Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 AM UTC

PDB ID	:	6MII / pdb_00006mii
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:

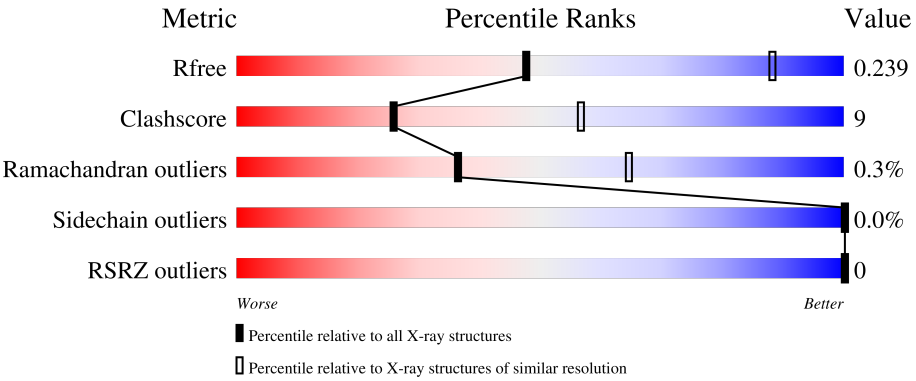
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 <=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	70% 26% .
1	B	610	76% 21% .
1	C	610	72% 24% .
1	D	610	78% 18% .
1	E	610	75% 22% .

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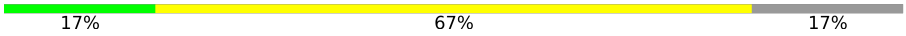
Mol	Chain	Length	Quality of chain
1	F	610	
2	X	12	

2 Entry composition (i)

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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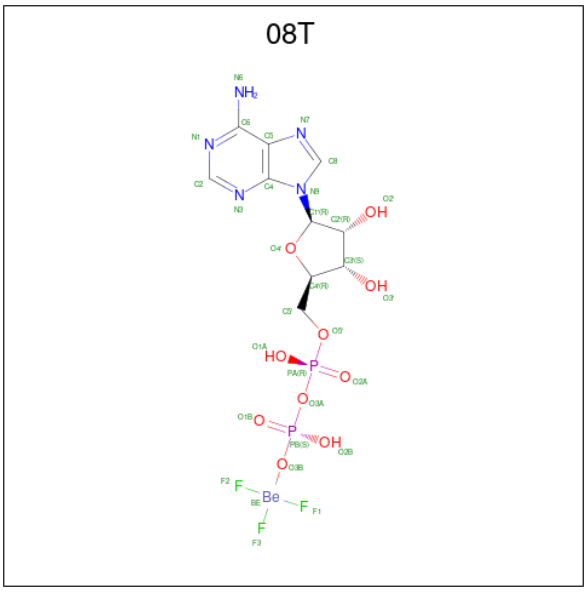
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LEU	-	expression tag	UNP Q9UXG1
C	269	GLY	-	linker	UNP Q9UXG1
C	270	GLY	-	linker	UNP Q9UXG1
C	271	SER	-	linker	UNP Q9UXG1
C	272	GLY	-	linker	UNP Q9UXG1
C	273	GLY	-	linker	UNP Q9UXG1
C	274	SER	-	linker	UNP Q9UXG1
D	0	SER	-	expression tag	UNP Q9UXG1
D	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*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 (CCD ID: 08T) (formula: $C_{10}H_{14}BeF_3N_5O_{10}P_2$) (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		

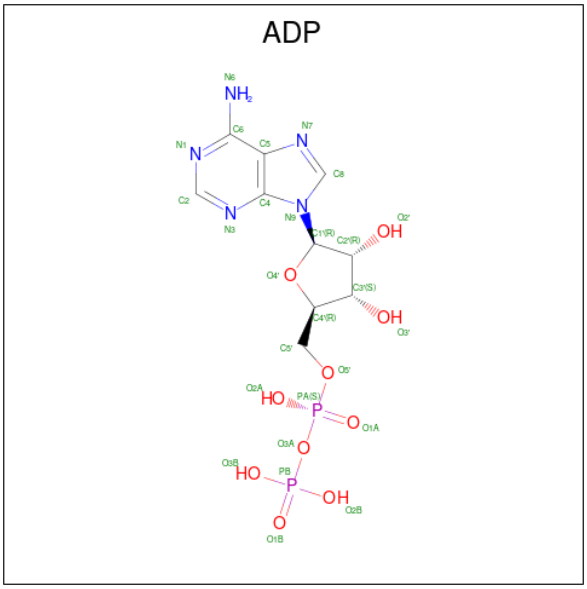
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: 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 (CCD ID: 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.

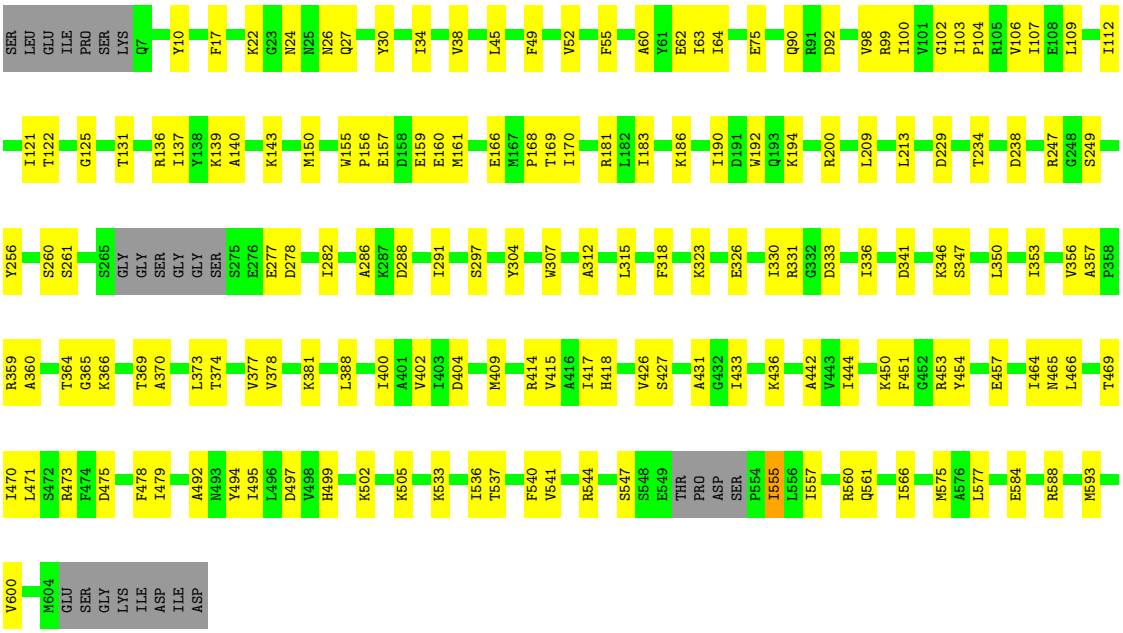
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	2	Total O 2 2	0	0
7	C	3	Total O 3 3	0	0
7	D	4	Total O 4 4	0	0
7	E	3	Total O 3 3	0	0
7	F	3	Total O 3 3	0	0

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 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.

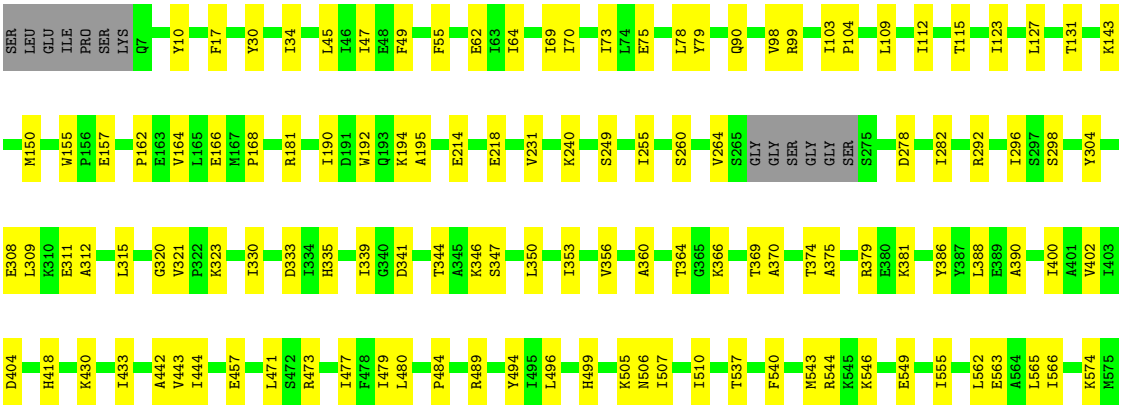
• Molecule 1: Minichromosome maintenance protein MCM

Chain A:



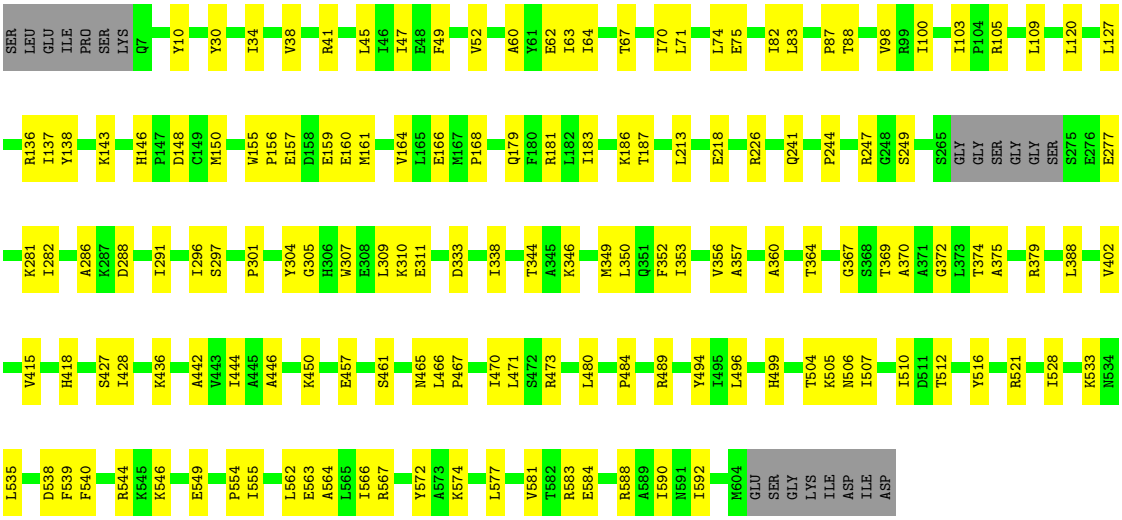
• Molecule 1: Minichromosome maintenance protein MCM

