Full wwPDB EM Validation Report ⓘ

Feb 27, 2025 – 06:10 pm GMT

PDB ID	:	9GM5
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:

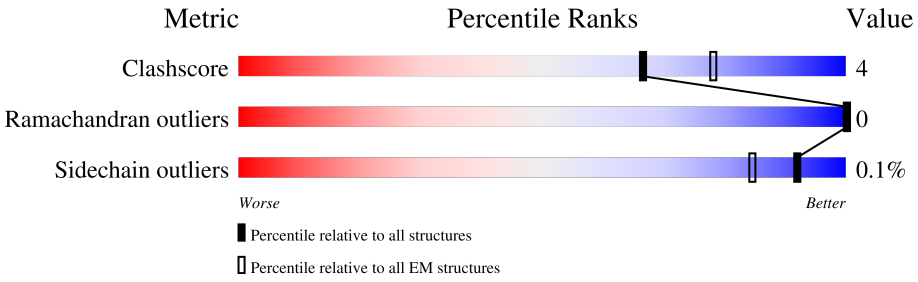
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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)
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 <=5%

Mol	Chain	Length	Quality of chain
1	2	868	65% 8% 27%
2	3	1006	53% 5% 42%
3	4	933	59% 9% 33%
4	5	775	73% 9% 18%
5	6	1017	56% 11% 33%
6	7	845	64% · 32%
7	8	604	77% 7% 16%
8	A	949	41% · 56%
9	B	560	36% · 60%

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

2 Entry composition (i)

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		

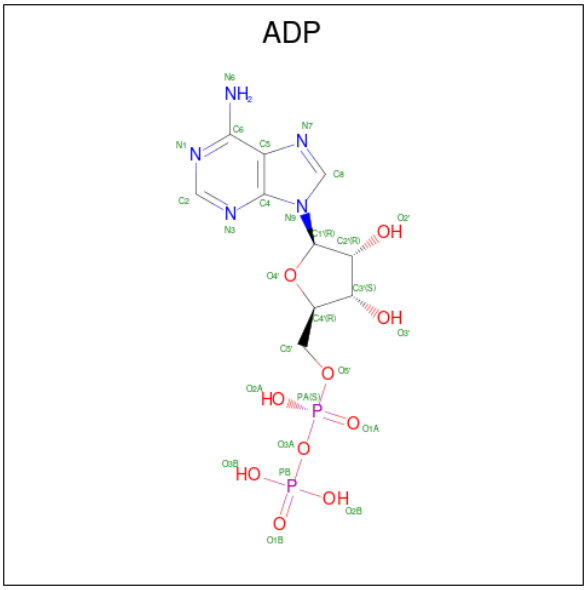
- Molecule 13 is a protein called Origin recognition complex subunit 6.

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 (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	
16	5	1	Total	Zn	0
			1	1	

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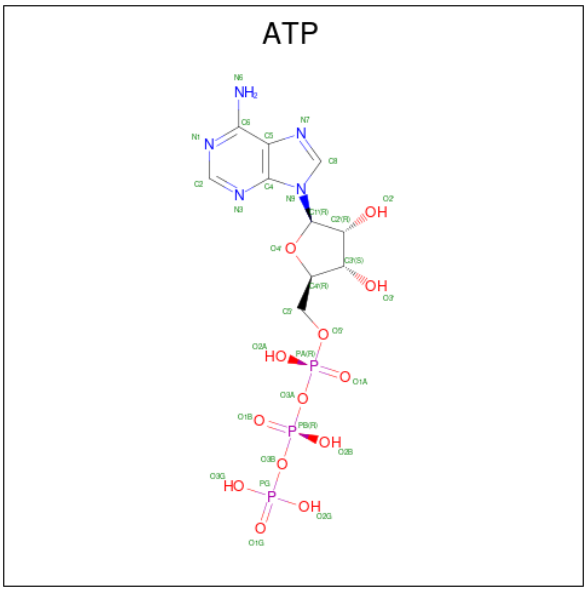
Mol	Chain	Residues	Atoms	AltConf
16	6	1	Total Zn 1 1	0
16	7	1	Total Zn 1 1	0

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



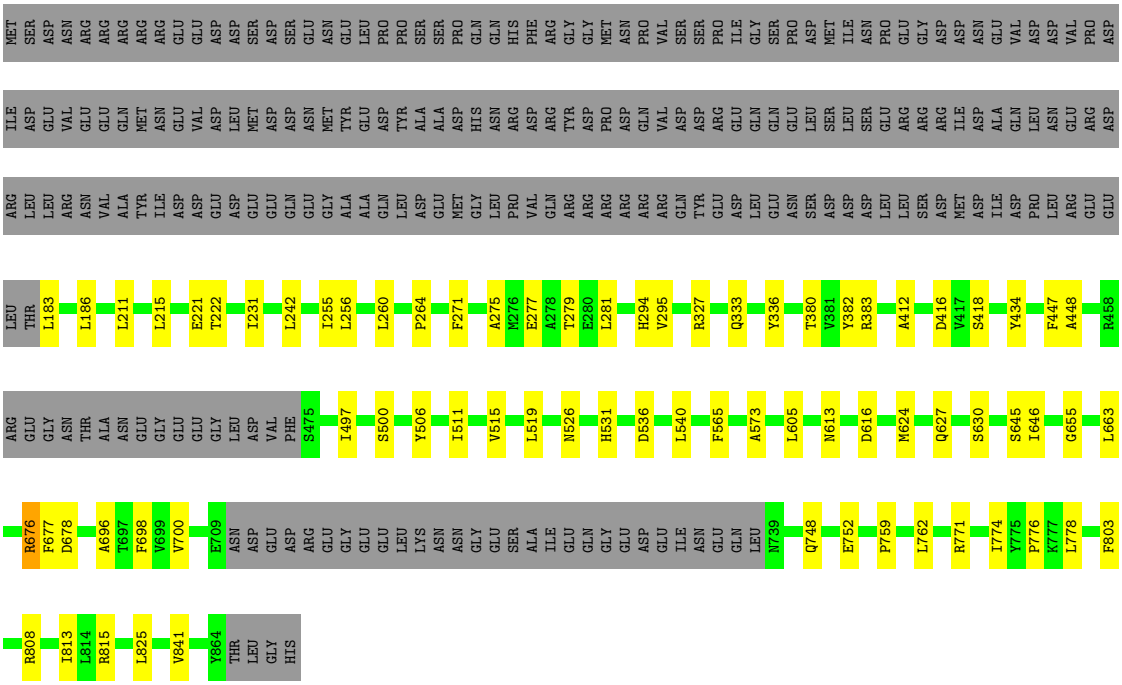
Mol	Chain	Residues	Atoms	AltConf
17	D	1	Total C N O P 31 10 5 13 3	0
17	E	1	Total C N O P 31 10 5 13 3	0

3 Residue-property plots (i)

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

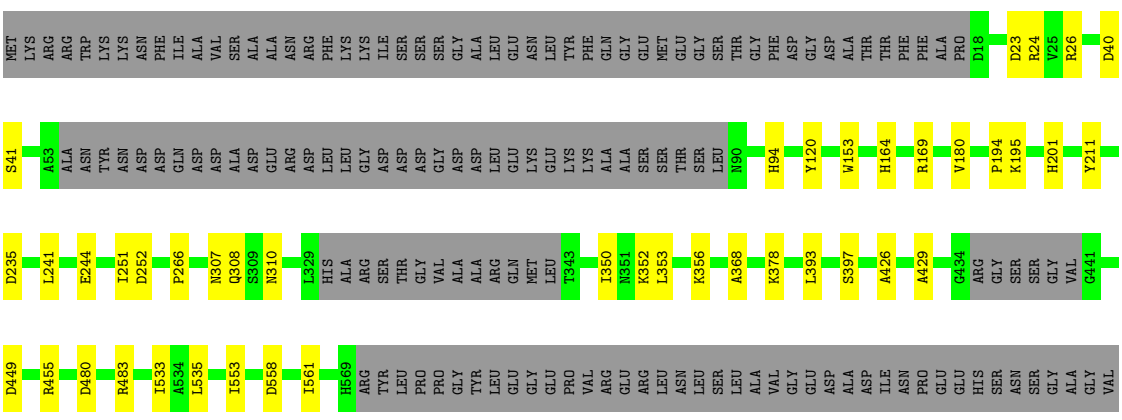
- Molecule 1: DNA replication licensing factor MCM2

