



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2024 – 11:56 AM EST

PDB ID : 6VDD  
Title : POL domain of PolI from *M. smegmatis* complex with DNA primer-template and dNTP  
Authors : Shuman, S.; Goldgur, Y.; Ghosh, S.  
Deposited on : 2019-12-24  
Resolution : 1.90 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](mailto: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>.

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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  
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

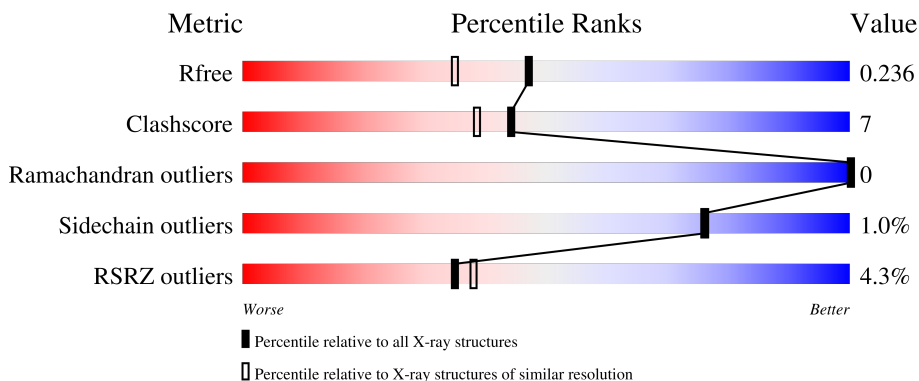
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	605	 3% 81% 12% • 6%
1	D	605	 5% 80% 14% • 6%
2	B	11	 64% 18% 18%
2	E	11	 36% 55% 9%
3	C	14	 57% 43%

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Mol	Chain	Length	Quality of chain
4	F	16	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '12%', a large green segment labeled '75%', a small yellow segment labeled '6%', and a grey segment on the right labeled '19%'.</p>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10595 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 DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	567	Total	C	N	O	S	0	0	0
			4377	2731	786	847	13			
1	D	567	Total	C	N	O	S	0	0	0
			4375	2730	784	848	13			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*GP\*TP\*A\*(DCT))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	Total	C	N	O	P	0	0	0
			222	107	43	62	10			
2	E	11	Total	C	N	O	P	0	0	0
			222	107	43	62	10			

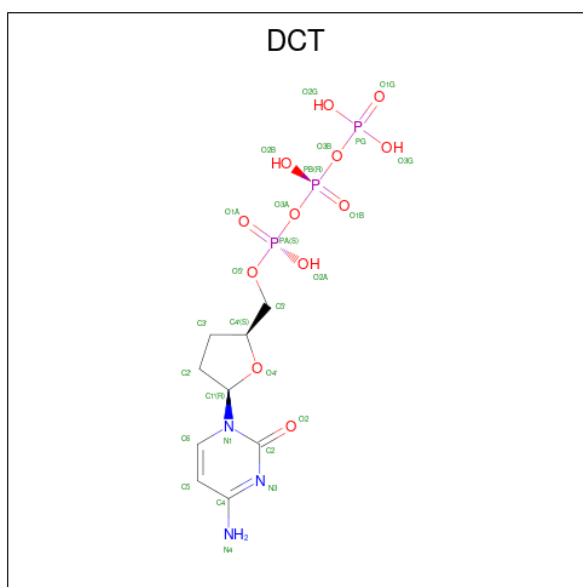
- Molecule 3 is a DNA chain called DNA (5'-D(P\*CP\*GP\*TP\*AP\*CP\*GP\*TP\*GP\*AP\*TP\*CP\*GP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	14	Total	C	N	O	P	0	0	0
			287	136	53	84	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*TP\*AP\*CP\*GP\*TP\*GP\*AP\*TP\*CP\*GP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	13	Total	C	N	O	P	0	0	0
			268	127	50	78	13			

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O P	0	0
			13	10 3		
5	D	1	Total	O P	0	0
			13	10 3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		
6	B	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	397	Total	O	0	0
			397	397		
7	B	26	Total	O	0	0
			26	26		
7	C	33	Total	O	0	0
			33	33		
7	D	300	Total	O	0	0
			300	300		

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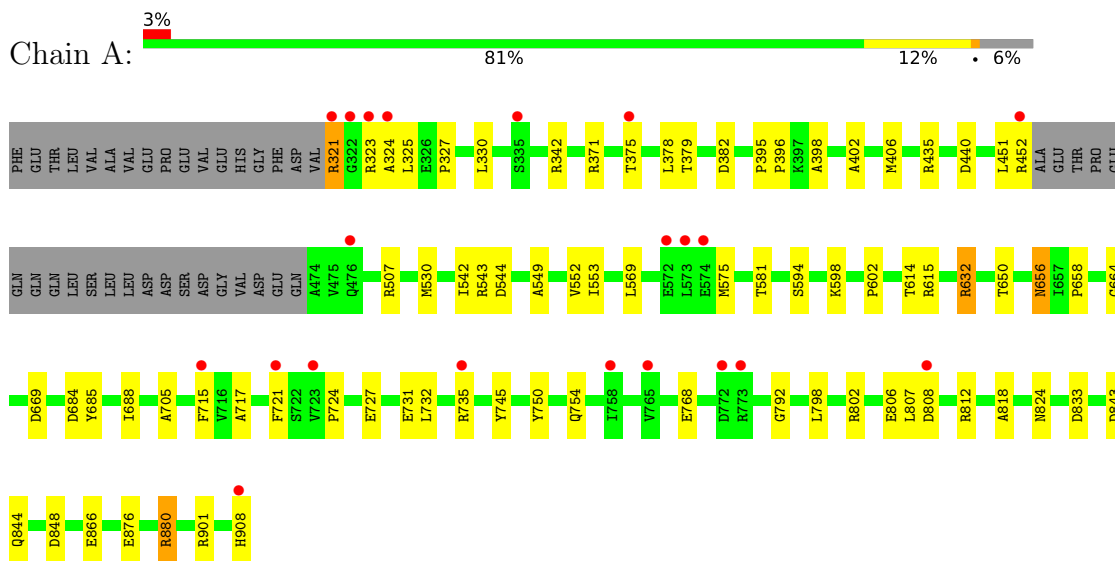
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	E	20	Total	O	0	0
			20	20		
7	F	36	Total	O	0	0
			36	36		

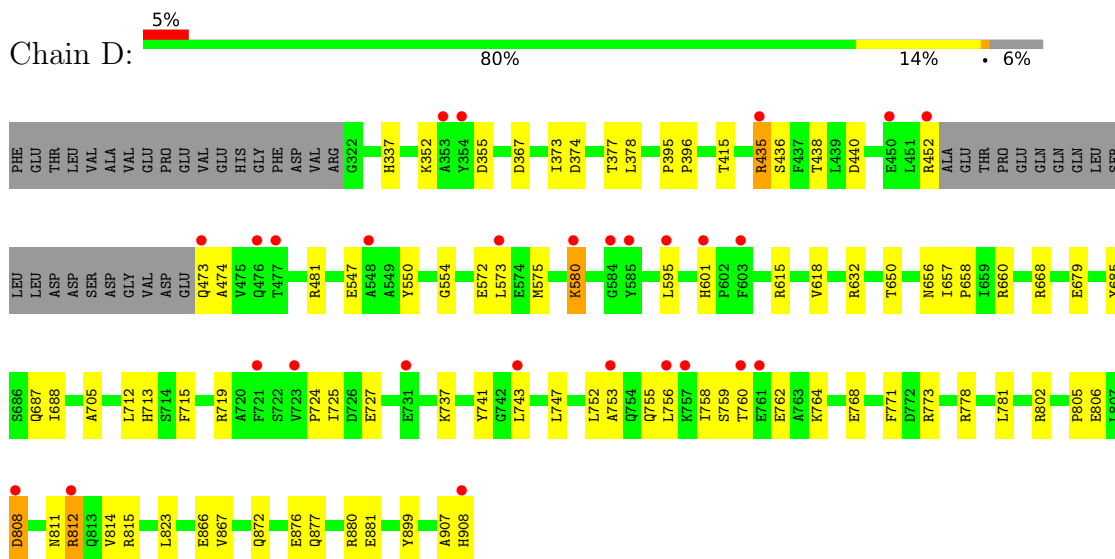
### 3 Residue-property plots

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: DNA polymerase I



- Molecule 1: DNA polymerase I



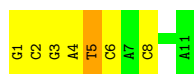
- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*GP\*TP\*A\*(DCT))-3')

