



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:50 AM BST

PDB ID : 6U77  
Title : yGsy2p in complex with small molecule  
Authors : Tang, B.; Hurley, T.D.  
Deposited on : 2019-08-31  
Resolution : 2.85 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 : 2.13.1  
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) : 2.13.1

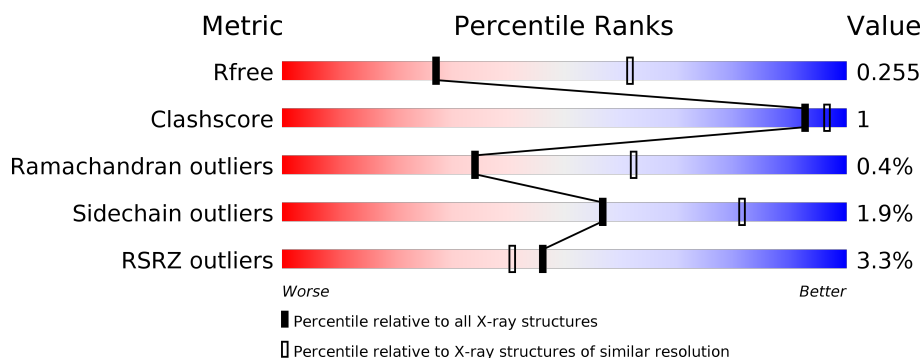
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	705	<div> <div></div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	705	<div> <div></div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	C	705	<div> <div></div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>
1	D	705	<div> <div></div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20692 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.

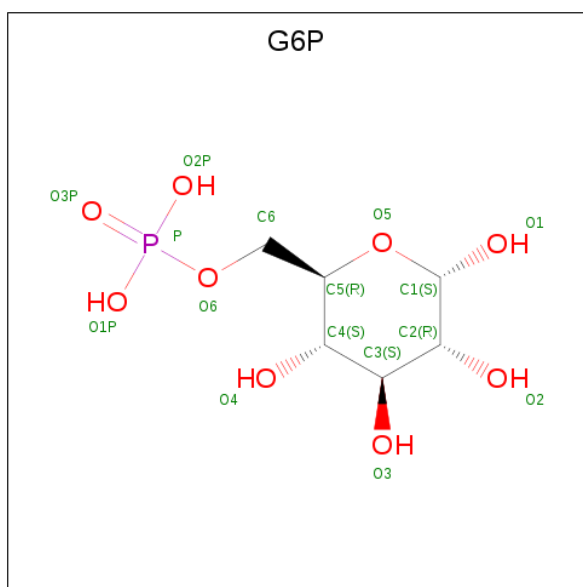
- Molecule 1 is a protein called Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	C	646	Total	C	N	O	S	0	0	0
			5200	3322	907	952	19			
1	D	624	Total	C	N	O	S	0	0	0
			5038	3222	880	918	18			

There are 4 discrepancies between the modelled and reference sequences:

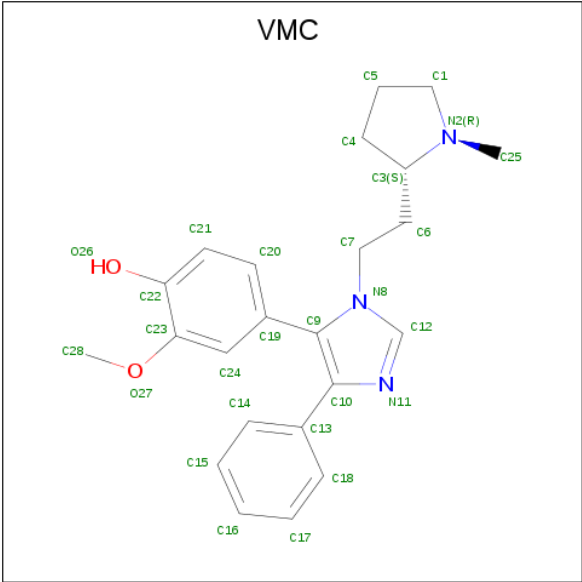
Chain	Residue	Modelled	Actual	Comment	Reference
A	535	SER	ALA	conflict	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
C	535	SER	ALA	conflict	UNP P27472
D	535	SER	ALA	conflict	UNP P27472

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is 2-methoxy-4-(1-{2-[(2S)-1-methylpyrrolidin-2-yl]ethyl}-4-phenyl-1H-imidazol-5-yl)phenol (three-letter code: VMC) (formula: C<sub>23</sub>H<sub>27</sub>N<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).

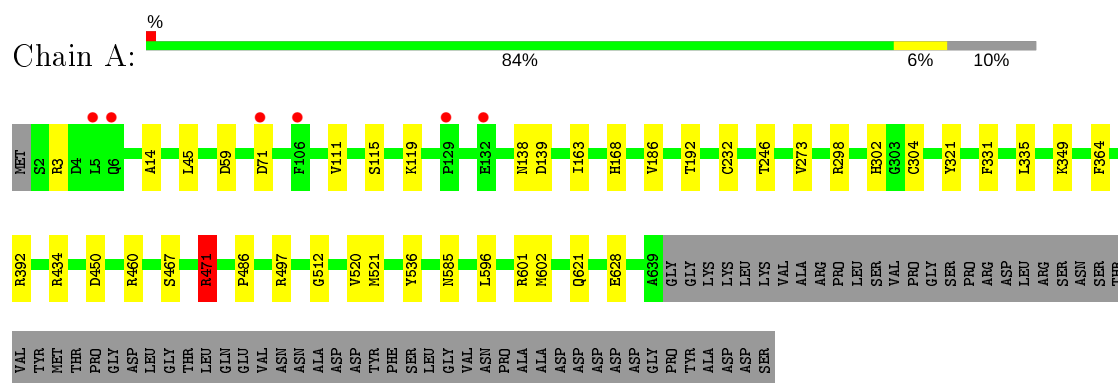


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	23	3	2		
3	C	1	Total	C	N	O	0	0
			28	23	3	2		
3	D	1	Total	C	N	O	0	0
			28	23	3	2		

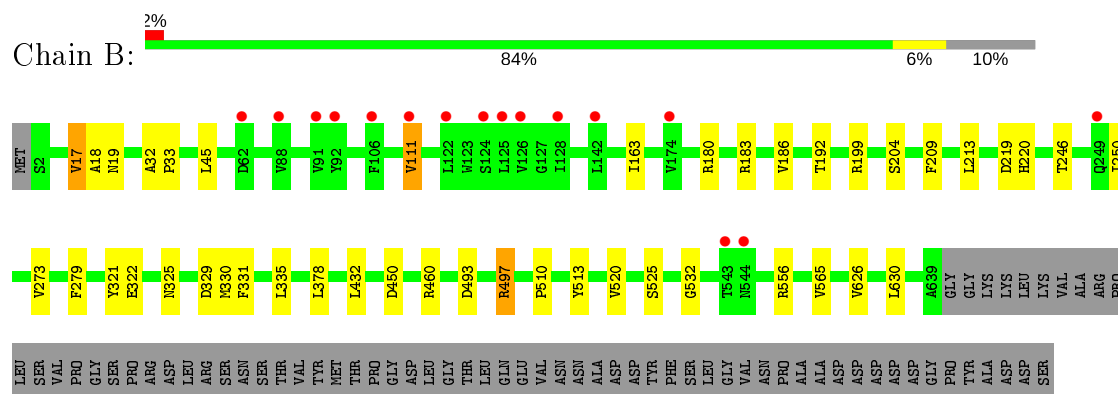
### 3 Residue-property plots [i](#)

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.

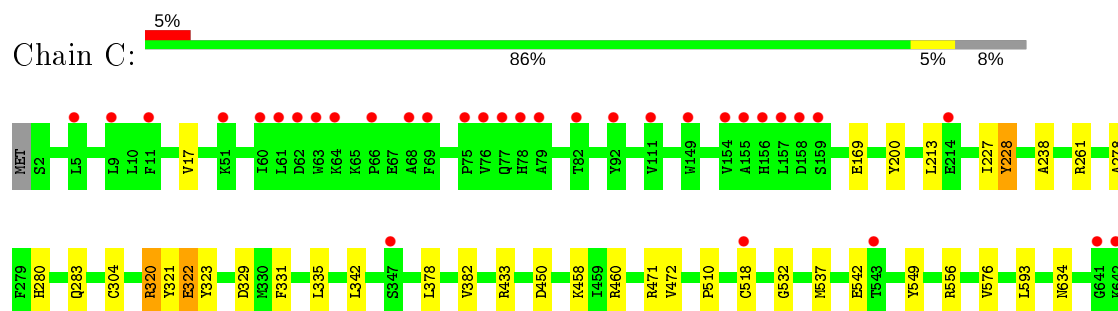
- Molecule 1: Glycogen [starch] synthase isoform 2