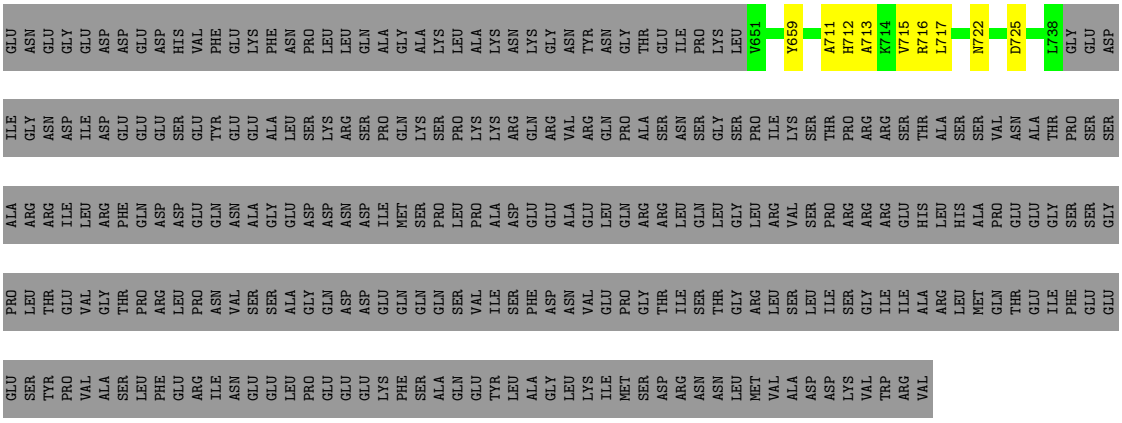
Chain 2:



- Molecule 2: DNA replication licensing factor MCM3

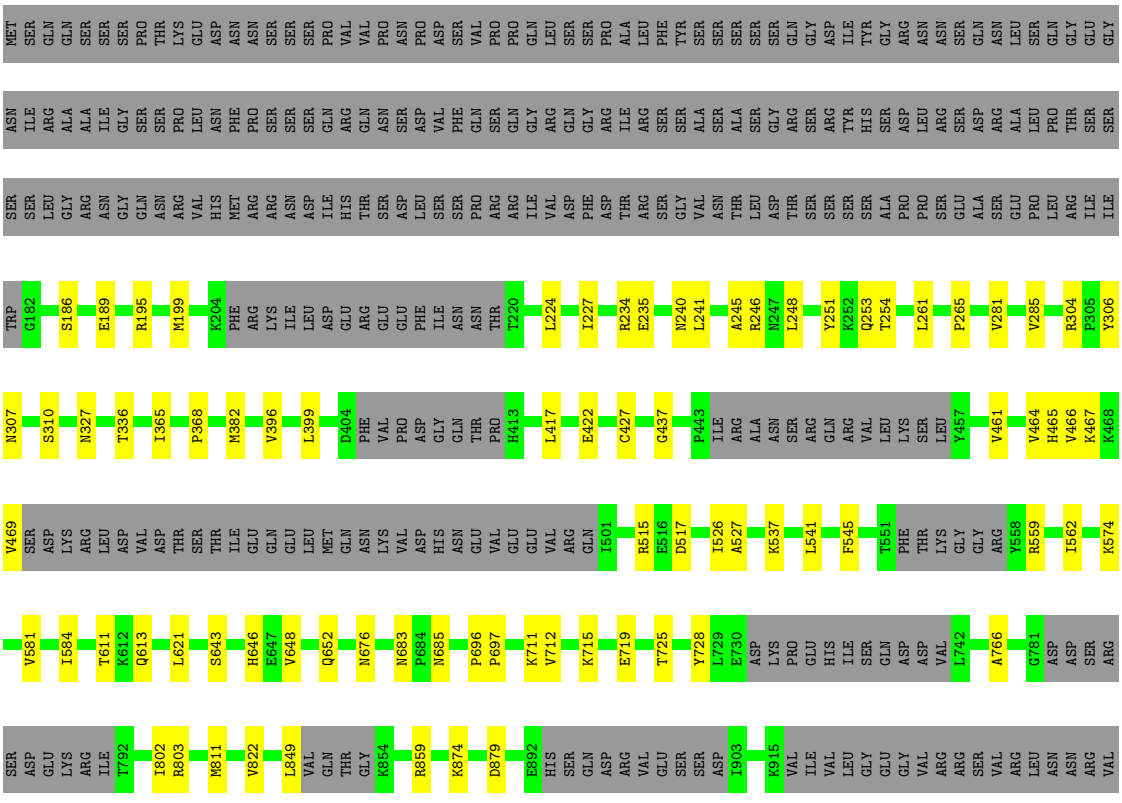
Chain 3:





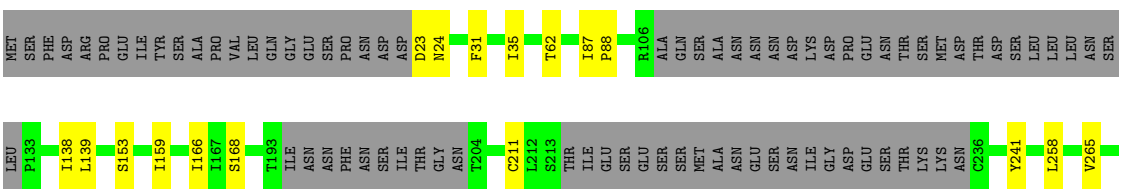
• Molecule 3: DNA replication licensing factor MCM4

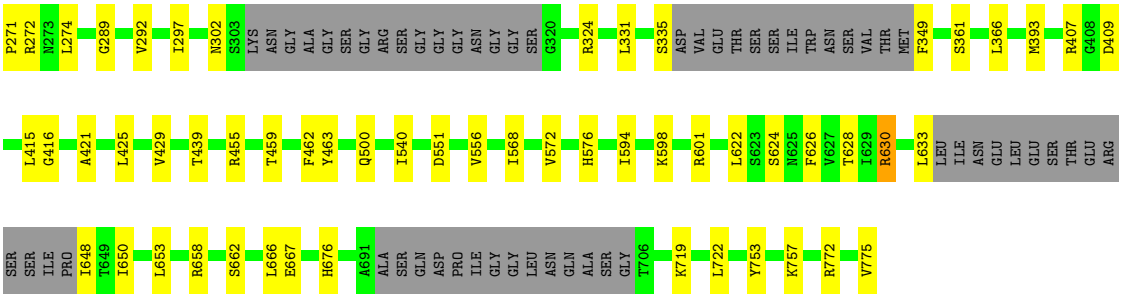
Chain 4:



• Molecule 4: Minichromosome maintenance protein 5

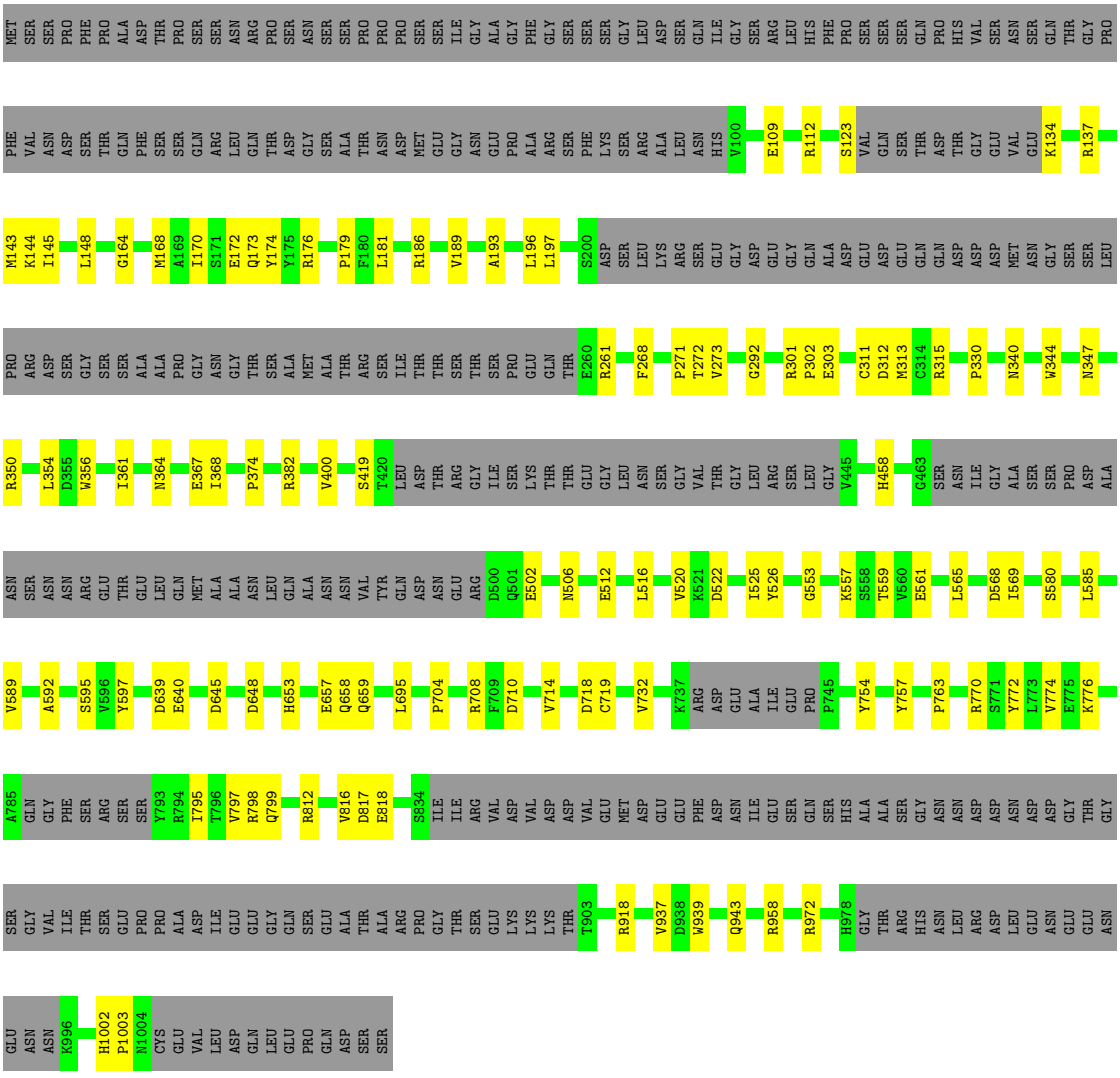
Chain 5:





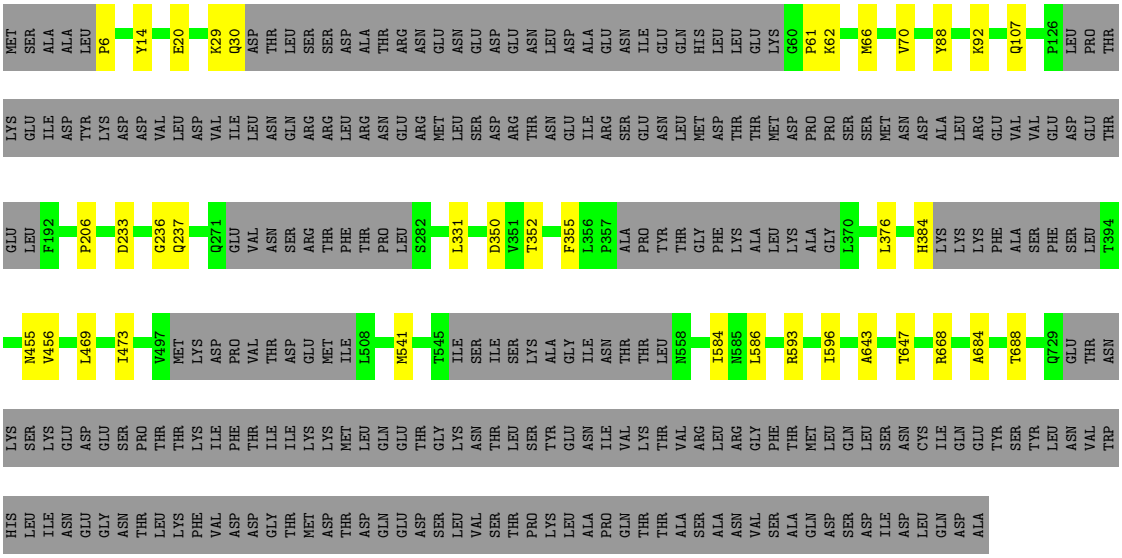
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



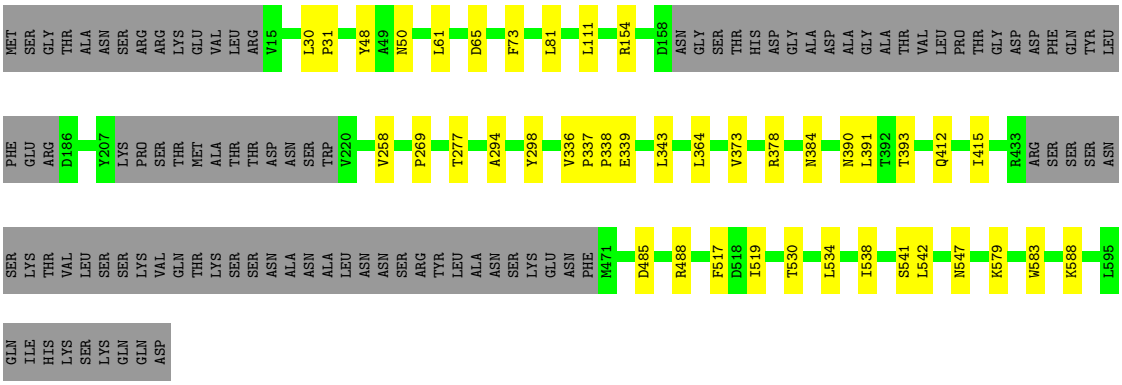
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