Chain B:  64% 18% 18%



- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*GP\*TP\*A\*(DCT))-3')

Chain E:  36% 55% 9%




- Molecule 3: DNA (5'-D(P\*CP\*GP\*TP\*AP\*CP\*GP\*TP\*GP\*AP\*TP\*CP\*GP\*CP\*A)-3')

Chain C:  57% 43%



- Molecule 4: DNA (5'-D(P\*GP\*TP\*AP\*CP\*GP\*TP\*GP\*AP\*TP\*CP\*GP\*CP\*A)-3')

Chain F:  12% 75% 6% 19%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.66Å 233.81Å 169.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 1.90 48.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.53-1.90) 95.0 (48.53-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472+SVN, PHENIX 1.15.2_3472+SVN	Depositor
R, $R_{free}$	0.191 , 0.237 0.191 , 0.236	Depositor DCC
$R_{free}$ test set	2000 reflections (1.92%)	wwPDB-VI
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10595	wwPDB-VI
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VI

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DCT, MG

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	0.40	0/4447	0.60	4/6023 (0.1%)
1	D	0.47	4/4445 (0.1%)	0.61	8/6021 (0.1%)
2	B	1.07	1/249 (0.4%)	1.21	3/382 (0.8%)
2	E	1.06	0/249	1.84	5/382 (1.3%)
3	C	0.85	0/321	0.97	0/493
4	F	0.85	0/300	0.99	0/461
All	All	0.52	5/10011 (0.0%)	0.72	20/13762 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	808	ASP	CB-CG	11.26	1.75	1.51
1	D	580	LYS	CE-NZ	7.75	1.68	1.49
1	D	435	ARG	CB-CG	-7.60	1.32	1.52
1	D	435	ARG	NE-CZ	-6.09	1.25	1.33
2	B	4	DA	N9-C4	-5.03	1.34	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	DT	O5 <sup>1</sup> -P-OP1	-26.89	78.43	110.70
2	B	4	DA	O5 <sup>1</sup> -P-OP2	-8.26	98.27	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	ARG	NE-CZ-NH1	8.11	124.36	120.30
2	E	5	DT	O5'-P-OP2	8.00	120.30	110.70
1	D	435	ARG	CG-CD-NE	-7.82	95.38	111.80
2	B	8	DC	O4'-C1'-N1	6.81	112.77	108.00
2	E	4	DA	OP2-P-O3'	6.60	119.73	105.20
1	D	812	ARG	CG-CD-NE	-6.31	98.55	111.80
1	D	435	ARG	N-CA-CB	6.25	121.86	110.60
1	D	435	ARG	CB-CG-CD	-6.09	95.77	111.60
1	A	632	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	D	435	ARG	CA-CB-CG	5.94	126.47	113.40
1	D	435	ARG	CB-CA-C	-5.91	98.59	110.40
1	A	812	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	E	8	DC	O4'-C1'-N1	5.39	111.78	108.00
2	E	5	DT	C1'-O4'-C4'	-5.30	104.80	110.10
1	D	435	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	808	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	880	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	B	4	DA	P-O3'-C3'	5.02	125.73	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	756	LEU	Peptide

## 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	4377	0	4348	52	1
1	D	4375	0	4343	64	1
2	B	222	0	123	5	0
2	E	222	0	123	3	1
3	C	287	0	158	4	0
4	F	268	0	147	1	0
5	A	13	0	0	0	0
5	D	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	D	2	0	0	0	0
7	A	397	0	0	14	0
7	B	26	0	0	0	0
7	C	33	0	0	0	0
7	D	300	0	0	10	0
7	E	20	0	0	0	0
7	F	36	0	0	0	0
All	All	10595	0	9242	124	2

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 7.

