



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:56 pm BST

PDB ID : 6BNJ  
Title : Human hypoxanthine guanine phosphoribosyltransferase in complex with [3R,4R]-4-guanin-9-yl-3-((R)-2-hydroxy-2-phosphonoethyl)oxy-1-N-(phosphonopropionyl)pyrrolidine  
Authors : Keough, D.T.; Rejman, D.; Guddat, L.W.  
Deposited on : 2017-11-16  
Resolution : 1.91 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

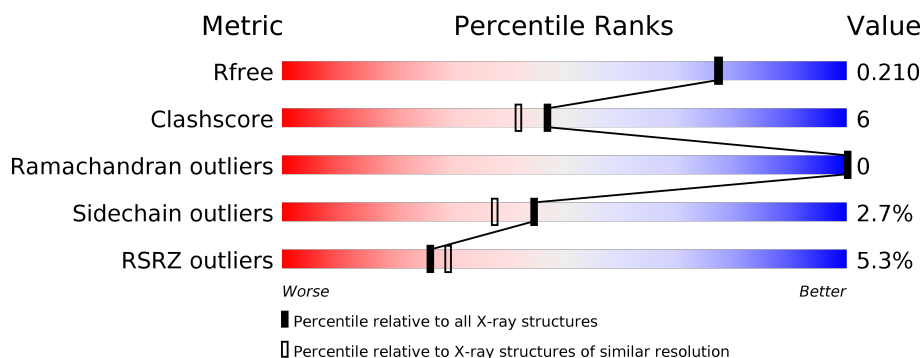
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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 on 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	218	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>
1	B	218	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	218	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 6%</div> </div> </div>
1	D	218	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7429 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.

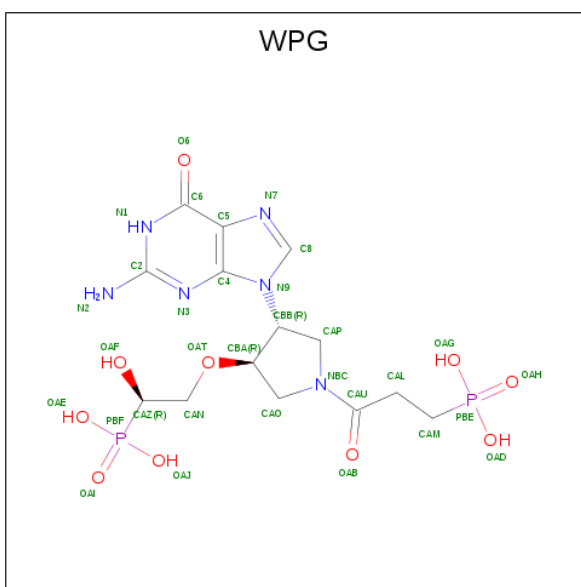
- Molecule 1 is a protein called Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	13	0
			1643	1060	276	299	8			
1	B	207	Total	C	N	O	S	0	13	0
			1700	1101	280	312	7			
1	C	204	Total	C	N	O	S	0	15	0
			1698	1098	281	311	8			
1	D	208	Total	C	N	O	S	0	12	0
			1716	1111	286	311	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	engineered mutation	UNP P00492
A	205	ALA	CYS	engineered mutation	UNP P00492
B	22	ALA	CYS	engineered mutation	UNP P00492
B	205	ALA	CYS	engineered mutation	UNP P00492
C	22	ALA	CYS	engineered mutation	UNP P00492
C	205	ALA	CYS	engineered mutation	UNP P00492
D	22	ALA	CYS	engineered mutation	UNP P00492
D	205	ALA	CYS	engineered mutation	UNP P00492

- Molecule 2 is (3-[(3R,4R)-3-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-4-[(2R)-2-hydroxy-2-phosphonoethoxy]pyrrolidin-1-yl]-3-oxopropyl)phosphonic acid (three-letter code: WPG) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>6</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 14	N 6	O 10	P 2	0	0
2	B	1	Total 32	C 14	N 6	O 10	P 2	0	0
2	C	1	Total 32	C 14	N 6	O 10	P 2	0	0
2	D	1	Total 32	C 14	N 6	O 10	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	143	Total O 143 143	0	0

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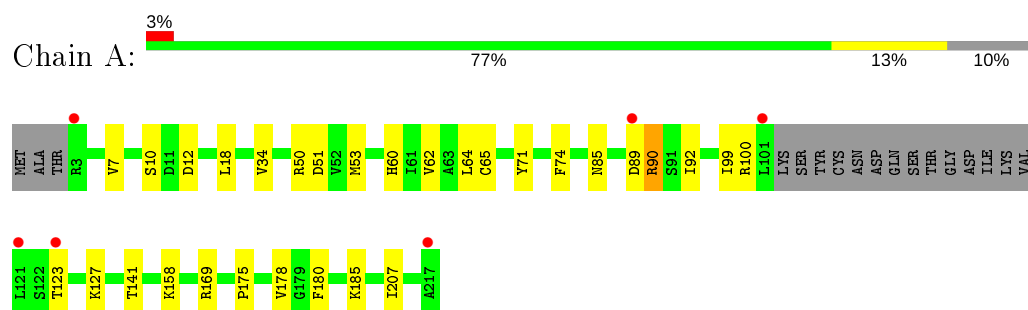
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	114	Total 114	O 114	0	0
4	C	154	Total 154	O 154	0	0
4	D	125	Total 125	O 125	0	0

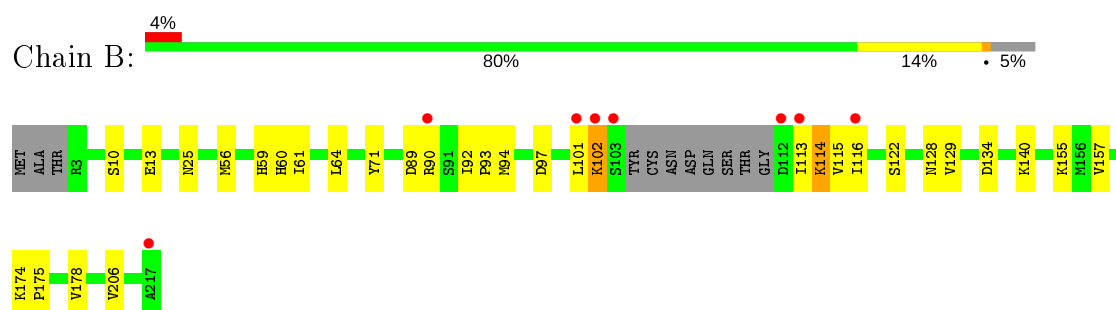
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