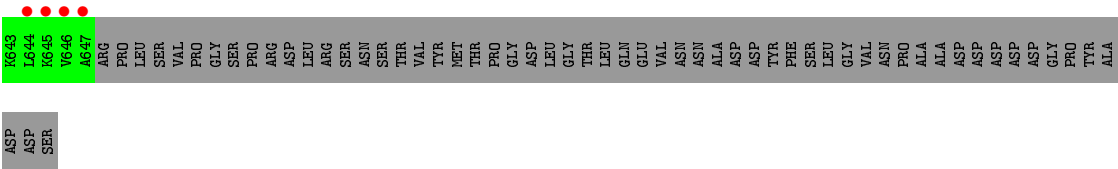


- Molecule 1: Glycogen [starch] synthase isoform 2

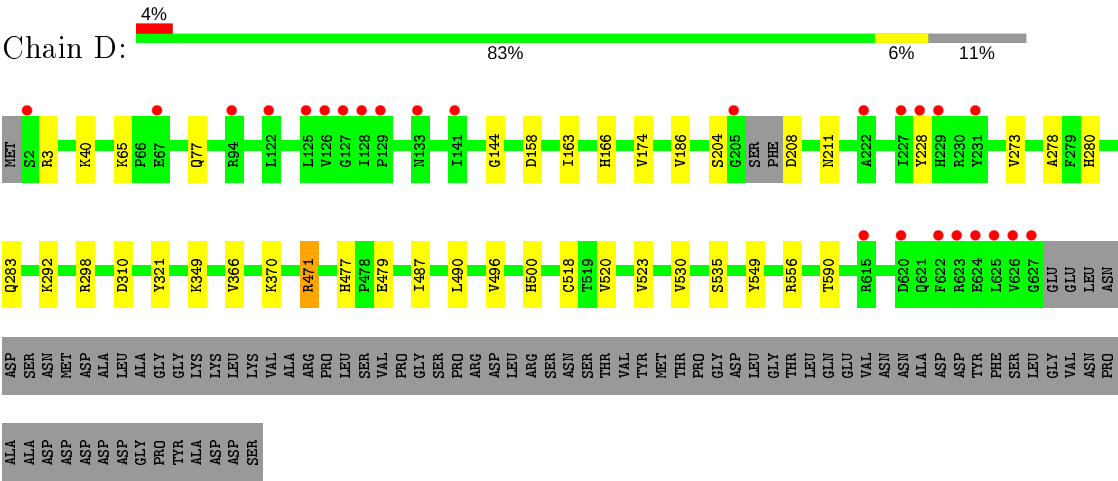


- Molecule 1: Glycogen [starch] synthase isoform 2





● Molecule 1: Glycogen [starch] synthase isoform 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.26 Å   206.56 Å   205.03 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	145.52 – 2.85 48.51 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (145.52-2.85) 99.8 (48.51-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.199 , 0.259 0.198 , 0.255	Depositor DCC
$R_{free}$ test set	4888 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: G6P, VMC

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	0.54	0/5270	0.74	4/7141 (0.1%)
1	B	0.53	0/5270	0.75	3/7141 (0.0%)
1	C	0.50	0/5325	0.70	1/7212 (0.0%)
1	D	0.53	0/5161	0.74	2/6992 (0.0%)
All	All	0.52	0/21026	0.73	10/28486 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	298	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	471	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	497	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	471	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	329	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	320	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	392	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	298	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	180	ARG	NE-CZ-NH1	5.05	122.82	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	5145	0	5048	15	0
1	B	5145	0	5048	16	0
1	C	5200	0	5118	15	0
1	D	5038	0	4955	18	0
2	A	16	0	11	0	0
2	B	32	0	22	1	0
2	C	16	0	11	1	0
2	D	16	0	11	1	0
3	A	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
All	All	20692	0	20224	61	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 1.

All (61) 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:A:349:LYS:O	1:A:471:ARG:HD3	1.95	0.65
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.30	0.64
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.32	0.64
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.32	0.62
1:C:283:GLN:HG2	1:D:280:HIS:CE1	2.36	0.60
1:B:322:GLU:HG3	1:B:325:ASN:HB2	1.82	0.60
1:B:273:VAL:HG13	1:B:520:VAL:HG13	1.83	0.59
1:B:199:ARG:NH2	2:B:902:G6P:O3P	2.37	0.57
1:C:510:PRO:O	1:C:532:GLY:HA3	2.07	0.54
1:B:626:VAL:HG11	1:B:630:LEU:HD11	1.89	0.54
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.44	0.53
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.92	0.52
1:C:283:GLN:HG3	2:C:901:G6P:O1	2.10	0.51
1:D:349:LYS:O	1:D:471:ARG:HD3	2.10	0.50
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.46	0.50
1:D:3:ARG:NH1	1:D:158:ASP:O	2.46	0.49
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.49	0.47
1:A:585:ASN:HD21	1:B:279:PHE:HE1	1.57	0.47
1:D:292:LYS:HD2	1:D:490:LEU:HD21	1.98	0.46
1:A:364:PHE:CE2	1:A:486:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG12	1:B:18:ALA:N	2.30	0.46
1:B:192:THR:CG2	1:B:246:THR:HG22	2.45	0.46
1:A:536:TYR:CZ	1:A:602:MET:HE1	2.51	0.46
1:D:549:TYR:O	1:D:590:THR:HG22	2.15	0.45
1:A:119:LYS:NZ	1:A:138:ASN:OD1	2.50	0.45
1:D:208:ASP:OD2	1:D:211:ASN:ND2	2.49	0.45
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.51	0.45
1:C:549:TYR:HB3	1:C:593:LEU:HD11	1.99	0.44
1:A:163:ILE:HB	1:A:186:VAL:HG12	1.97	0.44
1:D:477:HIS:O	1:D:479:GLU:N	2.49	0.44
1:A:302:HIS:O	1:A:434:ARG:HD2	2.17	0.44
1:D:496:VAL:HG12	1:D:523:VAL:HG21	1.99	0.44
1:A:192:THR:HG22	1:A:246:THR:HG22	1.98	0.44
1:D:65:LYS:O	1:D:77:GLN:NE2	2.51	0.43
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.53	0.43
1:B:493:ASP:O	1:B:497:ARG:HG3	2.18	0.43
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.50	0.43
1:C:320:ARG:NH1	1:C:322:GLU:OE1	2.51	0.43
1:D:500:HIS:NE2	2:D:901:G6P:O2P	2.46	0.43
1:A:3:ARG:O	1:A:621:GLN:NE2	2.52	0.43
1:A:273:VAL:HG13	1:A:520:VAL:HG13	2.01	0.42
1:C:378:LEU:O	1:C:382:VAL:HG23	2.19	0.42
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.01	0.42
1:D:292:LYS:CD	1:D:490:LEU:HD21	2.49	0.42
1:B:209:PHE:O	1:B:213:LEU:HB3	2.20	0.42
1:B:510:PRO:O	1:B:532:GLY:HA3	2.20	0.42
1:B:378:LEU:HD22	1:B:432:LEU:HD11	2.00	0.42
1:A:497:ARG:NH1	1:A:521:MET:SD	2.93	0.42
1:A:331:PHE:CZ	1:A:335:LEU:HD11	2.55	0.42
1:B:330:MET:HG2	1:B:565:VAL:HG22	2.02	0.42
1:A:596:LEU:HA	1:A:601:ARG:HD3	2.02	0.41
1:C:227:ILE:O	1:C:228:TYR:C	2.58	0.41
1:C:200:TYR:CD1	1:C:227:ILE:HD11	2.56	0.41
1:D:487:ILE:HA	1:D:487:ILE:HD13	1.91	0.41
1:C:342:LEU:HD21	1:C:576:VAL:HG11	2.03	0.41
1:D:273:VAL:HG13	1:D:520:VAL:HG13	2.03	0.41
1:C:238:ALA:O	1:C:261:ARG:NH1	2.53	0.41
1:D:366:VAL:O	1:D:370:LYS:HB2	2.21	0.41
1:A:14:ALA:HB2	1:A:168:HIS:HB2	2.02	0.41
1:B:32:ALA:N	1:B:33:PRO:CD	2.83	0.40
1:D:163:ILE:HB	1:D:186:VAL:HG12	2.03	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	636/705 (90%)	608 (96%)	26 (4%)	2 (0%)	41	68
1	B	636/705 (90%)	600 (94%)	33 (5%)	3 (0%)	29	57
1	C	644/705 (91%)	611 (95%)	30 (5%)	3 (0%)	29	57
1	D	620/705 (88%)	583 (94%)	34 (6%)	3 (0%)	29	57
All	All	2536/2820 (90%)	2402 (95%)	123 (5%)	11 (0%)	34	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	VAL
1	B	204	SER
1	D	40	LYS
1	D	228	TYR
1	B	17	VAL
1	D	204	SER
1	C	169	GLU
1	A	115	SER
1	C	228	TYR
1	C	17	VAL
1	A	512	GLY

### 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	551/608 (91%)	540 (98%)	11 (2%)	55	80
1	B	551/608 (91%)	540 (98%)	11 (2%)	55	80
1	C	556/608 (91%)	543 (98%)	13 (2%)	50	78
1	D	539/608 (89%)	532 (99%)	7 (1%)	69	88
All	All	2197/2432 (90%)	2155 (98%)	42 (2%)	57	81

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	59	ASP
1	A	71	ASP
1	A	111	VAL
1	A	139	ASP
1	A	232	CYS
1	A	304	CYS
1	A	321	TYR
1	A	467	SER
1	A	471	ARG
1	A	628	GLU
1	B	19	ASN
1	B	45	LEU
1	B	111	VAL
1	B	183	ARG
1	B	219	ASP
1	B	220	HIS
1	B	250	ILE
1	B	321	TYR
1	B	513	TYR
1	B	525	SER
1	B	556	ARG
1	C	213	LEU
1	C	304	CYS
1	C	321	TYR
1	C	322	GLU
1	C	433	ARG
1	C	458	LYS
1	C	471	ARG
1	C	472	VAL
1	C	518	CYS
1	C	537	MET
1	C	542	GLU

