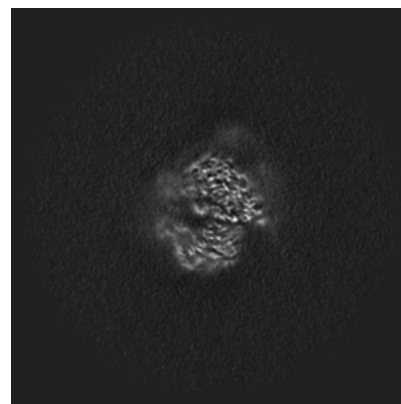
6.2.1 Primary map



X Index: 220



Y Index: 220

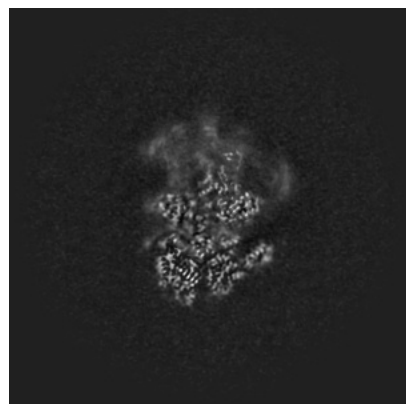


Z Index: 220

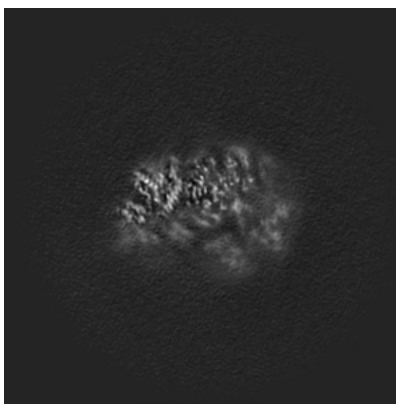
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

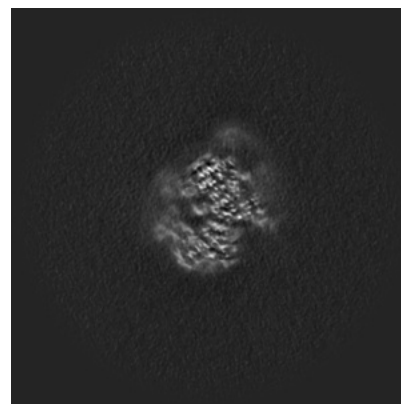
6.3.1 Primary map



X Index: 221



Y Index: 220

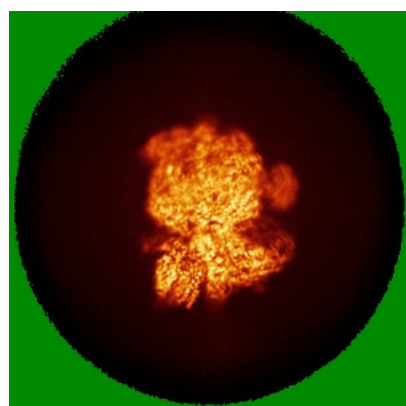


Z Index: 223

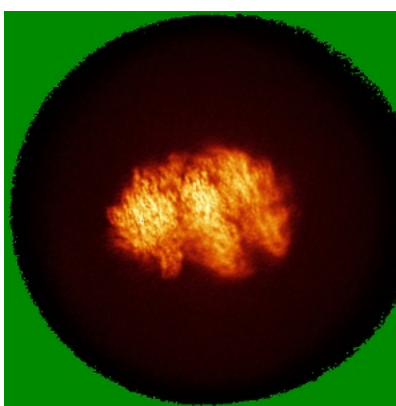
The images above show the largest variance slices of the map in three orthogonal directions.

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

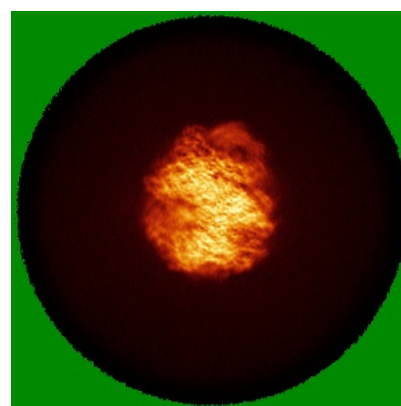
6.4.1 Primary map



X



Y



Z

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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