All (124) 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:D:808:ASP:CB	1:D:808:ASP:CG	1.75	1.52
1:D:580:LYS:CE	1:D:580:LYS:NZ	1.68	1.51
1:A:656:ASN:ND2	7:A:1101:HOH:O	1.95	0.99
1:A:876:GLU:OE1	1:A:880:ARG:NH1	1.98	0.96
1:A:615:ARG:NH2	2:B:8:DC:O2	2.07	0.87
1:D:719:ARG:HE	1:D:773:ARG:HD2	1.40	0.86
1:A:321:ARG:NH2	7:A:1103:HOH:O	2.10	0.81
2:B:4:DA:H2''	2:B:5:DT:O5'	1.84	0.75
1:A:451:LEU:O	1:A:452:ARG:NH1	2.20	0.75
1:A:342:ARG:HD3	1:A:398:ALA:HB2	1.66	0.74
1:D:580:LYS:NZ	1:D:580:LYS:CD	2.52	0.72
1:D:554:GLY:N	7:D:1103:HOH:O	2.18	0.72
1:D:778:ARG:NH1	7:D:1102:HOH:O	2.23	0.72
1:D:473:GLN:N	7:D:1105:HOH:O	2.22	0.70
1:A:440:ASP:OD1	7:A:1102:HOH:O	2.09	0.70
1:D:758:ILE:HD12	1:D:762:GLU:HB3	1.73	0.69
1:D:812:ARG:HG3	1:D:815:ARG:NH2	2.09	0.66
1:D:805:PRO:O	1:D:808:ASP:HB2	1.96	0.65
1:A:324:ALA:N	7:A:1114:HOH:O	2.30	0.64
1:D:355:ASP:O	7:D:1101:HOH:O	2.15	0.64
1:A:656:ASN:ND2	1:A:656:ASN:O	2.32	0.62
1:A:594:SER:O	1:A:598:LYS:HG3	1.99	0.62
1:D:573:LEU:HD12	1:D:573:LEU:O	2.01	0.61
1:D:867:VAL:HG11	1:D:872:GLN:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:768:GLU:OE1	7:D:1102:HOH:O	2.17	0.60
1:A:745:TYR:CE2	1:A:824:ASN:ND2	2.71	0.58
1:A:543:ARG:NH1	1:A:544:ASP:OD1	2.36	0.58
1:A:325:LEU:HD21	1:A:330:LEU:HB2	1.84	0.58
1:A:669:ASP:O	7:A:1105:HOH:O	2.17	0.58
1:D:452:ARG:HD2	1:D:481:ARG:NH1	2.19	0.58
1:D:658:PRO:O	1:D:668:ARG:HD2	2.04	0.57
1:D:715:PHE:HA	1:D:725:ILE:HD12	1.86	0.57
1:A:552:VAL:HG21	1:A:602:PRO:HG2	1.86	0.57
2:B:4:DA:H2'	2:B:5:DT:H72	1.86	0.56
1:D:719:ARG:NE	1:D:773:ARG:HD2	2.16	0.56
1:A:382:ASP:OD2	7:A:1106:HOH:O	2.18	0.55
1:D:743:LEU:HD12	1:D:747:LEU:HB3	1.87	0.55
1:D:907:ALA:O	1:D:908:HIS:ND1	2.39	0.55
1:D:452:ARG:HD2	1:D:481:ARG:HH12	1.71	0.55
1:A:745:TYR:CZ	1:A:824:ASN:ND2	2.73	0.55
1:D:575:MET:HE1	1:D:595:LEU:HB3	1.89	0.55
1:D:808:ASP:CG	1:D:808:ASP:CA	2.71	0.54
1:D:632:ARG:NH2	1:D:866:GLU:OE2	2.38	0.54
1:D:760:THR:O	1:D:764:LYS:HG3	2.08	0.54
1:D:806:GLU:C	1:D:808:ASP:N	2.60	0.53
1:A:685:TYR:HB3	1:A:688:ILE:HB	1.90	0.53
1:A:901:ARG:NH1	7:A:1105:HOH:O	2.42	0.53
1:A:798:LEU:HD12	1:A:833:ASP:HB3	1.90	0.53
1:D:806:GLU:C	1:D:808:ASP:H	2.10	0.53
1:D:724:PRO:HG2	1:D:727:GLU:HB2	1.91	0.52
1:A:806:GLU:HB2	1:A:818:ALA:HB2	1.91	0.52
2:E:1:DG:H2'	2:E:2:DC:C6	2.45	0.52
1:A:908:HIS:O	7:A:1107:HOH:O	2.19	0.52
1:A:375:THR:HA	1:A:378:LEU:HD23	1.93	0.51
1:A:402:ALA:O	1:A:406:MET:HG3	2.11	0.50
1:A:724:PRO:HG2	1:A:727:GLU:HG3	1.91	0.50
1:D:808:ASP:CB	1:D:808:ASP:OD1	2.50	0.50
1:A:323:ARG:O	1:A:371:ARG:HA	2.11	0.50
1:A:802:ARG:NH1	3:C:10:DA:OP1	2.31	0.49
3:C:17:DC:H2''	3:C:18:DG:C8	2.46	0.49
1:D:632:ARG:HH22	1:D:866:GLU:CD	2.15	0.49
1:A:549:ALA:O	1:A:553:ILE:HG12	2.12	0.49
2:B:4:DA:H2'	2:B:5:DT:C7	2.42	0.49
2:E:5:DT:H2''	2:E:6:DC:O4'	2.12	0.48
3:C:19:DC:H2''	3:C:20:DA:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:THR:HG22	1:D:440:ASP:H	1.77	0.48
1:D:438:THR:HG22	1:D:440:ASP:N	2.29	0.48
1:A:375:THR:HA	1:A:378:LEU:CD2	2.44	0.48
1:A:732:LEU:HD12	1:A:735:ARG:HH21	1.79	0.47
1:D:880:ARG:NH1	7:D:1107:HOH:O	2.47	0.47
1:A:731:GLU:OE1	1:A:735:ARG:NH2	2.48	0.47
1:A:684:ASP:HB2	7:A:1432:HOH:O	2.14	0.46
1:A:569:LEU:O	1:A:575:MET:HB3	2.16	0.46
1:D:741:TYR:OH	5:D:1001:DCT:O1B	2.16	0.46
1:A:802:ARG:NH1	7:A:1133:HOH:O	2.46	0.46
1:D:687:GLN:HE21	1:D:712:LEU:HB3	1.81	0.46
1:A:327:PRO:HB3	1:A:379:THR:HG21	1.98	0.45
1:D:781:LEU:HD22	1:D:823:LEU:HD22	1.98	0.45
1:D:415:THR:HG23	7:D:1246:HOH:O	2.16	0.45
1:D:573:LEU:HD22	1:D:601:HIS:NE2	2.32	0.45
1:D:877:GLN:NE2	1:D:881:GLU:OE1	2.50	0.45
1:A:549:ALA:O	1:A:552:VAL:HG12	2.16	0.44
1:D:876:GLU:HB2	1:D:899:TYR:OH	2.17	0.44
1:D:705:ALA:HB2	1:D:715:PHE:CD1	2.53	0.44
1:D:374:ASP:HB3	1:D:377:THR:OG1	2.17	0.44
2:E:2:DC:H2''	2:E:3:DG:C8	2.53	0.44
1:A:507:ARG:HG2	7:A:1386:HOH:O	2.17	0.44
1:A:325:LEU:O	7:A:1108:HOH:O	2.21	0.43
1:D:440:ASP:OD2	1:D:452:ARG:NH1	2.51	0.43
1:A:530:MET:HE2	7:A:1225:HOH:O	2.16	0.43
1:A:632:ARG:NH2	1:A:866:GLU:OE2	2.48	0.43
1:A:792:GLY:HA2	7:A:1358:HOH:O	2.18	0.43
1:D:650:THR:HG22	4:F:12:DG:H3'	2.00	0.43
1:D:753:ALA:HB2	1:D:760:THR:HA	2.00	0.43
1:D:752:LEU:HA	1:D:755:GLN:HB2	2.01	0.43
1:A:717:ALA:O	1:A:721:PHE:HB2	2.19	0.43
1:D:876:GLU:OE1	1:D:880:ARG:NH2	2.44	0.43
1:D:473:GLN:HG2	1:D:474:ALA:N	2.33	0.43
1:A:581:THR:HB	2:B:6:DC:OP1	2.18	0.43
1:D:657:ILE:O	1:D:668:ARG:NH1	2.52	0.43
1:A:807:LEU:HA	1:A:807:LEU:HD23	1.83	0.42
1:D:572:GLU:O	1:D:573:LEU:C	2.57	0.42
1:A:650:THR:HG22	3:C:12:DG:H3'	2.01	0.42
1:D:373:ILE:HG23	1:D:378:LEU:HD21	2.01	0.42
1:D:685:TYR:HB3	1:D:688:ILE:HB	2.00	0.42
1:D:713:HIS:CE1	1:D:737:LYS:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ALA:HB2	1:A:715:PHE:CD1	2.54	0.42
1:D:656:ASN:ND2	7:D:1132:HOH:O	2.51	0.42
1:D:715:PHE:HA	1:D:725:ILE:CD1	2.50	0.42
1:D:806:GLU:OE1	7:D:1104:HOH:O	2.21	0.42
1:D:436:SER:HA	7:D:1234:HOH:O	2.19	0.42
1:D:547:GLU:HA	1:D:550:TYR:HB2	2.00	0.41
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.91	0.41
1:A:632:ARG:HH22	1:A:866:GLU:CD	2.23	0.41
1:D:811:ASN:OD1	1:D:814:VAL:HG23	2.20	0.41
1:A:750:TYR:O	1:A:754:GLN:HG2	2.20	0.41
1:D:615:ARG:HA	1:D:618:VAL:HG22	2.01	0.41
1:A:844:GLN:NE2	1:A:848:ASP:OD1	2.53	0.41
1:D:395:PRO:HA	1:D:396:PRO:HD3	1.91	0.41
1:A:542:ILE:HD11	1:A:614:THR:HA	2.02	0.41
1:A:658:PRO:HB2	1:A:664:GLY:HA3	2.02	0.41
1:D:337:HIS:NE2	1:D:367:ASP:OD2	2.53	0.40
1:D:771:PHE:CD1	1:D:778:ARG:HB2	2.56	0.40
1:D:679:GLU:OE2	1:D:872:GLN:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:NH2	1:A:808:ASP:O[3_454]	1.06	1.14
1:D:812:ARG:NH1	2:E:5:DT:OP1[3_454]	1.58	0.62