Chain B:



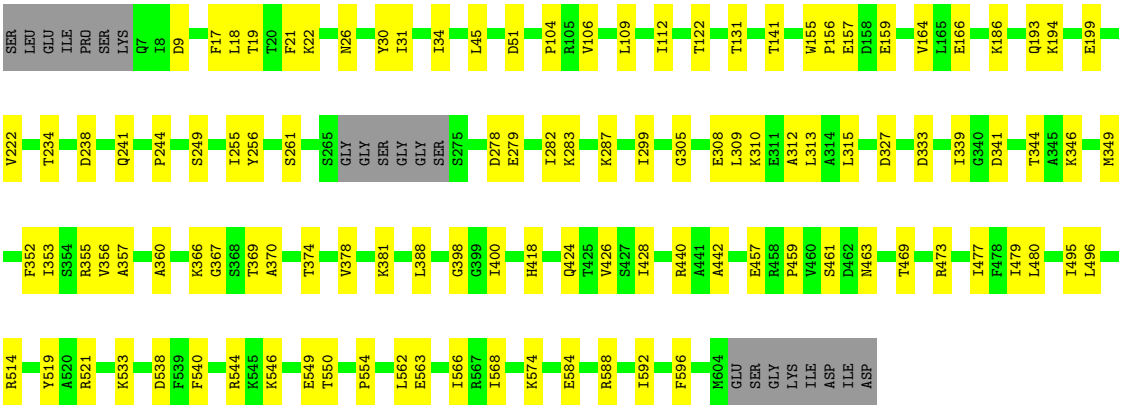
• Molecule 1: Minichromosome maintenance protein MCM

Chain C:



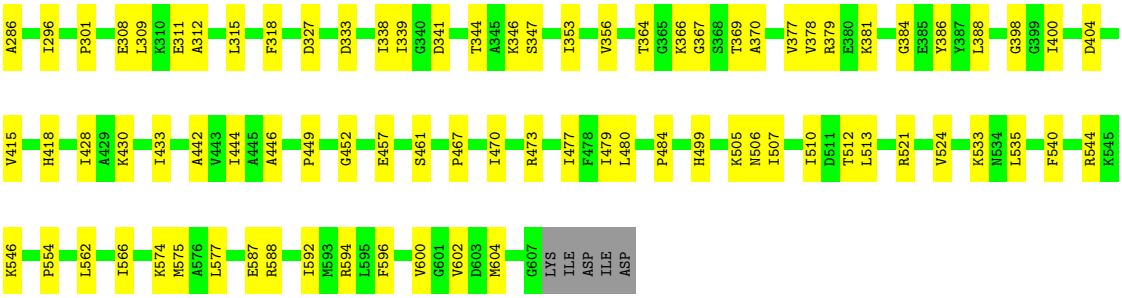
• Molecule 1: Minichromosome maintenance protein MCM

Chain D:



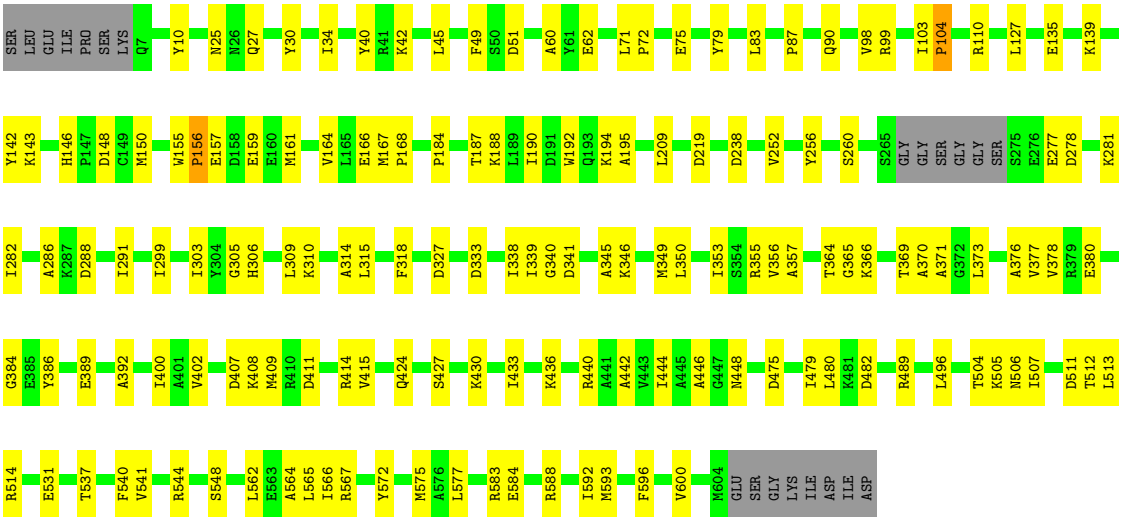
• Molecule 1: Minichromosome maintenance protein MCM

Chain E:



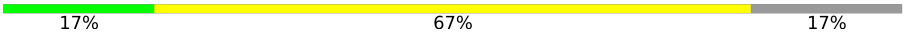
• Molecule 1: Minichromosome maintenance protein MCM

Chain F:



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

Chain X:



4 Data and refinement statistics (i)

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 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.70-3.15) 97.3 (44.70-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.188 , 0.241 0.191 , 0.239	Depositor DCC
R_{free} test set	4259 reflections (4.90%)	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)	0.29 , 85.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/4732	0.63	0/6393
1	B	0.36	0/4762	0.61	0/6438
1	C	0.29	0/4762	0.54	0/6438
1	D	0.25	0/4762	0.53	0/6438
1	E	0.27	0/4781	0.54	0/6463
1	F	0.31	0/4762	0.59	0/6438
2	X	0.42	0/220	0.65	0/336
All	All	0.31	0/28781	0.57	0/38944

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	A	4655	0	4797	118	0
1	B	4683	0	4820	95	0
1	C	4683	0	4820	109	0
1	D	4683	0	4820	77	0
1	E	4702	0	4834	99	0
1	F	4683	0	4820	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	545	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 (545) 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:A:373:LEU:HD11	1:A:409:MET:HE1	1.58	0.85
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:309:LEU:HD13	1:F:349:MET:HE1	1.73	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
1:C:183:ILE:HG22	1:C:186:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:214:GLU:OE2	1:E:240:LYS:NZ	2.30	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:F:184:PRO:C	1:F:187:THR:HG22	2.29	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: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:E:136:ARG:HH21	1:E:218:GLU:CD	2.13	0.56
1:F:377:VAL:HG22	1:F:433:ILE:HD11	1.86	0.56
1:B:543:MET:HA	1:B:604:MET:HE1	1.87	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:A:497:ASP:CG	1:A:502:LYS:HD2	2.32	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:565:LEU:HG	1:B:593:MET:HE3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:LEU:HD13	1:D:349:MET:HE1	1.91	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
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: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:A:373:LEU:CD1	1:A:409:MET:HE1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:99:ARG:HD3	1:F:260:SER:O	2.12	0.49
1:F:407:ASP:CG	1:F:448:ASN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:142:TYR:HE2	1:F:167:MET:HE2	1.80	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: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:F:565:LEU:HG	1:F:593:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:161:MET:HE1	1:C:166:GLU:O	2.16	0.45
1:C:415:VAL:HA	1:C:418:HIS:CE1	2.52	0.45
1:D:30:TYR:OH	1:D:51:ASP:OD2	2.24	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:GLU:N	1:F:277:GLU:OE1	2.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:409:MET:HE2	1:F:409:MET:HB3	1.68	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: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
1:F:25:ASN:H	1:F:27:GLN:CD	2.26	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:A:90:GLN:C	1:A:92:ASP:H	2.26	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.82	0.42
1:C:309:LEU:HB3	1:C:349:MET:HE1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HD13	1:B:218:GLU:OE1	2.20	0.42
1:C:146:HIS:C	1:C:148:ASP:H	2.27	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
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:146:HIS:C	1:E:148:ASP:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:282:ILE:HD12	1:F:282:ILE:C	2.46	0.41
1:F:357:ALA:HB1	1:F:400:ILE:HD13	2.02	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:593:MET:HE2	1:A:593:MET:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24 55
1	B	585/610 (96%)	552 (94%)	33 (6%)	0	100 100
1	C	585/610 (96%)	552 (94%)	32 (6%)	1 (0%)	43 71
1	D	585/610 (96%)	556 (95%)	26 (4%)	3 (0%)	24 55
1	E	588/610 (96%)	557 (95%)	31 (5%)	0	100 100
1	F	585/610 (96%)	552 (94%)	31 (5%)	2 (0%)	36 64
All	All	3507/3660 (96%)	3314 (94%)	184 (5%)	9 (0%)	36 64