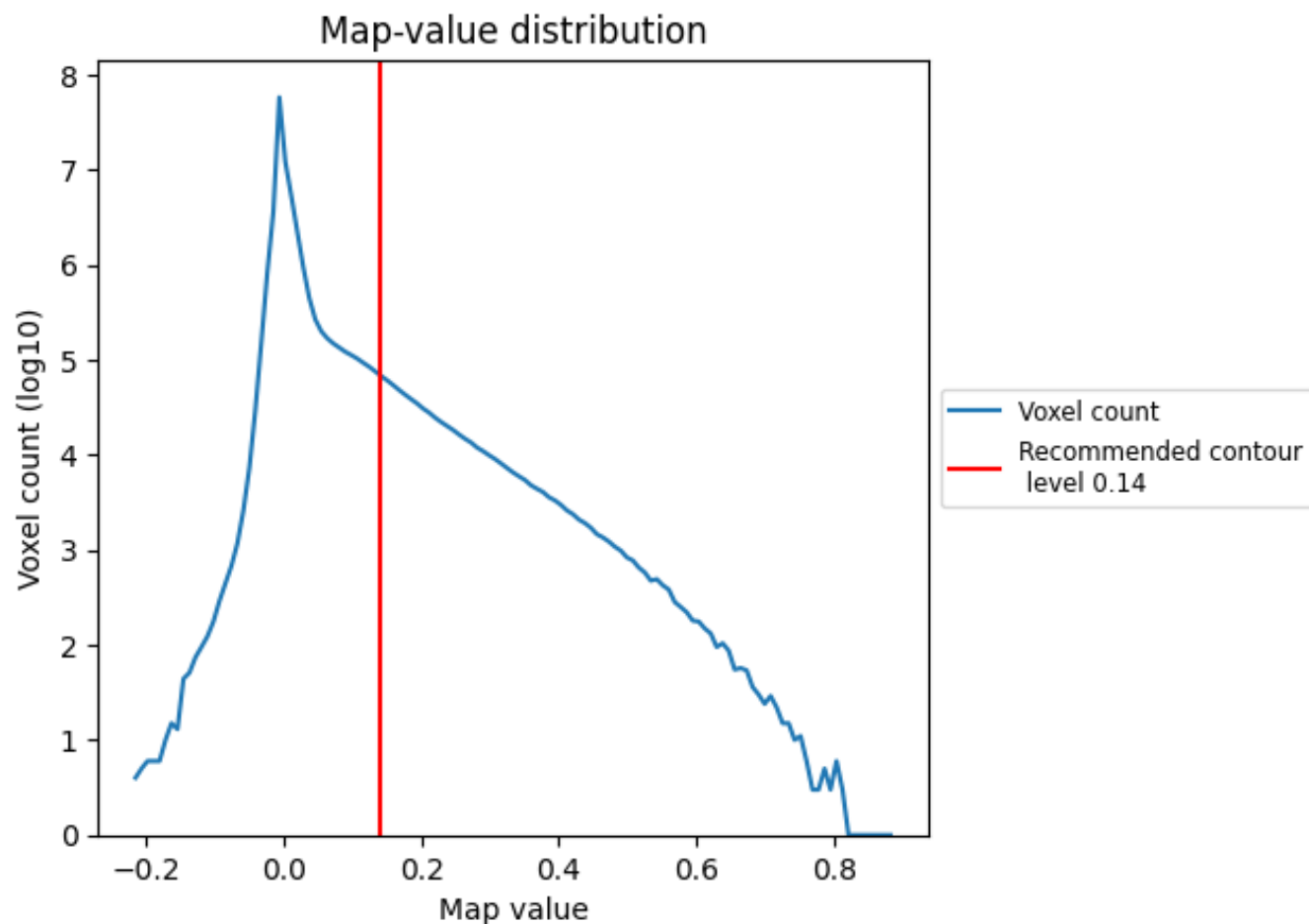
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