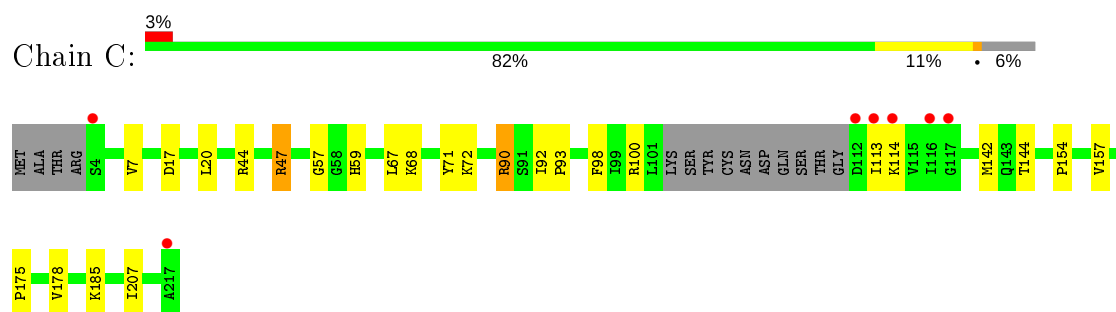
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

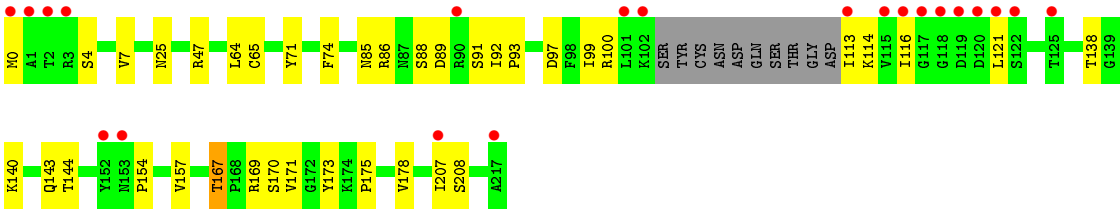


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.62Å 93.94Å 130.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.40 – 1.91 47.52 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.40-1.91) 99.8 (47.52-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.176 , 0.208 0.178 , 0.210	Depositor DCC
$R_{free}$ test set	2000 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.3	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	7429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, WPG

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	0.68	0/1714	0.74	1/2314 (0.0%)
1	B	0.69	0/1771	0.75	1/2396 (0.0%)
1	C	0.72	0/1774	0.74	1/2393 (0.0%)
1	D	0.69	0/1783	0.76	0/2406
All	All	0.70	0/7042	0.75	3/9509 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	47	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	51	ASP	CB-CG-OD1	5.59	123.33	118.30

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	1643	0	1695	20	0
1	B	1700	0	1755	24	0
1	C	1698	0	1762	18	0
1	D	1716	0	1794	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	143	0	0	8	0
4	B	114	0	0	2	0
4	C	154	0	0	3	0
4	D	125	0	0	2	0
All	All	7429	0	7006	86	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 6.

All (86) 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:68:LYS:HE3	1:C:100[B]:ARG:HH21	1.39	0.84
1:B:114:LYS:HE2	1:B:115:VAL:H	1.46	0.81
1:B:64[B]:LEU:HD23	1:B:97:ASP:HB3	1.63	0.80
4:B:434:HOH:O	1:D:25:ASN:HB2	1.83	0.78
1:A:100:ARG:HD2	4:A:443:HOH:O	1.84	0.77
1:A:175:PRO:HG2	1:A:178:VAL:HG22	1.70	0.73
1:A:10[B]:SER:OG	1:A:12[B]:ASP:OD1	2.07	0.72
1:D:113:ILE:HD13	1:D:144:THR:HG21	1.69	0.72
1:B:92[A]:ILE:HG13	1:B:93:PRO:HD2	1.72	0.70
1:D:143:GLN:NE2	1:D:171:VAL:HG11	2.08	0.68
1:C:175:PRO:HG2	1:C:178[A]:VAL:HG22	1.76	0.68
1:D:169:ARG:NH1	4:D:401:HOH:O	2.22	0.68
1:D:175:PRO:HG2	1:D:178:VAL:HG22	1.77	0.66
1:B:61[A]:ILE:HB	1:B:94:MET:HG2	1.77	0.65
1:D:207[B]:ILE:HG22	4:D:402:HOH:O	1.97	0.64
1:B:129:VAL:HB	1:B:157[B]:VAL:HG12	1.81	0.63
1:C:175:PRO:HG2	1:C:178[B]:VAL:HG12	1.81	0.62
1:A:185:LYS:NZ	4:A:402:HOH:O	2.24	0.62
1:C:113:ILE:HB	1:C:144:THR:CG2	2.30	0.61
1:C:113:ILE:HB	1:C:144:THR:HG22	1.81	0.61
1:B:56:MET:O	1:B:61[A]:ILE:HD11	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HE2	1:B:174:LYS:HA	1.82	0.60
1:C:175:PRO:HG2	1:C:178[B]:VAL:CG1	2.32	0.60
1:A:207:ILE:HG22	4:A:409:HOH:O	2.05	0.57
1:A:89[A]:ASP:OD1	1:A:90:ARG:N	2.38	0.57
1:C:57:GLY:O	1:C:90[B]:ARG:NH2	2.29	0.55
1:C:92:ILE:HG13	1:C:93:PRO:HD2	1.87	0.55
1:A:141:THR:HG21	4:A:456:HOH:O	2.05	0.55
1:B:206:VAL:HG13	4:B:404:HOH:O	2.05	0.55
1:B:25[A]:ASN:ND2	1:D:89:ASP:O	2.40	0.55
1:D:171:VAL:HG13	1:D:173:TYR:H	1.72	0.55
1:D:65:CYS:HB2	1:D:74:PHE:CD1	2.42	0.54
