



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 02:50 PM EDT

PDB ID : 6MII
Title : Crystal structure of minichromosome maintenance protein MCM/DNA complex
Authors : Enemark, E.J.; Meagher, M.; Epling, L.B.
Deposited on : 2018-09-19
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

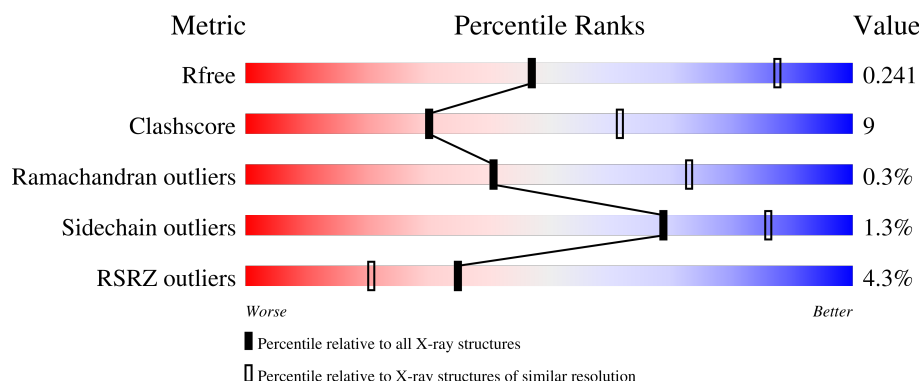
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


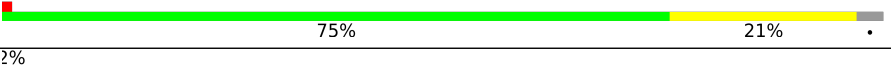
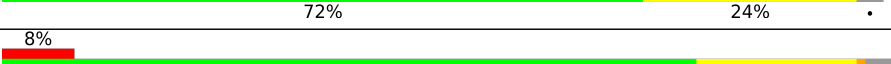
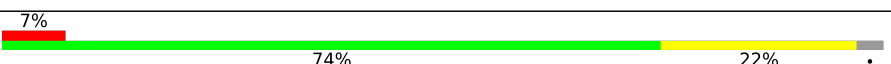

The reported resolution of this entry is 3.15 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	610	
1	B	610	
1	C	610	
1	D	610	
1	E	610	

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Mol	Chain	Length	Quality of chain
1	F	610	<div><div></div><div>4%</div><div>71%</div><div>25%</div><div></div></div>
2	X	12	<div><div></div><div>17%</div><div>58%</div><div>8%</div><div>17%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28494 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Minichromosome maintenance protein MCM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4655	2969	799	873	14			
1	B	589	Total	C	N	O	S	0	0	0
			4683	2985	803	881	14			
1	C	589	Total	C	N	O	S	0	0	0
			4683	2985	803	881	14			
1	D	589	Total	C	N	O	S	0	0	0
			4683	2985	803	881	14			
1	E	592	Total	C	N	O	S	0	0	0
			4702	2995	806	887	14			
1	F	589	Total	C	N	O	S	0	0	0
			4683	2985	803	881	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UXG1
A	1	LEU	-	expression tag	UNP Q9UXG1
A	269	GLY	-	linker	UNP Q9UXG1
A	270	GLY	-	linker	UNP Q9UXG1
A	271	SER	-	linker	UNP Q9UXG1
A	272	GLY	-	linker	UNP Q9UXG1
A	273	GLY	-	linker	UNP Q9UXG1
A	274	SER	-	linker	UNP Q9UXG1
B	0	SER	-	expression tag	UNP Q9UXG1
B	1	LEU	-	expression tag	UNP Q9UXG1
B	269	GLY	-	linker	UNP Q9UXG1
B	270	GLY	-	linker	UNP Q9UXG1
B	271	SER	-	linker	UNP Q9UXG1
B	272	GLY	-	linker	UNP Q9UXG1
B	273	GLY	-	linker	UNP Q9UXG1
B	274	SER	-	linker	UNP Q9UXG1
C	0	SER	-	expression tag	UNP Q9UXG1

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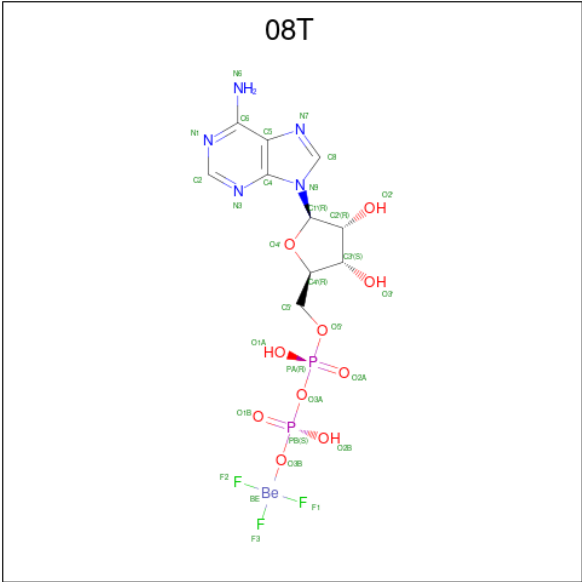
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LEU	-	expression tag	UNP Q9UXG1
C	269	GLY	-	linker	UNP Q9UXG1
C	270	GLY	-	linker	UNP Q9UXG1
C	271	SER	-	linker	UNP Q9UXG1
C	272	GLY	-	linker	UNP Q9UXG1
C	273	GLY	-	linker	UNP Q9UXG1
C	274	SER	-	linker	UNP Q9UXG1
D	0	SER	-	expression tag	UNP Q9UXG1
D	1	LEU	-	expression tag	UNP Q9UXG1
D	269	GLY	-	linker	UNP Q9UXG1
D	270	GLY	-	linker	UNP Q9UXG1
D	271	SER	-	linker	UNP Q9UXG1
D	272	GLY	-	linker	UNP Q9UXG1
D	273	GLY	-	linker	UNP Q9UXG1
D	274	SER	-	linker	UNP Q9UXG1
E	0	SER	-	expression tag	UNP Q9UXG1
E	1	LEU	-	expression tag	UNP Q9UXG1
E	269	GLY	-	linker	UNP Q9UXG1
E	270	GLY	-	linker	UNP Q9UXG1
E	271	SER	-	linker	UNP Q9UXG1
E	272	GLY	-	linker	UNP Q9UXG1
E	273	GLY	-	linker	UNP Q9UXG1
E	274	SER	-	linker	UNP Q9UXG1
F	0	SER	-	expression tag	UNP Q9UXG1
F	1	LEU	-	expression tag	UNP Q9UXG1
F	269	GLY	-	linker	UNP Q9UXG1
F	270	GLY	-	linker	UNP Q9UXG1
F	271	SER	-	linker	UNP Q9UXG1
F	272	GLY	-	linker	UNP Q9UXG1
F	273	GLY	-	linker	UNP Q9UXG1
F	274	SER	-	linker	UNP Q9UXG1

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	10	Total	C	N	O	P	0	0	0
			201	100	20	71	10			

- Molecule 3 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (three-letter code: 08T) (formula: C₁₀H₁₄BeF₃N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
3	B	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
3	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

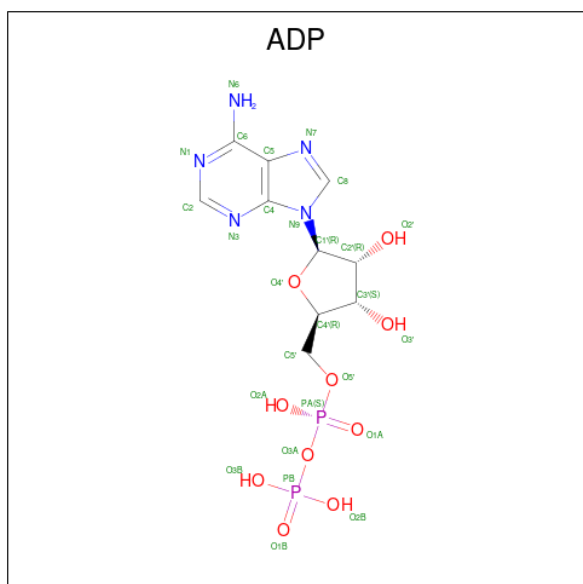
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O P 27 10 5 10 2	0	0
6	E	1	Total C N O P 27 10 5 10 2	0	0
6	F	1	Total C N O P 27 10 5 10 2	0	0

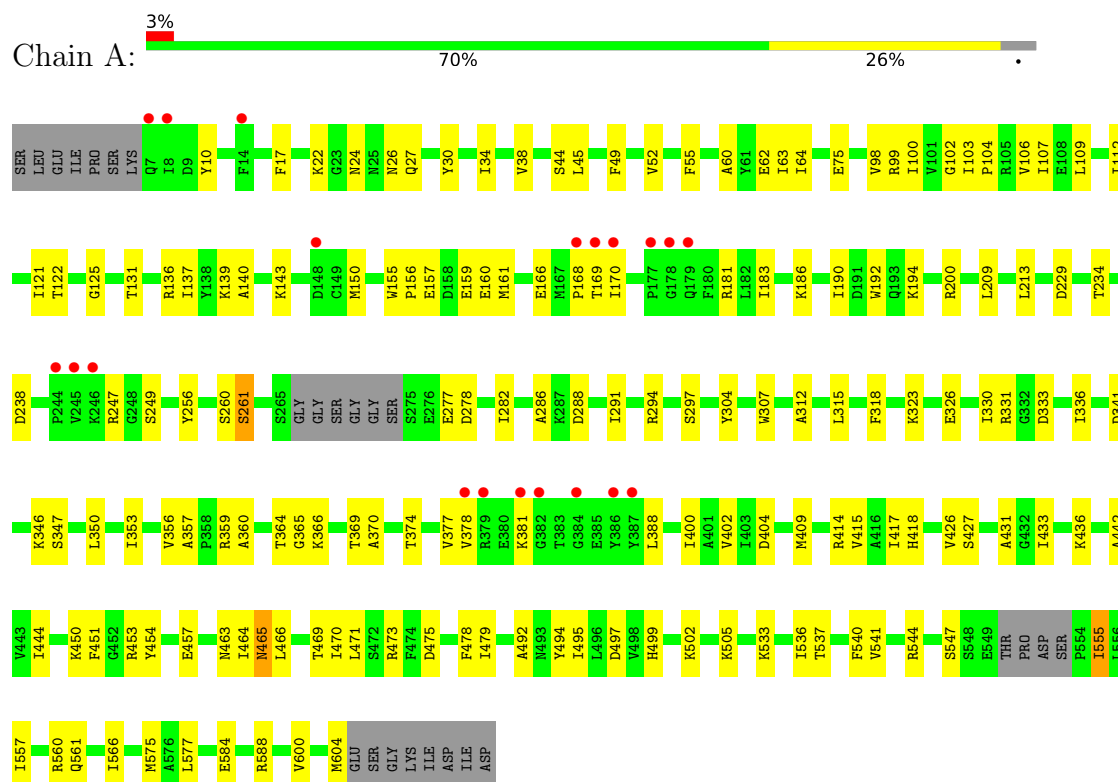
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	O 3	0	0
7	B	2	Total 2	O 2	0	0
7	C	3	Total 3	O 3	0	0
7	D	4	Total 4	O 4	0	0
7	E	3	Total 3	O 3	0	0
7	F	3	Total 3	O 3	0	0

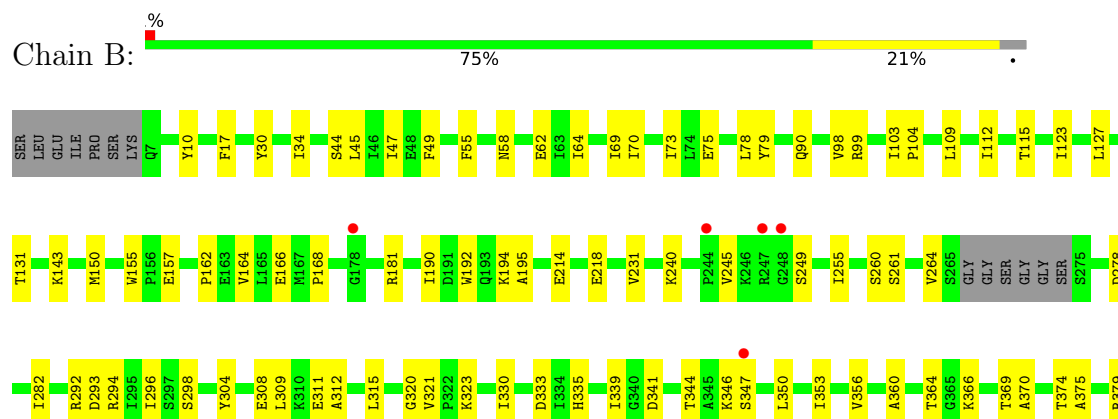
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

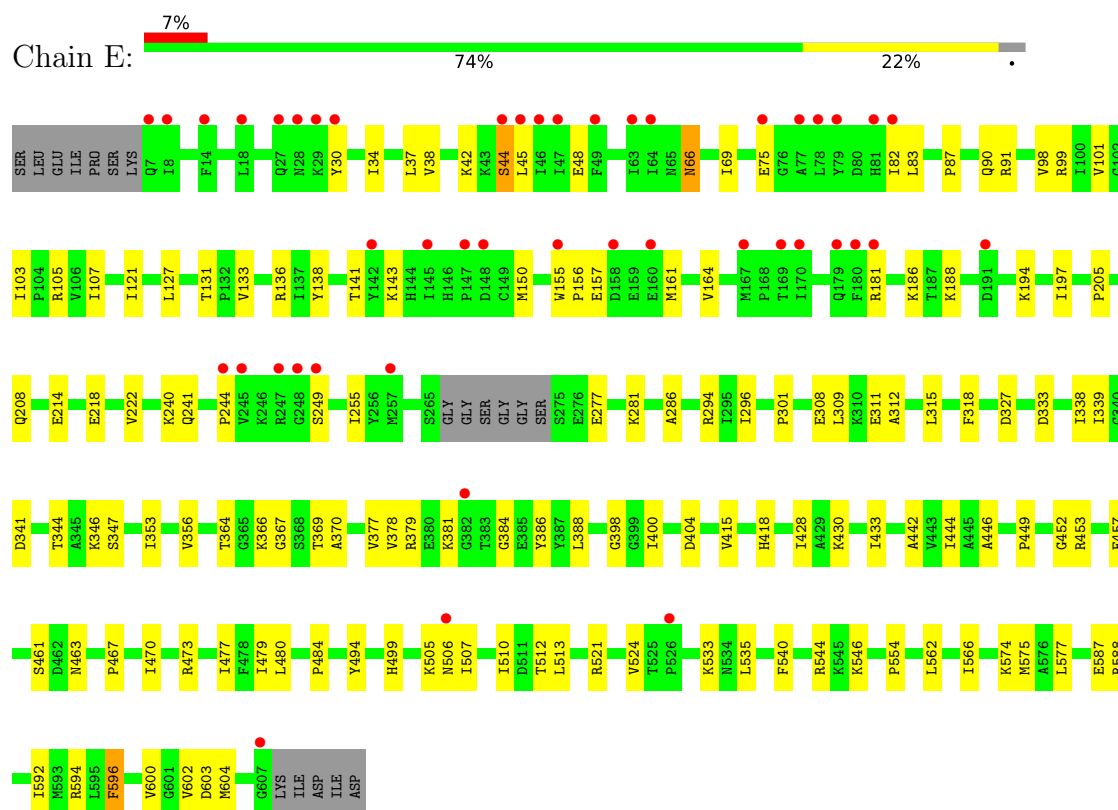
• Molecule 1: Minichromosome maintenance protein MCM