## 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	563/605 (93%)	548 (97%)	15 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	563/605 (93%)	545 (97%)	18 (3%)	0	100	100
All	All	1126/1210 (93%)	1093 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	453/487 (93%)	449 (99%)	4 (1%)	78	79
1	D	453/487 (93%)	448 (99%)	5 (1%)	73	73
All	All	906/974 (93%)	897 (99%)	9 (1%)	76	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ARG
1	A	656	ASN
1	A	768	GLU
1	A	843	ASP
1	D	352	LYS
1	D	435	ARG
1	D	660	ARG
1	D	759	SER
1	D	802	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
5	DCT	A	1001	6	8,12,28	1.44	1 (12%)	15,20,43	1.07	1 (6%)
5	DCT	D	1001	6	8,12,28	1.38	1 (12%)	15,20,43	1.42	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DCT	A	1001	6	-	5/12/12/31	-
5	DCT	D	1001	6	-	6/12/12/31	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	DCT	PA-O1A	3.58	1.62	1.50
5	D	1001	DCT	PA-O1A	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001	DCT	PB-O3B-PG	-3.44	121.03	132.83
5	D	1001	DCT	O5'-PA-O3A	2.70	113.69	104.64
5	A	1001	DCT	PB-O3B-PG	-2.24	125.14	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

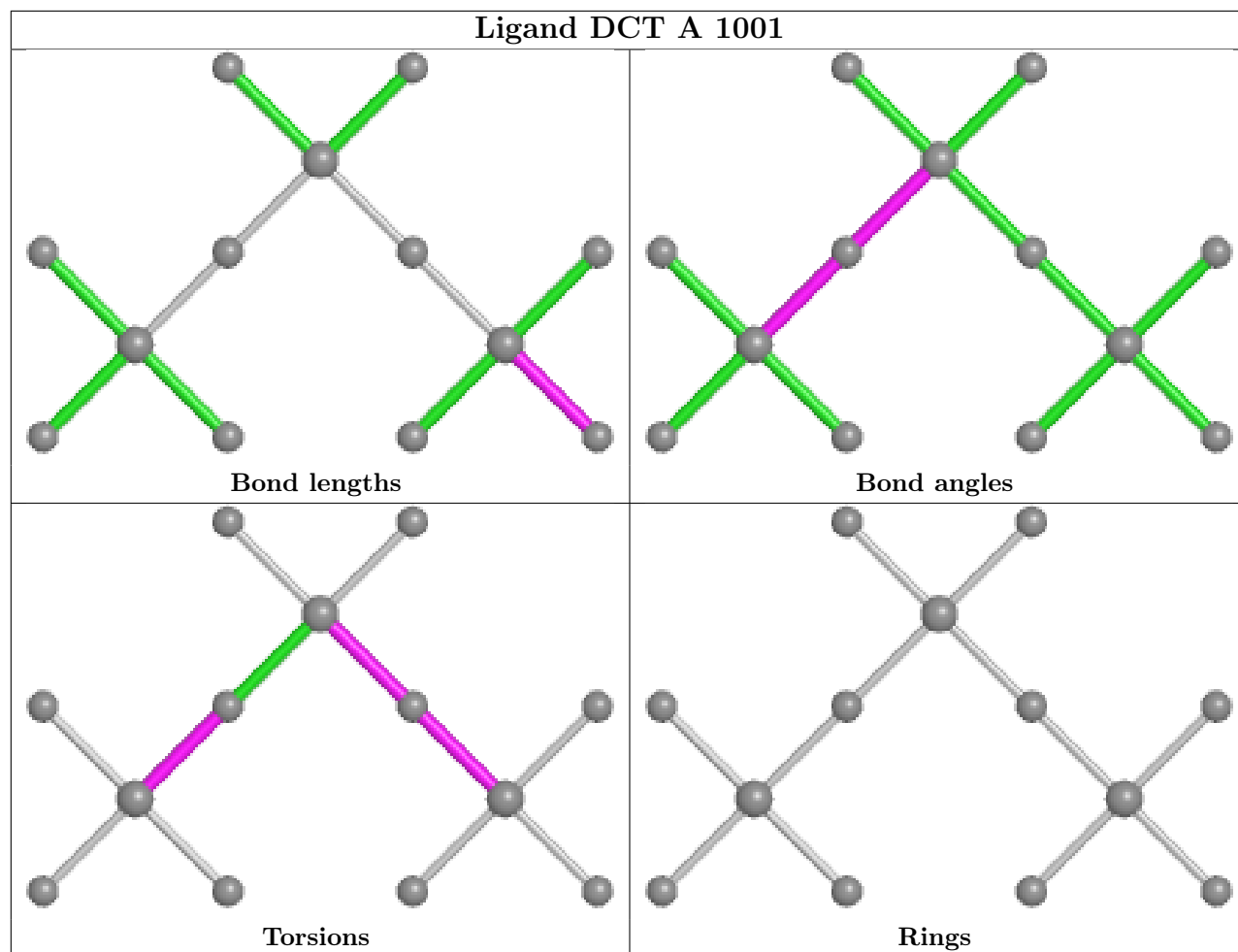
Mol	Chain	Res	Type	Atoms
5	A	1001	DCT	PB-O3B-PG-O3G
5	D	1001	DCT	PB-O3A-PA-O5'
5	D	1001	DCT	PB-O3A-PA-O2A
5	A	1001	DCT	PB-O3A-PA-O5'
5	A	1001	DCT	PA-O3A-PB-O2B
5	D	1001	DCT	PA-O3A-PB-O2B
5	D	1001	DCT	PB-O3B-PG-O1G
5	A	1001	DCT	PB-O3B-PG-O1G
5	A	1001	DCT	PB-O3A-PA-O2A
5	D	1001	DCT	PA-O3A-PB-O1B
5	D	1001	DCT	PB-O3A-PA-O1A