1:B:114:LYS:CE	1:B:115:VAL:H	2.15	0.54
1:B:89:ASP:O	1:D:25:ASN:ND2	2.36	0.54
1:B:102:LYS:HB3	1:B:116:ILE:HD12	1.91	0.53
1:A:60:HIS:CD2	1:A:127:LYS:HD3	2.43	0.53
1:C:185:LYS:NZ	4:C:404:HOH:O	2.41	0.52
1:D:64[A]:LEU:HD11	1:D:99:ILE:HG23	1.91	0.52
1:A:62:VAL:HG21	1:A:123:THR:O	2.08	0.52
1:D:207[A]:ILE:HG22	1:D:208:SER:O	2.10	0.52
1:B:61[A]:ILE:HD13	1:B:128:ASN:HB2	1.92	0.52
1:D:143:GLN:HE22	1:D:171:VAL:HG11	1.74	0.52
1:B:10:SER:OG	1:B:13[A]:GLU:HG3	2.11	0.51
1:B:61[B]:ILE:HB	1:B:94:MET:HG2	1.93	0.50
1:B:101:LEU:HB3	1:B:113:ILE:HG21	1.93	0.50
1:B:175:PRO:HG2	1:B:178:VAL:HG22	1.93	0.49
1:D:85:ASN:OD1	1:D:91:SER:HB2	2.13	0.49
1:D:100:ARG:HB3	1:D:116[B]:ILE:CG2	2.43	0.48
1:B:64[B]:LEU:CD2	1:B:97:ASP:HB3	2.37	0.48
1:D:88[B]:SER:OG	1:D:89:ASP:N	2.46	0.48
1:C:68:LYS:HE3	1:C:100[B]:ARG:NH2	2.20	0.47
1:D:100:ARG:O	1:D:116[B]:ILE:HG22	2.15	0.47
1:C:17:ASP:HA	4:C:481:HOH:O	2.15	0.46
1:A:169:ARG:NH1	4:A:403:HOH:O	2.28	0.46
1:C:67:LEU:HB2	1:C:100[A]:ARG:HG2	1.96	0.46
1:A:53[B]:MET:SD	1:A:92[B]:ILE:HD11	2.55	0.46
1:A:65:CYS:HB2	1:A:74:PHE:CD1	2.51	0.45
1:C:207:ILE:HG22	4:C:411:HOH:O	2.15	0.45
1:D:154:PRO:HG3	1:D:157:VAL:HG22	1.99	0.45
1:D:171:VAL:HG22	1:D:171:VAL:O	2.18	0.44
1:D:0:MET:HB3	1:D:47:ARG:HH22	1.82	0.44
1:D:0:MET:HB3	1:D:47:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:NH1	1:D:86:ARG:O	2.51	0.44
1:A:7:VAL:HB	1:A:180:PHE:CD2	2.53	0.43
1:D:138:THR:OG1	1:D:140:LYS:HG3	2.18	0.43
1:A:18:LEU:HD23	1:A:34:VAL:HG23	1.99	0.43
1:B:102:LYS:HE2	1:B:102:LYS:HB2	1.80	0.43
1:B:101:LEU:HB3	1:B:113:ILE:CG2	2.48	0.43
1:B:59[B]:HIS:CD2	1:B:155:LYS:HE2	2.53	0.43
1:B:60:HIS:C	1:B:60:HIS:CD2	2.92	0.43
1:A:64:LEU:HD11	1:A:99[A]:ILE:HG23	2.01	0.42
1:C:154:PRO:HG3	1:C:157:VAL:HG22	2.00	0.42
1:B:64[B]:LEU:CD1	1:B:129:VAL:HG13	2.49	0.42
1:D:167:THR:HG23	1:D:170:SER:HB3	2.01	0.42
1:C:67:LEU:HD11	1:C:98:PHE:HB3	2.01	0.42
1:D:65:CYS:HB2	1:D:74:PHE:CG	2.54	0.42
1:A:85:ASN:ND2	4:A:417:HOH:O	2.54	0.41
1:B:64[B]:LEU:HD12	1:B:129:VAL:HG13	2.01	0.41
1:C:20:LEU:HD13	1:D:7:VAL:HG22	2.02	0.41
1:C:7:VAL:HG23	1:C:44:ARG:HD3	2.02	0.41
1:D:64[B]:LEU:CD2	1:D:97:ASP:HB3	2.51	0.41
1:A:50:ARG:NH2	4:A:416:HOH:O	2.54	0.41
1:A:175:PRO:HG2	1:A:178:VAL:CG2	2.45	0.41
1:C:59:HIS:C	1:C:92:ILE:HG12	2.41	0.41
1:D:92[B]:ILE:HG13	1:D:93:PRO:HD2	2.03	0.41
1:A:158:LYS:HE2	4:A:520:HOH:O	2.20	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	206/218 (94%)	200 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
1	C	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
1	D	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	853/872 (98%)	832 (98%)	21 (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	186/190 (98%)	184 (99%)	2 (1%)	73	73
1	B	192/190 (101%)	185 (96%)	7 (4%)	35	26
1	C	192/190 (101%)	184 (96%)	8 (4%)	30	20
1	D	193/190 (102%)	188 (97%)	5 (3%)	46	39
All	All	763/760 (100%)	741 (97%)	22 (3%)	44	35