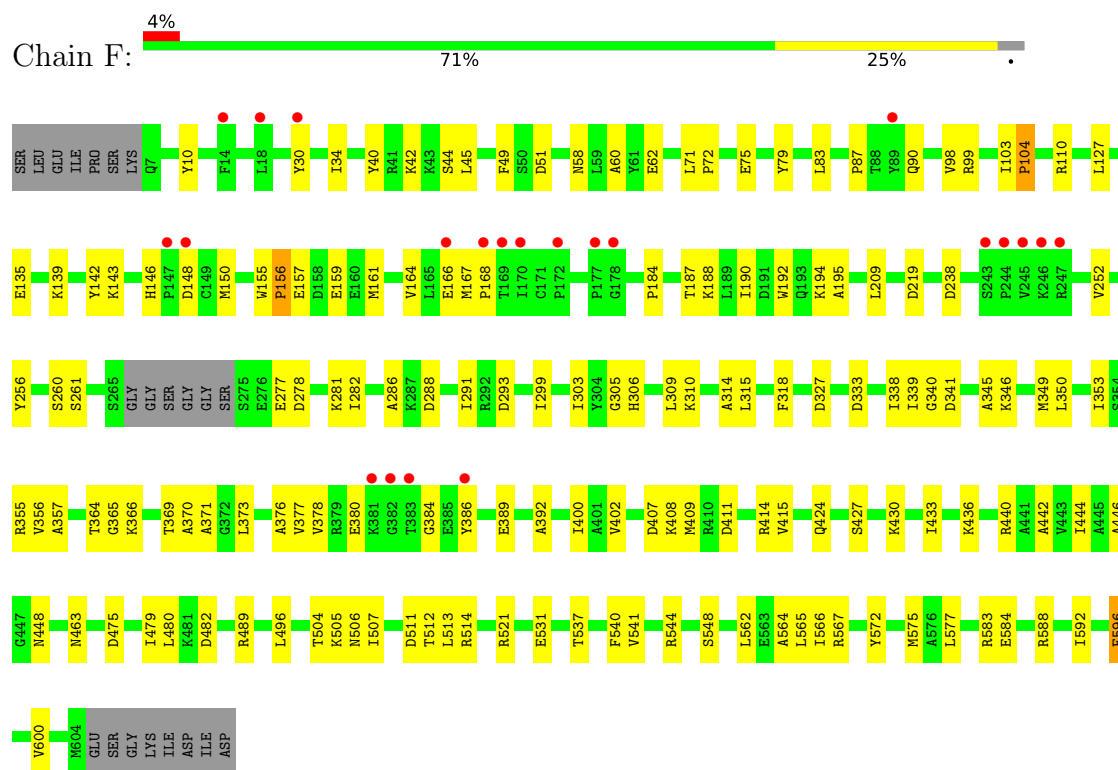
• Molecule 1: Minichromosome maintenance protein MCM



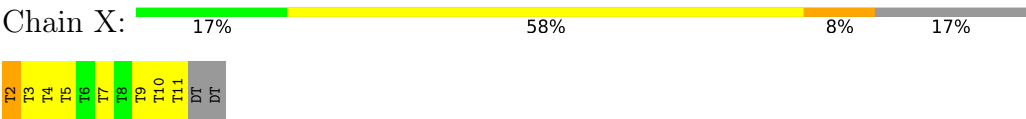
• Molecule 1: Minichromosome maintenance protein MCM



• Molecule 1: Minichromosome maintenance protein MCM



• Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	186.66Å 186.66Å 281.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.70 – 3.15 44.70 – 3.14	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.70-3.15) 96.9 (44.70-3.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.188 , 0.241 0.190 , 0.241	Depositor DCC
R_{free} test set	4259 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	120.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28494	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ADP, 08T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/4732	0.64	0/6393
1	B	0.39	0/4762	0.63	0/6438
1	C	0.35	0/4762	0.57	0/6438
1	D	0.31	0/4762	0.54	0/6438
1	E	0.33	0/4781	0.56	0/6463
1	F	0.37	0/4762	0.59	0/6438
2	X	1.20	1/220 (0.5%)	1.33	0/336
All	All	0.38	1/28781 (0.0%)	0.60	0/38944

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	2	DT	OP3-P	-10.35	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4655	0	4797	114	0
1	B	4683	0	4820	94	0
1	C	4683	0	4820	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4683	0	4820	77	0
1	E	4702	0	4834	98	0
1	F	4683	0	4820	105	0
2	X	201	0	121	9	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	0	0
6	E	27	0	12	0	0
6	F	27	0	12	1	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	3	0	0	0	0
7	D	4	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
All	All	28494	0	29107	534	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 9.