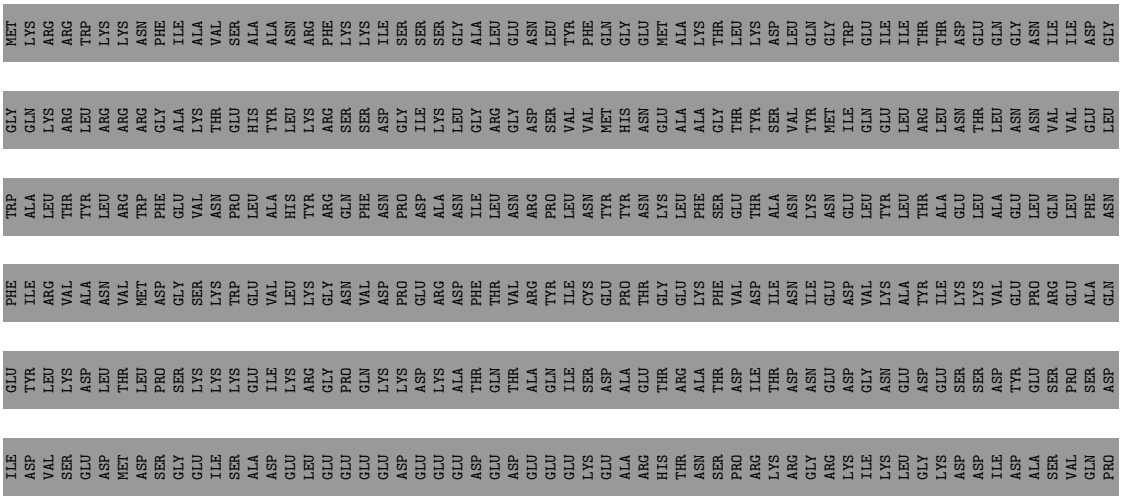
• Molecule 7: Cell division cycle protein CDT1

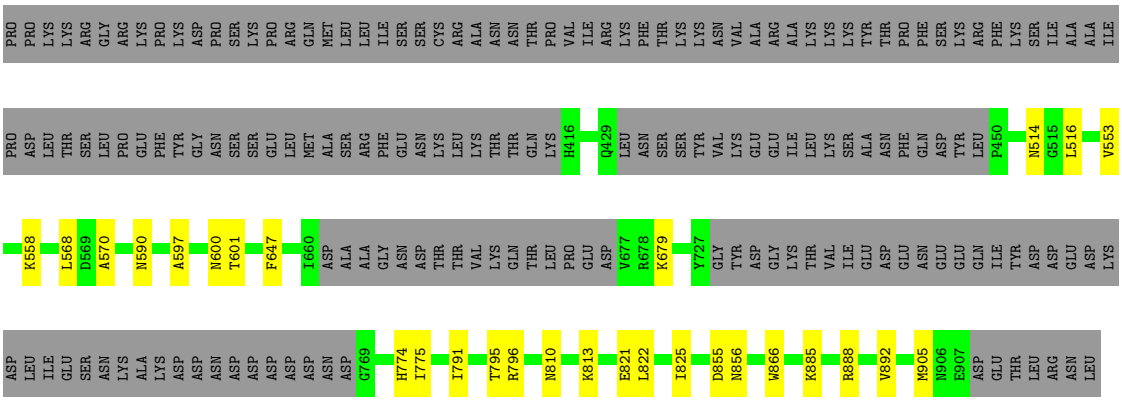
Chain 8:



• Molecule 8: Origin recognition complex subunit 1

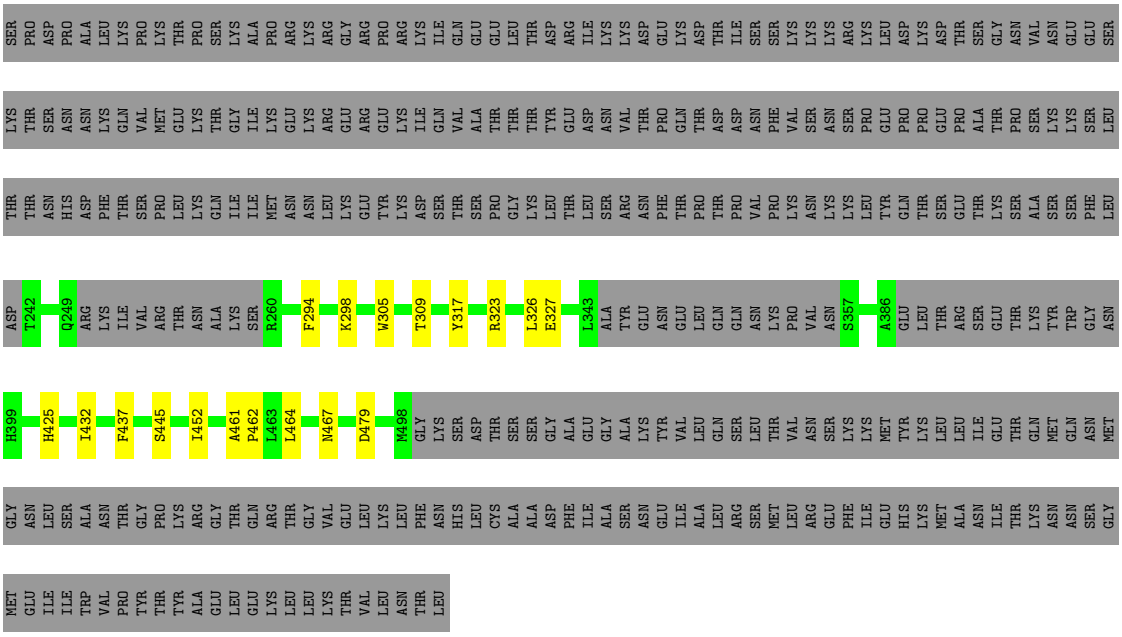
Chain A:





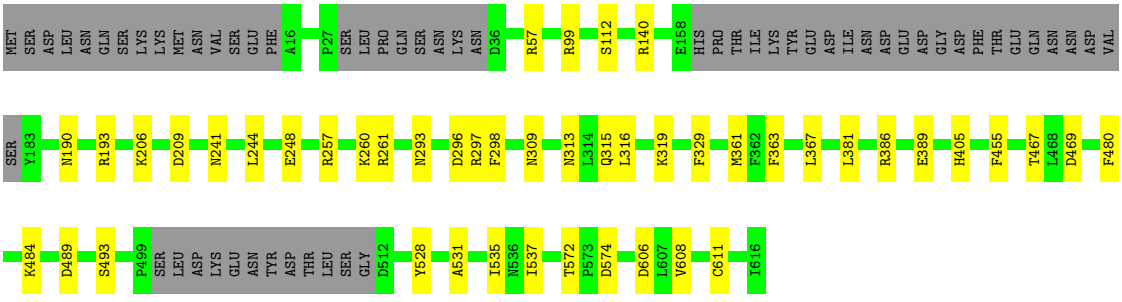
• Molecule 9: Origin recognition complex subunit 2

Chain B:



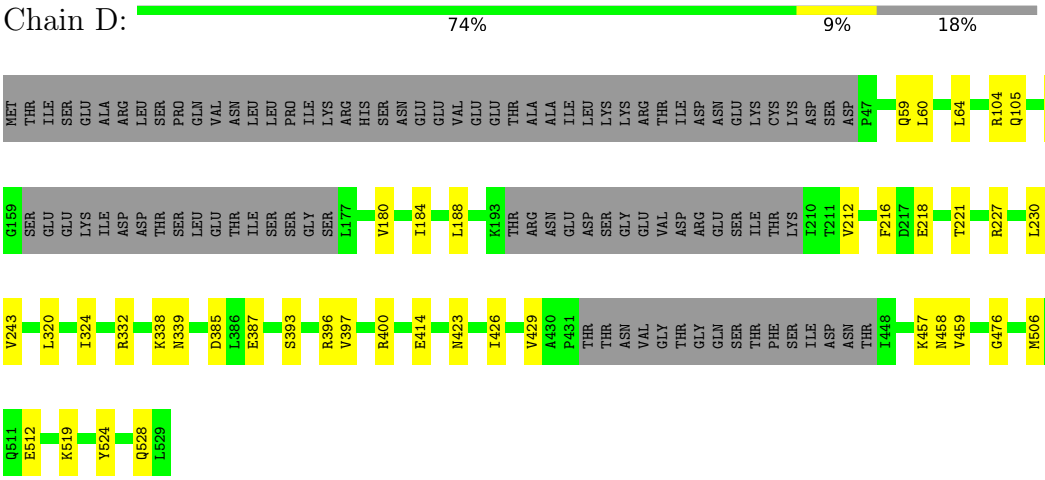
• Molecule 10: Origin recognition complex subunit 3

