



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 06:02 PM EDT

PDB ID : 7NA1
Title : HDM2 in complex with compound 2
Authors : Scapin, G.
Deposited on : 2021-06-19
Resolution : 2.30 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 : 2.23.2
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) : 2.23.2

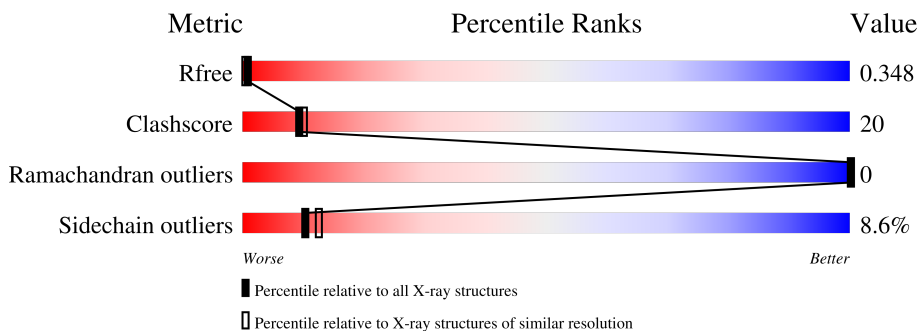
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	109	 61% 16% 5% 18%
1	B	109	 52% 27% • 18%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 1675 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.

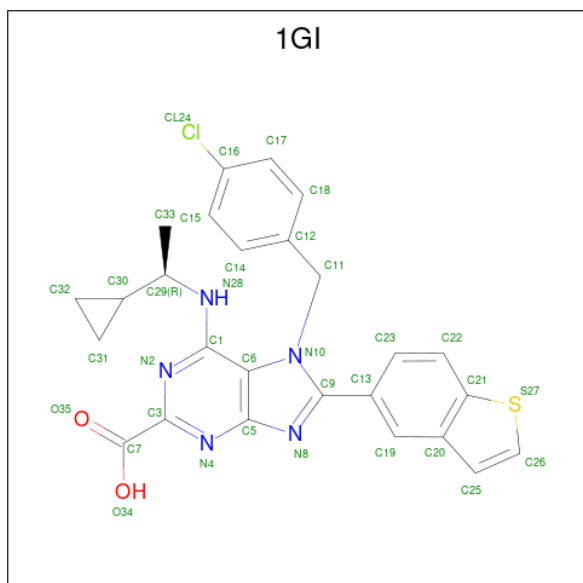
- Molecule 1 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	89	Total 745	C 485	N 127	O 128	S 5	0	3	0
1	B	89	Total 729	C 476	N 121	O 127	S 5	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	TYR	PHE	engineered mutation	UNP Q00987
A	76	HIS	TYR	engineered mutation	UNP Q00987
B	55	TYR	PHE	engineered mutation	UNP Q00987
B	76	HIS	TYR	engineered mutation	UNP Q00987

- Molecule 2 is 8-(1-benzothiophen-5-yl)-7-[(4-chlorophenyl)methyl]-6-[[[(1R)-1-cyclopropylethyl]amino]-7H-purine-2-carboxylic acid (three-letter code: 1GI) (formula: C₂₆H₂₂ClN₅O₂S) (labeled as "Ligand of Interest" by depositor).



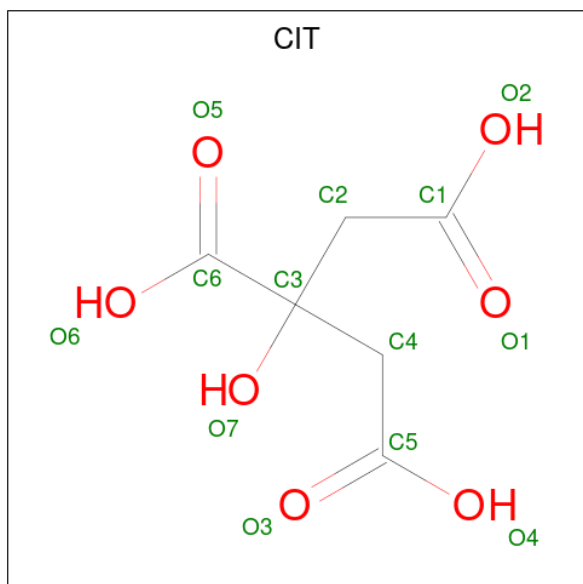
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	Cl	N	O	S	0	0
			35	26	1	5	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			35	26	1	5	2	1		

