



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 9G85 / pdb\_00009g85  
Title : Structure of Response regulator PleD in complex with c-diGMP and ppGpp  
Authors : Jaboulay, C.; Dugelay, C.; Guzzo, M.; Terradot, L.  
Deposited on : 2024-07-23  
Resolution : 2.90 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 : 4-5-2 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

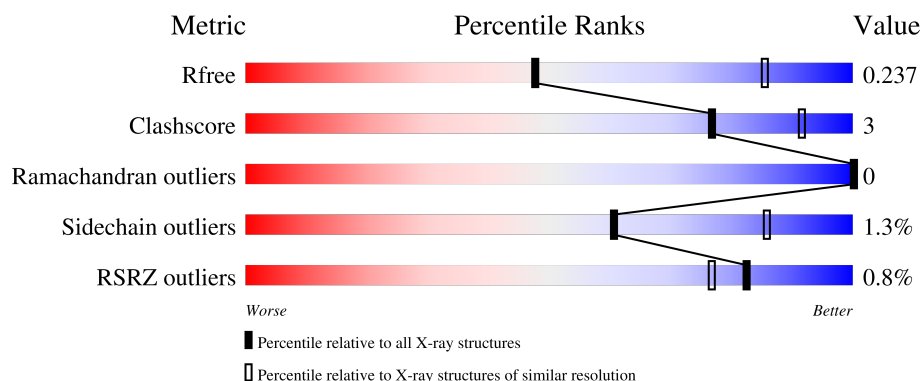
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	454	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	454	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	454	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>..</div> </div> </div>
1	D	454	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

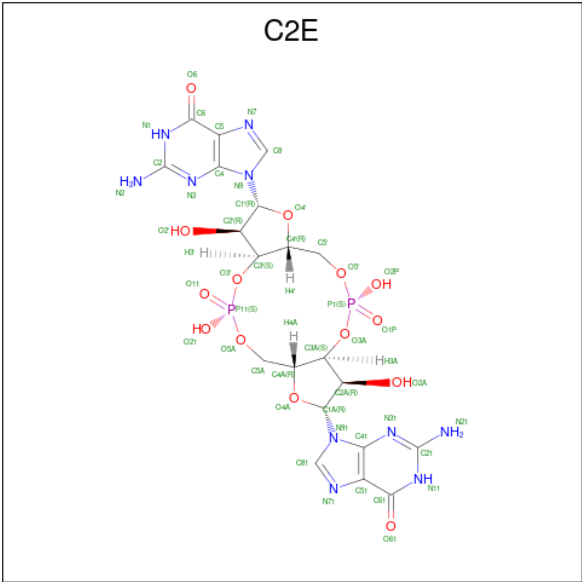
There are 5 unique types of molecules in this entry. The entry contains 14051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Response regulator PleD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	13	0	0
			3403	2120	614	654	15			
1	B	441	Total	C	N	O	S	16	0	0
			3353	2091	603	645	14			
1	C	439	Total	C	N	O	S	11	0	0
			3340	2083	600	643	14			
1	D	447	Total	C	N	O	S	11	0	0
			3401	2118	617	651	15			

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



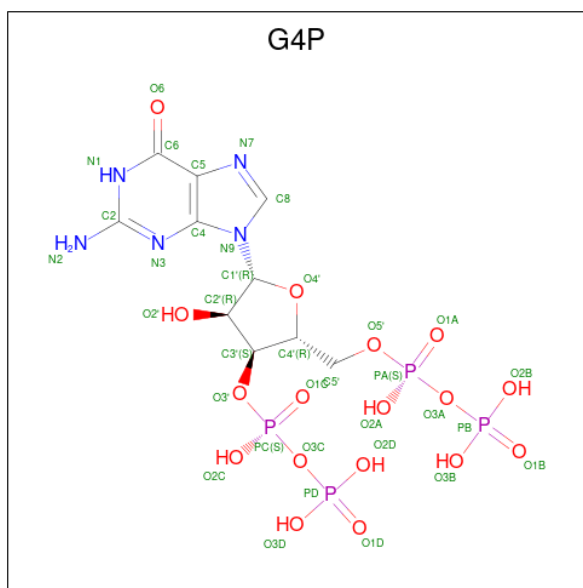
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 3 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula:  $C_{10}H_{17}N_5O_{17}P_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
3	B	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
3	C	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
3	D	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	B	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0
4	D	2	Total 2	Mg 2	0	0

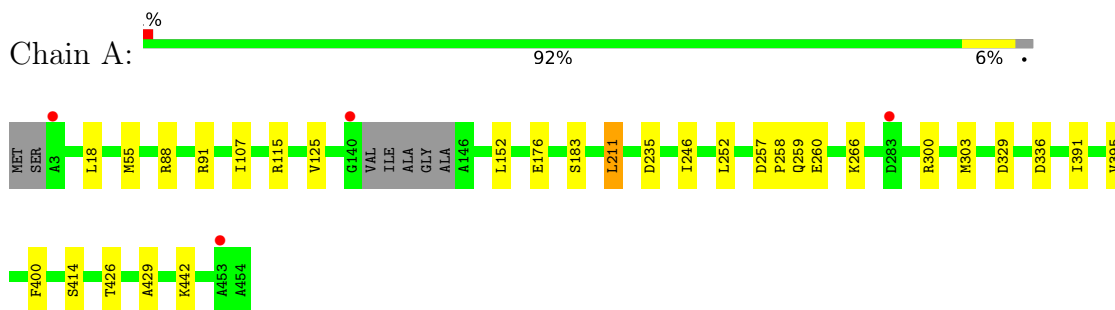
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	9	Total 9	O 9	0	0
5	C	6	Total 6	O 6	0	0
5	D	12	Total 12	O 12	0	0

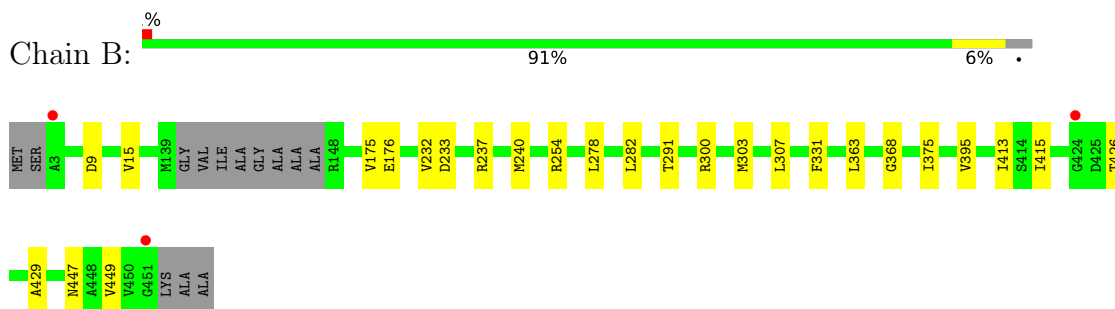
### 3 Residue-property plots [i](#)

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.

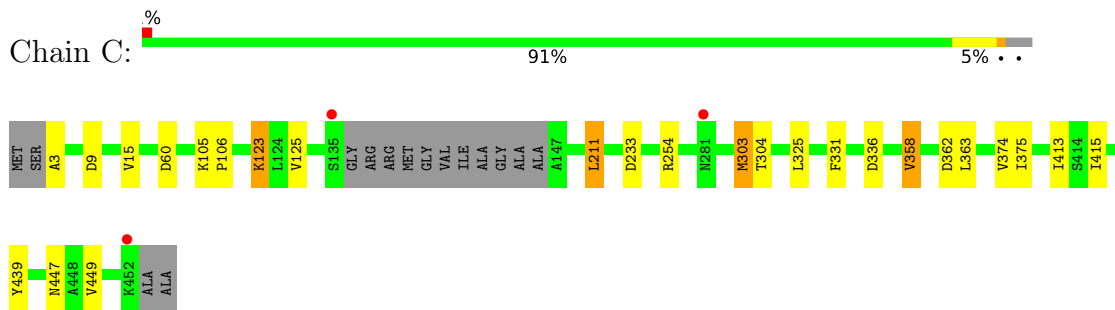
- Molecule 1: Response regulator PleD



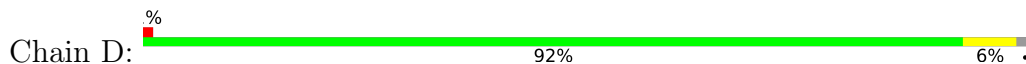
- Molecule 1: Response regulator PleD

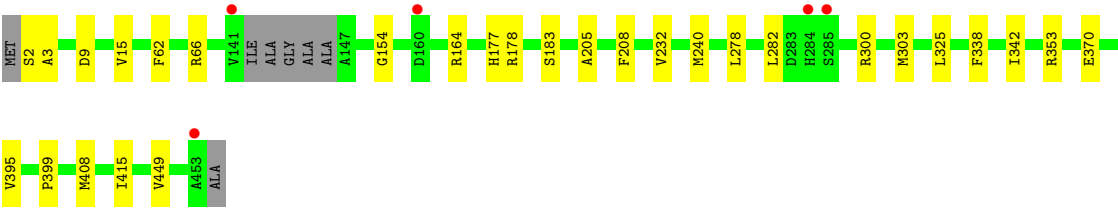


- Molecule 1: Response regulator PleD



- Molecule 1: Response regulator PleD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.00Å 133.00Å 510.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.70 – 2.90 47.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.70-2.90) 99.8 (47.70-2.90)	Depositor EDS
$R_{merge}$	0.43	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.201 , 0.239 0.201 , 0.237	Depositor DCC
$R_{free}$ test set	3014 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: C2E, G4P, 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	0.12	0/3445	0.30	0/4660
1	B	0.13	0/3395	0.30	0/4598
1	C	0.13	0/3382	0.31	0/4582
1	D	0.13	0/3442	0.32	0/4657
All	All	0.13	0/13664	0.31	0/18497

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 [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	3403	0	3441	18	0
1	B	3353	0	3374	16	0
1	C	3340	0	3361	17	0
1	D	3401	0	3437	17	0
2	A	46	0	18	2	0
2	B	138	0	60	3	0
2	C	138	0	59	3	0
2	D	46	0	21	3	0
3	A	36	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	9	4	0
3	C	36	0	9	3	0
3	D	36	0	9	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	7	0	0	0	0
5	B	9	0	0	0	0
5	C	6	0	0	1	0
5	D	12	0	0	0	0
All	All	14051	0	13808	79	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 3.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:C2E:C4A	2:D:502:C2E:O4A	1.63	1.22
2:B:504:C2E:O4A	2:B:504:C2E:C4A	1.64	1.19
2:C:502:C2E:O4A	2:C:502:C2E:C4A	1.63	1.16
2:A:501:C2E:C4A	2:A:501:C2E:O4A	1.63	1.16
1:A:88:ARG:HH12	1:A:258:PRO:HD2	1.27	0.98
1:A:18:LEU:HD11	1:A:107:ILE:HD12	1.67	0.77
1:A:88:ARG:NH1	1:A:258:PRO:HD2	2.02	0.75
1:B:237:ARG:HA	1:B:240:MET:HE3	1.77	0.67
3:A:502:G4P:O2C	1:B:300:ARG:NH2	2.25	0.67
1:D:399:PRO:HB2	1:D:408:MET:HE2	1.79	0.62
1:A:426:THR:HG23	1:A:429:ALA:H	1.64	0.62
1:B:233:ASP:HB2	1:B:254:ARG:HH21	1.65	0.61
1:A:152:LEU:HD21	1:A:266:LYS:HE2	1.85	0.58
2:B:502:C2E:O11	1:D:178:ARG:NH1	2.37	0.58
1:C:3:ALA:N	5:C:601:HOH:O	2.36	0.57
1:A:300:ARG:HH22	3:B:503:G4P:PC	2.26	0.56
1:B:278:LEU:HD23	1:B:282:LEU:HD12	1.86	0.55
1:C:439:TYR:OH	3:D:503:G4P:O1B	2.25	0.55
1:C:233:ASP:OD1	1:C:254:ARG:NH1	2.41	0.54
1:A:395:VAL:HG23	1:A:400:PHE:HZ	1.73	0.53
2:C:503:C2E:H2'	2:C:504:C2E:N11	2.23	0.53
1:A:88:ARG:HH12	1:A:258:PRO:CD	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HB	1:B:449:VAL:HG12	1.93	0.51
1:D:278:LEU:HD23	1:D:282:LEU:HD12	1.91	0.51
3:C:505:G4P:PC	1:D:300:ARG:HH22	2.34	0.51
1:A:336:ASP:CG	1:B:300:ARG:HH12	2.19	0.50
1:C:415:ILE:HB	1:C:449:VAL:HG12	1.95	0.49
1:B:331:PHE:N	3:B:503:G4P:O2A	2.44	0.49
3:D:503:G4P:O2C	3:D:503:G4P:O2'	2.25	0.49
1:D:370:GLU:CG	3:D:503:G4P:H5''	2.43	0.49
1:D:154:GLY:H	1:D:177:HIS:HD2	1.61	0.48
1:A:391:ILE:O	1:A:395:VAL:HG12	2.13	0.48
2:A:501:C2E:O4A	2:A:501:C2E:C5A	2.54	0.48
1:D:338:PHE:O	1:D:342:ILE:HD13	2.14	0.48
1:D:62:PHE:O	1:D:66:ARG:HG3	2.15	0.47
1:A:55:MET:HA	1:A:55:MET:HE2	1.97	0.47
1:D:2:SER:OG	1:D:3:ALA:N	2.48	0.47
1:D:370:GLU:HG2	3:D:503:G4P:H5''	1.97	0.47
1:B:363:LEU:HB2	1:B:375:ILE:HB	1.97	0.47
3:B:503:G4P:O3C	3:B:503:G4P:O2'	2.31	0.46
3:A:502:G4P:O1C	1:B:368:GLY:HA2	2.15	0.46
1:C:60:ASP:N	1:C:60:ASP:OD1	2.47	0.46
1:D:9:ASP:HB3	1:D:15:VAL:HG23	1.98	0.46
1:C:413:ILE:O	1:C:447:ASN:HA	2.15	0.45
1:D:232:VAL:HG21	1:D:240:MET:HG2	1.97	0.45
1:B:175:VAL:HG13	1:B:176:GLU:HG3	1.99	0.45
3:B:503:G4P:PC	3:B:503:G4P:O2'	2.76	0.43
1:C:303:MET:HE2	1:C:303:MET:HB3	1.74	0.43
1:B:9:ASP:HB3	1:B:15:VAL:HG23	2.01	0.43
1:C:9:ASP:HB3	1:C:15:VAL:HG23	2.00	0.43
1:D:415:ILE:HB	1:D:449:VAL:HG12	2.01	0.43
1:B:232:VAL:HG21	1:B:240:MET:HG2	2.00	0.43
2:C:502:C2E:O4A	2:C:502:C2E:C5A	2.57	0.43
1:A:91:ARG:NH1	1:A:257:ASP:OD2	2.51	0.43
1:A:257:ASP:OD1	1:A:259:GLN:N	2.52	0.43
1:A:414:SER:HB2	1:A:442:LYS:HE2	2.01	0.43
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.86	0.42
1:C:336:ASP:OD1	1:D:300:ARG:NH1	2.52	0.42
1:B:303:MET:HE3	1:B:303:MET:HB3	1.80	0.42
1:A:152:LEU:HD22	1:A:176:GLU:HB3	2.02	0.42
2:B:504:C2E:N1	2:D:502:C2E:H2A	2.35	0.42
1:D:325:LEU:HD23	1:D:325:LEU:HA	1.92	0.42
1:A:329:ASP:OD1	1:A:442:LYS:NZ	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LYS:HD3	1:C:123:LYS:O	2.21	0.41
1:C:358:VAL:HG21	1:C:374:VAL:HG11	2.03	0.41
1:B:413:ILE:O	1:B:447:ASN:HA	2.20	0.41
1:D:353:ARG:NH2	1:D:399:PRO:O	2.54	0.41
1:A:211:LEU:HD13	1:A:246:ILE:HD12	2.02	0.41
2:D:502:C2E:O4A	2:D:502:C2E:C5A	2.57	0.41
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.95	0.41
1:A:257:ASP:HB3	1:A:260:GLU:HB2	2.03	0.41
1:B:426:THR:HG23	1:B:429:ALA:H	1.86	0.41
1:C:105:LYS:HA	1:C:106:PRO:C	2.46	0.41
1:C:211:LEU:HD23	1:C:211:LEU:HA	1.85	0.41
1:C:331:PHE:HB3	3:C:505:G4P:O5'	2.21	0.40
3:C:505:G4P:PC	3:C:505:G4P:O2'	2.80	0.40
1:D:205:ALA:HB3	1:D:208:PHE:O	2.20	0.40
1:C:363:LEU:HB2	1:C:375:ILE:HB	2.03	0.40
1:C:358:VAL:HG22	1:C:362:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	443/454 (98%)	435 (98%)	8 (2%)	0	100	100
1	B	437/454 (96%)	429 (98%)	8 (2%)	0	100	100
1	C	435/454 (96%)	428 (98%)	7 (2%)	0	100	100
1	D	443/454 (98%)	437 (99%)	6 (1%)	0	100	100
All	All	1758/1816 (97%)	1729 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	359/369 (97%)	352 (98%)	7 (2%)	50	79
1	B	354/369 (96%)	352 (99%)	2 (1%)	78	93
1	C	353/369 (96%)	347 (98%)	6 (2%)	53	82
1	D	358/369 (97%)	354 (99%)	4 (1%)	65	88
All	All	1424/1476 (96%)	1405 (99%)	19 (1%)	61	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	125	VAL
1	A	183	SER
1	A	211	LEU
1	A	235	ASP
1	A	252	LEU
1	A	303	MET
1	B	291	THR
1	B	395	VAL
1	C	123	LYS
1	C	125	VAL
1	C	211	LEU
1	C	303	MET
1	C	304	THR
1	C	358	VAL
1	D	164	ARG
1	D	183	SER
1	D	303	MET
1	D	395	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	357	ASN
1	A	404	HIS
1	B	177	HIS
1	B	268	GLN
1	B	281	ASN
1	B	306	GLN
1	B	340	HIS
1	B	357	ASN
1	C	177	HIS
1	C	268	GLN
1	C	306	GLN
1	C	357	ASN
1	D	207	ASN
1	D	268	GLN
1	D	306	GLN
1	D	340	HIS
1	D	357	ASN
1	D	410	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	G4P	B	503	4	36,38,38	3.88	20 (55%)	56,61,61	2.61	21 (37%)
2	C2E	D	502	-	52,52,52	3.87	31 (59%)	78,82,82	1.96	25 (32%)
2	C2E	C	504	-	52,52,52	3.85	30 (57%)	78,82,82	1.94	22 (28%)
3	G4P	C	505	4	36,38,38	3.98	20 (55%)	56,61,61	2.59	22 (39%)
2	C2E	B	504	-	52,52,52	3.88	30 (57%)	78,82,82	1.94	21 (26%)
3	G4P	D	503	4	36,38,38	3.91	20 (55%)	56,61,61	2.54	21 (37%)
2	C2E	C	502	-	52,52,52	4.00	29 (55%)	78,82,82	2.13	22 (28%)
3	G4P	A	502	4	36,38,38	4.05	18 (50%)	56,61,61	2.61	16 (28%)
2	C2E	B	501	-	52,52,52	3.84	31 (59%)	78,82,82	1.95	22 (28%)
2	C2E	C	503	-	52,52,52	3.86	31 (59%)	78,82,82	1.93	22 (28%)
2	C2E	B	502	-	52,52,52	3.84	30 (57%)	78,82,82	1.94	22 (28%)
2	C2E	A	501	-	52,52,52	4.01	29 (55%)	78,82,82	2.14	23 (29%)

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	G4P	B	503	4	-	7/27/43/43	0/3/3/3
2	C2E	D	502	-	-	5/30/62/62	0/6/7/7
2	C2E	C	504	-	-	3/30/62/62	0/6/7/7
3	G4P	C	505	4	-	4/27/43/43	0/3/3/3
2	C2E	B	504	-	-	2/30/62/62	0/6/7/7
3	G4P	D	503	4	-	8/27/43/43	0/3/3/3
2	C2E	C	502	-	-	2/30/62/62	0/6/7/7
3	G4P	A	502	4	-	11/27/43/43	0/3/3/3
2	C2E	B	501	-	-	3/30/62/62	0/6/7/7
2	C2E	C	503	-	-	4/30/62/62	0/6/7/7
2	C2E	B	502	-	-	3/30/62/62	0/6/7/7
2	C2E	A	501	-	-	4/30/62/62	0/6/7/7