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Mol	Chain	Res	Type
1	C	556	ARG
1	C	634	ASN
1	D	166	HIS
1	D	310	ASP
1	D	321	TYR
1	D	518	CYS
1	D	530	VAL
1	D	535	SER
1	D	556	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	545	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	G6P	B	901	-	16,16,16	0.65	0	24,24,24	0.99	0
3	VMC	A	902	-	27,31,31	0.80	1 (3%)	30,43,43	2.48	5 (16%)
2	G6P	D	901	-	16,16,16	0.69	0	24,24,24	1.56	3 (12%)
3	VMC	C	902	-	27,31,31	0.76	1 (3%)	30,43,43	1.55	5 (16%)
2	G6P	B	902	-	16,16,16	0.62	0	24,24,24	1.13	2 (8%)
2	G6P	C	901	-	16,16,16	0.58	0	24,24,24	0.93	0
3	VMC	D	902	-	27,31,31	0.77	1 (3%)	30,43,43	1.50	5 (16%)
2	G6P	A	901	-	16,16,16	0.63	0	24,24,24	1.02	1 (4%)

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	G6P	B	901	-	-	1/6/26/26	0/1/1/1
3	VMC	A	902	-	-	8/15/25/25	0/4/4/4
2	G6P	D	901	-	-	5/6/26/26	0/1/1/1
3	VMC	C	902	-	-	9/15/25/25	0/4/4/4
2	G6P	B	902	-	-	4/6/26/26	0/1/1/1
2	G6P	C	901	-	-	2/6/26/26	0/1/1/1
3	VMC	D	902	-	-	6/15/25/25	0/4/4/4
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	VMC	C9-C10	2.68	1.49	1.43
3	A	902	VMC	C9-C10	2.58	1.49	1.43
3	D	902	VMC	C9-C10	2.46	1.49	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	VMC	O27-C23-C22	7.95	126.08	114.57
3	A	902	VMC	C28-O27-C23	7.83	129.35	117.53
3	A	902	VMC	O27-C23-C24	-4.99	115.54	124.12
2	D	901	G6P	O2P-P-O6	-4.50	94.76	106.73
3	C	902	VMC	O27-C23-C22	4.40	120.95	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	VMC	C10-C9-N8	-3.84	105.71	108.07
3	D	902	VMC	O27-C23-C22	3.82	120.10	114.57
3	C	902	VMC	C28-O27-C23	3.38	122.64	117.53
3	C	902	VMC	C10-C9-N8	-3.37	106.00	108.07
3	C	902	VMC	C12-N11-C10	3.28	109.23	102.99
2	D	901	G6P	O5-C5-C4	-3.27	103.76	109.69
3	A	902	VMC	C10-C9-N8	-3.15	106.13	108.07
3	D	902	VMC	C12-N11-C10	3.12	108.93	102.99
3	D	902	VMC	C28-O27-C23	3.11	122.22	117.53
3	A	902	VMC	C12-N11-C10	2.91	108.54	102.99
2	D	901	G6P	O2P-P-O1P	2.73	118.06	107.64
2	B	902	G6P	O5-C5-C6	2.69	112.09	106.67
3	C	902	VMC	O27-C23-C24	-2.66	119.55	124.12
3	D	902	VMC	O27-C23-C24	-2.37	120.04	124.12
2	A	901	G6P	C1-O5-C5	2.29	117.98	113.66
2	B	902	G6P	P-O6-C6	2.25	124.49	118.30

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	G6P	C4-C5-C6-O6
3	A	902	VMC	C20-C19-C9-N8
3	A	902	VMC	C24-C19-C9-N8
3	A	902	VMC	C3-C6-C7-N8
2	D	901	G6P	C4-C5-C6-O6
2	D	901	G6P	O5-C5-C6-O6
2	D	901	G6P	C6-O6-P-O1P
2	D	901	G6P	C6-O6-P-O2P
2	D	901	G6P	C6-O6-P-O3P
3	C	902	VMC	C20-C19-C9-N8
3	C	902	VMC	C24-C19-C9-N8
3	C	902	VMC	C3-C6-C7-N8
2	B	902	G6P	C6-O6-P-O1P
2	B	902	G6P	C6-O6-P-O2P
3	D	902	VMC	C3-C6-C7-N8
3	A	902	VMC	C24-C23-O27-C28
3	A	902	VMC	C22-C23-O27-C28
3	C	902	VMC	C22-C23-O27-C28
3	C	902	VMC	C24-C23-O27-C28
3	D	902	VMC	C24-C23-O27-C28
3	D	902	VMC	C22-C23-O27-C28

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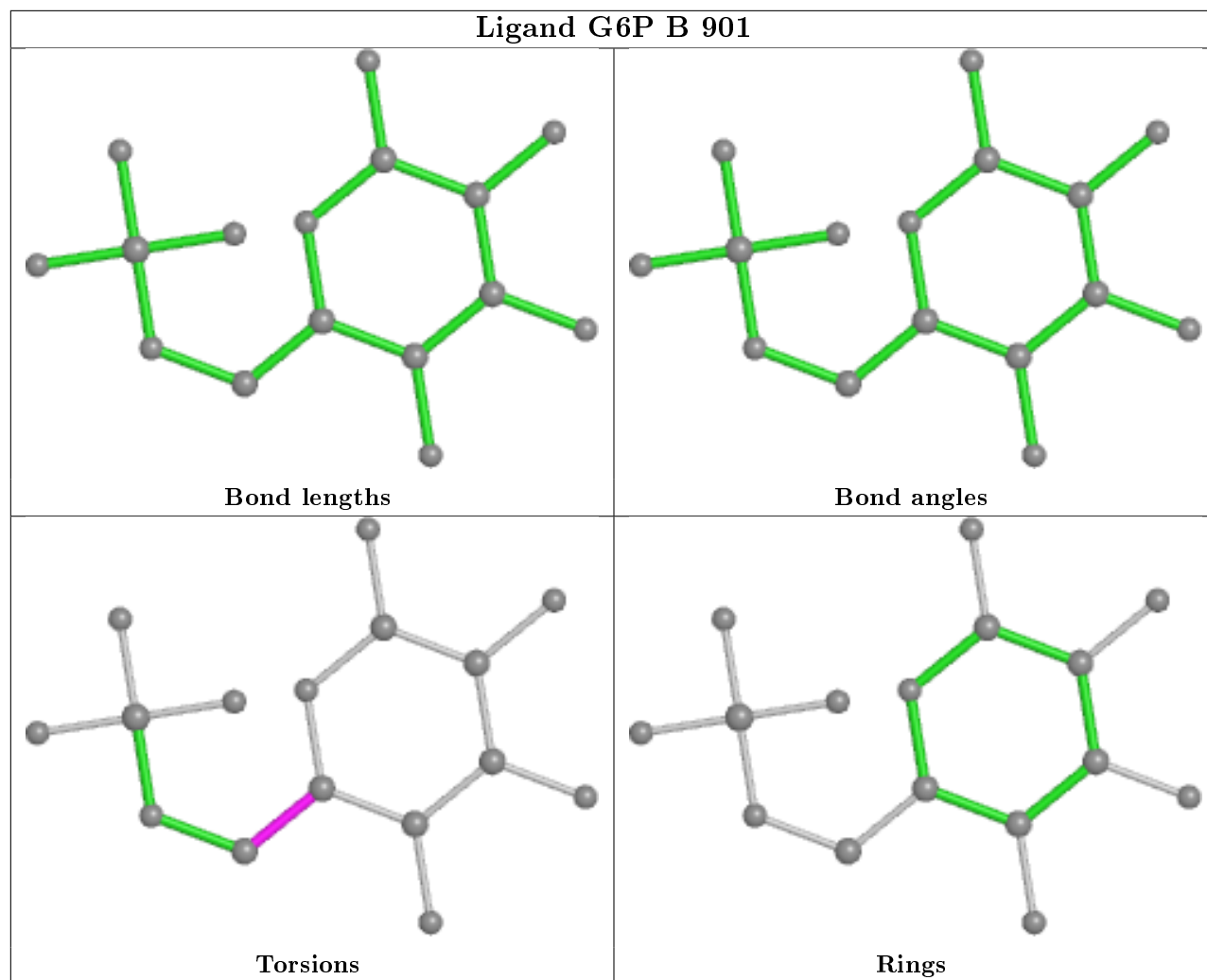
Mol	Chain	Res	Type	Atoms
3	D	902	VMC	N11-C10-C13-C18
2	B	902	G6P	C6-O6-P-O3P
2	C	901	G6P	C6-O6-P-O1P
2	C	901	G6P	C6-O6-P-O2P
3	D	902	VMC	N11-C10-C13-C14
3	A	902	VMC	C24-C19-C9-C10
3	C	902	VMC	C20-C19-C9-C10
3	C	902	VMC	C24-C19-C9-C10
2	B	902	G6P	C5-C6-O6-P
3	A	902	VMC	C20-C19-C9-C10
3	C	902	VMC	N11-C10-C13-C18
3	D	902	VMC	C24-C19-C9-N8
3	A	902	VMC	N11-C10-C13-C18
3	C	902	VMC	N11-C10-C13-C14