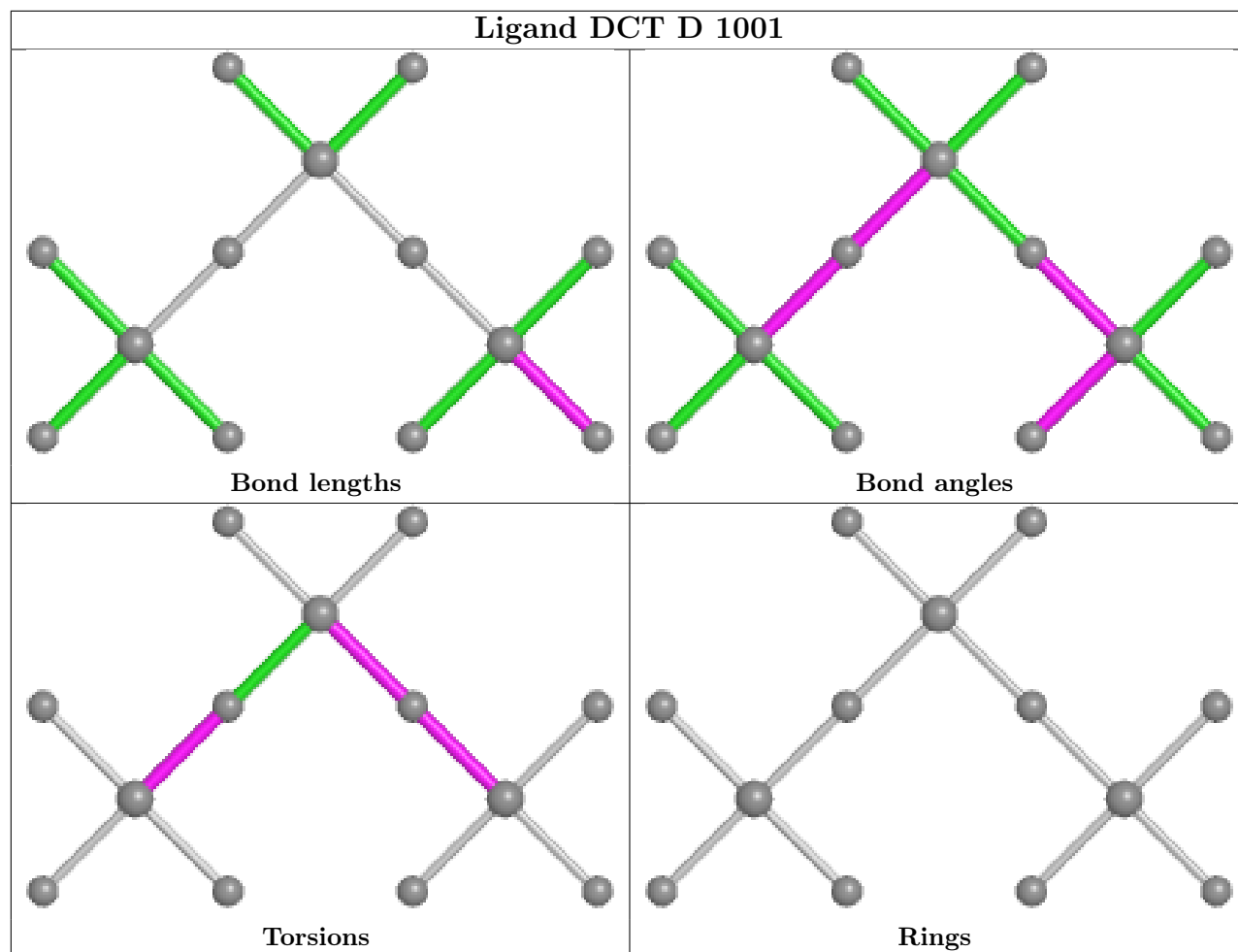
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	DCT	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	567/605 (93%)	0.26	21 (3%) 41 44	25, 46, 79, 113	0
1	D	567/605 (93%)	0.34	28 (4%) 29 33	27, 50, 87, 130	0
2	B	11/11 (100%)	-0.20	0 100 100	33, 40, 93, 109	0
2	E	11/11 (100%)	-0.05	0 100 100	36, 43, 117, 118	0
3	C	14/14 (100%)	-0.06	0 100 100	31, 48, 105, 128	0
4	F	13/16 (81%)	0.18	2 (15%) 2 2	33, 47, 142, 162	0
All	All	1183/1262 (93%)	0.28	51 (4%) 35 38	25, 48, 85, 162	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	808	ASP	7.1
1	D	452	ARG	6.7
1	A	908	HIS	5.3
1	A	721	PHE	5.1
4	F	20	DA	3.9
1	A	322	GLY	3.9
1	D	908	HIS	3.8
1	D	756	LEU	3.8
1	D	585	TYR	3.5
1	D	573	LEU	3.5
1	D	753	ALA	3.5
1	A	452	ARG	3.4
1	D	757	LYS	3.4
1	A	772	ASP	3.3
1	D	435	ARG	3.3
1	D	584	GLY	3.2
1	A	324	ALA	3.2
1	D	761	GLU	3.1
1	D	723	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	603	PHE	2.9
1	A	321	ARG	2.9
1	D	473	GLN	2.8
1	D	812	ARG	2.8
1	A	723	VAL	2.8
1	D	580	LYS	2.7
1	D	721	PHE	2.7
1	A	808	ASP	2.7
1	A	765	VAL	2.7
1	D	760	THR	2.6
1	A	323	ARG	2.6
1	A	572	GLU	2.5
1	A	758	ILE	2.5
1	A	735	ARG	2.5
1	D	353	ALA	2.4
1	D	743	LEU	2.4
4	F	19	DC	2.3
1	D	595	LEU	2.3
1	A	335	SER	2.2
1	A	773	ARG	2.2
1	D	354	TYR	2.2
1	A	715	PHE	2.2
1	A	476	GLN	2.2
1	D	450	GLU	2.1
1	D	731	GLU	2.1
1	D	476	GLN	2.1
1	D	548	ALA	2.1
1	D	477	THR	2.1
1	A	573	LEU	2.1
1	D	601	HIS	2.0
1	A	574	GLU	2.0
1	A	375	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

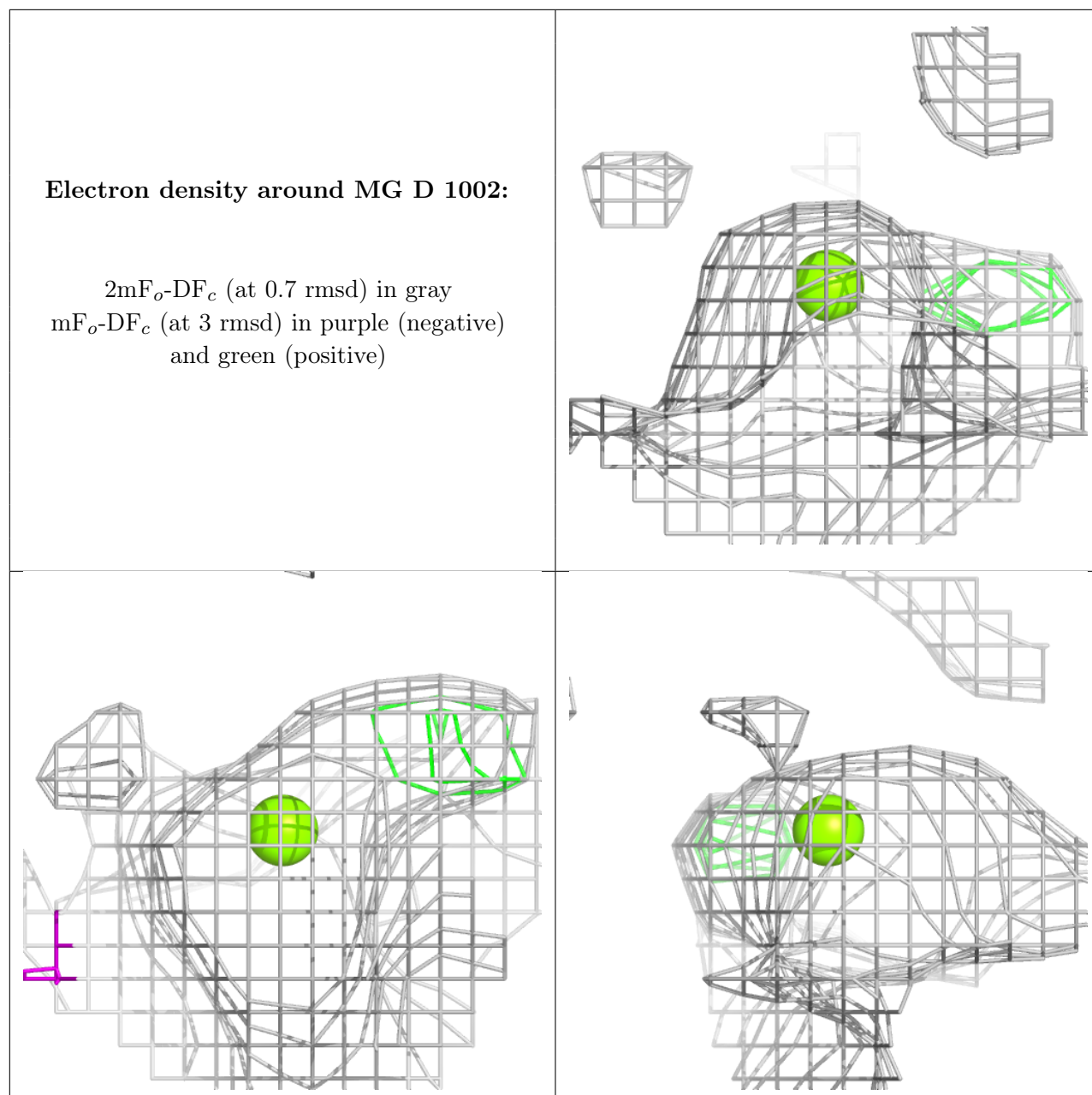
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	MG	D	1002	1/1	0.58	0.13	84,84,84,84	0
5	DCT	D	1001	13/27	0.89	0.10	62,81,94,96	0
6	MG	A	1003	1/1	0.93	0.06	54,54,54,54	0
6	MG	A	1002	1/1	0.94	0.05	44,44,44,44	0
5	DCT	A	1001	13/27	0.95	0.10	34,47,54,57	0
6	MG	B	101	1/1	0.96	0.03	49,49,49,49	0
6	MG	D	1003	1/1	0.96	0.07	42,42,42,42	0
6	MG	A	1004	1/1	0.98	0.04	34,34,34,34	0