All (319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	G4P	C2'-C3'	-13.90	1.22	1.53
3	D	503	G4P	C2'-C3'	-13.38	1.23	1.53
3	B	503	G4P	C2'-C3'	-13.36	1.23	1.53
3	C	505	G4P	C2'-C3'	-13.14	1.24	1.53
2	A	501	C2E	C3'-C4'	-11.42	1.23	1.52
2	C	502	C2E	C3'-C4'	-11.36	1.23	1.52
2	C	502	C2E	C3A-C4A	-11.13	1.24	1.52
2	A	501	C2E	C3A-C4A	-11.11	1.24	1.52
2	B	504	C2E	C3'-C4'	-10.67	1.25	1.52
2	D	502	C2E	C3'-C4'	-10.64	1.25	1.52
2	B	501	C2E	C3'-C4'	-10.61	1.25	1.52
2	C	504	C2E	C3'-C4'	-10.60	1.25	1.52
2	B	502	C2E	C3'-C4'	-10.56	1.25	1.52
2	C	503	C2E	C3'-C4'	-10.56	1.25	1.52
2	B	502	C2E	C3A-C4A	-10.38	1.26	1.52
2	C	504	C2E	C3A-C4A	-10.35	1.26	1.52
2	C	503	C2E	C3A-C4A	-10.33	1.26	1.52
2	D	502	C2E	C3A-C4A	-10.31	1.26	1.52
2	B	501	C2E	C3A-C4A	-10.28	1.26	1.52
2	B	504	C2E	C3A-C4A	-10.17	1.26	1.52
2	B	504	C2E	O4A-C4A	8.61	1.64	1.45
2	A	501	C2E	O4A-C4A	8.51	1.63	1.45
2	C	502	C2E	O4A-C4A	8.44	1.63	1.45
2	D	502	C2E	O4A-C4A	8.43	1.63	1.45
2	C	502	C2E	O4'-C4'	8.29	1.63	1.45
2	B	502	C2E	O4A-C4A	8.26	1.63	1.45
2	C	504	C2E	O4A-C4A	8.25	1.63	1.45
2	B	504	C2E	O4'-C4'	8.21	1.63	1.45
2	C	503	C2E	O4A-C4A	8.21	1.63	1.45
2	B	501	C2E	O4A-C4A	8.16	1.63	1.45
2	C	503	C2E	O4'-C4'	8.10	1.63	1.45
2	A	501	C2E	O4'-C4'	8.09	1.63	1.45
2	C	504	C2E	O4'-C4'	8.07	1.62	1.45
2	D	502	C2E	O4'-C4'	8.04	1.62	1.45
2	B	502	C2E	O4'-C4'	7.90	1.62	1.45
2	B	501	C2E	O4'-C4'	7.75	1.62	1.45
3	D	503	G4P	O4'-C4'	-7.46	1.28	1.45
3	A	502	G4P	PC-O3C	7.37	1.67	1.59
3	A	502	G4P	O4'-C4'	-7.33	1.28	1.45
3	C	505	G4P	O4'-C4'	-7.31	1.28	1.45
3	C	505	G4P	PC-O3C	7.28	1.67	1.59
3	B	503	G4P	O4'-C4'	-6.97	1.29	1.45
2	C	502	C2E	C4-N3	6.80	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C2E	C41-N31	6.76	1.49	1.34
2	B	504	C2E	C41-N31	6.75	1.49	1.34
2	C	504	C2E	C4-N3	6.75	1.49	1.34
2	C	503	C2E	C4-N3	6.75	1.49	1.34
2	B	502	C2E	C4-N3	6.74	1.49	1.34
2	B	504	C2E	C4-N3	6.74	1.49	1.34
2	A	501	C2E	C4-N3	6.73	1.49	1.34
2	B	501	C2E	C4-N3	6.73	1.49	1.34
2	D	502	C2E	C4-N3	6.69	1.49	1.34
2	D	502	C2E	C41-N31	6.67	1.49	1.34
2	A	501	C2E	C41-N31	6.66	1.49	1.34
2	B	502	C2E	C41-N31	6.66	1.49	1.34
2	C	503	C2E	C41-N31	6.63	1.49	1.34
3	A	502	G4P	C4-N3	6.59	1.49	1.34
3	D	503	G4P	C4-N3	6.55	1.49	1.34
2	C	502	C2E	C41-N31	6.52	1.49	1.34
2	C	504	C2E	C41-N31	6.52	1.49	1.34
3	C	505	G4P	C4-N3	6.48	1.49	1.34
3	B	503	G4P	C4-N3	6.47	1.49	1.34
3	B	503	G4P	PC-O3C	6.37	1.66	1.59
3	D	503	G4P	PA-O3A	5.97	1.65	1.59
2	A	501	C2E	C21-N31	5.91	1.47	1.33
3	C	505	G4P	PA-O3A	5.85	1.65	1.59
2	C	502	C2E	C2-N3	5.82	1.47	1.33
2	C	502	C2E	C21-N31	5.78	1.47	1.33
2	B	504	C2E	C21-N31	5.76	1.47	1.33
3	D	503	G4P	C3'-C4'	5.76	1.67	1.52
2	B	501	C2E	C21-N31	5.72	1.47	1.33
2	C	504	C2E	C2-N3	5.71	1.47	1.33
2	B	504	C2E	C2-N3	5.70	1.47	1.33
2	D	502	C2E	C21-N31	5.69	1.47	1.33
2	A	501	C2E	C2-N3	5.69	1.47	1.33
2	B	501	C2E	C2-N3	5.65	1.46	1.33
2	C	503	C2E	C2-N3	5.64	1.46	1.33
2	B	502	C2E	C21-N31	5.64	1.46	1.33
2	C	503	C2E	C21-N31	5.63	1.46	1.33
2	C	504	C2E	C21-N31	5.63	1.46	1.33
2	B	502	C2E	C2-N3	5.61	1.46	1.33
2	D	502	C2E	C2-N3	5.61	1.46	1.33
3	A	502	G4P	C3'-C4'	5.60	1.67	1.52
3	A	502	G4P	PA-O3A	5.53	1.65	1.59
2	A	501	C2E	C21-N21	5.48	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	G4P	C2-N3	5.47	1.46	1.33
3	A	502	G4P	C2-N3	5.42	1.46	1.33
2	C	502	C2E	P11-O3'	5.33	1.75	1.59
3	C	505	G4P	C2-N3	5.31	1.46	1.33
3	B	503	G4P	PA-O3A	5.30	1.65	1.59
2	C	502	C2E	C21-N21	5.28	1.46	1.34
3	C	505	G4P	C3'-C4'	5.27	1.66	1.52
3	B	503	G4P	C2-N3	5.25	1.45	1.33
2	C	503	C2E	O4A-C1A	-5.19	1.30	1.42
2	C	504	C2E	O4A-C1A	-5.13	1.30	1.42
2	B	501	C2E	O4A-C1A	-5.13	1.30	1.42
2	A	501	C2E	P11-O3'	5.11	1.74	1.59
2	C	502	C2E	C2-N2	5.08	1.46	1.34
2	D	502	C2E	O4A-C1A	-5.07	1.30	1.42
2	B	504	C2E	O4A-C1A	-5.05	1.30	1.42
2	B	502	C2E	O4A-C1A	-5.04	1.30	1.42
2	B	504	C2E	C21-N21	5.03	1.45	1.34
2	B	501	C2E	C21-N21	5.00	1.45	1.34
2	C	503	C2E	C21-N21	4.99	1.45	1.34
2	C	504	C2E	C21-N21	4.98	1.45	1.34
3	A	502	G4P	C1'-N9	-4.96	1.33	1.47
2	B	502	C2E	O4'-C1'	-4.96	1.30	1.42
2	D	502	C2E	C21-N21	4.92	1.45	1.34
2	A	501	C2E	C2-N2	4.92	1.45	1.34
2	B	502	C2E	C21-N21	4.91	1.45	1.34
3	B	503	G4P	C3'-C4'	4.90	1.65	1.52
2	C	504	C2E	O4'-C1'	-4.86	1.30	1.42
2	B	501	C2E	O4'-C1'	-4.86	1.30	1.42
2	D	502	C2E	O4'-C1'	-4.83	1.30	1.42
3	A	502	G4P	O4'-C1'	4.83	1.53	1.42
2	C	503	C2E	O4'-C1'	-4.83	1.30	1.42
2	B	504	C2E	O4'-C1'	-4.78	1.31	1.42
3	C	505	G4P	C1'-N9	-4.78	1.34	1.47
3	B	503	G4P	C1'-N9	-4.77	1.34	1.47
2	B	502	C2E	C2-N2	4.72	1.45	1.34
2	C	504	C2E	C2-N2	4.71	1.45	1.34
3	D	503	G4P	PC-O3C	4.69	1.64	1.59
2	B	501	C2E	C2-N2	4.69	1.45	1.34
2	B	504	C2E	C2-N2	4.68	1.45	1.34
2	C	502	C2E	O4A-C1A	-4.68	1.31	1.42
3	C	505	G4P	C2-N2	4.66	1.45	1.34
2	D	502	C2E	C2-N2	4.66	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	G4P	C2-N2	4.59	1.44	1.34
3	B	503	G4P	C2-N2	4.58	1.44	1.34
2	C	503	C2E	C2-N2	4.55	1.44	1.34
2	A	501	C2E	O4A-C1A	-4.54	1.31	1.42
2	A	501	C2E	P1-O3A	4.51	1.73	1.59
3	A	502	G4P	C2-N2	4.50	1.44	1.34
2	A	501	C2E	O4'-C1'	-4.46	1.31	1.42
3	D	503	G4P	PC-O3'	4.45	1.72	1.59
2	C	502	C2E	O4'-C1'	-4.35	1.32	1.42
2	D	502	C2E	P11-O3'	4.33	1.72	1.59
2	C	503	C2E	P11-O3'	4.33	1.72	1.59
2	C	502	C2E	P1-O3A	4.28	1.72	1.59
2	B	504	C2E	P11-O3'	4.22	1.72	1.59
2	C	504	C2E	P11-O3'	4.21	1.72	1.59
3	D	503	G4P	C1'-N9	-4.21	1.35	1.47
2	B	501	C2E	P11-O3'	4.17	1.71	1.59
2	B	502	C2E	P11-O3'	4.13	1.71	1.59
2	C	502	C2E	O3'-C3'	3.82	1.57	1.44
3	B	503	G4P	O4'-C1'	3.80	1.50	1.42
3	D	503	G4P	O4'-C1'	3.78	1.50	1.42
2	A	501	C2E	O3'-C3'	3.74	1.56	1.44
3	C	505	G4P	PC-O3'	3.70	1.70	1.59
2	D	502	C2E	O3'-C3'	3.62	1.56	1.44
3	C	505	G4P	C6-N1	3.59	1.45	1.38
2	B	502	C2E	O3'-C3'	3.59	1.56	1.44
2	A	501	C2E	O3A-C3A	3.58	1.56	1.44
2	C	503	C2E	P1-O3A	3.57	1.70	1.59
3	B	503	G4P	C6-N1	3.57	1.45	1.38
2	C	503	C2E	O3'-C3'	3.55	1.56	1.44
2	B	504	C2E	P1-O3A	3.53	1.70	1.59
3	A	502	G4P	C6-N1	3.53	1.45	1.38
2	D	502	C2E	P1-O3A	3.51	1.69	1.59
2	B	501	C2E	O3'-C3'	3.51	1.56	1.44
2	B	504	C2E	O3A-C3A	3.50	1.56	1.44
2	B	501	C2E	P1-O3A	3.50	1.69	1.59
2	C	504	C2E	O3'-C3'	3.49	1.56	1.44
2	C	503	C2E	O3A-C3A	3.49	1.56	1.44
3	C	505	G4P	C2'-C1'	3.48	1.64	1.53
2	B	501	C2E	O3A-C3A	3.48	1.55	1.44
2	D	502	C2E	O3A-C3A	3.46	1.55	1.44
2	C	504	C2E	P1-O3A	3.44	1.69	1.59
2	B	504	C2E	O3'-C3'	3.43	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	C2E	O3A-C3A	3.40	1.55	1.44
3	C	505	G4P	O4'-C1'	3.36	1.49	1.42
2	C	504	C2E	O3A-C3A	3.35	1.55	1.44
2	B	502	C2E	P1-O3A	3.28	1.69	1.59
3	C	505	G4P	C4-N9	-3.28	1.29	1.38
2	B	502	C2E	O3A-C3A	3.26	1.55	1.44
3	B	503	G4P	C4-N9	-3.24	1.29	1.38
3	D	503	G4P	C6-N1	3.24	1.44	1.38
3	A	502	G4P	PC-O3'	3.23	1.69	1.59
3	A	502	G4P	O2'-C2'	3.21	1.50	1.43
3	B	503	G4P	PC-O3'	3.12	1.68	1.59
2	C	502	C2E	O2A-C2A	-3.02	1.35	1.43
2	B	504	C2E	C2-N1	2.99	1.44	1.37
2	B	501	C2E	C2-N1	2.99	1.44	1.37
2	A	501	C2E	O2A-C2A	-2.98	1.35	1.43
2	C	503	C2E	C2-N1	2.96	1.44	1.37
2	C	504	C2E	C2-N1	2.96	1.44	1.37
3	B	503	G4P	C2'-C1'	2.95	1.62	1.53
3	D	503	G4P	C2'-C1'	2.94	1.62	1.53
2	B	502	C2E	C2-N1	2.93	1.44	1.37
3	B	503	G4P	C5-C6	2.93	1.55	1.44
2	C	502	C2E	C61-N11	2.89	1.44	1.38
2	A	501	C2E	O2'-C2'	-2.89	1.35	1.43
2	A	501	C2E	C61-N11	2.89	1.44	1.38
2	C	502	C2E	O2'-C2'	-2.89	1.35	1.43
3	C	505	G4P	C5-C6	2.88	1.55	1.44
3	A	502	G4P	C2-N1	2.88	1.44	1.37
3	C	505	G4P	C2-N1	2.86	1.44	1.37
3	D	503	G4P	O2'-C2'	2.84	1.50	1.43
2	D	502	C2E	C2-N1	2.83	1.44	1.37
3	B	503	G4P	C2-N1	2.83	1.44	1.37
3	B	503	G4P	O2'-C2'	2.82	1.49	1.43
3	C	505	G4P	O2'-C2'	2.78	1.49	1.43
3	D	503	G4P	C5-C6	2.78	1.54	1.44
2	A	501	C2E	C6-N1	2.77	1.44	1.38
3	A	502	G4P	C4-N9	-2.77	1.31	1.38
2	B	504	C2E	C21-N11	2.76	1.44	1.37
2	C	502	C2E	C6-N1	2.76	1.44	1.38
2	B	502	C2E	C21-N11	2.76	1.44	1.37
2	C	502	C2E	P11-O5A	2.75	1.70	1.59
3	A	502	G4P	C5-C6	2.74	1.54	1.44
2	A	501	C2E	P11-O5A	2.74	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	C2E	C21-N11	2.72	1.44	1.37
2	C	504	C2E	C21-N11	2.71	1.44	1.37
2	C	503	C2E	C21-N11	2.71	1.44	1.37
2	D	502	C2E	O2A-C2A	-2.66	1.36	1.43
2	B	501	C2E	O2A-C2A	-2.66	1.36	1.43
2	C	504	C2E	C51-N71	-2.63	1.33	1.39
3	D	503	G4P	C2-N1	2.62	1.44	1.37
2	B	501	C2E	C21-N11	2.61	1.44	1.37
2	A	501	C2E	C2-N1	2.61	1.44	1.37
2	C	503	C2E	O2A-C2A	-2.61	1.36	1.43
2	C	504	C2E	O2A-C2A	-2.61	1.36	1.43
2	D	502	C2E	C5-C6	2.60	1.54	1.44
2	B	502	C2E	C51-N71	-2.60	1.33	1.39
2	B	504	C2E	O2A-C2A	-2.60	1.36	1.43
2	B	502	C2E	O2A-C2A	-2.59	1.36	1.43
3	D	503	G4P	C4-N9	-2.58	1.31	1.38
2	C	503	C2E	C51-C61	2.57	1.54	1.44
2	B	501	C2E	O61-C61	-2.56	1.18	1.23
2	D	502	C2E	C51-C61	2.56	1.54	1.44
2	B	504	C2E	O61-C61	-2.56	1.18	1.23
2	C	502	C2E	O6-C6	-2.56	1.18	1.23
2	D	502	C2E	O61-C61	-2.55	1.18	1.23
2	B	504	C2E	C51-C61	2.55	1.53	1.44
2	D	502	C2E	P11-O5A	2.55	1.69	1.59
2	B	504	C2E	C61-N11	2.54	1.43	1.38
2	C	502	C2E	C2-N1	2.54	1.43	1.37
2	B	504	C2E	O2'-C2'	-2.54	1.36	1.43
2	D	502	C2E	C51-N71	-2.54	1.34	1.39
2	B	504	C2E	P11-O5A	2.53	1.69	1.59
2	A	501	C2E	O6-C6	-2.53	1.18	1.23
2	C	504	C2E	O6-C6	-2.52	1.18	1.23
2	B	501	C2E	C5-C6	2.52	1.53	1.44
2	B	502	C2E	C61-N11	2.52	1.43	1.38
2	B	501	C2E	P11-O5A	2.51	1.69	1.59
2	B	502	C2E	O6-C6	-2.51	1.18	1.23
2	B	501	C2E	O2'-C2'	-2.51	1.36	1.43
2	C	503	C2E	C5-C6	2.51	1.53	1.44
2	B	504	C2E	C5-C6	2.51	1.53	1.44
3	D	503	G4P	O3'-C3'	2.50	1.52	1.44
2	C	503	C2E	O61-C61	-2.50	1.18	1.23
2	B	502	C2E	C51-C61	2.50	1.53	1.44
2	C	504	C2E	O2'-C2'	-2.50	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C2E	C51-N71	-2.50	1.34	1.39
2	C	504	C2E	C51-C61	2.49	1.53	1.44
2	B	502	C2E	O61-C61	-2.49	1.18	1.23
2	C	504	C2E	C5-C6	2.49	1.53	1.44
2	B	504	C2E	O6-C6	-2.48	1.18	1.23
2	B	501	C2E	C51-C61	2.47	1.53	1.44
2	B	504	C2E	C51-N71	-2.47	1.34	1.39
2	D	502	C2E	C61-N11	2.47	1.43	1.38
2	B	502	C2E	O2'-C2'	-2.47	1.36	1.43
2	C	504	C2E	C61-N11	2.47	1.43	1.38
2	C	503	C2E	O2'-C2'	-2.46	1.36	1.43
2	B	502	C2E	P11-O5A	2.46	1.69	1.59
2	B	502	C2E	C5-C6	2.46	1.53	1.44
2	C	504	C2E	P11-O5A	2.45	1.69	1.59
2	D	502	C2E	O2'-C2'	-2.45	1.36	1.43
2	D	502	C2E	O6-C6	-2.45	1.18	1.23
2	A	501	C2E	C51-C61	2.45	1.53	1.44
2	C	503	C2E	P11-O5A	2.44	1.69	1.59
3	C	505	G4P	O3'-C3'	2.44	1.52	1.44
2	B	501	C2E	C61-N11	2.44	1.43	1.38
2	B	501	C2E	O6-C6	-2.43	1.19	1.23
2	C	503	C2E	C51-N71	-2.43	1.34	1.39
2	C	502	C2E	C51-C61	2.43	1.53	1.44
2	C	504	C2E	O61-C61	-2.42	1.19	1.23
2	C	503	C2E	C5-N7	-2.42	1.34	1.39
2	A	501	C2E	C5-C6	2.41	1.53	1.44
2	B	504	C2E	P1-O5'	2.40	1.68	1.59
2	A	501	C2E	P1-O5'	2.40	1.68	1.59
2	A	501	C2E	O61-C61	-2.40	1.19	1.23
2	C	502	C2E	C5-C6	2.39	1.53	1.44
2	C	503	C2E	O6-C6	-2.38	1.19	1.23
2	C	502	C2E	C21-N11	2.37	1.43	1.37
2	A	501	C2E	C21-N11	2.37	1.43	1.37
2	C	503	C2E	C6-N1	2.37	1.43	1.38
2	C	503	C2E	C61-N11	2.36	1.43	1.38
2	D	502	C2E	P1-O5'	2.36	1.68	1.59
2	B	502	C2E	C5-N7	-2.36	1.34	1.39
2	B	504	C2E	C5-N7	-2.35	1.34	1.39
2	C	502	C2E	O61-C61	-2.35	1.19	1.23
2	C	503	C2E	P1-O5'	2.35	1.68	1.59
2	C	504	C2E	C5-N7	-2.35	1.34	1.39
2	B	501	C2E	C5-N7	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	C2E	P1-O5'	2.33	1.68	1.59
2	B	501	C2E	P1-O5'	2.31	1.68	1.59
2	C	504	C2E	C6-N1	2.31	1.43	1.38
2	B	501	C2E	C6-N1	2.31	1.43	1.38
2	C	504	C2E	P1-O5'	2.30	1.68	1.59
3	B	503	G4P	C8-N7	2.28	1.38	1.32
2	B	502	C2E	C6-N1	2.27	1.43	1.38
3	D	503	G4P	C8-N7	2.27	1.38	1.32
2	D	502	C2E	C5-N7	-2.27	1.34	1.39
2	B	504	C2E	C6-N1	2.26	1.43	1.38
2	D	502	C2E	C6-N1	2.25	1.43	1.38
2	B	502	C2E	P1-O5'	2.24	1.68	1.59
3	C	505	G4P	C8-N7	2.22	1.38	1.32
3	D	503	G4P	O6-C6	-2.20	1.19	1.23
2	A	501	C2E	C51-N71	-2.20	1.34	1.39
3	B	503	G4P	O3'-C3'	2.15	1.51	1.44
2	C	502	C2E	C51-N71	-2.13	1.34	1.39
3	A	502	G4P	O3'-C3'	2.13	1.51	1.44
3	A	502	G4P	C2'-C1'	2.12	1.60	1.53
2	D	502	C2E	C2'-C3'	2.11	1.57	1.53
2	B	501	C2E	C2'-C3'	2.06	1.57	1.53
2	C	503	C2E	C2'-C3'	2.04	1.57	1.53
3	C	505	G4P	O6-C6	-2.03	1.19	1.23
3	B	503	G4P	O6-C6	-2.02	1.19	1.23

