



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:22 PM BST

PDB ID : 3G72  
Title : Design and Preparation of Potent, Non-Peptidic, Bioavailable Renin Inhibitors  
Authors : Bezencon, O.; Bur, D.; Prade, L.; Weller, T.; Boss, C.; Fischli, W.  
Deposited on : 2009-02-09  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

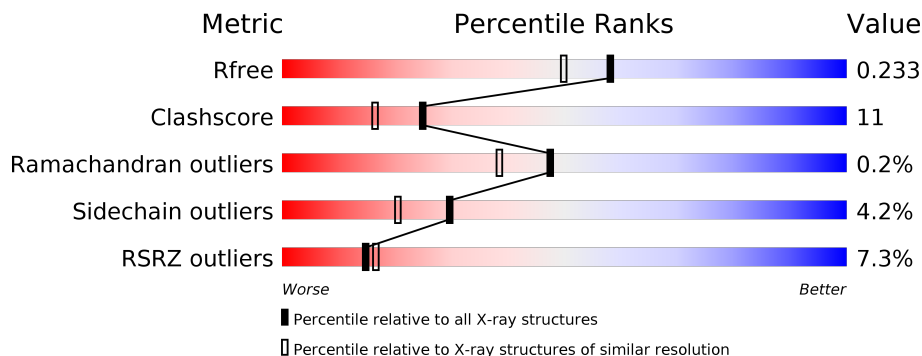
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	340	 <p>9% 78% 18% ..</p>
1	B	340	 <p>5% 77% 19% ..</p>

## 2 Entry composition [i](#)

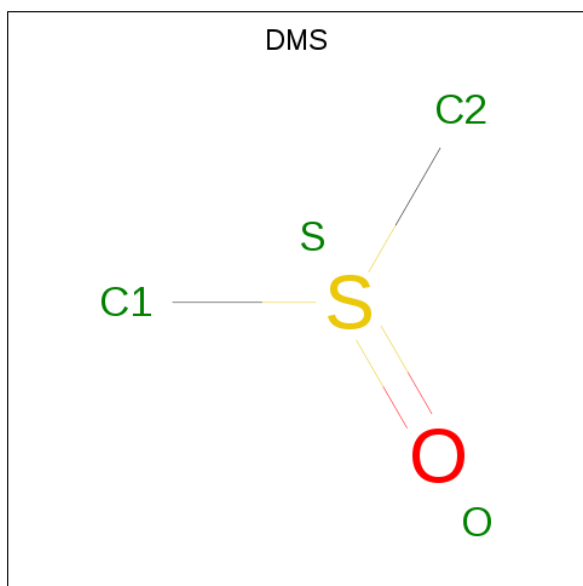
There are 5 unique types of molecules in this entry. The entry contains 5885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	Total 2584	C 1653	N 417	O 500	S 14	0	2	0
1	B	336	Total 2589	C 1655	N 418	O 502	S 14	0	0	0

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



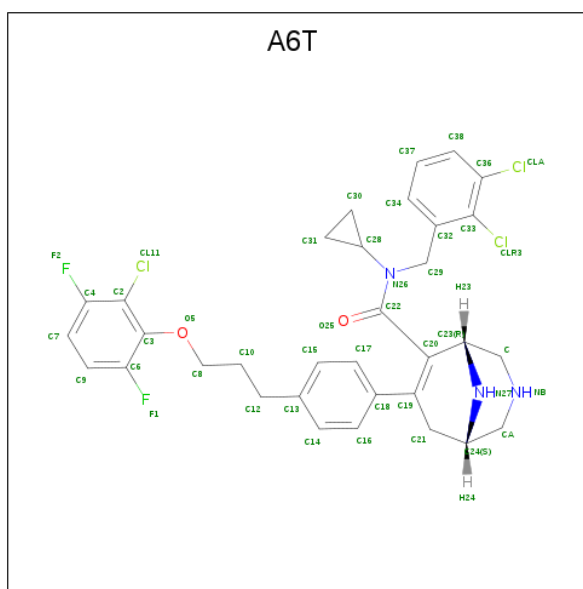
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0