Chain C:



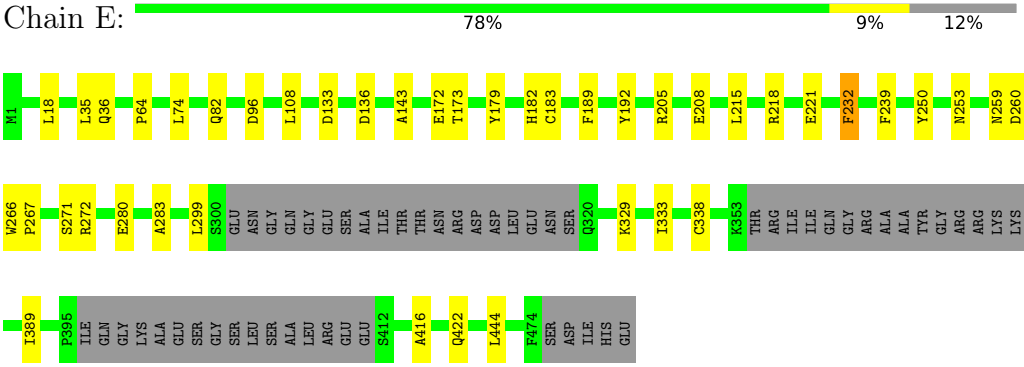
• Molecule 11: Origin recognition complex subunit 4

Chain D:



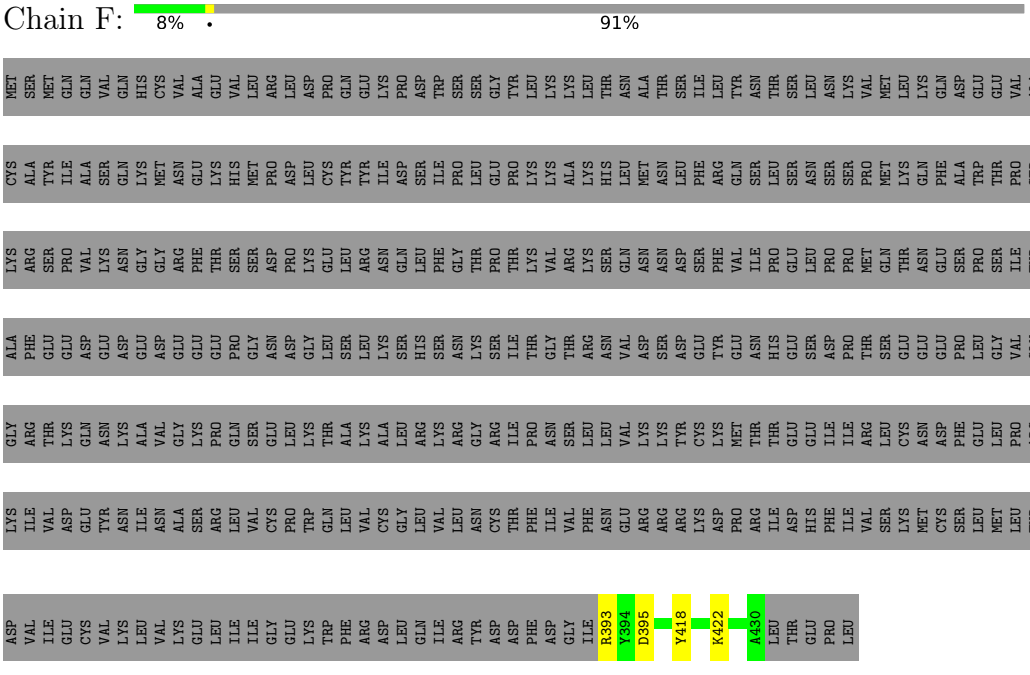
• Molecule 12: Origin recognition complex subunit 5

Chain E:



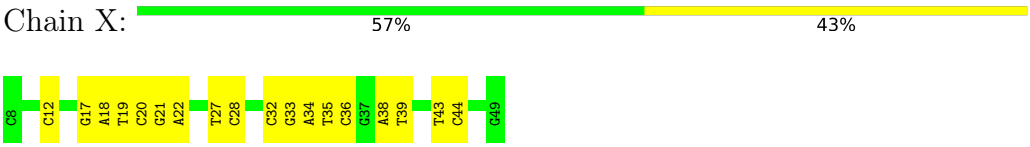
• Molecule 13: Origin recognition complex subunit 6

Chain F:



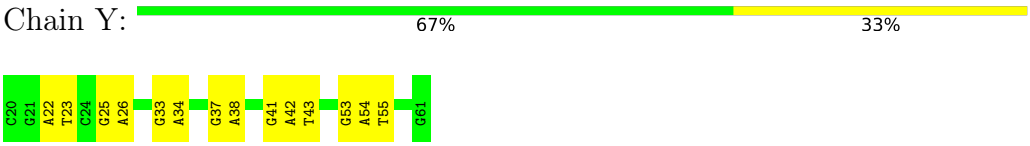
• Molecule 14: DNA

Chain X:



• Molecule 14: DNA

Chain Y:



4 Experimental information (i)

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 ($e^-/Å^2$)	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

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	0.25	0/5145	0.51	0/6945
2	3	0.24	0/4661	0.49	0/6323
3	4	0.24	0/5024	0.48	0/6775
4	5	0.24	0/5131	0.48	0/6921
5	6	0.25	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	0.24	0/3358	0.45	0/4519
9	B	0.25	0/1892	0.44	0/2556
10	C	0.25	0/4717	0.44	0/6364
11	D	0.25	0/3606	0.45	0/4873
12	E	0.25	0/3526	0.44	0/4791
13	F	0.22	0/328	0.47	0/440
14	X	0.52	0/965	0.96	0/1487
14	Y	0.53	0/965	0.98	0/1487
All	All	0.26	0/53545	0.50	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