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	G4P	C1'-N9-C8	-9.22	100.53	126.73
3	D	503	G4P	C1'-N9-C8	-8.18	103.48	126.73
3	B	503	G4P	C1'-N9-C8	-7.85	104.42	126.73
3	C	505	G4P	C1'-N9-C8	-7.69	104.89	126.73
3	A	502	G4P	C1'-N9-C4	7.40	148.35	126.49
3	D	503	G4P	C1'-N9-C4	6.22	144.85	126.49
2	A	501	C2E	C21-N31-C41	5.92	122.50	112.30
3	D	503	G4P	C2-N3-C4	5.81	122.31	112.30
3	B	503	G4P	C1'-N9-C4	5.70	143.31	126.49
2	C	502	C2E	C21-N31-C41	5.69	122.11	112.30
3	B	503	G4P	C2-N3-C4	5.60	121.94	112.30
2	C	502	C2E	C2-N3-C4	5.58	121.91	112.30
3	C	505	G4P	C2-N3-C4	5.58	121.91	112.30
3	B	503	G4P	O4'-C1'-N9	5.55	120.94	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	G4P	O4'-C1'-N9	5.50	120.81	108.36
3	C	505	G4P	C1'-N9-C4	5.35	142.28	126.49
3	A	502	G4P	C2-N3-C4	5.34	121.50	112.30
3	A	502	G4P	C4'-O4'-C1'	-5.31	97.74	109.47
2	A	501	C2E	C51-C41-N31	-5.30	119.96	128.39
2	A	501	C2E	C2-N3-C4	5.28	121.40	112.30
2	C	502	C2E	C51-C41-N31	-5.13	120.22	128.39
3	D	503	G4P	O4'-C1'-N9	5.01	119.71	108.36
2	D	502	C2E	C51-C41-N31	-4.96	120.50	128.39
2	C	504	C2E	C51-C41-N31	-4.94	120.53	128.39
3	C	505	G4P	N9-C8-N7	-4.94	104.25	113.40
2	B	504	C2E	C51-C41-N31	-4.93	120.54	128.39
2	D	502	C2E	C5-C4-N3	-4.90	120.59	128.39
2	B	501	C2E	C51-C41-N31	-4.87	120.64	128.39
2	B	502	C2E	C51-C41-N31	-4.86	120.66	128.39
2	C	504	C2E	C5-C4-N3	-4.84	120.68	128.39
2	C	502	C2E	C5-C4-N3	-4.80	120.74	128.39
2	B	504	C2E	C5-C4-N3	-4.79	120.77	128.39
2	C	503	C2E	C51-C41-N31	-4.79	120.77	128.39
3	D	503	G4P	N9-C8-N7	-4.75	104.59	113.40
3	B	503	G4P	N9-C8-N7	-4.73	104.63	113.40
2	B	502	C2E	C5-C4-N3	-4.72	120.88	128.39
2	C	503	C2E	C5-C4-N3	-4.72	120.88	128.39
2	B	501	C2E	C5-C4-N3	-4.68	120.94	128.39
2	B	501	C2E	N9-C8-N7	-4.64	104.79	113.40
3	C	505	G4P	O4'-C1'-N9	4.61	118.80	108.36
2	C	502	C2E	N9-C4-N3	4.56	135.07	125.95
3	C	505	G4P	C4'-O4'-C1'	-4.54	99.44	109.47
2	B	502	C2E	N9-C8-N7	-4.51	105.03	113.40
2	A	501	C2E	C5-C4-N3	-4.46	121.29	128.39
2	B	504	C2E	C21-N31-C41	4.45	119.96	112.30
2	C	503	C2E	N9-C8-N7	-4.41	105.22	113.40
2	B	501	C2E	C21-N31-C41	4.41	119.89	112.30
3	A	502	G4P	N9-C8-N7	-4.39	105.27	113.40
2	D	502	C2E	C21-N31-C41	4.37	119.83	112.30
2	D	502	C2E	N9-C8-N7	-4.36	105.32	113.40
2	C	504	C2E	C21-N31-C41	4.33	119.76	112.30
3	C	505	G4P	N2-C2-N1	4.32	125.87	116.76
2	C	504	C2E	N9-C8-N7	-4.31	105.40	113.40
2	C	503	C2E	C21-N31-C41	4.31	119.72	112.30
2	D	502	C2E	C2-N3-C4	4.29	119.69	112.30
2	B	502	C2E	C21-N31-C41	4.27	119.65	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	C2E	N9-C8-N7	-4.24	105.53	113.40
2	A	501	C2E	N9-C4-N3	4.19	134.32	125.95
2	B	501	C2E	N9-C4-N3	4.17	134.29	125.95
3	B	503	G4P	N2-C2-N1	4.17	125.55	116.76
2	B	504	C2E	N9-C4-N3	4.16	134.27	125.95
2	C	504	C2E	C2-N3-C4	4.16	119.46	112.30
2	B	502	C2E	C2-N3-C4	4.15	119.45	112.30
2	C	504	C2E	N9-C4-N3	4.15	134.25	125.95
2	A	501	C2E	N91-C41-N31	4.11	134.17	125.95
2	B	502	C2E	N9-C4-N3	4.11	134.16	125.95
3	D	503	G4P	C5-C4-N3	-4.07	121.91	128.39
3	B	503	G4P	C4'-O4'-C1'	-4.07	100.48	109.47
2	C	503	C2E	N9-C4-N3	4.05	134.04	125.95
3	C	505	G4P	C6-C5-N7	4.05	137.65	130.29
2	B	504	C2E	C2-N3-C4	4.02	119.23	112.30
2	B	501	C2E	C2-N3-C4	4.02	119.22	112.30
2	C	502	C2E	N91-C41-N31	4.02	133.99	125.95
2	D	502	C2E	C1'-N9-C4	-3.96	114.78	126.49
3	B	503	G4P	C6-C5-N7	3.94	137.45	130.29
2	C	503	C2E	C2-N3-C4	3.92	119.06	112.30
2	D	502	C2E	N9-C4-N3	3.92	133.80	125.95
2	C	503	C2E	C1'-N9-C4	-3.91	114.94	126.49
2	C	502	C2E	C5-C6-N1	3.91	123.20	113.25
2	B	501	C2E	C1'-N9-C4	-3.85	115.11	126.49
2	B	502	C2E	C1'-N9-C4	-3.82	115.21	126.49
2	A	501	C2E	C5-C6-N1	3.80	122.93	113.25
2	A	501	C2E	C51-C61-N11	3.78	122.87	113.25
2	C	504	C2E	C1'-N9-C4	-3.77	115.35	126.49
3	D	503	G4P	C5-C6-N1	3.77	122.84	113.25
3	A	502	G4P	N2-C2-N1	3.75	124.67	116.76
2	C	502	C2E	C51-C61-N11	3.72	122.72	113.25
3	D	503	G4P	N2-C2-N1	3.71	124.58	116.76
2	B	501	C2E	N91-C81-N71	-3.68	106.58	113.40
2	B	504	C2E	N91-C81-N71	-3.68	106.58	113.40
2	B	502	C2E	N91-C81-N71	-3.66	106.61	113.40
2	C	504	C2E	N91-C81-N71	-3.66	106.61	113.40
3	B	503	G4P	C5-C6-N1	3.66	122.57	113.25
3	A	502	G4P	C5-C6-N1	3.66	122.57	113.25
3	C	505	G4P	C5-C6-N1	3.65	122.55	113.25
3	A	502	G4P	C5-C4-N3	-3.65	122.58	128.39
2	B	504	C2E	C1'-N9-C4	-3.64	115.72	126.49
2	D	502	C2E	N91-C81-N71	-3.64	106.65	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	C2E	N91-C81-N71	-3.63	106.66	113.40
3	C	505	G4P	O4'-C4'-C3'	3.59	112.49	104.92
2	B	501	C2E	N91-C41-N31	3.50	132.96	125.95
2	B	502	C2E	N91-C41-N31	3.50	132.96	125.95
2	B	501	C2E	C8-N9-C4	3.50	112.59	106.03
2	C	504	C2E	N91-C41-N31	3.50	132.95	125.95
3	C	505	G4P	C2'-C1'-N9	3.50	122.98	113.25
3	C	505	G4P	C8-N9-C4	3.47	112.53	106.03
2	C	502	C2E	C21-N11-C61	-3.45	118.86	125.11
2	B	504	C2E	N91-C41-N31	3.44	132.84	125.95
3	D	503	G4P	C6-C5-N7	3.44	136.55	130.29
3	D	503	G4P	C4'-O4'-C1'	-3.43	101.89	109.47
2	D	502	C2E	N91-C41-N31	3.42	132.78	125.95
2	A	501	C2E	C1'-N9-C4	-3.41	116.42	126.49
2	A	501	C2E	C21-N11-C61	-3.36	119.03	125.11
3	B	503	G4P	C5-C4-N3	-3.35	123.06	128.39
2	B	502	C2E	C8-N9-C4	3.32	112.25	106.03
3	C	505	G4P	N1-C2-N3	-3.31	117.25	123.32
2	C	502	C2E	C2-N1-C6	-3.31	119.10	125.11
2	C	503	C2E	N91-C41-N31	3.29	132.53	125.95
3	A	502	G4P	C6-C5-N7	3.28	136.27	130.29
3	B	503	G4P	C8-N9-C4	3.28	112.17	106.03
2	A	501	C2E	C2-N1-C6	-3.27	119.19	125.11
3	D	503	G4P	C2'-C1'-N9	3.24	122.27	113.25
3	A	502	G4P	C2-N1-C6	-3.24	119.24	125.11
2	B	504	C2E	C8-N9-C4	3.23	112.09	106.03
2	C	503	C2E	C8-N9-C4	3.23	112.08	106.03
3	D	503	G4P	C2-N1-C6	-3.18	119.34	125.11
2	C	502	C2E	N9-C8-N7	-3.18	107.50	113.40
3	C	505	G4P	C5-C4-N3	-3.17	123.34	128.39
2	C	504	C2E	C8-N9-C4	3.17	111.96	106.03
2	C	502	C2E	O6-C6-C5	-3.16	118.18	126.53
3	D	503	G4P	C5'-C4'-C3'	-3.15	103.89	114.38
3	B	503	G4P	O3'-C3'-C4'	-3.15	98.93	110.03
3	B	503	G4P	N1-C2-N3	-3.14	117.58	123.32
2	C	502	C2E	C1'-N9-C4	-3.12	117.26	126.49
3	D	503	G4P	N1-C2-N3	-3.12	117.62	123.32
2	A	501	C2E	N9-C8-N7	-3.11	107.62	113.40
3	B	503	G4P	C2-N1-C6	-3.06	119.56	125.11
2	D	502	C2E	C21-N11-C61	-3.05	119.57	125.11
2	D	502	C2E	C8-N9-C4	3.05	111.75	106.03
2	B	504	C2E	C21-N11-C61	-3.04	119.60	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	G4P	C3'-C2'-C1'	3.03	106.55	99.89
2	C	504	C2E	C2-N1-C6	-3.02	119.64	125.11
3	D	503	G4P	C8-N9-C4	3.00	111.66	106.03
2	A	501	C2E	O6-C6-C5	-3.00	118.61	126.53
2	B	502	C2E	C21-N11-C61	-3.00	119.67	125.11
2	D	502	C2E	C2-N1-C6	-3.00	119.67	125.11
2	C	504	C2E	C21-N11-C61	-2.98	119.70	125.11
3	B	503	G4P	O4'-C4'-C3'	2.97	111.19	104.92
2	C	503	C2E	C2-N1-C6	-2.97	119.72	125.11
2	B	504	C2E	C2-N1-C6	-2.96	119.74	125.11
2	B	501	C2E	C2-N1-C6	-2.94	119.78	125.11
2	C	503	C2E	C21-N11-C61	-2.93	119.80	125.11
3	C	505	G4P	C2-N1-C6	-2.93	119.80	125.11
2	C	502	C2E	O61-C61-C51	-2.93	118.81	126.53
2	A	501	C2E	O61-C61-C51	-2.90	118.87	126.53
2	B	502	C2E	C2-N1-C6	-2.89	119.88	125.11
2	A	501	C2E	N11-C21-N31	-2.89	118.04	123.32
2	B	501	C2E	C21-N11-C61	-2.86	119.92	125.11
2	C	502	C2E	C8-N9-C4	2.86	111.38	106.03
2	C	502	C2E	N1-C2-N3	-2.83	118.14	123.32
2	A	501	C2E	C8-N9-C4	2.82	111.31	106.03
3	A	502	G4P	N1-C2-N3	-2.82	118.17	123.32
2	B	504	C2E	C51-C61-N11	2.79	120.36	113.25
3	B	503	G4P	O2'-C2'-C3'	2.78	118.97	111.19
2	B	501	C2E	C8-N7-C5	2.76	109.18	104.26
2	B	501	C2E	C51-C61-N11	2.75	120.26	113.25
2	D	502	C2E	C51-C61-N11	2.72	120.17	113.25
3	A	502	G4P	C8-N9-C4	2.72	111.12	106.03
2	C	504	C2E	C5-C6-N1	2.71	120.14	113.25
2	D	502	C2E	C5-C6-N1	2.70	120.11	113.25
2	C	503	C2E	C51-C61-N11	2.69	120.10	113.25
3	B	503	G4P	C2'-C1'-N9	2.68	120.70	113.25
3	C	505	G4P	O2'-C2'-C1'	2.67	119.31	110.10
2	B	502	C2E	C8-N7-C5	2.67	109.01	104.26
2	B	502	C2E	C5-C6-N1	2.67	120.04	113.25
2	A	501	C2E	N1-C2-N3	-2.66	118.46	123.32
2	B	502	C2E	C51-C61-N11	2.64	119.98	113.25
2	C	504	C2E	O6-C6-C5	-2.63	119.58	126.53
2	C	502	C2E	N11-C21-N31	-2.63	118.51	123.32
2	D	502	C2E	C8-N7-C5	2.63	108.94	104.26
2	B	504	C2E	C5-C6-N1	2.61	119.91	113.25
2	B	501	C2E	O61-C61-C51	-2.60	119.66	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C2E	C5-C6-N1	2.60	119.87	113.25
2	C	503	C2E	C8-N7-C5	2.59	108.88	104.26
2	C	504	C2E	C51-C61-N11	2.59	119.83	113.25
2	B	502	C2E	O6-C6-C5	-2.58	119.72	126.53
2	B	502	C2E	O61-C61-C51	-2.57	119.74	126.53
3	A	502	G4P	O6-C6-C5	-2.57	119.74	126.53
2	B	504	C2E	O61-C61-C51	-2.56	119.78	126.53
2	A	501	C2E	N91-C81-N71	-2.56	108.66	113.40
2	C	503	C2E	O6-C6-C5	-2.55	119.79	126.53
2	C	503	C2E	C5-C6-N1	2.55	119.75	113.25
2	B	504	C2E	O6-C6-C5	-2.55	119.81	126.53
2	C	504	C2E	O61-C61-C51	-2.54	119.82	126.53
2	B	501	C2E	O6-C6-C5	-2.52	119.89	126.53
2	B	501	C2E	C1A-N91-C41	-2.49	119.14	126.49
2	D	502	C2E	O61-C61-C51	-2.48	119.99	126.53
2	C	504	C2E	C8-N7-C5	2.47	108.66	104.26
2	C	503	C2E	C1A-N91-C41	-2.47	119.20	126.49
3	C	505	G4P	C6-C5-C4	-2.45	115.14	118.83
2	B	504	C2E	C8-N7-C5	2.44	108.61	104.26
2	B	504	C2E	C1A-N91-C41	-2.44	119.28	126.49
3	C	505	G4P	O2'-C2'-C3'	2.42	117.96	111.19
3	D	503	G4P	O4'-C4'-C3'	2.42	110.01	104.92
2	D	502	C2E	C1A-N91-C41	-2.41	119.36	126.49
3	D	503	G4P	O6-C6-C5	-2.40	120.20	126.53
3	C	505	G4P	O3'-C3'-C4'	-2.39	101.59	110.03
2	C	503	C2E	O61-C61-C51	-2.39	120.23	126.53
3	D	503	G4P	C8-N7-C5	2.38	108.50	104.26
2	D	502	C2E	C81-N71-C51	2.37	108.49	104.26
2	D	502	C2E	O6-C6-C5	-2.37	120.28	126.53
3	B	503	G4P	C6-C5-C4	-2.36	115.28	118.83
2	D	502	C2E	C1'-N9-C8	2.36	133.43	126.73
3	B	503	G4P	O6-C6-C5	-2.34	120.35	126.53
2	B	504	C2E	C81-N71-C51	2.34	108.43	104.26
3	C	505	G4P	O6-C6-C5	-2.34	120.37	126.53
2	C	504	C2E	C81-N71-C51	2.33	108.41	104.26
2	B	502	C2E	C81-N71-C51	2.33	108.41	104.26
2	C	502	C2E	N91-C81-N71	-2.33	109.09	113.40
2	A	501	C2E	O5A-P11-O11	2.30	118.06	108.94
2	C	503	C2E	C81-N71-C51	2.30	108.36	104.26
2	B	501	C2E	C81-N71-C51	2.26	108.28	104.26
2	B	502	C2E	C81-N91-C41	2.24	110.23	106.03
2	B	502	C2E	C1A-N91-C41	-2.24	119.86	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	C2E	O3'-P11-O11	2.21	116.88	109.81
2	C	504	C2E	C81-N91-C41	2.21	110.17	106.03
3	A	502	G4P	C8-N7-C5	2.21	108.19	104.26
2	A	501	C2E	C3'-C2'-C1'	2.21	104.74	99.89
2	A	501	C2E	O3'-P11-O11	2.21	116.85	109.81
2	B	501	C2E	C81-N91-C41	2.20	110.15	106.03
2	B	504	C2E	C5'-C4'-C3'	-2.20	107.05	114.38
2	C	503	C2E	C1'-N9-C8	2.20	132.97	126.73
3	D	503	G4P	C2'-C3'-C4'	2.19	107.08	103.24
3	C	505	G4P	C4-C5-N7	-2.19	107.20	110.67
2	A	501	C2E	C3A-C2A-C1A	2.19	104.70	99.89
2	C	502	C2E	O5A-P11-O11	2.18	117.58	108.94
2	D	502	C2E	O3'-P11-O11	2.18	116.78	109.81
3	C	505	G4P	C8-N7-C5	2.18	108.14	104.26
3	D	503	G4P	N9-C4-N3	2.17	130.30	125.95
3	B	503	G4P	C4-C5-N7	-2.15	107.27	110.67
2	B	504	C2E	C81-N91-C41	2.14	110.04	106.03
2	C	502	C2E	C3'-C2'-C1'	2.13	104.57	99.89
2	D	502	C2E	C3'-C2'-C1'	2.12	104.55	99.89
2	C	504	C2E	C1A-N91-C41	-2.12	120.23	126.49
2	D	502	C2E	O5A-P11-O11	2.11	117.31	108.94
2	C	503	C2E	C81-N91-C41	2.11	109.97	106.03
2	C	504	C2E	C1'-N9-C8	2.10	132.69	126.73
2	C	503	C2E	C3A-C2A-C1A	2.09	104.48	99.89
2	C	502	C2E	O3'-P11-O11	2.08	116.44	109.81
2	D	502	C2E	C81-N91-C41	2.06	109.89	106.03
3	B	503	G4P	C8-N7-C5	2.06	107.93	104.26
2	D	502	C2E	C3A-C2A-C1A	2.05	104.40	99.89
2	B	502	C2E	C1'-N9-C8	2.04	132.53	126.73
2	A	501	C2E	N21-C21-N11	2.03	121.04	116.76
2	B	501	C2E	O5A-P11-O11	2.02	116.95	108.94
3	D	503	G4P	C4-C5-N7	-2.02	107.47	110.67
2	C	502	C2E	N21-C21-N11	2.01	121.01	116.76
2	C	504	C2E	O3'-P11-O11	2.01	116.22	109.81
2	B	501	C2E	C3A-C2A-C1A	2.00	104.30	99.89