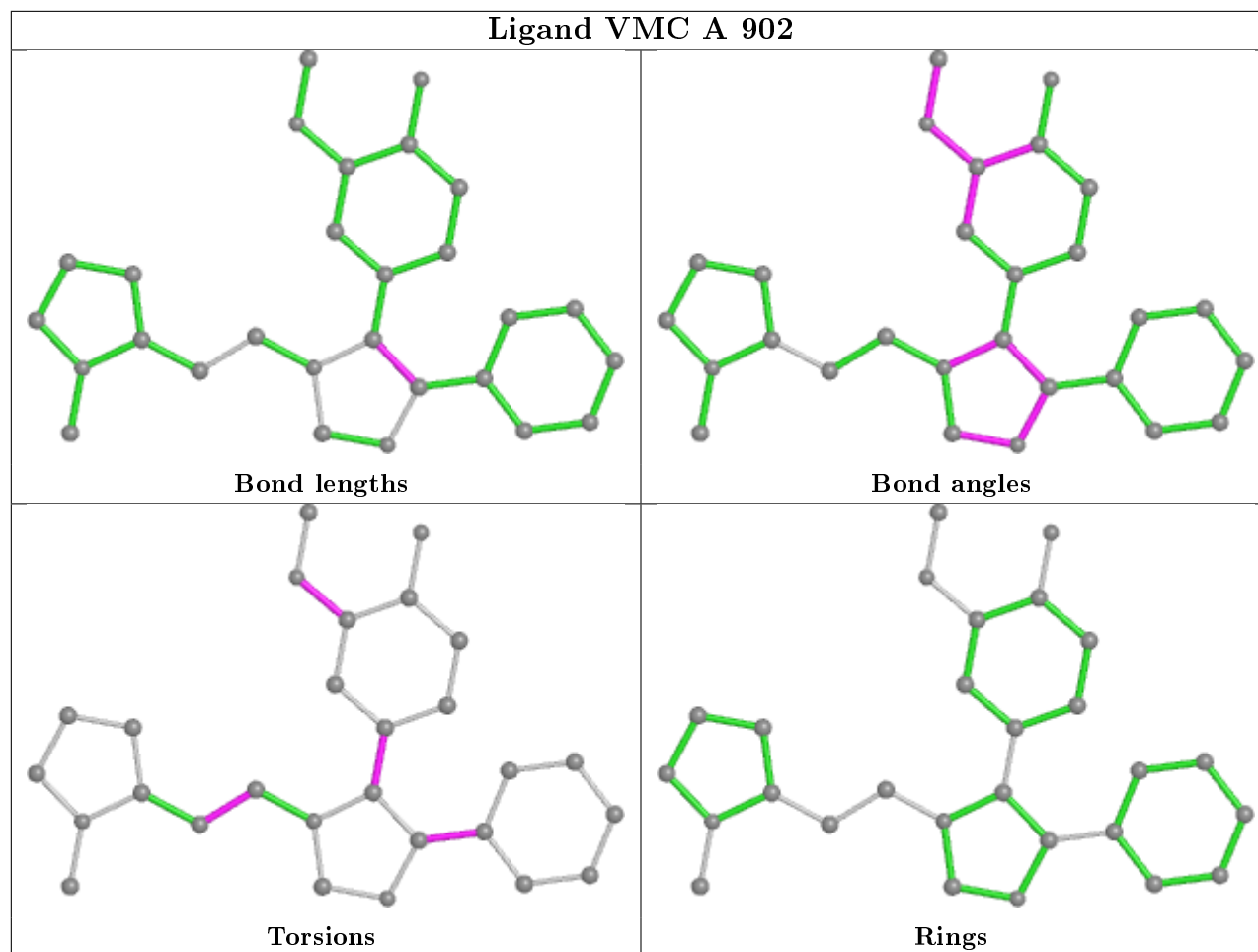
There are no ring outliers.

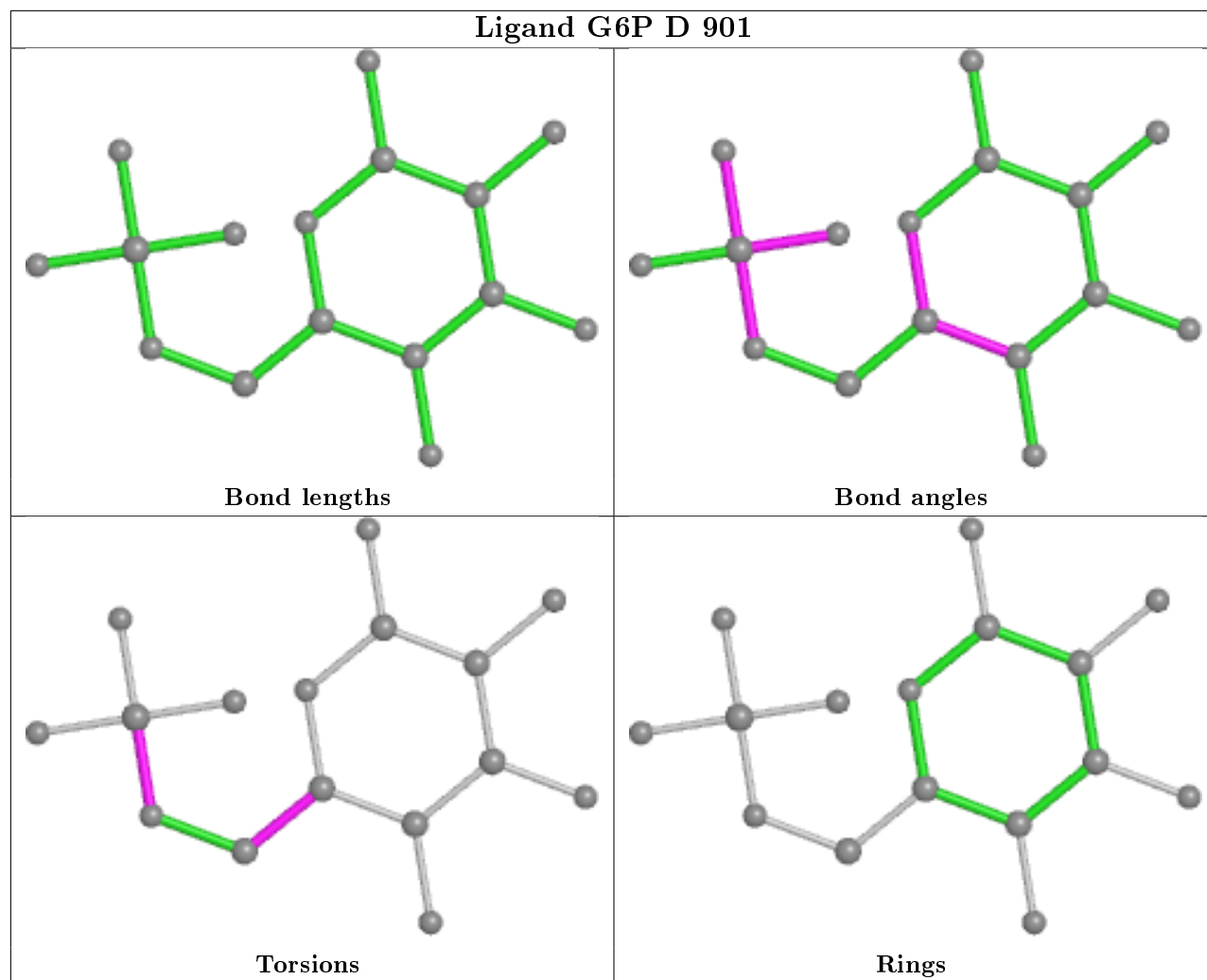
3 monomers are involved in 3 short contacts:

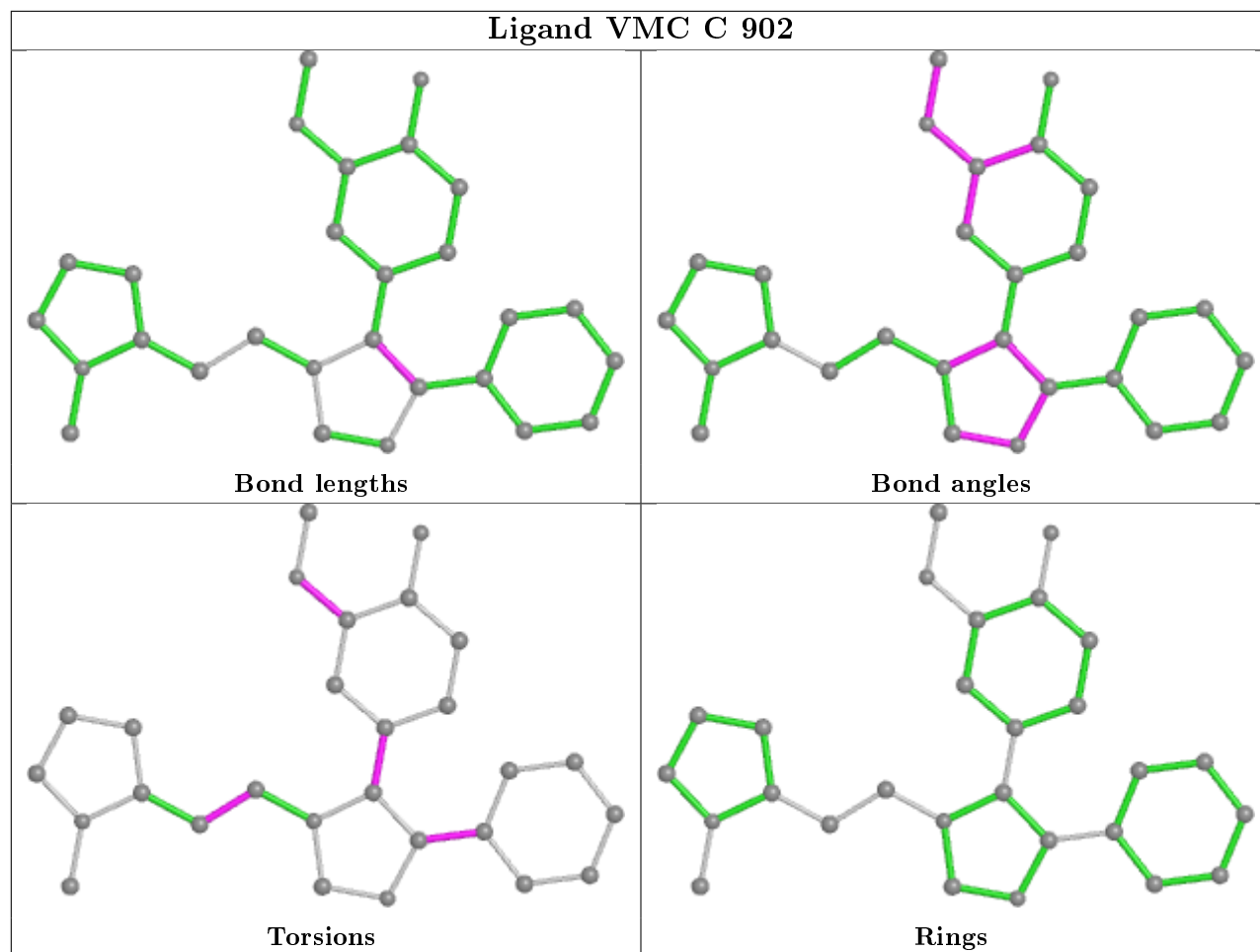
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	G6P	1	0
2	B	902	G6P	1	0
2	C	901	G6P	1	0

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.