- Molecule 4 is (1S,5R)-7-{4-[3-(2-chloro-3,6-difluorophenoxy)propyl]phenyl}-N-cyclopropyl-N-(2,3-dichlorobenzyl)-3,9-diazabicyclo[3.3.1]non-6-ene-6-carboxamide (three-letter code: A6T) (formula: C<sub>33</sub>H<sub>32</sub>Cl<sub>3</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
4	A	1	43	33	3	2	3	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
4	B	1	43	33	3	2	3	2	0	0

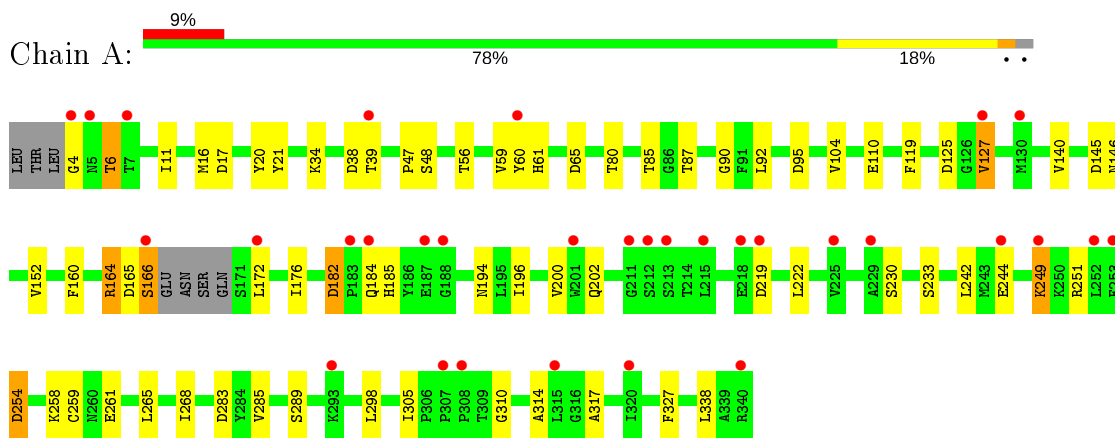
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	319	Total	O	0	0
			319	319		
5	B	271	Total	O	0	0
			271	271		

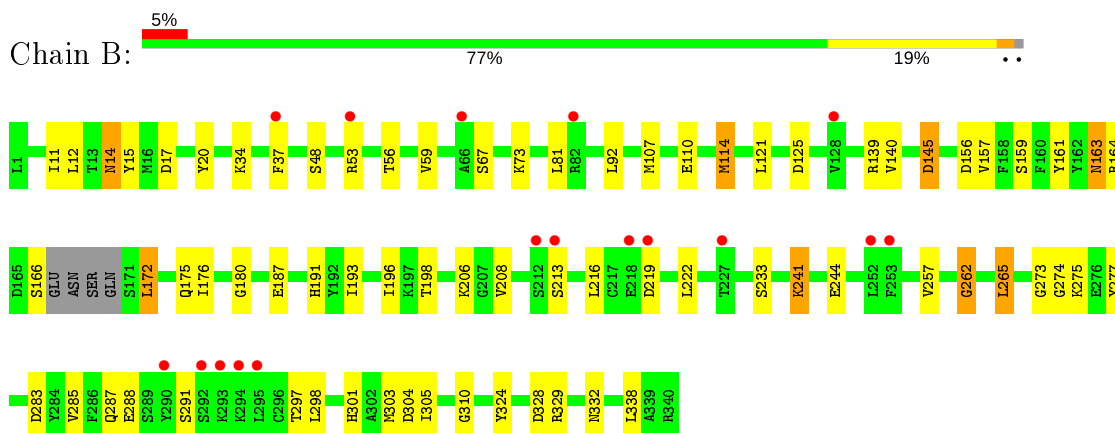
### 3 Residue-property plots [i](#)

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: Renin



- Molecule 1: Renin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.79Å 87.53Å 116.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.82 – 1.90 30.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.82-1.90) 96.8 (30.82-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.183 , 0.235 0.183 , 0.233	Depositor DCC
$R_{free}$ test set	2628 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.151	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A6T, DMS, NAG