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



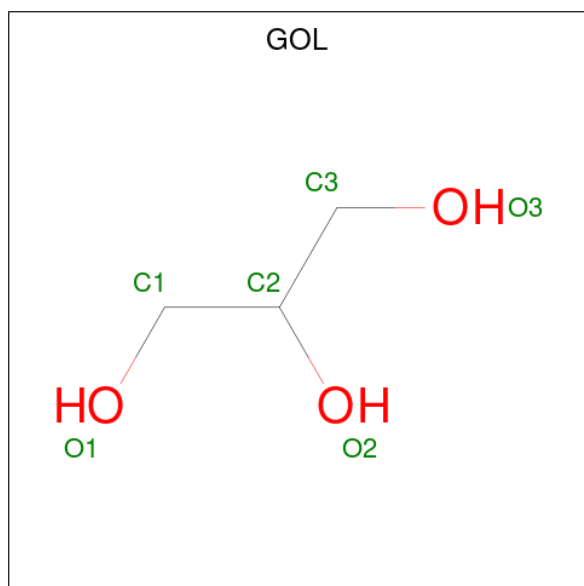
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

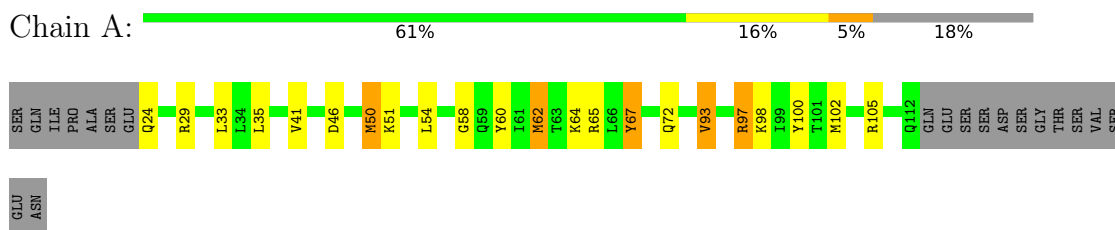
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	64	Total	O	0	0
			64	64		

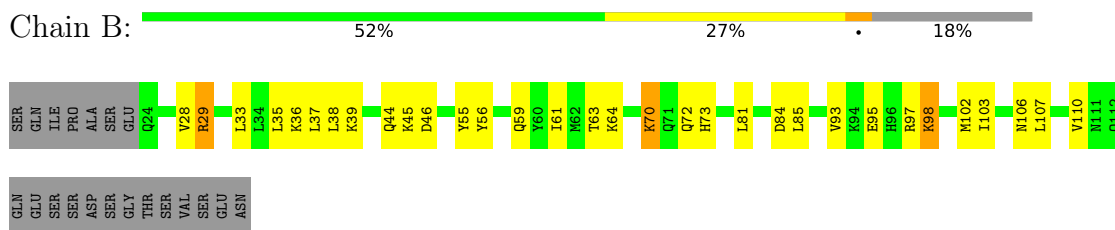
3 Residue-property plots

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. 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. 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: E3 ubiquitin-protein ligase Mdm2



- Molecule 1: E3 ubiquitin-protein ligase Mdm2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.35Å 39.43Å 160.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 31.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.30) 99.2 (31.69-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.255 , 0.354 0.260 , 0.348	Depositor DCC
R_{free} test set	551 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtrriage
Anisotropy	0.422	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	0.379 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1675	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CIT, GOL, 1GI

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	0.62	0/768	0.70	0/1034
1	B	0.65	0/749	0.73	0/1010
All	All	0.64	0/1517	0.72	0/2044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	745	0	786	28	0
1	B	729	0	759	31	0
2	A	35	0	0	5	0
2	B	35	0	0	3	0
3	A	5	0	0	0	0
4	A	13	0	5	2	0
5	B	6	0	8	3	0
6	A	43	0	0	0	0
6	B	64	0	0	3	0
All	All	1675	0	1558	62	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 20.

