



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2022 – 12:42 am BST

PDB ID : 7P9J
Title : Prim-Pol Domain of CRISPR-associated Prim-Pol (CAPP) from *Marinitoga* sp. 1137 - Primer Initiation Complex
Authors : Li, A.W.H.; Doherty, A.J.
Deposited on : 2021-07-27
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

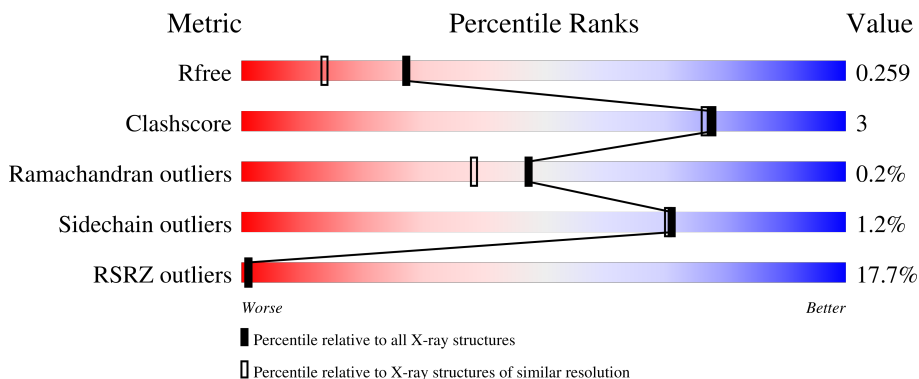
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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	219	
1	B	219	
1	C	219	
2	D	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5813 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 TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1810	1170	307	330	3	0	1	0
1	B	218	1793	1161	305	323	4	0	1	0
1	C	215	1777	1151	302	321	3	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	ALA	variant	UNP H2J4R1
A	148	GLN	HIS	variant	UNP H2J4R1
A	152	ASN	ASP	variant	UNP H2J4R1
A	214	THR	ILE	variant	UNP H2J4R1
A	319	ASN	ASP	variant	UNP H2J4R1
B	110	GLY	ALA	variant	UNP H2J4R1
B	148	GLN	HIS	variant	UNP H2J4R1
B	152	ASN	ASP	variant	UNP H2J4R1
B	214	THR	ILE	variant	UNP H2J4R1
B	319	ASN	ASP	variant	UNP H2J4R1
C	110	GLY	ALA	variant	UNP H2J4R1
C	148	GLN	HIS	variant	UNP H2J4R1
C	152	ASN	ASP	variant	UNP H2J4R1
C	214	THR	ILE	variant	UNP H2J4R1
C	319	ASN	ASP	variant	UNP H2J4R1

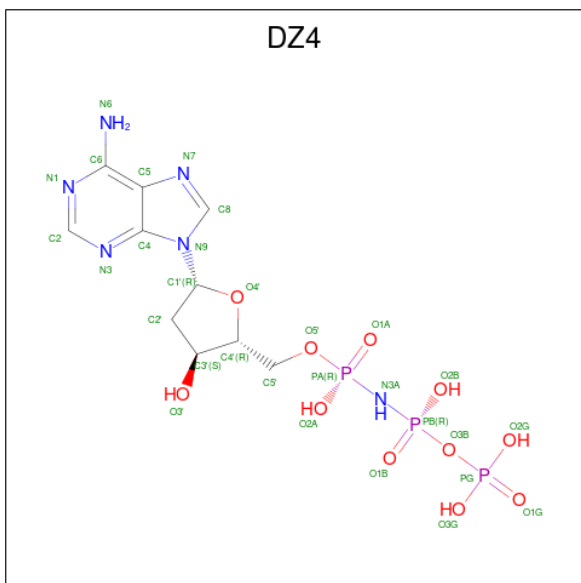
- Molecule 2 is a DNA chain called Templating strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	6	120	59	25	31	5	0	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Co 2 2	0	0
3	B	3	Total Co 3 3	0	0
3	C	2	Total Co 2 2	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 30 10 6 11 3	0	0
4	B	1	Total C N O P 30 10 6 11 3	0	0
4	B	1	Total C N O P 30 10 6 11 3	0	0
4	C	1	Total C N O P 30 10 6 11 3	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	32	10	5	14	3	0	0

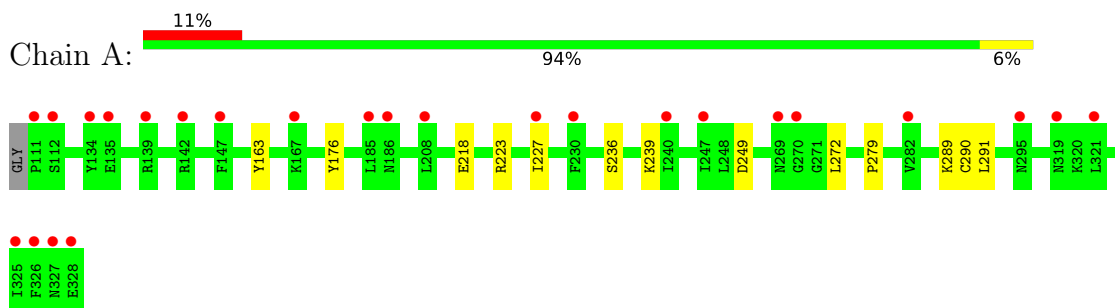
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	46	Total	O	0	0
			46	46		
6	C	42	Total	O	0	0
			42	42		

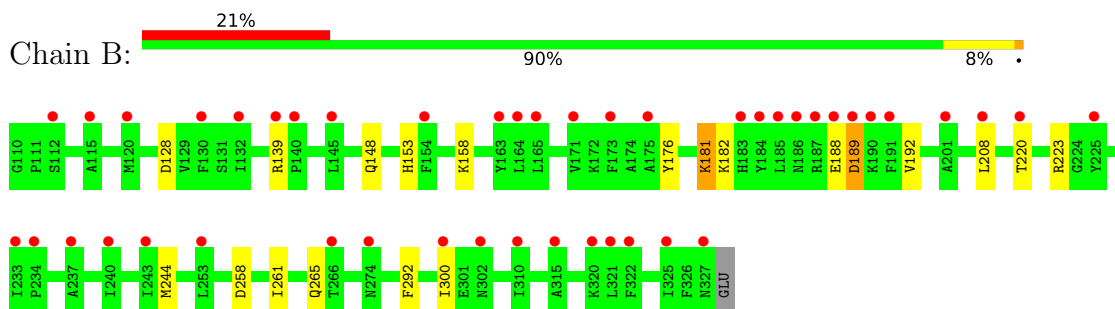
3 Residue-property plots [i](#)

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.

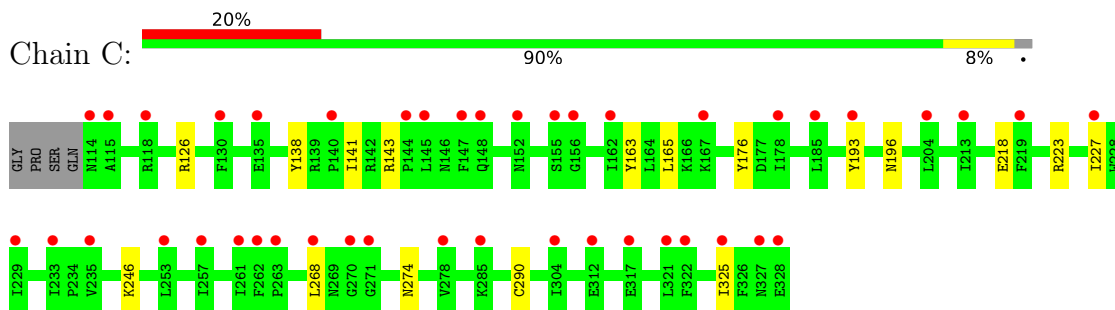
- Molecule 1: TPR_REGION domain-containing protein



- Molecule 1: TPR_REGION domain-containing protein

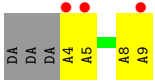


- Molecule 1: TPR_REGION domain-containing protein



- Molecule 2: Templating strand





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	227.82Å 39.50Å 74.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.35 – 1.90 45.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	76.2 (45.35-1.90) 76.2 (45.35-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.228 , 0.259 0.226 , 0.259	Depositor DCC
R_{free} test set	2145 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5813	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DZ4, CO, GTP

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	0.48	0/1849	0.68	0/2486
1	B	0.47	0/1831	0.70	0/2461
1	C	0.47	0/1815	0.67	0/2439
2	D	0.32	0/135	0.63	0/206
All	All	0.47	0/5630	0.68	0/7592