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	0.72	0/2644	0.89	7/3586 (0.2%)
1	B	0.73	0/2648	0.90	5/3590 (0.1%)
All	All	0.72	0/5292	0.89	12/7176 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	283	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	38	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	145	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	145	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	125	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	254	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	304	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	95	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	219	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	182	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	283	ASP	CB-CG-OD2	5.33	123.09	118.30

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	2584	0	2513	52	0
1	B	2589	0	2529	59	0
2	A	4	0	6	1	0
2	B	4	0	6	1	0
3	A	14	0	13	1	0
3	B	14	0	13	6	0
4	A	43	0	32	2	0
4	B	43	0	32	1	0
5	A	319	0	0	6	1
5	B	271	0	0	6	1
All	All	5885	0	5144	113	1

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 11.

All (113) 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:B:14:ASN:HD21	1:B:17:ASP:H	1.25	0.84
1:A:21[B]:TYR:CE2	1:A:34:LYS:HD3	2.13	0.83
1:A:196:ILE:CD1	1:A:222:LEU:HD22	2.13	0.79
1:A:249:LYS:HE2	5:A:466:HOH:O	1.82	0.78
1:B:107:MET:HE1	3:B:342:NAG:O5	1.85	0.77
1:B:53:ARG:HE	1:B:59:VAL:HG12	1.48	0.77
1:A:196:ILE:HD13	1:A:222:LEU:HD22	1.71	0.73
1:B:196:ILE:HD13	1:B:222:LEU:HD22	1.71	0.72
1:B:163:ASN:HD22	1:B:164:ARG:H	1.37	0.71
1:B:20:TYR:N	2:B:341:DMS:O	2.18	0.71
1:B:14:ASN:HD22	1:B:14:ASN:C	1.92	0.70
1:B:285:VAL:HG22	1:B:298:LEU:HD22	1.73	0.70
3:A:342:NAG:O7	5:A:462:HOH:O	2.12	0.66
1:B:196:ILE:CD1	1:B:222:LEU:HD22	2.26	0.66
1:B:56:THR:HA	1:B:59:VAL:HG22	1.77	0.66
1:A:48:SER:HB2	1:A:110:GLU:HB3	1.76	0.66
1:B:48:SER:HB2	1:B:110:GLU:HB3	1.78	0.65
1:A:164:ARG:NH1	5:A:362:HOH:O	2.28	0.65
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.09	0.65
1:B:206:LYS:HE3	1:B:274:GLY:H	1.62	0.65
1:B:206:LYS:HE3	1:B:274:GLY:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASN:HD21	1:B:17:ASP:N	1.95	0.64
1:B:257:VAL:HG11	1:B:265:LEU:HD21	1.78	0.64
1:A:21[B]:TYR:HE2	1:A:34:LYS:HD3	1.61	0.63
1:B:175:GLN:NE2	5:B:374:HOH:O	2.32	0.63
1:A:4:GLY:HA2	5:A:412:HOH:O	1.99	0.62
1:B:140:VAL:HG23	5:B:524:HOH:O	2.02	0.60
1:B:107:MET:HE1	3:B:342:NAG:O6	2.02	0.60
1:A:80:THR:HG23	1:A:87:THR:CG2	2.32	0.59
1:A:185:HIS:HE1	5:A:593:HOH:O	1.84	0.59
1:A:21[B]:TYR:CD2	1:A:34:LYS:HB3	2.39	0.58
1:A:6:THR:OG1	1:A:152:VAL:O	2.20	0.57
1:A:20:TYR:N	2:A:341:DMS:O	2.22	0.57
1:B:163:ASN:ND2	1:B:164:ARG:H	2.02	0.57
1:B:14:ASN:ND2	1:B:17:ASP:H	1.99	0.57
1:B:92:LEU:CD2	1:B:107:MET:HE3	2.35	0.56
1:B:14:ASN:C	1:B:14:ASN:ND2	2.58	0.56
1:B:275:LYS:HD3	1:B:277:TYR:CZ	2.42	0.55
1:A:305:ILE:O	1:A:310:GLY:HA3	2.08	0.54
1:B:107:MET:HE1	3:B:342:NAG:C6	2.37	0.54
1:B:114:MET:HE1	4:B:343:A6T:H8A	1.89	0.54
1:B:159:SER:HB3	1:B:324:TYR:CE1	2.42	0.54
1:A:164:ARG:NH1	1:A:164:ARG:HG3	2.23	0.54
1:A:11:ILE:HD12	1:A:172:LEU:CD1	2.38	0.53