All (534) 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)
1:F:369:THR:HG22	1:F:370:ALA:H	1.25	0.98
1:E:381:LYS:HB2	1:F:384:GLY:HA2	1.52	0.90
1:D:496:LEU:HD13	1:E:533:LYS:HG3	1.61	0.80
1:A:365:GLY:HA2	1:A:409:MET:SD	2.23	0.78
1:B:418:HIS:HB3	1:B:473:ARG:HH21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:VAL:HG21	1:F:489:ARG:HG2	1.68	0.75
1:B:471:LEU:HD13	1:B:555:ILE:HD13	1.68	0.75
1:A:143:LYS:HE2	1:A:150:MET:HG3	1.69	0.74
1:A:374:THR:HB	1:A:426:VAL:HG11	1.70	0.72
1:A:209:LEU:HD11	1:B:390:ALA:HB2	1.70	0.71
1:D:549:GLU:HG2	1:D:550:THR:HG23	1.73	0.71
1:E:133:VAL:HG13	1:E:222:VAL:HG11	1.71	0.70
1:D:521:ARG:HA	1:D:574:LYS:HE2	1.71	0.70
1:F:184:PRO:O	1:F:187:THR:HG22	1.92	0.70
1:B:249:SER:HA	1:C:164:VAL:HA	1.72	0.70
1:D:333:ASP:HB3	1:D:442:ALA:HB2	1.74	0.69
1:E:249:SER:HA	1:F:164:VAL:HA	1.73	0.69
1:A:454:TYR:CE2	1:A:479:ILE:HD13	2.28	0.68
1:A:381:LYS:HG3	1:B:379:ARG:NH1	2.07	0.68
1:D:22:LYS:HB2	1:D:26:ASN:HA	1.74	0.68
1:B:496:LEU:HD13	1:C:533:LYS:HG3	1.76	0.68
1:D:388:LEU:HD11	1:D:428:ILE:HD11	1.76	0.67
1:A:566:ILE:HD11	1:F:496:LEU:HD21	1.78	0.67
1:D:418:HIS:HB3	1:D:473:ARG:HH21	1.60	0.66
1:E:83:LEU:HD21	1:E:90:GLN:HB2	1.76	0.66
1:C:83:LEU:HD23	1:C:87:PRO:HA	1.78	0.66
1:A:427:SER:HB3	1:A:436:LYS:HG3	1.77	0.66
1:C:388:LEU:HD11	1:C:428:ILE:HD11	1.76	0.66
1:F:369:THR:HG22	1:F:370:ALA:N	2.04	0.65
1:A:107:ILE:HD11	1:A:121:ILE:HD13	1.77	0.65
1:F:155:TRP:O	1:F:157:GLU:N	2.30	0.65
1:C:504:THR:HB	1:C:507:ILE:HD12	1.78	0.65
1:F:376:ALA:HB3	1:F:389:GLU:HB2	1.77	0.65
1:F:184:PRO:HA	1:F:187:THR:CG2	2.27	0.65
1:D:398:GLY:O	1:D:521:ARG:NH2	2.29	0.65
1:B:34:ILE:HD11	1:B:45:LEU:HD22	1.79	0.65
1:B:356:VAL:HG23	1:B:510:ILE:HG13	1.78	0.65
1:E:38:VAL:HG22	1:E:82:ILE:HG23	1.79	0.65
1:D:249:SER:HA	1:E:164:VAL:HA	1.79	0.65
1:A:155:TRP:O	1:A:157:GLU:N	2.30	0.64
1:B:298:SER:HA	1:B:507:ILE:HD11	1.79	0.64
1:C:369:THR:HB	1:C:372:GLY:H	1.61	0.64
1:D:155:TRP:O	1:D:157:GLU:N	2.29	0.64
1:C:156:PRO:HG3	1:C:161:MET:HG2	1.79	0.64
1:A:465:ASN:O	1:A:465:ASN:ND2	2.31	0.64
1:C:418:HIS:HB3	1:C:473:ARG:HH21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ILE:HG22	1:C:186:LYS:H	1.63	0.63
1:F:40:TYR:HB2	1:F:42:LYS:HE2	1.79	0.63
1:A:377:VAL:HG22	1:A:433:ILE:HD11	1.80	0.63
1:B:499:HIS:NE2	1:C:563:GLU:OE1	2.30	0.63
1:A:181:ARG:NE	1:F:166:GLU:OE2	2.31	0.63
1:B:489:ARG:NH2	1:C:538:ASP:OD1	2.25	0.63
1:A:34:ILE:HD11	1:A:45:LEU:HD22	1.80	0.62
1:C:143:LYS:HE2	1:C:150:MET:HG3	1.81	0.62
1:D:312:ALA:HA	1:D:315:LEU:HD12	1.80	0.62
1:B:166:GLU:OE2	1:C:181:ARG:NE	2.33	0.62
1:F:511:ASP:OD1	1:F:514:ARG:NH2	2.33	0.62
1:E:477:ILE:O	1:E:596:PHE:HD1	1.82	0.62
1:A:381:LYS:HG3	1:B:379:ARG:HH12	1.64	0.62
1:C:10:TYR:CZ	1:C:62:GLU:HG3	2.34	0.61
1:B:540:PHE:CZ	1:B:544:ARG:HD2	2.35	0.61
1:F:350:LEU:HB3	1:F:402:VAL:HG11	1.82	0.61
1:F:411:ASP:OD2	1:F:414:ARG:NH2	2.33	0.60
1:E:83:LEU:HD23	1:E:87:PRO:HA	1.84	0.60
1:E:356:VAL:HG23	1:E:510:ILE:HG13	1.84	0.60
1:C:301:PRO:HB3	1:C:507:ILE:HD11	1.82	0.60
1:D:238:ASP:HB3	1:D:256:TYR:CE1	2.37	0.60
1:E:484:PRO:HG2	1:F:548:SER:HB3	1.83	0.60
1:E:90:GLN:HG3	1:E:91:ARG:HG3	1.84	0.59
1:D:341:ASP:O	1:D:346:LYS:NZ	2.34	0.59
1:C:34:ILE:HD11	1:C:45:LEU:HD22	1.83	0.59
1:E:369:THR:HG21	2:X:11:DT:OP2	2.02	0.59
1:A:464:ILE:HG21	1:A:471:LEU:HD11	1.85	0.59
1:E:461:SER:HA	1:E:554:PRO:HG3	1.84	0.58
1:F:371:ALA:HB1	1:F:376:ALA:HA	1.85	0.58
1:B:360:ALA:HA	1:B:400:ILE:O	2.02	0.58
1:A:400:ILE:HD13	1:A:442:ALA:HB3	1.84	0.58
1:E:34:ILE:HD11	1:E:45:LEU:HD22	1.86	0.58
1:B:155:TRP:O	1:B:157:GLU:N	2.37	0.58
1:E:366:LYS:HG2	1:F:415:VAL:HG23	1.85	0.58
1:F:143:LYS:HE2	1:F:150:MET:HG3	1.86	0.58
1:C:496:LEU:HD13	1:D:533:LYS:HG3	1.85	0.57
1:E:388:LEU:HD11	1:E:428:ILE:HD11	1.84	0.57
1:A:536:ILE:HD13	1:A:566:ILE:HD13	1.86	0.57
1:E:214:GLU:OE2	1:E:240:LYS:NZ	2.30	0.57
1:A:418:HIS:CE1	1:A:473:ARG:HE	2.22	0.57
1:E:377:VAL:HG22	1:E:433:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:TYR:CE2	1:B:62:GLU:HG3	2.40	0.57
1:C:38:VAL:O	1:C:41:ARG:NH1	2.38	0.57
1:E:141:THR:HG21	1:E:186:LYS:HB2	1.87	0.57
1:B:369:THR:HG21	2:X:5:DT:OP2	2.05	0.56
1:A:22:LYS:HB3	1:A:26:ASN:HA	1.87	0.56
1:F:377:VAL:HG22	1:F:433:ILE:HD11	1.86	0.56
1:A:229:ASP:OD1	1:A:359:ARG:NH2	2.30	0.56
1:C:136:ARG:NH1	1:C:218:GLU:OE2	2.38	0.56
1:C:418:HIS:HB3	1:C:473:ARG:NH2	2.20	0.56
1:A:469:THR:HG21	1:F:408:LYS:HD3	1.88	0.56
1:C:64:ILE:HD11	1:C:103:ILE:HB	1.88	0.56
1:A:136:ARG:HH21	1:A:190:ILE:HD12	1.71	0.56
1:A:166:GLU:OE2	1:B:181:ARG:NE	2.39	0.56
1:A:64:ILE:HD11	1:A:104:PRO:HD2	1.88	0.55
1:C:350:LEU:HB3	1:C:402:VAL:HG11	1.88	0.55
1:C:471:LEU:HD13	1:C:555:ILE:HD13	1.88	0.55
1:C:588:ARG:O	1:C:592:ILE:HG23	2.06	0.55
1:F:184:PRO:HA	1:F:187:THR:HG21	1.89	0.55
1:E:341:ASP:O	1:E:346:LYS:NZ	2.39	0.55
1:C:369:THR:HG21	2:X:7:DT:OP2	2.06	0.55
1:D:17:PHE:O	1:D:21:PHE:HB3	2.06	0.55
1:F:475:ASP:OD2	1:F:567:ARG:NH1	2.40	0.55
1:B:30:TYR:HE1	1:B:47:ILE:HA	1.72	0.55
1:F:30:TYR:OH	1:F:51:ASP:OD2	2.21	0.55
1:F:139:LYS:HB3	1:F:188:LYS:HB2	1.89	0.55
1:D:241:GLN:HB3	1:D:244:PRO:HG3	1.87	0.55
1:D:461:SER:HA	1:D:554:PRO:HG3	1.89	0.55
1:E:48:GLU:HA	1:E:101:VAL:HG12	1.89	0.54
1:C:109:LEU:HD11	1:C:213:LEU:HB3	1.90	0.54
1:D:562:LEU:O	1:D:566:ILE:HG12	2.08	0.54
1:A:557:ILE:HG23	1:A:561:GLN:HB2	1.89	0.54
1:D:353:ILE:HA	1:D:356:VAL:HG12	1.90	0.54
1:C:155:TRP:CE3	1:C:168:PRO:HB3	2.43	0.54
1:C:333:ASP:HB3	1:C:442:ALA:HB2	1.89	0.54
1:E:103:ILE:HG22	1:E:105:ARG:H	1.72	0.54
1:C:484:PRO:HB3	1:D:544:ARG:HE	1.72	0.54
1:F:505:LYS:HG2	1:F:506:ASN:H	1.73	0.54
1:B:292:ARG:HE	1:B:576:ALA:HB2	1.73	0.53
1:B:339:ILE:O	1:B:479:ILE:HA	2.09	0.53
1:A:136:ARG:NH2	1:A:190:ILE:HD12	2.24	0.53
1:A:312:ALA:HB1	1:A:336:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:3:DT:H5'	2:X:3:DT:C6	2.44	0.53
1:C:155:TRP:O	1:C:157:GLU:N	2.41	0.53
1:B:562:LEU:O	1:B:566:ILE:HG12	2.08	0.53
1:D:381:LYS:HB2	1:E:384:GLY:HA3	1.91	0.53
1:E:66:ASN:O	1:E:66:ASN:ND2	2.42	0.53
1:B:231:VAL:HG12	1:B:264:VAL:HG22	1.90	0.53
1:B:369:THR:HG22	1:B:370:ALA:H	1.74	0.53
1:B:540:PHE:CD1	1:B:562:LEU:HB2	2.43	0.53
1:A:353:ILE:HD12	1:A:444:ILE:HD13	1.91	0.53
1:C:535:LEU:HD11	1:C:583:ARG:HH21	1.74	0.53
1:E:301:PRO:HB3	1:E:507:ILE:HD11	1.91	0.53
1:A:249:SER:HA	1:B:164:VAL:HA	1.91	0.52
1:F:34:ILE:HD11	1:F:45:LEU:HD22	1.91	0.52
1:F:184:PRO:C	1:F:187:THR:HG22	2.29	0.52
1:A:533:LYS:HG2	1:F:496:LEU:HD22	1.91	0.52
1:B:109:LEU:HD12	1:B:123:ILE:HD13	1.90	0.52
1:E:562:LEU:O	1:E:566:ILE:HG12	2.09	0.52
1:A:492:ALA:HB3	1:B:537:THR:HG23	1.91	0.52
1:A:347:SER:OG	1:A:404:ASP:OD2	2.27	0.52
1:D:141:THR:HG21	1:D:186:LYS:HB2	1.92	0.52
1:D:378:VAL:HG23	1:E:386:TYR:HE1	1.73	0.52
1:F:184:PRO:HA	1:F:187:THR:HG22	1.90	0.52
1:C:241:GLN:HB3	1:C:244:PRO:HG3	1.92	0.52
1:E:136:ARG:HH21	1:E:218:GLU:CD	2.13	0.52
1:B:30:TYR:O	1:B:34:ILE:HG12	2.10	0.52
1:B:350:LEU:HB3	1:B:402:VAL:HG11	1.92	0.52
1:C:562:LEU:O	1:C:566:ILE:HG12	2.09	0.52
1:A:278:ASP:O	1:A:282:ILE:HG23	2.10	0.52
1:B:131:THR:HG23	1:B:194:LYS:O	2.10	0.51
1:C:540:PHE:CZ	1:C:544:ARG:HD2	2.45	0.51
1:E:308:GLU:HG2	1:E:309:LEU:N	2.25	0.51
1:E:418:HIS:HB3	1:E:473:ARG:HH21	1.75	0.51
1:B:278:ASP:O	1:B:282:ILE:HG23	2.10	0.51
1:D:159:GLU:OE1	1:E:181:ARG:NH2	2.42	0.51
1:B:69:ILE:O	1:B:73:ILE:HD13	2.11	0.51
1:B:353:ILE:HA	1:B:356:VAL:HG12	1.93	0.51
1:E:381:LYS:HB2	1:F:384:GLY:CA	2.33	0.51
1:F:110:ARG:NH2	1:F:209:LEU:O	2.43	0.51
1:F:190:ILE:HD11	1:F:219:ASP:HB2	1.92	0.51
1:B:99:ARG:HD3	1:B:260:SER:O	2.11	0.51
1:A:377:VAL:HG11	1:A:431:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:PHE:CD1	1:C:562:LEU:HB2	2.45	0.51
1:A:288:ASP:HB3	1:A:291:ILE:HB	1.93	0.51
1:E:296:ILE:HG12	1:E:311:GLU:HA	1.92	0.51
1:F:572:TYR:OH	1:F:592:ILE:HG21	2.11	0.51
1:A:544:ARG:NH2	1:F:482:ASP:OD1	2.41	0.51
1:C:105:ARG:HD2	1:C:120:LEU:O	2.11	0.50
1:E:301:PRO:HD2	1:F:327:ASP:OD2	2.10	0.50
1:B:64:ILE:HD11	1:B:103:ILE:HD12	1.93	0.50
1:F:584:GLU:O	1:F:588:ARG:HG3	2.12	0.50
1:A:209:LEU:CD1	1:B:390:ALA:HB2	2.41	0.50
1:A:326:GLU:O	1:F:355:ARG:NH2	2.44	0.50
1:A:450:LYS:HB2	1:A:465:ASN:HB2	1.93	0.50
1:B:484:PRO:HB3	1:C:544:ARG:HE	1.77	0.50
1:C:286:ALA:HB2	1:C:577:LEU:HD22	1.94	0.50
1:C:388:LEU:HD11	1:C:428:ILE:CD1	2.42	0.50
1:A:131:THR:HG23	1:A:194:LYS:O	2.12	0.50
1:A:247:ARG:NH1	1:C:179:GLN:OE1	2.45	0.50
1:F:364:THR:HG22	1:F:366:LYS:H	1.76	0.50
1:A:312:ALA:HA	1:A:315:LEU:HD12	1.93	0.50
1:E:107:ILE:HD12	1:E:121:ILE:HD13	1.94	0.50
1:E:156:PRO:HG3	1:E:161:MET:HG2	1.93	0.50
1:E:333:ASP:HB3	1:E:442:ALA:HB2	1.92	0.50
1:A:304:TYR:HB2	1:A:494:TYR:CD2	2.47	0.50
1:A:497:ASP:CG	1:A:502:LYS:HD2	2.32	0.50
1:B:584:GLU:O	1:B:588:ARG:HG3	2.12	0.50
1:C:499:HIS:NE2	1:D:563:GLU:OE1	2.40	0.50
1:E:477:ILE:HB	1:E:596:PHE:CE1	2.47	0.50
1:A:547:SER:HB3	1:A:555:ILE:HA	1.94	0.50
1:D:540:PHE:CD1	1:D:562:LEU:HB2	2.47	0.50
1:F:427:SER:HB3	1:F:436:LYS:HG3	1.93	0.50
1:A:353:ILE:HA	1:A:356:VAL:HG12	1.93	0.49
1:D:584:GLU:O	1:D:588:ARG:HG3	2.13	0.49
1:C:521:ARG:HA	1:C:574:LYS:HE2	1.94	0.49
1:F:353:ILE:HD11	1:F:444:ILE:HG21	1.95	0.49
1:B:296:ILE:HG12	1:B:311:GLU:HA	1.94	0.49
1:B:341:ASP:O	1:B:346:LYS:NZ	2.45	0.49
1:D:367:GLY:O	1:E:430:LYS:HE3	2.12	0.49
1:E:338:ILE:O	1:E:446:ALA:HA	2.13	0.49
1:B:484:PRO:HB3	1:C:544:ARG:NE	2.27	0.49
1:C:277:GLU:N	1:C:277:GLU:OE1	2.46	0.49
1:D:313:LEU:HD22	1:D:353:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ARG:HD3	1:F:260:SER:O	2.12	0.49
1:D:234:THR:HB	1:D:261:SER:HB3	1.95	0.49
1:A:30:TYR:O	1:A:34:ILE:HG12	2.13	0.49
1:D:339:ILE:O	1:D:479:ILE:HA	2.12	0.49
1:F:303:ILE:HD12	1:F:345:ALA:HB1	1.95	0.49
1:B:155:TRP:CZ3	1:B:168:PRO:HB3	2.48	0.49
1:D:131:THR:HG21	1:D:194:LYS:HB3	1.95	0.49
1:F:338:ILE:O	1:F:446:ALA:HA	2.13	0.49
1:C:249:SER:HA	1:D:164:VAL:HA	1.95	0.49
1:E:594:ARG:HG3	1:E:604:MET:HG3	1.95	0.49
1:A:155:TRP:CD1	1:A:168:PRO:HD3	2.48	0.48
1:A:155:TRP:CE3	1:A:168:PRO:HB3	2.48	0.48
1:A:560:ARG:HG2	6:F:2001:ADP:H5'1	1.94	0.48
1:C:41:ARG:HH21	1:C:88:THR:HB	1.78	0.48
1:E:155:TRP:O	1:E:157:GLU:N	2.46	0.48
1:F:155:TRP:CE3	1:F:168:PRO:HB3	2.47	0.48
1:F:333:ASP:HB3	1:F:442:ALA:HB2	1.94	0.48
1:F:339:ILE:O	1:F:479:ILE:HA	2.13	0.48
1:C:461:SER:HA	1:C:554:PRO:HG3	1.94	0.48
1:C:297:SER:HA	1:C:307:TRP:HZ3	1.78	0.48
1:E:37:LEU:HG	1:E:42:LYS:O	2.14	0.48
1:F:365:GLY:HA3	1:F:409:MET:HG2	1.94	0.48
1:B:364:THR:HG22	1:B:366:LYS:H	1.77	0.48
1:E:505:LYS:HG2	1:E:506:ASN:H	1.78	0.48
1:F:83:LEU:HD23	1:F:87:PRO:HA	1.96	0.48
1:D:366:LYS:HE3	1:E:415:VAL:CG2	2.44	0.48
1:F:192:TRP:CH2	1:F:194:LYS:HB2	2.49	0.48
1:C:30:TYR:O	1:C:34:ILE:HG12	2.13	0.48
2:X:2:DT:H5'	2:X:2:DT:C6	2.48	0.48
1:A:109:LEU:O	1:A:112:ILE:HG23	2.14	0.48
1:C:75:GLU:HG2	1:C:98:VAL:HG23	1.96	0.48
1:A:139:LYS:HG3	1:A:156:PRO:HG2	1.95	0.48
1:E:353:ILE:HD12	1:E:444:ILE:HD13	1.96	0.48
1:A:414:ARG:O	1:A:417:ILE:HG12	2.13	0.47
1:B:34:ILE:HD12	1:B:78:LEU:HD11	1.96	0.47
1:C:467:PRO:HG2	1:C:470:ILE:HG22	1.96	0.47
1:E:364:THR:HG22	1:E:367:GLY:H	1.79	0.47
1:E:369:THR:HG22	1:E:370:ALA:H	1.77	0.47
1:F:377:VAL:HG21	1:F:430:LYS:HB2	1.96	0.47
1:B:49:PHE:CE1	1:B:64:ILE:HG13	2.49	0.47
1:B:457:GLU:OE1	1:B:457:GLU:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HG2	1:B:98:VAL:HG23	1.96	0.47
1:C:288:ASP:HB3	1:C:291:ILE:HB	1.95	0.47
1:D:357:ALA:HB1	1:D:400:ILE:HD13	1.96	0.47
1:F:353:ILE:HD12	1:F:444:ILE:HD13	1.97	0.47
1:B:192:TRP:CH2	1:B:194:LYS:HB2	2.48	0.47
1:F:318:PHE:CE2	1:F:575:MET:HG3	2.49	0.47
1:B:103:ILE:HG23	1:B:104:PRO:HD2	1.96	0.47
1:D:369:THR:HG22	1:D:370:ALA:H	1.78	0.47
1:A:312:ALA:HB2	1:A:478:PHE:HE2	1.80	0.47
1:B:30:TYR:CE1	1:B:47:ILE:HA	2.50	0.47
1:C:47:ILE:HD11	1:C:100:ILE:HG13	1.96	0.47
1:D:546:LYS:O	1:D:549:GLU:HB3	2.15	0.47
1:A:499:HIS:NE2	1:B:563:GLU:OE1	2.47	0.47
1:C:309:LEU:HD22	1:C:338:ILE:HG12	1.96	0.47
1:E:524:VAL:O	1:E:574:LYS:HE3	2.14	0.47
1:F:49:PHE:CZ	1:F:60:ALA:HB1	2.49	0.47
1:C:155:TRP:CG	1:C:168:PRO:HD3	2.50	0.47
1:C:346:LYS:HD2	1:C:446:ALA:HB1	1.97	0.47
1:B:418:HIS:HB3	1:B:473:ARG:NH2	2.26	0.46
1:C:357:ALA:HB3	1:C:360:ALA:HB2	1.97	0.46
1:C:364:THR:HG22	1:C:367:GLY:H	1.80	0.46
1:F:537:THR:O	1:F:541:VAL:HG23	2.15	0.46
1:C:489:ARG:NH2	1:D:538:ASP:OD1	2.42	0.46
1:E:286:ALA:HB2	1:E:577:LEU:HD22	1.96	0.46
1:B:112:ILE:HD11	1:B:255:ILE:HD13	1.97	0.46