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	1810	0	1794	7	0
1	B	1793	0	1789	11	0
1	C	1777	0	1766	13	0
2	D	120	0	69	3	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
4	A	30	0	13	0	0
4	B	60	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	13	1	0
5	B	32	0	11	0	0
6	A	66	0	0	0	0
6	B	46	0	0	1	0
6	C	42	0	0	1	0
All	All	5813	0	5481	32	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 (32) 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:C:126:ARG:HG2	1:C:165:LEU:O	1.97	0.65
1:B:188:GLU:O	1:B:188:GLU:HG3	2.01	0.60
1:A:236:SER:HB2	1:A:239:LYS:HG3	1.88	0.55
1:C:126:ARG:CG	1:C:165:LEU:O	2.56	0.53
1:B:244:MET:HE2	1:B:261:ILE:HG23	1.91	0.52
1:C:193:TYR:HA	1:C:196:ASN:HB2	1.93	0.51
1:C:126:ARG:HH12	1:C:268:LEU:HD13	1.76	0.50
1:C:163:TYR:N	6:C:505:HOH:O	2.38	0.50
1:A:163:TYR:CZ	1:A:272:LEU:HD23	2.46	0.50
1:C:246:LYS:HD3	1:C:325:ILE:HG12	1.94	0.50
1:B:176:TYR:HE2	1:B:208:LEU:HD21	1.79	0.47
1:A:218:GLU:OE2	1:A:290:CYS:HB3	2.15	0.47
1:C:176:TYR:HB2	1:C:227:ILE:HB	1.97	0.46
1:C:141:ILE:HG22	1:C:143:ARG:HG2	1.98	0.46
1:A:289:LYS:HE3	1:A:291:LEU:HD21	1.98	0.46
1:B:220:THR:HG21	6:B:529:HOH:O	2.15	0.46
1:C:218:GLU:OE2	1:C:290:CYS:HB3	2.15	0.46
1:C:126:ARG:HD3	1:C:163:TYR:CB	2.46	0.46
1:B:153:HIS:HA	1:B:158:LYS:O	2.17	0.45
2:D:8:DA:H2'	2:D:9:DA:C8	2.51	0.45
1:B:139:ARG:HD3	2:D:5:DA:H1'	1.99	0.44
1:C:163:TYR:HA	1:C:274:ASN:O	2.18	0.43
1:A:176:TYR:HB2	1:A:227:ILE:HB	2.01	0.43
2:D:4:DA:H2''	2:D:5:DA:C8	2.54	0.43
1:B:128:ASP:N	1:B:128:ASP:OD1	2.52	0.43
1:B:189:ASP:O	1:B:192:VAL:HG12	2.19	0.42
1:B:181:LYS:HD2	1:B:181:LYS:HA	1.73	0.42
1:A:218:GLU:HG3	1:A:279:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HB3	1:C:268:LEU:HD21	2.03	0.41
1:A:249:ASP:OD1	1:B:148:GLN:HB2	2.21	0.41
1:B:292:PHE:O	1:B:300:ILE:HG12	2.20	0.41
1:C:138:TYR:CE1	4:C:403:DZ4:H2'	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
1	B	217/219 (99%)	208 (96%)	8 (4%)	1 (0%)	29	18
1	C	213/219 (97%)	210 (99%)	3 (1%)	0	100	100
All	All	647/657 (98%)	629 (97%)	17 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	182	LYS

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	195/199 (98%)	194 (100%)	1 (0%)	88	89
1	B	192/199 (96%)	187 (97%)	5 (3%)	46	39
1	C	190/199 (96%)	189 (100%)	1 (0%)	88	89
All	All	577/597 (97%)	570 (99%)	7 (1%)	71	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ARG
1	B	181	LYS
1	B	189	ASP
1	B	223	ARG
1	B	258	ASP
1	B	265	GLN
1	C	223	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 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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$
4	DZ4	B	403	3	29,32,32	2.22	13 (44%)	33,50,50	1.74	7 (21%)
5	GTP	B	404	3	26,34,34	0.98	3 (11%)	32,54,54	0.73	1 (3%)
4	DZ4	B	405	3	29,32,32	2.20	13 (44%)	33,50,50	1.71	9 (27%)
4	DZ4	C	403	3	29,32,32	2.00	13 (44%)	33,50,50	1.61	6 (18%)
4	DZ4	A	403	3	29,32,32	2.29	13 (44%)	33,50,50	1.78	8 (24%)

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
4	DZ4	B	403	3	-	4/15/34/34	0/3/3/3
5	GTP	B	404	3	-	3/18/38/38	0/3/3/3
4	DZ4	B	405	3	-	4/15/34/34	0/3/3/3
4	DZ4	C	403	3	-	2/15/34/34	0/3/3/3
4	DZ4	A	403	3	-	2/15/34/34	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	DZ4	PB-O3B	5.43	1.65	1.59
4	A	403	DZ4	PB-O2B	-5.22	1.42	1.56
4	B	403	DZ4	PB-O2B	-4.64	1.44	1.56
4	A	403	DZ4	PA-O2A	-4.59	1.44	1.56
4	B	403	DZ4	PA-O2A	-4.37	1.45	1.56
4	B	405	DZ4	PA-O2A	-3.77	1.46	1.56
4	B	405	DZ4	PB-O2B	-3.71	1.46	1.56
4	B	403	DZ4	PB-O3B	3.54	1.63	1.59
4	B	405	DZ4	C5-N7	3.46	1.52	1.39
4	C	403	DZ4	PB-O2B	-3.43	1.47	1.56
4	C	403	DZ4	C5-N7	3.32	1.51	1.39
4	C	403	DZ4	PB-O3B	3.32	1.63	1.59
4	C	403	DZ4	PA-O2A	-3.29	1.47	1.56
4	B	403	DZ4	C5-N7	3.27	1.51	1.39
4	C	403	DZ4	C6-N6	3.15	1.45	1.34
4	B	405	DZ4	PA-N3A	3.05	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	DZ4	C5-N7	3.04	1.50	1.39
4	A	403	DZ4	C6-N6	2.97	1.44	1.34
4	A	403	DZ4	PG-O2G	-2.96	1.43	1.54
4	B	405	DZ4	PB-N3A	2.94	1.71	1.63
4	A	403	DZ4	PG-O3G	-2.92	1.43	1.54
4	B	403	DZ4	C6-N6	2.91	1.44	1.34
4	B	403	DZ4	PG-O3G	-2.86	1.43	1.54
4	B	403	DZ4	PG-O2G	-2.84	1.43	1.54
4	A	403	DZ4	PB-O3B	2.84	1.62	1.59
4	B	405	DZ4	C6-N6	2.84	1.44	1.34
4	A	403	DZ4	PA-N3A	2.82	1.70	1.63
4	C	403	DZ4	C2-N3	2.76	1.36	1.32
5	B	404	GTP	C5-C6	-2.67	1.42	1.47
4	C	403	DZ4	PA-N3A	2.61	1.70	1.63
4	B	403	DZ4	C1'-N9	-2.57	1.41	1.49
4	B	405	DZ4	C2-N3	2.50	1.36	1.32
4	B	403	DZ4	PA-N3A	2.46	1.69	1.63
4	A	403	DZ4	C1'-N9	-2.43	1.42	1.49
4	B	403	DZ4	PB-N3A	2.42	1.69	1.63
4	A	403	DZ4	C4-N3	-2.40	1.32	1.35
4	B	403	DZ4	C6-C5	-2.31	1.34	1.43
4	C	403	DZ4	PB-N3A	2.27	1.69	1.63
4	A	403	DZ4	C6-C5	-2.23	1.35	1.43
4	B	405	DZ4	C1'-N9	-2.21	1.42	1.49
5	B	404	GTP	C8-N7	-2.19	1.31	1.35
4	C	403	DZ4	C1'-N9	-2.19	1.42	1.49
4	A	403	DZ4	C2-N3	2.19	1.35	1.32
4	B	405	DZ4	C6-C5	-2.17	1.35	1.43
4	C	403	DZ4	C6-C5	-2.17	1.35	1.43
4	B	405	DZ4	PG-O2G	-2.14	1.46	1.54
4	C	403	DZ4	PG-O3G	-2.12	1.46	1.54
4	A	403	DZ4	PB-N3A	2.11	1.68	1.63
4	B	403	DZ4	C2-N3	2.08	1.35	1.32
4	B	405	DZ4	PA-O5'	2.07	1.65	1.57
4	C	403	DZ4	C4-N3	-2.03	1.32	1.35
5	B	404	GTP	C5-C4	-2.03	1.37	1.43
4	C	403	DZ4	PA-O5'	2.02	1.65	1.57
4	B	405	DZ4	PG-O3G	-2.02	1.47	1.54
4	B	403	DZ4	C4-N3	-2.02	1.32	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	DZ4	O2A-PA-O1A	-4.97	99.50	109.92
4	A	403	DZ4	O2A-PA-O1A	-4.69	100.08	109.92
4	B	405	DZ4	O2B-PB-O1B	-4.22	101.07	109.92
4	B	403	DZ4	O2A-PA-O1A	-4.21	101.10	109.92
4	B	405	DZ4	O2A-PA-O1A	-4.19	101.14	109.92
4	B	403	DZ4	O2B-PB-O1B	-3.75	102.06	109.92
4	A	403	DZ4	PB-O3B-PG	-3.74	119.45	132.62
4	B	403	DZ4	PB-O3B-PG	-3.72	119.50	132.62
4	A	403	DZ4	O2B-PB-O1B	-3.43	102.72	109.92
4	B	403	DZ4	O3G-PG-O3B	3.29	115.66	104.64
4	C	403	DZ4	PB-O3B-PG	-3.25	121.16	132.62
4	A	403	DZ4	O2G-PG-O3B	3.07	114.93	104.64
4	B	405	DZ4	O3G-PG-O3B	3.05	114.85	104.64
4	B	403	DZ4	C2'-C1'-N9	-2.89	107.60	114.27
4	B	403	DZ4	O2G-PG-O3B	2.76	113.88	104.64
4	C	403	DZ4	O2G-PG-O3B	2.72	113.75	104.64
4	B	405	DZ4	O2G-PG-O3B	2.69	113.66	104.64
4	A	403	DZ4	O3G-PG-O3B	2.67	113.59	104.64
4	A	403	DZ4	O1A-PA-N3A	2.60	115.60	111.77
4	C	403	DZ4	O1A-PA-N3A	2.48	115.42	111.77
4	C	403	DZ4	O2A-PA-O5'	2.48	113.46	106.75
4	B	405	DZ4	O2B-PB-O3B	2.39	112.62	104.64
4	A	403	DZ4	C2'-C1'-N9	-2.25	109.07	114.27
4	C	403	DZ4	O3G-PG-O1G	-2.21	102.03	110.68
4	B	405	DZ4	C2'-C3'-C4'	2.18	107.29	102.76
4	B	405	DZ4	C5-C6-N6	-2.15	117.08	120.35
4	B	405	DZ4	O2G-PG-O1G	-2.07	102.58	110.68
4	A	403	DZ4	C4-C5-N7	-2.05	107.26	109.40
5	B	404	GTP	O6-C6-C5	2.04	128.36	124.37
4	B	403	DZ4	O1A-PA-N3A	2.02	114.75	111.77
4	B	405	DZ4	PB-O3B-PG	-2.02	125.51	132.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	DZ4	PA-N3A-PB-O1B
4	B	403	DZ4	PA-N3A-PB-O1B
4	B	405	DZ4	C5'-O5'-PA-O2A
4	B	405	DZ4	PA-N3A-PB-O1B
4	B	405	DZ4	PG-O3B-PB-O1B
4	B	405	DZ4	PG-O3B-PB-O2B
4	C	403	DZ4	PA-N3A-PB-O1B