1:A:258:LYS:O	1:A:261:GLU:HG2	2.09	0.53
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.72	0.53
1:B:11:ILE:HD12	1:B:172:LEU:HD11	1.91	0.52
1:A:61:HIS:HE1	1:A:119:PHE:O	1.92	0.52
1:B:163:ASN:HD22	1:B:164:ARG:N	2.05	0.52
1:B:244:GLU:HG2	5:B:546:HOH:O	2.09	0.52
1:A:127[B]:VAL:HG21	4:A:343:A6T:H15	1.91	0.51
1:A:80:THR:HG23	1:A:87:THR:HG23	1.92	0.51
1:B:92:LEU:HD21	1:B:107:MET:CE	2.42	0.50
4:A:343:A6T:H28	4:A:343:A6T:C18	2.42	0.49
1:B:303:MET:HG2	1:B:305:ILE:HG13	1.94	0.49
1:B:216:LEU:HD21	1:B:241:LYS:HB3	1.94	0.49
1:B:198:THR:HG22	1:B:332:ASN:CG	2.33	0.48
1:B:191:HIS:CE1	1:B:273:GLY:O	2.67	0.48
1:B:305:ILE:O	1:B:310:GLY:HA3	2.12	0.48
1:A:21[B]:TYR:HD2	1:A:34:LYS:HB3	1.77	0.48
1:B:233:SER:HA	1:B:301:HIS:O	2.12	0.48
1:B:157:VAL:HG12	1:B:328:ASP:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:HB2	1:B:176:ILE:HD11	1.96	0.47
1:B:191:HIS:HE1	1:B:273:GLY:O	1.95	0.47
1:A:39:THR:HG21	1:A:327:PHE:CZ	2.48	0.47
1:B:92:LEU:HD11	1:B:140:VAL:HG11	1.96	0.47
1:B:14:ASN:HD22	1:B:15:TYR:N	2.11	0.47
1:B:92:LEU:HD21	1:B:107:MET:HE3	1.96	0.47
1:A:11:ILE:HG23	1:A:172:LEU:CD1	2.45	0.46
1:A:165:ASP:HA	1:A:166:SER:HA	1.78	0.46
1:A:285:VAL:HG22	1:A:298:LEU:HD22	1.97	0.46
1:A:182:ASP:OD1	1:A:184:GLN:HG2	2.15	0.46
1:B:156:ASP:O	1:B:329:ARG:HB2	2.15	0.46
1:A:56:THR:HA	1:A:59:VAL:HG12	1.97	0.46
1:B:107:MET:CE	3:B:342:NAG:O6	2.64	0.46
1:B:187:GLU:CD	1:B:338:LEU:HD23	2.36	0.46
1:B:107:MET:CE	3:B:342:NAG:O5	2.60	0.46
1:A:265:LEU:HD12	1:A:285:VAL:CG2	2.46	0.46
3:B:342:NAG:O4	5:B:563:HOH:O	1.64	0.45
1:A:196:ILE:HD13	1:A:222:LEU:CD2	2.46	0.45
1:A:200:VAL:HG22	1:A:202:GLN:HB2	1.98	0.45
1:A:259:CYS:HB3	1:A:289:SER:O	2.17	0.45
1:B:163:ASN:ND2	1:B:164:ARG:N	2.64	0.45
1:A:249:LYS:HE3	1:A:249:LYS:HB2	1.71	0.44
1:A:230:SER:O	1:A:317:ALA:HB3	2.18	0.44
1:A:11:ILE:HD12	1:A:172:LEU:HD13	2.00	0.44
1:B:37:PHE:CG	1:B:176:ILE:CD1	3.01	0.44
1:A:251:ARG:HB2	1:A:254:ASP:OD1	2.18	0.44
1:B:37:PHE:CD1	1:B:176:ILE:HD12	2.53	0.44
1:A:16:MET:O	1:A:17:ASP:HB2	2.19	0.43
1:B:208:VAL:HB	1:B:216:LEU:HB2	2.00	0.43
1:B:161:TYR:HB2	1:B:324:TYR:CE2	2.54	0.43
1:B:12:LEU:HD11	1:B:176:ILE:HG13	2.01	0.43
1:A:11:ILE:HG23	1:A:172:LEU:HD12	2.01	0.42
1:A:56:THR:HA	1:A:59:VAL:CG1	2.49	0.42
1:A:59:VAL:HG22	1:A:60:TYR:CE2	2.54	0.42
1:B:193:ILE:N	1:B:193:ILE:HD12	2.35	0.42
1:A:92:LEU:HD21	1:A:140:VAL:HG21	2.00	0.42
1:A:242:LEU:HD11	1:A:268:ILE:HD13	2.02	0.42
1:A:233:SER:OG	1:A:314:ALA:HB3	2.19	0.42
1:B:241:LYS:HE2	5:B:449:HOH:O	2.20	0.42
1:A:80:THR:CG2	1:A:87:THR:HG23	2.49	0.42
1:B:67:SER:HA	5:B:569:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:CZ	1:A:176:ILE:HD12	2.55	0.41
1:A:85:THR:HB	1:B:121:LEU:HD22	2.02	0.41
1:B:159:SER:OG	1:B:180:GLY:O	2.29	0.41
1:B:262:GLY:O	1:B:265:LEU:HB2	2.20	0.41
1:B:262:GLY:HA3	1:B:287:GLN:HE22	1.86	0.41
1:A:90:GLY:HA3	1:A:110:GLU:O	2.21	0.41
1:A:104:VAL:CG2	1:A:146:ASN:HB3	2.51	0.40
1:A:47:PRO:HD3	1:A:125:ASP:O	2.21	0.40
1:A:65:ASP:OD1	5:A:568:HOH:O	2.22	0.40
1:A:265:LEU:HD12	1:A:285:VAL:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:357:HOH:O	5:B:610:HOH:O[3_554]	2.11	0.09