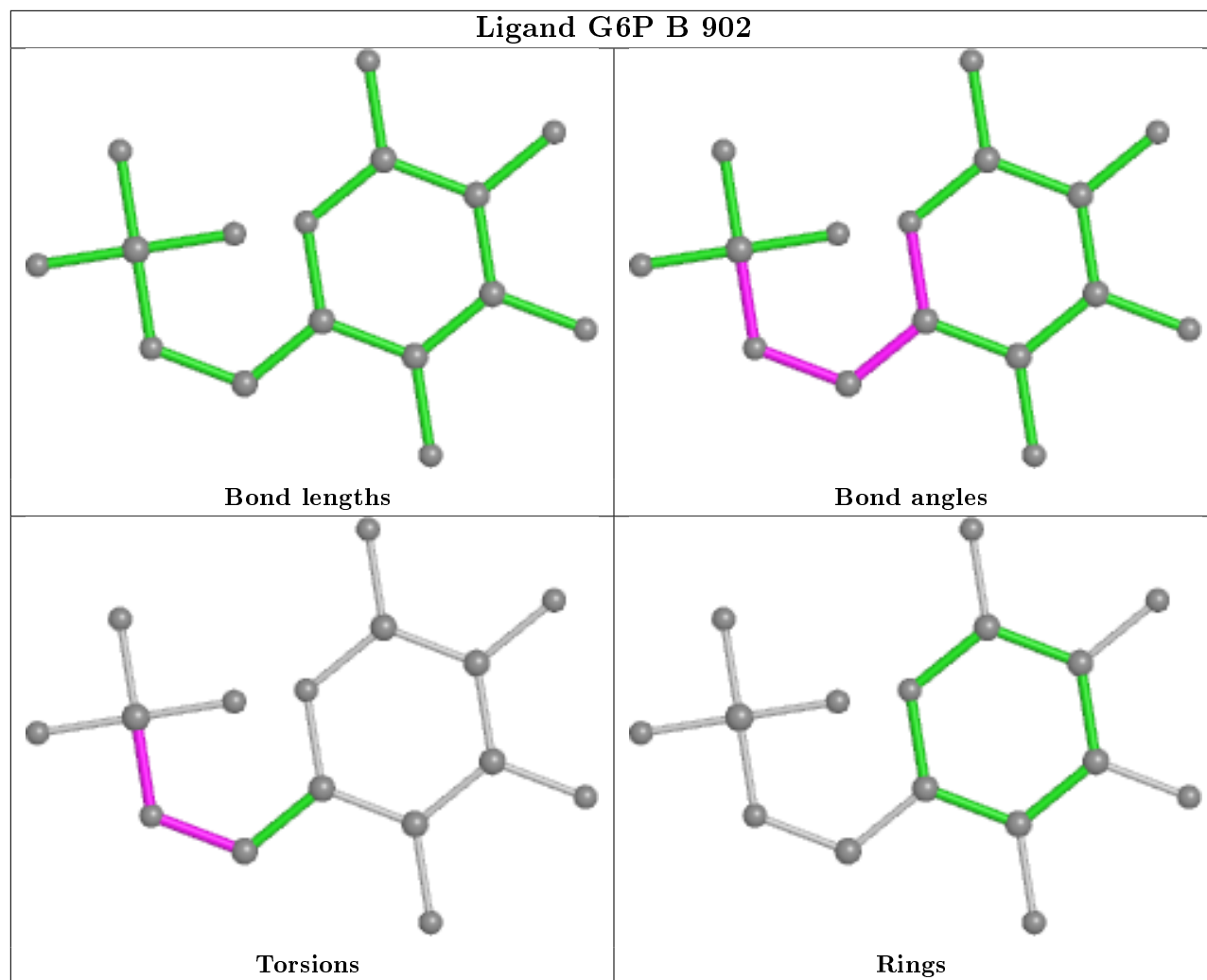


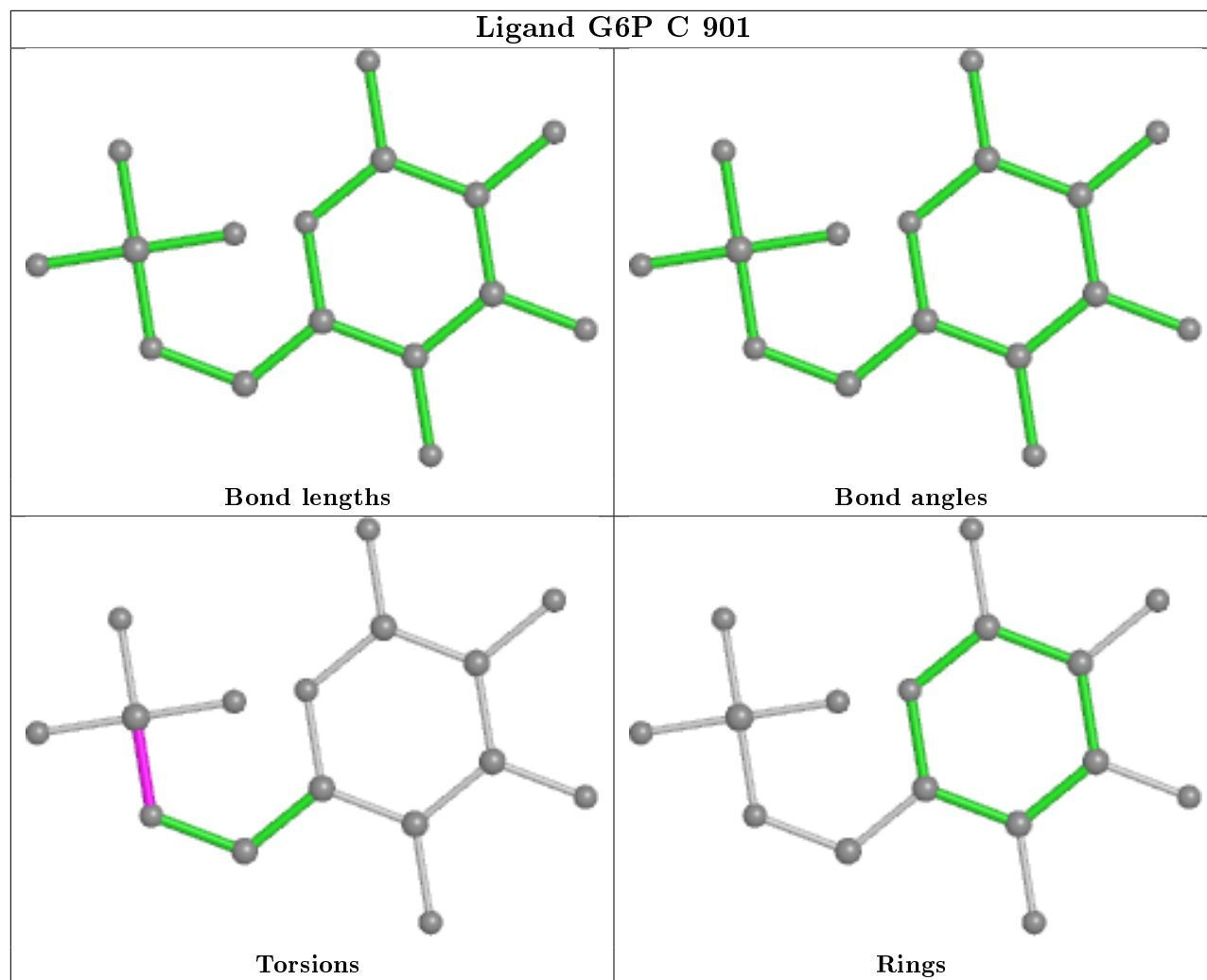


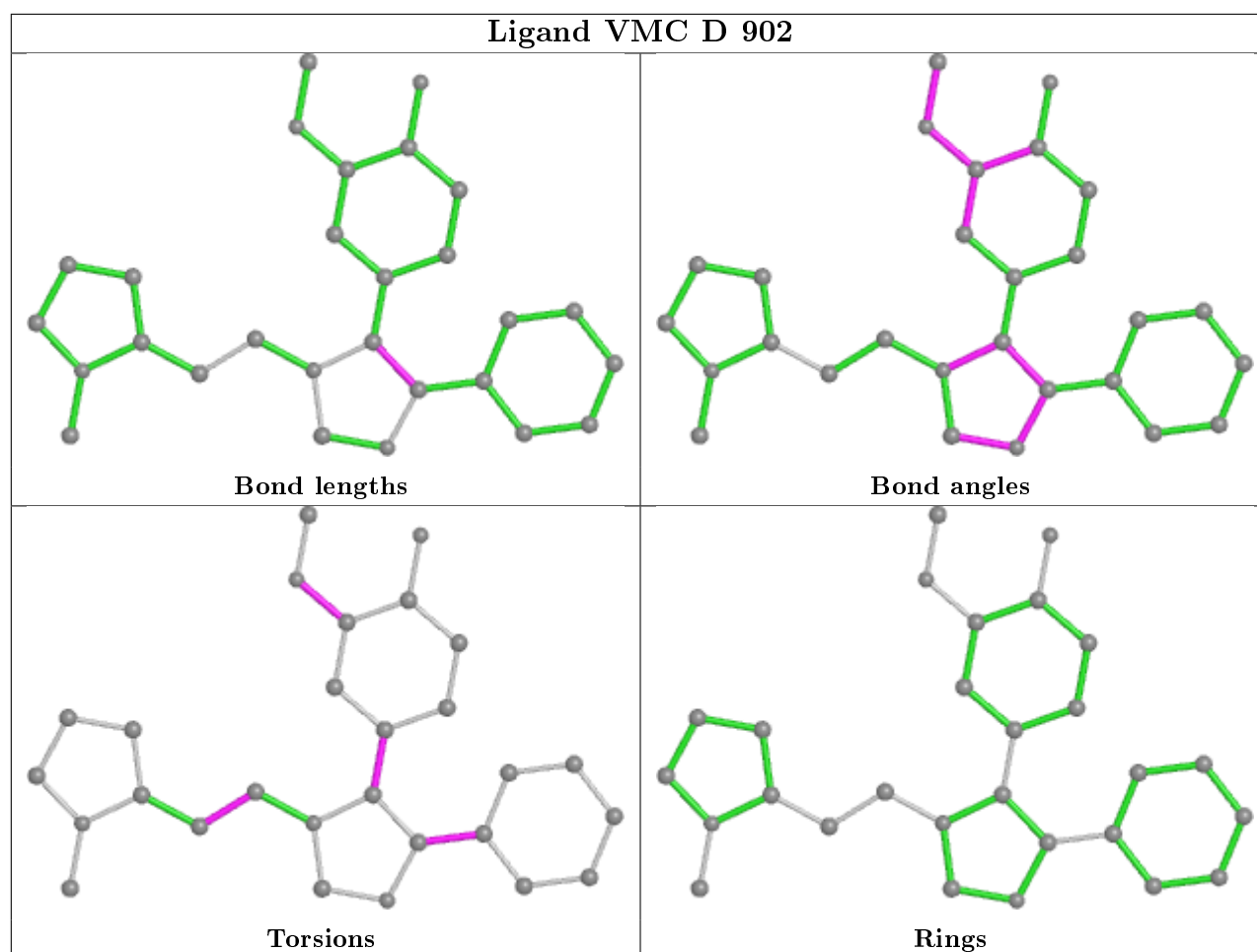




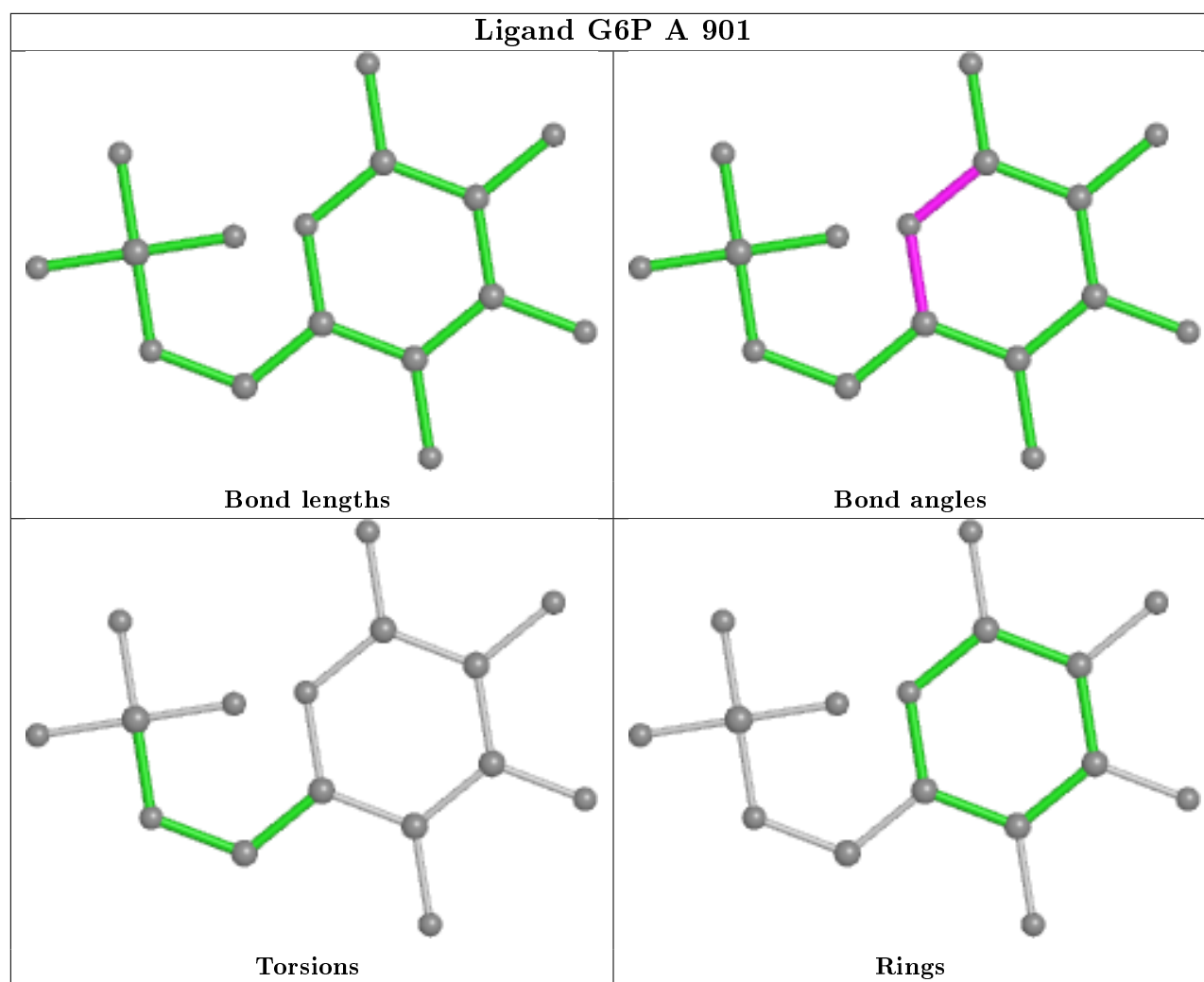
## Ligand G6P B 902











## 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	638/705 (90%)	-0.05	6 (0%) 84 84	46, 75, 123, 155	0
1	B	638/705 (90%)	0.04	16 (2%) 57 54	53, 79, 117, 140	0
1	C	646/705 (91%)	0.20	37 (5%) 23 19	55, 85, 133, 157	0
1	D	624/705 (88%)	0.16	25 (4%) 38 32	49, 85, 145, 174	0
All	All	2546/2820 (90%)	0.09	84 (3%) 46 41	46, 81, 136, 174	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	624	GLU	5.2
1	D	128	ILE	5.1
1	C	647	ALA	4.9
1	C	92	TYR	4.9
1	C	641	GLY	4.8
1	D	626	VAL	4.7
1	D	622	PHE	4.4
1	B	125	LEU	4.3
1	D	625	LEU	4.3
1	C	646	VAL	4.2
1	C	645	LYS	4.2
1	D	129	PRO	4.2
1	B	128	ILE	4.1
1	C	644	LEU	4.0
1	D	125	LEU	4.0
1	D	126	VAL	3.8
1	C	642	LYS	3.7
1	C	155	ALA	3.6
1	C	61	LEU	3.6
1	A	5	LEU	3.5
1	C	63	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	71	ASP	3.4
1	D	627	GLY	3.3
1	C	214	GLU	3.3