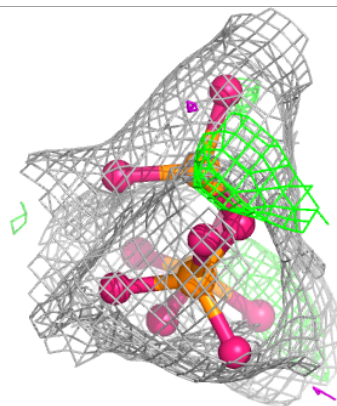
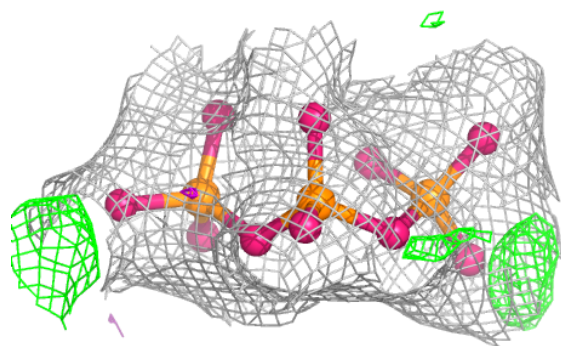
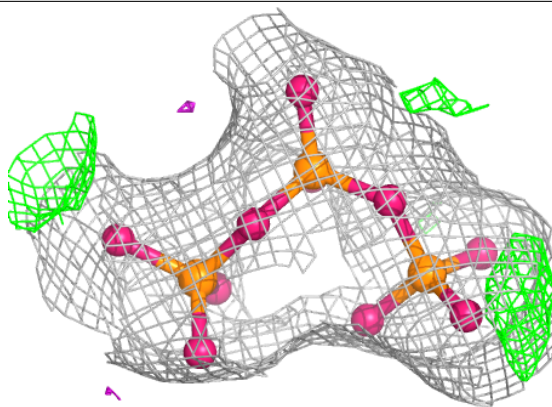
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





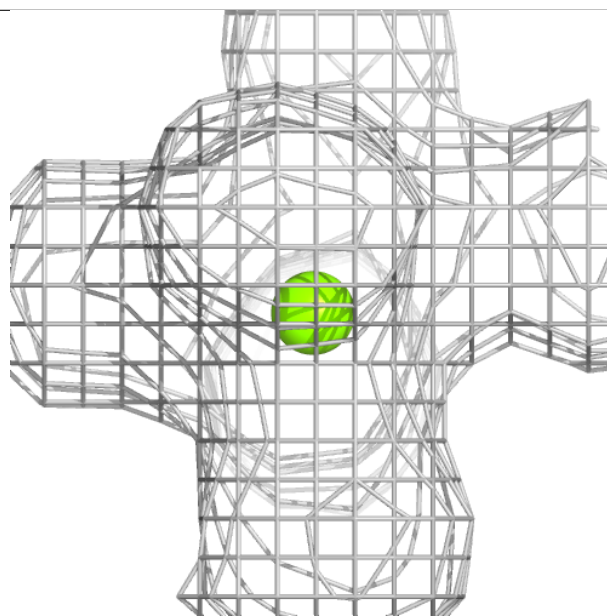
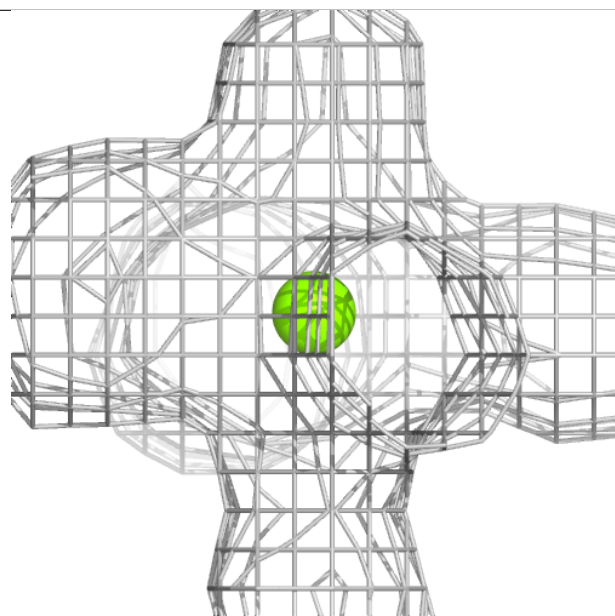
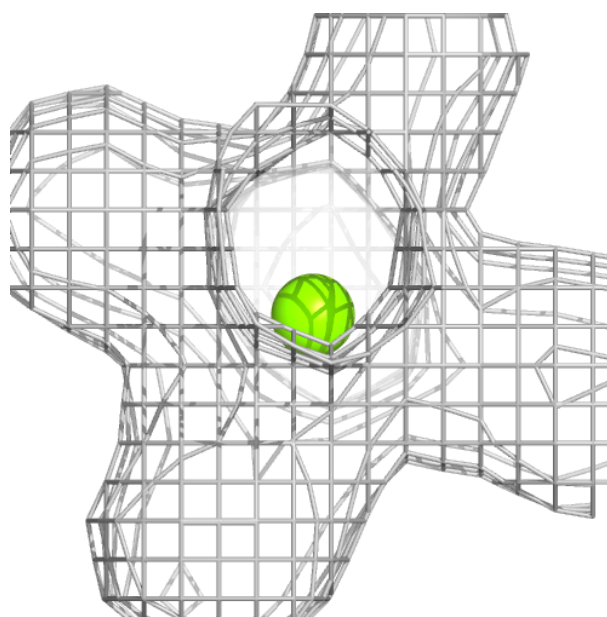
**Electron density around DCT D 1001:**