## 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	331/340 (97%)	327 (99%)	4 (1%)	0	100	100
1	B	332/340 (98%)	326 (98%)	5 (2%)	1 (0%)	41	31
All	All	663/680 (98%)	653 (98%)	9 (1%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	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	285/290 (98%)	276 (97%)	9 (3%)	39	30
1	B	286/290 (99%)	270 (94%)	16 (6%)	21	11
All	All	571/580 (98%)	546 (96%)	25 (4%)	30	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	127[A]	VAL
1	A	127[B]	VAL
1	A	164	ARG
1	A	166	SER
1	A	194	ASN
1	A	244	GLU
1	A	249	LYS
1	A	338	LEU
1	B	14	ASN
1	B	34	LYS
1	B	73	LYS
1	B	81	LEU
1	B	114	MET
1	B	139	ARG
1	B	145	ASP
1	B	163	ASN
1	B	166	SER
1	B	172	LEU
1	B	213	SER
1	B	241	LYS
1	B	265	LEU
1	B	288	GLU
1	B	291	SER
1	B	297	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	150	GLN
1	A	184	GLN
1	A	194	ASN
1	A	202	GLN
1	A	331	ASN
1	B	14	ASN
1	B	74	HIS
1	B	135	GLN
1	B	163	ASN
1	B	191	HIS
1	B	194	ASN
1	B	287	GLN
1	B	331	ASN