All (62) 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:97[A]:ARG:HH11	1:A:97[A]:ARG:HG3	1.32	0.93
4:A:203:CIT:O1	4:A:203:CIT:O6	1.98	0.82
1:A:50:MET:HE2	1:A:100:TYR:HD1	1.46	0.80
1:A:50:MET:HE2	1:A:100:TYR:CD1	2.21	0.76
1:A:64:LYS:HA	1:A:64:LYS:HE2	1.68	0.76
1:B:73:HIS:HD2	5:B:202:GOL:H31	1.53	0.74
1:A:97[B]:ARG:CD	1:A:97[B]:ARG:H	2.01	0.73
1:A:97[A]:ARG:HG3	1:A:97[A]:ARG:NH1	1.94	0.72
2:A:201:1GI:C26	1:B:59:GLN:NE2	2.52	0.71
1:B:95:GLU:HB3	1:B:98:LYS:HG2	1.72	0.69
1:A:50:MET:HE3	1:A:100:TYR:HE1	1.57	0.69
1:B:73:HIS:HA	5:B:202:GOL:H12	1.73	0.69
1:A:97[B]:ARG:H	1:A:97[B]:ARG:HD2	1.57	0.68
1:B:73:HIS:CD2	5:B:202:GOL:H31	2.30	0.65
1:A:93:VAL:HG22	2:A:201:1GI:C14	2.29	0.62
1:A:35:LEU:HD21	1:A:46:ASP:OD1	2.01	0.60
1:A:50:MET:HE3	1:A:100:TYR:CE1	2.35	0.60
1:B:29:ARG:HG2	1:B:46:ASP:O	2.03	0.58
1:B:93:VAL:HG13	2:B:201:1GI:N4	2.19	0.58
1:B:102:MET:O	1:B:106:ASN:ND2	2.38	0.57
1:B:97:ARG:NH1	6:B:301:HOH:O	2.37	0.57
1:A:50:MET:CE	1:A:100:TYR:CE1	2.88	0.57
1:A:98:LYS:O	1:A:102:MET:HG3	2.05	0.57
1:A:50:MET:CE	1:A:100:TYR:CD1	2.88	0.56
1:B:28:VAL:HB	1:B:107:LEU:HD13	1.87	0.56
1:B:61:ILE:HG13	6:B:305:HOH:O	2.06	0.55
1:B:98:LYS:HE2	1:B:98:LYS:H	1.71	0.55
1:A:93:VAL:HG13	2:A:201:1GI:C5	2.37	0.55
1:B:98:LYS:H	1:B:98:LYS:CE	2.21	0.53
1:B:29:ARG:HE	1:B:110:VAL:HG11	1.74	0.52
1:B:93:VAL:CG1	2:B:201:1GI:N4	2.74	0.51
1:B:35:LEU:HG	1:B:39:LYS:HE3	1.93	0.50
1:A:65:ARG:O	1:A:65:ARG:HG3	2.12	0.50
1:B:81:LEU:O	1:B:84:ASP:HB2	2.12	0.50
1:B:70:LYS:NZ	6:B:303:HOH:O	2.45	0.49
1:A:41:VAL:HG11	1:A:60:TYR:HA	1.95	0.48
1:B:55:TYR:O	1:B:59:GLN:HG2	2.14	0.48
1:A:97[A]:ARG:HH11	1:A:97[A]:ARG:CG	2.10	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:1GI:C11	2:A:201:1GI:C23	2.92	0.48
1:A:50:MET:CE	1:A:54:LEU:HD11	2.43	0.48
1:B:28:VAL:HG21	1:B:107:LEU:HD22	1.96	0.48
1:A:58:GLY:O	1:A:62[B]:MET:HG2	2.16	0.46
1:B:38:LEU:HD22	1:B:56:TYR:HB2	1.98	0.45
1:B:72:GLN:O	1:B:73:HIS:HB2	2.14	0.45
1:A:97[B]:ARG:H	1:A:97[B]:ARG:NE	2.15	0.44
1:B:81:LEU:O	1:B:81:LEU:HD12	2.18	0.44
1:B:81:LEU:HA	1:B:84:ASP:OD2	2.18	0.44
1:B:33:LEU:HD22	1:B:81:LEU:HD11	1.98	0.44
1:A:24:GLN:HB3	1:A:51:LYS:HG3	2.01	0.43
2:A:201:1GI:C26	1:B:59:GLN:HE21	2.29	0.43
1:B:103:ILE:HG22	1:B:107:LEU:HD23	1.99	0.43
1:B:93:VAL:HG13	2:B:201:1GI:C3	2.48	0.43
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.82	0.43
1:A:29:ARG:HH21	1:A:46:ASP:HB3	1.84	0.42
1:A:67:TYR:OH	1:A:72:GLN:O	2.24	0.42
1:B:95:GLU:HB3	1:B:98:LYS:CG	2.45	0.42
4:A:203:CIT:O6	4:A:203:CIT:C1	2.66	0.42
1:B:37:LEU:C	1:B:37:LEU:HD23	2.41	0.41
1:A:50:MET:HE3	1:A:54:LEU:HD11	2.02	0.41
1:B:33:LEU:HB3	1:B:85:LEU:HD11	2.03	0.41