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	G4P	C3'-O3'-PC-O3C
3	B	503	G4P	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	B	503	G4P	C5'-O5'-PA-O1A
3	B	503	G4P	C5'-O5'-PA-O2A
3	C	505	G4P	C5'-O5'-PA-O3A
3	C	505	G4P	C5'-O5'-PA-O2A
3	C	505	G4P	C2'-C3'-O3'-PC
3	D	503	G4P	C5'-O5'-PA-O3A
3	D	503	G4P	C5'-O5'-PA-O1A
3	D	503	G4P	C5'-O5'-PA-O2A
3	A	502	G4P	O4'-C4'-C5'-O5'
3	A	502	G4P	C2'-C3'-O3'-PC
3	B	503	G4P	C2'-C3'-O3'-PC
3	D	503	G4P	C2'-C3'-O3'-PC
3	A	502	G4P	C3'-C4'-C5'-O5'
3	D	503	G4P	O4'-C4'-C5'-O5'
3	D	503	G4P	C3'-C4'-C5'-O5'
3	C	505	G4P	C3'-C4'-C5'-O5'
3	A	502	G4P	C4'-C3'-O3'-PC
3	A	502	G4P	C4'-C5'-O5'-PA
2	A	501	C2E	C3A-O3A-P1-O1P
2	C	503	C2E	C3A-O3A-P1-O1P
2	D	502	C2E	C3A-O3A-P1-O1P
3	A	502	G4P	C3'-O3'-PC-O1C
2	A	501	C2E	C5'-O5'-P1-O1P
2	B	501	C2E	C5'-O5'-P1-O1P
2	B	502	C2E	C5'-O5'-P1-O1P
2	B	502	C2E	C5A-O5A-P11-O11
2	B	504	C2E	C5'-O5'-P1-O1P
2	C	502	C2E	C5'-O5'-P1-O1P
2	C	503	C2E	C5'-O5'-P1-O1P
2	C	504	C2E	C5'-O5'-P1-O1P
2	C	504	C2E	C5A-O5A-P11-O11
2	D	502	C2E	C5'-O5'-P1-O1P
2	D	502	C2E	C5A-O5A-P11-O21
2	D	502	C2E	C5A-O5A-P11-O11
3	D	503	G4P	C4'-C5'-O5'-PA
3	A	502	G4P	PD-O3C-PC-O2C
3	D	503	G4P	C4'-C3'-O3'-PC
3	A	502	G4P	PB-O3A-PA-O2A
3	B	503	G4P	C3'-C4'-C5'-O5'
3	B	503	G4P	C4'-C3'-O3'-PC
2	A	501	C2E	C3A-O3A-P1-O2P
2	A	501	C2E	C3'-O3'-P11-O11

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Mol	Chain	Res	Type	Atoms
2	B	501	C2E	C3A-O3A-P1-O1P
2	B	501	C2E	C3'-O3'-P11-O11
2	B	502	C2E	C3'-O3'-P11-O11
2	B	504	C2E	C3'-O3'-P11-O11
2	C	502	C2E	C3'-O3'-P11-O11
2	C	503	C2E	C3A-O3A-P1-O2P
2	C	503	C2E	C3'-O3'-P11-O11
2	C	504	C2E	C3'-O3'-P11-O11
2	D	502	C2E	C3A-O3A-P1-O2P
3	A	502	G4P	C3'-O3'-PC-O2C
3	A	502	G4P	PD-O3C-PC-O1C
3	B	503	G4P	PB-O3A-PA-O2A

There are no ring outliers.

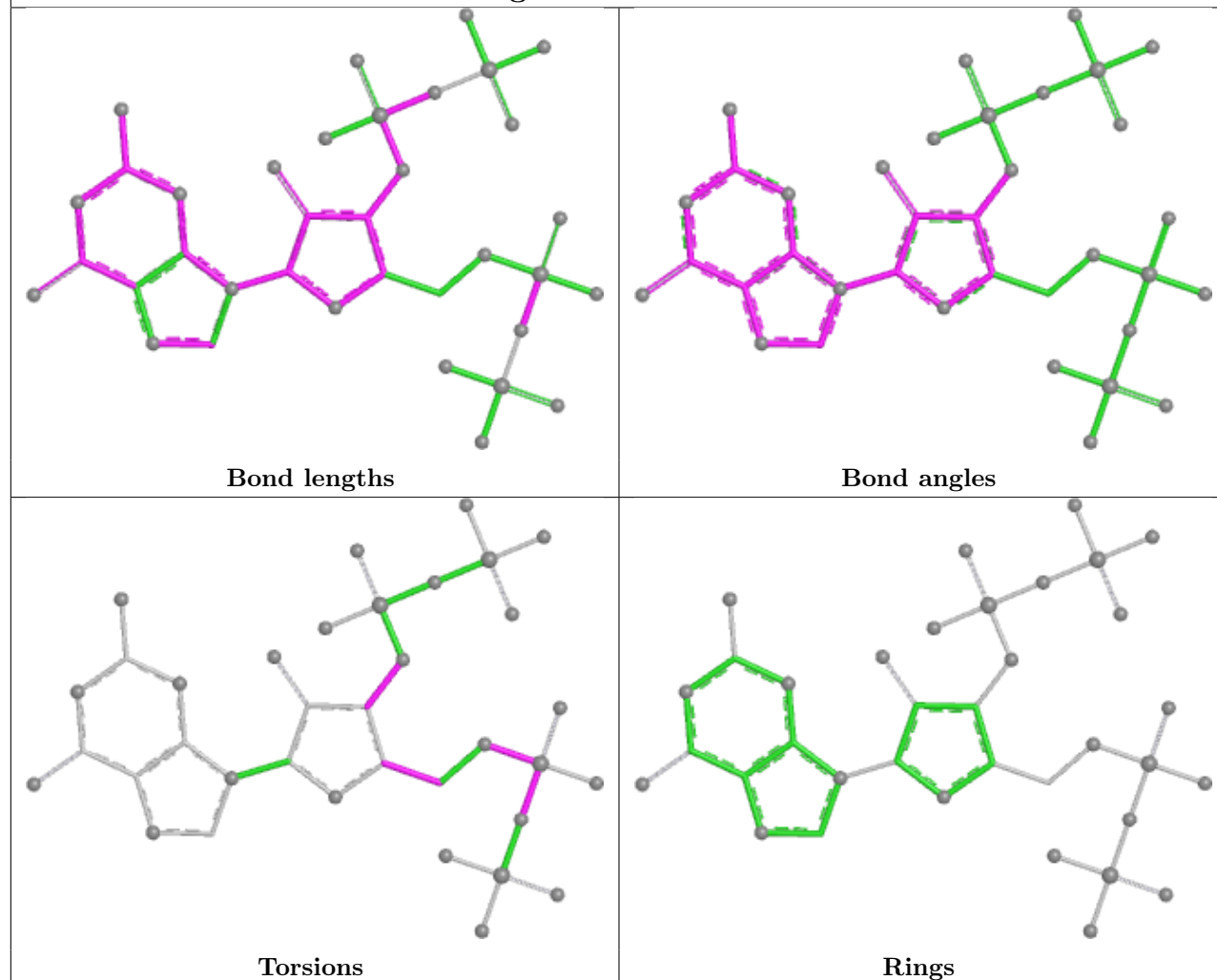
11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	G4P	4	0
2	D	502	C2E	3	0
2	C	504	C2E	1	0
3	C	505	G4P	3	0
2	B	504	C2E	2	0
3	D	503	G4P	4	0
2	C	502	C2E	2	0
3	A	502	G4P	2	0
2	C	503	C2E	1	0
2	B	502	C2E	1	0
2	A	501	C2E	2	0

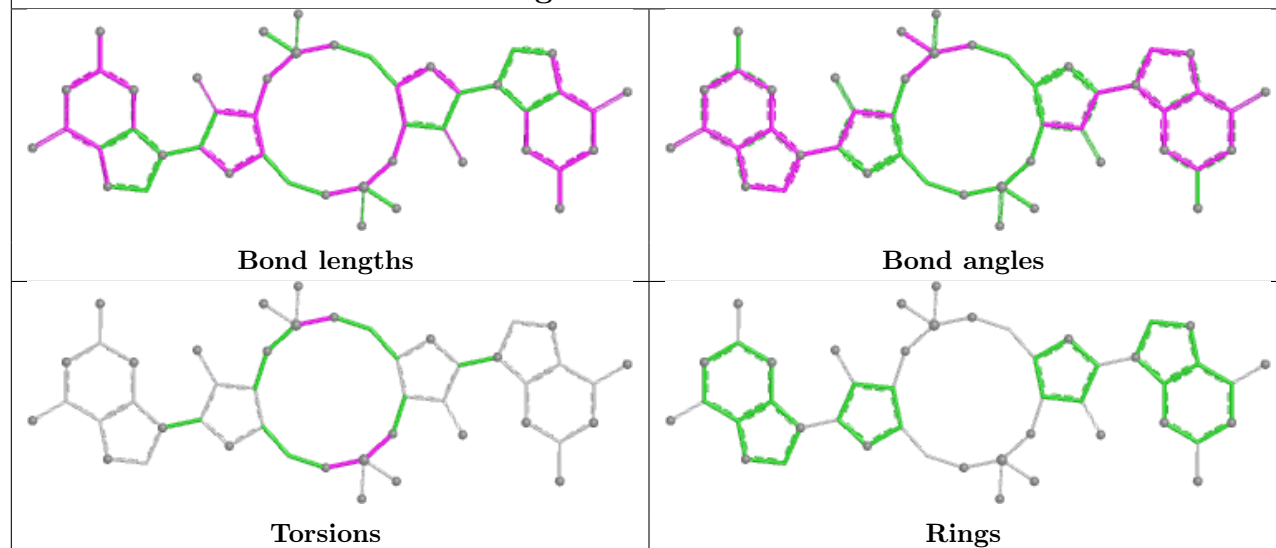
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand G4P B 503

