



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:52 am BST

PDB ID : 5YG5
Title : Crystal structure of ribose-1,5-bisphosphate isomerase from *Pyrococcus horikoshii* OT3 in complex with ribulose-1,5-bisphosphate and GMP
Authors : Gogoi, P.; Kanaujia, S.P.
Deposited on : 2017-09-22
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

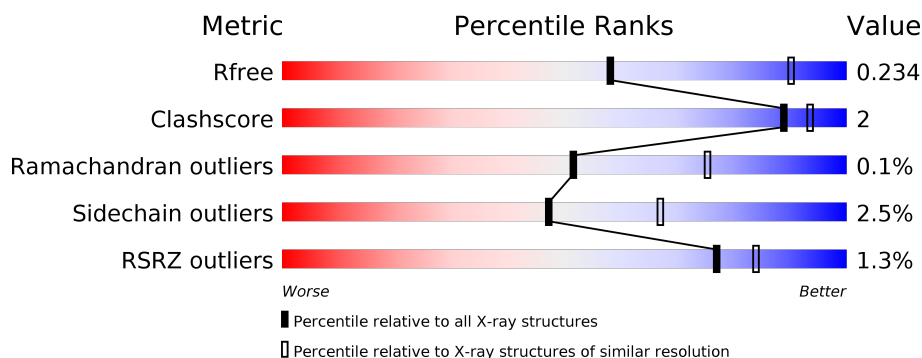
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	324	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	324	<div> <div></div> <div>92%</div> <div>8%</div> <div>•</div> </div>
1	C	324	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	G	B	406	-	-	-	X
6	G	C	404	-	-	-	X

2 Entry composition [i](#)

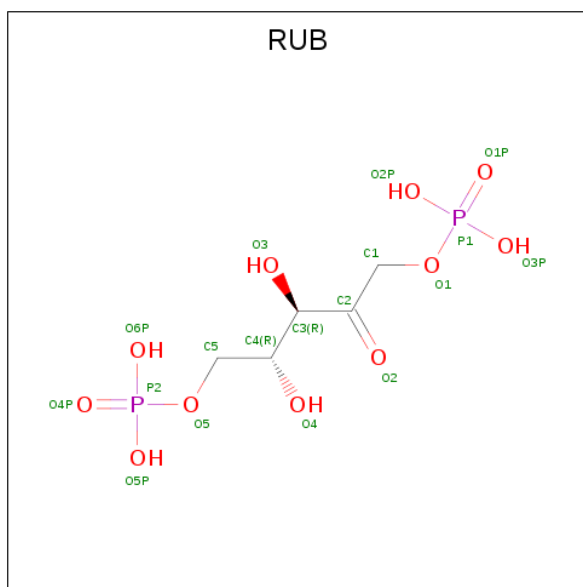
There are 7 unique types of molecules in this entry. The entry contains 8028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribose 1,5-bisphosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2551	1638	431	469	13			
1	B	322	Total	C	N	O	S	0	0	0
			2546	1635	430	468	13			
1	C	322	Total	C	N	O	S	0	0	0
			2546	1635	430	468	13			

- Molecule 2 is RIBULOSE-1,5-DIPHOSPHATE (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	5	11	2		
2	B	1	Total	C	O	P	0	0
			18	5	11	2		
2	C	1	Total	C	O	P	0	0
			18	5	11	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

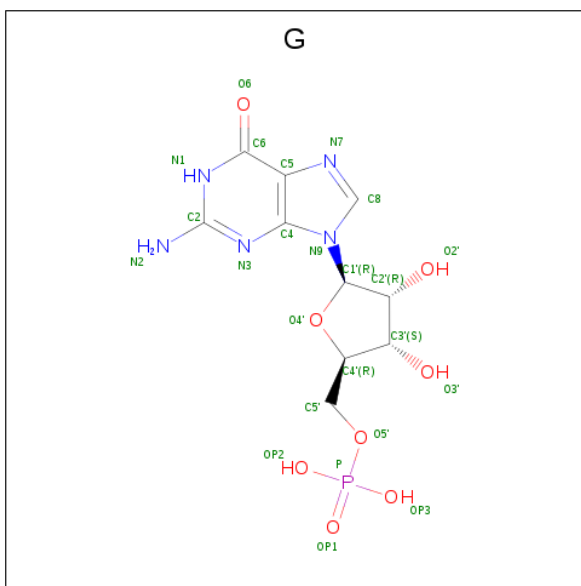
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
6	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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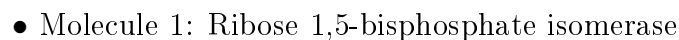
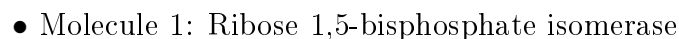
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
6	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
6	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	69	Total	O	0	0
			69	69		
7	B	79	Total	O	0	0
			79	79		
7	C	45	Total	O	0	0
			45	45		

- Molecule 1: Ribose 1,5-bisphosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	98.99 Å 98.99 Å 257.09 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.73 – 2.75 85.70 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (85.73-2.75) 100.0 (85.70-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.73 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.162 , 0.232 0.170 , 0.234	Depositor DCC
R_{free} test set	1848 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: RUB, K, PEG, MPD

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	0.69	0/2606	0.87	2/3527 (0.1%)
1	B	0.68	0/2598	0.83	4/3516 (0.1%)
1	C	0.65	0/2598	0.82	4/3516 (0.1%)
All	All	0.67	0/7802	0.84	10/10559 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	162	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	76	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	162	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	162	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	190	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	144	MET	CG-SD-CE	5.28	108.64	100.20
1	B	129	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	96	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	C	116	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2551	0	2619	13	0
1	B	2546	0	2613	9	0
1	C	2546	0	2613	8	0
2	A	18	0	8	0	0
2	B	18	0	8	0	0
2	C	18	0	8	0	0
3	A	8	0	14	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	7	0	10	0	0
6	B	72	0	36	0	0
6	C	48	0	24	0	0
7	A	69	0	0	0	0
7	B	79	0	0	1	0
7	C	45	0	0	0	0
All	All	8028	0	7953	30	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 2.