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	90/109 (83%)	83 (92%)	7 (8%)	0	100	100
1	B	89/109 (82%)	81 (91%)	8 (9%)	0	100	100
All	All	179/218 (82%)	164 (92%)	15 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	85/102 (83%)	77 (91%)	8 (9%)	8 10
1	B	82/102 (80%)	74 (90%)	8 (10%)	8 9
All	All	167/204 (82%)	151 (90%)	16 (10%)	10 10

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	MET
1	A	62[A]	MET
1	A	62[B]	MET
1	A	67	TYR
1	A	93	VAL
1	A	97[A]	ARG
1	A	97[B]	ARG
1	A	105	ARG
1	B	29	ARG
1	B	36	LYS
1	B	44	GLN
1	B	45	LYS
1	B	63	THR
1	B	64	LYS
1	B	70	LYS
1	B	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	B	59	GLN
1	B	73	HIS

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](#)

5 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	1GI	B	201	-	31,40,40	0.95	1 (3%)	34,59,59	1.56	6 (17%)
5	GOL	B	202	-	5,5,5	0.74	0	5,5,5	0.55	0
3	SO4	A	202	-	4,4,4	0.16	0	6,6,6	0.40	0
2	1GI	A	201	-	31,40,40	0.96	1 (3%)	34,59,59	1.84	11 (32%)
4	CIT	A	203	-	3,12,12	1.77	0	3,17,17	1.68	1 (33%)

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	1GI	B	201	-	-	3/16/22/22	0/6/6/6
5	GOL	B	202	-	-	2/4/4/4	-
2	1GI	A	201	-	-	3/16/22/22	0/6/6/6
4	CIT	A	203	-	-	2/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	1GI	C21-S27	-2.76	1.72	1.74
2	B	201	1GI	C21-S27	-2.67	1.72	1.74