1:D:309:LEU:HD13	1:D:349:MET:HE1	1.97	0.46
1:E:535:LEU:HD23	1:E:587:GLU:HG3	1.97	0.46
1:C:457:GLU:N	1:C:457:GLU:OE1	2.47	0.46
1:F:531:GLU:HB2	1:F:583:ARG:HG2	1.98	0.46
1:D:352:PHE:HD1	1:E:327:ASP:HB2	1.81	0.46
1:A:297:SER:HA	1:A:307:TRP:HZ3	1.81	0.46
1:C:572:TYR:OH	1:C:592:ILE:HG21	2.15	0.46
1:D:496:LEU:HD22	1:E:533:LYS:HB2	1.98	0.46
1:B:127:LEU:HD11	1:B:195:ALA:HB1	1.98	0.46
1:C:296:ILE:HG12	1:C:311:GLU:HA	1.98	0.46
1:E:312:ALA:HA	1:E:315:LEU:HD12	1.97	0.46
1:F:369:THR:CG2	1:F:370:ALA:H	2.09	0.46
1:B:505:LYS:HG2	1:B:506:ASN:H	1.80	0.46
1:D:283:LYS:O	1:D:287:LYS:HG2	2.15	0.46
1:F:127:LEU:HD11	1:F:195:ALA:HB1	1.97	0.46
1:F:156:PRO:HG3	1:F:161:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:LYS:NZ	1:F:512:THR:HG21	2.30	0.46
1:A:103:ILE:HG22	1:A:122:THR:OG1	2.16	0.45
1:A:415:VAL:HG11	1:F:366:LYS:CG	2.46	0.45
1:A:457:GLU:N	1:A:457:GLU:OE1	2.47	0.45
1:A:537:THR:O	1:A:541:VAL:HG23	2.16	0.45
1:C:450:LYS:HB2	1:C:465:ASN:HB2	1.97	0.45
1:E:499:HIS:ND1	1:F:566:ILE:HG21	2.31	0.45
1:A:159:GLU:OE1	1:B:181:ARG:NH2	2.46	0.45
1:E:449:PRO:HD2	1:E:452:GLY:O	2.16	0.45
1:C:338:ILE:O	1:C:446:ALA:HA	2.15	0.45
1:C:353:ILE:HA	1:C:356:VAL:HG12	1.98	0.45
1:F:504:THR:HB	1:F:507:ILE:HD12	1.98	0.45
1:A:415:VAL:HG11	1:F:366:LYS:HG2	1.98	0.45
1:C:388:LEU:HA	1:C:388:LEU:HD12	1.44	0.45
1:F:278:ASP:O	1:F:282:ILE:HG23	2.17	0.45
1:F:373:LEU:HD23	1:F:392:ALA:HB3	1.99	0.45
1:A:357:ALA:HB3	1:A:360:ALA:HB2	1.98	0.45
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.78	0.45
1:C:309:LEU:HB3	1:C:349:MET:HE1	1.99	0.45
1:C:415:VAL:HA	1:C:418:HIS:CE1	2.52	0.45
1:F:305:GLY:O	1:F:310:LYS:HE3	2.16	0.45
1:C:52:VAL:HG11	1:C:63:ILE:HD12	1.97	0.45
1:C:356:VAL:HG23	1:C:510:ILE:HG13	1.98	0.45
1:D:30:TYR:OH	1:D:51:ASP:OD2	2.24	0.45
1:E:484:PRO:HB3	1:F:544:ARG:NE	2.32	0.45
1:D:477:ILE:HB	1:D:596:PHE:HE1	1.80	0.45
1:F:356:VAL:HG21	1:F:513:LEU:HD23	1.97	0.45
1:B:471:LEU:HD13	1:B:555:ILE:CD1	2.43	0.45
1:F:142:TYR:HE2	1:F:167:MET:HE2	1.81	0.45
1:B:546:LYS:HD3	1:B:549:GLU:OE1	2.17	0.44
1:C:505:LYS:HG2	1:C:506:ASN:H	1.82	0.44
1:D:106:VAL:HG22	1:D:122:THR:HB	1.97	0.44
1:A:341:ASP:O	1:A:346:LYS:NZ	2.50	0.44
1:B:214:GLU:OE2	1:B:240:LYS:HE2	2.17	0.44
1:C:41:ARG:NH2	1:C:88:THR:HB	2.31	0.44
1:F:75:GLU:HG2	1:F:98:VAL:HG23	1.99	0.44
1:E:364:THR:HG22	1:E:366:LYS:H	1.83	0.44
1:F:277:GLU:N	1:F:277:GLU:OE1	2.51	0.44
1:F:407:ASP:CG	1:F:448:ASN:H	2.20	0.44
1:A:417:ILE:HD11	1:A:470:ILE:HD11	1.98	0.44
1:A:495:ILE:HD12	1:B:562:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ILE:HD11	1:D:255:ILE:HD13	1.99	0.44
1:E:75:GLU:HG2	1:E:98:VAL:HG23	2.00	0.44
1:F:540:PHE:CZ	1:F:544:ARG:HD2	2.51	0.44
1:A:169:THR:HB	1:A:170:ILE:HD12	1.99	0.44
1:A:181:ARG:NH2	1:F:159:GLU:OE1	2.49	0.44
1:C:34:ILE:O	1:C:38:VAL:HG23	2.18	0.44
1:D:568:ILE:HG21	1:D:592:ILE:HD11	2.00	0.44
1:E:484:PRO:HB3	1:F:544:ARG:HB3	1.99	0.44
1:D:424:GLN:HB3	1:D:440:ARG:HA	1.99	0.44
1:C:138:TYR:HA	1:C:161:MET:HB2	2.00	0.44
1:E:379:ARG:HB2	1:E:386:TYR:CE2	2.52	0.44
1:F:340:GLY:HA3	1:F:480:LEU:HB2	1.99	0.44
1:A:183:ILE:HG22	1:A:186:LYS:H	1.82	0.44
1:B:381:LYS:HG3	1:C:379:ARG:HH11	1.82	0.44
1:E:318:PHE:CE2	1:E:575:MET:HG3	2.53	0.44
1:B:112:ILE:O	1:B:112:ILE:HG13	2.16	0.44
1:C:352:PHE:HD1	1:D:327:ASP:HB2	1.83	0.44
1:D:357:ALA:HB3	1:D:360:ALA:HB2	1.99	0.44
1:D:457:GLU:OE1	1:D:457:GLU:N	2.51	0.44
1:E:127:LEU:HA	1:E:197:ILE:HG22	2.00	0.44
1:F:79:TYR:OH	1:F:90:GLN:OE1	2.35	0.44
1:F:596:PHE:O	1:F:600:VAL:HG22	2.17	0.44
1:A:333:ASP:HB3	1:A:442:ALA:HB2	2.00	0.43
1:C:484:PRO:HB3	1:D:544:ARG:NE	2.32	0.43
1:D:459:PRO:O	1:D:463:ASN:HB2	2.16	0.43
1:E:143:LYS:HE2	1:E:150:MET:HG3	1.98	0.43
1:B:344:THR:CG2	1:B:480:LEU:HD13	2.48	0.43
1:D:193:GLN:HB2	1:D:222:VAL:HG22	1.99	0.43
1:D:388:LEU:HD12	1:D:388:LEU:HA	1.69	0.43
1:A:584:GLU:O	1:A:588:ARG:HG3	2.18	0.43
1:B:320:GLY:O	1:B:574:LYS:NZ	2.50	0.43
1:D:278:ASP:O	1:D:282:ILE:HG23	2.19	0.43
1:E:398:GLY:O	1:E:521:ARG:NH2	2.51	0.43
1:E:524:VAL:HG11	1:E:574:LYS:HA	1.99	0.43
1:B:245:VAL:HG13	1:C:167:MET:HE1	2.01	0.43
1:B:298:SER:HA	1:B:507:ILE:CD1	2.47	0.43
1:E:34:ILE:O	1:E:38:VAL:HG23	2.17	0.43
1:E:277:GLU:OE1	1:E:277:GLU:N	2.52	0.43
1:F:378:VAL:HG22	1:F:380:GLU:HG2	2.01	0.43
1:A:106:VAL:HG22	1:A:122:THR:HB	2.00	0.43
1:D:355:ARG:O	1:D:514:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:TYR:CE1	1:E:188:LYS:HB3	2.54	0.43
1:E:281:LYS:NZ	1:E:512:THR:HG21	2.33	0.43
1:F:299:ILE:HD12	1:F:314:ALA:HB2	1.99	0.43
1:A:374:THR:HB	1:A:426:VAL:CG1	2.45	0.43
1:C:304:TYR:HB2	1:C:494:TYR:CD2	2.54	0.43
1:D:18:LEU:O	1:D:31:ILE:N	2.52	0.43
1:A:10:TYR:CZ	1:A:62:GLU:HG3	2.53	0.43
1:A:234:THR:HB	1:A:261:SER:HB3	2.01	0.43
1:A:277:GLU:N	1:A:277:GLU:OE1	2.52	0.43
1:B:70:ILE:HD12	1:B:70:ILE:HA	1.93	0.43
1:E:477:ILE:HB	1:E:596:PHE:HE1	1.84	0.43
1:F:288:ASP:HB3	1:F:291:ILE:HB	2.00	0.43
2:X:2:DT:C2	2:X:3:DT:C4	3.07	0.43
1:E:30:TYR:O	1:E:34:ILE:HG12	2.19	0.43
1:E:66:ASN:HD21	1:E:69:ILE:HG22	1.84	0.43
1:F:309:LEU:HD13	1:F:349:MET:HE1	1.99	0.43
1:F:565:LEU:HD23	1:F:565:LEU:HA	1.87	0.43
1:B:353:ILE:HD12	1:B:444:ILE:HD13	2.01	0.43
1:B:430:LYS:O	1:B:433:ILE:HG12	2.19	0.43
1:A:24:ASN:N	1:A:27:GLN:OE1	2.49	0.42
1:A:137:ILE:HG21	1:A:140:ALA:HB2	2.00	0.42
1:D:109:LEU:HB3	1:D:199:GLU:HB3	2.00	0.42
1:E:131:THR:HG23	1:E:194:LYS:O	2.19	0.42
1:A:286:ALA:HB2	1:A:577:LEU:HD22	2.00	0.42
1:A:505:LYS:HE2	1:A:505:LYS:HB3	1.82	0.42
2:X:9:DT:H1'	2:X:10:DT:H5'	2.00	0.42
1:A:75:GLU:HG2	1:A:98:VAL:HG23	2.00	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.82	0.42
1:C:540:PHE:CE1	1:C:562:LEU:HB2	2.55	0.42
1:D:374:THR:HB	1:D:426:VAL:HG11	2.01	0.42
1:E:388:LEU:CD1	1:E:428:ILE:HD11	2.49	0.42
1:F:155:TRP:CG	1:F:168:PRO:HD3	2.54	0.42
1:B:374:THR:OG1	1:B:375:ALA:N	2.51	0.42
1:A:331:ARG:NH2	1:A:475:ASP:OD1	2.52	0.42
1:A:350:LEU:HB3	1:A:402:VAL:HG11	2.00	0.42
1:B:34:ILE:HD13	1:B:45:LEU:HD13	2.02	0.42
1:B:190:ILE:HD13	1:B:218:GLU:OE1	2.20	0.42
1:C:159:GLU:HB3	1:C:160:GLU:H	1.61	0.42
1:D:279:GLU:HG3	1:D:519:TYR:CE2	2.54	0.42
1:E:546:LYS:HG3	1:E:604:MET:SD	2.59	0.42
1:A:540:PHE:CZ	1:A:544:ARG:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HD23	1:C:226:ARG:O	2.20	0.42
1:E:356:VAL:HG21	1:E:513:LEU:HD23	2.00	0.42
1:E:467:PRO:HG2	1:E:470:ILE:HG22	2.01	0.42
1:A:566:ILE:HD11	1:F:496:LEU:CD2	2.49	0.42
1:C:344:THR:CG2	1:C:480:LEU:HD13	2.50	0.42
1:E:457:GLU:OE1	1:E:457:GLU:N	2.50	0.42
1:F:341:ASP:O	1:F:346:LYS:NZ	2.52	0.42
1:A:49:PHE:CE1	1:A:60:ALA:HB1	2.54	0.42
1:C:369:THR:HG22	1:C:370:ALA:N	2.35	0.42
1:C:564:ALA:HA	1:C:567:ARG:NH1	2.35	0.42
1:D:352:PHE:CD1	1:E:327:ASP:HB2	2.55	0.42
1:E:540:PHE:CZ	1:E:544:ARG:HD2	2.55	0.42
1:A:388:LEU:HD13	1:A:433:ILE:HD11	2.01	0.42
1:B:115:THR:H	1:B:115:THR:HG23	1.63	0.42
1:B:540:PHE:CE1	1:B:562:LEU:HB2	2.54	0.42
1:C:67:THR:HA	1:C:70:ILE:HG22	2.01	0.42
1:D:469:THR:O	1:D:473:ARG:NH1	2.52	0.42
1:E:378:VAL:HG23	1:F:386:TYR:CE1	2.55	0.42
1:A:369:THR:HG21	2:X:3:DT:OP2	2.20	0.42
1:B:312:ALA:HA	1:B:315:LEU:HD12	2.02	0.42
1:D:540:PHE:CE1	1:D:562:LEU:HB2	2.55	0.42
1:F:71:LEU:N	1:F:72:PRO:HD2	2.35	0.42
1:A:52:VAL:HG12	1:A:60:ALA:HB2	2.00	0.41
1:A:318:PHE:CE2	1:A:575:MET:HG3	2.55	0.41
1:A:369:THR:OG1	1:B:430:LYS:HG2	2.20	0.41
1:B:308:GLU:HG2	1:B:309:LEU:N	2.35	0.41
1:B:477:ILE:O	1:B:596:PHE:HD1	2.03	0.41
1:C:427:SER:HA	1:C:436:LYS:HA	2.01	0.41
1:E:347:SER:OG	1:E:404:ASP:OD2	2.37	0.41
1:E:588:ARG:O	1:E:592:ILE:HG23	2.20	0.41
1:A:64:ILE:HG12	1:A:103:ILE:HD11	2.01	0.41
1:E:205:PRO:HB2	1:E:208:GLN:HG3	2.02	0.41
1:E:241:GLN:HB3	1:E:244:PRO:HG3	2.01	0.41
1:E:344:THR:HG21	1:E:480:LEU:HB3	2.03	0.41
1:A:192:TRP:CE3	1:F:252:VAL:HG11	2.55	0.41
1:B:347:SER:OG	1:B:404:ASP:OD2	2.38	0.41
1:C:374:THR:OG1	1:C:375:ALA:N	2.54	0.41
1:C:528:ILE:HA	1:C:581:VAL:HB	2.01	0.41
1:E:44:SER:OG	1:E:99:ARG:NE	2.54	0.41
1:E:600:VAL:HG23	1:E:602:VAL:HG23	2.02	0.41
1:F:357:ALA:HB1	1:F:400:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:PHE:CD1	1:F:562:LEU:HB2	2.55	0.41
1:B:17:PHE:HB2	1:B:55:PHE:CD2	2.55	0.41
1:B:321:VAL:HG12	1:B:323:LYS:HE3	2.03	0.41
1:C:309:LEU:HD11	1:C:480:LEU:HD11	2.03	0.41
1:D:34:ILE:HD11	1:D:45:LEU:HD22	2.02	0.41
1:A:125:GLY:HA2	1:A:200:ARG:HG2	2.03	0.41
1:C:137:ILE:HG22	1:C:161:MET:HG3	2.01	0.41
1:C:388:LEU:CD1	1:C:428:ILE:HD11	2.46	0.41
1:C:584:GLU:O	1:C:588:ARG:HG3	2.20	0.41
1:F:349:MET:HB3	1:F:349:MET:HE3	1.95	0.41
1:F:588:ARG:O	1:F:592:ILE:HG23	2.20	0.41
1:B:333:ASP:HB3	1:B:442:ALA:HB2	2.03	0.41
1:E:388:LEU:HD11	1:E:428:ILE:CD1	2.49	0.41
1:E:477:ILE:O	1:E:596:PHE:CD1	2.68	0.41
1:A:107:ILE:HD11	1:A:121:ILE:CD1	2.48	0.41
1:A:557:ILE:HG23	1:A:561:GLN:CB	2.51	0.41
1:B:79:TYR:OH	1:B:90:GLN:OE1	2.39	0.41
1:D:308:GLU:HG2	1:D:309:LEU:N	2.36	0.41
1:D:495:ILE:HD12	1:E:562:LEU:HD23	2.03	0.41
1:F:286:ALA:HB2	1:F:577:LEU:HD22	2.02	0.41
1:A:17:PHE:HB2	1:A:55:PHE:CD2	2.56	0.41
1:A:34:ILE:O	1:A:38:VAL:HG23	2.21	0.41
1:A:364:THR:HG22	1:A:366:LYS:H	1.85	0.41
1:A:369:THR:HG22	1:A:370:ALA:H	1.86	0.41
1:A:451:PHE:O	1:A:453:ARG:N	2.53	0.41
1:B:34:ILE:CD1	1:B:78:LEU:HD11	2.51	0.41
1:B:162:PRO:HG2	1:B:164:VAL:O	2.20	0.41
1:B:304:TYR:HB2	1:B:494:TYR:CG	2.56	0.41
1:C:369:THR:HG22	1:C:370:ALA:H	1.84	0.41
1:C:546:LYS:O	1:C:549:GLU:HB3	2.20	0.41
1:D:166:GLU:OE2	1:E:181:ARG:NE	2.49	0.41
1:D:378:VAL:HG23	1:E:386:TYR:CE1	2.54	0.41
1:D:477:ILE:HB	1:D:596:PHE:CE1	2.55	0.41
1:E:400:ILE:CG2	1:E:444:ILE:HD12	2.51	0.41
1:F:10:TYR:CE2	1:F:62:GLU:HG3	2.55	0.41
1:F:103:ILE:HB	1:F:104:PRO:HD2	2.02	0.41
1:A:99:ARG:HD3	1:A:260:SER:O	2.21	0.41
1:A:156:PRO:HG3	1:A:161:MET:HG2	2.03	0.41
1:B:369:THR:HG22	1:B:370:ALA:N	2.35	0.41
1:D:299:ILE:HD13	1:D:299:ILE:HA	1.92	0.41
2:X:4:DT:C2	2:X:5:DT:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:VAL:HG22	1:C:82:ILE:HG23	2.03	0.40
1:C:281:LYS:NZ	1:C:512:THR:HG21	2.36	0.40
1:C:301:PRO:HD2	1:D:327:ASP:OD2	2.21	0.40
1:D:477:ILE:O	1:D:596:PHE:HD1	2.03	0.40
1:E:255:ILE:HD11	1:F:135:GLU:HG2	2.03	0.40
1:F:146:HIS:ND1	1:F:148:ASP:HB2	2.37	0.40
1:F:238:ASP:HB3	1:F:256:TYR:CE1	2.56	0.40
1:F:315:LEU:HD11	1:F:572:TYR:CZ	2.56	0.40
1:F:480:LEU:HA	1:F:480:LEU:HD23	1.81	0.40
1:A:63:ILE:HG21	1:A:100:ILE:HG12	2.03	0.40
1:A:159:GLU:HB3	1:A:160:GLU:H	1.58	0.40
1:A:378:VAL:HG23	1:B:386:TYR:HE1	1.86	0.40
1:B:335:HIS:CE1	1:B:443:VAL:H	2.39	0.40
1:C:282:ILE:HB	1:C:516:TYR:CD2	2.57	0.40
1:C:305:GLY:O	1:C:310:LYS:HE3	2.21	0.40
1:C:353:ILE:HD12	1:C:444:ILE:HD13	2.03	0.40
1:A:109:LEU:HD11	1:A:213:LEU:HB3	2.02	0.40
1:A:433:ILE:HD13	1:A:433:ILE:HG21	1.86	0.40
1:A:499:HIS:NE2	1:B:330:ILE:HG21	2.37	0.40
1:C:49:PHE:CZ	1:C:60:ALA:HB1	2.56	0.40
1:D:131:THR:CG2	1:D:194:LYS:HB3	2.51	0.40
1:F:424:GLN:HB3	1:F:440:ARG:HA	2.02	0.40
1:A:238:ASP:HB3	1:A:256:TYR:CE1	2.56	0.40
1:B:388:LEU:HA	1:B:388:LEU:HD12	1.59	0.40
1:C:70:ILE:O	1:C:74:LEU:HG	2.20	0.40
1:C:465:ASN:O	1:C:465:ASN:ND2	2.55	0.40
1:C:466:LEU:HD23	1:C:466:LEU:HA	1.90	0.40
1:D:19:THR:HA	1:D:31:ILE:HB	2.04	0.40
1:D:344:THR:HG21	1:D:480:LEU:HB3	2.04	0.40
1:A:323:LYS:HB2	1:A:330:ILE:HB	2.03	0.40
1:B:143:LYS:CE	1:B:150:MET:HG3	2.52	0.40
1:C:535:LEU:HD11	1:C:583:ARG:NH2	2.35	0.40
1:C:539:PHE:CD2	1:C:590:ILE:HG23	2.57	0.40
1:D:305:GLY:O	1:D:310:LYS:HE3	2.22	0.40
1:E:339:ILE:O	1:E:479:ILE:HA	2.21	0.40
1:F:306:HIS:O	1:F:310:LYS:HD2	2.22	0.40
1:F:564:ALA:HA	1:F:567:ARG:NH1	2.37	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/610 (95%)	545 (94%)	31 (5%)	3 (0%)	29	65
1	B	585/610 (96%)	552 (94%)	33 (6%)	0	100	100
1	C	585/610 (96%)	552 (94%)	32 (6%)	1 (0%)	47	78
1	D	585/610 (96%)	556 (95%)	26 (4%)	3 (0%)	29	65
1	E	588/610 (96%)	557 (95%)	31 (5%)	0	100	100
1	F	585/610 (96%)	552 (94%)	31 (5%)	2 (0%)	41	73
All	All	3507/3660 (96%)	3314 (94%)	184 (5%)	9 (0%)	41	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	ILE
1	A	600	VAL
1	D	104	PRO
1	D	9	ASP
1	F	104	PRO
1	C	247	ARG
1	A	102	GLY
1	D	156	PRO
1	F	156	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/530 (96%)	504 (99%)	6 (1%)	71	87
1	B	514/530 (97%)	507 (99%)	7 (1%)	67	85
1	C	514/530 (97%)	507 (99%)	7 (1%)	67	85
1	D	514/530 (97%)	508 (99%)	6 (1%)	71	87
1	E	516/530 (97%)	508 (98%)	8 (2%)	62	83
1	F	514/530 (97%)	507 (99%)	7 (1%)	67	85
All	All	3082/3180 (97%)	3041 (99%)	41 (1%)	69	86