All (30) 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:145:LYS:HD3	1:C:177:TYR:CD2	2.32	0.64
1:B:124:ARG:NH1	7:B:501:HOH:O	2.35	0.59
1:C:319:LYS:NZ	1:C:324:ASP:O	2.40	0.54
1:A:259:THR:HA	1:A:262:ILE:O	2.09	0.52
1:B:258:PRO:HB3	1:B:276:VAL:HB	1.92	0.52
1:A:38:GLN:HE21	1:A:53:GLU:HB3	1.77	0.49
1:A:241:PHE:HB3	1:A:308:LEU:HD21	1.94	0.49
1:A:6:VAL:HG22	1:A:38:GLN:OE1	2.12	0.49
1:C:44:ALA:HB1	1:C:49:GLU:HB3	1.95	0.48
1:C:145:LYS:HD3	1:C:177:TYR:CE2	2.50	0.47
1:B:50:LEU:HD23	1:B:95:LEU:HD23	1.96	0.47
1:A:145:LYS:NZ	1:A:149:GLU:OE2	2.48	0.46
1:A:257:ASP:OD2	1:A:259:THR:OG1	2.24	0.46
1:C:8:GLU:HG2	1:C:37:ILE:HG21	1.97	0.46
1:A:86:TYR:HB2	1:A:95:LEU:HD11	1.97	0.46
1:B:107:ILE:O	1:B:111:GLU:HG3	2.17	0.44
1:C:320:GLU:HG2	1:C:322:TRP:CZ2	2.53	0.44
1:C:259:THR:HA	1:C:262:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLU:HG2	1:A:322:TRP:CZ2	2.53	0.43
1:A:82:VAL:HG21	1:A:99:ALA:HB2	2.00	0.43
1:B:236:ALA:O	1:B:294:THR:HA	2.18	0.43
1:B:44:ALA:HB1	1:B:49:GLU:HB3	2.01	0.42
1:C:160:GLU:HB2	1:C:183:TYR:OH	2.20	0.42
1:A:69:VAL:HB	1:A:242:HIS:CD2	2.55	0.42
1:A:42:SER:OG	1:A:53:GLU:OE2	2.36	0.41
1:B:320:GLU:HG2	1:B:322:TRP:CZ2	2.55	0.41
1:A:201:MET:CE	1:A:218:THR:HG23	2.50	0.41
1:A:246:MET:SD	1:A:308:LEU:HB3	2.60	0.40
1:B:51:TRP:CH2	1:B:83:LYS:HG3	2.57	0.40
1:B:213:ILE:HG12	1:B:283:VAL:HG22	2.04	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	321/324 (99%)	308 (96%)	12 (4%)	1 (0%)	41	60
1	B	320/324 (99%)	302 (94%)	18 (6%)	0	100	100
1	C	320/324 (99%)	306 (96%)	14 (4%)	0	100	100
All	All	961/972 (99%)	916 (95%)	44 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLY

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	268/268 (100%)	262 (98%)	6 (2%)	52	70
1	B	267/268 (100%)	262 (98%)	5 (2%)	57	73
1	C	267/268 (100%)	258 (97%)	9 (3%)	37	58
All	All	802/804 (100%)	782 (98%)	20 (2%)	47	67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	91	ASP
1	A	112	LYS
1	A	124	ARG
1	A	138	LYS
1	A	311	GLU
1	B	137	SER
1	B	194	LYS
1	B	195	MET
1	B	272	LYS
1	B	296	ARG
1	C	43	LYS
1	C	45	LYS
1	C	48	GLU
1	C	71	LEU
1	C	116	ARG
1	C	160	GLU
1	C	296	ARG
1	C	311	GLU
1	C	317	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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
2	RUB	A	401	-	15,17,17	1.26	2 (13%)	16,25,25	1.09	1 (6%)
2	RUB	B	401	-	15,17,17	0.96	2 (13%)	16,25,25	1.52	3 (18%)
2	RUB	C	401	-	15,17,17	0.86	0	16,25,25	1.50	4 (25%)
6	G	B	405	-	22,26,26	1.09	2 (9%)	27,40,40	2.33	7 (25%)
5	PEG	B	403	-	6,6,6	0.84	0	5,5,5	0.68	0
6	G	C	403	-	22,26,26	1.16	2 (9%)	27,40,40	2.38	6 (22%)
6	G	B	404	-	22,26,26	1.13	2 (9%)	27,40,40	2.34	6 (22%)
6	G	B	406	-	22,26,26	1.12	2 (9%)	27,40,40	2.34	6 (22%)
3	MPD	A	402	-	7,7,7	0.58	0	9,10,10	1.23	1 (11%)
6	G	C	404	-	22,26,26	1.14	2 (9%)	27,40,40	2.33	6 (22%)

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
2	RUB	A	401	-	-	5/20/20/20	-
2	RUB	B	401	-	-	8/20/20/20	-
2	RUB	C	401	-	-	3/20/20/20	-
6	G	B	405	-	-	3/6/26/26	0/3/3/3
5	PEG	B	403	-	-	2/4/4/4	-
6	G	C	403	-	-	2/6/26/26	0/3/3/3
6	G	B	404	-	-	2/6/26/26	0/3/3/3
6	G	B	406	-	-	3/6/26/26	0/3/3/3
3	MPD	A	402	-	-	2/5/5/5	-
6	G	C	404	-	-	4/6/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	G	C6-N1	3.86	1.39	1.33
6	B	404	G	C6-N1	3.85	1.39	1.33
6	C	404	G	C6-N1	3.85	1.39	1.33
6	B	405	G	C6-N1	3.79	1.39	1.33
6	B	406	G	C6-N1	3.73	1.39	1.33
2	A	401	RUB	O1-C1	3.60	1.45	1.43
2	B	401	RUB	O1-C1	2.30	1.44	1.43
2	A	401	RUB	O3-C3	2.18	1.46	1.42
6	C	403	G	C8-N7	-2.11	1.30	1.34
6	C	404	G	C8-N7	-2.10	1.31	1.34
6	B	405	G	C8-N7	-2.08	1.31	1.34
2	B	401	RUB	O3-C3	2.08	1.46	1.42
6	B	404	G	C8-N7	-2.08	1.31	1.34
6	B	406	G	C8-N7	-2.04	1.31	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	403	G	C5-C6-N1	-8.73	111.49	123.43
6	B	404	G	C5-C6-N1	-8.70	111.53	123.43
6	C	404	G	C5-C6-N1	-8.69	111.54	123.43
6	B	406	G	C5-C6-N1	-8.61	111.65	123.43
6	B	405	G	C5-C6-N1	-8.60	111.67	123.43
6	B	404	G	C6-N1-C2	5.81	125.16	115.93
6	C	403	G	C6-N1-C2	5.80	125.14	115.93
6	C	404	G	C6-N1-C2	5.77	125.10	115.93
6	B	406	G	C6-N1-C2	5.77	125.10	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	405	G	C6-N1-C2	5.77	125.09	115.93
6	B	404	G	C2-N3-C4	-2.98	111.96	115.36
2	C	401	RUB	O6P-P2-O5	-2.97	98.82	106.73
6	C	403	G	C2-N3-C4	-2.96	111.98	115.36
6	B	405	G	C2-N3-C4	-2.95	111.98	115.36
6	B	406	G	C2-N3-C4	-2.95	111.99	115.36
2	C	401	RUB	O5P-P2-O5	-2.94	98.91	106.73
6	C	403	G	OP2-P-OP3	2.94	118.86	107.64
6	C	404	G	C2-N3-C4	-2.90	112.05	115.36
6	B	406	G	O2'-C2'-C1'	2.58	120.39	110.85
6	B	404	G	N3-C2-N1	-2.55	123.82	127.22
6	B	405	G	N3-C2-N1	-2.51	123.87	127.22
6	C	403	G	N3-C2-N1	-2.51	123.87	127.22
6	B	406	G	N3-C2-N1	-2.51	123.88	127.22
6	C	404	G	N3-C2-N1	-2.47	123.92	127.22
2	B	401	RUB	O1-P1-O1P	-2.36	99.86	106.47
6	B	405	G	OP2-P-OP1	2.34	119.83	110.68
2	A	401	RUB	O5P-P2-O4P	2.33	119.81	110.68
6	C	404	G	OP2-P-OP1	2.31	119.74	110.68
3	A	402	MPD	O2-C2-CM	2.27	115.38	108.08
2	B	401	RUB	O5-C5-C4	2.22	115.29	109.36
6	B	406	G	OP2-P-OP1	2.20	119.29	110.68
2	C	401	RUB	O6P-P2-O5P	2.17	115.92	107.64
2	B	401	RUB	O5-P2-O4P	-2.16	100.43	106.47
6	C	403	G	C6-C5-C4	-2.08	118.81	120.80
6	B	404	G	C6-C5-C4	-2.04	118.85	120.80
6	B	404	G	OP2-P-OP1	2.04	118.68	110.68
2	C	401	RUB	O6P-P2-O4P	2.02	118.59	110.68
6	B	405	G	C6-C5-C4	-2.02	118.87	120.80
6	B	405	G	O2'-C2'-C1'	2.01	118.28	110.85
6	C	404	G	C6-C5-C4	-2.00	118.89	120.80