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%)	510 (100%)	0	100 100
1	B	514/530 (97%)	514 (100%)	0	100 100
1	C	514/530 (97%)	513 (100%)	1 (0%)	87 87
1	D	514/530 (97%)	514 (100%)	0	100 100
1	E	516/530 (97%)	516 (100%)	0	100 100
1	F	514/530 (97%)	514 (100%)	0	100 100
All	All	3082/3180 (97%)	3081 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
1	C	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	B	97	HIS
1	B	179	GLN
1	B	306	HIS
1	B	348	GLN
1	C	25	ASN
1	C	465	ASN
1	D	28	ASN
1	D	56	ASN
1	D	58	ASN
1	D	465	ASN
1	E	58	ASN
1	E	66	ASN
1	E	348	GLN
1	E	506	ASN
1	F	448	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 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	$\#\|Z\| > 2$
3	08T	C	2001	5	31,33,33	1.48	4 (12%)	41,52,52	1.86	9 (21%)
3	08T	A	2001	5	31,33,33	1.36	4 (12%)	41,52,52	1.96	13 (31%)
6	ADP	F	2001	5	28,29,29	1.42	6 (21%)	43,45,45	1.70	8 (18%)
3	08T	B	2001	5	31,33,33	1.44	6 (19%)	41,52,52	1.75	7 (17%)
6	ADP	D	2001	5	28,29,29	1.46	5 (17%)	43,45,45	1.79	10 (23%)
6	ADP	E	2001	5	28,29,29	1.51	5 (17%)	43,45,45	1.73	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	08T	C	2001	5	-	4/16/38/38	0/3/3/3
3	08T	A	2001	5	-	2/16/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	F	2001	5	-	7/16/32/32	0/3/3/3
3	08T	B	2001	5	-	4/16/38/38	0/3/3/3
6	ADP	D	2001	5	-	6/16/32/32	0/3/3/3
6	ADP	E	2001	5	-	2/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	08T	C5-C4	5.06	1.48	1.39
6	E	2001	ADP	C5-C4	4.86	1.47	1.39
6	D	2001	ADP	C5-C4	4.64	1.47	1.39
3	B	2001	08T	C5-C4	4.53	1.47	1.39
6	F	2001	ADP	C5-C4	4.45	1.47	1.39
3	A	2001	08T	C5-C4	4.33	1.46	1.39
6	E	2001	ADP	PA-O3A	3.22	1.63	1.59
6	F	2001	ADP	C5-N7	-2.80	1.34	1.39
6	D	2001	ADP	C5-N7	-2.78	1.34	1.39
6	D	2001	ADP	PA-O3A	2.76	1.62	1.59
3	C	2001	08T	C5-C6	2.70	1.48	1.41
3	A	2001	08T	C8-N7	2.67	1.36	1.31
3	B	2001	08T	C5-C6	2.53	1.48	1.41
3	A	2001	08T	C5-N7	-2.51	1.34	1.39
6	E	2001	ADP	C5-C6	2.48	1.47	1.41
3	C	2001	08T	C5-N7	-2.44	1.34	1.39
3	C	2001	08T	C8-N7	2.43	1.36	1.31
3	B	2001	08T	C5-N7	-2.40	1.34	1.39
6	E	2001	ADP	C5-N7	-2.38	1.34	1.39
6	F	2001	ADP	C5-C6	2.36	1.47	1.41
6	E	2001	ADP	C8-N7	2.32	1.36	1.31
6	F	2001	ADP	C8-N7	2.31	1.36	1.31
3	B	2001	08T	C8-N7	2.30	1.36	1.31
3	A	2001	08T	C5-C6	2.25	1.47	1.41
6	F	2001	ADP	C4-N9	-2.23	1.33	1.37
6	D	2001	ADP	C4-N9	-2.20	1.33	1.37
3	B	2001	08T	PB-O3A	2.12	1.61	1.59
3	B	2001	08T	C4-N9	-2.11	1.33	1.37
6	D	2001	ADP	C8-N7	2.08	1.35	1.31
6	F	2001	ADP	PA-O3A	2.04	1.61	1.59

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	08T	C5-C4-N3	-5.76	118.79	126.72
6	F	2001	ADP	C5-C4-N3	-5.74	118.82	126.72
3	C	2001	08T	C5-C4-N3	-5.70	118.87	126.72
3	B	2001	08T	C5-C4-N3	-5.43	119.24	126.72
6	E	2001	ADP	C5-C4-N3	-4.98	119.86	126.72
6	D	2001	ADP	C5-C4-N3	-4.98	119.86	126.72
6	D	2001	ADP	N3-C4-N9	4.84	135.40	127.17
3	C	2001	08T	N3-C4-N9	4.51	134.83	127.17
6	F	2001	ADP	N3-C4-N9	4.37	134.60	127.17
6	E	2001	ADP	N3-C4-N9	4.30	134.49	127.17
3	A	2001	08T	N3-C4-N9	4.30	134.47	127.17
3	B	2001	08T	N3-C4-N9	4.28	134.45	127.17
6	D	2001	ADP	C4-N9-C8	3.53	109.44	105.74
3	A	2001	08T	C2-N3-C4	3.50	120.39	111.83
3	A	2001	08T	C4-C5-N7	-3.48	106.60	110.58
3	B	2001	08T	C2-N3-C4	3.47	120.31	111.83
3	C	2001	08T	C2-N3-C4	3.44	120.23	111.83
3	C	2001	08T	C4-C5-N7	-3.40	106.69	110.58
6	F	2001	ADP	C2-N3-C4	3.26	119.78	111.83
3	A	2001	08T	O3A-PB-O1B	-3.11	101.34	110.70
3	A	2001	08T	N3-C2-N1	-3.08	123.92	128.58
6	F	2001	ADP	C4-C5-N7	-3.08	107.07	110.58
3	C	2001	08T	N3-C2-N1	-3.07	123.93	128.58
3	B	2001	08T	N3-C2-N1	-3.05	123.96	128.58
6	E	2001	ADP	C4-N9-C8	3.02	108.90	105.74
6	D	2001	ADP	C2-N3-C4	2.99	119.14	111.83
3	B	2001	08T	C4-C5-N7	-2.99	107.17	110.58
6	D	2001	ADP	N3-C2-N1	-2.97	124.08	128.58
6	E	2001	ADP	C2-N3-C4	2.92	118.96	111.83
6	E	2001	ADP	C4-C5-N7	-2.90	107.26	110.58
6	D	2001	ADP	N6-C6-N1	2.75	124.51	118.38
6	E	2001	ADP	N3-C2-N1	-2.58	124.68	128.58
3	A	2001	08T	C5-N7-C8	2.42	107.25	103.45
3	A	2001	08T	C4-N9-C8	2.42	108.28	105.74
3	A	2001	08T	C3'-C2'-C1'	2.40	106.00	101.46
3	C	2001	08T	C5-N7-C8	2.39	107.21	103.45
3	A	2001	08T	O3B-PB-O1B	-2.33	105.00	111.52
3	B	2001	08T	C4-N9-C8	2.32	108.17	105.74
6	F	2001	ADP	N3-C2-N1	-2.32	125.07	128.58
6	F	2001	ADP	O3A-PB-O1B	-2.32	98.85	111.04
6	D	2001	ADP	C2'-C1'-N9	-2.30	107.58	113.30
3	C	2001	08T	O2B-PB-O1B	2.24	122.89	112.44
3	A	2001	08T	C2'-C1'-N9	-2.24	107.75	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2001	ADP	C5-N7-C8	2.23	106.95	103.45
6	D	2001	ADP	O3B-PB-O2B	2.19	116.02	107.80
3	C	2001	08T	C2-N1-C6	2.19	122.32	118.73
3	C	2001	08T	C4-N9-C8	2.18	108.02	105.74
6	E	2001	ADP	C2-N1-C6	2.18	122.31	118.73
6	F	2001	ADP	C5-N7-C8	2.16	106.84	103.45
6	E	2001	ADP	O3A-PB-O1B	-2.12	99.88	111.04
3	A	2001	08T	C6-C5-N7	2.12	136.17	132.09
3	A	2001	08T	O2B-PB-O1B	2.11	122.26	112.44
6	D	2001	ADP	C4-C5-N7	-2.07	108.21	110.58
6	F	2001	ADP	C4-N9-C8	2.07	107.91	105.74
6	D	2001	ADP	C2-N1-C6	2.05	122.09	118.73
3	B	2001	08T	C3'-C2'-C1'	2.02	105.28	101.46

There are no chirality outliers.

All (25) 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
3	C	2001	08T	C5'-O5'-PA-O3A
6	D	2001	ADP	PA-O3A-PB-O3B
6	D	2001	ADP	C5'-O5'-PA-O1A
6	D	2001	ADP	C5'-O5'-PA-O3A
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
6	F	2001	ADP	C5'-O5'-PA-O3A
3	B	2001	08T	C5'-O5'-PA-O2A
3	B	2001	08T	C5'-O5'-PA-O3A
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	PA-O3A-PB-O1B
6	F	2001	ADP	PA-O3A-PB-O1B
6	F	2001	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	B	2001	08T	PA-O3A-PB-O1B

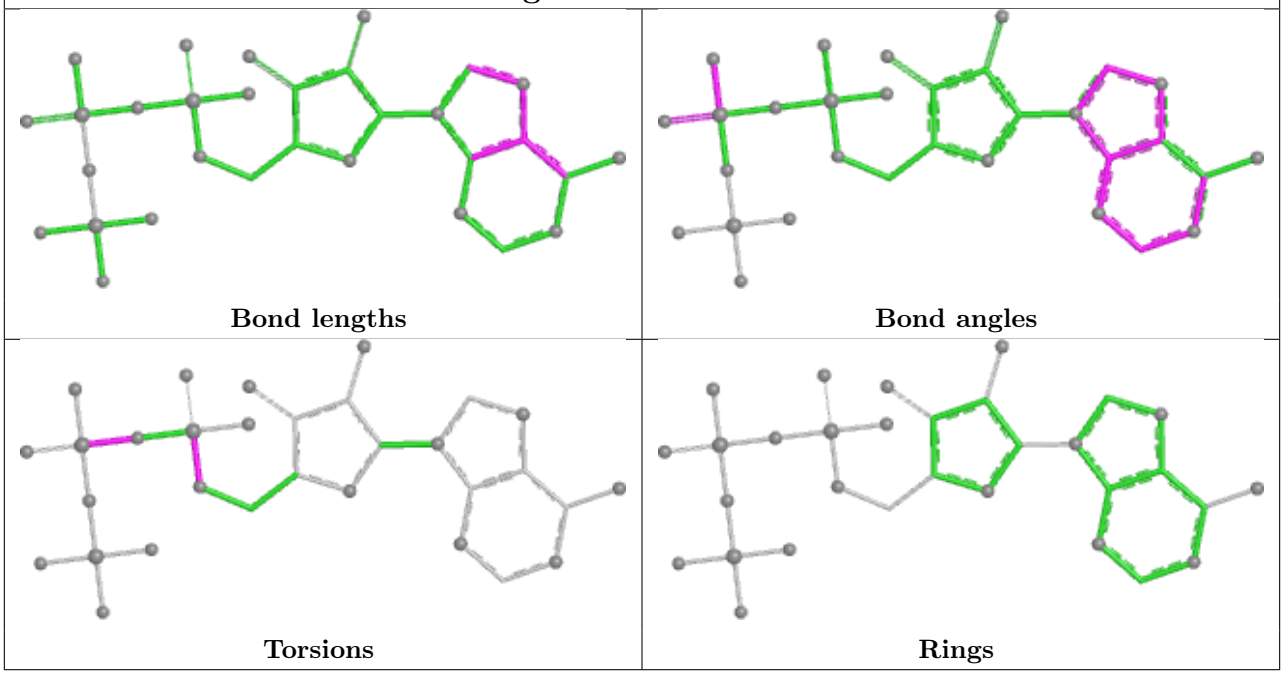
There are no ring outliers.