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	201	1GI	C12-C11-N10	5.59	121.31	112.63
2	B	201	1GI	C32-C30-C29	5.26	127.92	119.16
4	A	203	CIT	C3-C2-C1	2.71	119.32	114.98
2	A	201	1GI	C3-N4-C5	-2.70	111.72	115.08
2	A	201	1GI	C33-C29-N28	-2.57	104.28	110.78
2	A	201	1GI	C19-C13-C9	-2.56	116.56	120.49
2	A	201	1GI	C23-C13-C19	2.47	121.96	118.09
2	A	201	1GI	N4-C3-N2	2.34	127.95	126.11
2	B	201	1GI	C12-C11-N10	2.33	116.25	112.63
2	A	201	1GI	C25-C20-C19	-2.30	128.31	136.62
2	A	201	1GI	N28-C1-N2	2.29	123.77	118.90
2	A	201	1GI	C11-C12-C18	-2.28	116.06	120.40
2	B	201	1GI	C25-C20-C19	-2.21	128.65	136.62
2	A	201	1GI	C15-C14-C12	-2.18	118.03	121.03
2	A	201	1GI	C13-C19-C20	-2.16	117.79	121.53
2	B	201	1GI	C19-C13-C9	-2.15	117.18	120.49
2	B	201	1GI	N8-C9-N10	-2.06	109.95	115.11
2	B	201	1GI	C11-C12-C18	-2.02	116.56	120.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

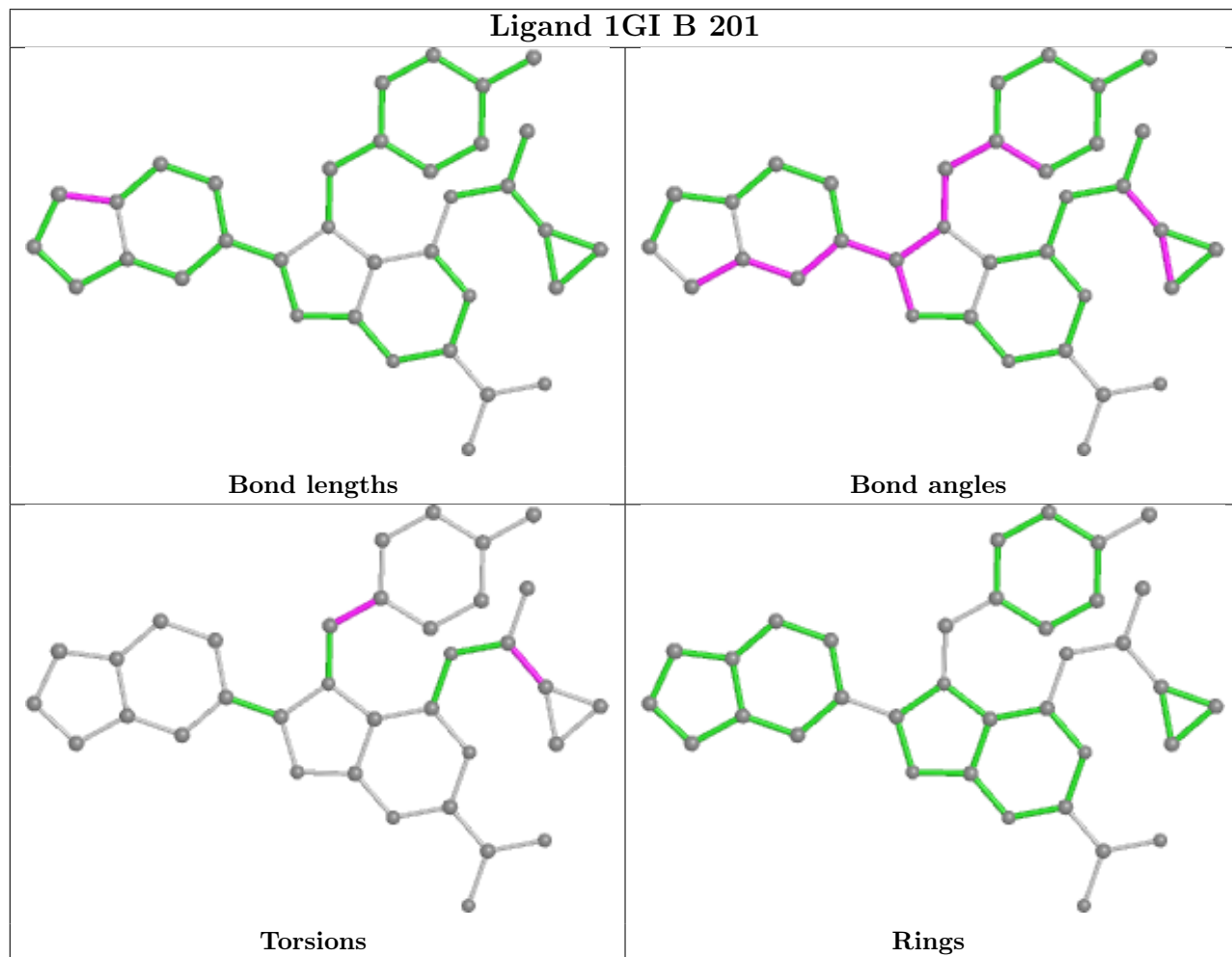
Mol	Chain	Res	Type	Atoms
2	B	201	1GI	N28-C29-C30-C32
5	B	202	GOL	O1-C1-C2-C3
2	B	201	1GI	N10-C11-C12-C14
2	A	201	1GI	N10-C11-C12-C14
2	B	201	1GI	N10-C11-C12-C18
2	A	201	1GI	N10-C11-C12-C18
2	A	201	1GI	N28-C29-C30-C32
4	A	203	CIT	C1-C2-C3-C6
4	A	203	CIT	C2-C3-C4-C5
5	B	202	GOL	C1-C2-C3-O3