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	90	ARG
1	B	71	TYR
1	B	90	ARG
1	B	102	LYS
1	B	114	LYS
1	B	122[A]	SER
1	B	122[B]	SER
1	B	140	LYS
1	C	47	ARG
1	C	71	TYR
1	C	72	LYS
1	C	90[A]	ARG

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Mol	Chain	Res	Type
1	C	90[B]	ARG
1	C	114	LYS
1	C	142[A]	MET
1	C	142[B]	MET
1	D	4	SER
1	D	71	TYR
1	D	114	LYS
1	D	121	LEU
1	D	167	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	GLN
1	D	151	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	WPG	B	301	3	28,34,34	2.57	10 (35%)	33,52,52	2.63	16 (48%)
2	WPG	C	301	3	28,34,34	2.66	9 (32%)	33,52,52	2.37	11 (33%)
2	WPG	A	301	3	28,34,34	2.71	12 (42%)	33,52,52	2.44	13 (39%)
2	WPG	D	301	3	28,34,34	2.99	12 (42%)	33,52,52	2.53	12 (36%)

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	WPG	B	301	3	-	3/17/37/37	0/3/3/3
2	WPG	C	301	3	-	3/17/37/37	0/3/3/3
2	WPG	A	301	3	-	3/17/37/37	0/3/3/3
2	WPG	D	301	3	-	3/17/37/37	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	WPG	PBF-OAE	-8.57	1.41	1.54
2	D	301	WPG	OAF-CAZ	-7.08	1.33	1.41
2	C	301	WPG	PBE-CAM	6.49	1.85	1.78
2	A	301	WPG	PBE-CAM	6.42	1.85	1.78
2	C	301	WPG	O6-C6	5.43	1.38	1.24
2	A	301	WPG	O6-C6	5.39	1.38	1.24
2	B	301	WPG	PBE-CAM	5.35	1.84	1.78
2	B	301	WPG	O6-C6	5.25	1.37	1.24
2	A	301	WPG	C2-N2	5.24	1.44	1.33
2	A	301	WPG	PBF-OAI	5.13	1.58	1.49
2	B	301	WPG	CAU-NBC	5.12	1.45	1.35
2	C	301	WPG	CAU-NBC	4.83	1.45	1.35
2	A	301	WPG	CAU-NBC	4.71	1.44	1.35
2	D	301	WPG	CAU-NBC	4.54	1.44	1.35
2	C	301	WPG	PBF-OAI	4.53	1.57	1.49
2	C	301	WPG	C2-N2	4.53	1.43	1.33
2	B	301	WPG	C2-N2	4.25	1.42	1.33
2	B	301	WPG	PBF-OAI	4.20	1.56	1.49
2	D	301	WPG	PBF-OAJ	-4.03	1.48	1.54
2	A	301	WPG	PBE-OAH	3.91	1.58	1.50
2	D	301	WPG	O6-C6	3.80	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	WPG	PBE-CAM	3.79	1.82	1.78
2	B	301	WPG	PBE-OAH	3.59	1.57	1.50
2	C	301	WPG	PBE-OAH	3.49	1.57	1.50
2	D	301	WPG	PBE-OAD	-3.26	1.47	1.54
2	B	301	WPG	PBF-OAE	-3.26	1.49	1.54
2	C	301	WPG	C4-N3	3.14	1.40	1.35
2	B	301	WPG	OAF-CAZ	-3.04	1.38	1.41
2	D	301	WPG	OAT-CBA	-2.97	1.37	1.43
2	D	301	WPG	CAO-CBA	-2.86	1.46	1.52
2	D	301	WPG	C2-N2	2.79	1.39	1.33
2	A	301	WPG	OAF-CAZ	-2.79	1.38	1.41
2	A	301	WPG	C4-N3	2.59	1.39	1.35
2	D	301	WPG	CAP-CBB	-2.54	1.47	1.54
2	C	301	WPG	PBF-OAE	-2.45	1.51	1.54
2	B	301	WPG	C4-N3	2.39	1.39	1.35
2	B	301	WPG	PBF-OAJ	2.37	1.58	1.54
2	A	301	WPG	CAO-CBA	-2.34	1.47	1.52
2	D	301	WPG	OAT-CAN	-2.31	1.39	1.43
2	A	301	WPG	C6-N1	2.12	1.36	1.33
2	C	301	WPG	PBE-OAD	-2.07	1.50	1.54
2	A	301	WPG	PBF-OAE	-2.04	1.51	1.54
2	A	301	WPG	OAT-CBA	-2.03	1.39	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	WPG	OAT-CAN-CAZ	5.88	119.16	108.39
2	C	301	WPG	OAT-CAN-CAZ	5.30	118.10	108.39
2	A	301	WPG	N3-C2-N1	-5.15	120.35	127.22
2	C	301	WPG	N3-C2-N1	-5.07	120.46	127.22
2	B	301	WPG	N3-C2-N1	-4.98	120.58	127.22
2	D	301	WPG	N3-C2-N1	-4.86	120.73	127.22
2	C	301	WPG	C6-N1-C2	4.76	123.50	115.93
2	B	301	WPG	C6-N1-C2	4.74	123.45	115.93
2	A	301	WPG	CAP-CBB-N9	4.73	122.89	113.33
2	C	301	WPG	CAP-CBB-N9	4.61	122.64	113.33
2	B	301	WPG	OAT-CAN-CAZ	4.58	116.80	108.39
2	D	301	WPG	CAP-CBB-N9	4.54	122.51	113.33
2	B	301	WPG	CAN-OAT-CBA	4.44	121.56	115.15
2	A	301	WPG	OAT-CAN-CAZ	4.44	116.53	108.39
2	A	301	WPG	C2-N3-C4	4.41	120.39	115.36
2	D	301	WPG	C6-N1-C2	4.40	122.92	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	WPG	CAN-OAT-CBA	4.32	121.38	115.15
2	C	301	WPG	C5-C6-N1	-4.30	117.55	123.43
2	B	301	WPG	CAP-CBB-N9	4.20	121.82	113.33
2	D	301	WPG	C2-N3-C4	4.17	120.12	115.36
2	B	301	WPG	C5-C6-N1	-4.09	117.83	123.43
2	A	301	WPG	C6-N1-C2	4.01	122.31	115.93
2	D	301	WPG	C5-C6-N1	-3.97	118.00	123.43
2	A	301	WPG	OAH-PBE-CAM	-3.76	104.45	111.40
2	C	301	WPG	C2-N3-C4	3.53	119.39	115.36
2	B	301	WPG	OAH-PBE-CAM	-3.41	105.08	111.40
2	B	301	WPG	C6-C5-C4	-3.35	117.60	120.80
2	B	301	WPG	OAI-PBF-CAZ	-3.29	104.96	112.94
2	B	301	WPG	C2-N3-C4	3.29	119.11	115.36
2	A	301	WPG	C5-C6-N1	-3.27	118.95	123.43
2	A	301	WPG	OAI-PBF-CAZ	-3.26	105.01	112.94
2	B	301	WPG	PBF-CAZ-CAN	3.14	116.71	111.51
2	C	301	WPG	OAD-PBE-CAM	3.14	114.34	106.95
2	A	301	WPG	C6-C5-C4	-3.12	117.82	120.80
2	B	301	WPG	CAP-NBC-CAO	-3.09	106.72	112.81
2	B	301	WPG	OAB-CAU-NBC	-2.99	116.22	122.05
2	B	301	WPG	CAL-CAU-NBC	2.94	122.60	118.01
2	C	301	WPG	OAI-PBF-CAZ	-2.91	105.88	112.94
2	A	301	WPG	CAN-OAT-CBA	2.80	119.20	115.15
2	B	301	WPG	OAG-PBE-CAM	2.58	113.02	106.95
2	A	301	WPG	OAT-CBA-CAO	-2.49	106.90	112.02
2	D	301	WPG	OAH-PBE-CAM	2.47	115.97	111.40
2	A	301	WPG	OAD-PBE-CAM	2.45	112.70	106.95
2	C	301	WPG	C6-C5-C4	-2.38	118.52	120.80
2	D	301	WPG	CAP-NBC-CAO	-2.30	108.27	112.81
2	D	301	WPG	C6-C5-C4	-2.28	118.62	120.80
2	D	301	WPG	OAD-PBE-OAH	-2.25	106.45	112.39
2	A	301	WPG	CAP-NBC-CAO	-2.13	108.62	112.81
2	C	301	WPG	OAB-CAU-NBC	-2.06	118.04	122.05
2	C	301	WPG	CAP-NBC-CAO	-2.05	108.76	112.81
2	D	301	WPG	OAG-PBE-CAM	2.01	111.69	106.95
2	B	301	WPG	CAO-NBC-CAU	2.00	129.35	123.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	WPG	CBB-CBA-OAT-CAN