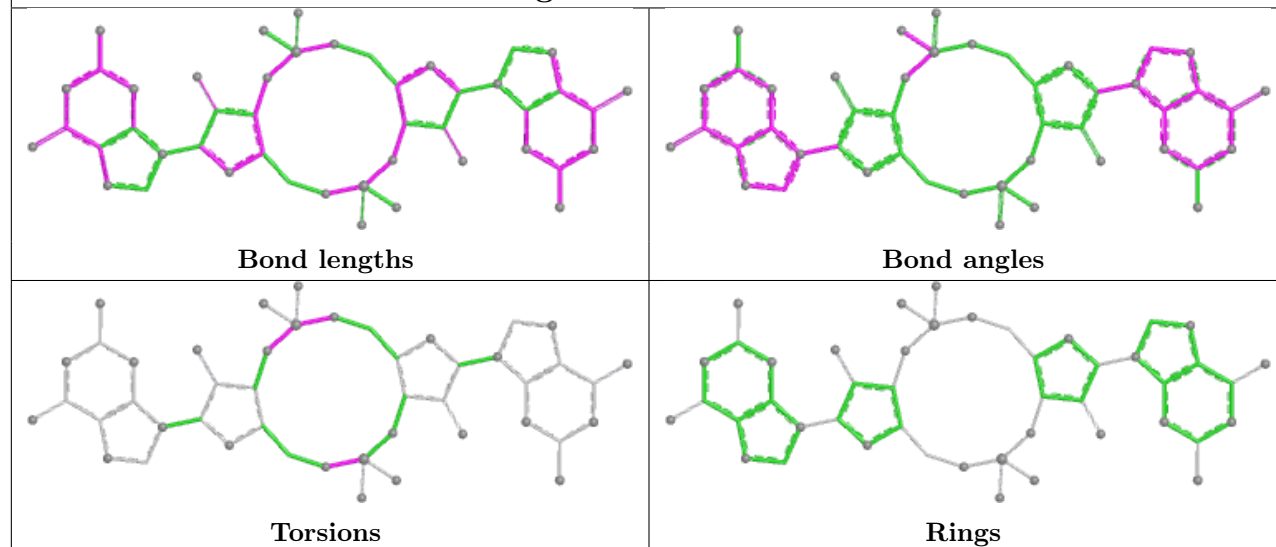


## Ligand C2E D 502

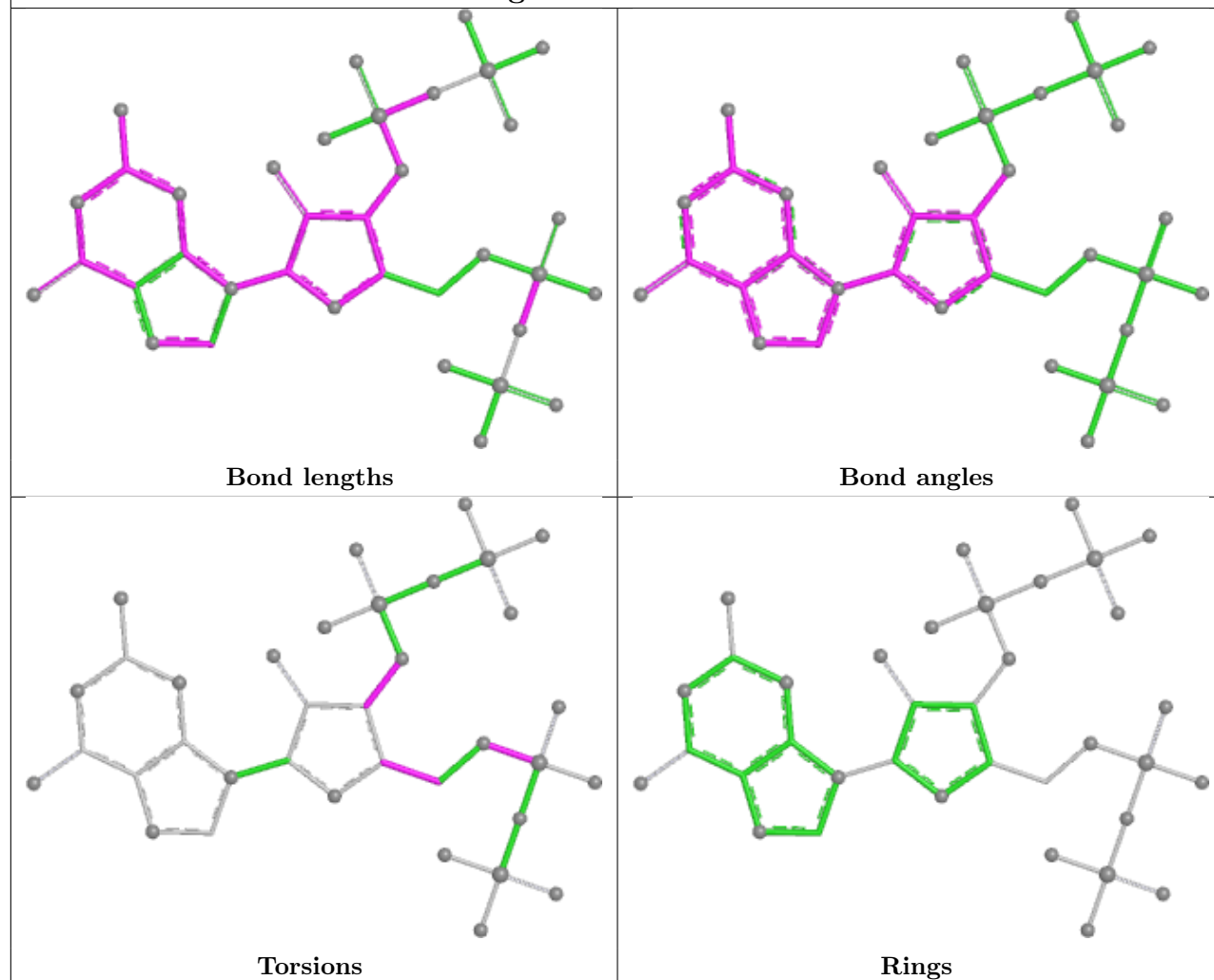




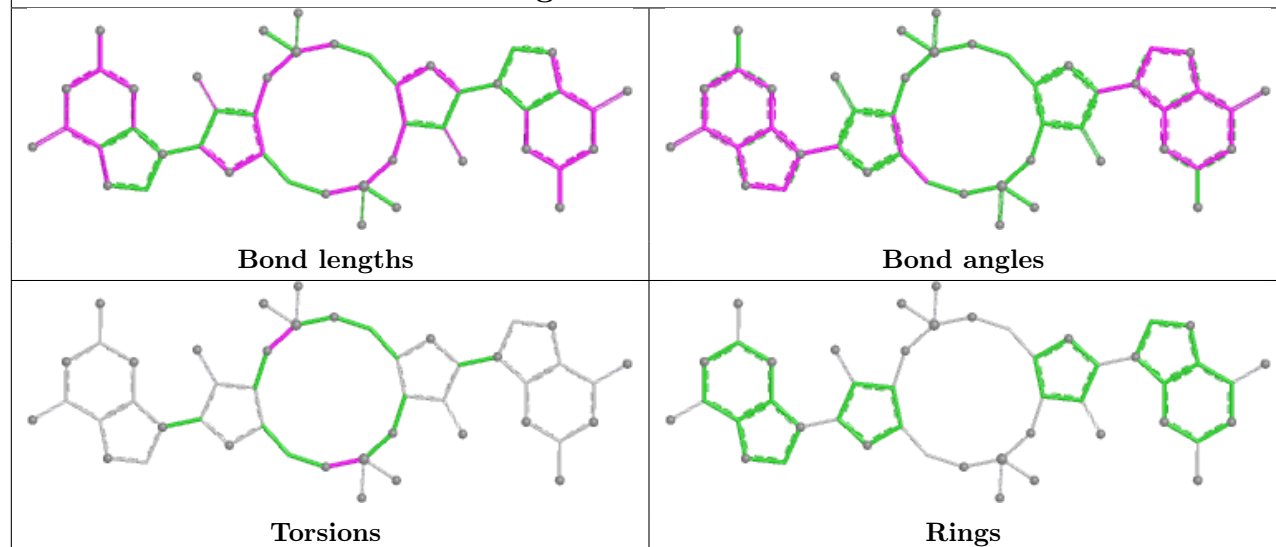
## Ligand C2E C 504



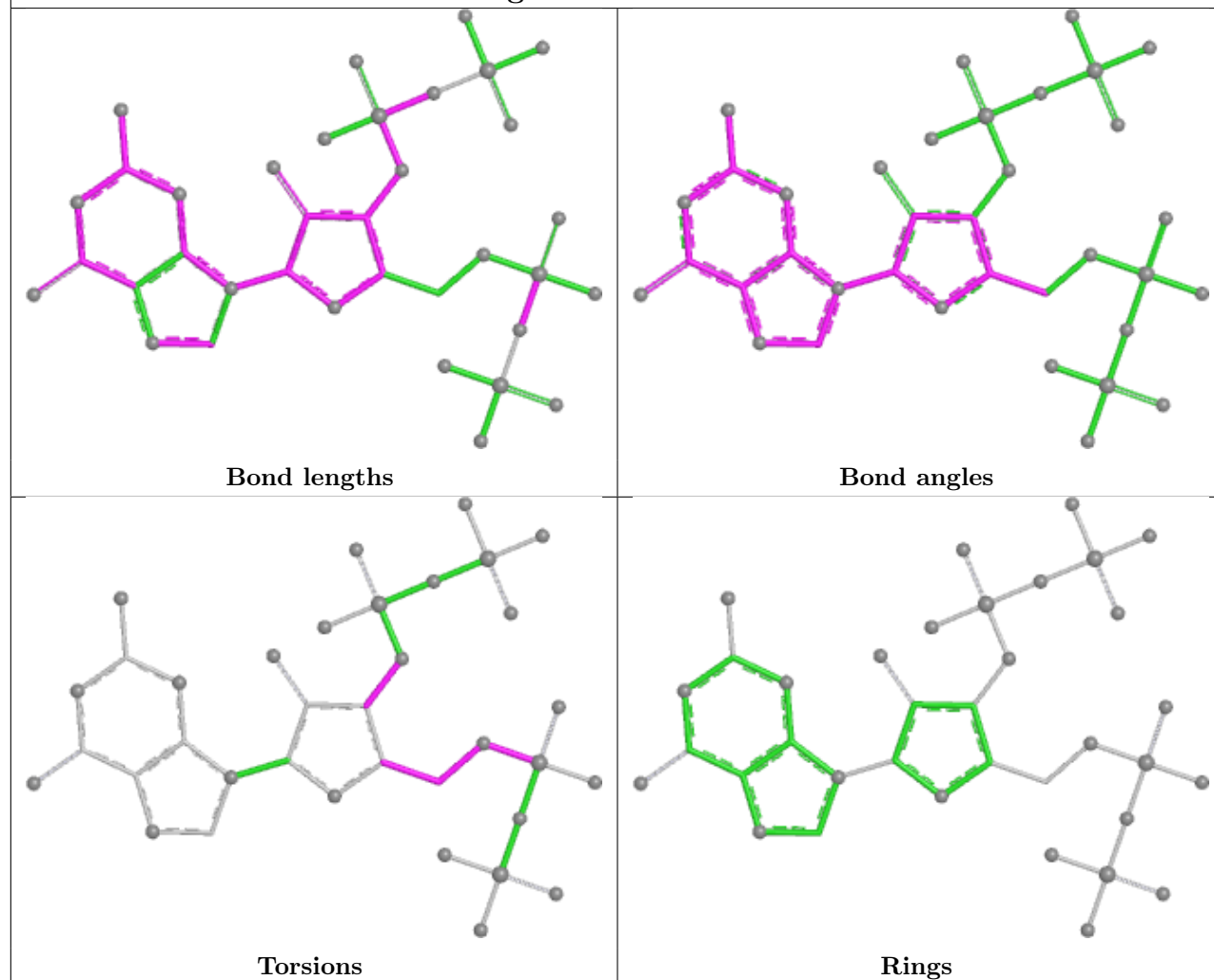
## Ligand G4P C 505



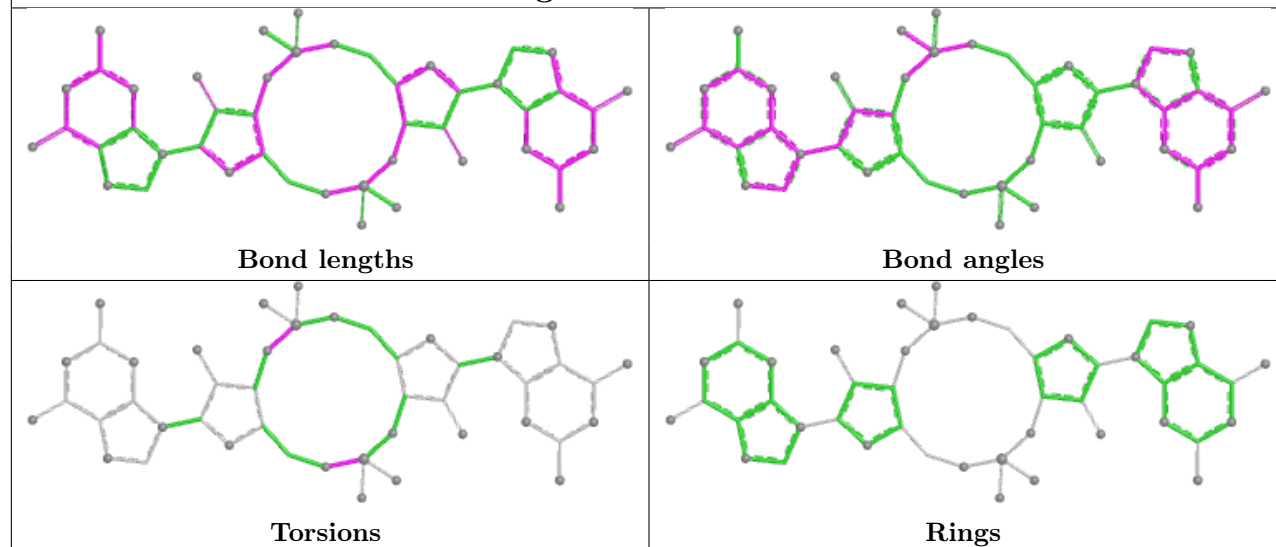
## Ligand C2E B 504



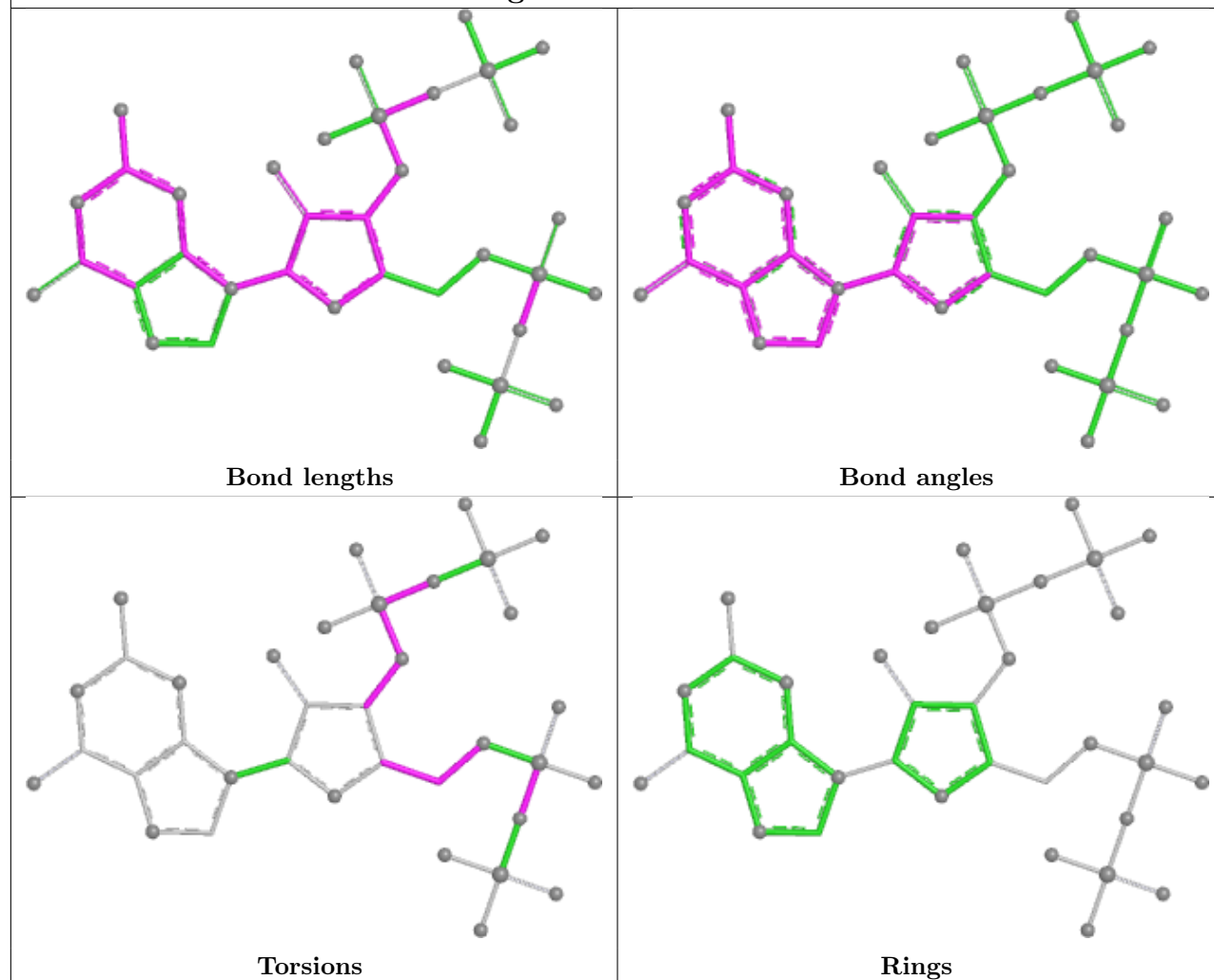
## Ligand G4P D 503



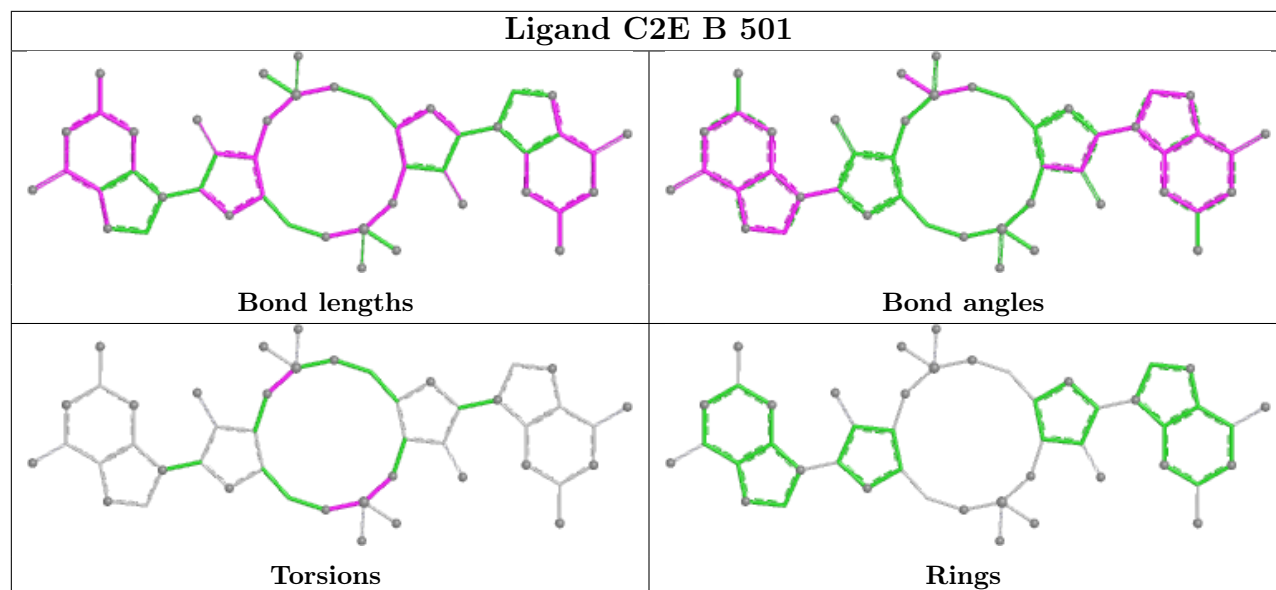
## Ligand C2E C 502



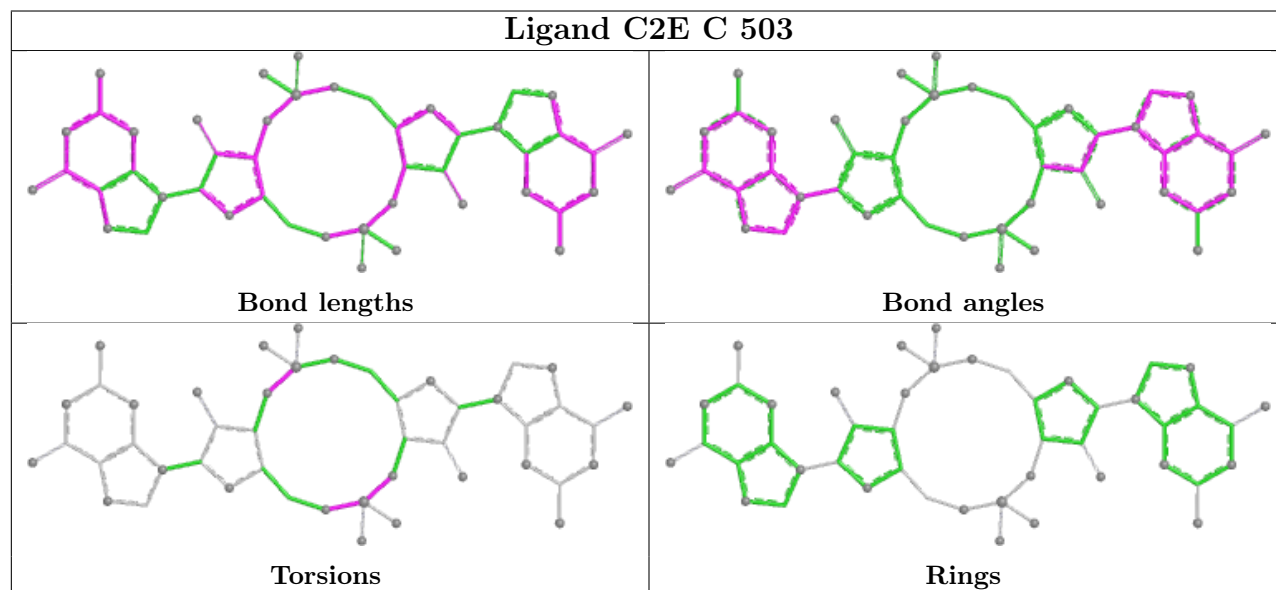
## Ligand G4P A 502



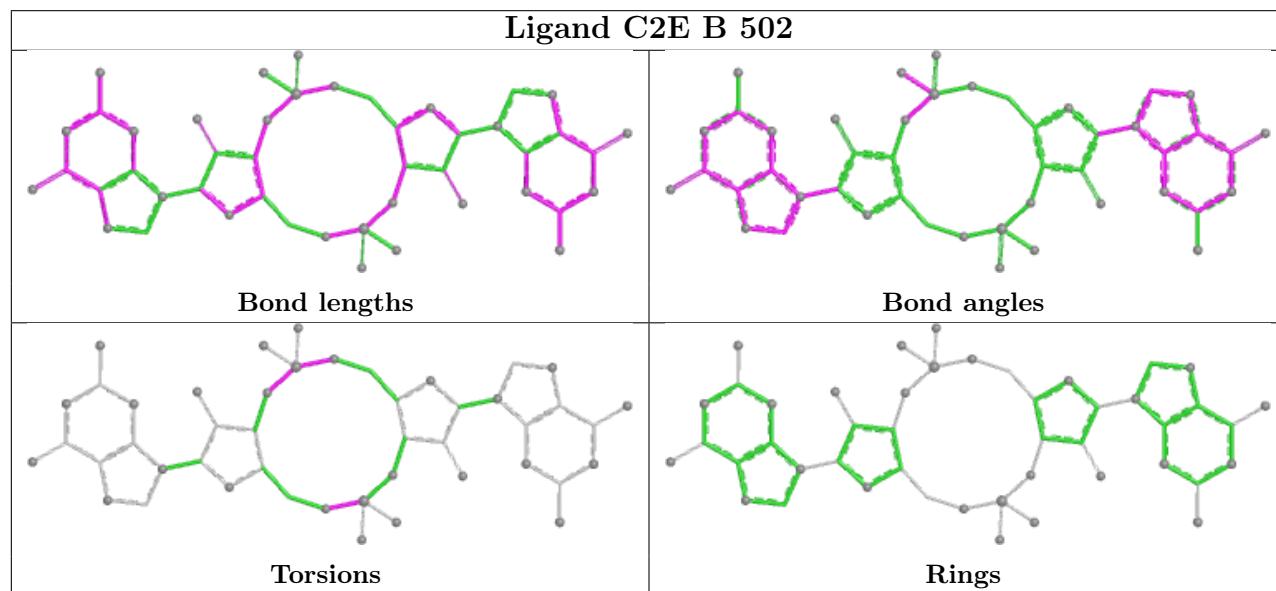
## Ligand C2E B 501

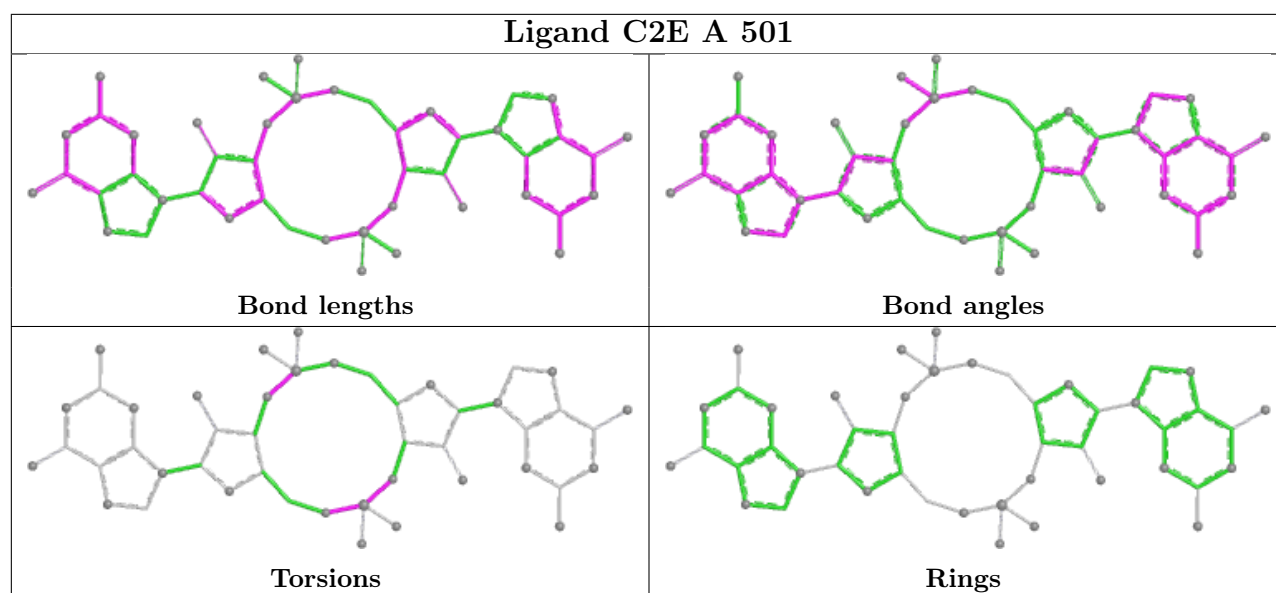


## Ligand C2E C 503



## Ligand C2E B 502





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	447/454 (98%)	-0.34	4 (0%) 81 75	40, 71, 100, 127	5 (1%)
1	B	441/454 (97%)	-0.25	3 (0%) 84 79	42, 83, 114, 136	6 (1%)
1	C	439/454 (96%)	-0.29	3 (0%) 84 79	44, 77, 104, 128	3 (0%)
1	D	447/454 (98%)	-0.27	5 (1%) 78 71	46, 74, 110, 133	3 (0%)
All	All	1774/1816 (97%)	-0.29	15 (0%) 82 77	40, 77, 110, 136	17 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	VAL	4.5
1	D	160	ASP	3.9
1	C	281	ASN	3.6
1	D	285	SER	3.4
1	C	452	LYS	3.3
1	A	3	ALA	3.2
1	B	451	GLY	3.1
1	A	140	GLY	2.8
1	B	3	ALA	2.4
1	A	283	ASP	2.4
1	C	135	SER	2.4
1	D	453	ALA	2.3
1	A	453	ALA	2.2
1	B	424	GLY	2.2
1	D	284	HIS	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

There are no oligosaccharides in this entry.