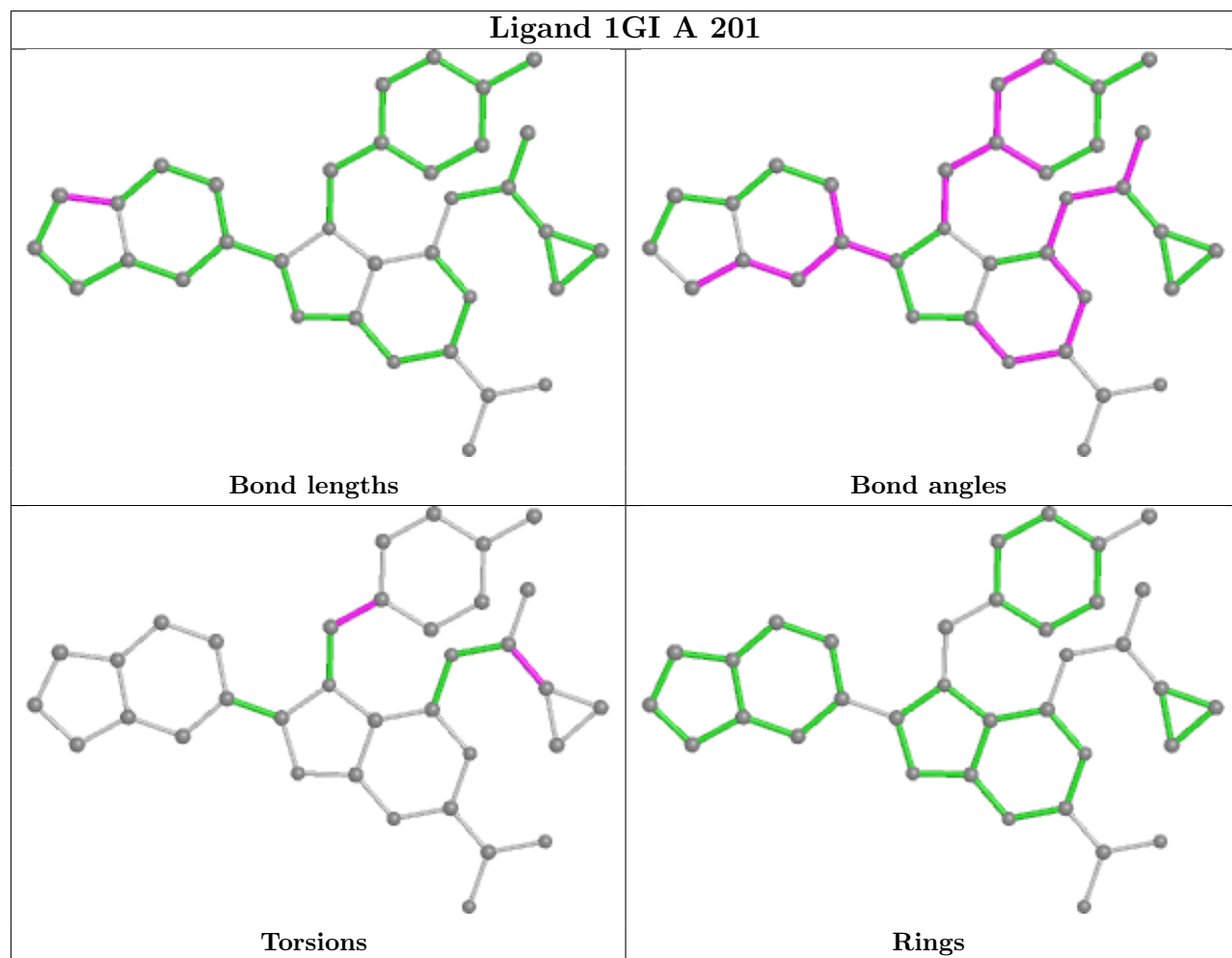
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	1GI	3	0
5	B	202	GOL	3	0
2	A	201	1GI	5	0
4	A	203	CIT	2	0