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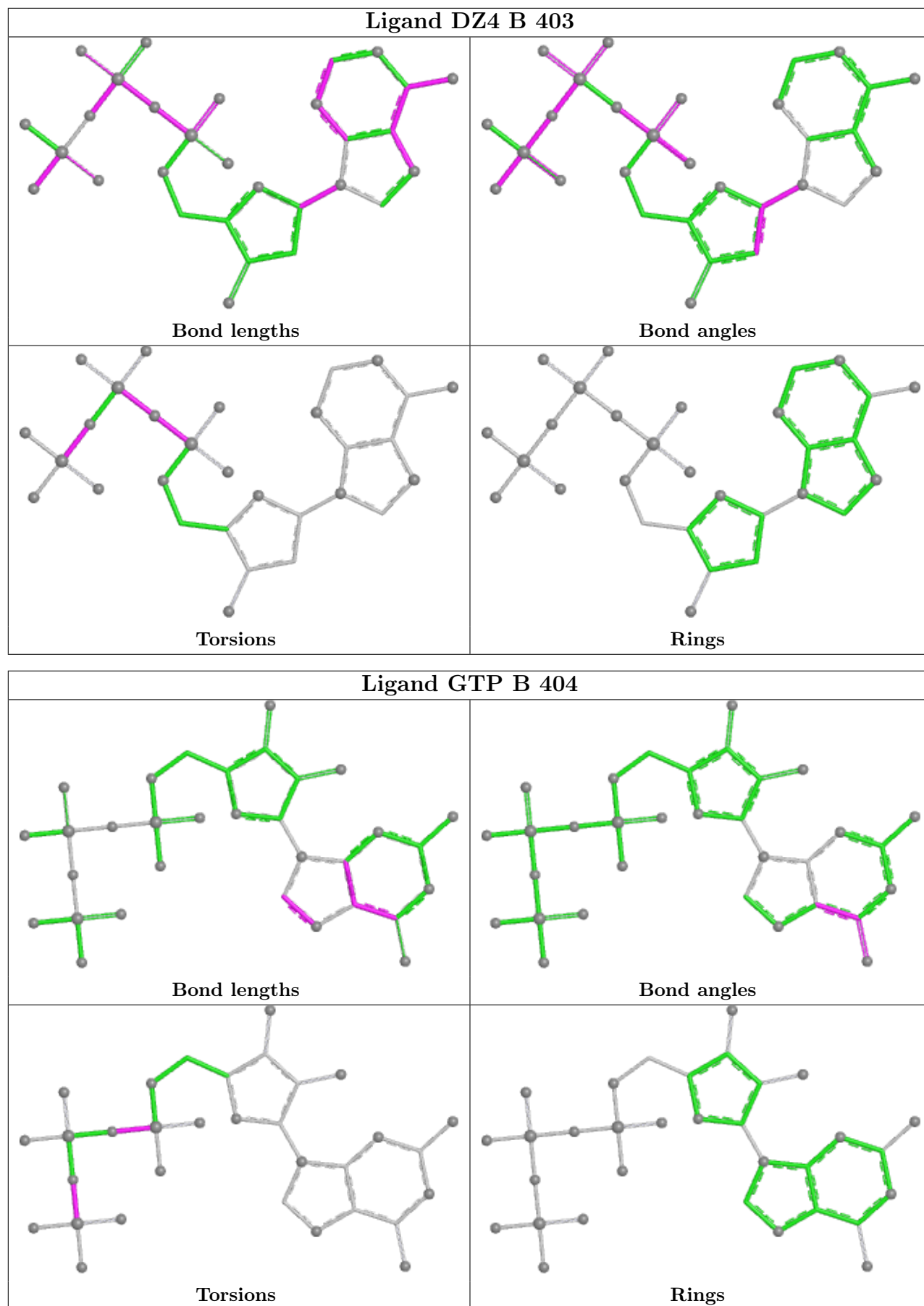
Mol	Chain	Res	Type	Atoms
4	C	403	DZ4	PB-O3B-PG-O2G
5	B	404	GTP	PB-O3B-PG-O2G
4	B	403	DZ4	PB-O3B-PG-O2G
4	B	403	DZ4	PB-N3A-PA-O5'
5	B	404	GTP	PB-O3A-PA-O1A
4	B	403	DZ4	PB-N3A-PA-O1A
5	B	404	GTP	PB-O3B-PG-O1G
4	A	403	DZ4	PB-O3B-PG-O2G