## 6.4 Ligands

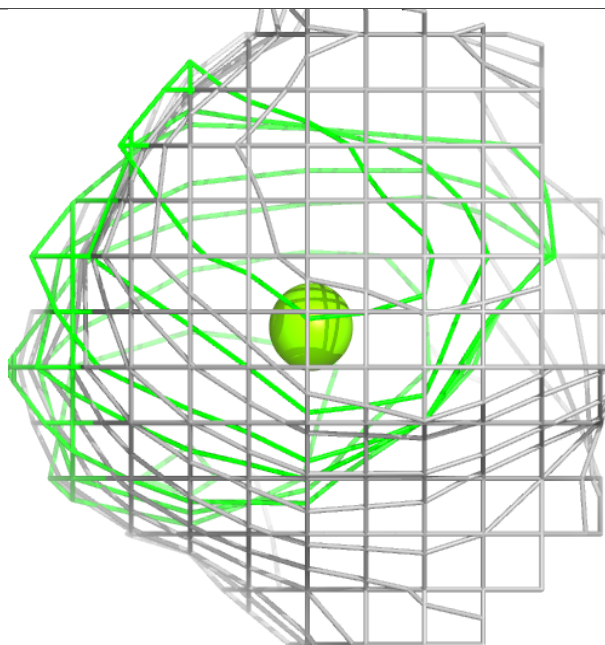
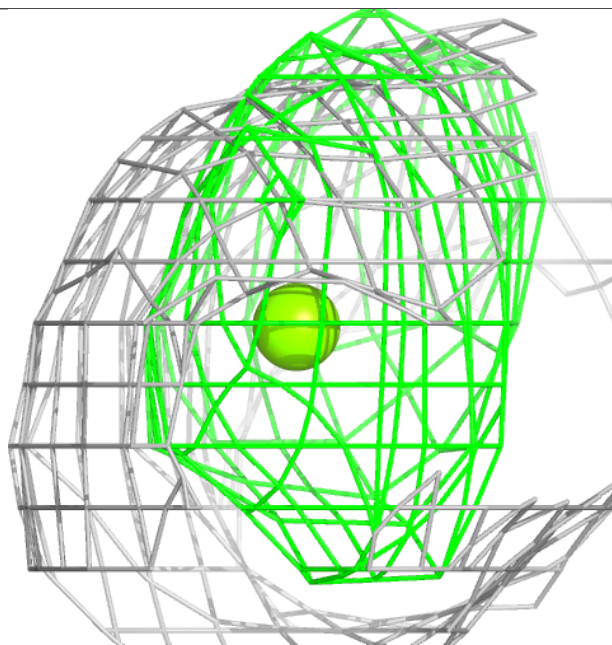
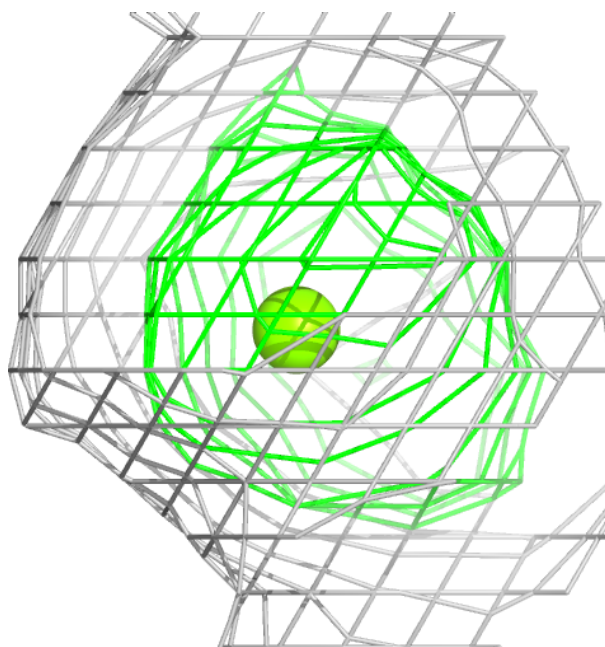
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	D	501	1/1	0.79	0.24	92,92,92,92	0
3	G4P	A	502	36/36	0.82	0.14	58,89,140,150	0
3	G4P	D	503	36/36	0.85	0.12	66,88,141,179	0
3	G4P	B	503	36/36	0.88	0.12	62,82,128,147	0
3	G4P	C	505	36/36	0.88	0.11	67,89,185,196	0
4	MG	B	506	1/1	0.91	0.18	81,81,81,81	0
4	MG	B	505	1/1	0.91	0.14	81,81,81,81	0
2	C2E	D	502	46/46	0.92	0.07	72,87,96,103	0
4	MG	C	501	1/1	0.93	0.16	73,73,73,73	0
2	C2E	B	504	46/46	0.93	0.07	69,88,96,109	0
2	C2E	C	503	46/46	0.94	0.06	55,69,76,86	0
4	MG	A	504	1/1	0.94	0.05	65,65,65,65	0
2	C2E	C	504	46/46	0.94	0.06	52,67,74,89	0
4	MG	A	503	1/1	0.95	0.17	70,70,70,70	0
2	C2E	A	501	46/46	0.95	0.06	43,61,70,82	0
2	C2E	B	501	46/46	0.95	0.06	59,67,78,84	0
2	C2E	C	502	46/46	0.96	0.05	40,57,64,71	0
4	MG	C	506	1/1	0.96	0.09	82,82,82,82	0
2	C2E	B	502	46/46	0.96	0.06	53,61,72,79	0
4	MG	D	504	1/1	0.97	0.04	82,82,82,82	0

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

**Electron density around MG D 501:**

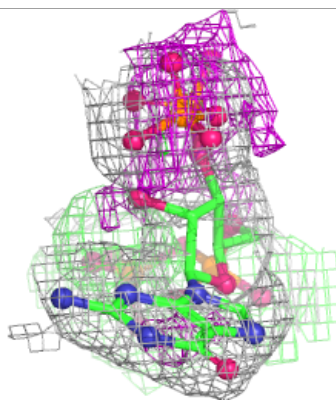
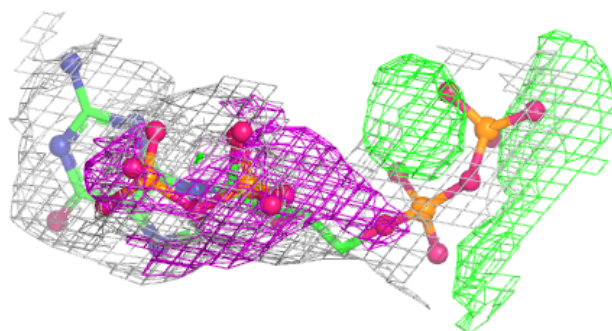
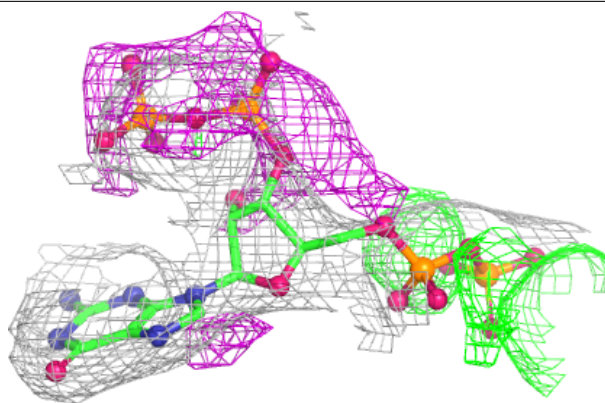
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



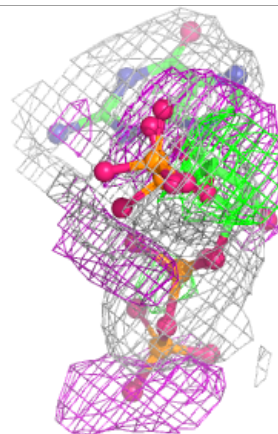
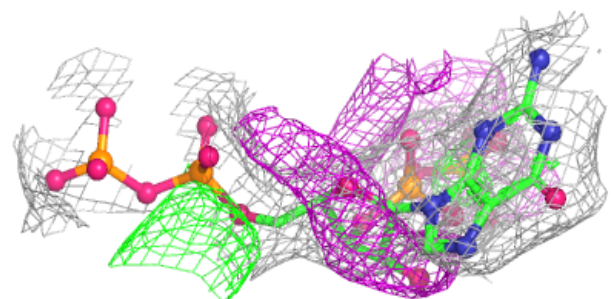
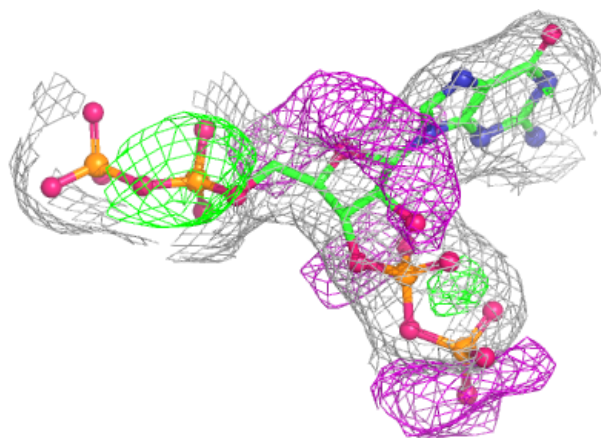


**Electron density around G4P A 502:**

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

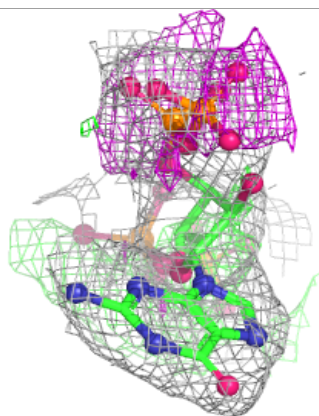
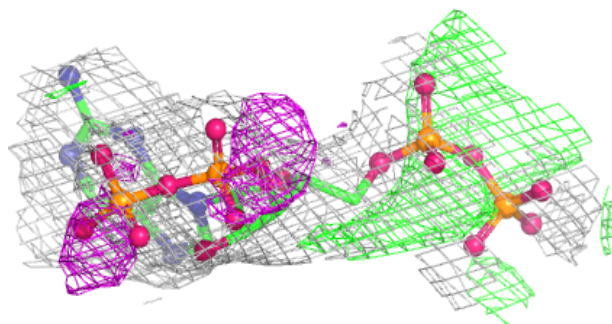
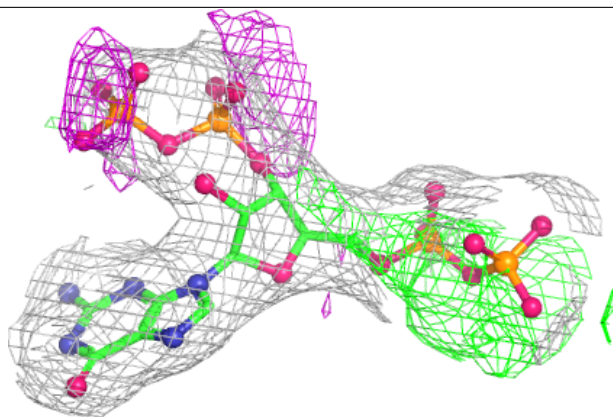
**Electron density around G4P D 503:**

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

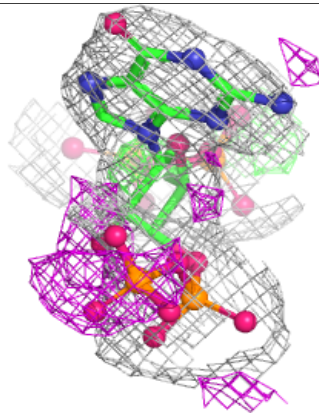
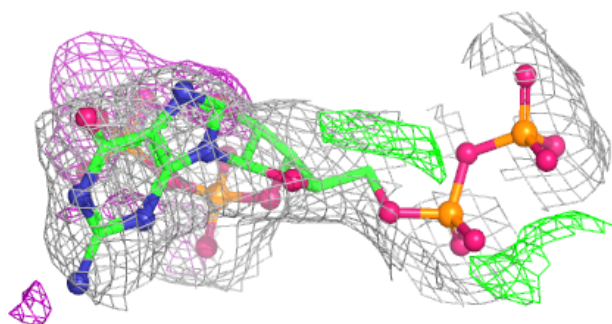
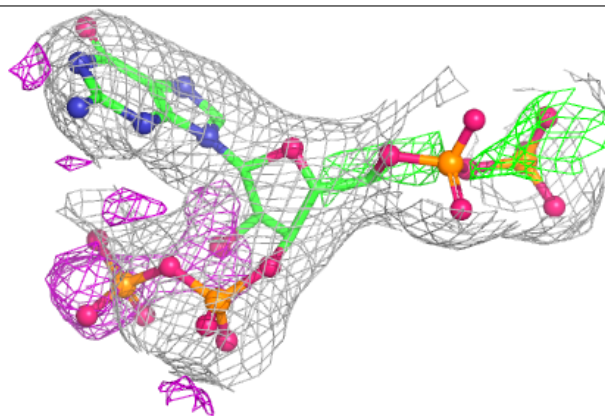


**Electron density around G4P B 503:**

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

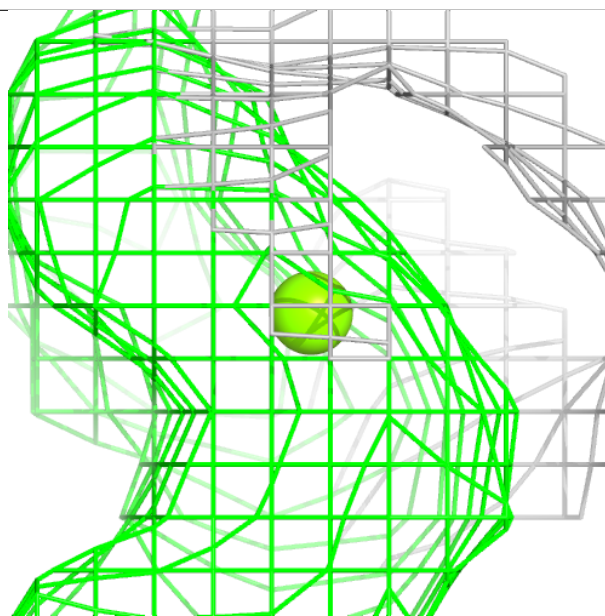
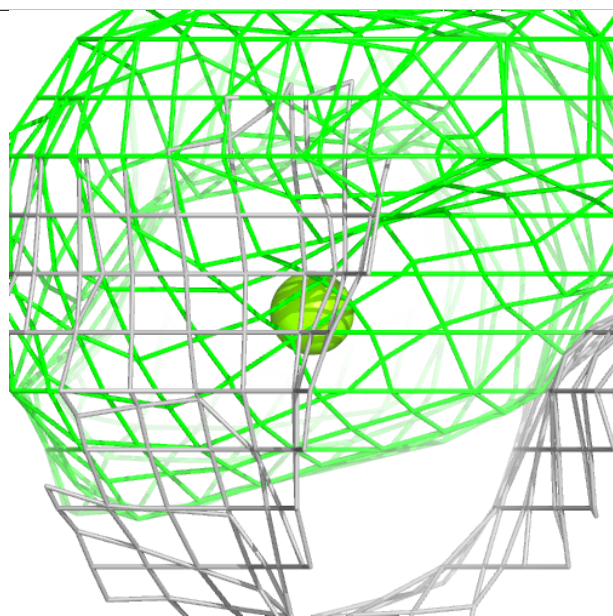
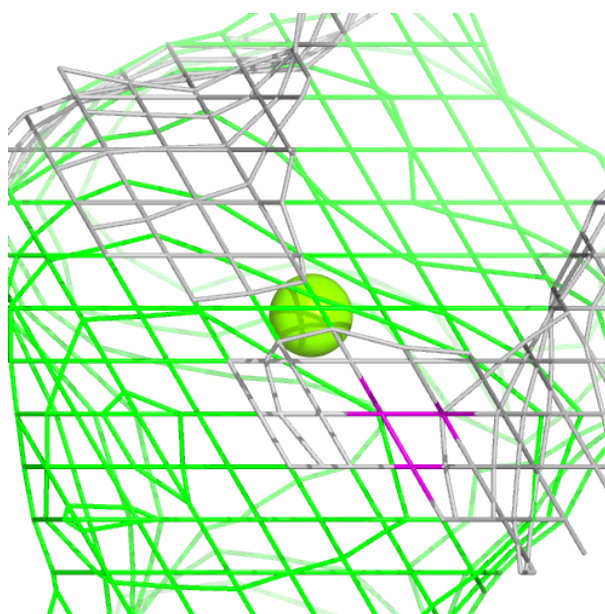
**Electron density around G4P C 505:**

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



**Electron density around MG B 506:**

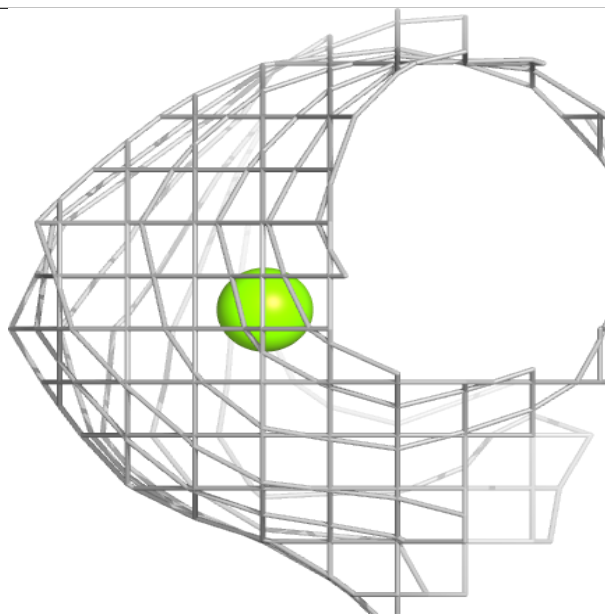
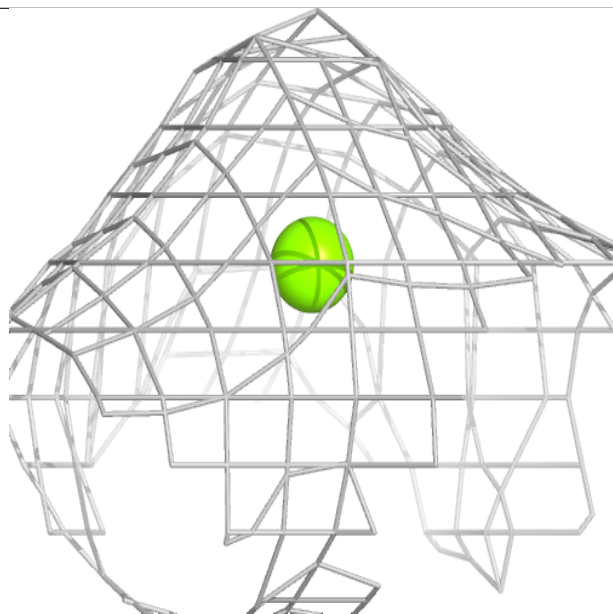
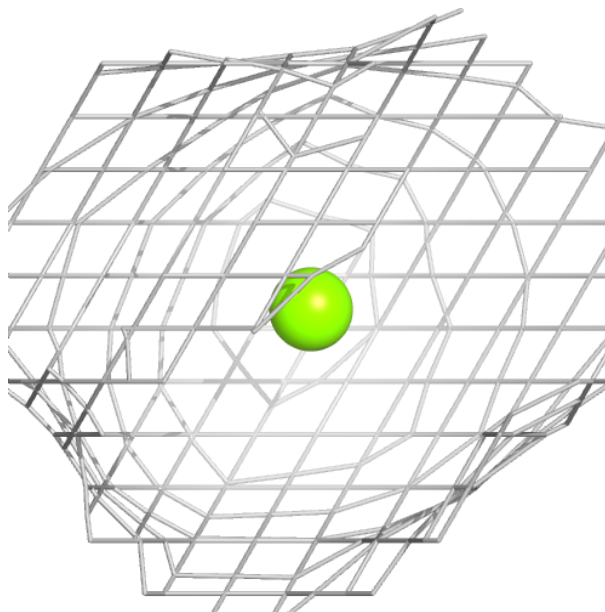
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