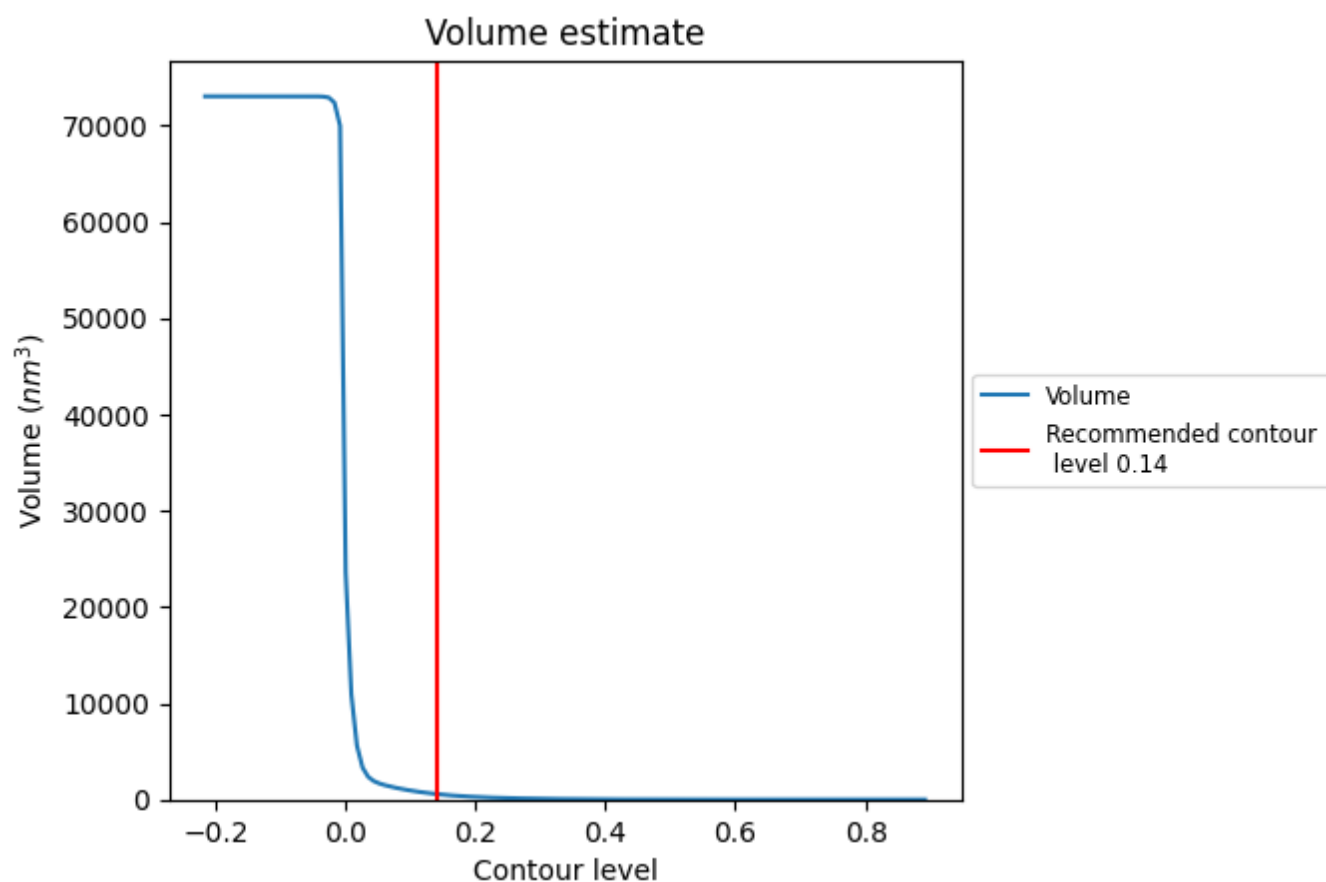
This section contains the results of statistical analysis of the map.

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.