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	30	0
3	4	4964	0	5031	45	0
4	5	5059	0	5144	45	0
5	6	5408	0	5458	72	0
6	7	4541	0	4583	21	0
7	8	4047	0	4117	24	0
8	A	3310	0	3406	19	0
9	B	1845	0	1815	10	0
10	C	4618	0	4589	29	0
11	D	3542	0	3610	33	0
12	E	3444	0	3463	31	0
13	F	324	0	330	3	0
14	X	861	0	473	13	0
14	Y	861	0	473	10	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	391	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 (391) 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)
3:4:399: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
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
8:A:558:LYS:NZ	8:A:590:ASN:O	2.27	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
3:4:874:LYS:NZ	3:4:879:ASP:OD1	2.36	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
4:5:258:LEU:O	4:5:274:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
14:X:33:DG:H2"	14:X:34:DA:H8	1.78	0.47
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
4:5:459:THR:HG1	4:5:463:TYR:HH	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:7:684: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
5:6:123:SER:HG	5:6:134:LYS:N	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:4:336:THR:HG1	3:4:396:VAL:H	1.63	0.42
9:B:305:TRP:CZ3	9:B:309:THR:HG21	2.54	0.42
14:Y:42:DA:C8	14:Y:43:DT:H72	2.54	0.42
1:2:676:ARG:HG3	1:2:808:ARG:NH2	2.35	0.42
4:5:626:PHE:CZ	4:5:650:ILE:HA	2.54	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:7:20:GLU:OE1	6:7:92:LYS:NZ	2.45	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
8:A:888:ARG:HH12	11:D:512:GLU:CD	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:D:400:ARG:HH12	11:D:414:GLU:CD	2.23	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
1:2:497:ILE:O	1:2:500:SER:OG	2.34	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
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
10:C:528:TYR:HH	10:C:611:CYS:H	1.69	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	567 (100%)	0	100	100
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%)	458 (100%)	1 (0%)	92	96
8	A	366/842 (44%)	366 (100%)	0	100	100
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%)	391 (100%)	1 (0%)	91	94
13	F	36/406 (9%)	36 (100%)	0	100	100
All	All	5690/8622 (66%)	5686 (100%)	4 (0%)	92	96

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

Mol	Chain	Res	Type
1	2	676	ARG
4	5	630	ARG
7	8	583	TRP
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
5	6	340	ASN
11	D	458	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	$\#\|Z\| > 2$
17	ATP	E	501	-	26,33,33	0.62	0	31,52,52	0.81	2 (6%)
15	ADP	5	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
15	ADP	2	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	ATP	D	601	-	26,33,33	0.60	0	31,52,52	0.79	1 (3%)
15	ADP	6	1101	-	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)
15	ADP	4	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.33	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ATP	E	501	-	-	5/18/38/38	0/3/3/3
15	ADP	5	901	-	-	1/12/32/32	0/3/3/3
15	ADP	2	901	-	-	5/12/32/32	0/3/3/3
17	ATP	D	601	-	-	5/18/38/38	0/3/3/3
15	ADP	6	1101	-	-	3/12/32/32	0/3/3/3
15	ADP	4	1001	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5	901	ADP	C5-C4	2.49	1.47	1.40
15	6	1101	ADP	C5-C4	2.47	1.47	1.40
15	4	1001	ADP	C5-C4	2.47	1.47	1.40
15	2	901	ADP	C5-C4	2.44	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	5	901	ADP	PA-O3A-PB	-3.86	119.59	132.83
15	6	1101	ADP	C3'-C2'-C1'	3.75	106.62	100.98
15	6	1101	ADP	PA-O3A-PB	-3.62	120.41	132.83
15	2	901	ADP	C3'-C2'-C1'	3.56	106.34	100.98
15	2	901	ADP	PA-O3A-PB	-3.51	120.78	132.83
15	5	901	ADP	N3-C2-N1	-3.15	123.75	128.68
15	5	901	ADP	C3'-C2'-C1'	3.14	105.71	100.98
15	4	1001	ADP	N3-C2-N1	-3.12	123.81	128.68
15	6	1101	ADP	N3-C2-N1	-3.08	123.86	128.68
15	2	901	ADP	N3-C2-N1	-3.02	123.95	128.68
15	4	1001	ADP	C3'-C2'-C1'	2.96	105.44	100.98
15	6	1101	ADP	C4-C5-N7	-2.77	106.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	5	901	ADP	C4-C5-N7	-2.73	106.55	109.40
15	4	1001	ADP	C4-C5-N7	-2.66	106.63	109.40
15	4	1001	ADP	PA-O3A-PB	-2.44	124.45	132.83
17	D	601	ATP	C5-C6-N6	2.32	123.88	120.35
17	E	501	ATP	C5-C6-N6	2.28	123.81	120.35
15	2	901	ADP	C4-C5-N7	-2.25	107.06	109.40
17	E	501	ATP	PB-O3B-PG	2.02	139.77	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

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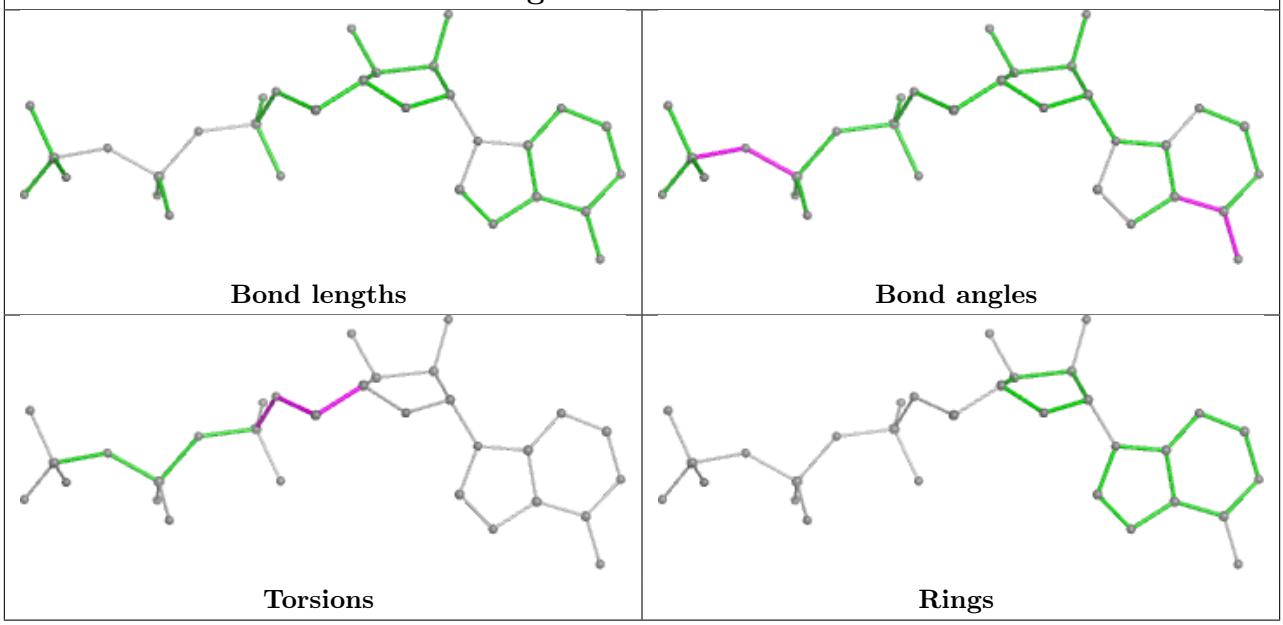
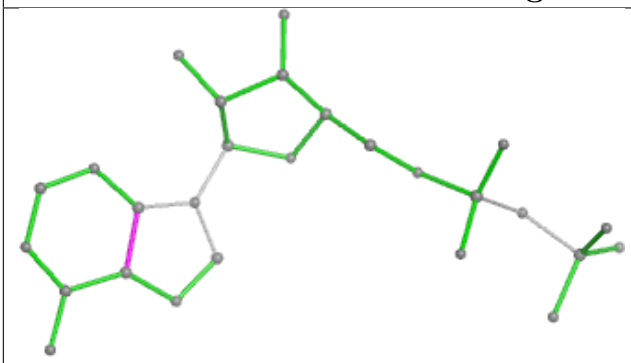
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	6	1101	ADP	1	0
15	4	1001	ADP	1	0

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 then 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.