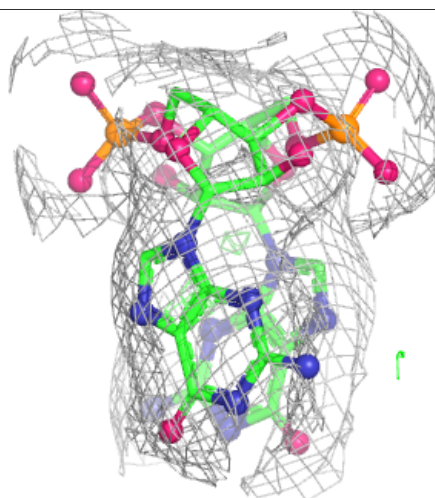
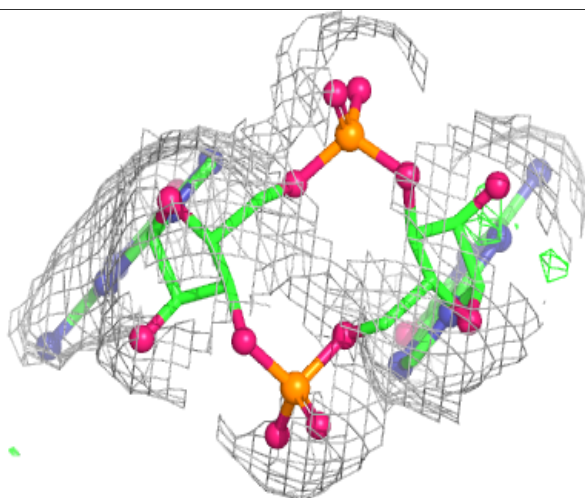
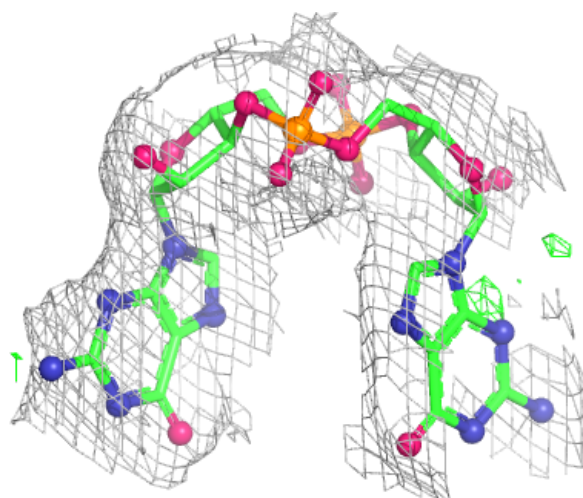
**Electron density around MG B 505:**

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



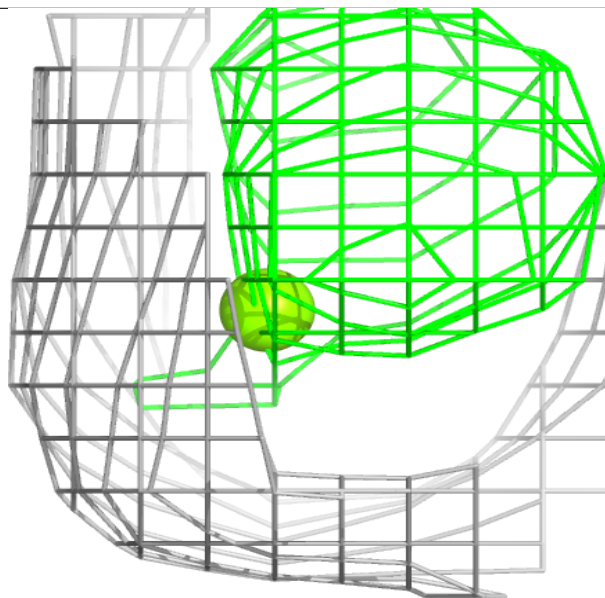
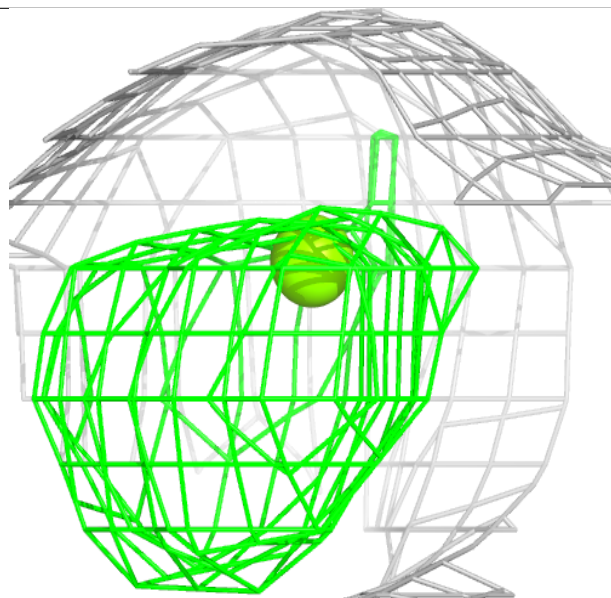
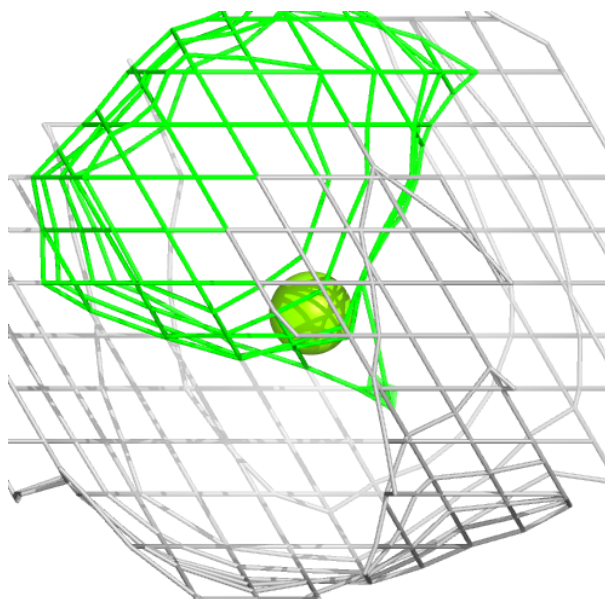
**Electron density around C2E D 502:**

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



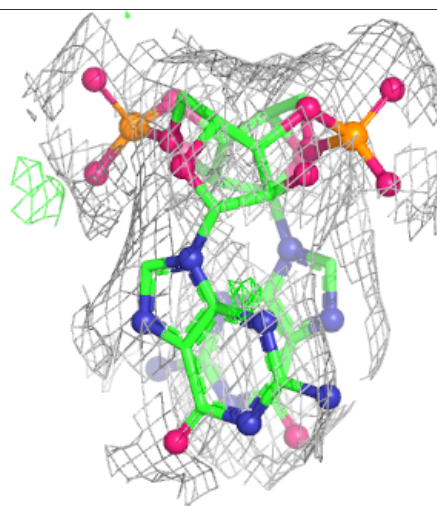
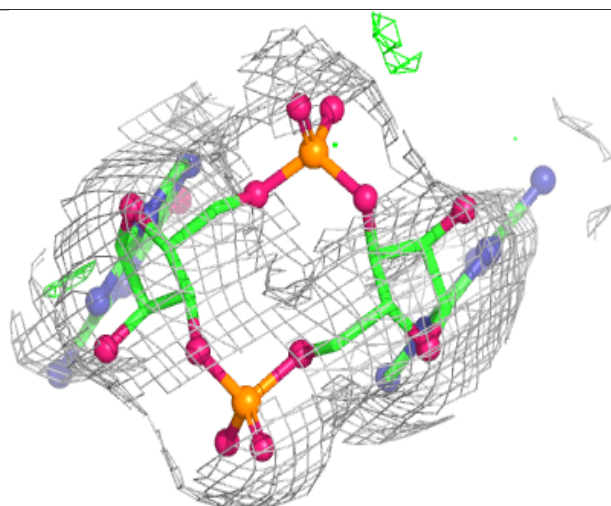
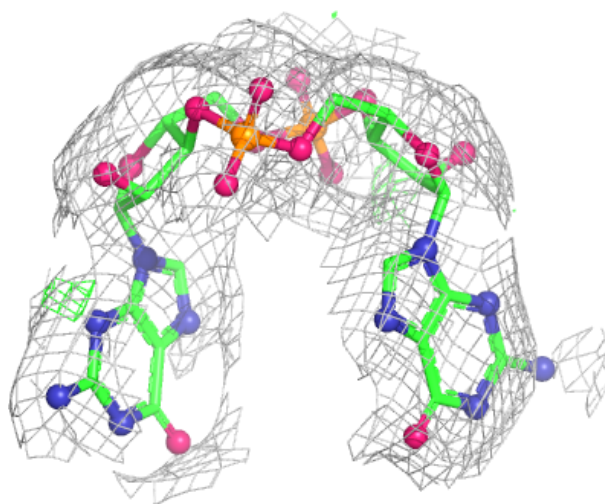
**Electron density around MG C 501:**

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



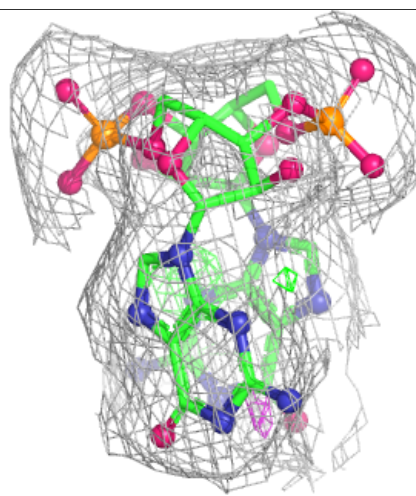
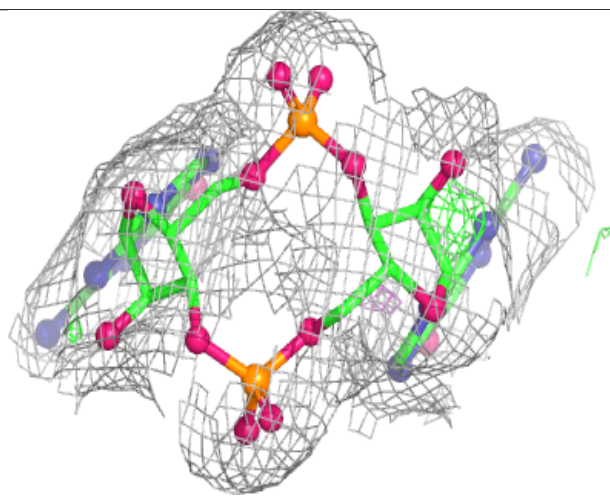
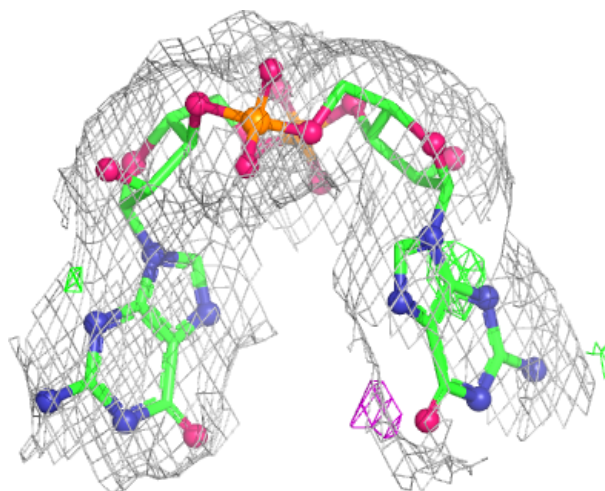
**Electron density around C2E B 504:**

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



**Electron density around C2E C 503:**

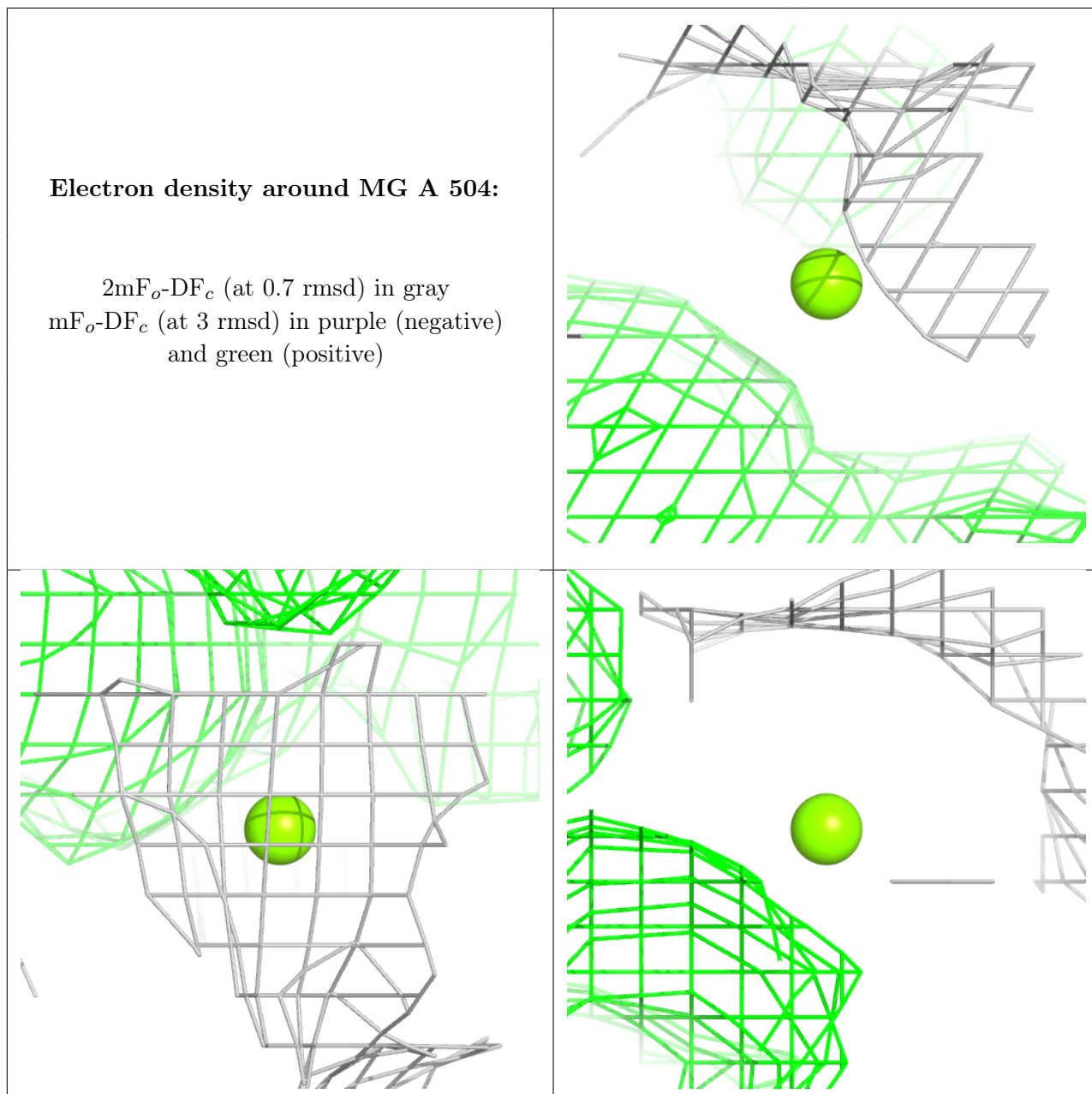
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





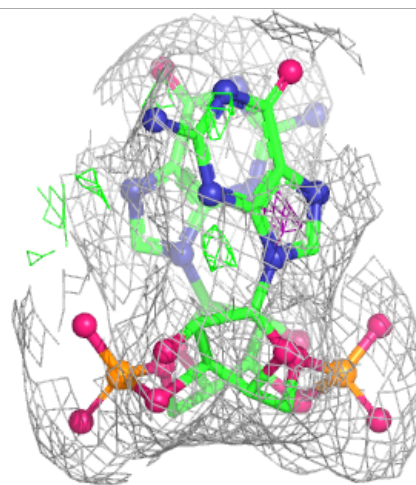
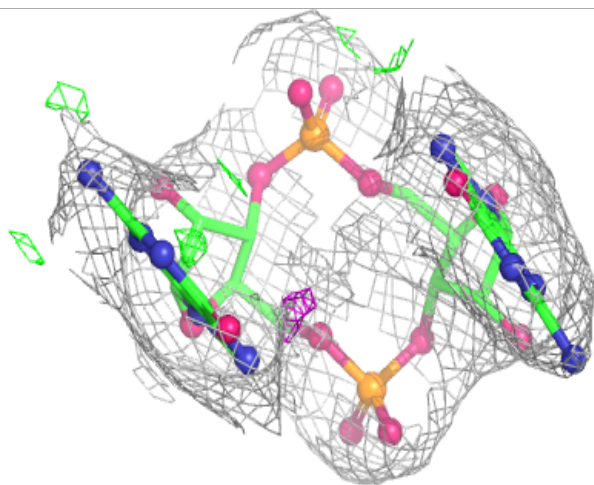
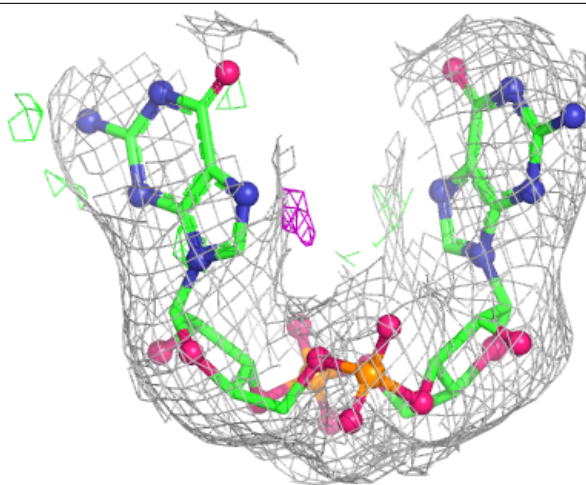
**Electron density around MG A 504:**