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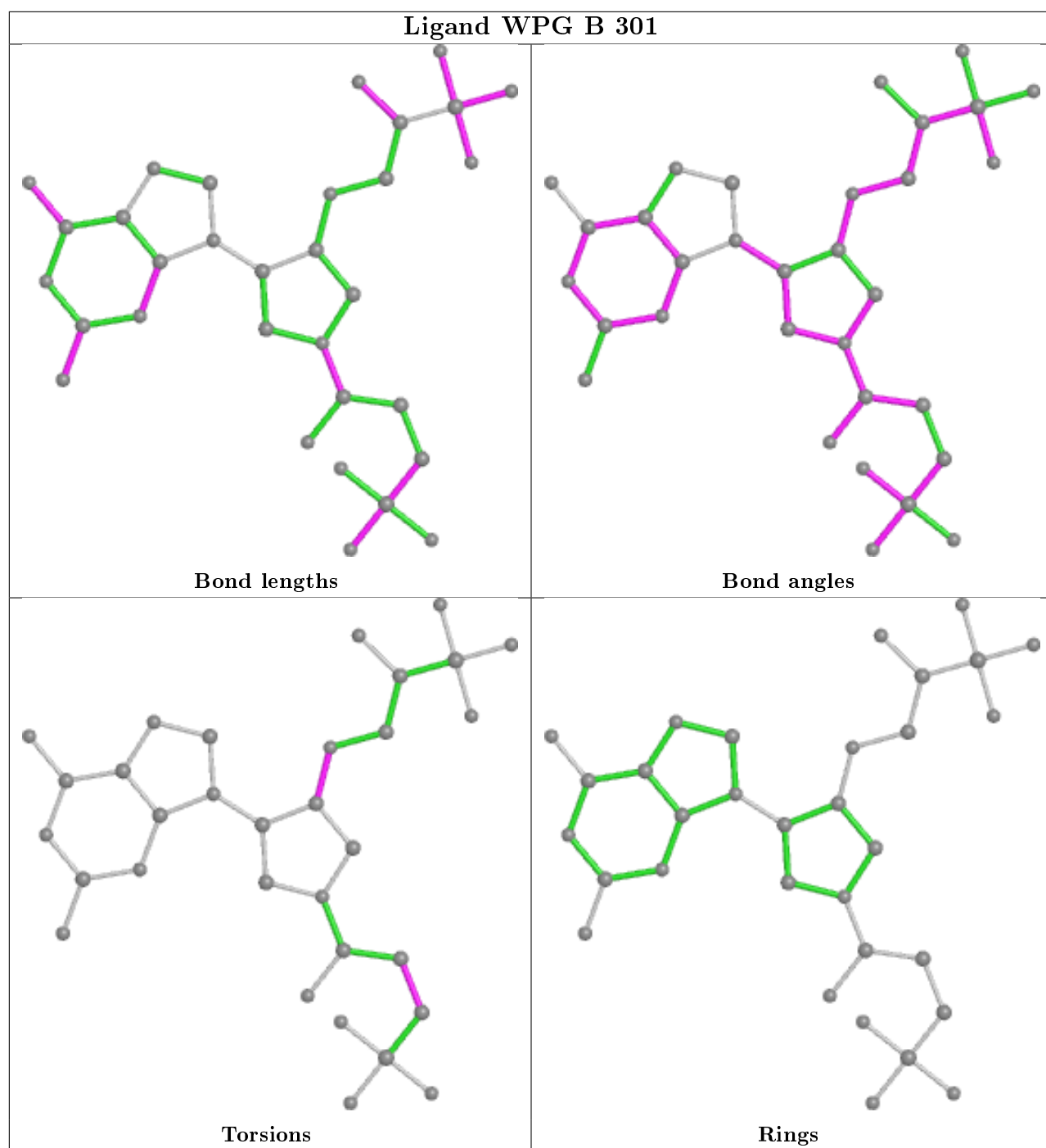
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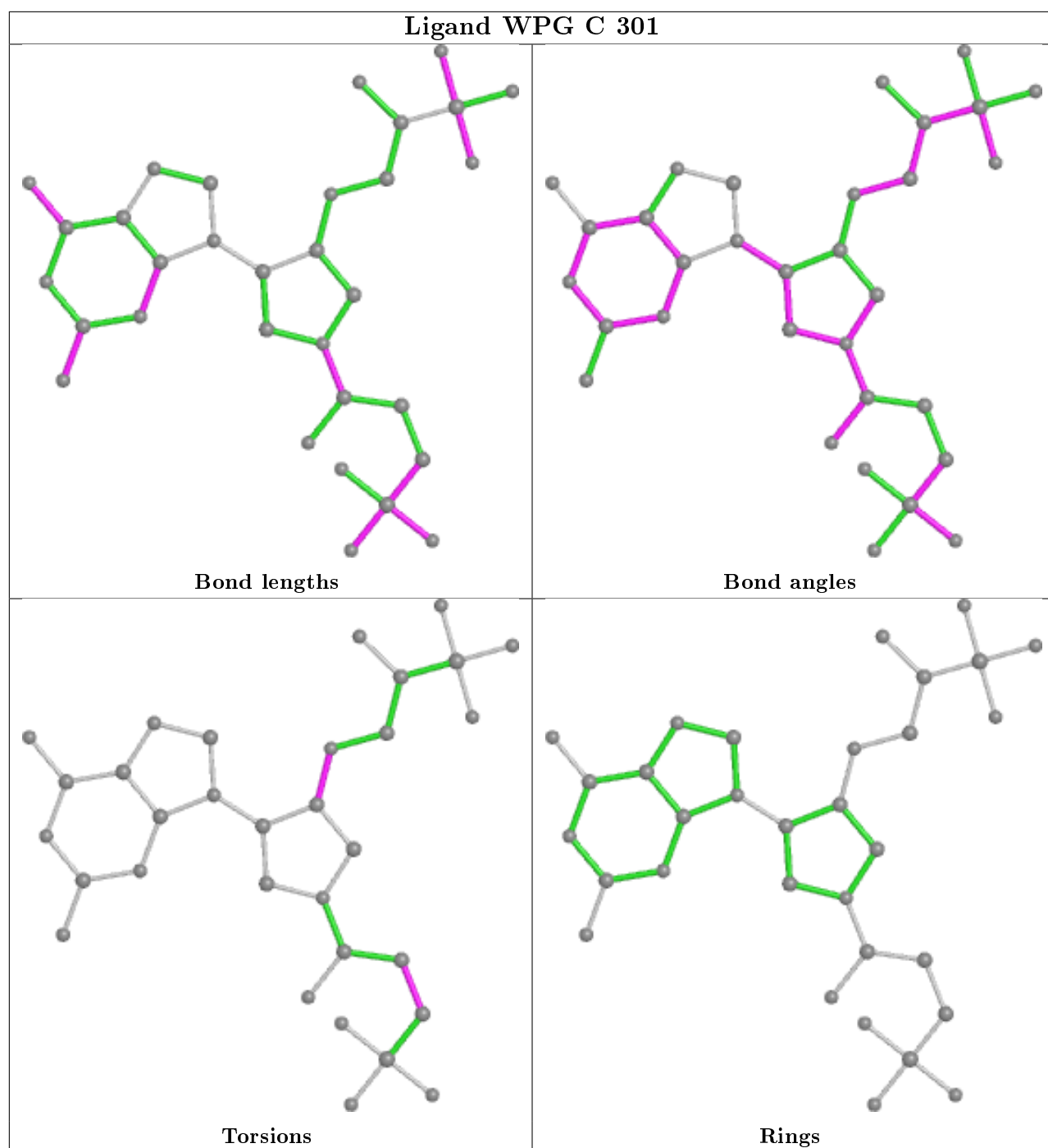
Mol	Chain	Res	Type	Atoms
2	C	301	WPG	CAU-CAL-CAM-PBE
2	D	301	WPG	CAU-CAL-CAM-PBE
2	C	301	WPG	CAO-CBA-OAT-CAN
2	A	301	WPG	CAO-CBA-OAT-CAN
2	B	301	WPG	CAO-CBA-OAT-CAN
2	D	301	WPG	CAO-CBA-OAT-CAN
2	A	301	WPG	CAU-CAL-CAM-PBE
2	B	301	WPG	CAU-CAL-CAM-PBE
2	A	301	WPG	CBB-CBA-OAT-CAN
2	B	301	WPG	CBB-CBA-OAT-CAN
2	D	301	WPG	CBB-CBA-OAT-CAN