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	RUB	C1-C2-C3-O3
2	A	401	RUB	C1-O1-P1-O2P
2	A	401	RUB	C1-O1-P1-O3P
2	B	401	RUB	C1-C2-C3-O3
2	B	401	RUB	O2-C2-C3-O3
2	B	401	RUB	O3-C3-C4-O4

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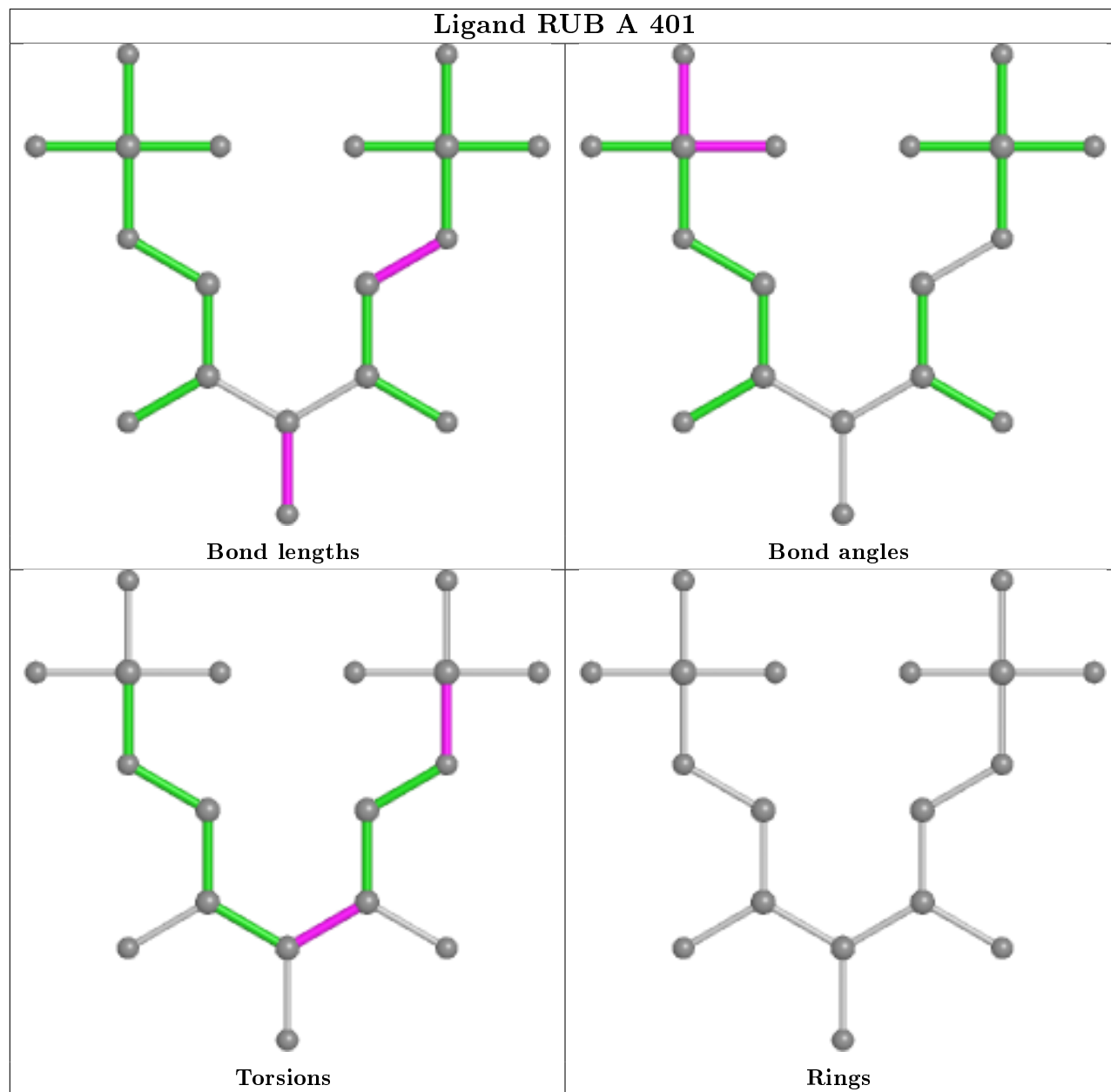
Mol	Chain	Res	Type	Atoms
2	B	401	RUB	C5-O5-P2-O4P
2	B	401	RUB	C5-O5-P2-O6P
2	C	401	RUB	C1-C2-C3-O3
6	B	405	G	C5'-O5'-P-OP1
6	C	403	G	O4'-C4'-C5'-O5'
6	B	404	G	C5'-O5'-P-OP3
6	B	406	G	O4'-C4'-C5'-O5'
6	C	404	G	C5'-O5'-P-OP1
6	C	404	G	O4'-C4'-C5'-O5'
6	C	404	G	C3'-C4'-C5'-O5'
6	B	406	G	C3'-C4'-C5'-O5'
5	B	403	PEG	O1-C1-C2-O2
2	A	401	RUB	C1-O1-P1-O1P
6	B	406	G	C5'-O5'-P-OP1
2	B	401	RUB	C1-O1-P1-O3P
2	B	401	RUB	C5-O5-P2-O5P
6	B	405	G	C5'-O5'-P-OP3
6	B	404	G	C5'-O5'-P-OP2
2	A	401	RUB	O2-C2-C3-O3
2	C	401	RUB	O2-C2-C3-O3
5	B	403	PEG	C1-C2-O2-C3
2	B	401	RUB	C1-O1-P1-O2P
6	C	403	G	C5'-O5'-P-OP2
6	C	404	G	C5'-O5'-P-OP3
2	C	401	RUB	O3-C3-C4-O4
3	A	402	MPD	C2-C3-C4-C5
6	B	405	G	O4'-C4'-C5'-O5'
3	A	402	MPD	C2-C3-C4-O4