1	C	78	HIS	3.2
1	C	11	PHE	3.2
1	C	159	SER	3.2
1	C	157	LEU	3.2
1	B	126	VAL	3.1
1	C	158	ASP	3.0
1	C	156	HIS	3.0
1	A	6	GLN	3.0
1	B	124	SER	3.0
1	D	127	GLY	3.0
1	C	76	VAL	3.0
1	C	69	PHE	2.9
1	C	75	PRO	2.9
1	C	62	ASP	2.9
1	C	9	LEU	2.9
1	B	544	ASN	2.8
1	C	543	THR	2.8
1	D	141	ILE	2.8
1	C	66	PRO	2.8
1	D	2	SER	2.7
1	D	228	TYR	2.7
1	B	91	VAL	2.7
1	D	620	ASP	2.7
1	D	623	ARG	2.7
1	B	142	LEU	2.6
1	D	231	TYR	2.6
1	D	94	ARG	2.5
1	C	77	GLN	2.5
1	A	106	PHE	2.5
1	C	60	ILE	2.5
1	A	132	GLU	2.4
1	B	62	ASP	2.4
1	B	174	VAL	2.4
1	D	205	GLY	2.4
1	B	122	LEU	2.4
1	C	5	LEU	2.4
1	C	154	VAL	2.4
1	D	227	ILE	2.4
1	C	51	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	PHE	2.3
1	C	111	VAL	2.3
1	D	229	HIS	2.3
1	C	64	LYS	2.3
1	C	68	ALA	2.2
1	B	543	THR	2.2
1	B	88	VAL	2.2
1	D	615	ARG	2.2
1	D	122	LEU	2.1
1	A	129	PRO	2.1
1	D	133	ASN	2.1
1	D	222	ALA	2.1
1	B	92	TYR	2.1
1	C	82	THR	2.1
1	D	67	GLU	2.1
1	C	149	TRP	2.0
1	B	249	GLN	2.0
1	C	347	SER	2.0
1	C	518	CYS	2.0
1	C	79	ALA	2.0
1	B	111	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