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





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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

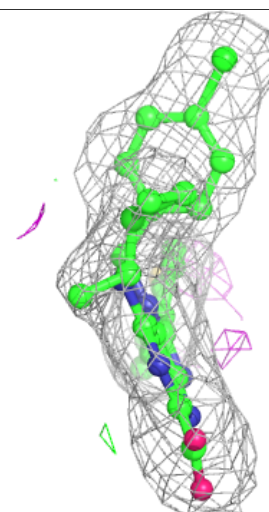
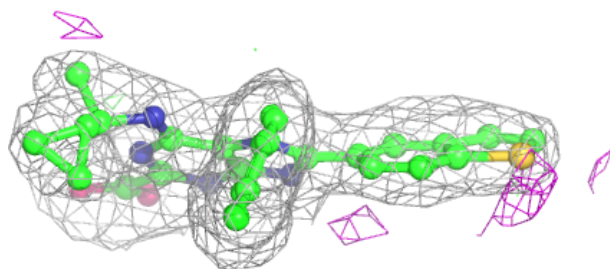
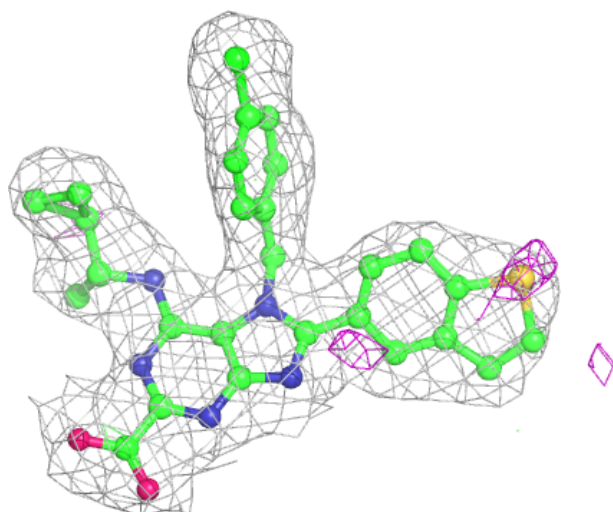
6.4 Ligands