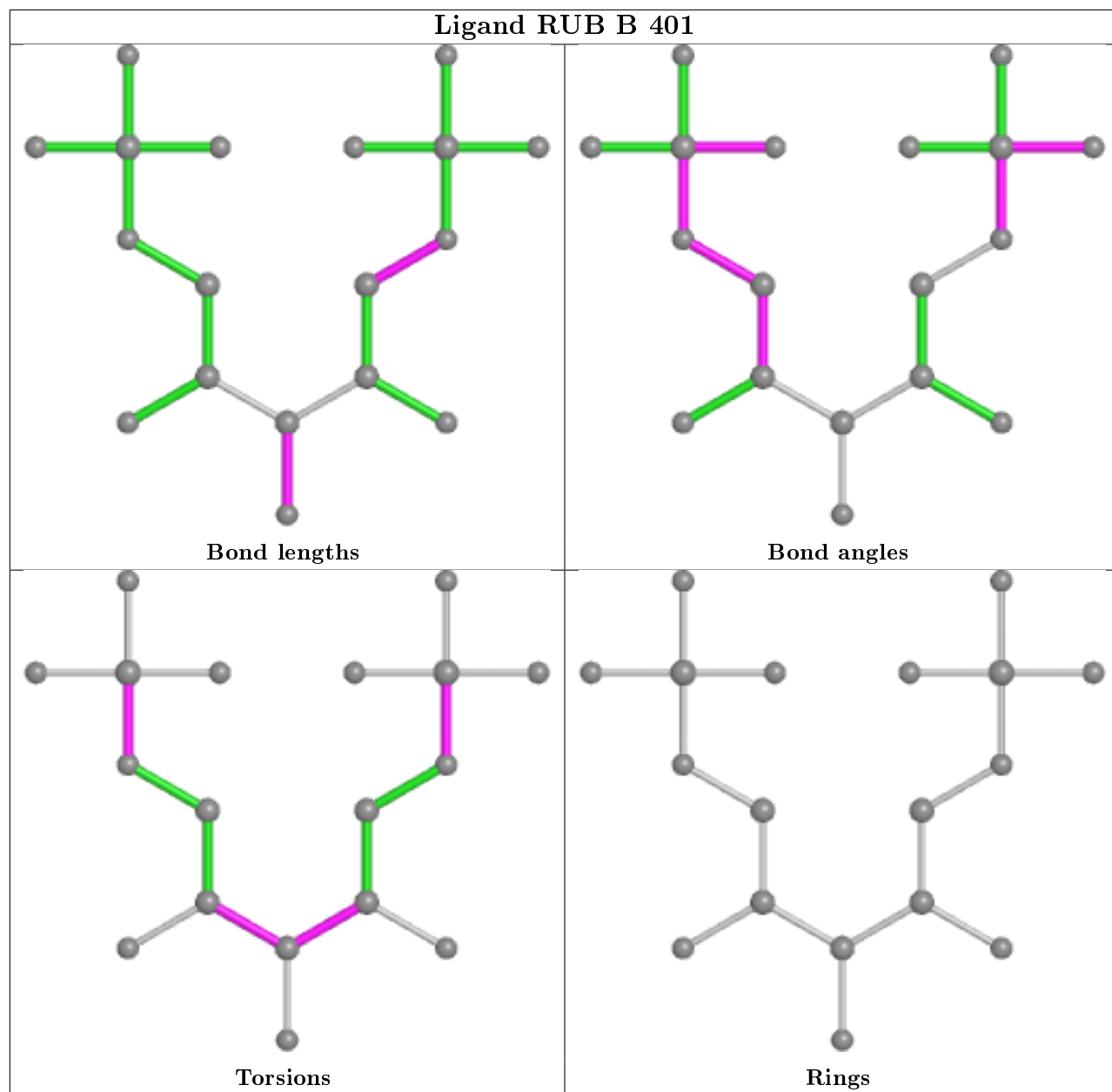
There are no ring outliers.

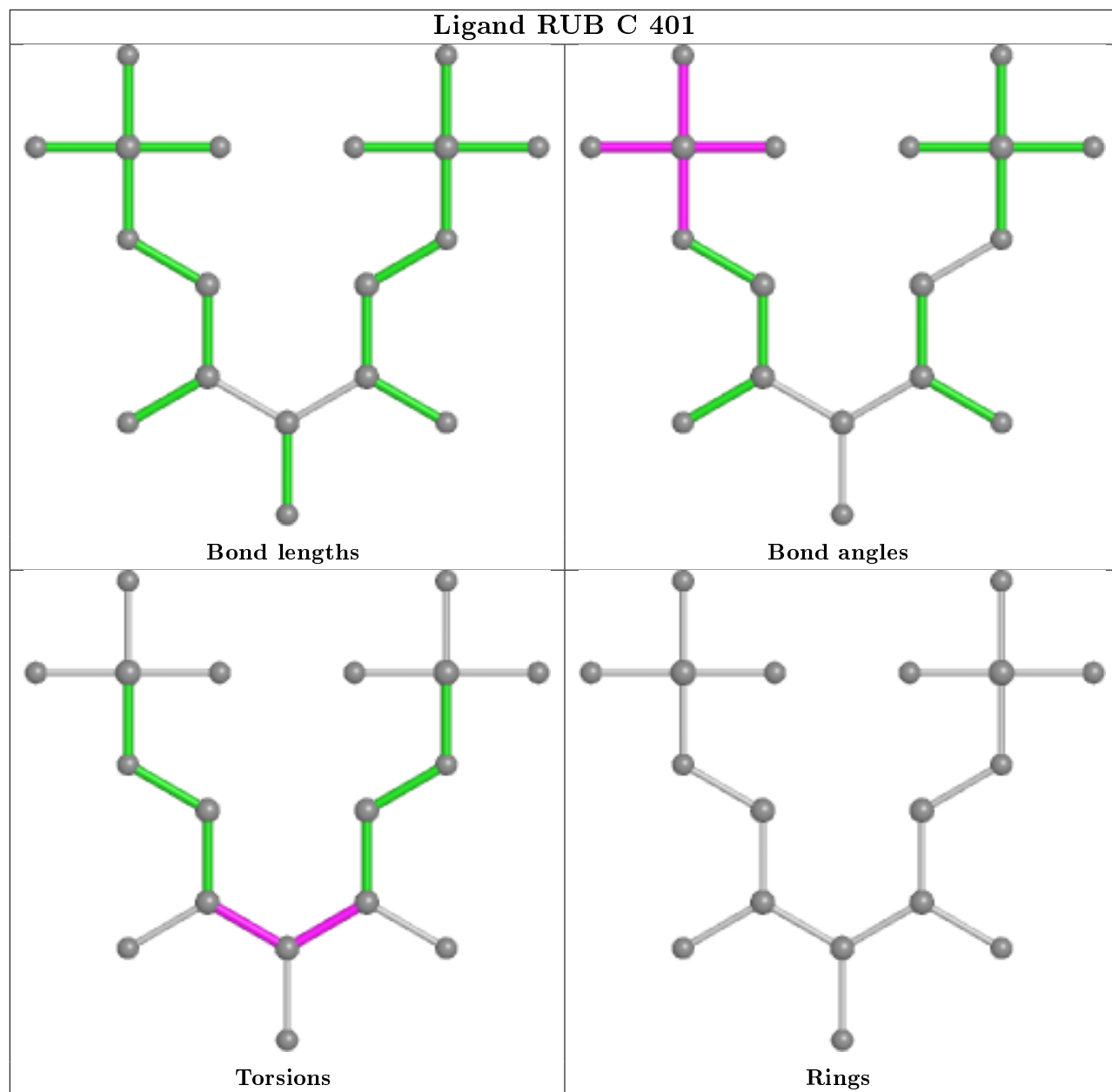
No monomer is involved in short contacts.