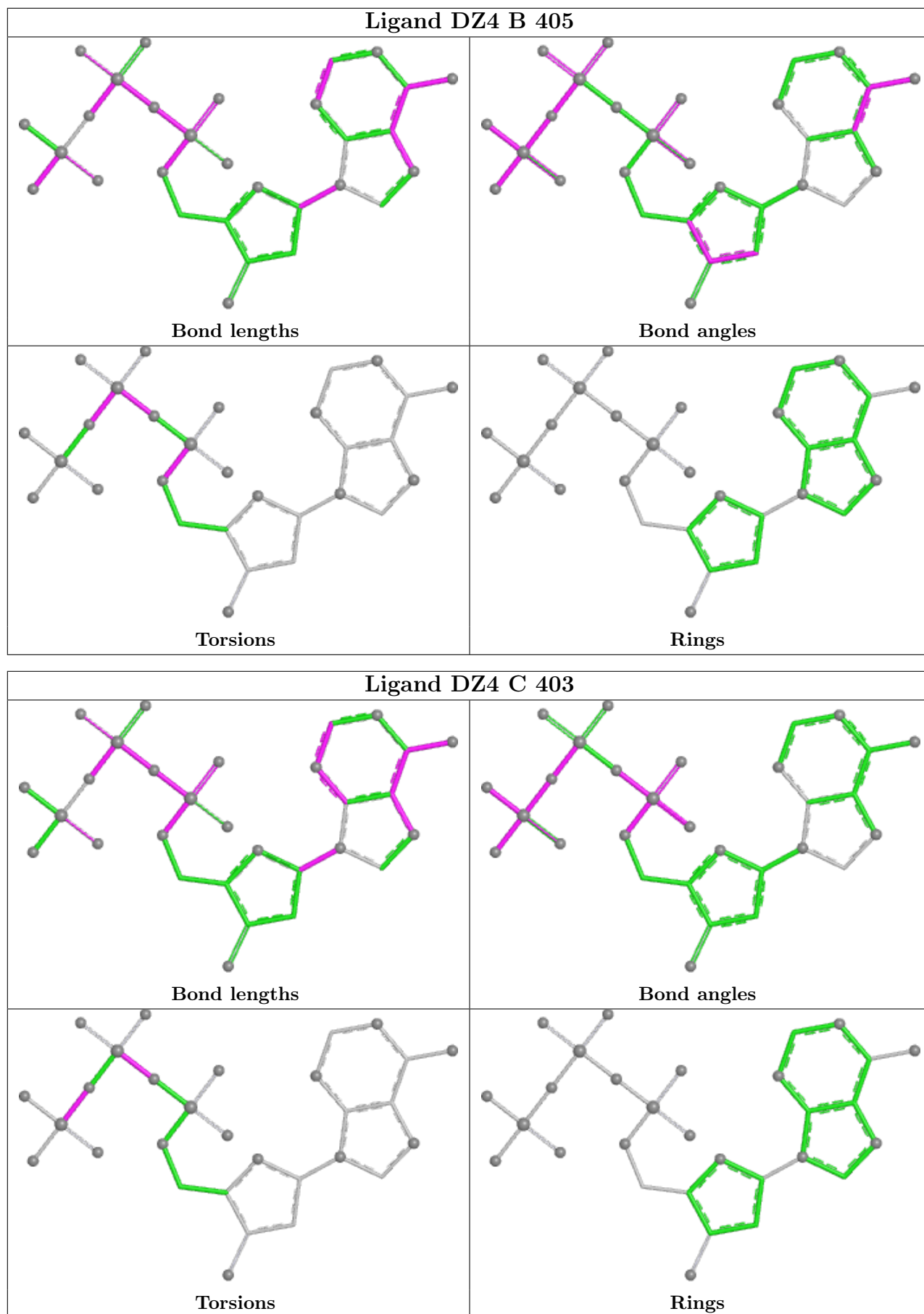
There are no ring outliers.

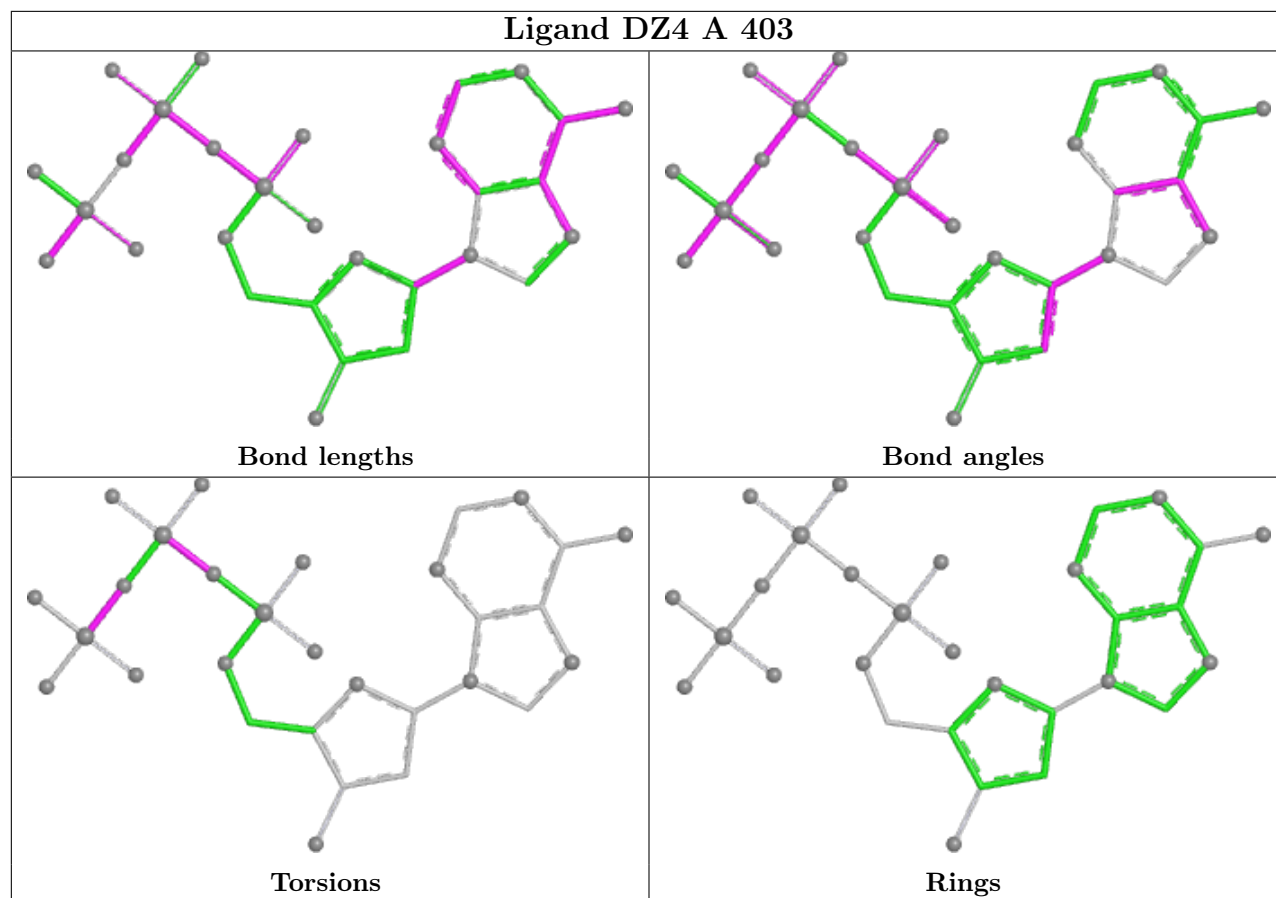
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	DZ4	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/219 (99%)	1.21	25 (11%) 4 5	32, 41, 56, 71	0
1	B	218/219 (99%)	1.49	45 (20%) 1 1	32, 44, 71, 103	0
1	C	215/219 (98%)	1.32	43 (20%) 1 1	31, 43, 61, 79	0
2	D	6/9 (66%)	2.50	3 (50%) 0 0	63, 71, 94, 113	0
All	All	657/666 (98%)	1.35	116 (17%) 1 1	31, 43, 63, 113	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	TYR	9.9
1	B	186	ASN	8.7
1	B	189	ASP	7.6
1	B	325	ILE	7.4
1	B	185	LEU	6.3
1	A	270	GLY	6.2
2	D	4	DA	6.1
1	B	208	LEU	6.1
1	C	114	ASN	6.1
1	B	188	GLU	6.0
1	C	115	ALA	5.8
1	B	191	PHE	4.7
1	B	322	PHE	4.5
1	A	327	ASN	4.2
1	B	233	ILE	4.2
1	A	134	TYR	4.1
1	C	261	ILE	3.8
1	C	140	PRO	3.8
1	A	111	PRO	3.8
1	B	300	ILE	3.7
1	B	266	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	227	ILE	3.7
1	B	187	ARG	3.6
1	C	148	GLN	3.6
1	A	185	LEU	3.6
1	B	165	LEU	3.6
1	C	233	ILE	3.5
2	D	5	DA	3.5
1	C	130	PHE	3.5
1	A	325	ILE	3.4
1	C	145	LEU	3.4
1	A	295	ASN	3.3
1	C	325	ILE	3.3
1	C	321	LEU	3.3
1	A	186	ASN	3.3
1	C	268	LEU	3.2
1	B	321	LEU	3.2
1	C	328	GLU	3.1
1	C	270	GLY	3.1
1	A	139	ARG	3.1
1	A	247	ILE	3.1
1	A	319	ASN	3.1
1	B	302	ASN	3.1
1	C	253	LEU	3.1
1	B	139	ARG	3.1
2	D	9	DA	3.0
1	B	225	TYR	3.0
1	A	269	ASN	3.0
1	B	115	ALA	3.0
1	C	262	PHE	3.0
1	C	193	TYR	2.9
1	A	326	PHE	2.9
1	B	163	TYR	2.8
1	A	135	GLU	2.8
1	C	204	LEU	2.8
1	A	142	ARG	2.7
1	C	185	LEU	2.7
1	B	274	ASN	2.7
1	C	162	ILE	2.7
1	B	201	ALA	2.7
1	B	243	ILE	2.7
1	C	156	GLY	2.7
1	C	152	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	235	VAL	2.6
1	C	304	ILE	2.6
1	C	147	PHE	2.6
1	B	145	LEU	2.5
1	C	271	GLY	2.5
1	B	171	VAL	2.5
1	A	328	GLU	2.5
1	B	310	ILE	2.4
1	A	208	LEU	2.4
1	B	173	PHE	2.4
1	B	320	LYS	2.4
1	B	130	PHE	2.4
1	B	140	PRO	2.4
1	B	120[A]	MET	2.3
1	B	315	ALA	2.3
1	A	112	SER	2.3
1	A	282	VAL	2.3
1	C	118	ARG	2.3
1	C	278	VAL	2.3
1	C	312	GLU	2.3
1	B	112	SER	2.3
1	A	230	PHE	2.2
1	A	240	ILE	2.2
1	C	155	SER	2.2
1	C	178	ILE	2.2
1	B	183	HIS	2.2
1	A	167	LYS	2.2
1	C	213	ILE	2.2
1	C	257	ILE	2.2
1	A	321	LEU	2.2
1	B	253	LEU	2.2
1	C	322	PHE	2.2
1	C	263	PRO	2.2
1	C	229	ILE	2.2
1	A	147	PHE	2.2
1	C	219	PHE	2.2
1	B	164	LEU	2.1
1	B	154	PHE	2.1
1	C	227	ILE	2.1
1	B	234	PRO	2.1
1	C	317	GLU	2.1
1	C	144	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	327	ASN	2.1
1	B	220	THR	2.1
1	C	167	LYS	2.1
1	B	237	ALA	2.1
1	B	240	ILE	2.1
1	C	285	LYS	2.0
1	B	132	ILE	2.0
1	C	135	GLU	2.0
1	B	190	LYS	2.0
1	B	175	ALA	2.0
1	B	327	ASN	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](#)