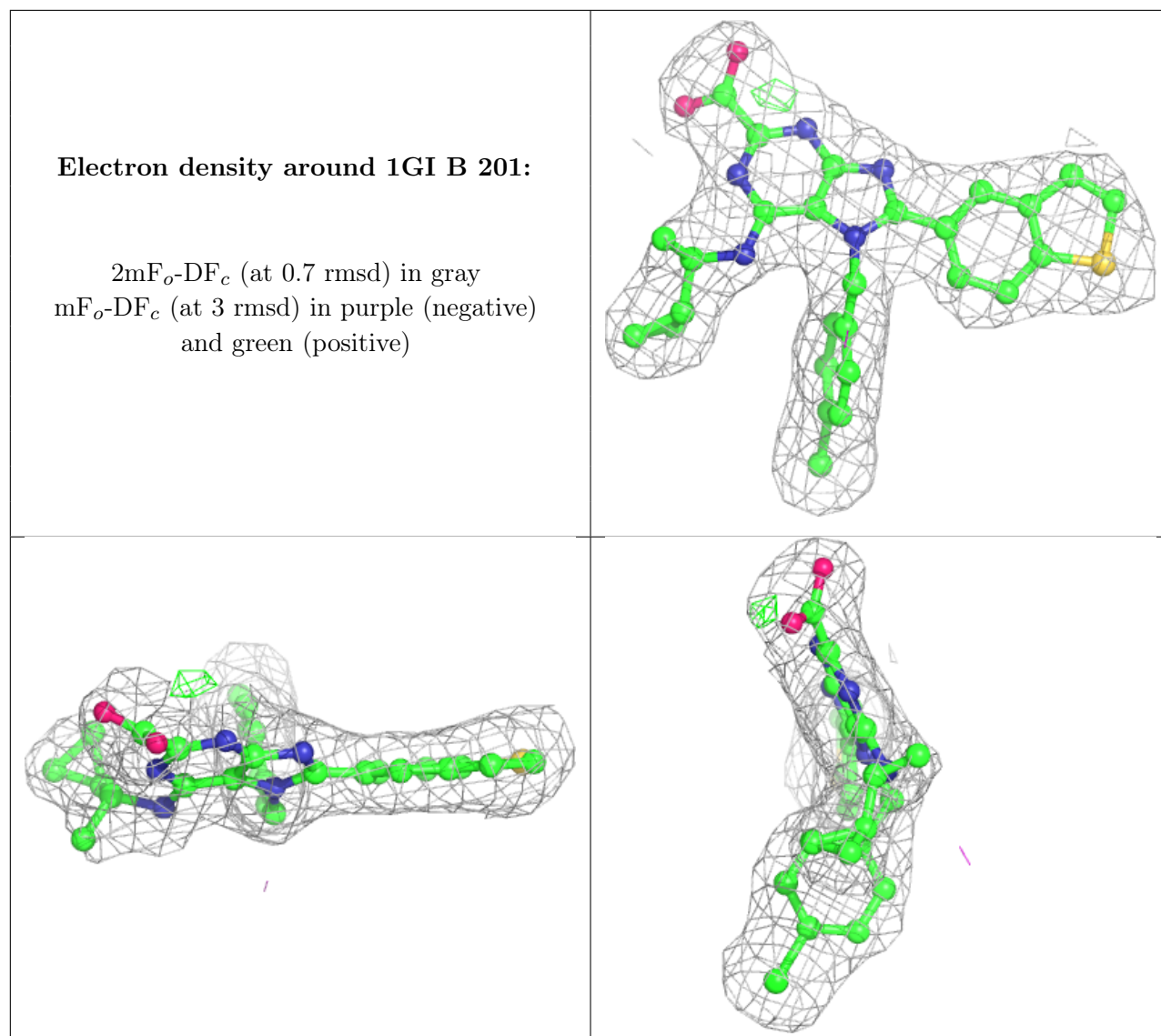
Unable to reproduce the depositors R factor - this section is therefore empty.

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 1GI A 201:

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





6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.