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

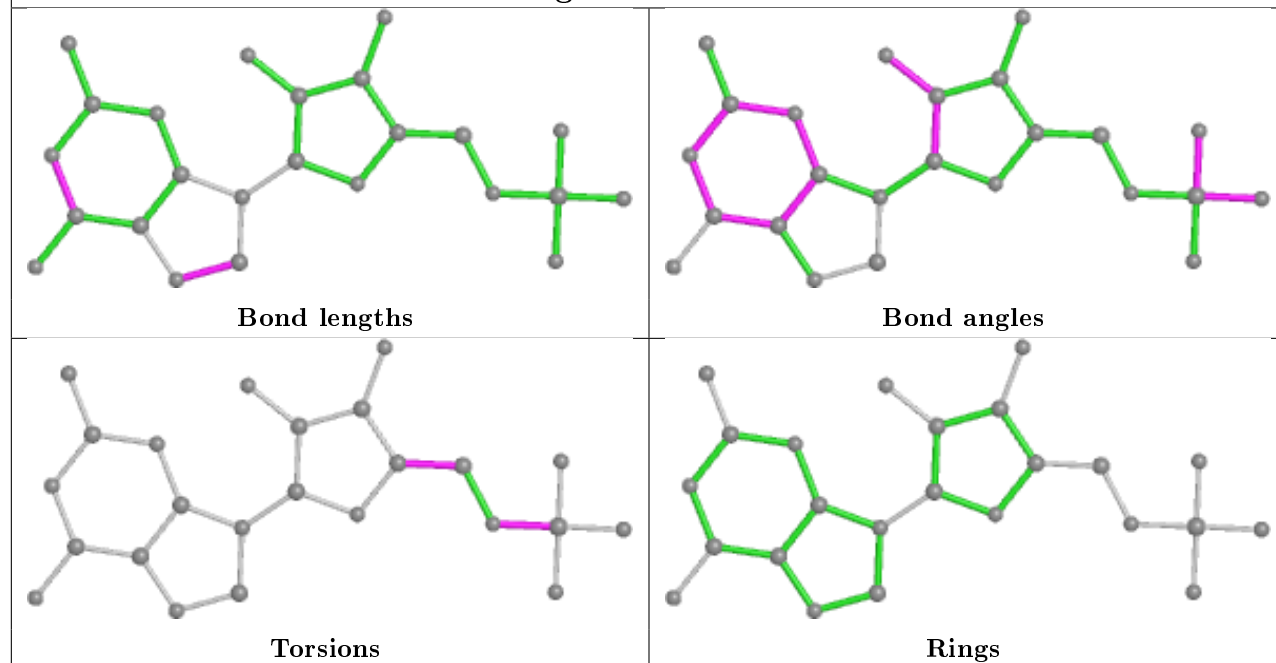
equivalents in the CSD to analyse the geometry.