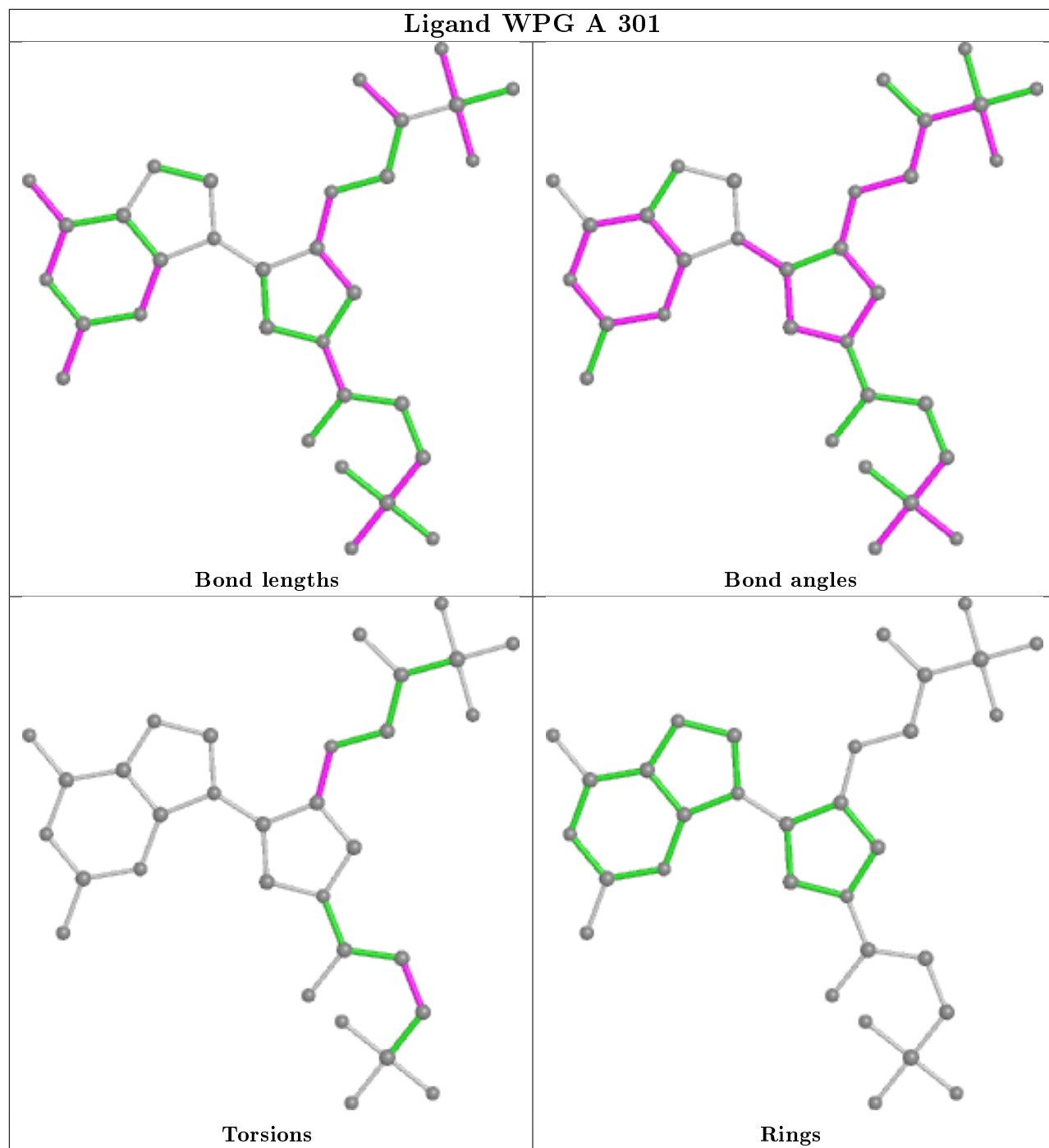
There are no ring outliers.

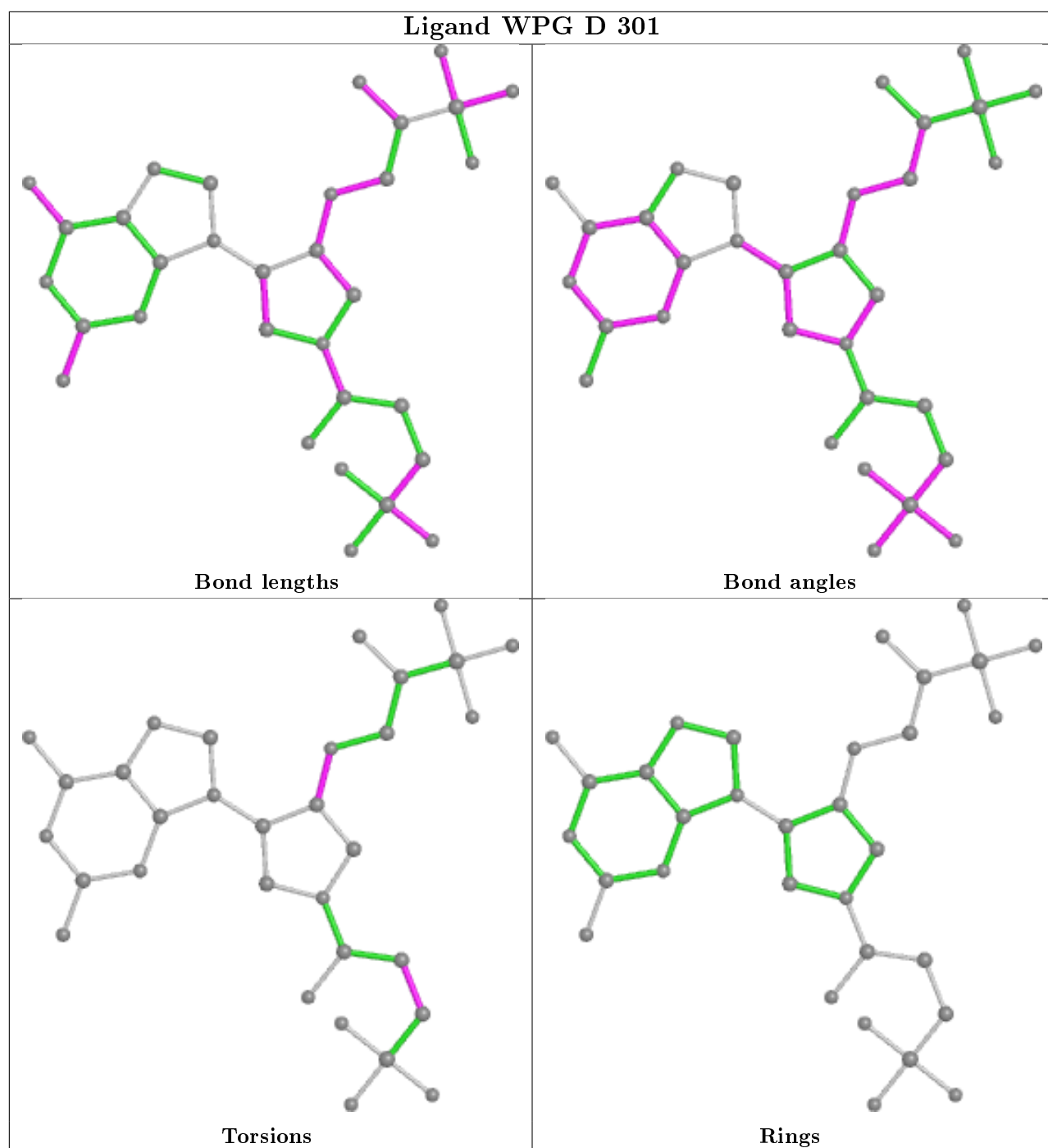
No monomer is involved in short contacts.