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



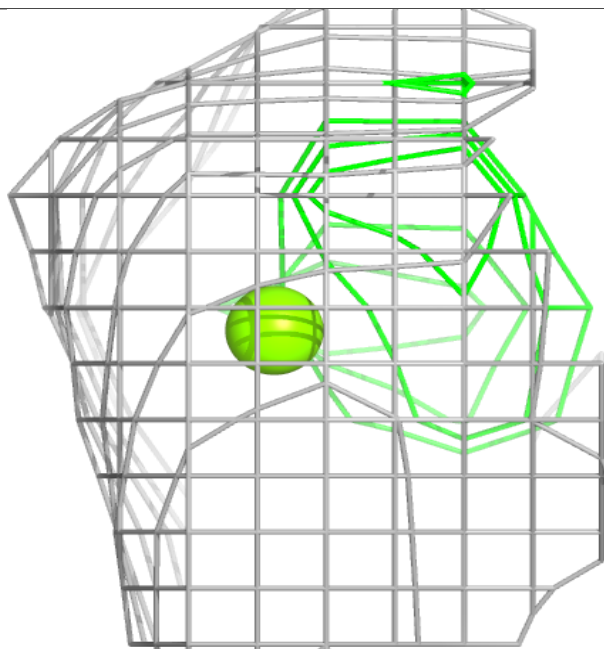
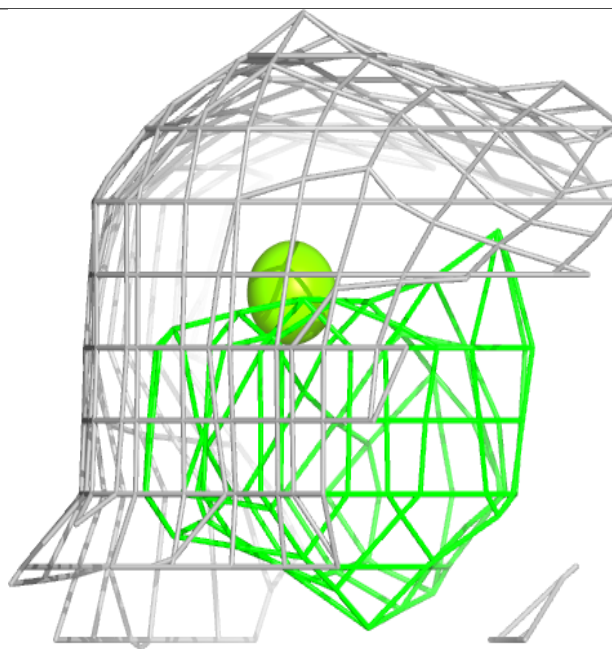
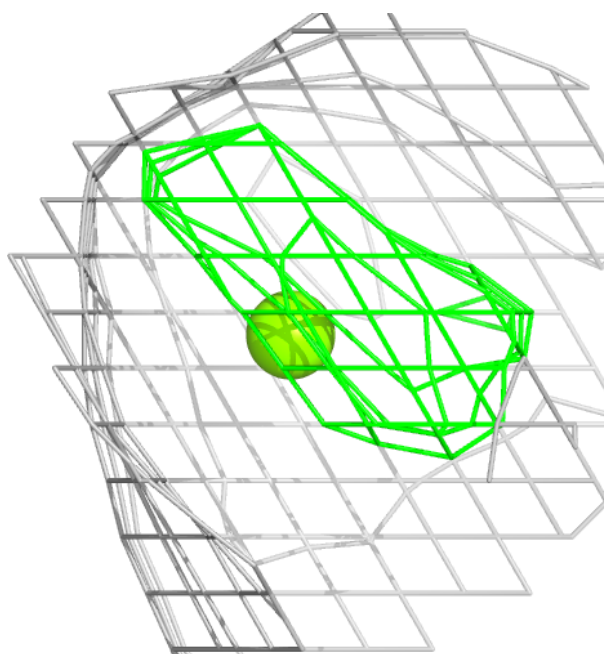
**Electron density around C2E C 504:**

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



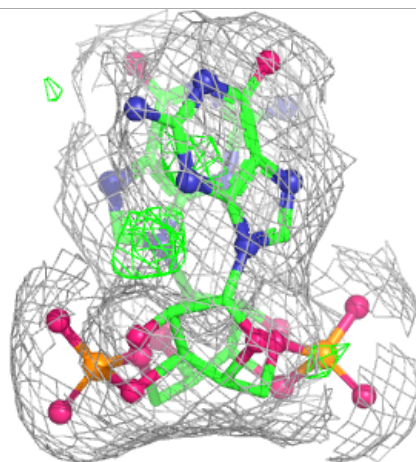
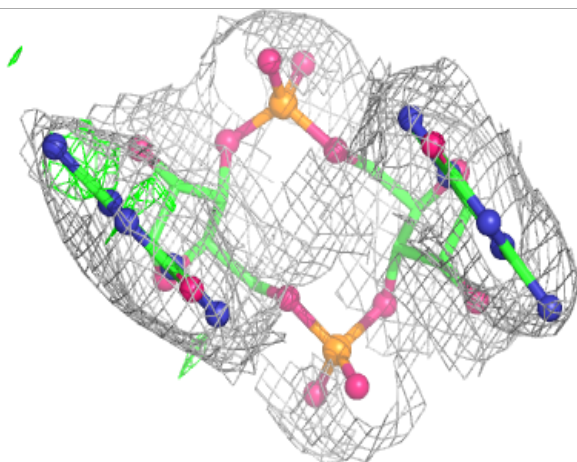
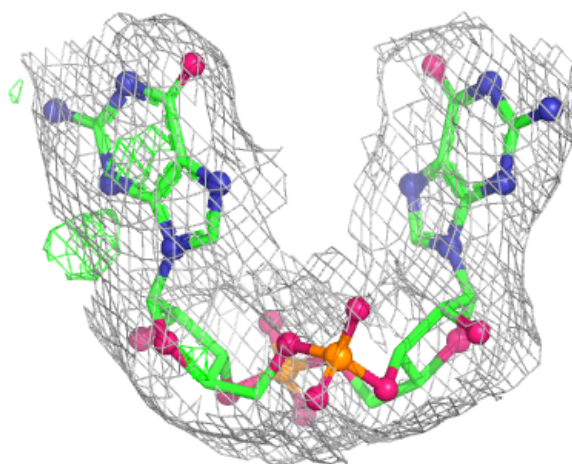
**Electron density around MG A 503:**

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



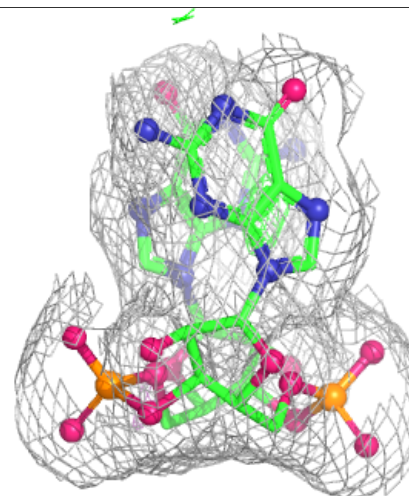
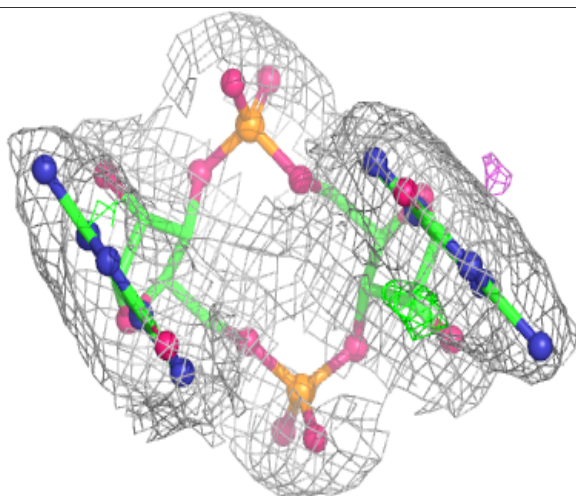
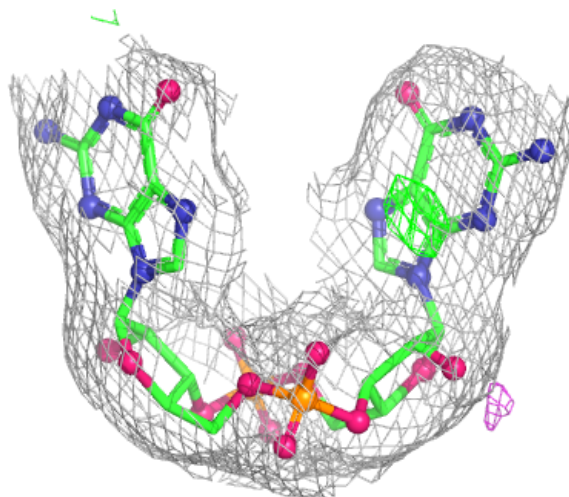
**Electron density around C2E A 501:**

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



**Electron density around C2E B 501:**

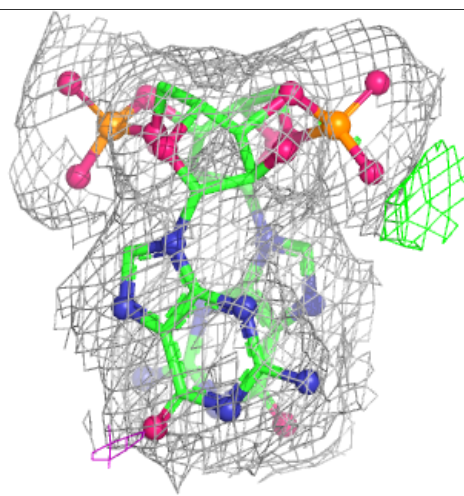
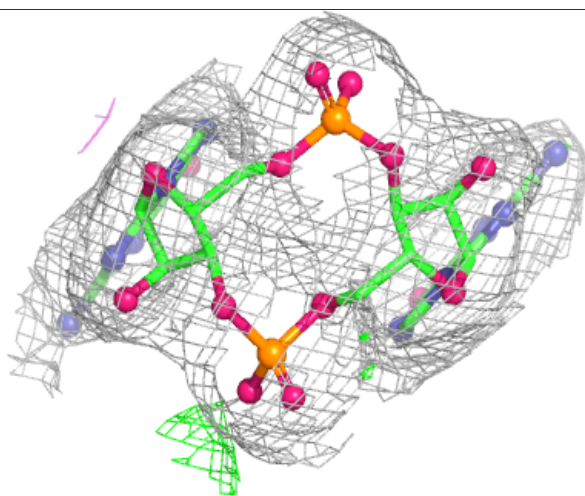
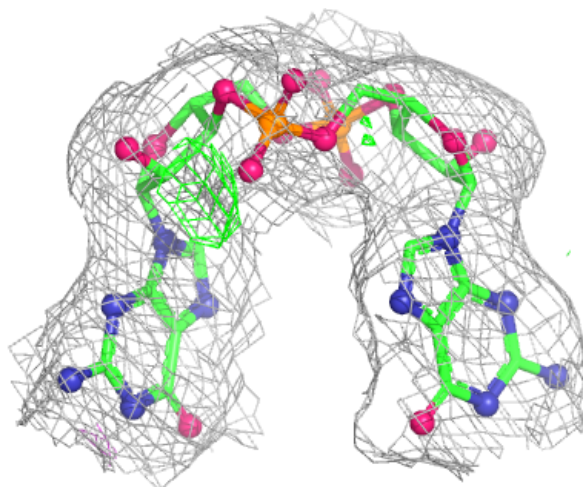
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





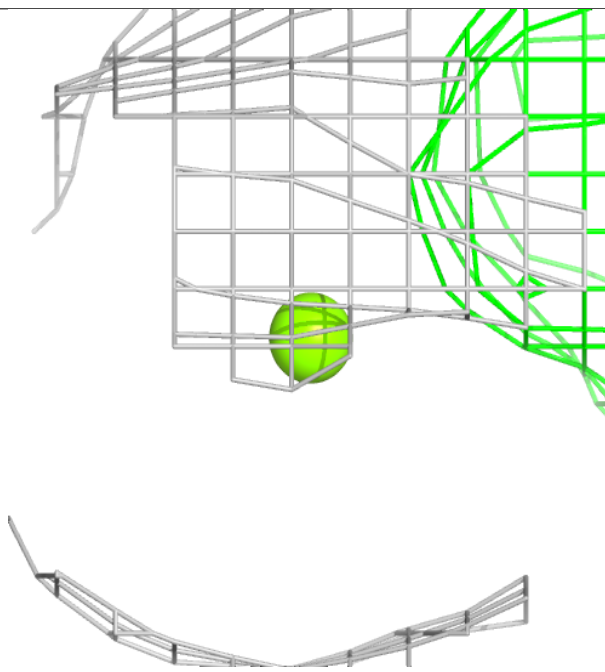
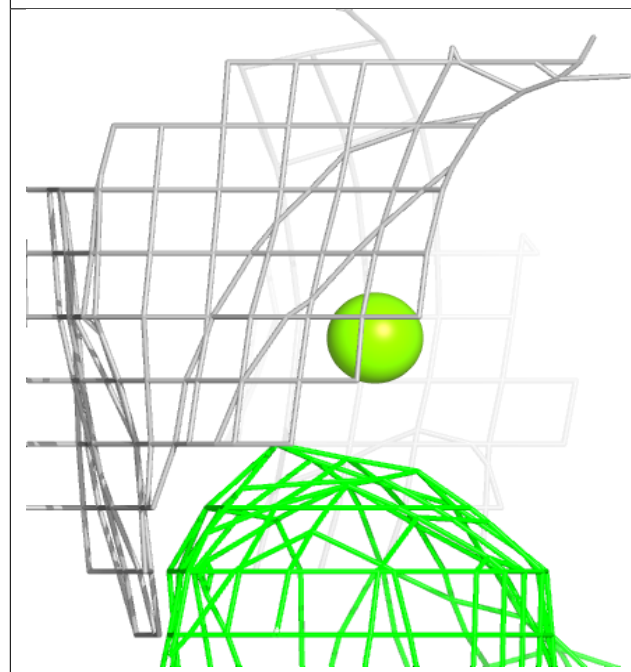
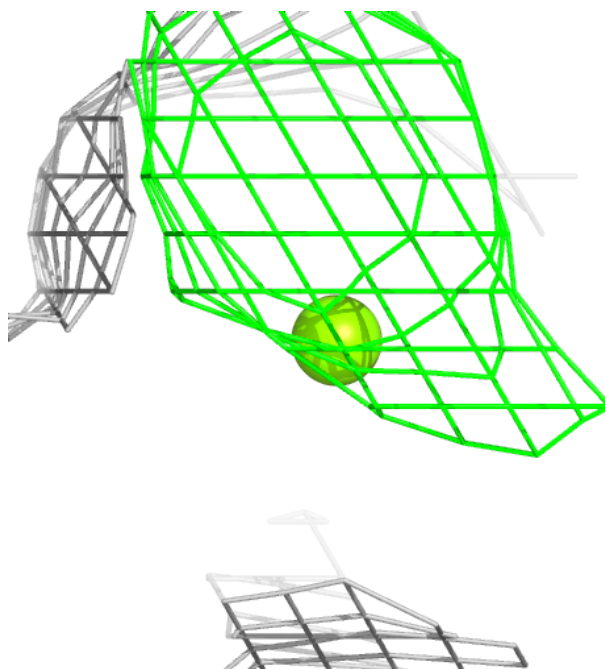
**Electron density around C2E C 502:**

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



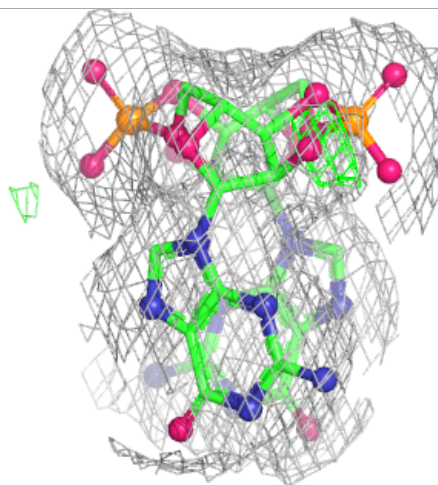
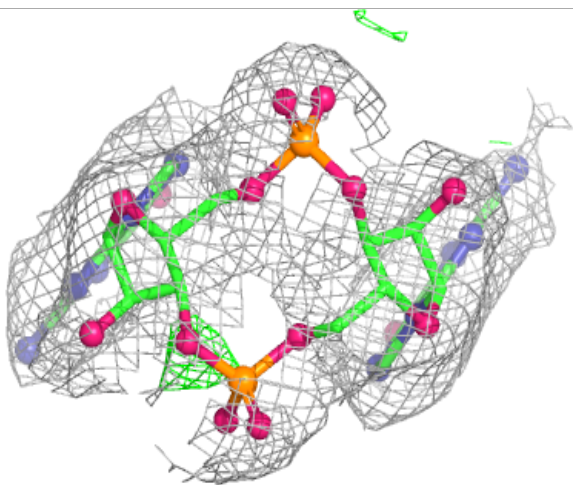
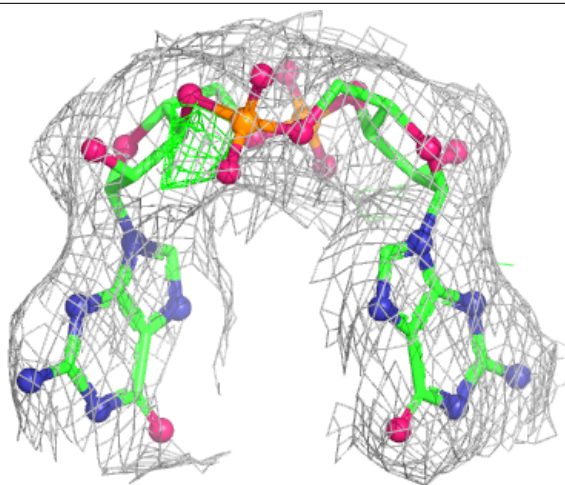
**Electron density around MG C 506:**

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

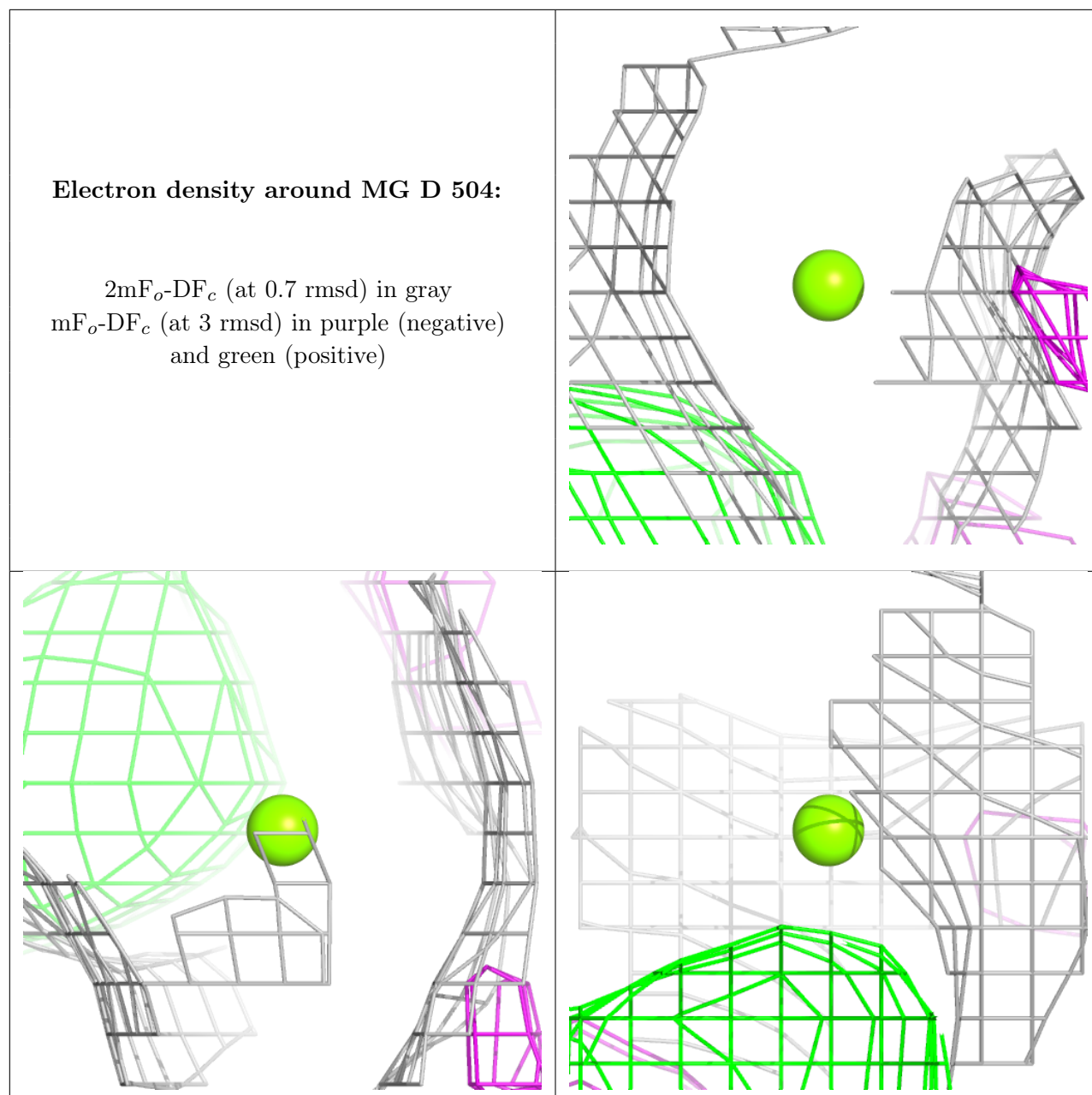


**Electron density around C2E B 502:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.