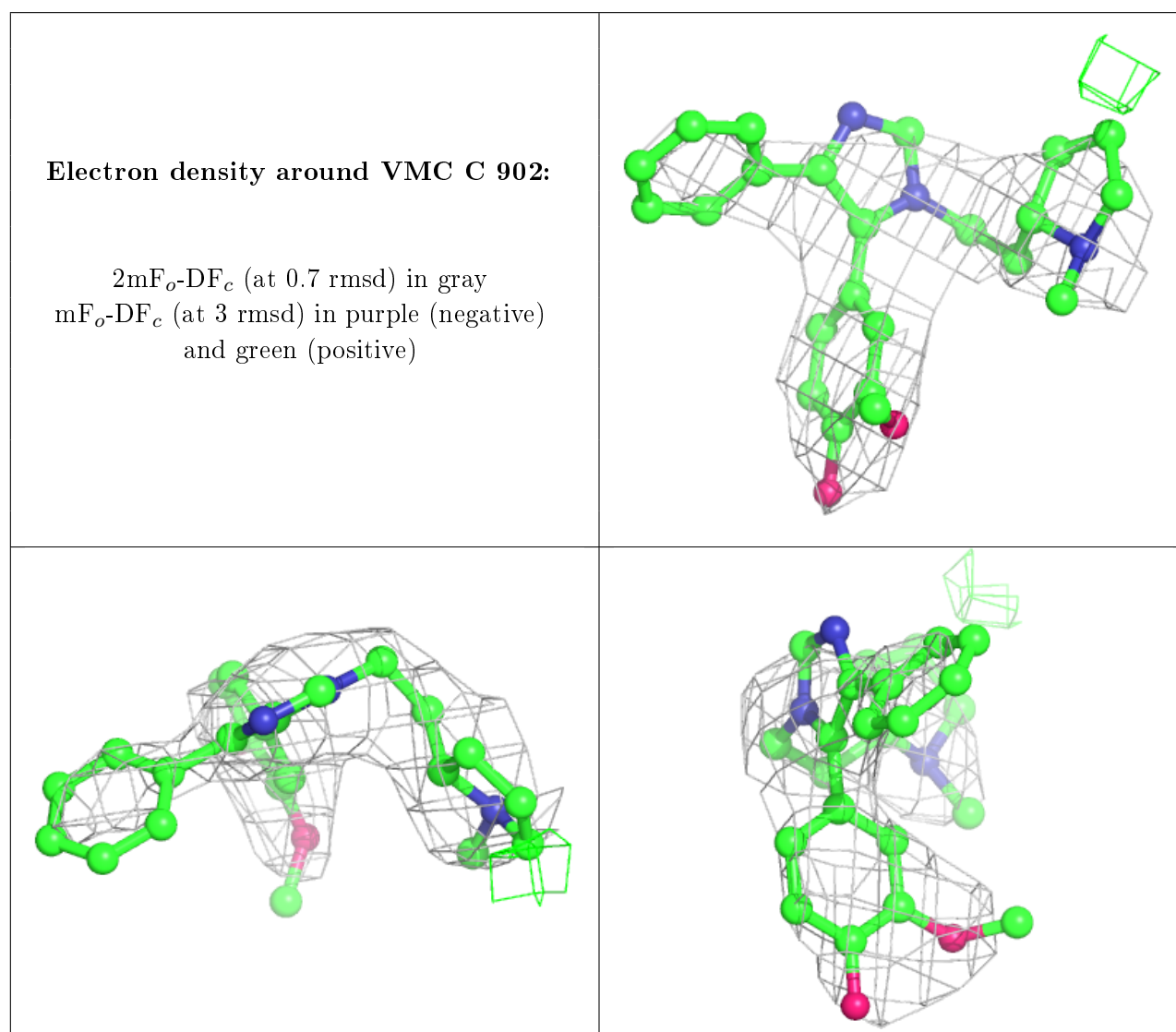
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	VMC	C	902	28/28	0.87	0.30	117,128,134,135	0
3	VMC	A	902	28/28	0.88	0.33	95,101,110,111	0

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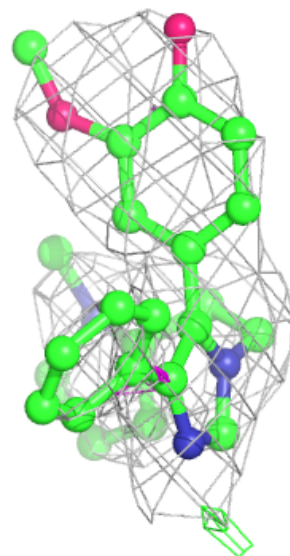
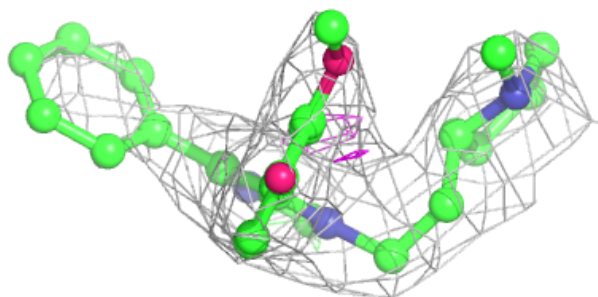
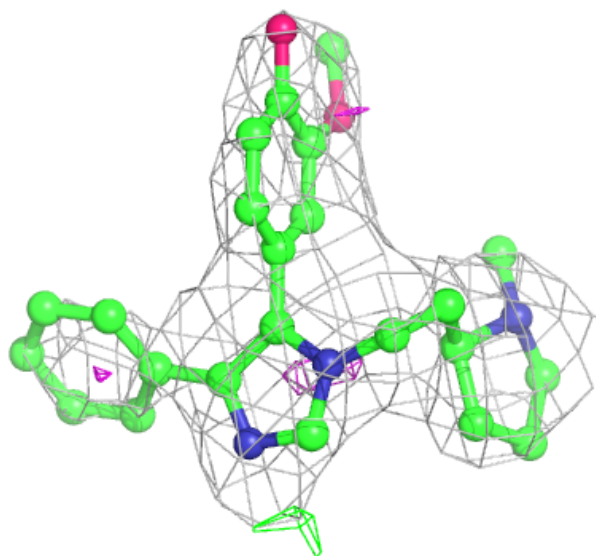
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	VMC	D	902	28/28	0.89	0.38	101,109,122,124	0
2	G6P	B	902	16/16	0.94	0.19	79,88,91,91	0
2	G6P	D	901	16/16	0.98	0.16	45,48,51,53	0
2	G6P	C	901	16/16	0.98	0.18	61,65,66,69	0
2	G6P	B	901	16/16	0.98	0.15	52,57,59,61	0
2	G6P	A	901	16/16	0.98	0.19	47,53,57,58	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.



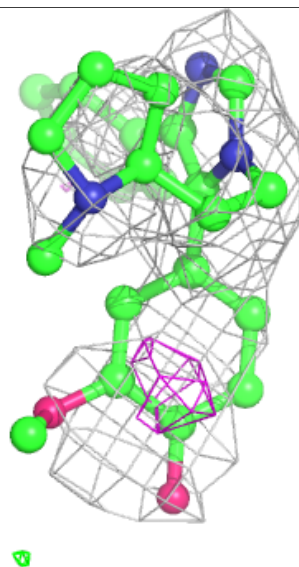
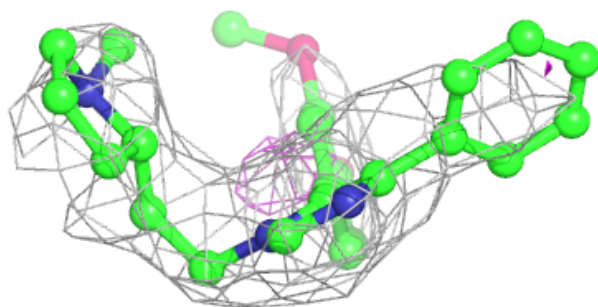
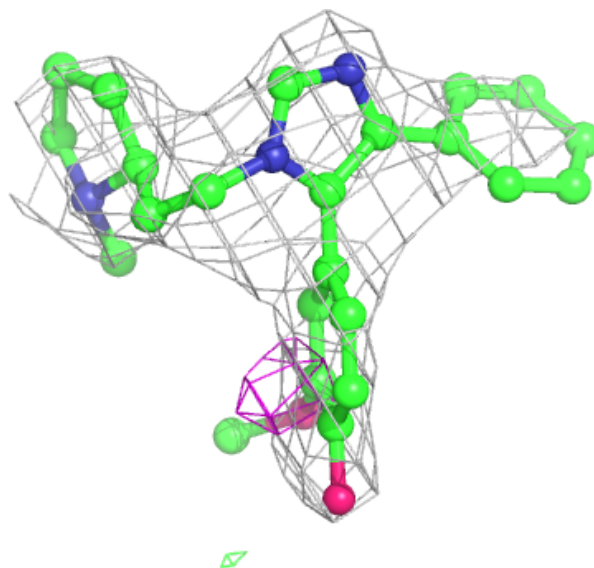
**Electron density around VMC A 902:**