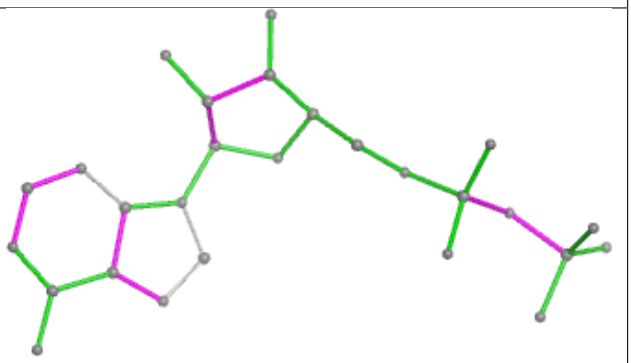
Ligand ATP E 501



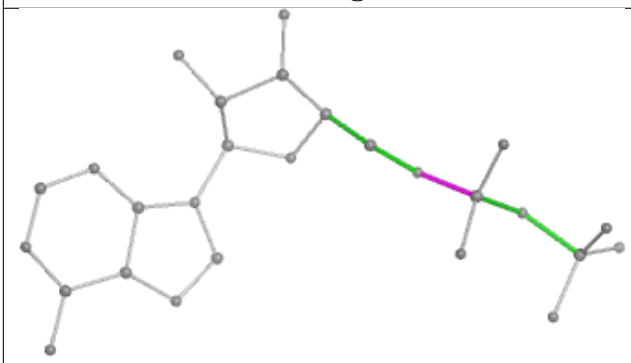
Ligand ADP 5 901



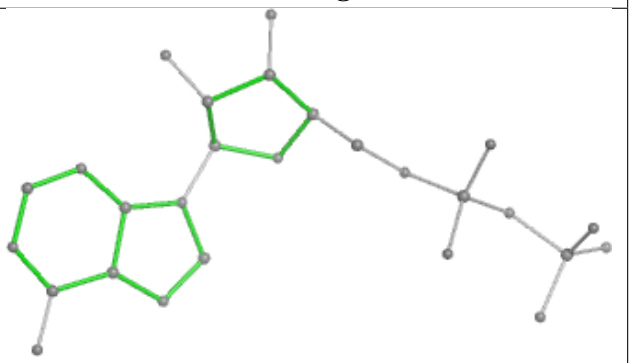
Bond lengths



Bond angles

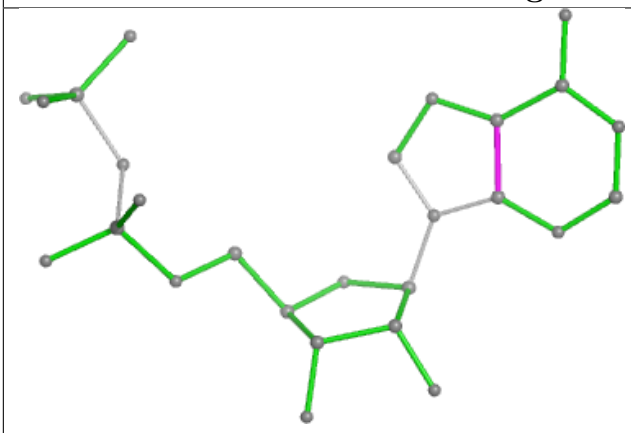


Torsions

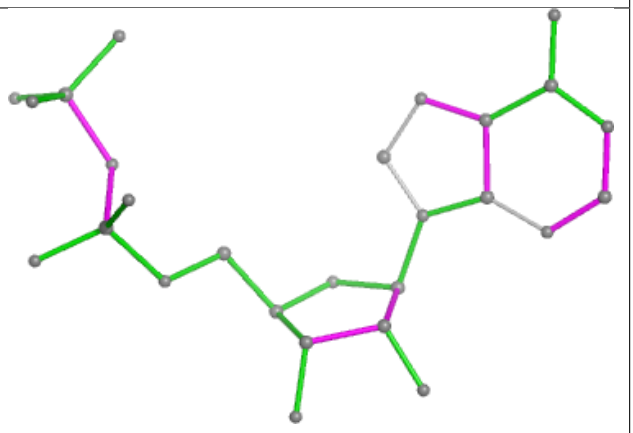


Rings

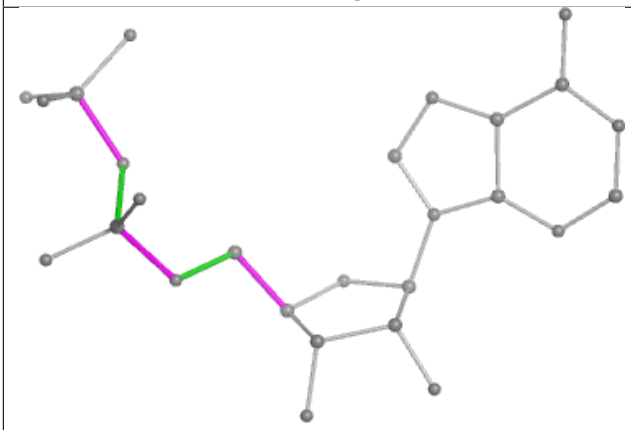
Ligand ADP 2 901



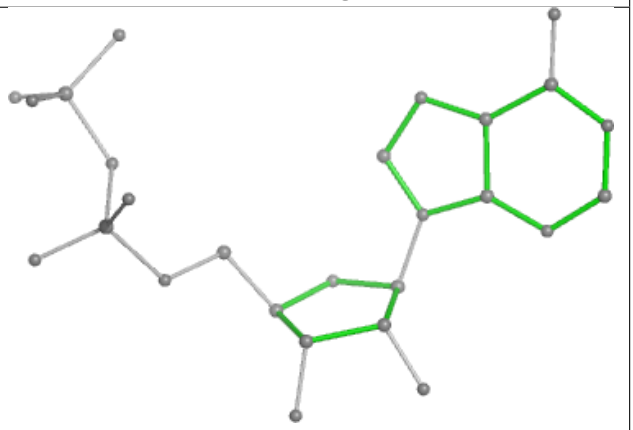