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	197/218 (90%)	0.02	7 (3%) 42 45	10, 19, 41, 59	0
1	B	207/218 (94%)	0.13	8 (3%) 39 42	10, 22, 43, 74	0
1	C	204/218 (93%)	0.06	7 (3%) 45 48	9, 19, 40, 52	0
1	D	208/218 (95%)	0.37	21 (10%) 7 8	9, 22, 51, 62	0
All	All	816/872 (93%)	0.15	43 (5%) 26 29	9, 21, 45, 74	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	121	LEU	7.1
1	B	217	ALA	6.8
1	C	4	SER	6.4
1	C	217	ALA	4.7
1	D	152	TYR	4.6
1	D	113	ILE	4.4
1	D	119	ASP	4.4
1	D	217	ALA	3.9
1	B	112	ASP	3.9
1	D	120	ASP	3.8
1	C	113	ILE	3.7
1	A	120	ASP	3.6
1	A	101	LEU	3.6
1	C	117	GLY	3.3
1	D	0	MET	3.2
1	B	113	ILE	3.1
1	D	2	THR	3.1
1	D	101	LEU	3.0
1	C	114	LYS	3.0
1	D	116[A]	ILE	2.9
1	D	153	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	102	LYS	2.9
1	D	118	GLY	2.8
1	A	121	LEU	2.8
1	D	122	SER	2.7
1	A	217	ALA	2.6
1	D	1	ALA	2.6
1	D	90[A]	ARG	2.6
1	B	116	ILE	2.6
1	B	101	LEU	2.5
1	C	112	ASP	2.5
1	A	123	THR	2.4
1	D	117	GLY	2.4
1	A	89[A]	ASP	2.4
1	B	102	LYS	2.4
1	D	207[A]	ILE	2.3
1	B	90	ARG	2.3
1	D	3	ARG	2.3
1	D	115	VAL	2.2
1	B	103	SER	2.2
1	D	125	THR	2.0
1	A	3	ARG	2.0
1	C	116	ILE	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 carbohydrates 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, 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
3	MG	B	302	1/1	0.71	0.18	41,41,41,41	0

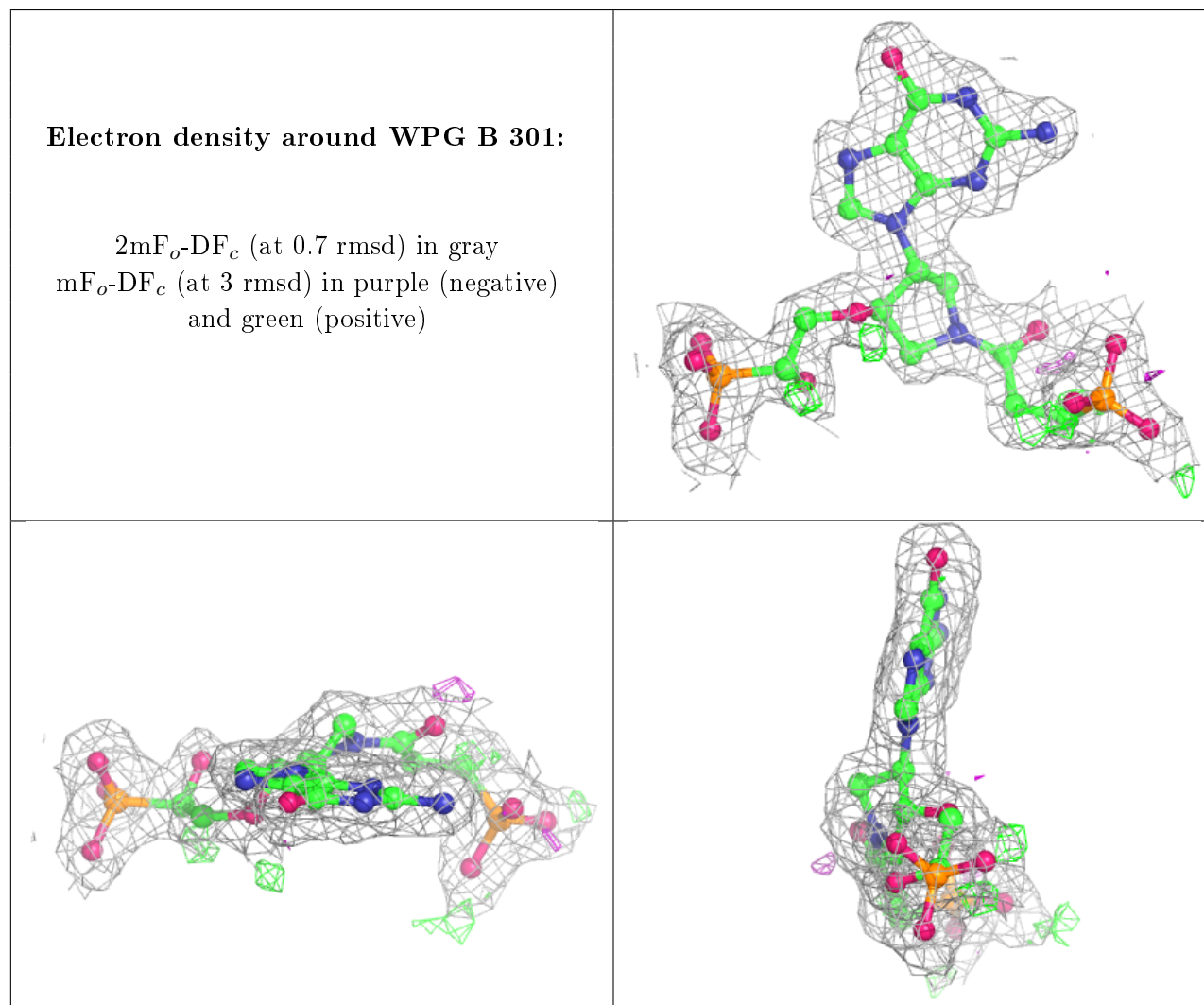
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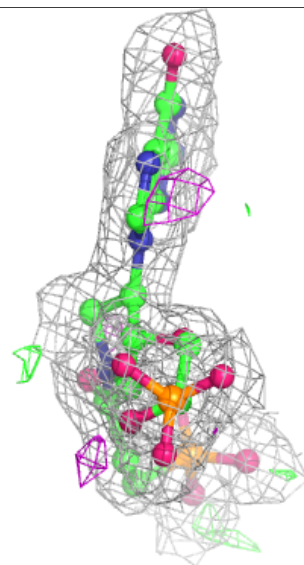
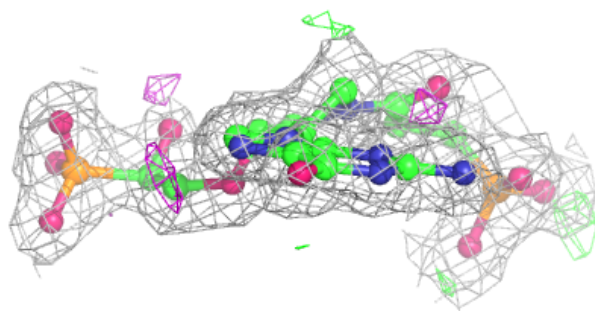
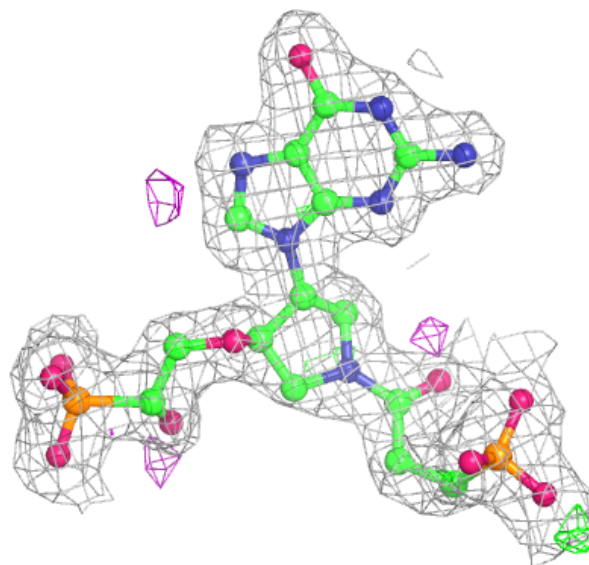
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	WPG	B	301	32/32	0.95	0.11	20,26,37,41	0
2	WPG	D	301	32/32	0.95	0.12	18,28,35,37	0
2	WPG	A	301	32/32	0.96	0.10	18,25,29,31	0
3	MG	C	303	1/1	0.96	0.10	27,27,27,27	0
3	MG	B	303	1/1	0.96	0.05	33,33,33,33	0
2	WPG	C	301	32/32	0.97	0.10	15,22,25,28	0
3	MG	D	303	1/1	0.97	0.08	29,29,29,29	0
3	MG	A	302	1/1	0.98	0.10	29,29,29,29	0
3	MG	D	302	1/1	0.98	0.06	31,31,31,31	0
3	MG	A	303	1/1	0.99	0.07	26,26,26,26	0
3	MG	C	302	1/1	0.99	0.08	24,24,24,24	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.