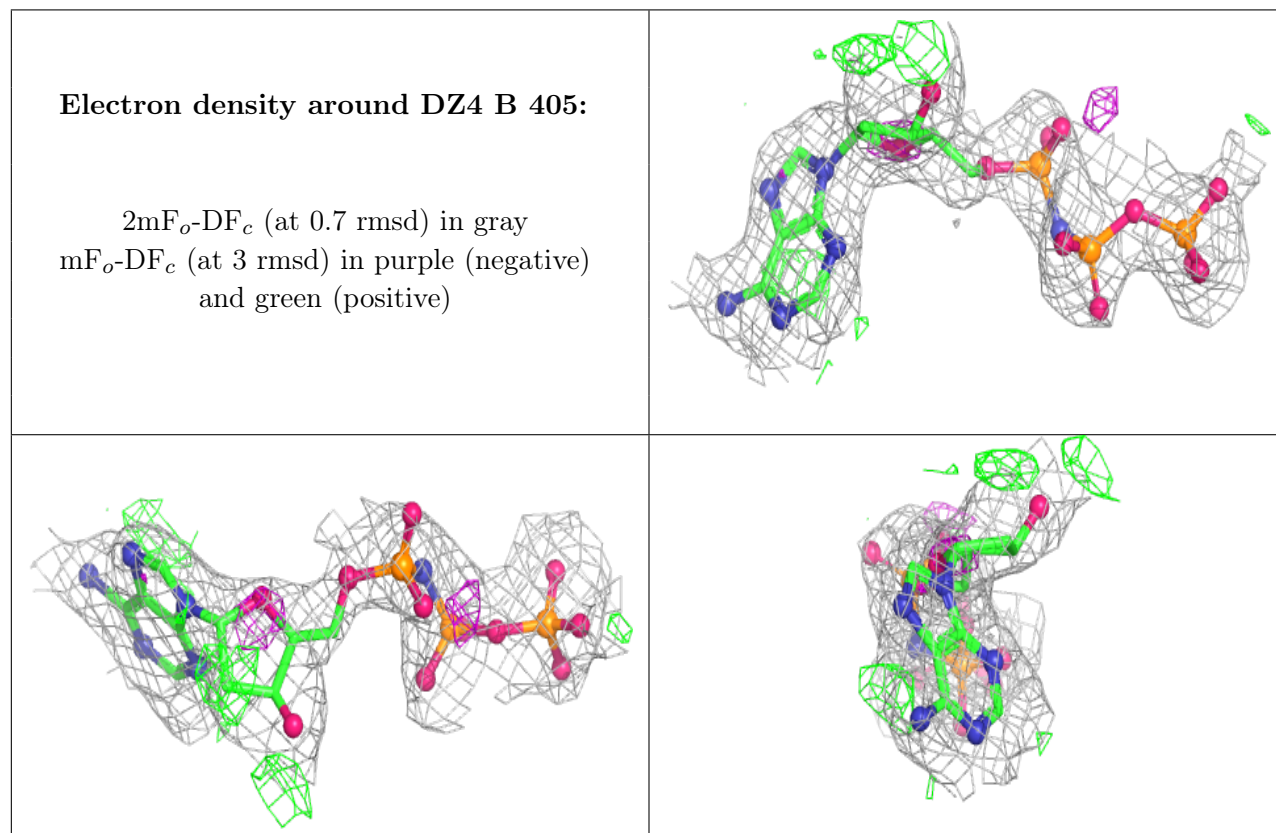
There are no monosaccharides in this entry.

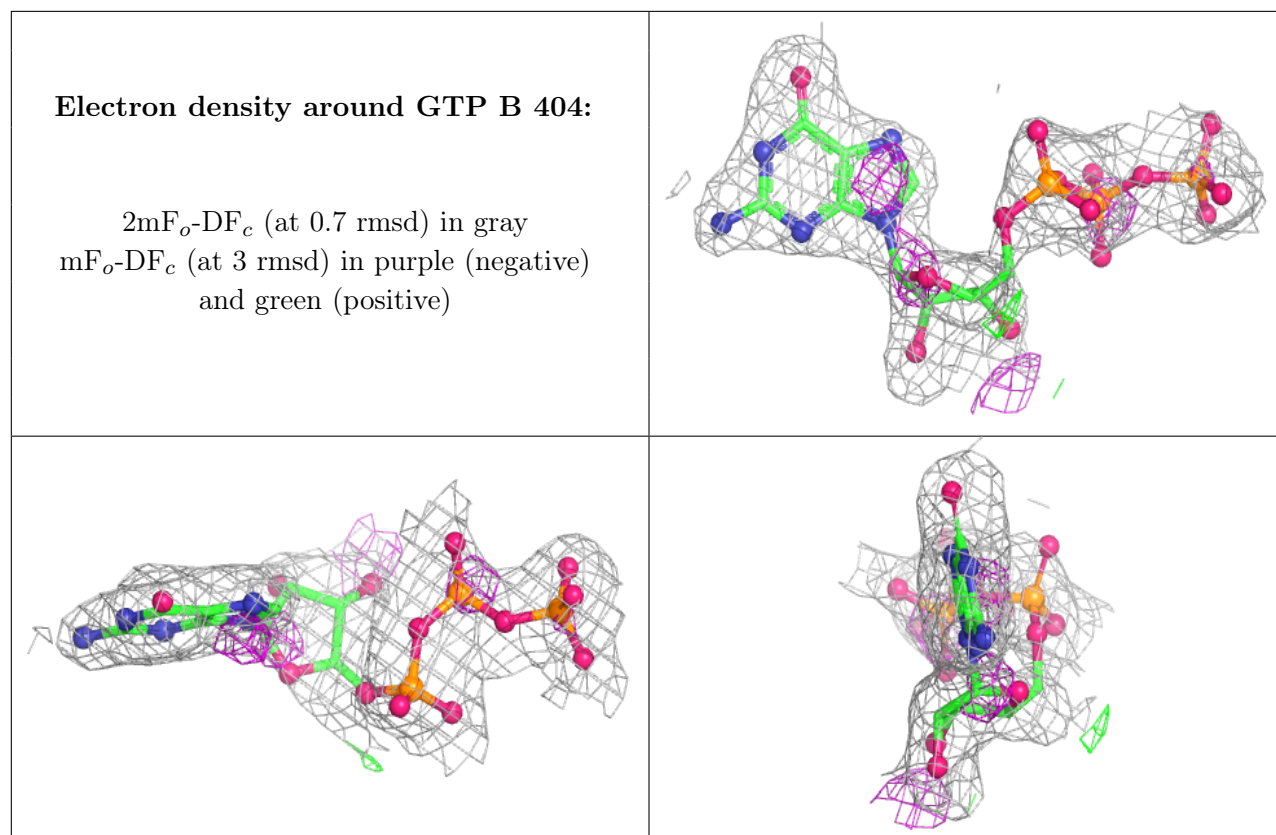
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DZ4	B	405	30/30	0.73	0.20	36,64,79,83	0
5	GTP	B	404	32/32	0.74	0.23	51,57,83,91	0
3	CO	A	402	1/1	0.81	0.31	68,68,68,68	0
3	CO	C	402	1/1	0.84	0.13	57,57,57,57	0
4	DZ4	C	403	30/30	0.86	0.16	34,37,42,44	0
4	DZ4	B	403	30/30	0.87	0.15	31,42,45,46	0
3	CO	B	402	1/1	0.87	0.08	62,62,62,62	0
4	DZ4	A	403	30/30	0.88	0.17	31,39,46,51	0
3	CO	B	406	1/1	0.92	0.06	78,78,78,78	0
3	CO	C	401	1/1	0.93	0.11	39,39,39,39	0
3	CO	B	401	1/1	0.96	0.10	44,44,44,44	0
3	CO	A	401	1/1	0.99	0.07	41,41,41,41	0