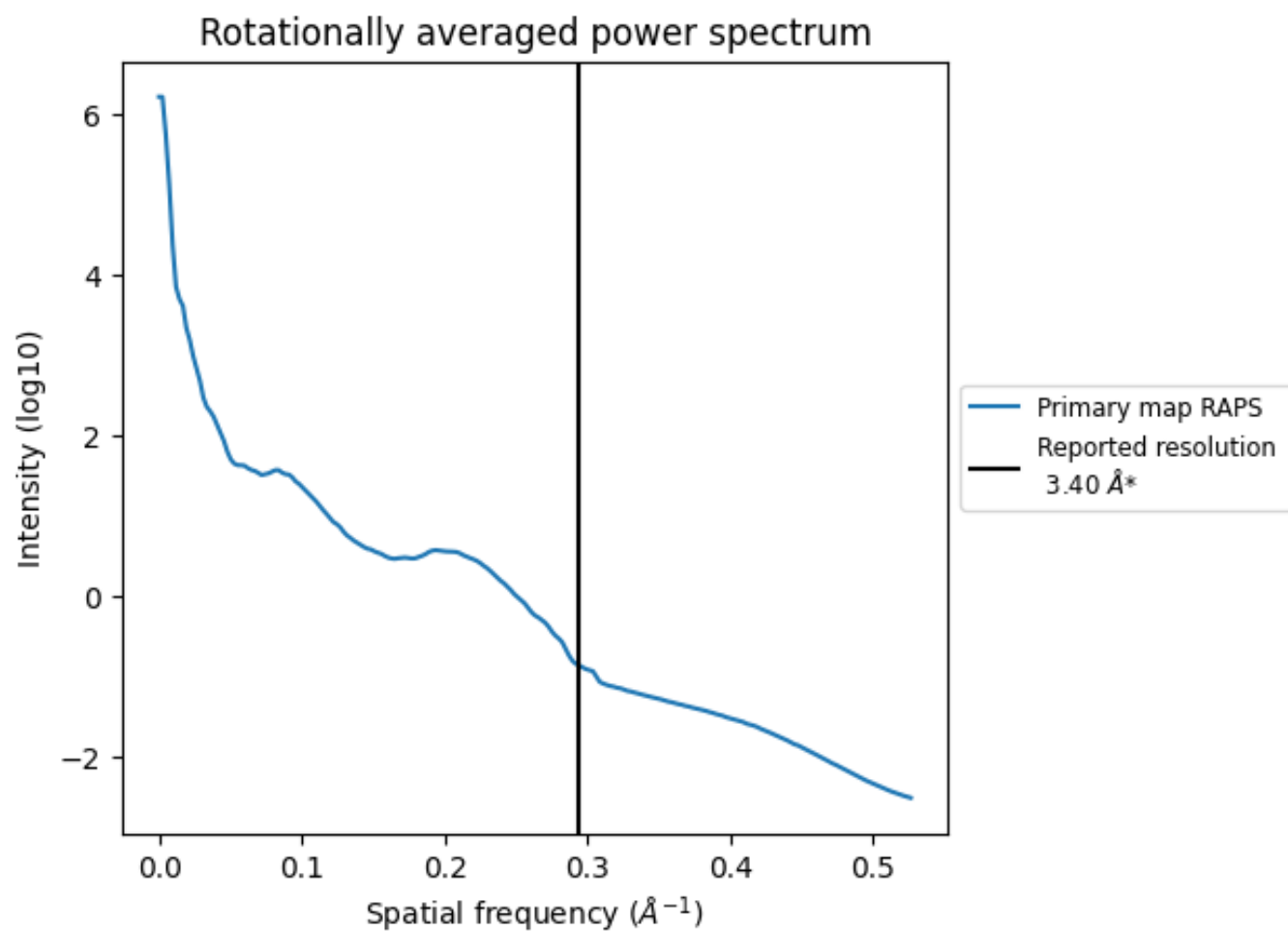
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 574 nm^3 ; this corresponds to an approximate mass of 519 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 0.294 Å⁻¹

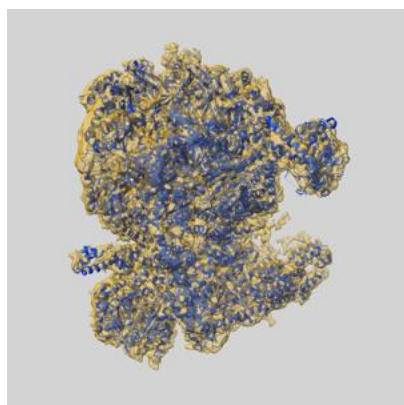
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

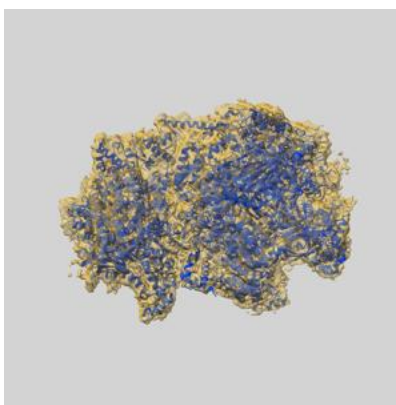
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51401 and PDB model 9GJP. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