1 monomer is involved in 1 short contact:

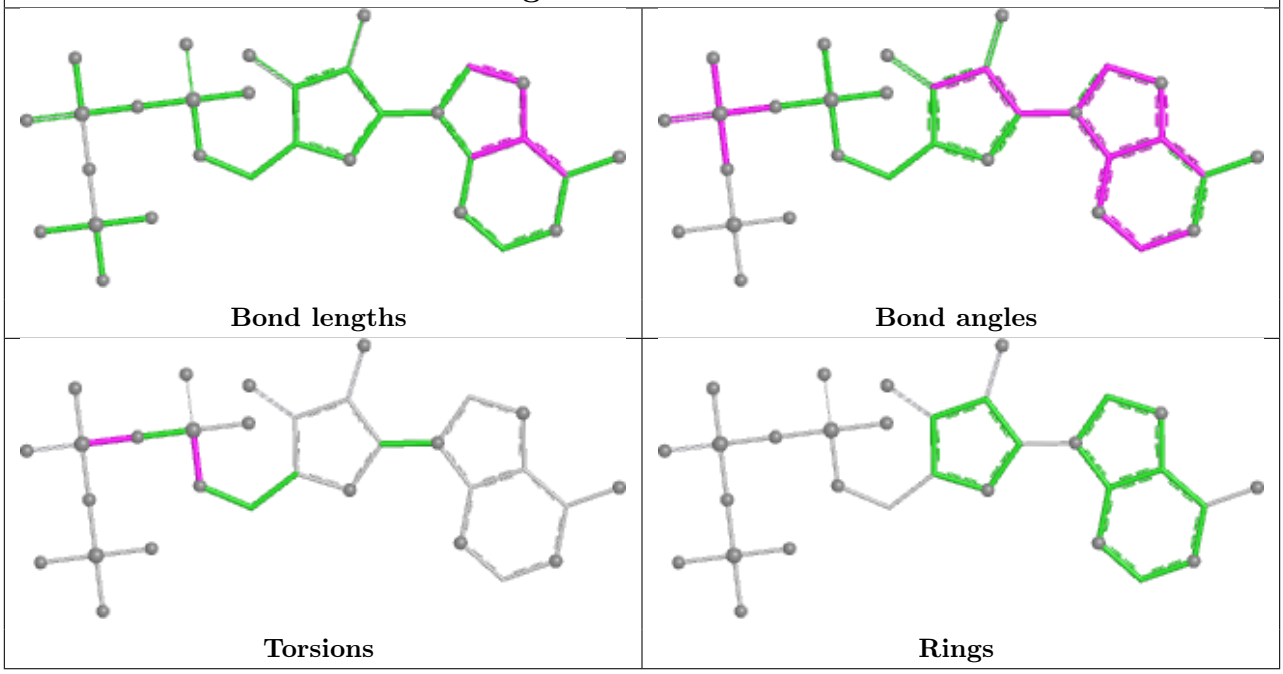
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2001	ADP	1	0

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 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.

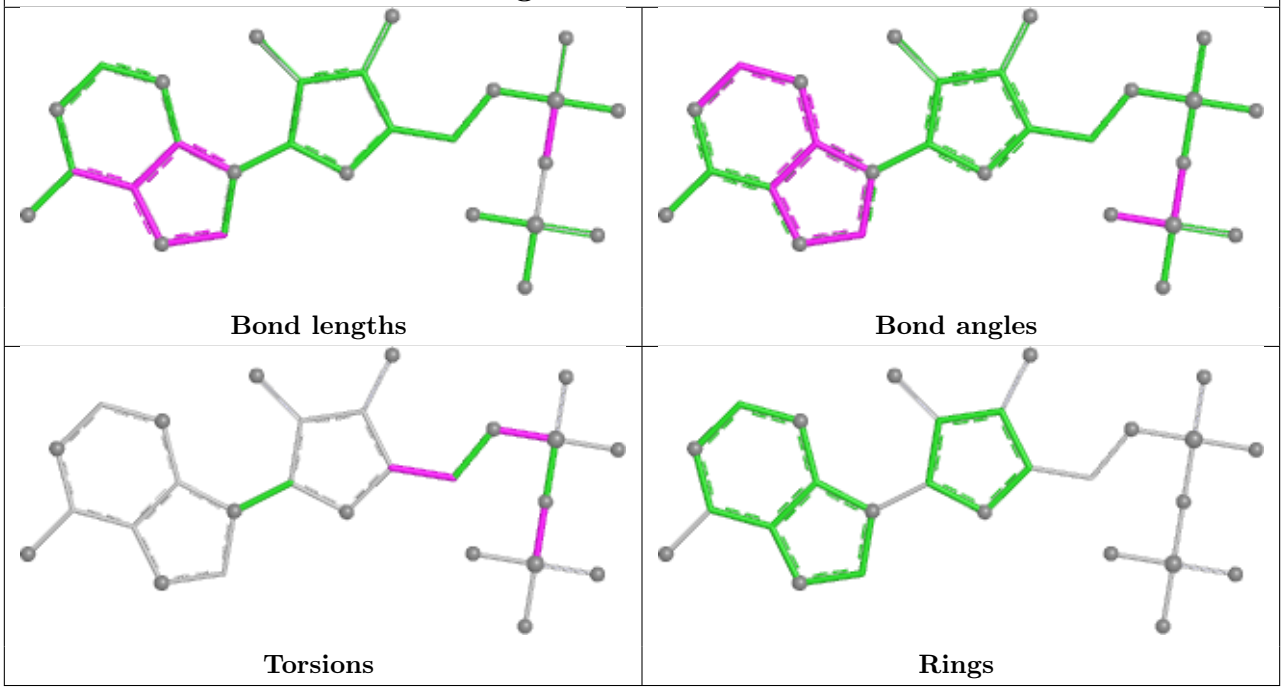
Ligand 08T C 2001



Ligand 08T A 2001



Ligand ADP F 2001



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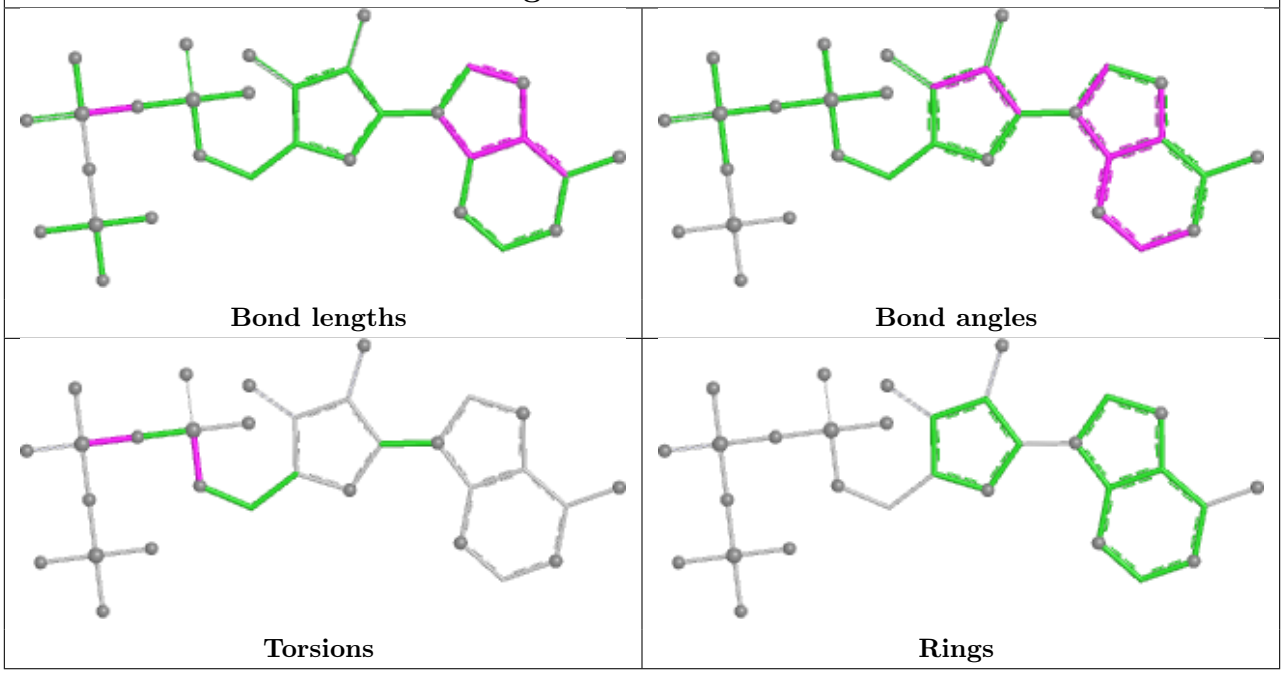