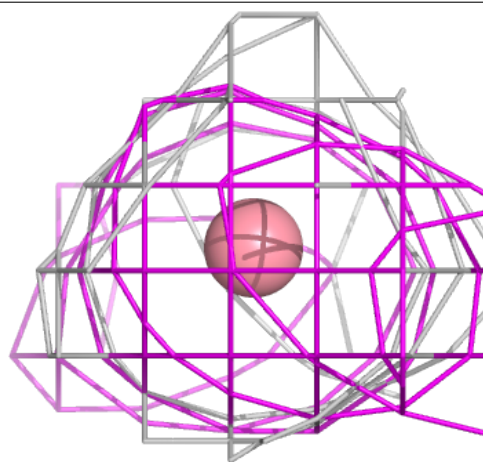
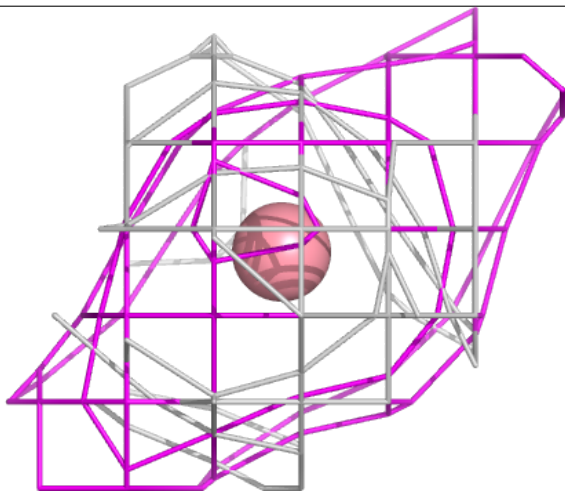
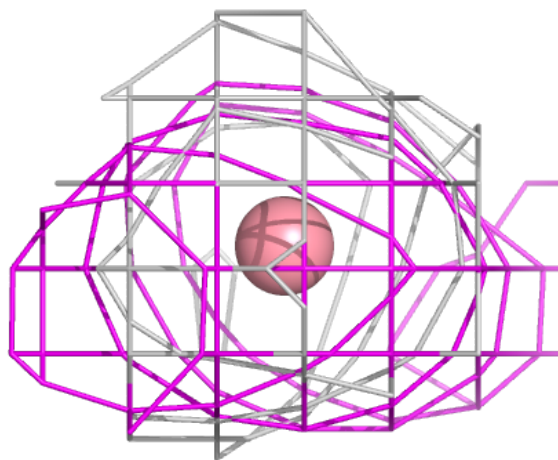
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





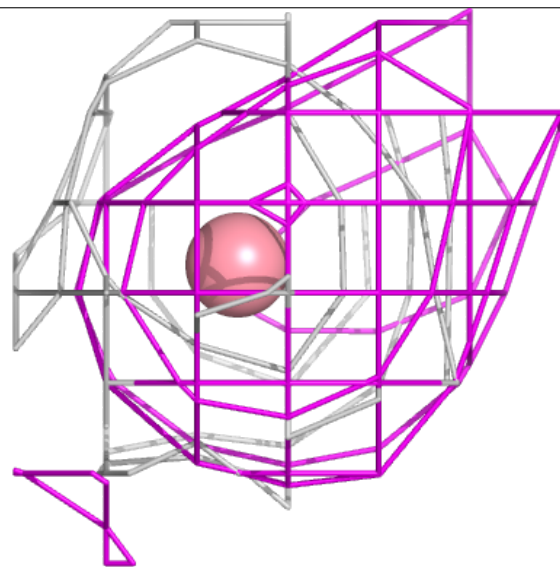
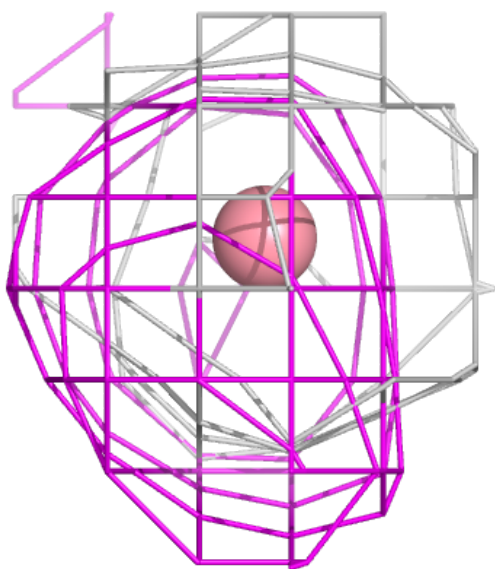
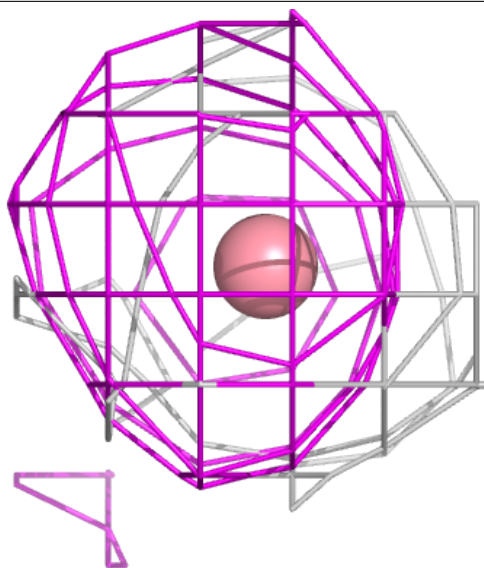
Electron density around CO A 402:

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



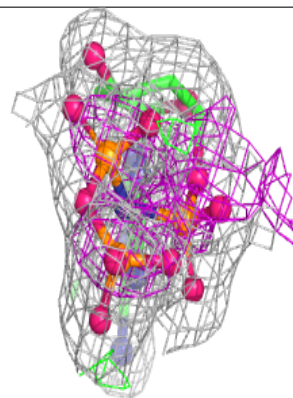
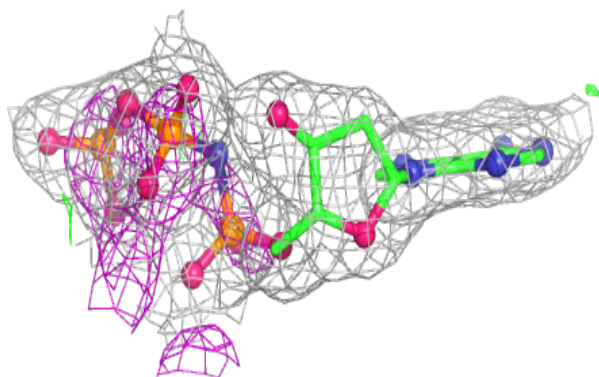
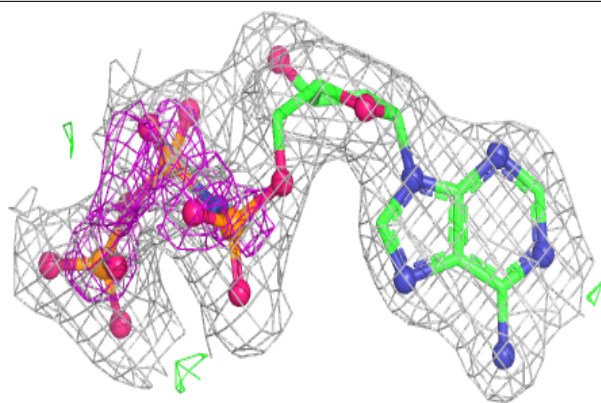
Electron density around CO C 402:

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

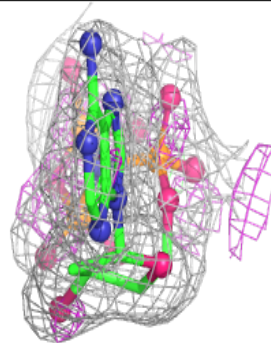
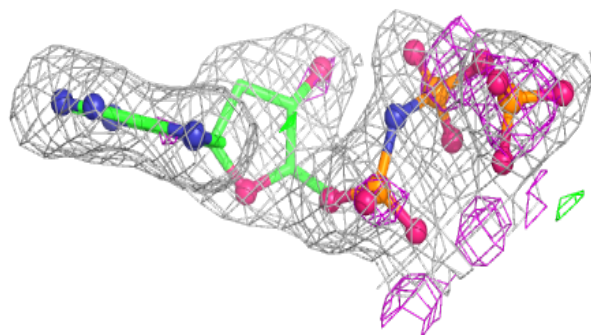
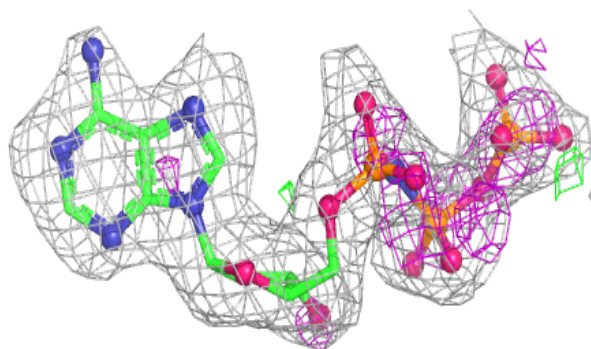