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	261	SER
1	A	294	ARG
1	A	463	ASN
1	A	465	ASN
1	A	604	MET
1	B	44	SER
1	B	58	ASN
1	B	261	SER
1	B	293	ASP
1	B	294	ARG
1	B	463	ASN
1	B	596	PHE
1	C	44	SER
1	C	261	SER
1	C	294	ARG
1	C	418	HIS
1	C	463	ASN
1	C	494	TYR
1	C	596	PHE
1	D	44	SER
1	D	261	SER
1	D	418	HIS
1	D	453	ARG
1	D	463	ASN
1	D	596	PHE
1	E	44	SER
1	E	66	ASN
1	E	294	ARG
1	E	453	ARG

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Mol	Chain	Res	Type
1	E	463	ASN
1	E	494	TYR
1	E	596	PHE
1	E	603	ASP
1	F	44	SER
1	F	58	ASN
1	F	261	SER
1	F	293	ASP
1	F	463	ASN
1	F	521	ARG
1	F	596	PHE

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

Mol	Chain	Res	Type
1	B	423	GLN
1	D	493	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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	$\# Z > 2$
6	ADP	D	2001	5	24,29,29	0.95	1 (4%)	29,45,45	1.33	4 (13%)
6	ADP	E	2001	5	24,29,29	0.91	1 (4%)	29,45,45	1.39	5 (17%)
3	08T	B	2001	5	26,33,33	0.93	1 (3%)	25,52,52	1.41	4 (16%)
3	08T	C	2001	5	26,33,33	1.02	1 (3%)	25,52,52	1.47	6 (24%)
6	ADP	F	2001	5	24,29,29	0.95	1 (4%)	29,45,45	1.37	5 (17%)
3	08T	A	2001	5	26,33,33	0.85	1 (3%)	25,52,52	1.54	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	D	2001	5	-	6/12/32/32	0/3/3/3
6	ADP	E	2001	5	-	3/12/32/32	0/3/3/3
3	08T	B	2001	5	-	3/12/38/38	0/3/3/3
3	08T	C	2001	5	-	4/12/38/38	0/3/3/3
6	ADP	F	2001	5	-	6/12/32/32	0/3/3/3
3	08T	A	2001	5	-	4/12/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	08T	C5-C4	2.72	1.48	1.40
6	E	2001	ADP	C5-C4	2.58	1.47	1.40
6	D	2001	ADP	C5-C4	2.43	1.47	1.40
3	B	2001	08T	C5-C4	2.36	1.47	1.40
6	F	2001	ADP	C5-C4	2.30	1.47	1.40
3	A	2001	08T	C5-C4	2.22	1.46	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	08T	C3'-C2'-C1'	3.33	106.00	100.98
3	A	2001	08T	N3-C2-N1	-3.05	123.92	128.68
3	C	2001	08T	N3-C2-N1	-3.04	123.93	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	08T	N3-C2-N1	-3.02	123.96	128.68
6	F	2001	ADP	PA-O3A-PB	-2.97	122.62	132.83
6	D	2001	ADP	N3-C2-N1	-2.94	124.08	128.68
3	B	2001	08T	C3'-C2'-C1'	2.86	105.28	100.98
6	D	2001	ADP	N6-C6-N1	2.86	124.51	118.57
6	F	2001	ADP	C3'-C2'-C1'	2.69	105.02	100.98
3	A	2001	08T	C4-C5-N7	-2.68	106.60	109.40
3	C	2001	08T	C4-C5-N7	-2.60	106.69	109.40
6	E	2001	ADP	N3-C2-N1	-2.56	124.68	128.68
3	C	2001	08T	C3'-C2'-C1'	2.55	104.81	100.98
6	E	2001	ADP	PA-O3A-PB	-2.50	124.26	132.83
3	A	2001	08T	O3B-PB-O1B	-2.33	105.00	111.52
6	F	2001	ADP	N3-C2-N1	-2.31	125.07	128.68
6	F	2001	ADP	C4-C5-N7	-2.24	107.07	109.40
6	F	2001	ADP	O3A-PB-O1B	-2.22	98.85	111.19
6	D	2001	ADP	O3B-PB-O2B	2.19	116.02	107.64
3	C	2001	08T	O2B-PB-O1B	2.15	122.89	112.24
3	B	2001	08T	C4-C5-N7	-2.14	107.17	109.40
3	C	2001	08T	PB-O3A-PA	-2.14	125.48	132.83
3	C	2001	08T	C2-N1-C6	2.09	122.32	118.75
6	E	2001	ADP	C2-N1-C6	2.08	122.31	118.75
6	D	2001	ADP	C3'-C2'-C1'	2.05	104.07	100.98
6	E	2001	ADP	C4-C5-N7	-2.05	107.26	109.40
6	E	2001	ADP	O3A-PB-O1B	-2.04	99.88	111.19
3	A	2001	08T	O2B-PB-O1B	2.03	122.26	112.24
3	B	2001	08T	PB-O3A-PA	-2.00	125.95	132.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	08T	C5'-O5'-PA-O1A
3	B	2001	08T	C5'-O5'-PA-O1A
3	C	2001	08T	C5'-O5'-PA-O2A
6	D	2001	ADP	PA-O3A-PB-O3B
6	D	2001	ADP	C5'-O5'-PA-O1A
6	E	2001	ADP	PA-O3A-PB-O2B
6	F	2001	ADP	PA-O3A-PB-O2B
6	F	2001	ADP	PA-O3A-PB-O3B
6	F	2001	ADP	C5'-O5'-PA-O1A
6	F	2001	ADP	C5'-O5'-PA-O2A
3	B	2001	08T	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
6	D	2001	ADP	C5'-O5'-PA-O3A
6	F	2001	ADP	C5'-O5'-PA-O3A
3	B	2001	08T	C5'-O5'-PA-O2A
3	C	2001	08T	C5'-O5'-PA-O1A
6	D	2001	ADP	C5'-O5'-PA-O2A
3	C	2001	08T	PA-O3A-PB-O2B
6	D	2001	ADP	O4'-C4'-C5'-O5'
6	D	2001	ADP	PA-O3A-PB-O2B
6	E	2001	ADP	PA-O3A-PB-O3B
3	A	2001	08T	C5'-O5'-PA-O3A
3	C	2001	08T	C5'-O5'-PA-O3A
6	E	2001	ADP	C5'-O5'-PA-O3A
3	A	2001	08T	PA-O3A-PB-O1B
3	A	2001	08T	C5'-O5'-PA-O2A
6	F	2001	ADP	PA-O3A-PB-O1B

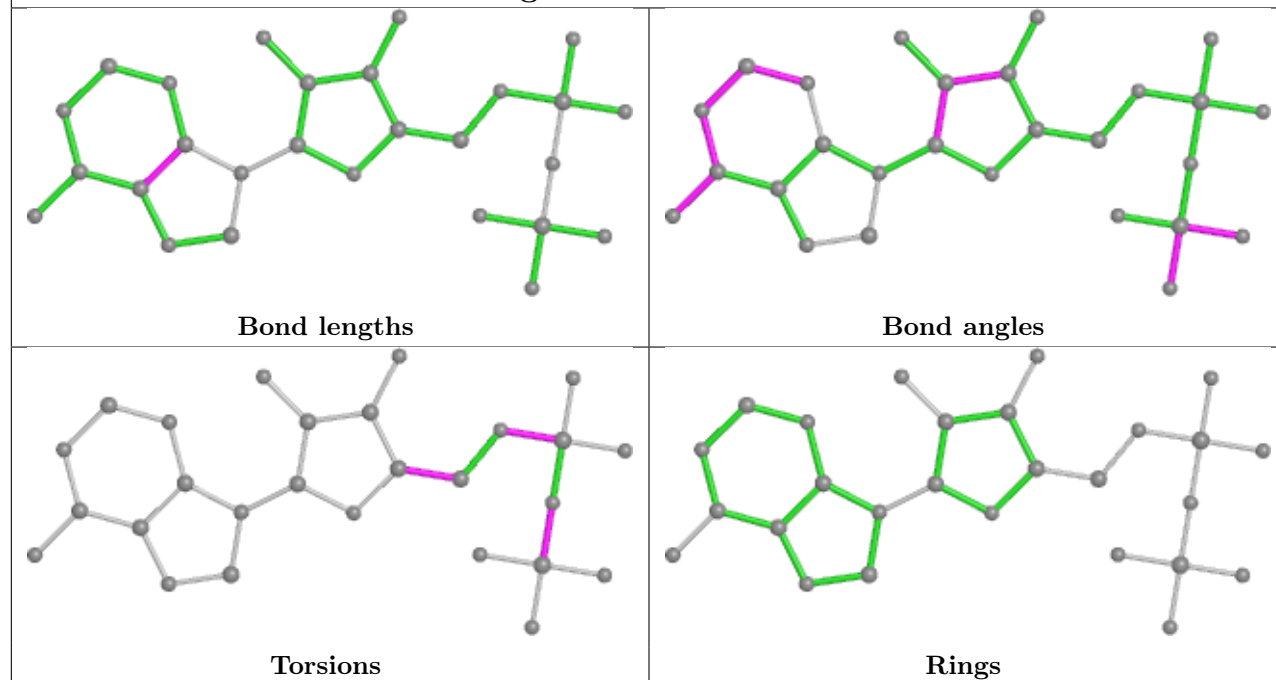
There are no ring outliers.

1 monomer is involved in 1 short contact:

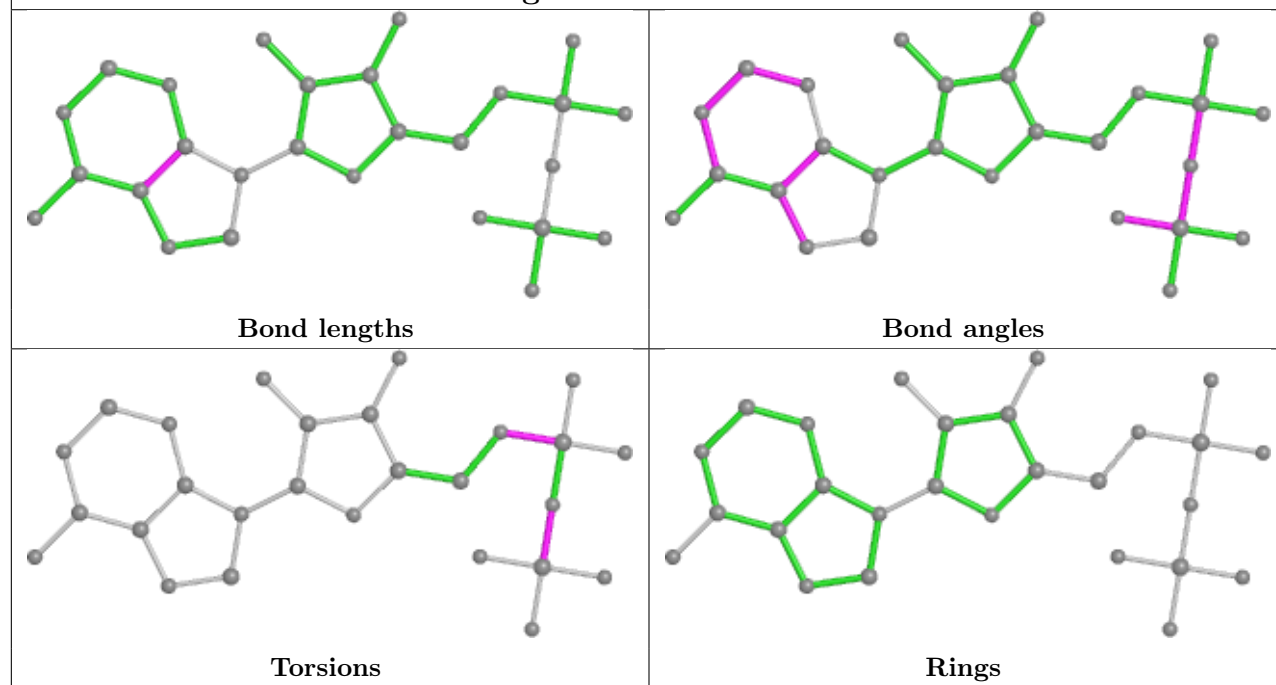
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