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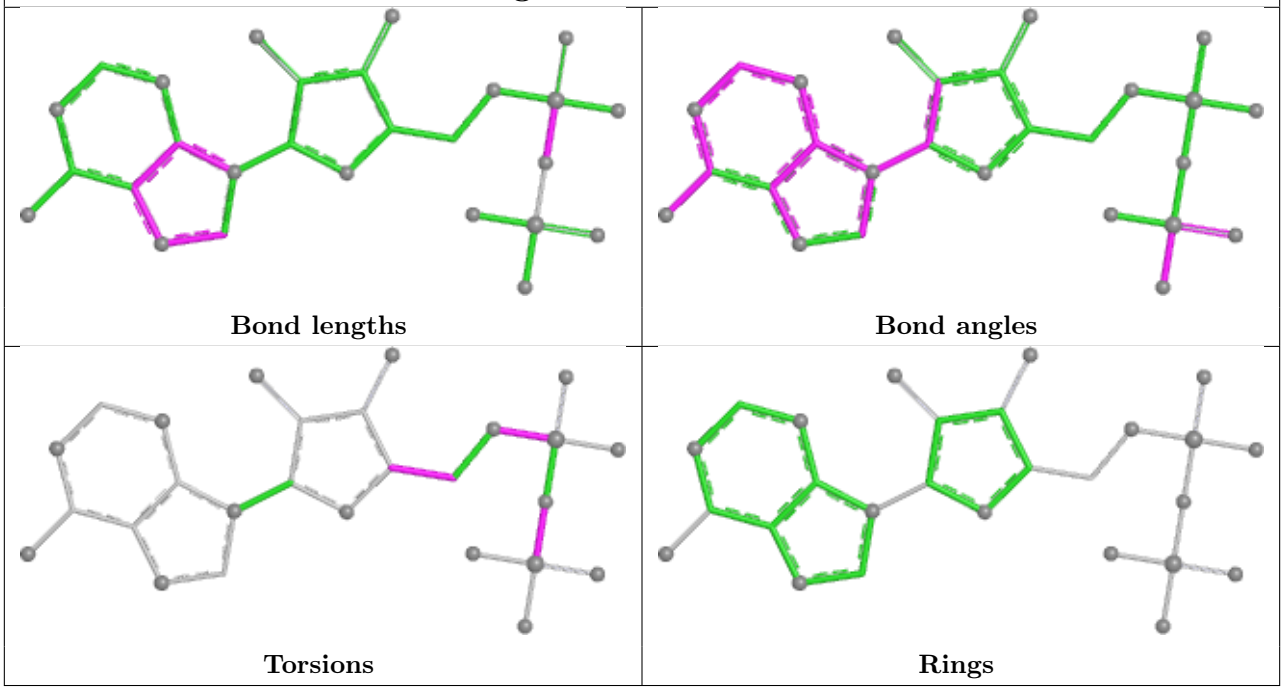
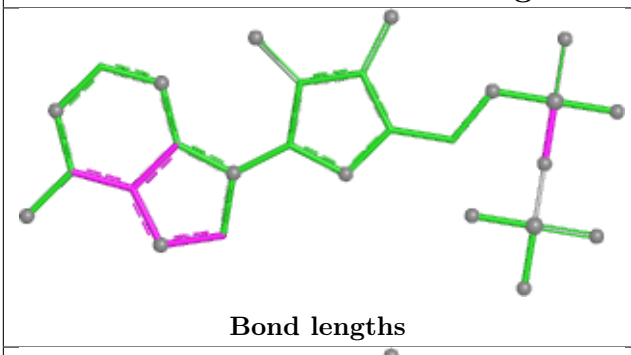
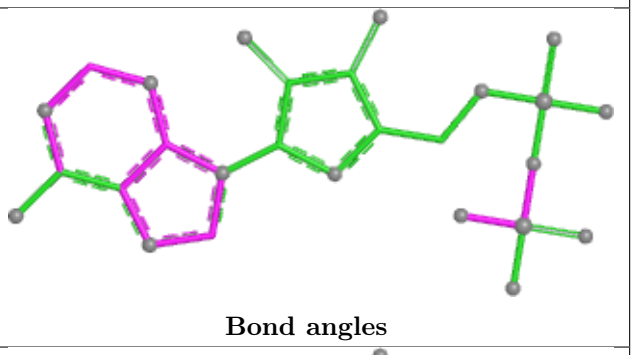


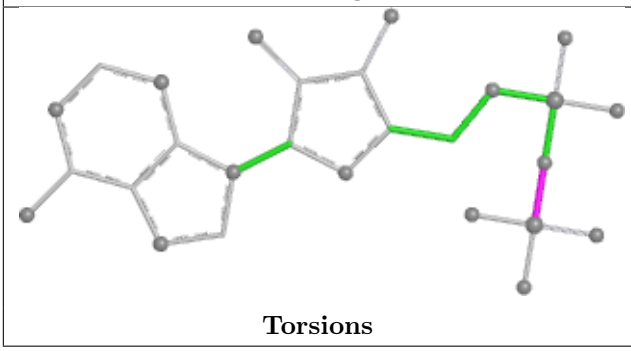
Ligand ADP E 2001



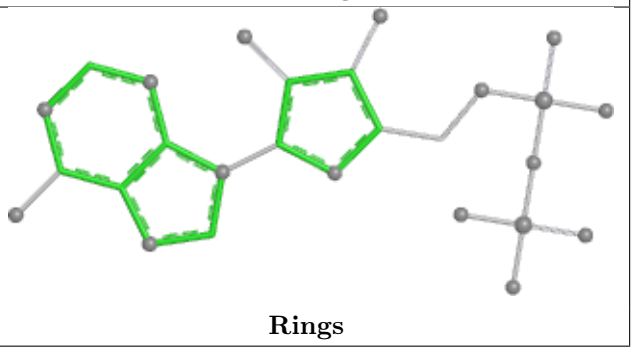
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	-0.77	0	100	100	72, 113, 209, 257	0
1	B	589/610 (96%)	-0.84	0	100	100	70, 107, 192, 244	0
1	C	589/610 (96%)	-0.84	0	100	100	84, 136, 204, 253	0
1	D	589/610 (96%)	-0.69	0	100	100	110, 169, 262, 303	0
1	E	592/610 (97%)	-0.64	0	100	100	105, 156, 262, 298	0
1	F	589/610 (96%)	-0.67	0	100	100	80, 127, 228, 269	0
2	X	10/12 (83%)	-0.60	0	100	100	124, 158, 180, 182	0
All	All	3543/3672 (96%)	-0.74	0	100	100	70, 136, 242, 303	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands

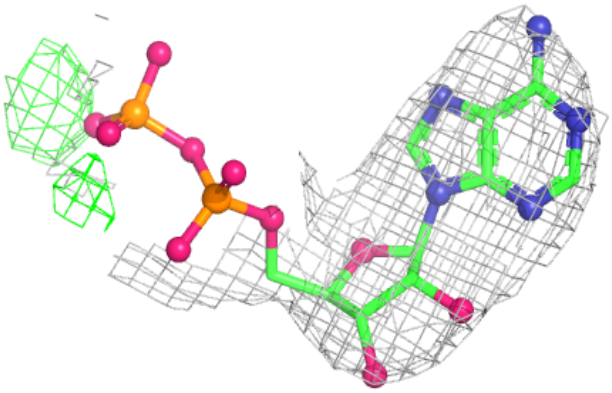
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

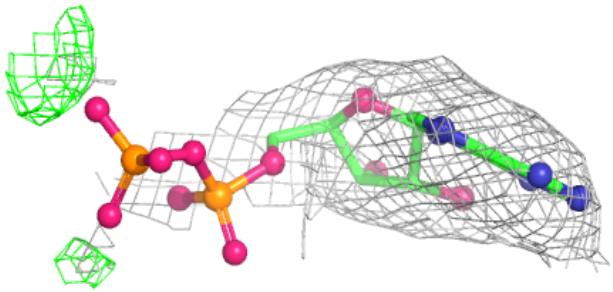
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	D	2002	1/1	0.94	0.04	255,255,255,255	0
4	ZN	A	2002	1/1	0.95	0.06	239,239,239,239	0
4	ZN	F	2002	1/1	0.95	0.05	247,247,247,247	0
6	ADP	D	2001	27/27	0.95	0.06	129,142,147,158	0
6	ADP	E	2001	27/27	0.95	0.07	105,115,124,138	0
6	ADP	F	2001	27/27	0.96	0.05	91,109,117,127	0
5	MG	D	2003	1/1	0.97	0.06	176,176,176,176	0
5	MG	E	2003	1/1	0.97	0.09	153,153,153,153	0
3	08T	C	2001	31/31	0.97	0.06	97,117,141,142	0
4	ZN	E	2002	1/1	0.97	0.03	270,270,270,270	0
3	08T	A	2001	31/31	0.97	0.05	75,82,109,115	0
4	ZN	B	2002	1/1	0.98	0.04	211,211,211,211	0
3	08T	B	2001	31/31	0.98	0.05	81,100,114,128	0
5	MG	F	2003	1/1	0.98	0.09	161,161,161,161	0
5	MG	B	2003	1/1	0.99	0.03	119,119,119,119	0
5	MG	C	2003	1/1	0.99	0.08	157,157,157,157	0
4	ZN	C	2002	1/1	0.99	0.03	182,182,182,182	0
5	MG	A	2003	1/1	0.99	0.05	115,115,115,115	0

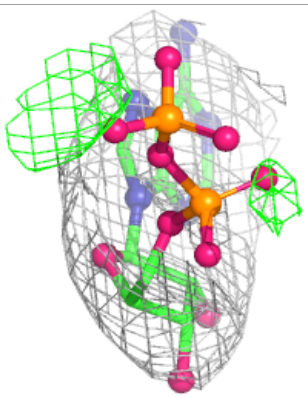
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

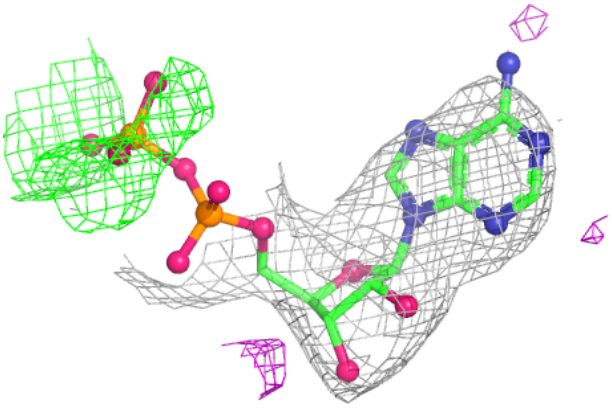


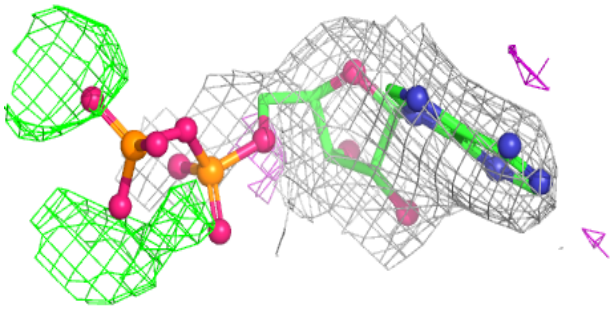


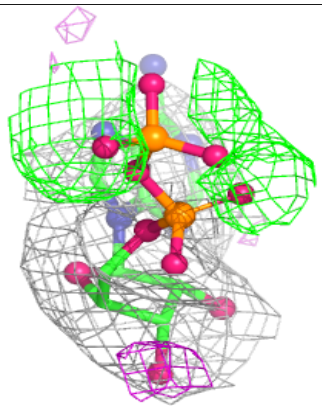


Electron density around ADP E 2001:

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

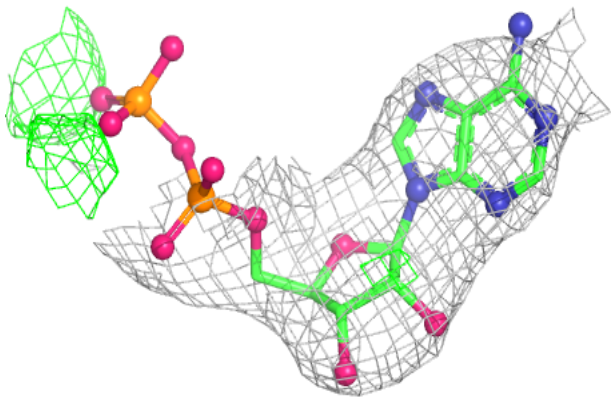


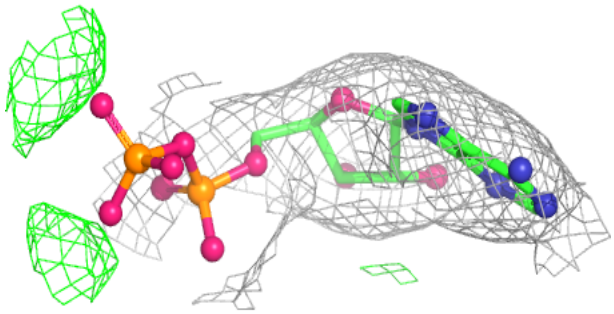


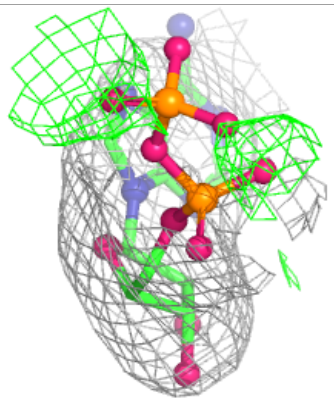


Electron density around ADP F 2001:

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

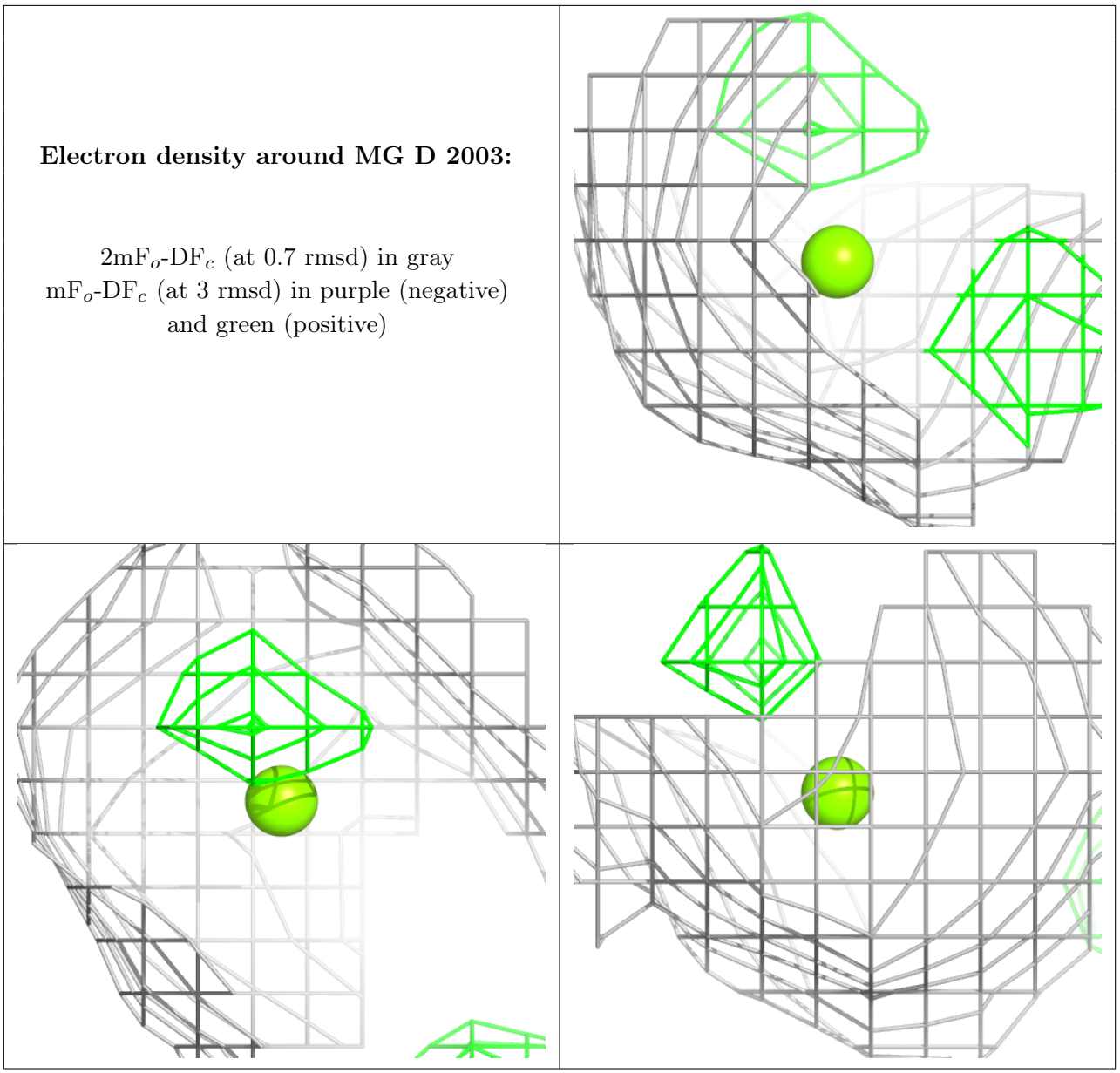






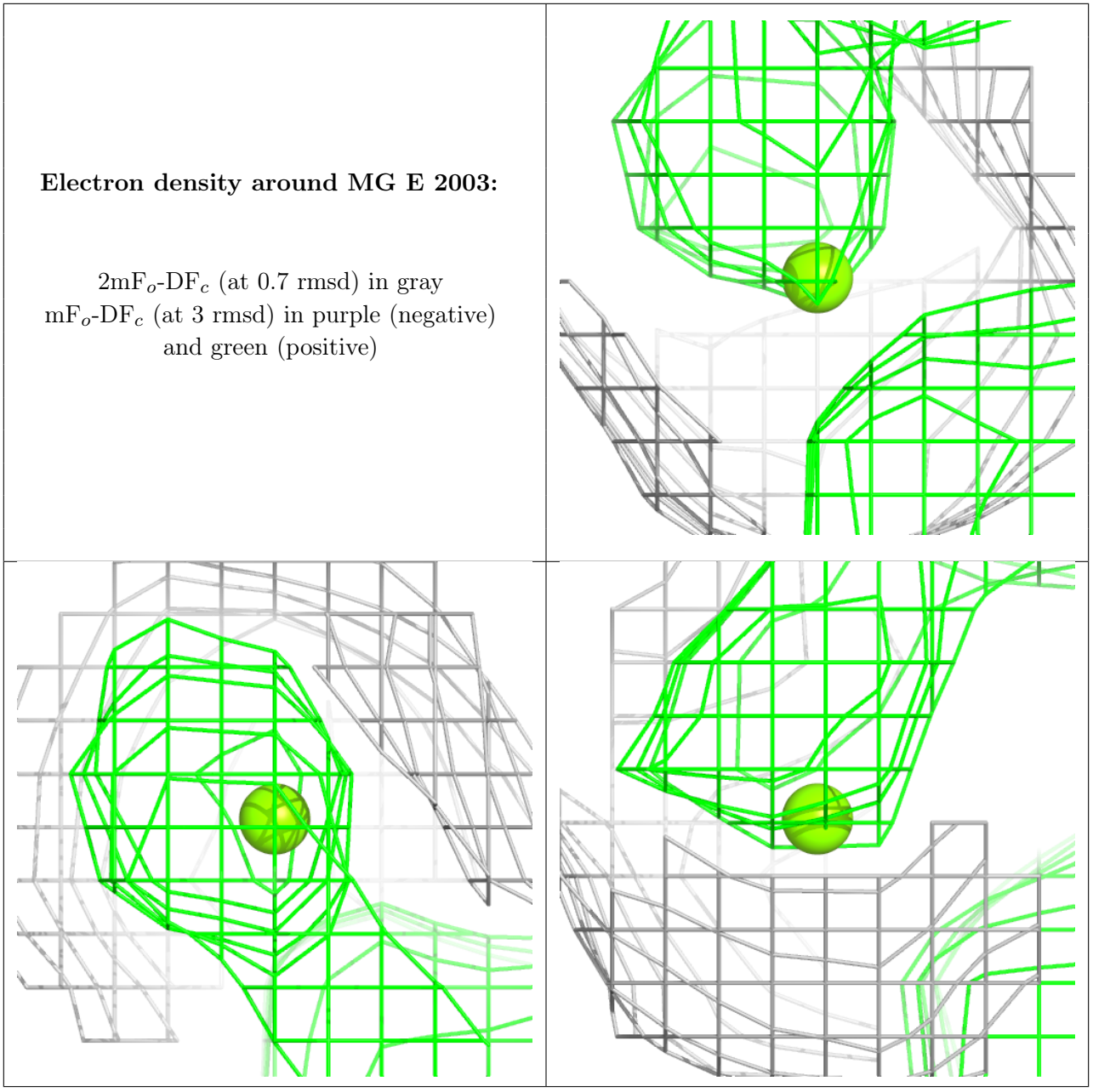
Electron density around MG D 2003:

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



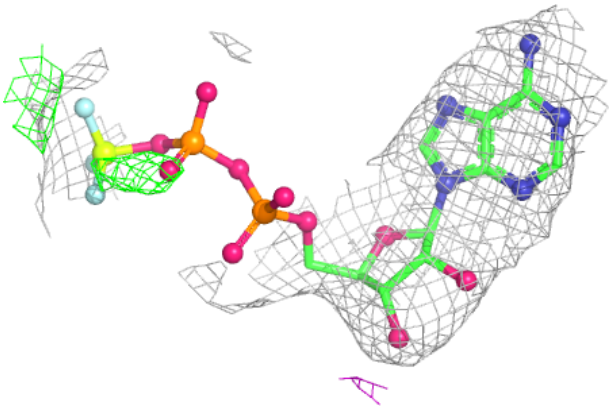
Electron density around MG E 2003:

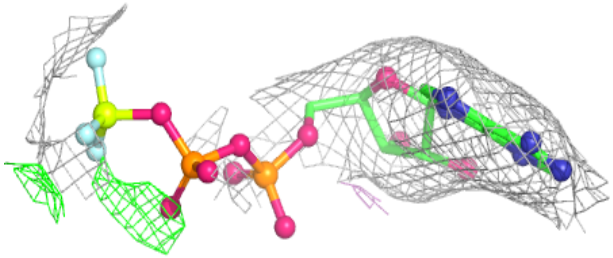
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

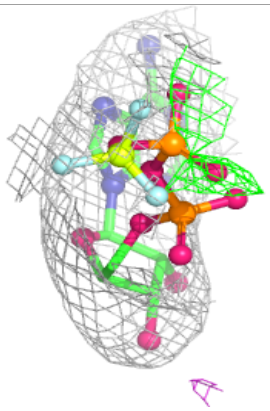


Electron density around 08T C 2001:

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

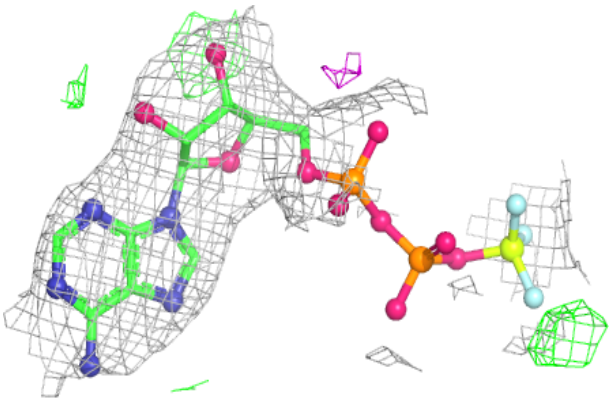


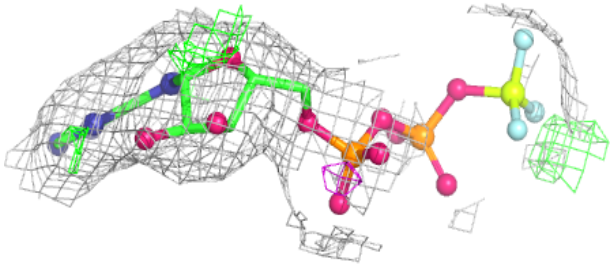


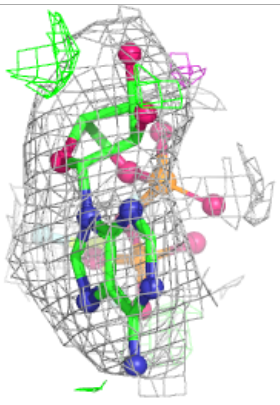


Electron density around 08T A 2001:

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

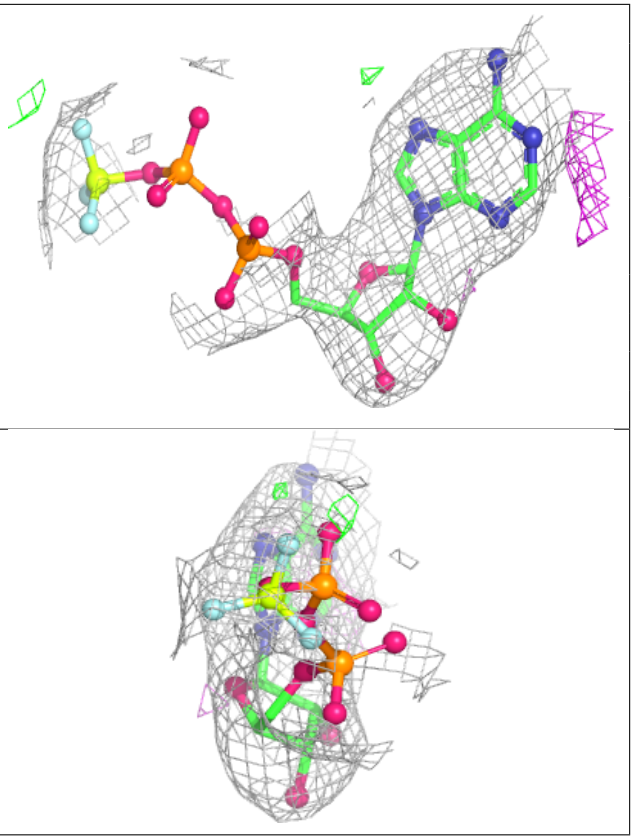


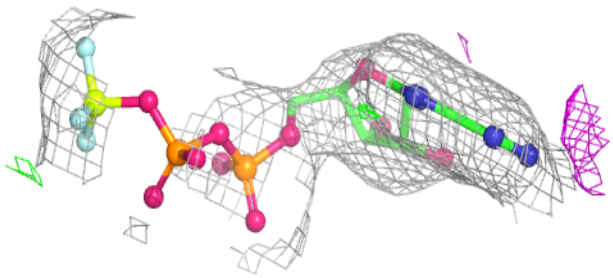




Electron density around 08T B 2001:

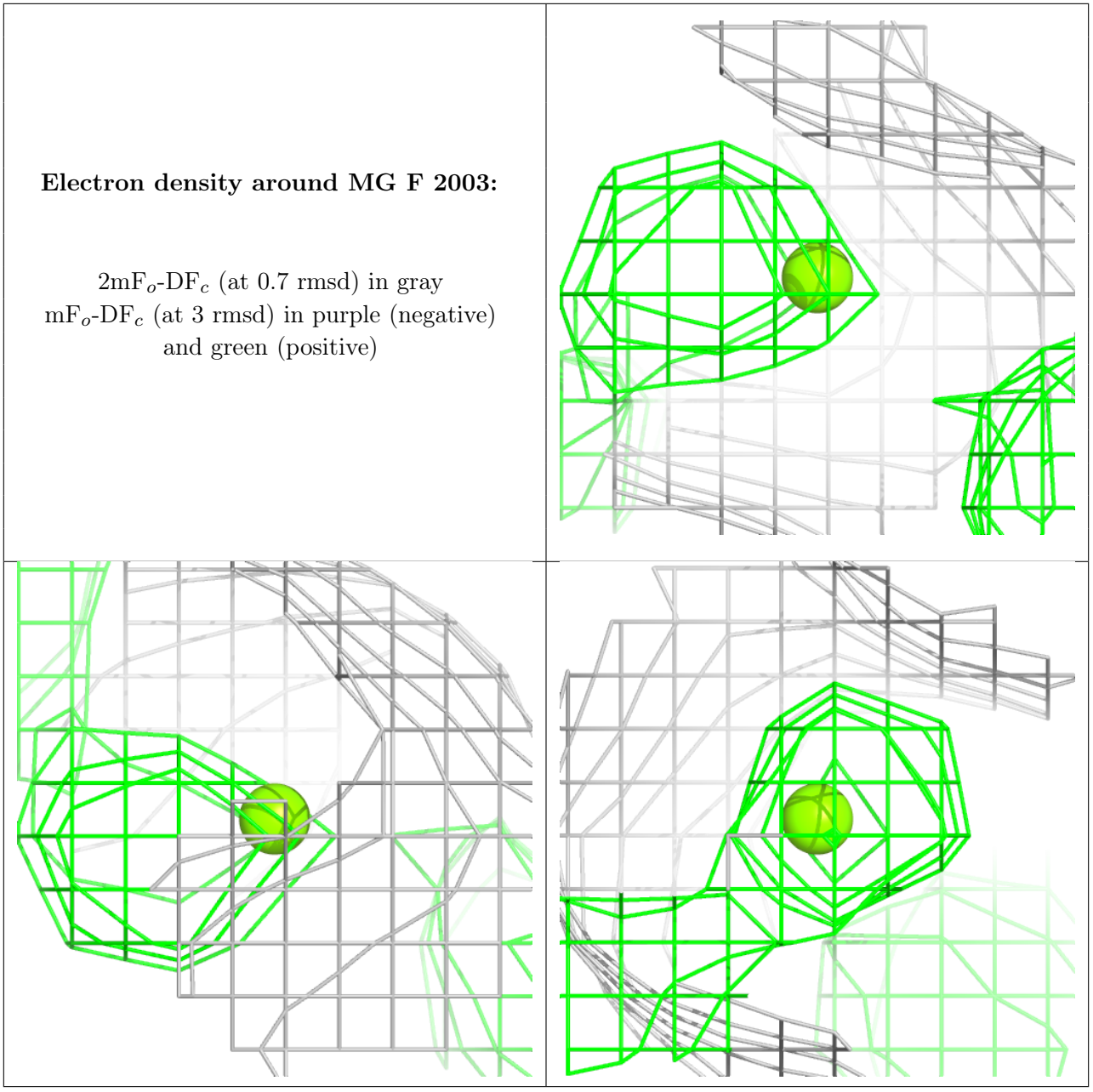
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