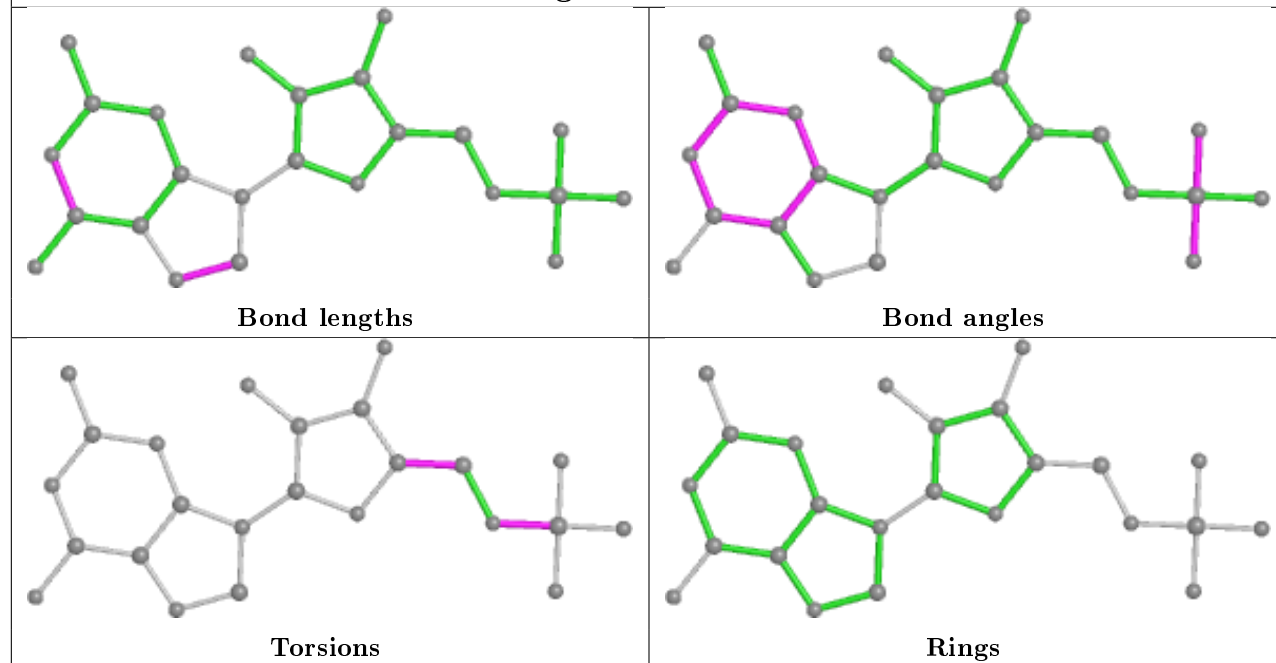




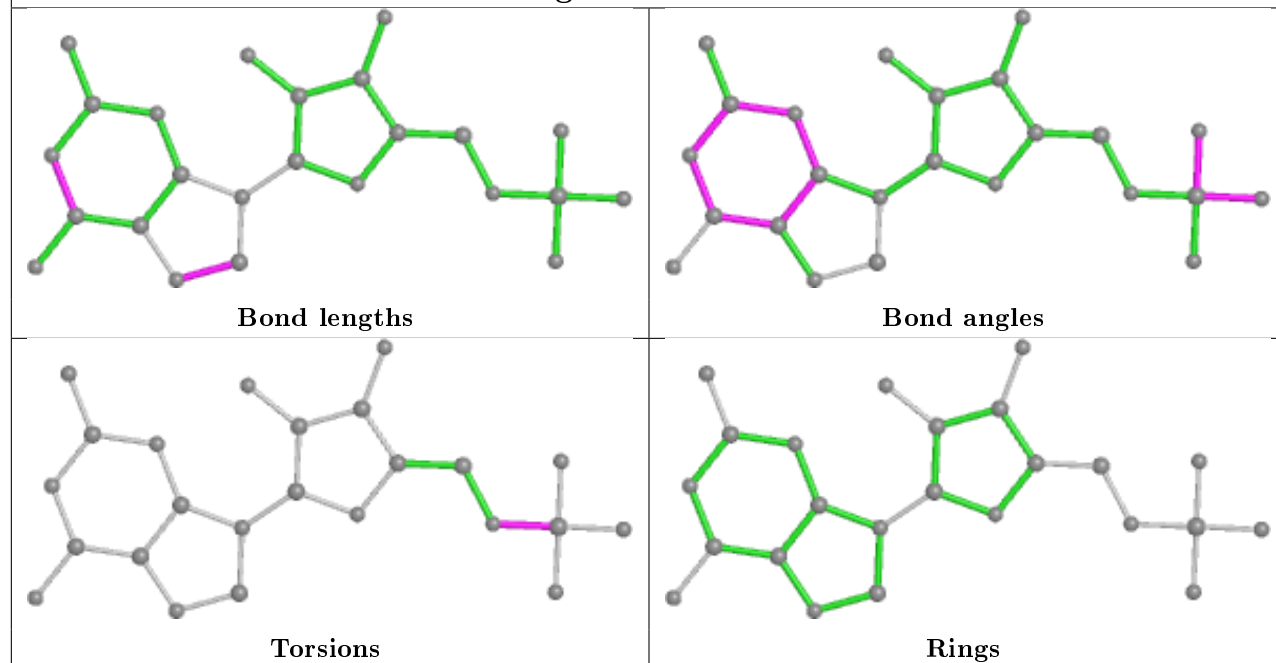
Ligand G B 405



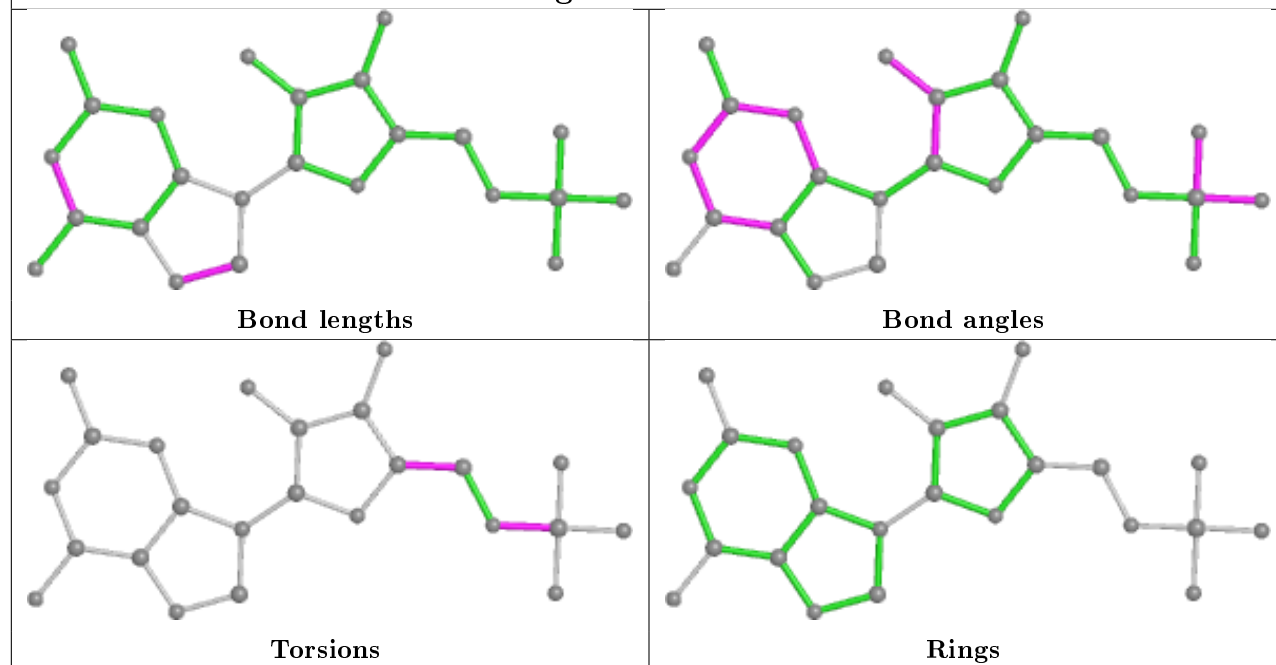
Ligand G C 403

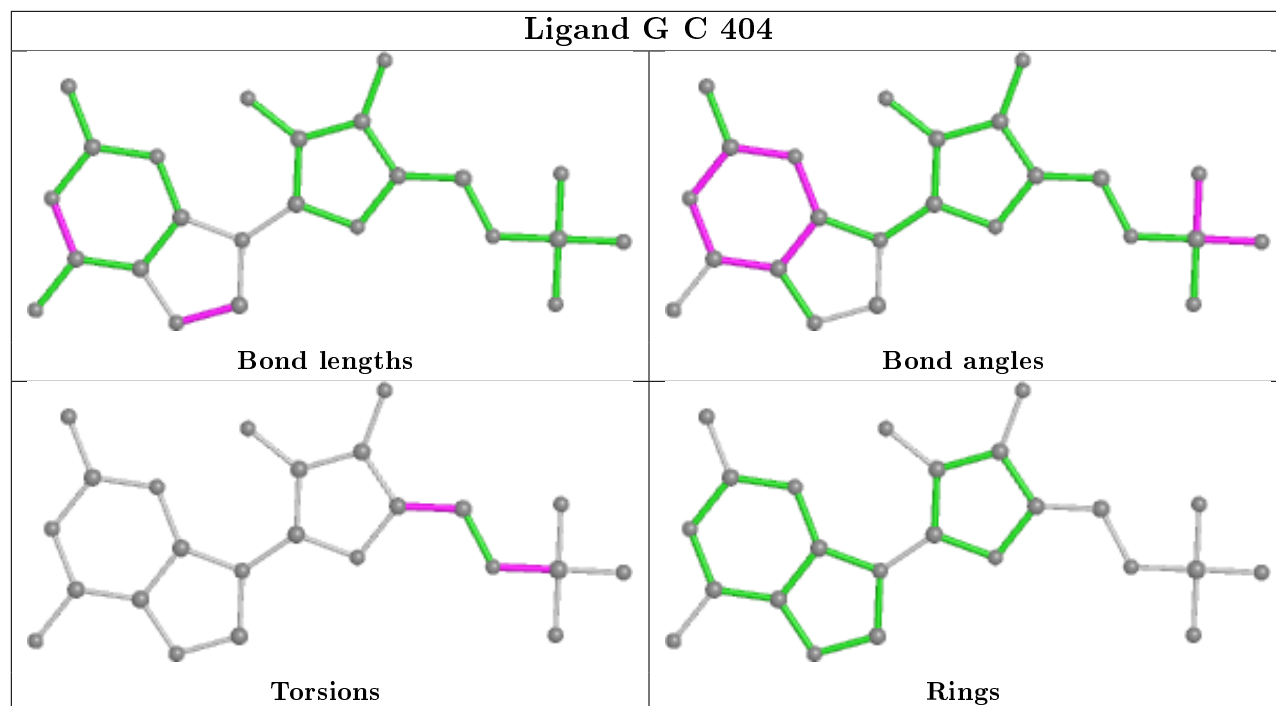


Ligand G B 404



Ligand G B 406





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	322/324 (99%)	-0.05	2 (0%) 89 92	22, 37, 70, 94	0
1	B	322/324 (99%)	-0.21	0 100 100	22, 36, 67, 93	0
1	C	322/324 (99%)	0.16	11 (3%) 45 53	27, 43, 73, 93	0
All	All	966/972 (99%)	-0.04	13 (1%) 77 84	22, 39, 71, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	PHE	3.4
1	C	314	TRP	2.9
1	A	89	GLY	2.6
1	C	102	SER	2.6
1	C	101	ASN	2.3
1	C	100	ILE	2.3
1	C	92	LEU	2.2
1	A	314	TRP	2.2
1	C	94	THR	2.2
1	C	40	GLU	2.2
1	C	99	ALA	2.1
1	C	310	GLU	2.1
1	C	95	LEU	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