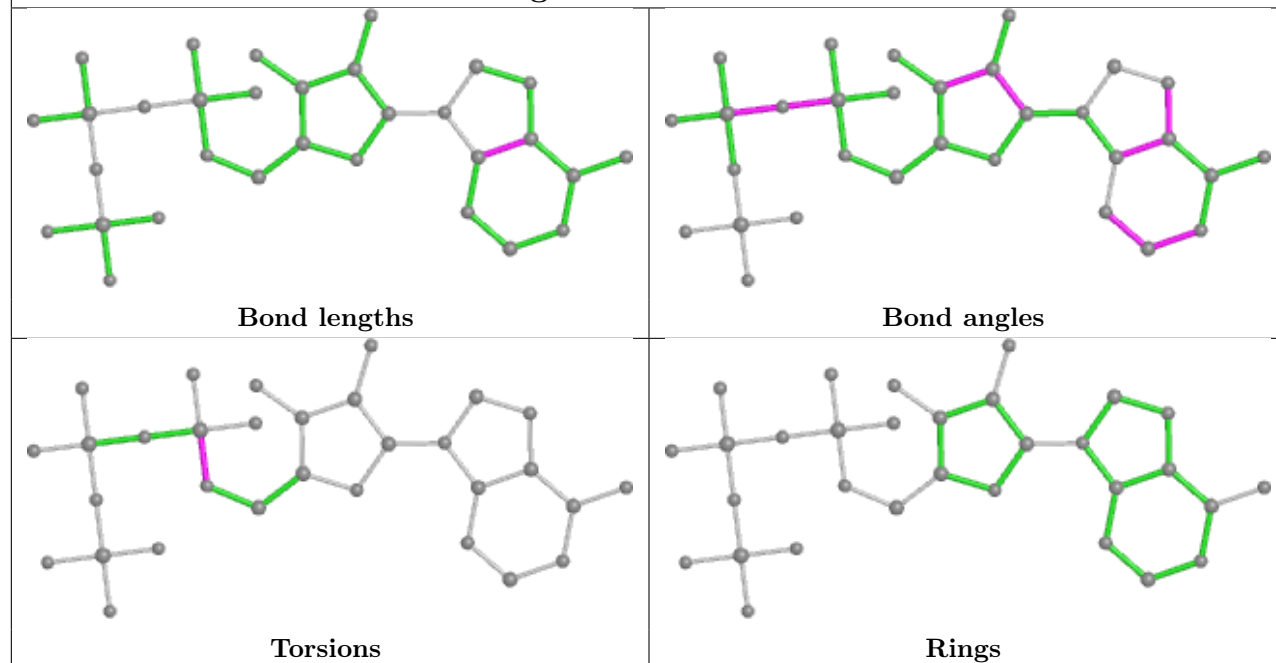
Ligand ADP D 2001



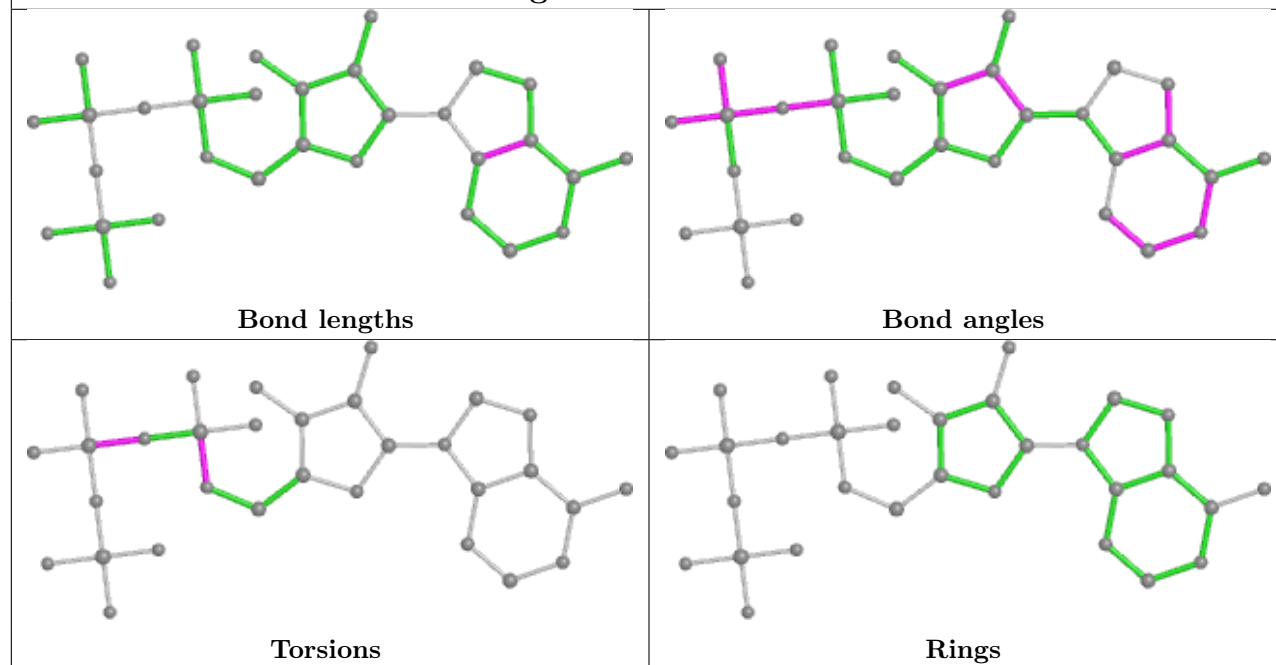
Ligand ADP E 2001

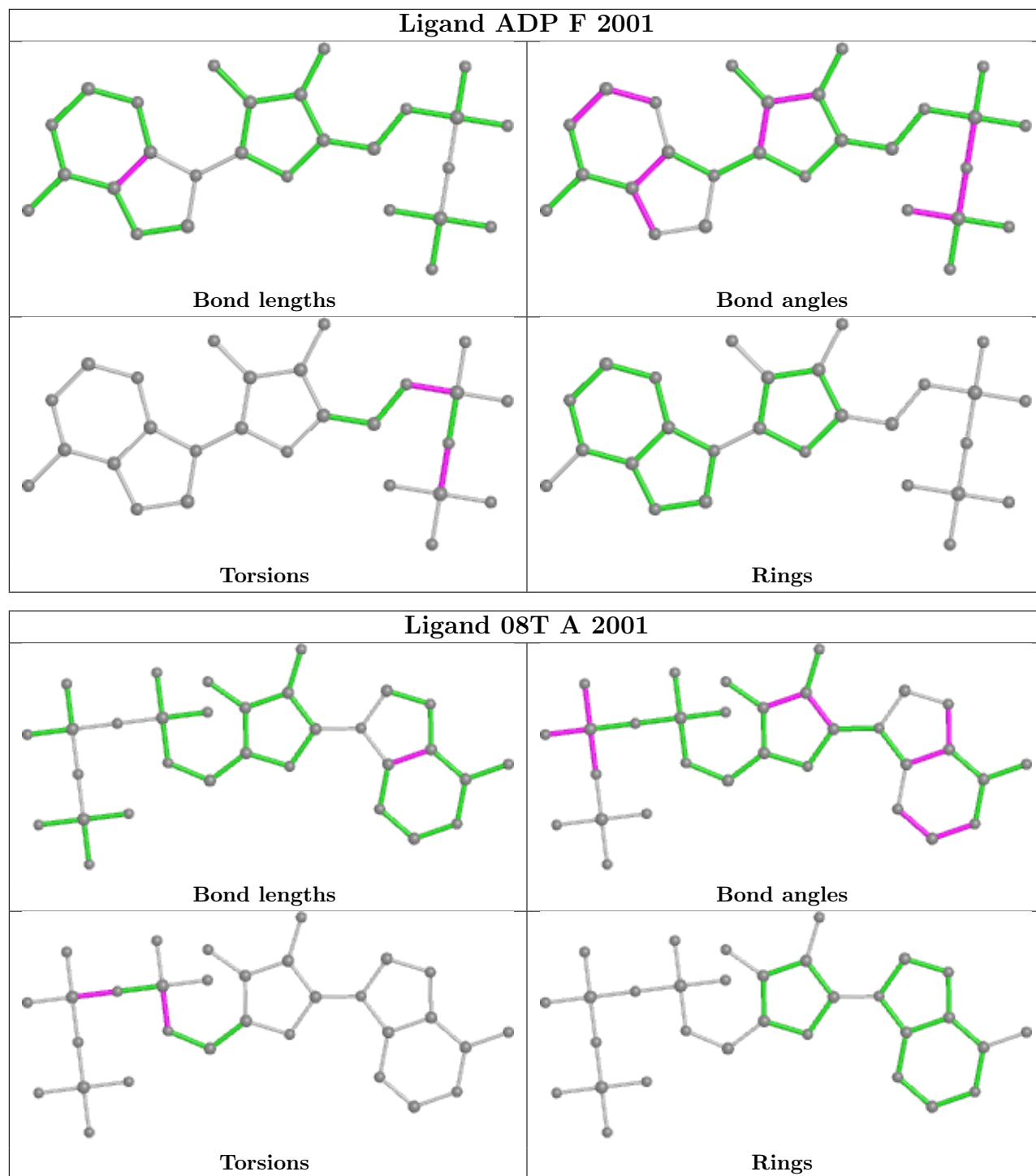


Ligand 08T B 2001



Ligand 08T C 2001





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	585/610 (95%)	-0.12	20 (3%)	45	28	72, 113, 209, 257	0
1	B	589/610 (96%)	-0.25	5 (0%)	86	78	70, 107, 192, 244	0
1	C	589/610 (96%)	-0.13	11 (1%)	66	53	84, 136, 204, 253	0
1	D	589/610 (96%)	0.25	48 (8%)	12	6	110, 169, 262, 303	0
1	E	592/610 (97%)	0.18	45 (7%)	13	7	105, 156, 262, 298	0
1	F	589/610 (96%)	-0.01	22 (3%)	41	25	80, 127, 228, 269	0
2	X	10/12 (83%)	-0.20	0	100	100	124, 158, 180, 182	0
All	All	3543/3672 (96%)	-0.01	151 (4%)	35	21	70, 136, 242, 303	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	245	VAL	10.3
1	E	248	GLY	8.4
1	F	244	PRO	8.4
1	E	249	SER	7.1
1	E	244	PRO	6.6
1	F	246	LYS	6.3
1	D	100	ILE	6.1
1	E	158	ASP	6.1
1	D	78	LEU	6.0
1	A	382	GLY	5.7
1	E	30	TYR	5.7
1	D	45	LEU	5.5
1	D	47	ILE	5.5
1	E	7	GLN	5.5
1	E	169	THR	5.3
1	F	247	ARG	5.2
1	E	180	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	382	GLY	4.9
1	D	99	ARG	4.9
1	D	59	LEU	4.8
1	C	245	VAL	4.6
1	E	179	GLN	4.5
1	E	245	VAL	4.5
1	D	8	ILE	4.5
1	B	247	ARG	4.4
1	E	247	ARG	4.4
1	F	30	TYR	4.2
1	D	54	SER	4.0
1	D	7	GLN	3.9
1	D	63	ILE	3.9
1	E	8	ILE	3.9
1	E	47	ILE	3.8
1	E	145	ILE	3.8
1	A	387	TYR	3.7
1	D	53	LEU	3.7
1	C	14	PHE	3.7
1	C	247	ARG	3.7
1	A	386	TYR	3.6
1	E	18	LEU	3.5
1	E	78	LEU	3.5
1	E	29	LYS	3.4
1	F	170	ILE	3.4
1	C	244	PRO	3.4
1	D	168	PRO	3.4
1	D	79	TYR	3.4
1	E	28	ASN	3.3
1	E	77	ALA	3.3
1	F	169	THR	3.2
1	A	381	LYS	3.2
1	D	93	ILE	3.1
1	E	79	TYR	3.1
1	E	14	PHE	3.1
1	D	60	ALA	3.1
1	D	152	GLU	3.1
1	E	170	ILE	3.1
1	D	82	ILE	3.0
1	D	179	GLN	3.0
1	E	148	ASP	3.0
1	D	14	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	170	ILE	3.0
1	A	245	VAL	3.0
1	D	245	VAL	3.0
1	D	77	ALA	2.9
1	F	383	THR	2.9
1	A	7	GLN	2.9
1	A	169	THR	2.9
1	D	257	MET	2.9
1	E	64	ILE	2.8
1	E	147	PRO	2.8
1	F	178	GLY	2.8
1	E	506	ASN	2.8
1	F	147	PRO	2.8
1	D	237	LEU	2.8
1	D	166	GLU	2.8
1	A	379	ARG	2.8
1	D	575	MET	2.8
1	F	381	LYS	2.8
1	D	142	TYR	2.7
1	A	177	PRO	2.7
1	D	265	SER	2.7
1	F	168	PRO	2.7
1	A	148	ASP	2.7
1	E	63	ILE	2.7
1	A	179	GLN	2.7
1	F	386	TYR	2.7
1	D	81	HIS	2.7
1	D	147	PRO	2.7
1	D	61	TYR	2.7
1	F	166	GLU	2.6
1	E	27	GLN	2.6
1	B	244	PRO	2.6
1	C	177	PRO	2.6
1	A	246	LYS	2.6
1	E	191	ASP	2.6
1	D	247	ARG	2.6
1	A	378	VAL	2.6
1	E	257	MET	2.6
1	D	46	ILE	2.5
1	D	43	LYS	2.5
1	E	46	ILE	2.5
1	F	172	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	2.5
1	C	8	ILE	2.5
1	D	163	GLU	2.5
1	F	177	PRO	2.5
1	A	384	GLY	2.5
1	E	49	PHE	2.5
1	F	243	SER	2.5
1	E	82	ILE	2.5
1	E	160	GLU	2.5
1	D	26	ASN	2.4
1	C	382	GLY	2.4
1	E	44	SER	2.4
1	D	244	PRO	2.4
1	D	28	ASN	2.4
1	E	181	ARG	2.4
1	F	89	TYR	2.4
1	E	45	LEU	2.4
1	A	178	GLY	2.3
1	D	177	PRO	2.3
1	D	165	LEU	2.3
1	E	142	TYR	2.3
1	D	96	VAL	2.3
1	D	49	PHE	2.3
1	E	607	GLY	2.3
1	E	75	GLU	2.3
1	F	18	LEU	2.3
1	B	178	GLY	2.3
1	A	244	PRO	2.3
1	D	182	LEU	2.3
1	D	89	TYR	2.3
1	D	74	LEU	2.2
1	B	248	GLY	2.2
1	D	58	ASN	2.2
1	D	55	PHE	2.2
1	E	382	GLY	2.2
1	C	248	GLY	2.2
1	A	14	PHE	2.2
1	A	8	ILE	2.1
1	F	148	ASP	2.1
1	C	74	LEU	2.1
1	A	168	PRO	2.1
1	F	14	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	554	PRO	2.1
1	B	347	SER	2.1
1	D	576	ALA	2.1
1	E	167	MET	2.1
1	E	155	TRP	2.0
1	C	152	GLU	2.0
1	E	526	PRO	2.0
1	E	81	HIS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