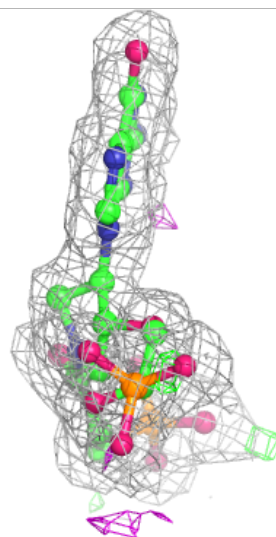
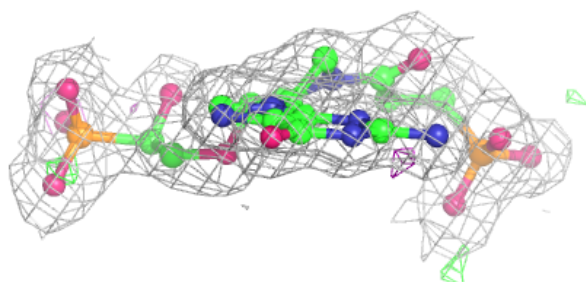
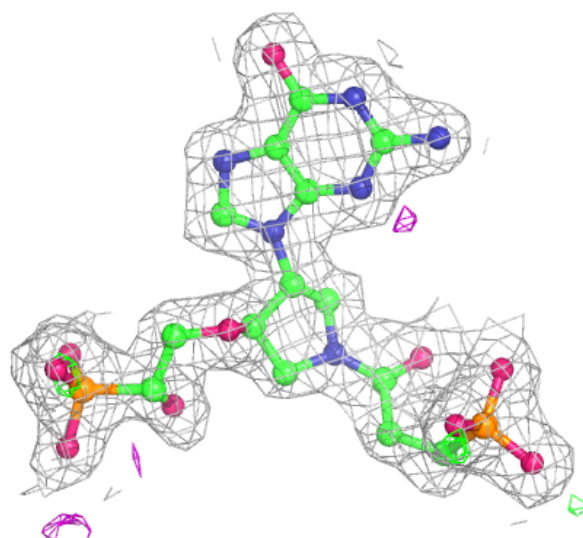
**Electron density around WPG D 301:**

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



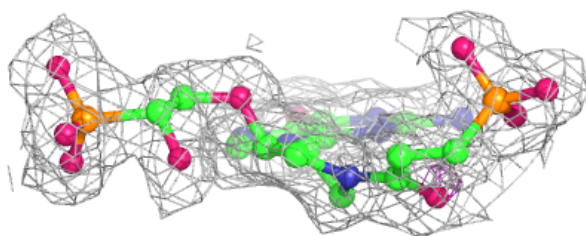
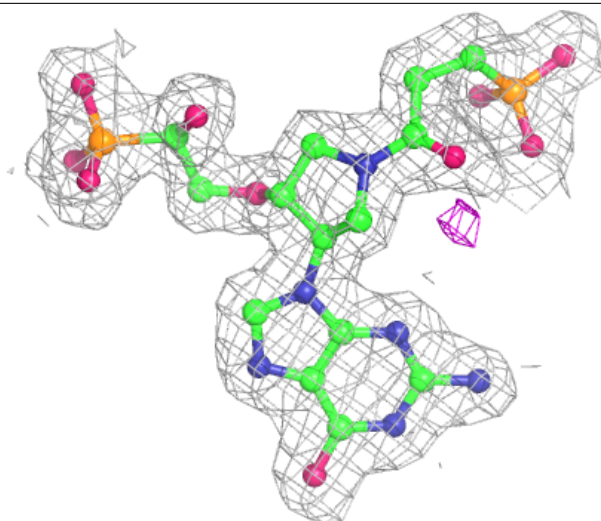
**Electron density around WPG A 301:**

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



**Electron density around WPG C 301:**

$2mF_o-DF_c$  (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.