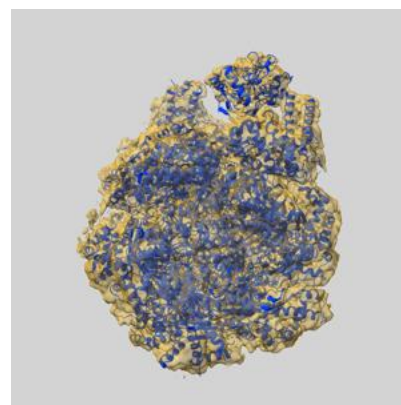
9.1 Map-model overlay [i](#)



X



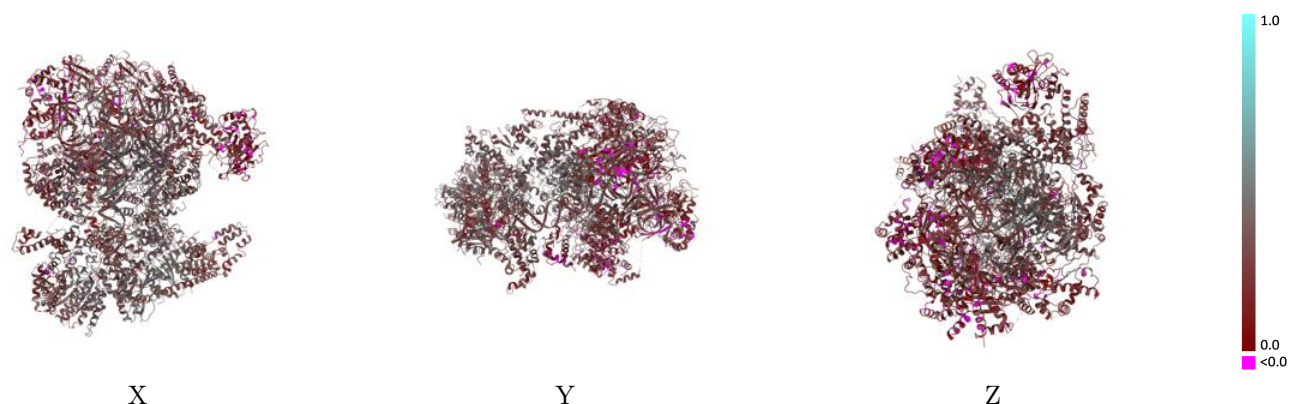
Y



Z

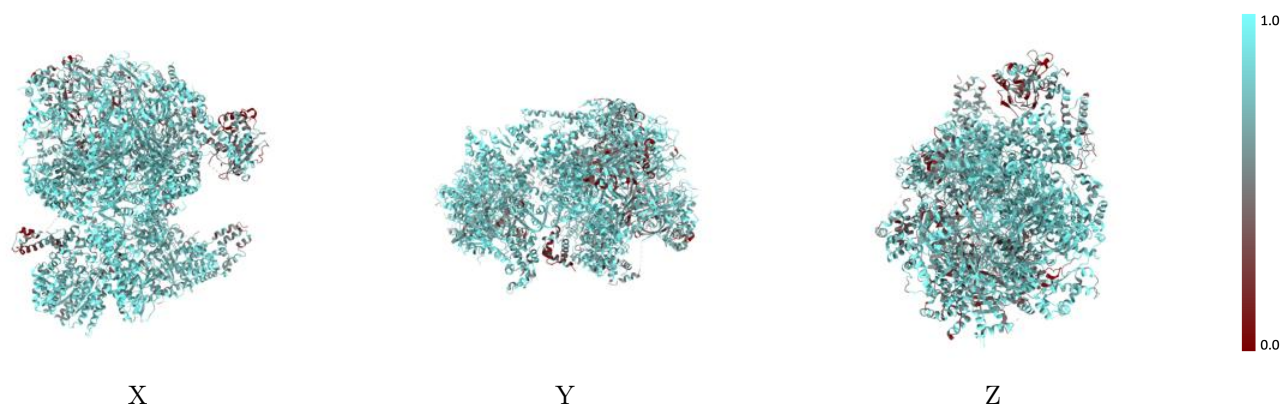
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