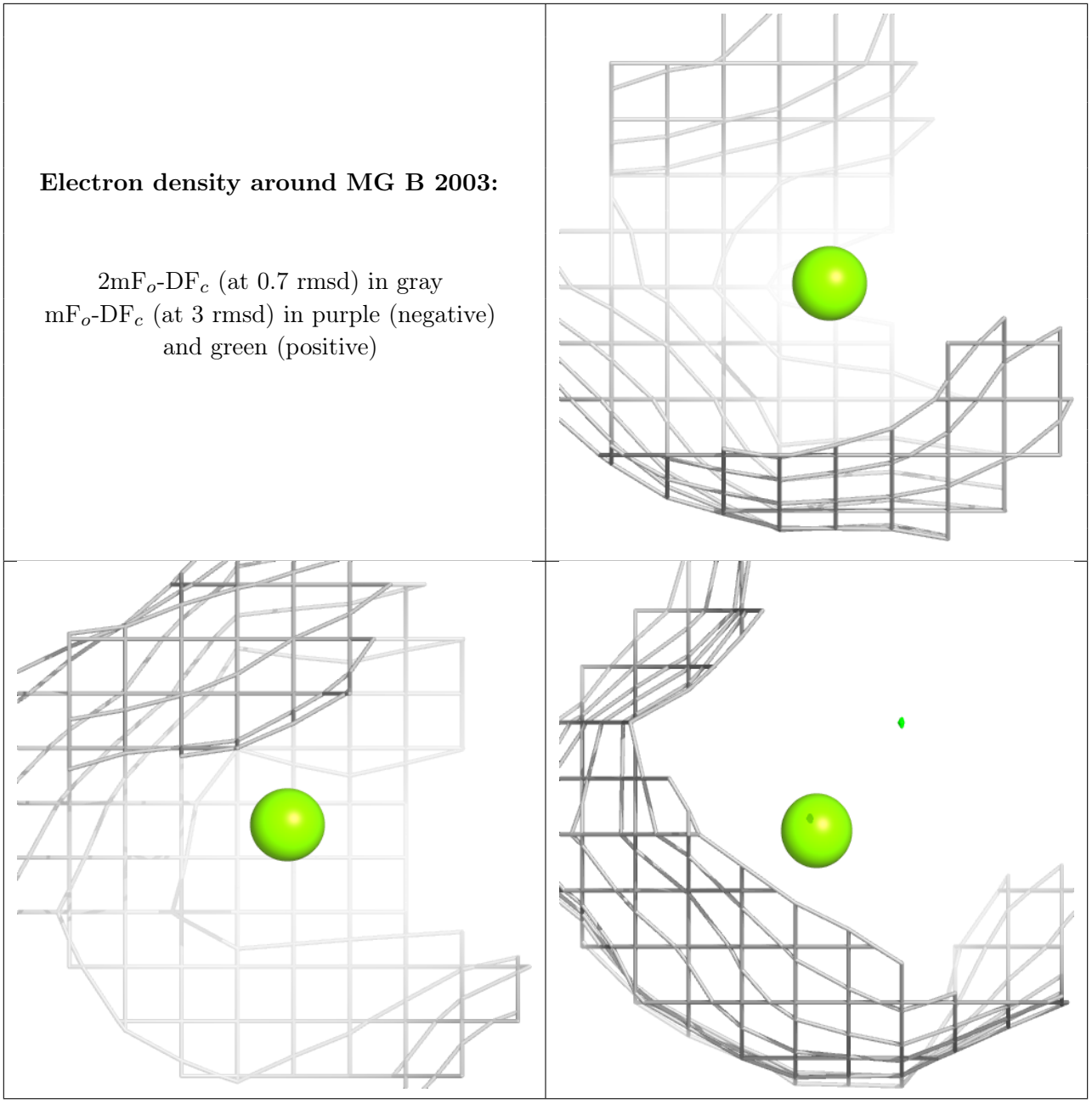
Electron density around MG F 2003:

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



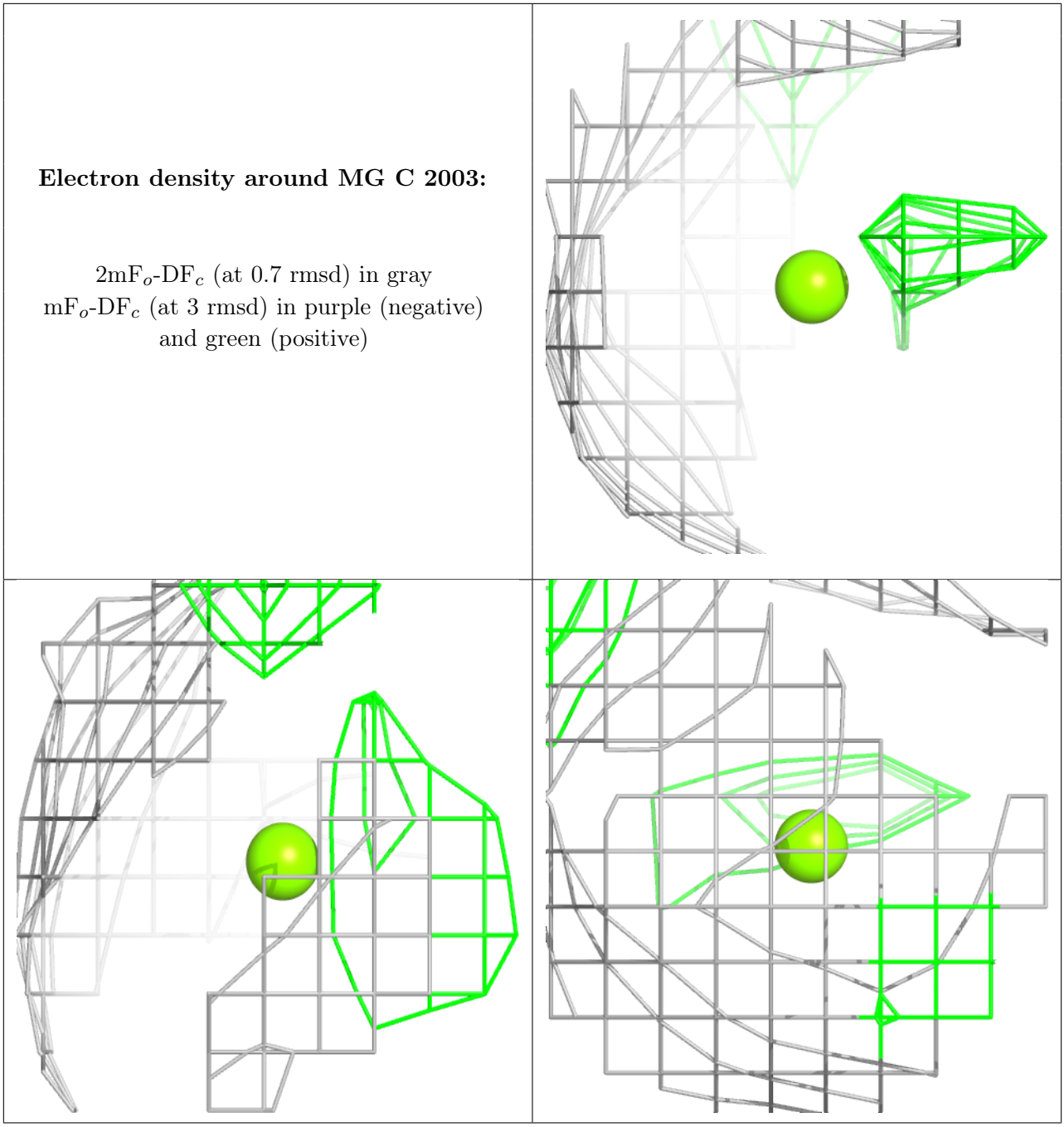
Electron density around MG B 2003:

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



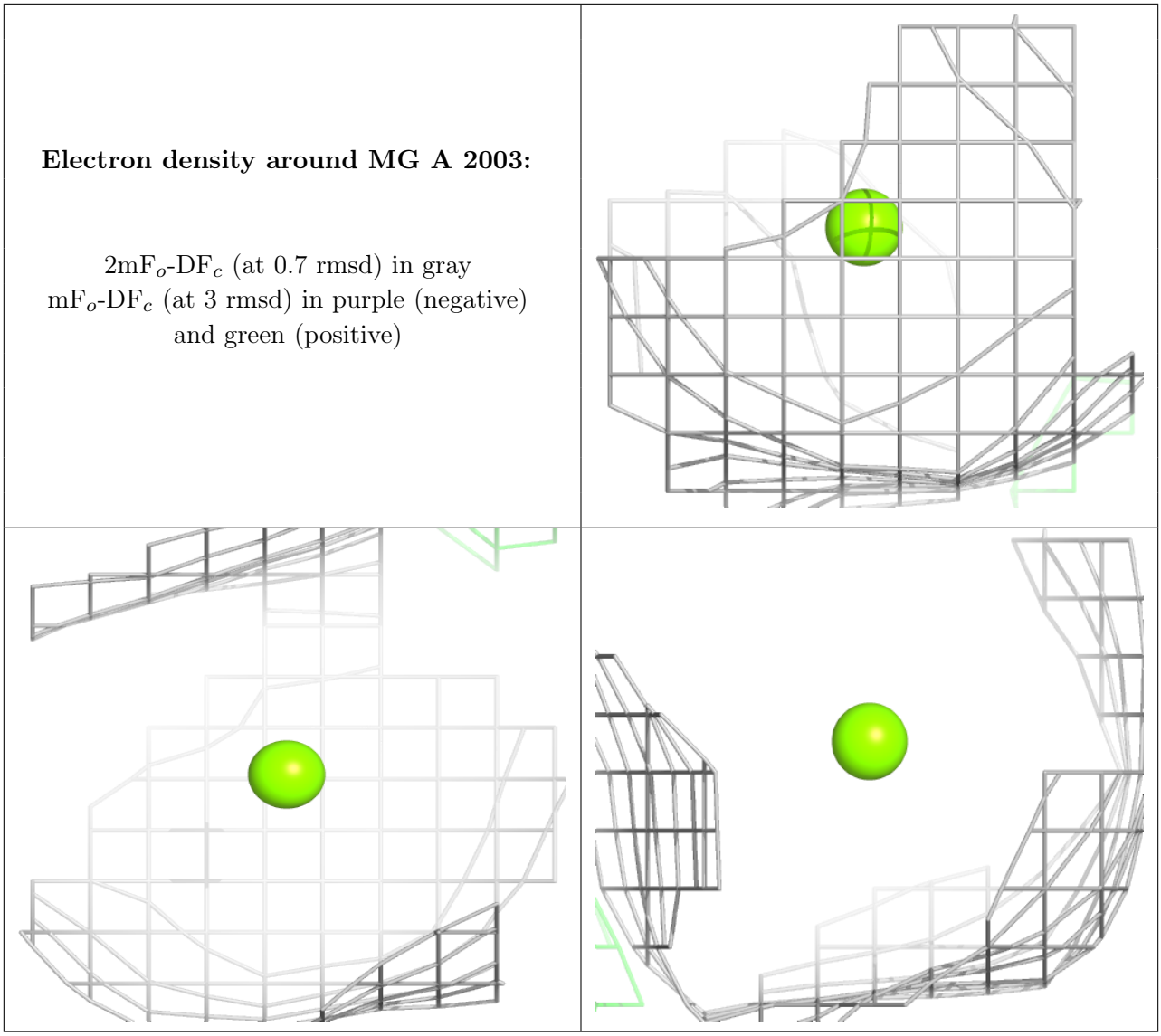
Electron density around MG C 2003:

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



Electron density around MG A 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 (i)

There are no such residues in this entry.