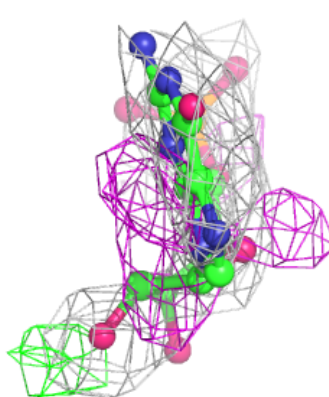
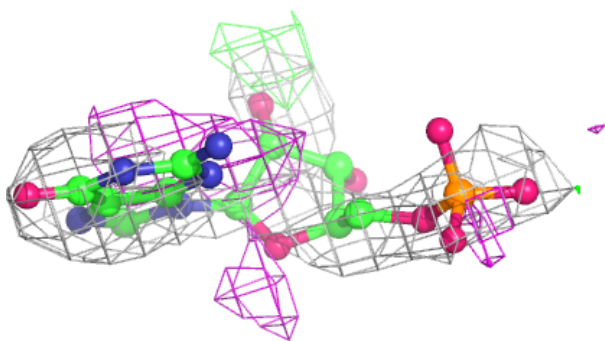
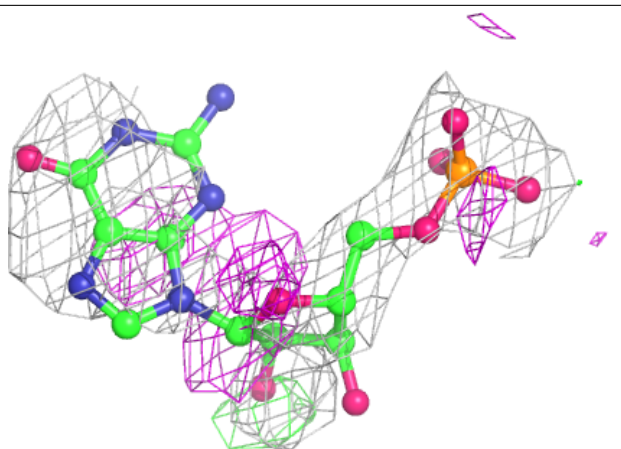
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	G	B	406	24/24	0.67	0.49	67,112,120,126	0
6	G	C	404	24/24	0.67	0.44	79,114,123,126	0
6	G	B	404	24/24	0.73	0.33	73,118,127,130	0
5	PEG	B	403	7/7	0.78	0.27	56,64,72,74	0
6	G	B	405	24/24	0.80	0.34	72,102,119,127	0
6	G	C	403	24/24	0.86	0.27	62,96,135,143	0
4	K	C	402	1/1	0.90	0.13	41,41,41,41	0
3	MPD	A	402	8/8	0.94	0.22	43,46,49,50	0
4	K	B	402	1/1	0.96	0.20	46,46,46,46	0
4	K	A	403	1/1	0.97	0.07	46,46,46,46	0
2	RUB	B	401	18/18	0.99	0.14	23,27,36,37	0
2	RUB	C	401	18/18	0.99	0.14	33,36,41,42	0
2	RUB	A	401	18/18	0.99	0.14	28,32,34,36	0

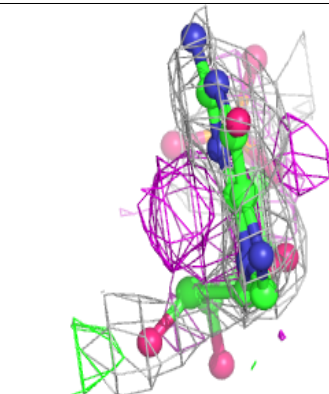
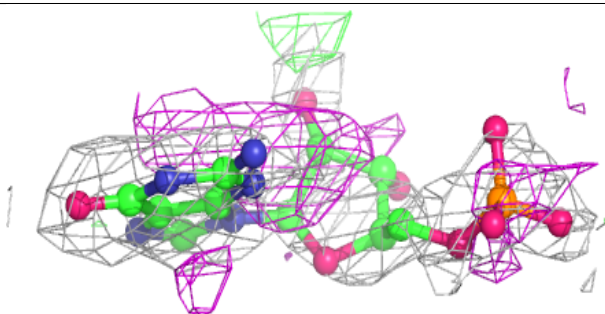
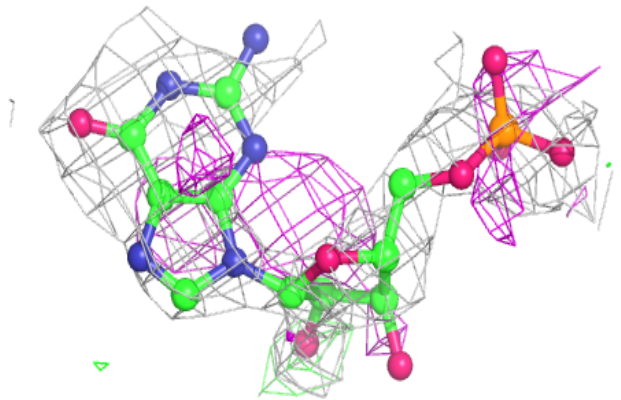
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G 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)

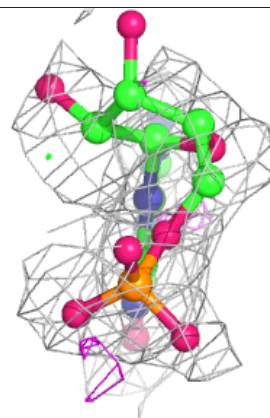
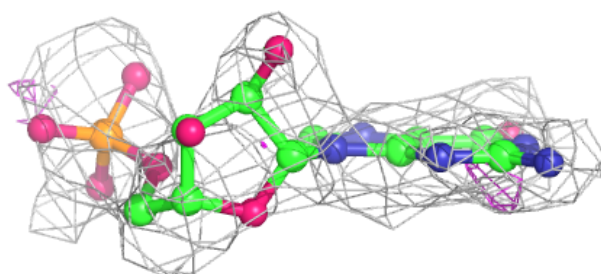
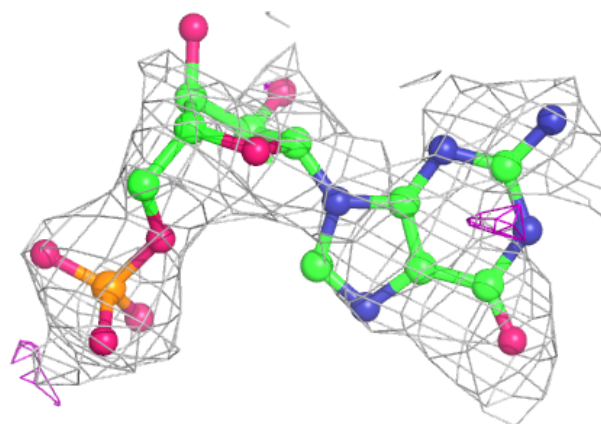
**Electron density around G C 404:**

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

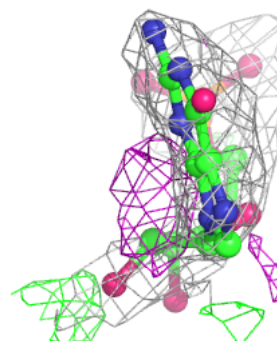
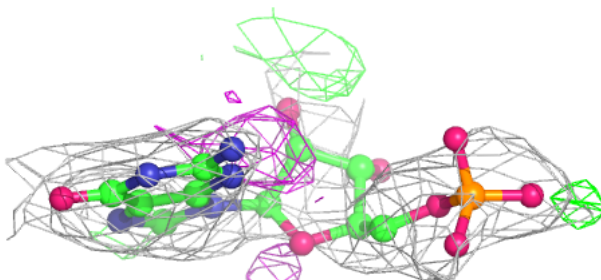
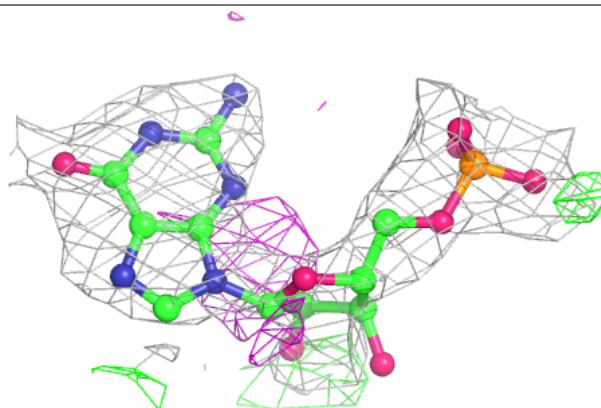


Electron density around G B 404:

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

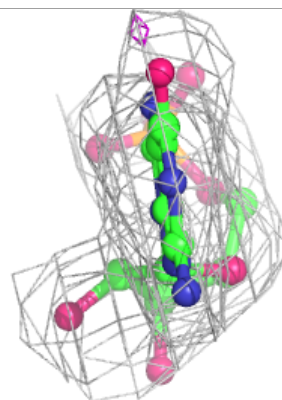
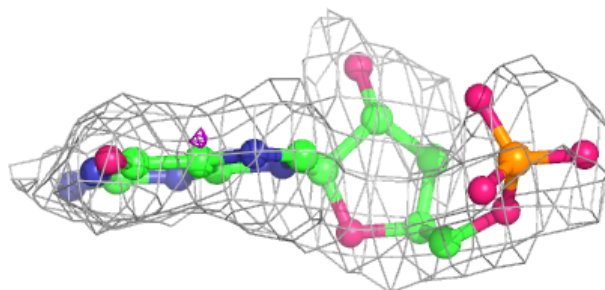
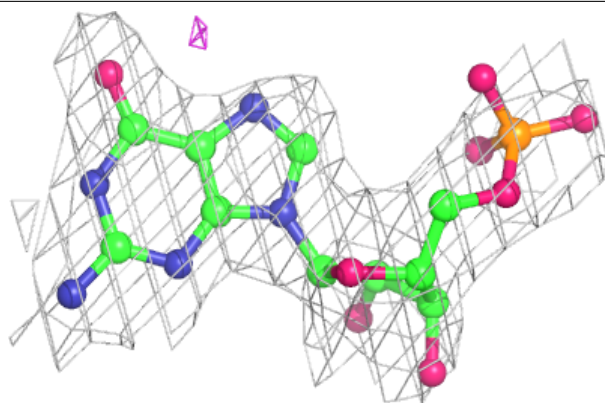
**Electron density around G B 405:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

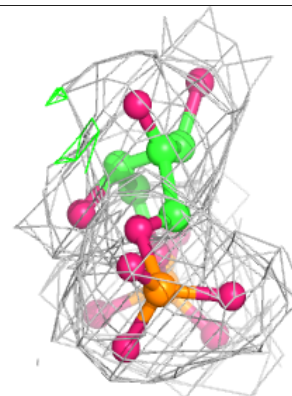
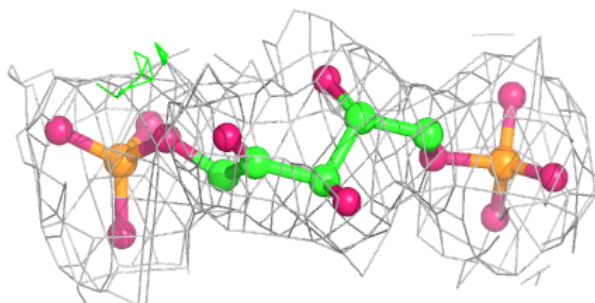
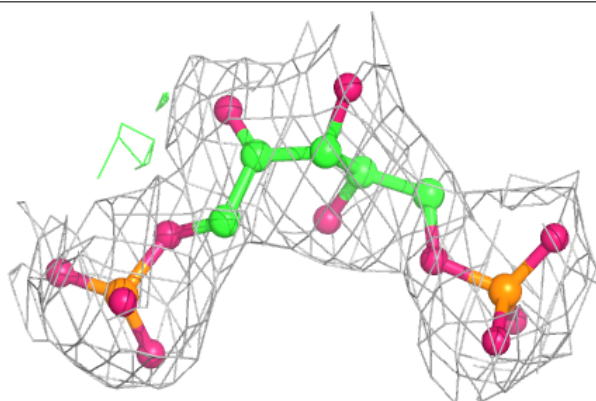


Electron density around G C 403:

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

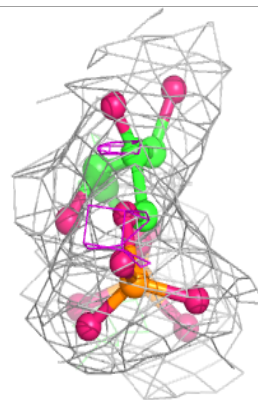
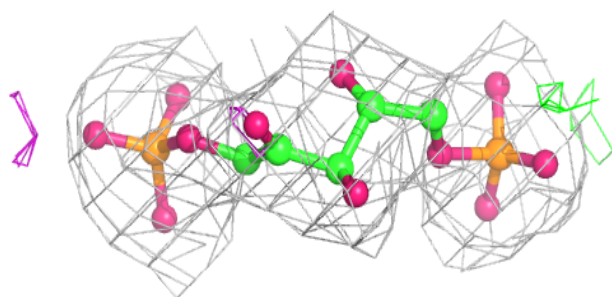
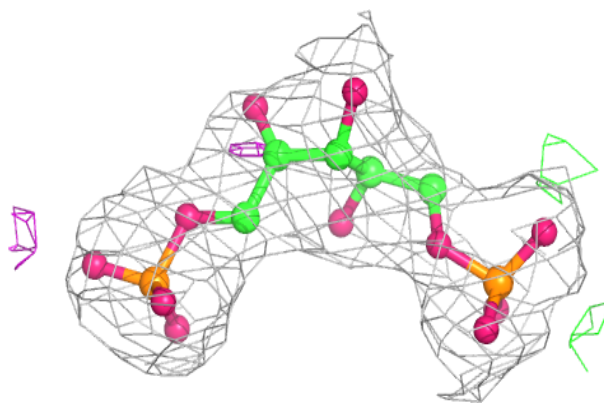
**Electron density around RUB B 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

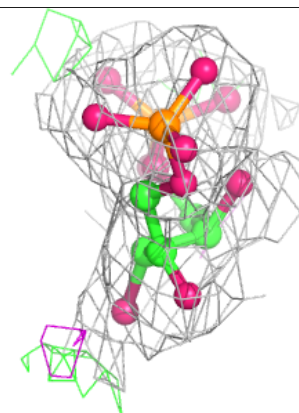
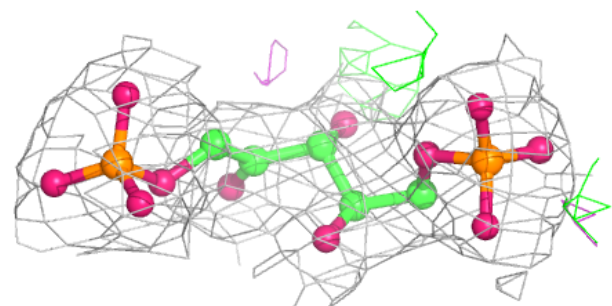
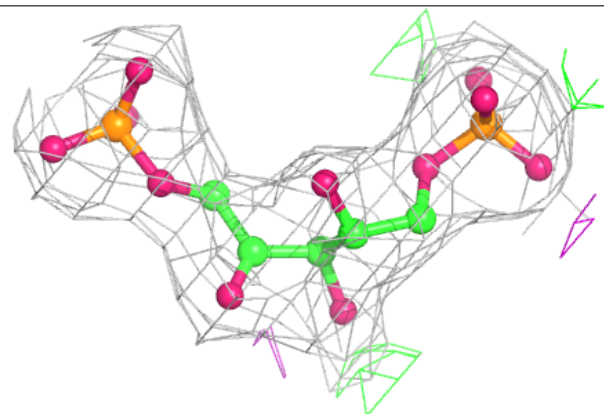


Electron density around RUB C 401:

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

**Electron density around RUB A 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

There are no such residues in this entry.