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



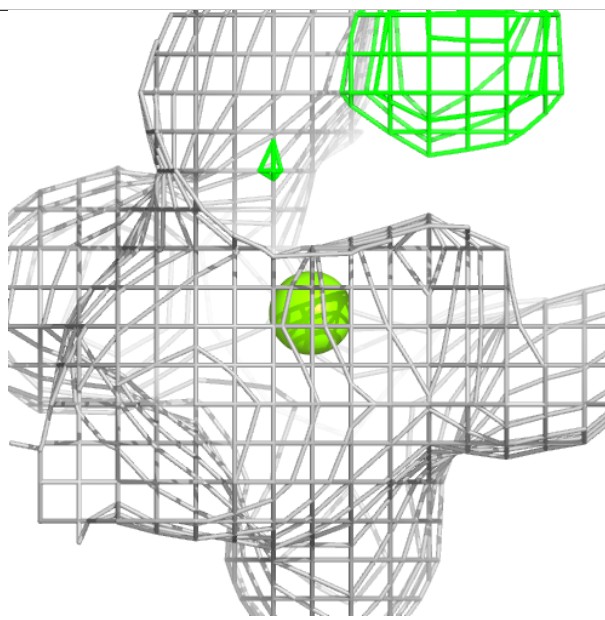
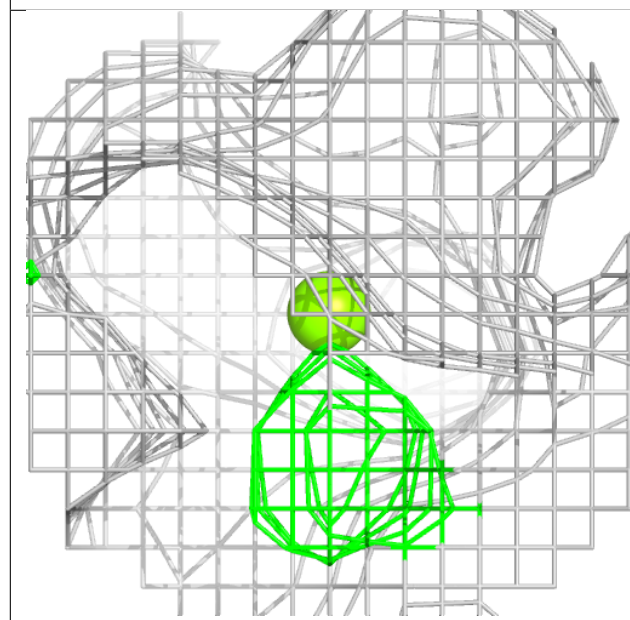
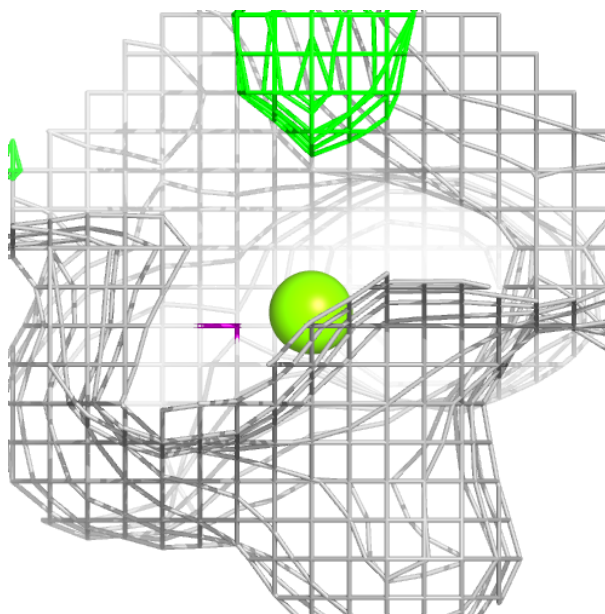
**Electron density around MG A 1003:**

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



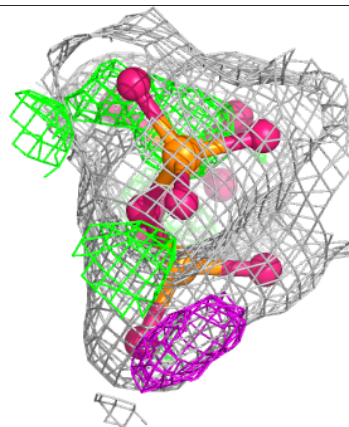
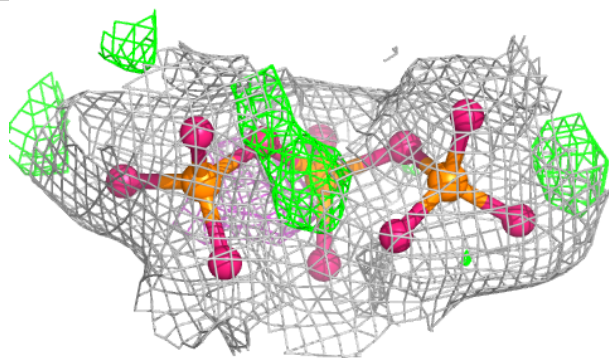
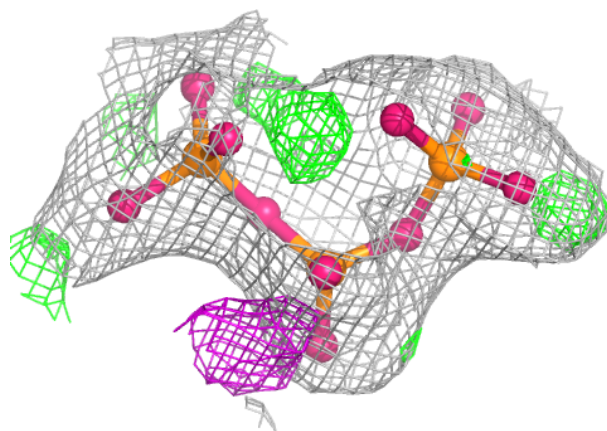
**Electron density around MG A 1002:**

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



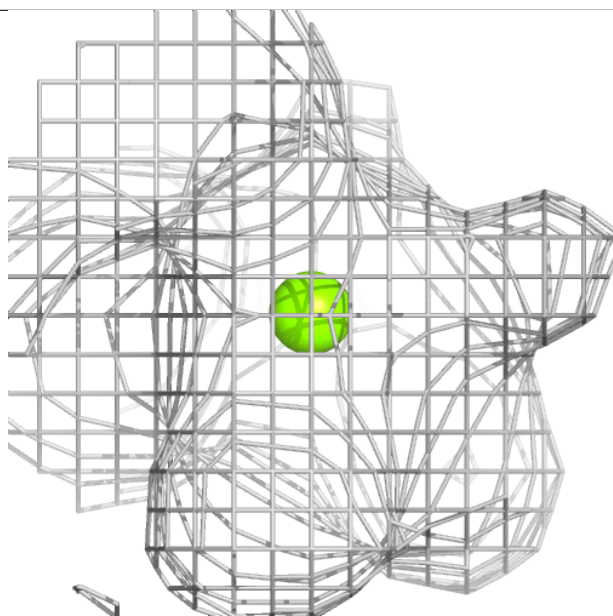
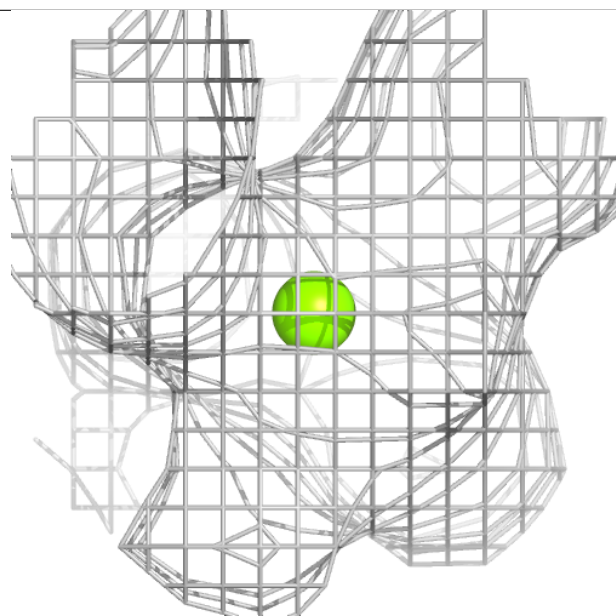
**Electron density around DCT A 1001:**