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



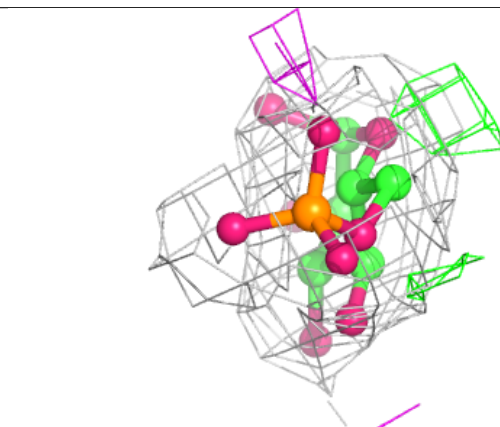
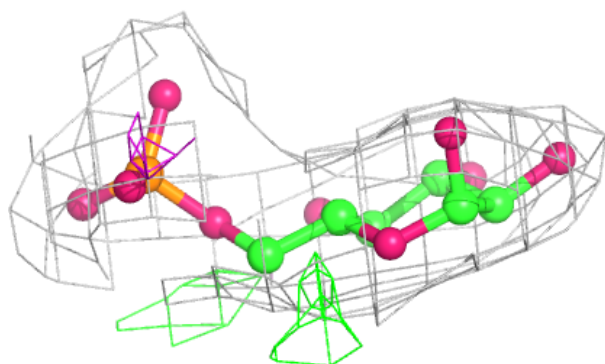
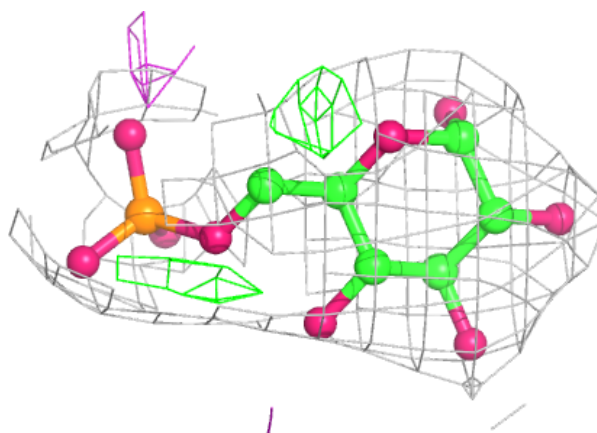
**Electron density around VMC D 902:**

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

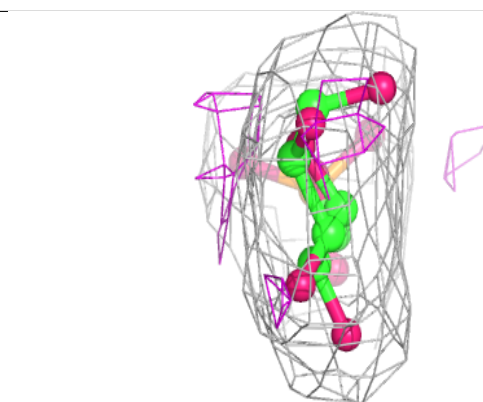
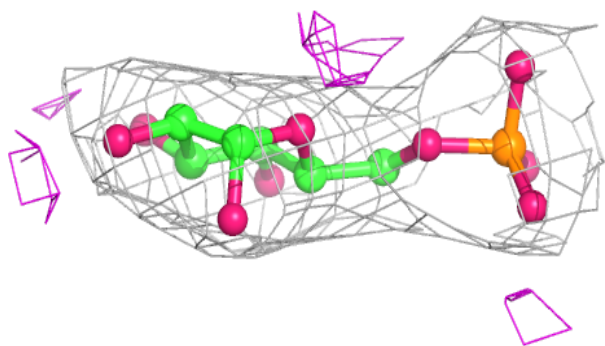
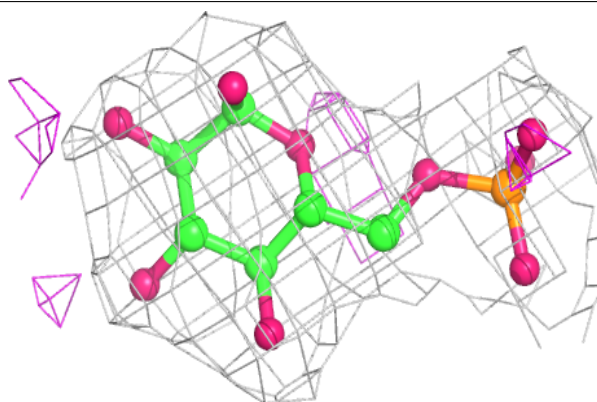


**Electron density around G6P B 902:**

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

**Electron density around G6P D 901:**

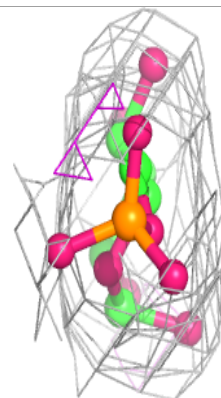
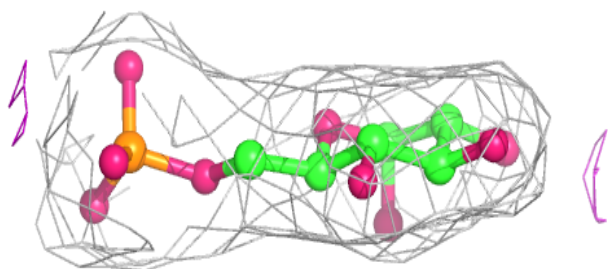
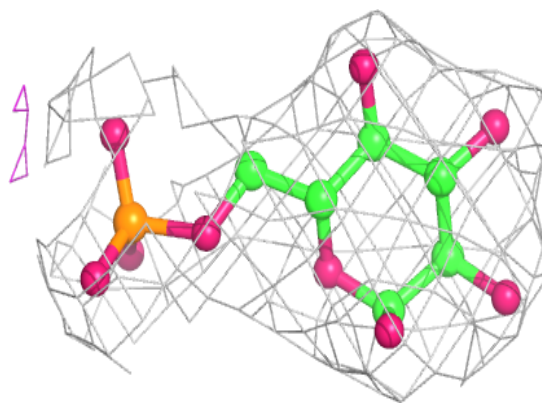
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



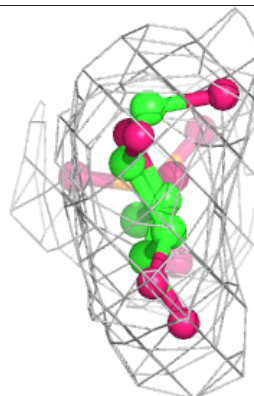
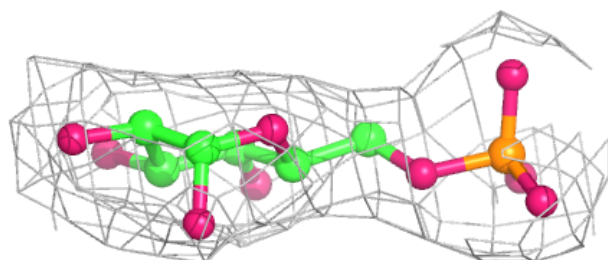
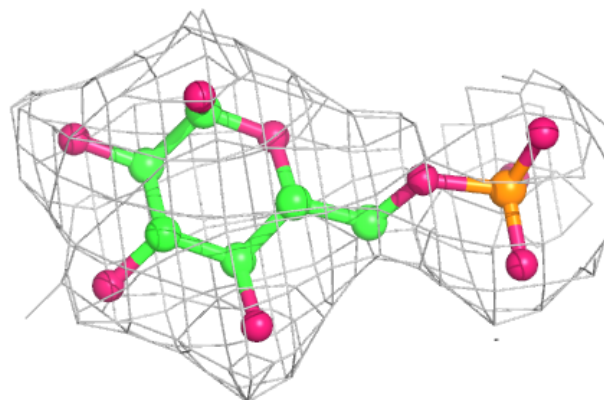


**Electron density around G6P C 901:**

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

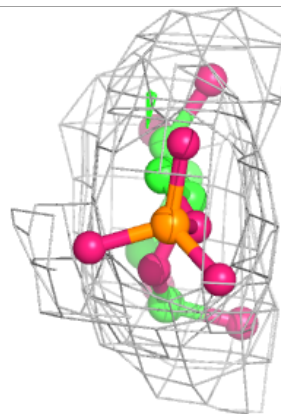
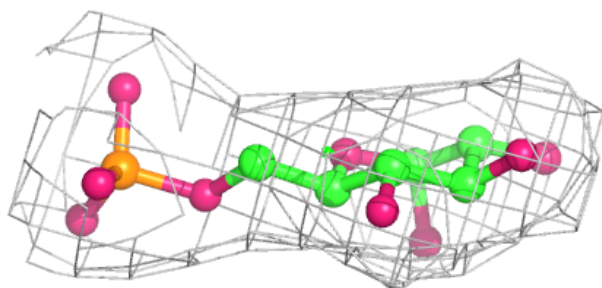
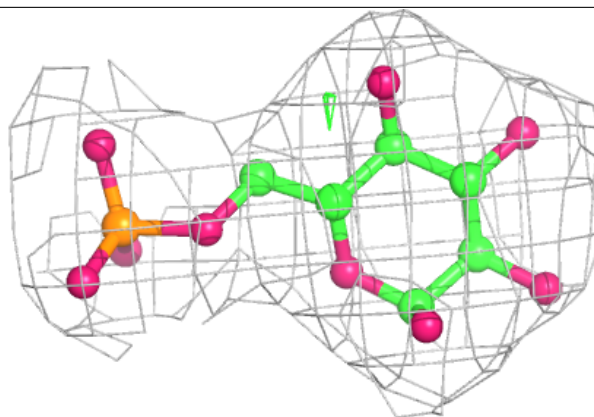
**Electron density around G6P B 901:**

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



**Electron density around G6P A 901:**

$2mF_o - DF_c$  (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.