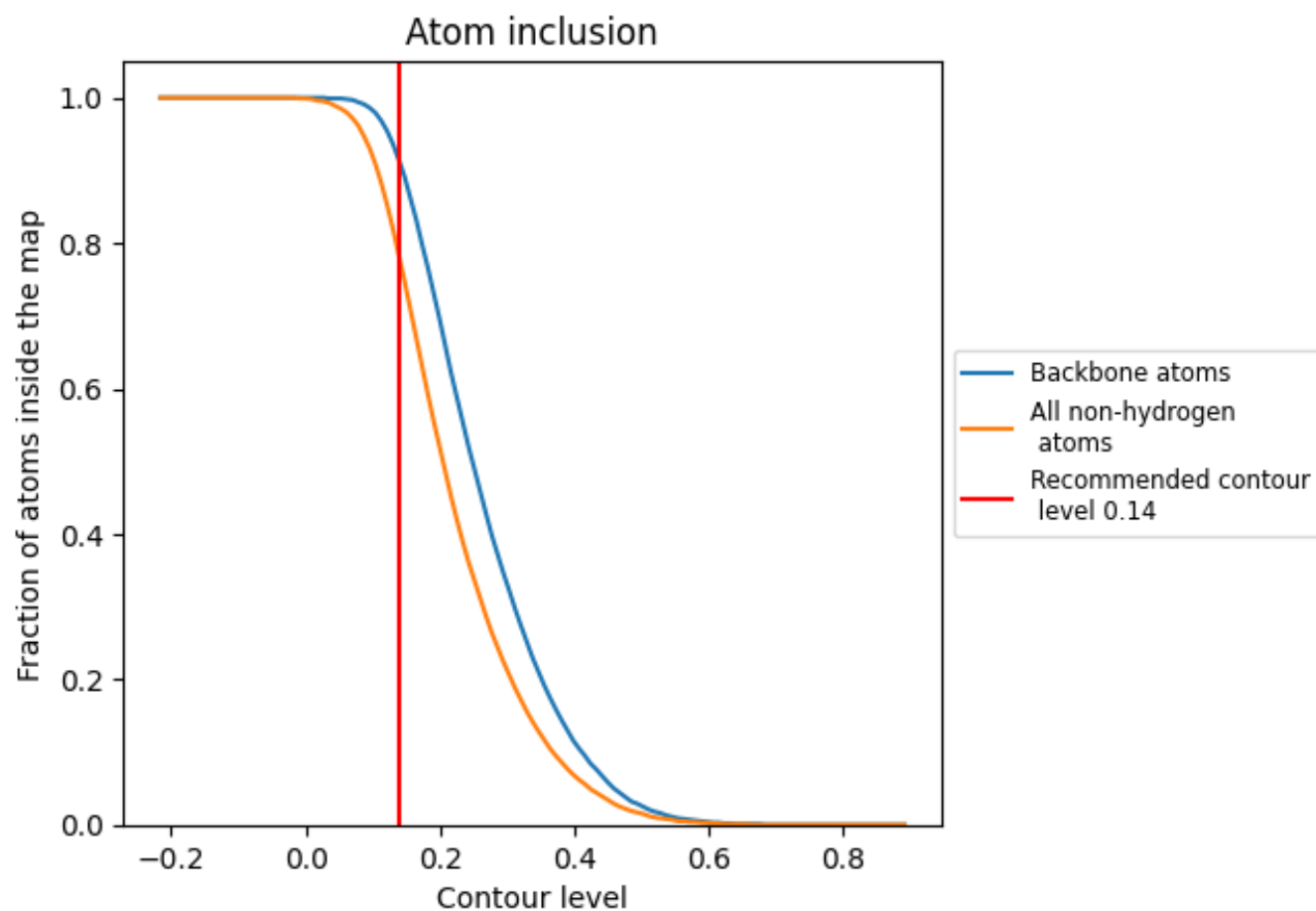
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

































9.4 Atom inclusion ⓘ



At the recommended contour level, 91% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.2930
2	 0.8630	 0.3660
3	 0.6680	 0.1990
4	 0.7940	 0.2780
5	 0.7560	 0.2420
6	 0.8560	 0.3510
7	 0.7210	 0.2080
8	 0.6060	 0.2100
A	 0.7750	 0.3420
B	 0.8350	 0.3660
C	 0.7910	 0.3350
D	 0.8220	 0.3340
E	 0.8630	 0.3870
F	 0.6250	 0.3000
X	 0.8620	 0.2620
Y	 0.8480	 0.2700