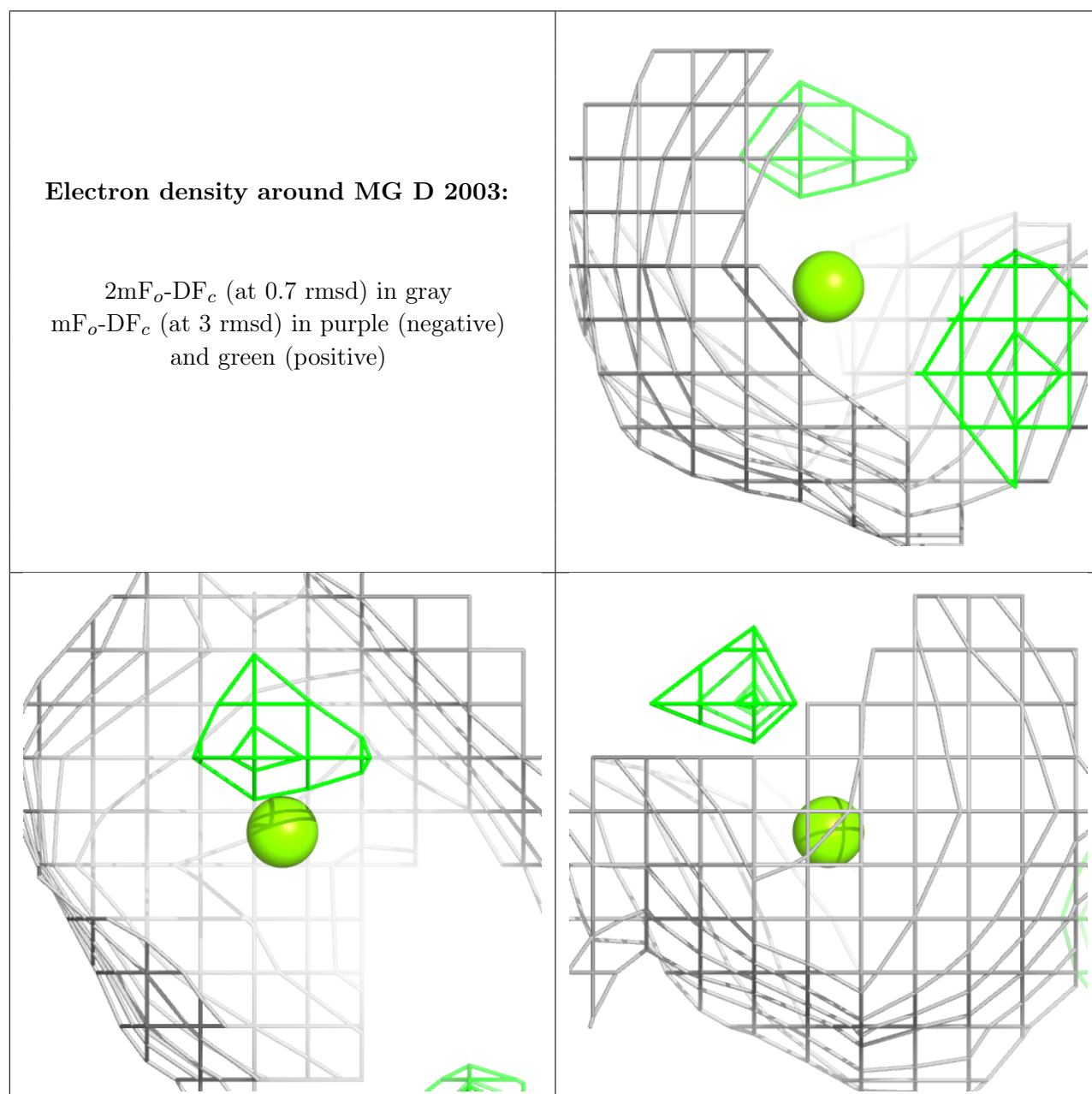
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	A	2002	1/1	0.68	0.06	239,239,239,239	0
4	ZN	D	2002	1/1	0.68	0.05	255,255,255,255	0
4	ZN	F	2002	1/1	0.80	0.14	247,247,247,247	0
4	ZN	E	2002	1/1	0.83	0.05	270,270,270,270	0
5	MG	D	2003	1/1	0.84	0.26	176,176,176,176	0
4	ZN	B	2002	1/1	0.91	0.04	211,211,211,211	0
5	MG	F	2003	1/1	0.92	0.35	161,161,161,161	0
6	ADP	E	2001	27/27	0.92	0.28	105,115,124,138	0
3	08T	C	2001	31/31	0.94	0.27	97,117,141,142	0
3	08T	B	2001	31/31	0.95	0.27	81,100,114,128	0
6	ADP	F	2001	27/27	0.95	0.26	91,109,117,127	0
6	ADP	D	2001	27/27	0.96	0.23	129,142,147,158	0
5	MG	E	2003	1/1	0.97	0.38	153,153,153,153	0
3	08T	A	2001	31/31	0.97	0.27	75,82,109,115	0
5	MG	B	2003	1/1	0.97	0.29	119,119,119,119	0

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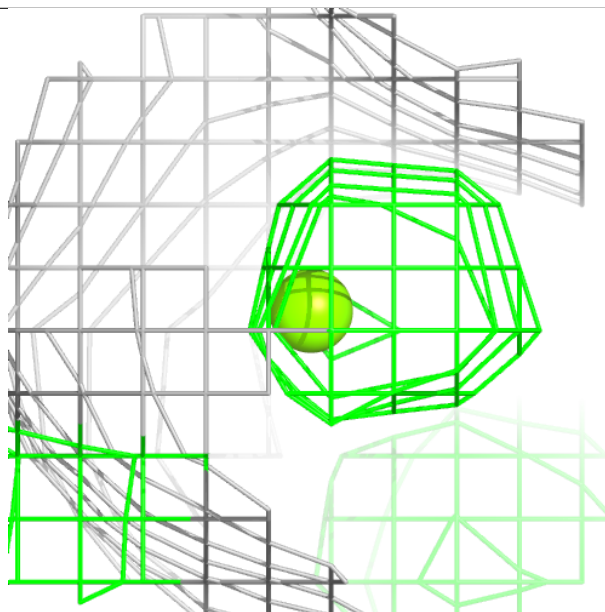
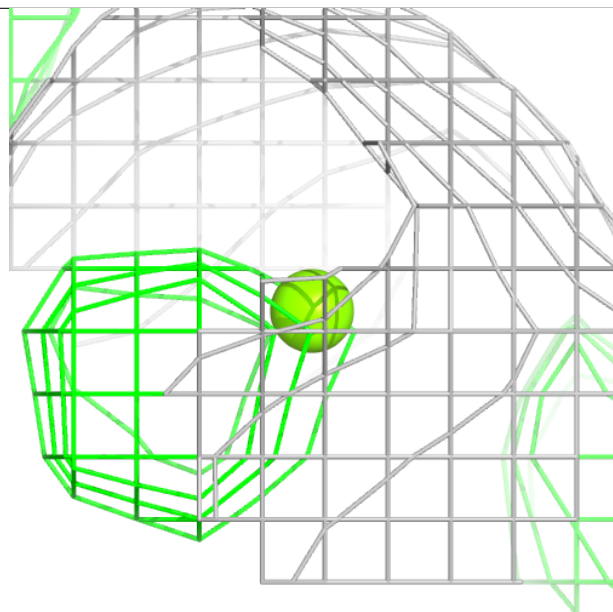
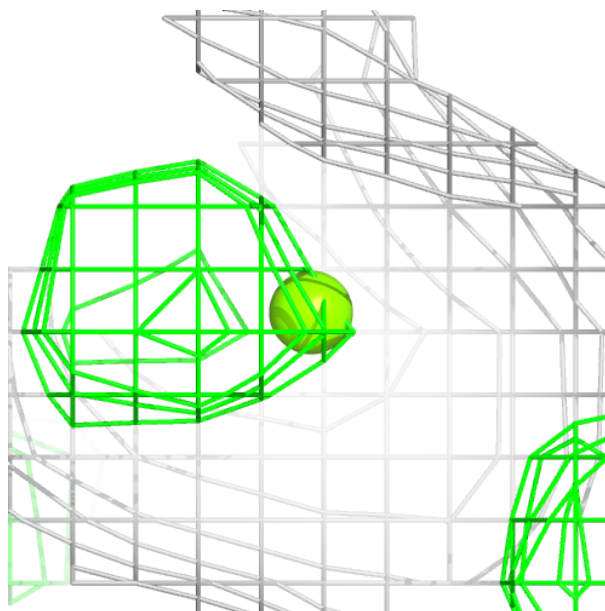
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	2003	1/1	0.97	0.32	157,157,157,157	0
4	ZN	C	2002	1/1	0.97	0.05	182,182,182,182	0
5	MG	A	2003	1/1	0.99	0.28	115,115,115,115	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



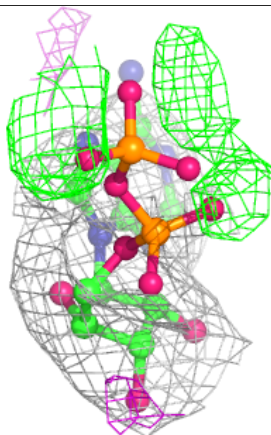
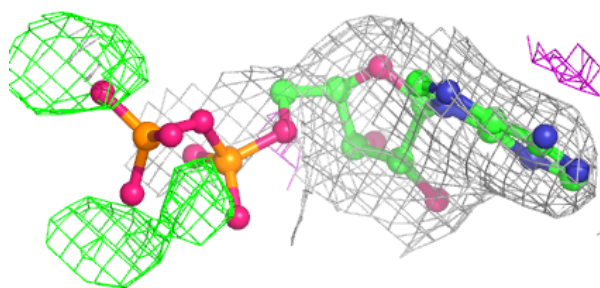
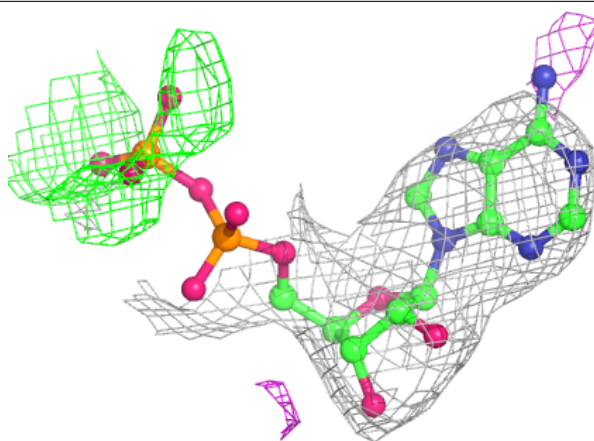
Electron density around MG F 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

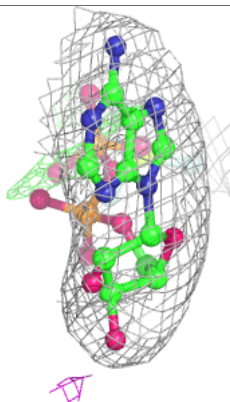
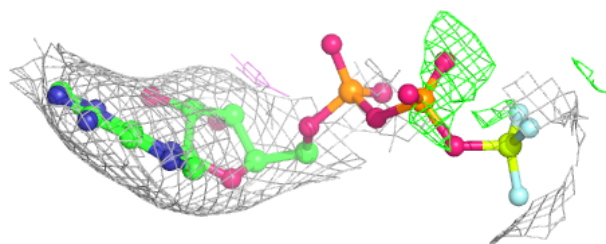
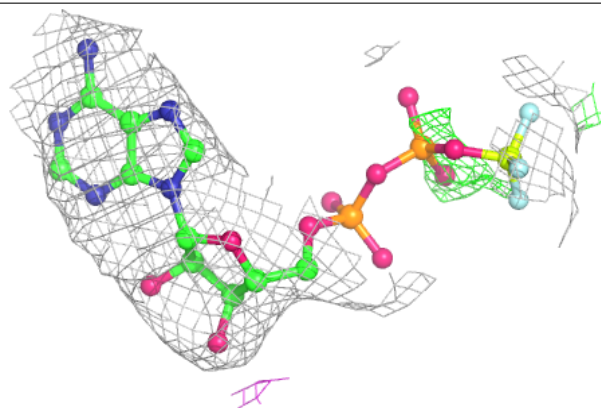


Electron density around ADP E 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

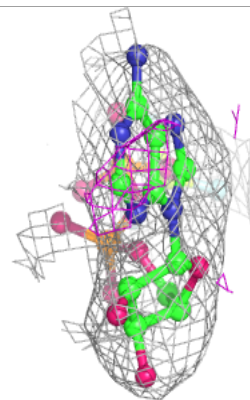
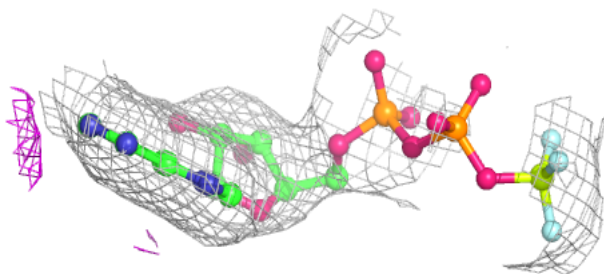
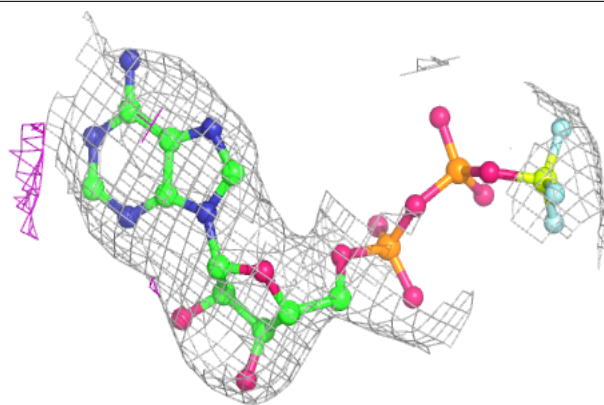
**Electron density around 08T C 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

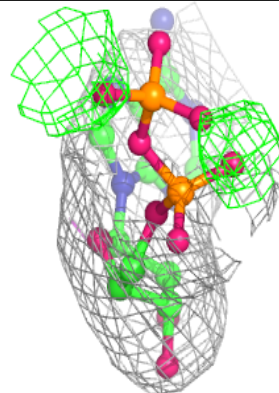
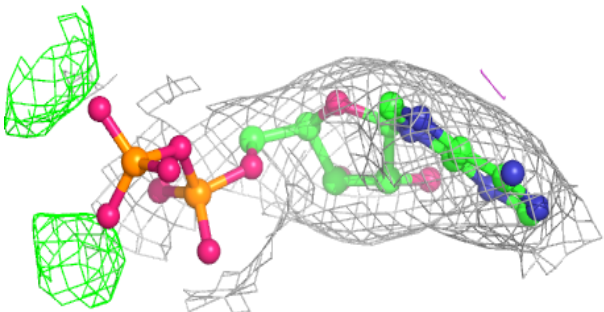
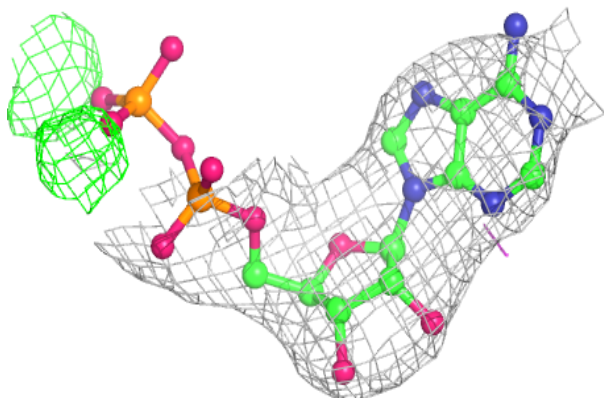


Electron density around 08T B 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

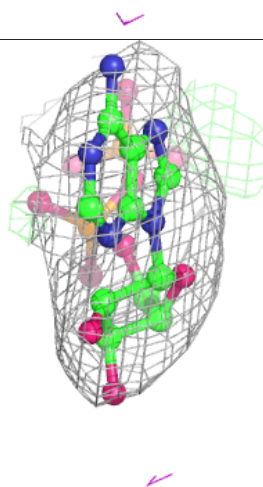
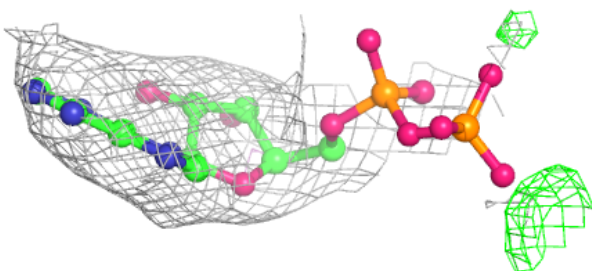
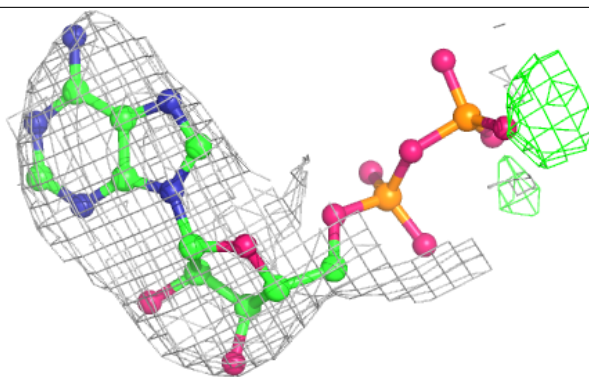
**Electron density around ADP F 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