Bond lengths



Bond angles

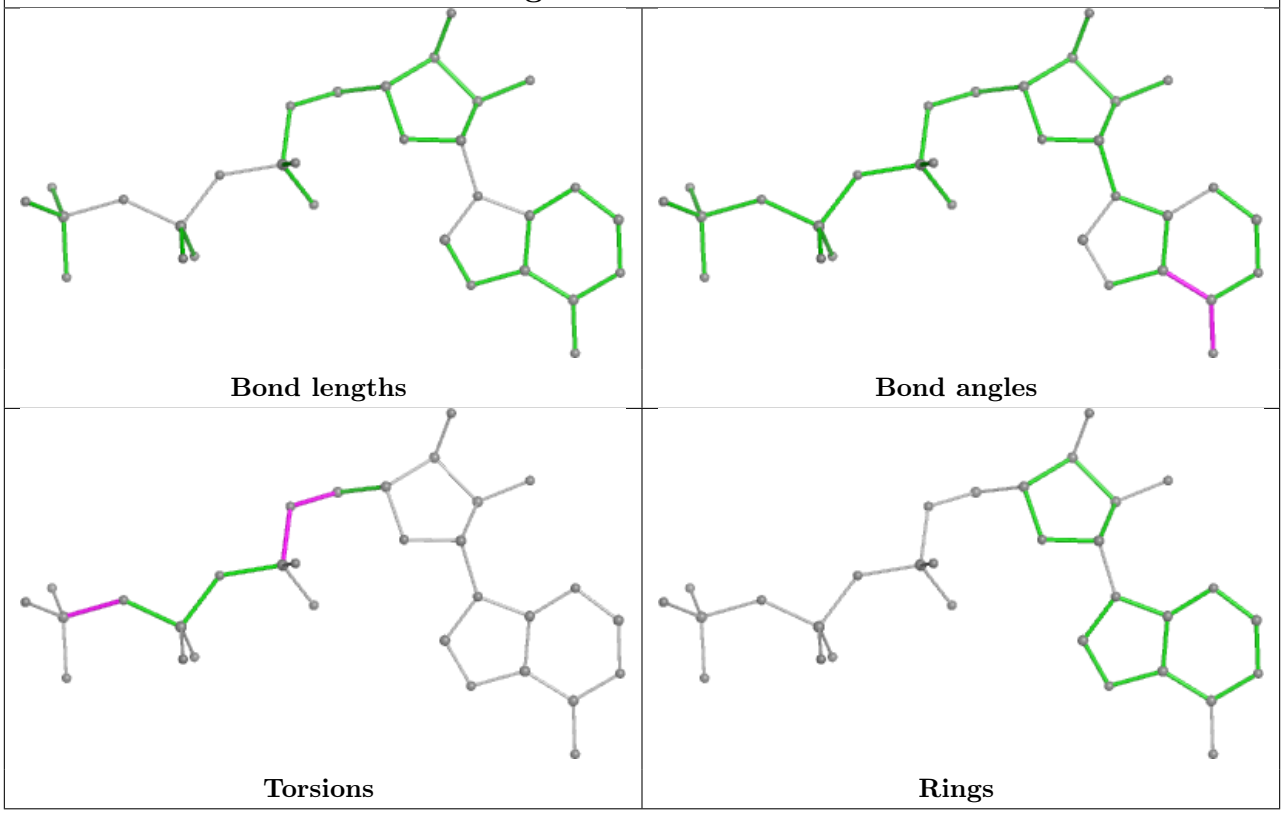


Torsions

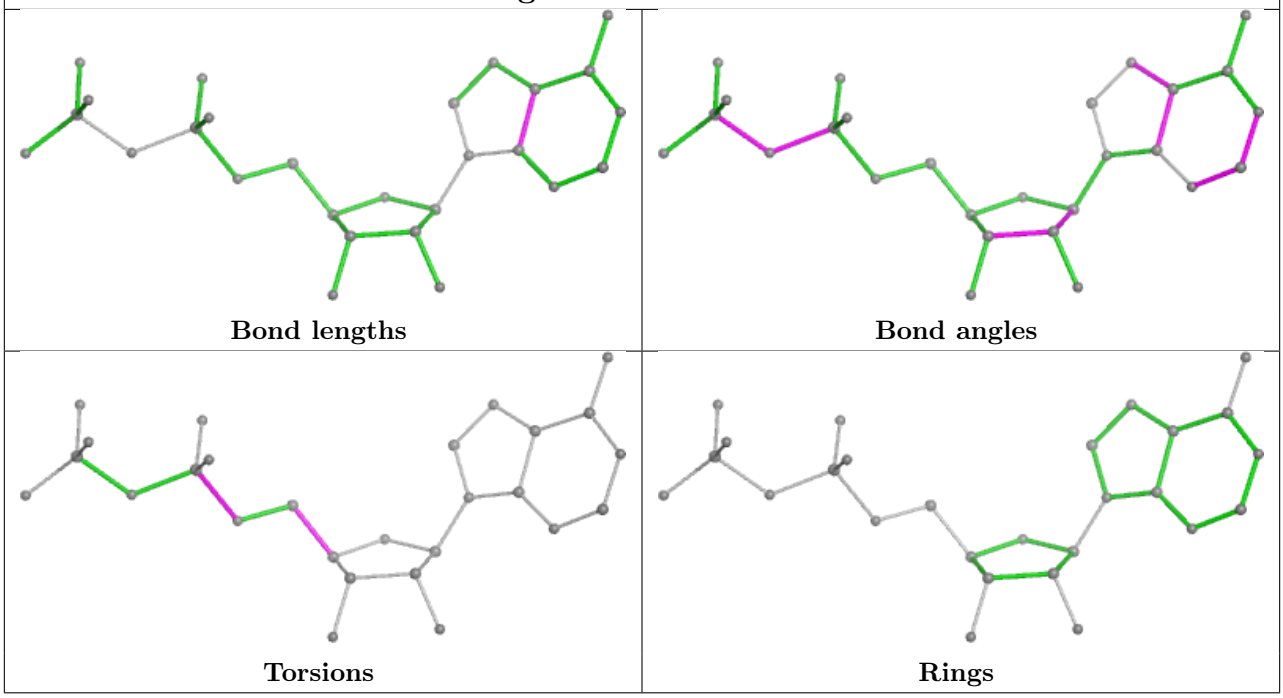


Rings

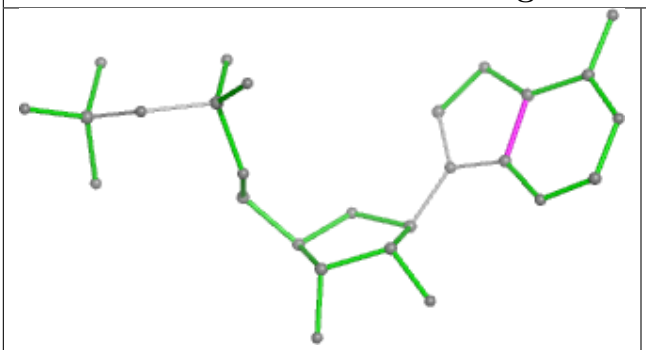
Ligand ATP D 601



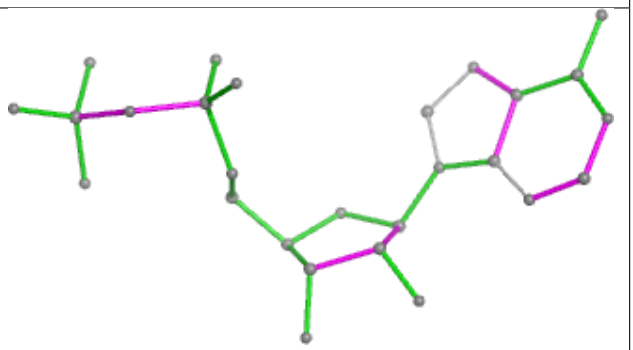
Ligand ADP 6 1101



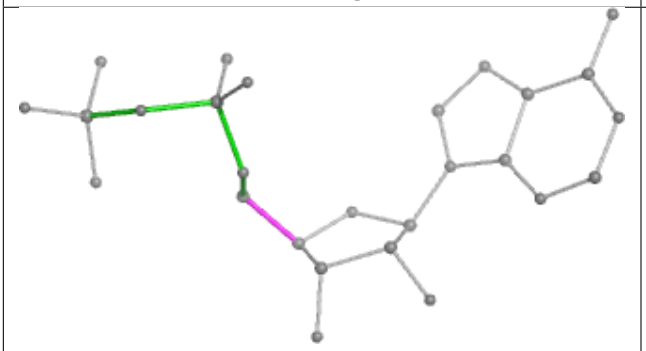
Ligand ADP 4 1001



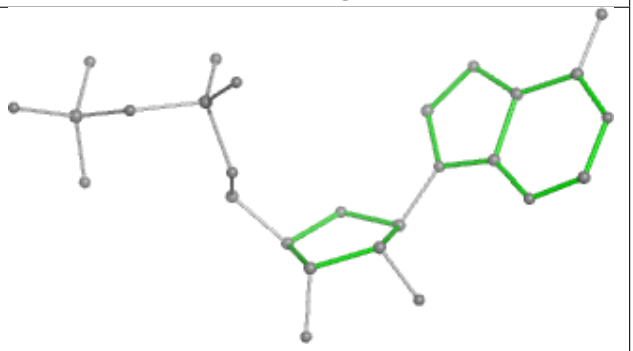
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.