Electron density around DZ4 C 403:

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

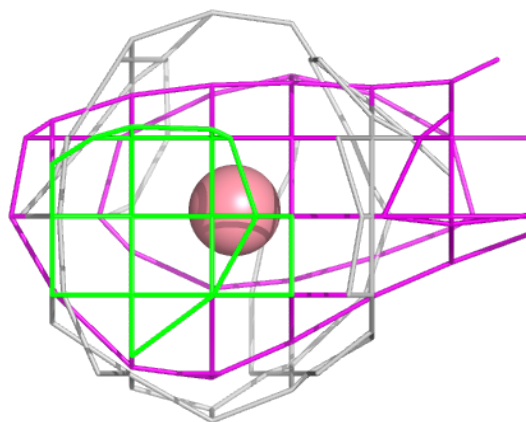
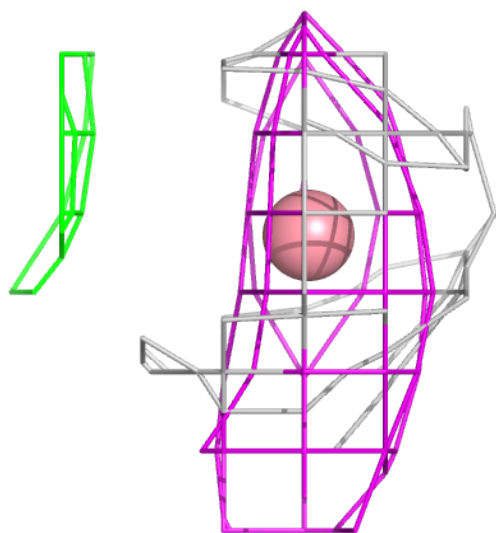
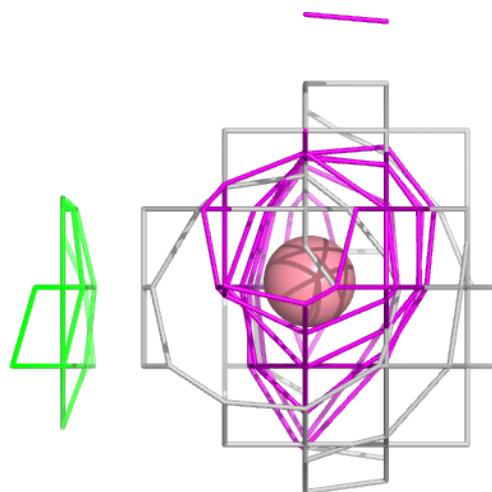
**Electron density around DZ4 B 403:**

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



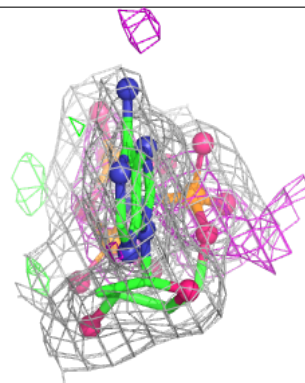
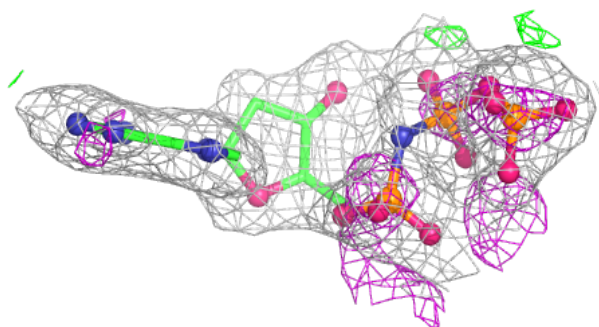
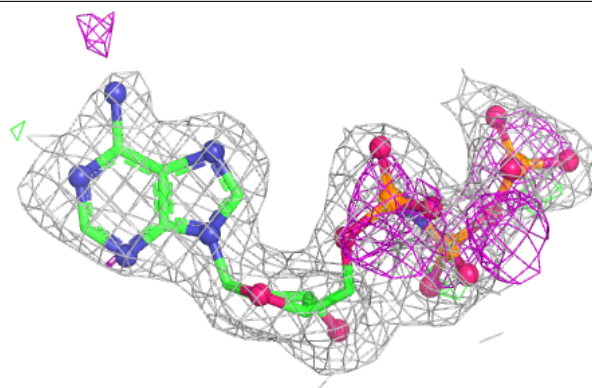
Electron density around CO B 402:

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



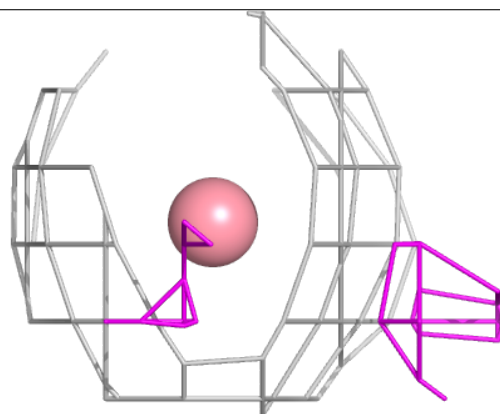
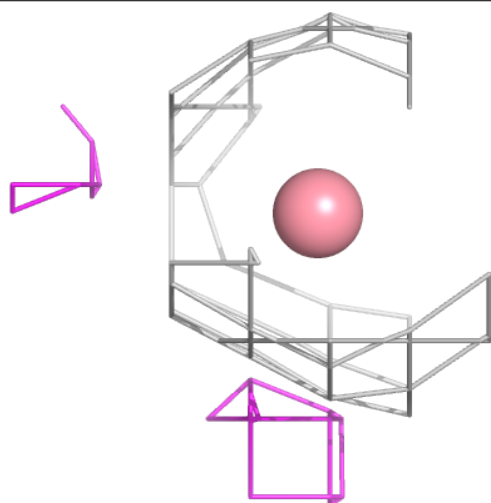
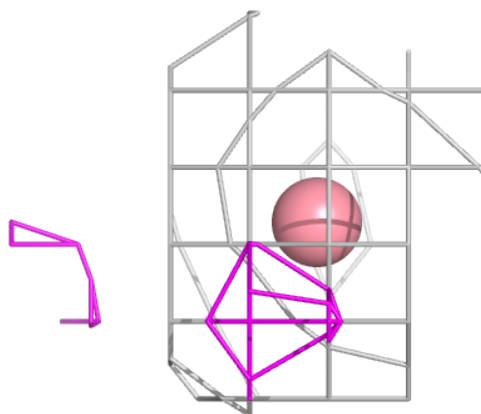
Electron density around DZ4 A 403:

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



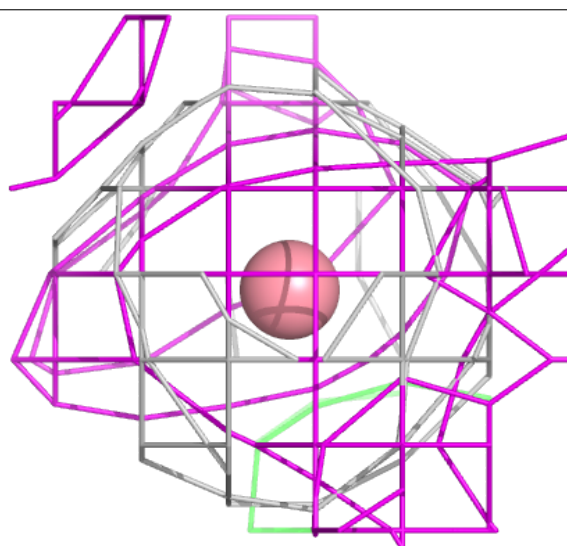
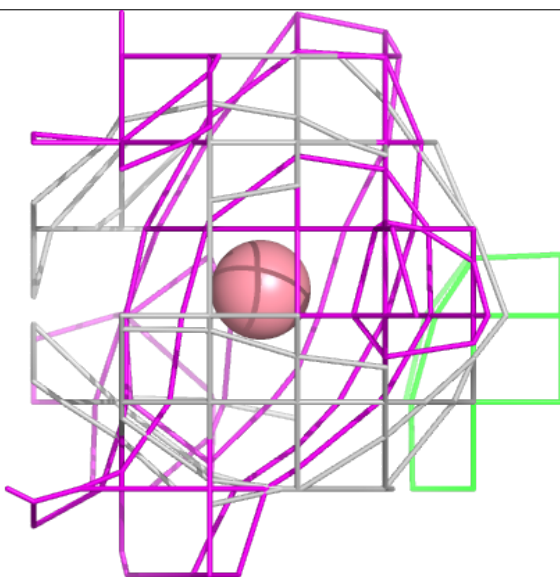
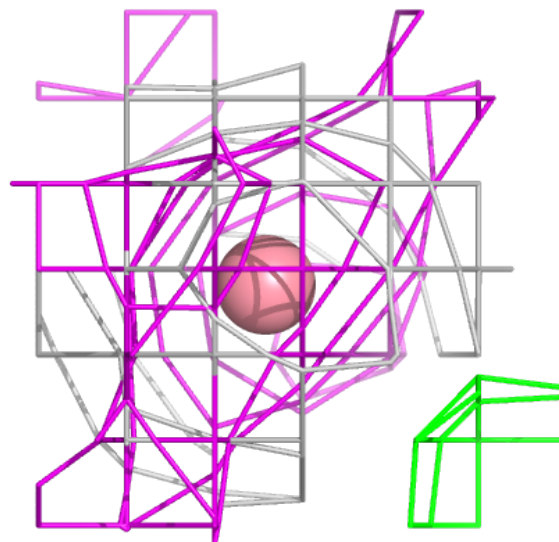
Electron density around CO B 406:

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



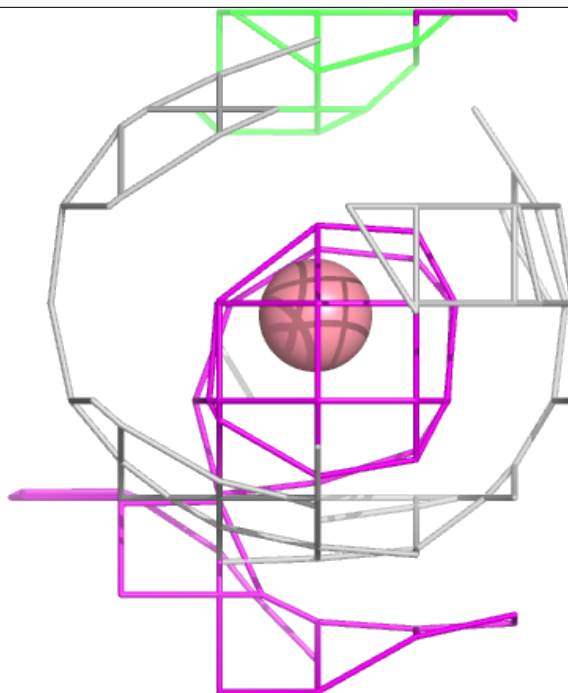
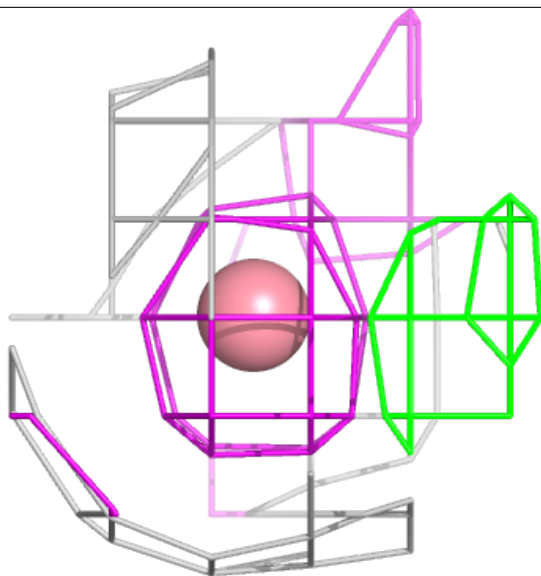
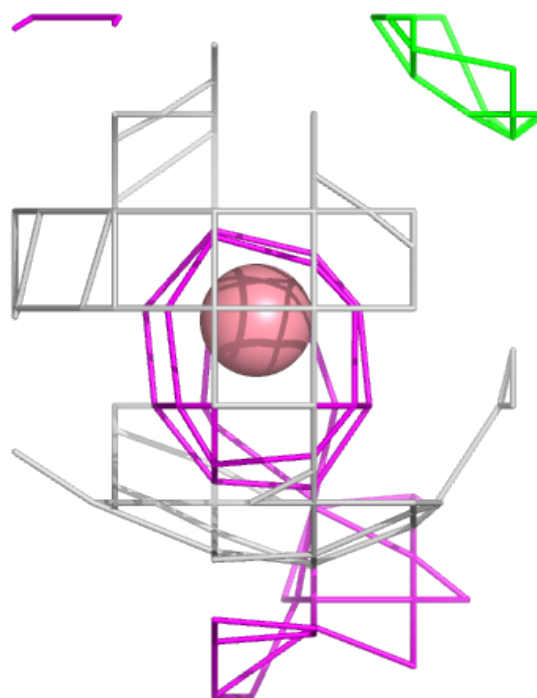
Electron density around CO C 401:

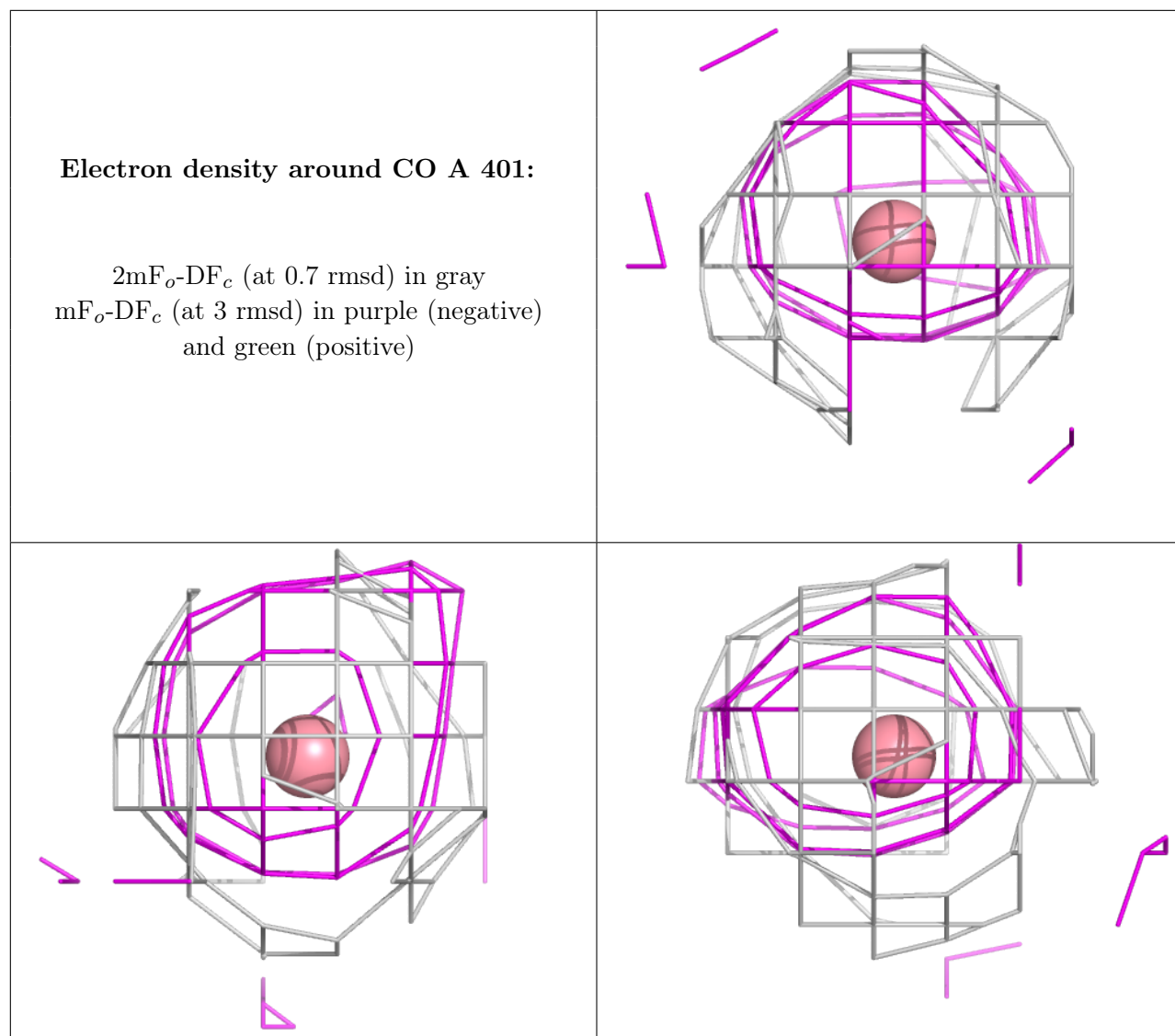
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CO B 401:

$2mF_o-DF_c$ (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.