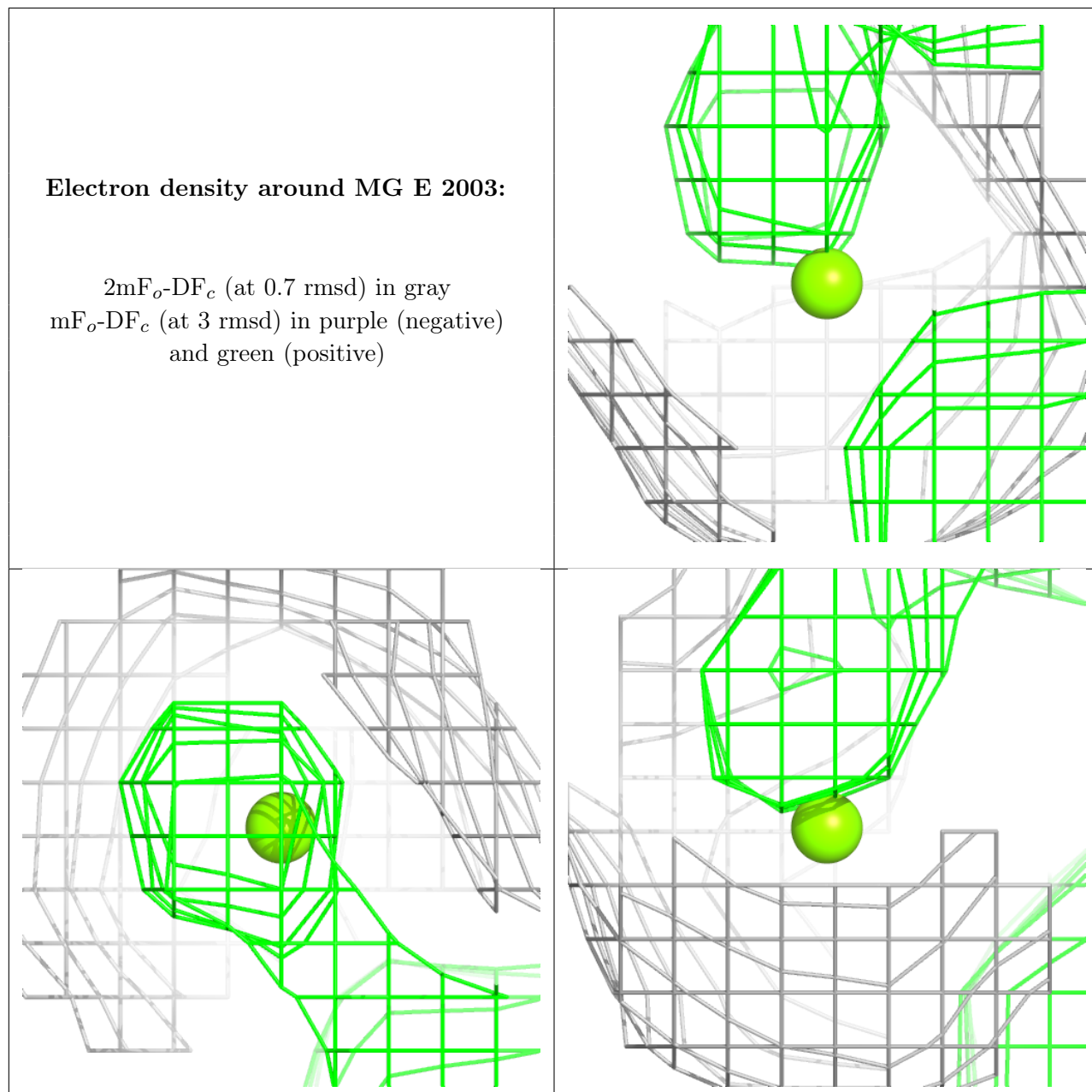
Electron density around ADP D 2001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



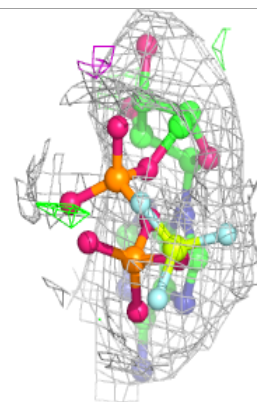
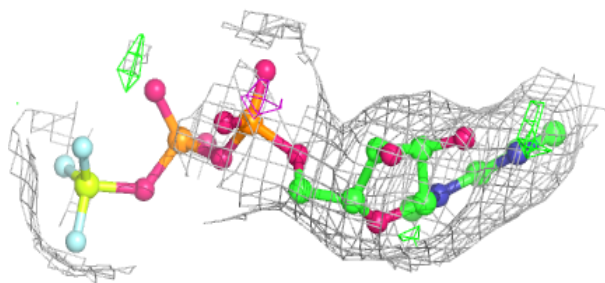
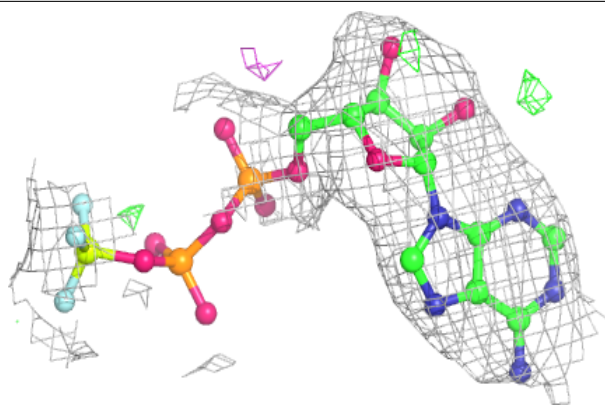
Electron density around MG E 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



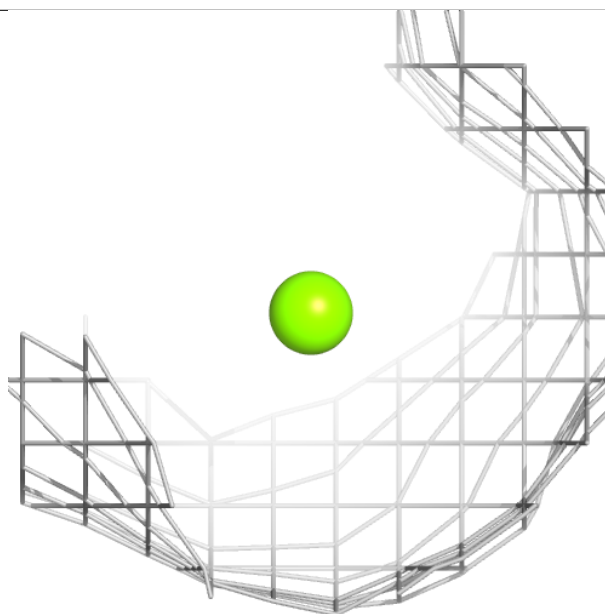
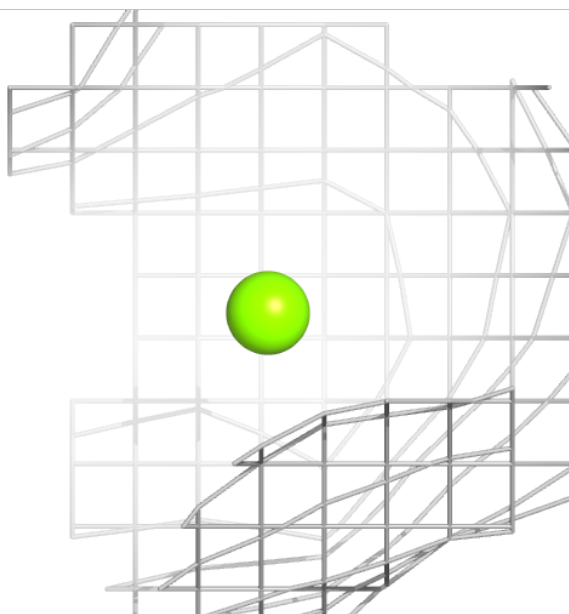
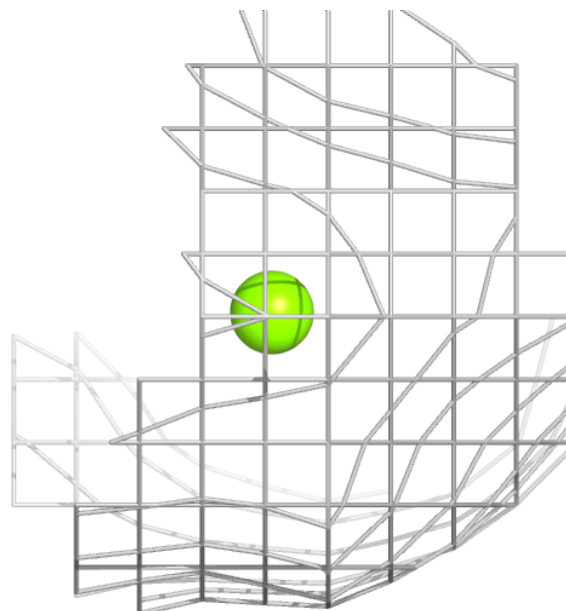
Electron density around 08T A 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



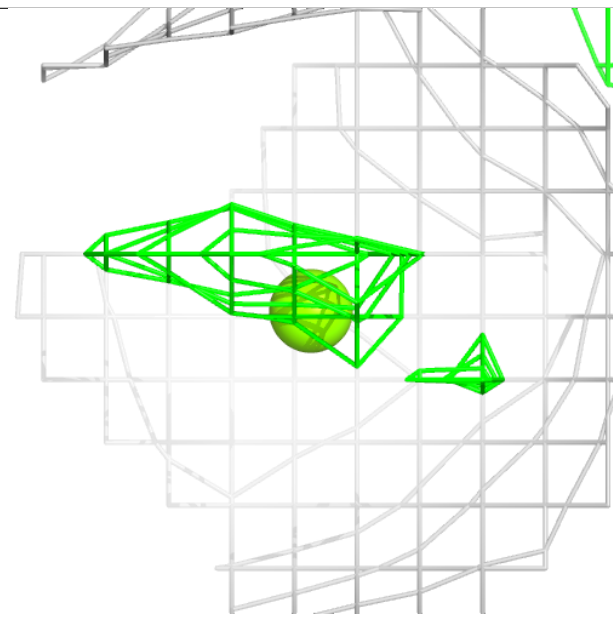
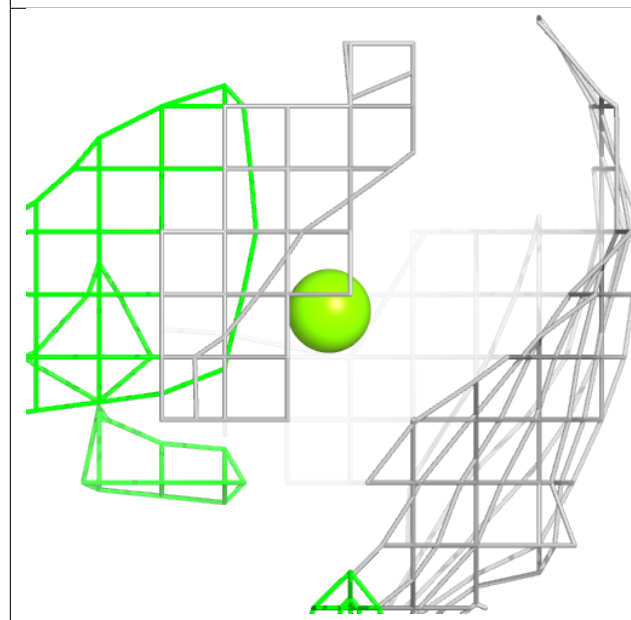
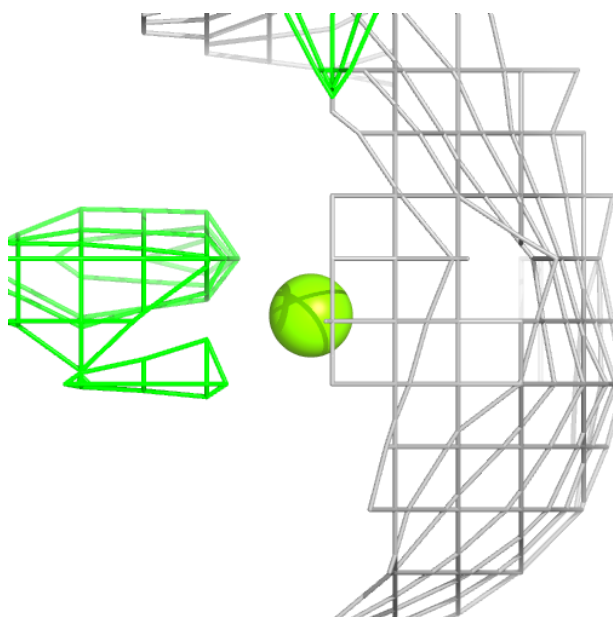
Electron density around MG B 2003:

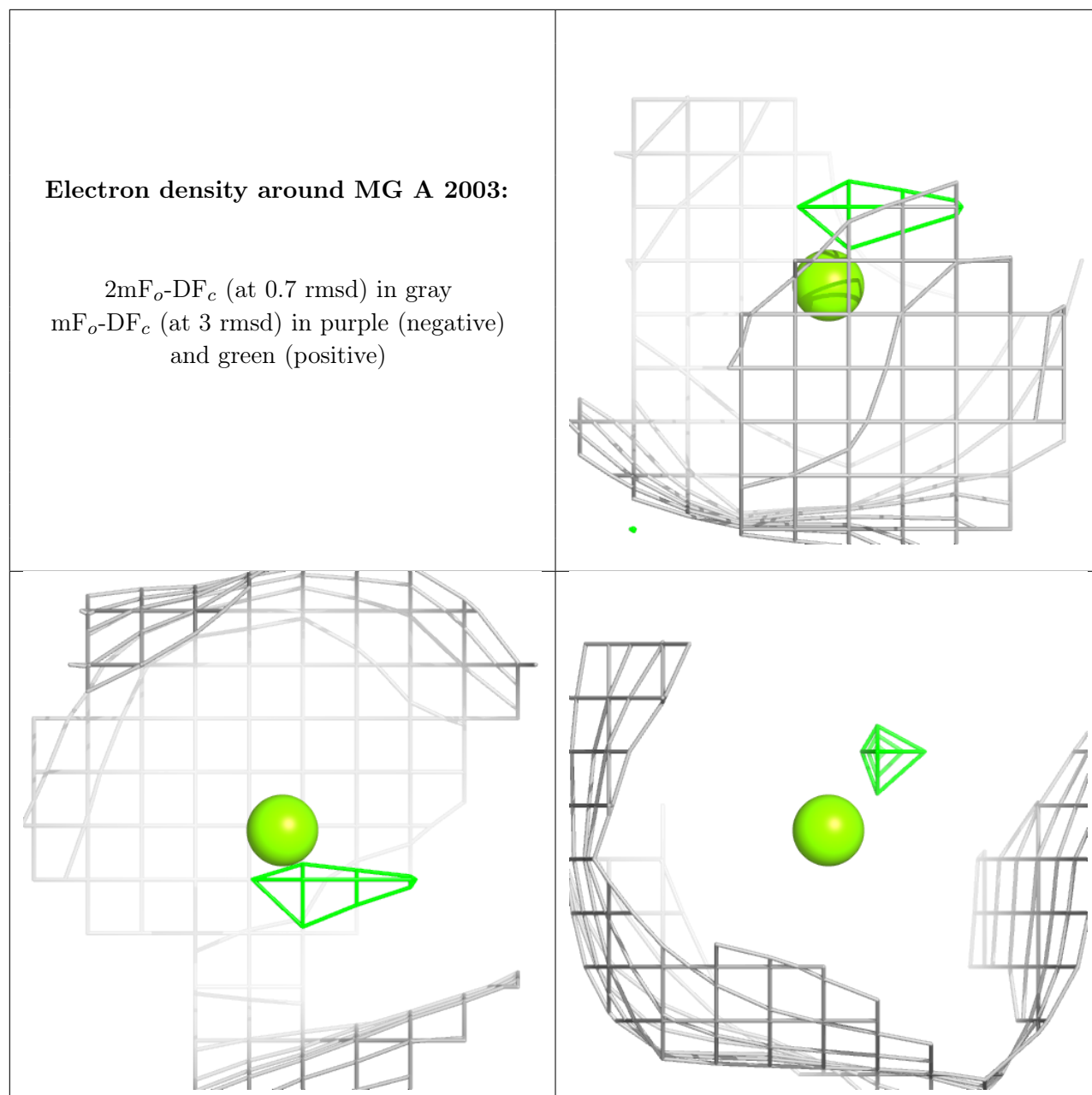
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG C 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.