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



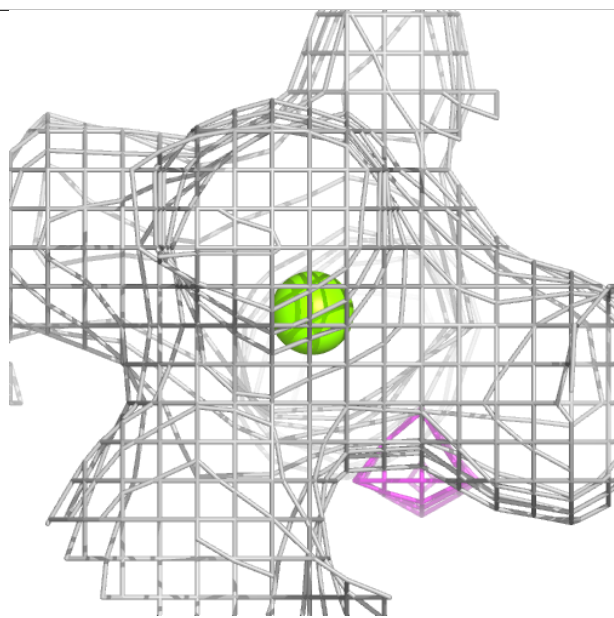
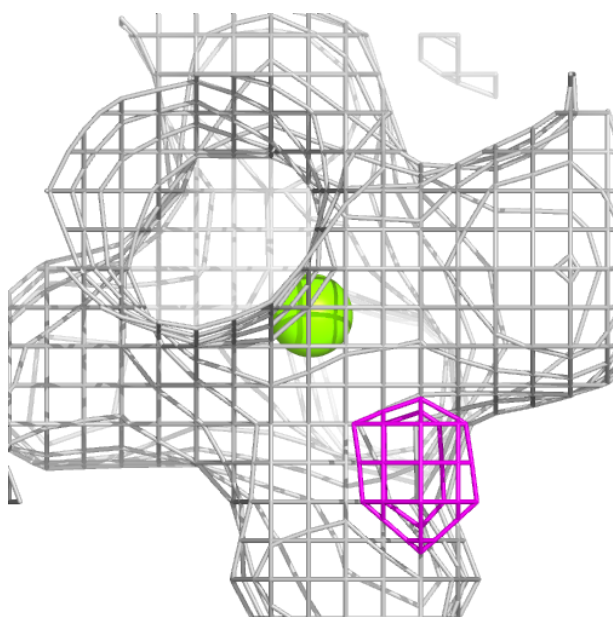
**Electron density around MG B 101:**

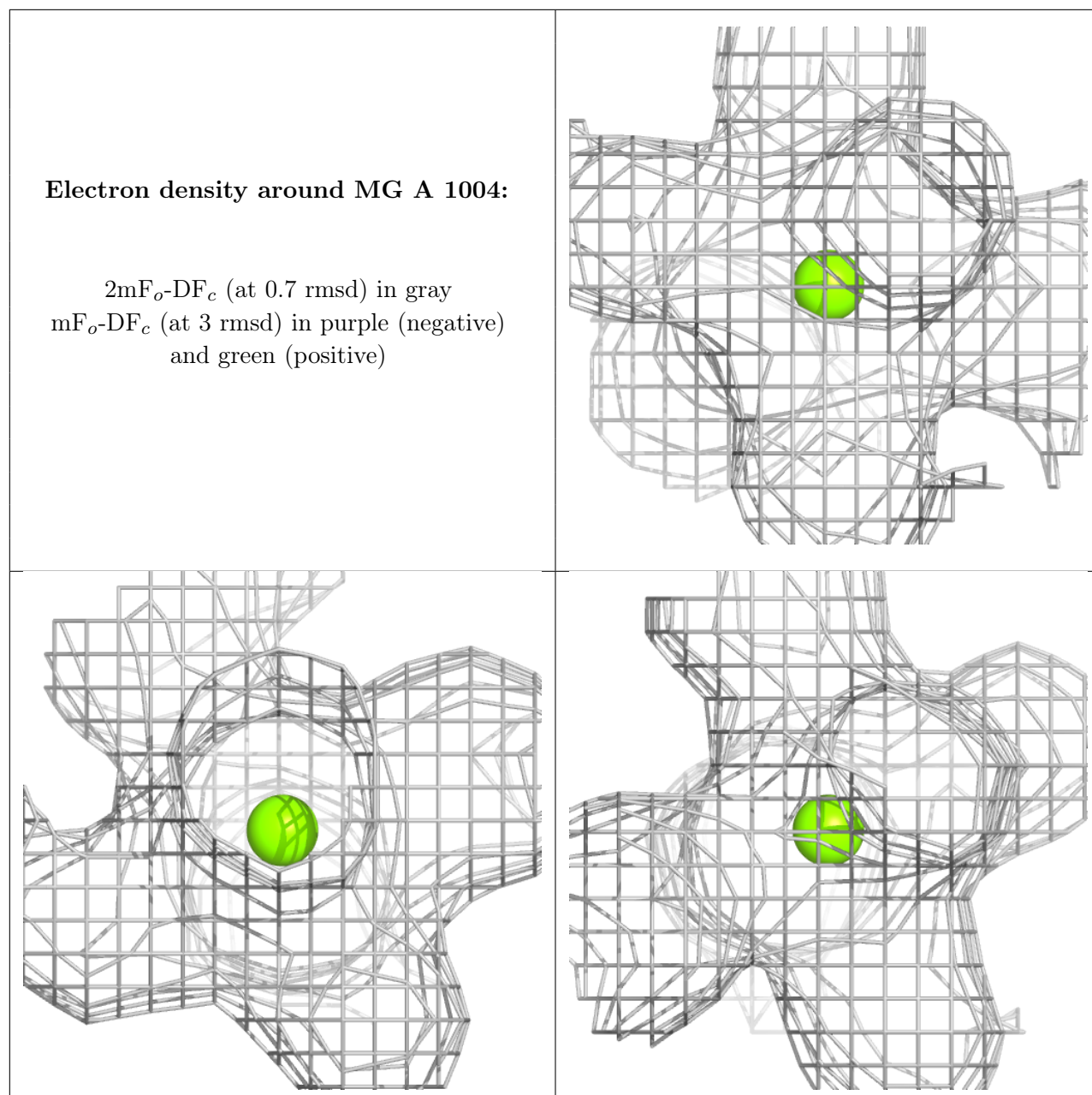
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG D 1003:**

$2mF_o-DF_c$  (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.