### 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](#)

6 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
3	NAG	A	342	1	14,14,15	0.47	0	17,19,21	1.67	3 (17%)
3	NAG	B	342	1	14,14,15	0.93	1 (7%)	17,19,21	1.15	2 (11%)
2	DMS	B	341	-	3,3,3	2.53	1 (33%)	3,3,3	0.87	0
4	A6T	A	343	-	45,48,48	1.42	7 (15%)	59,69,69	1.87	16 (27%)
2	DMS	A	341	-	3,3,3	2.55	1 (33%)	3,3,3	1.26	0
4	A6T	B	343	-	45,48,48	1.46	8 (17%)	59,69,69	2.12	16 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A6T	A	343	-	-	1/27/51/51	0/6/6/6
3	NAG	A	342	1	-	4/6/23/26	0/1/1/1
3	NAG	B	342	1	-	0/6/23/26	0/1/1/1
4	A6T	B	343	-	-	1/27/51/51	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	DMS	O-S	4.26	1.79	1.50
2	A	341	DMS	O-S	4.25	1.78	1.50
4	A	343	A6T	C10-C12	-3.94	1.33	1.52
4	B	343	A6T	C10-C12	-3.76	1.34	1.52
4	A	343	A6T	C2-CL11	3.74	1.80	1.72
4	B	343	A6T	C33-CLR3	3.63	1.80	1.72
4	B	343	A6T	C24-N27	-3.22	1.45	1.47
4	A	343	A6T	C30-C28	3.16	1.55	1.48
4	B	343	A6T	C36-CLA	2.95	1.80	1.73
4	A	343	A6T	C33-CLR3	2.89	1.79	1.72
4	B	343	A6T	C2-CL11	2.87	1.79	1.72
3	B	342	NAG	O7-C7	2.75	1.29	1.23
4	B	343	A6T	C30-C28	2.68	1.54	1.48
4	A	343	A6T	C21-C19	2.55	1.53	1.50
4	A	343	A6T	C22-C20	-2.34	1.46	1.49
4	B	343	A6T	C21-C19	2.21	1.53	1.50
4	A	343	A6T	C36-C33	-2.16	1.36	1.39
4	B	343	A6T	C31-C28	2.02	1.53	1.48

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	343	A6T	C20-C22-N26	7.65	127.61	119.66
4	B	343	A6T	C32-C29-N26	6.16	122.17	113.34
4	A	343	A6T	C20-C22-N26	5.43	125.31	119.66
4	B	343	A6T	C33-C36-CLA	-5.09	115.56	120.52
4	A	343	A6T	C32-C29-N26	4.70	120.07	113.34
4	A	343	A6T	CA-NB-C	4.54	116.68	111.70
3	A	342	NAG	C2-N2-C7	4.14	128.80	122.90
4	B	343	A6T	C-C23-C20	3.69	116.40	111.89
4	B	343	A6T	C29-N26-C28	-3.63	114.54	118.33
4	B	343	A6T	C29-C32-C33	-3.44	116.00	121.73
4	A	343	A6T	CA-C24-C21	-3.38	108.74	112.62
4	A	343	A6T	C20-C23-N27	-3.31	104.81	108.91
4	A	343	A6T	C29-N26-C28	-3.30	114.89	118.33
4	B	343	A6T	O25-C22-N26	-3.26	115.26	122.15
3	B	342	NAG	C2-N2-C7	-3.04	118.57	122.90
4	B	343	A6T	C34-C32-C33	3.03	119.57	117.43
4	A	343	A6T	C29-C32-C33	-2.97	116.78	121.73
4	A	343	A6T	C-C23-C20	2.93	115.47	111.89
3	A	342	NAG	O5-C5-C6	2.93	111.79	107.20
4	B	343	A6T	C20-C23-N27	-2.87	105.35	108.91
4	B	343	A6T	C38-C36-CLA	2.86	124.15	118.41
4	B	343	A6T	C3-C2-C4	2.86	120.36	117.93
4	A	343	A6T	C33-C36-CLA	-2.78	117.82	120.52
4	A	343	A6T	C21-C19-C18	-2.53	111.85	115.94
4	B	343	A6T	C10-C12-C13	2.50	123.09	113.68
4	A	343	A6T	O25-C22-C20	-2.43	113.79	119.94
4	A	343	A6T	O5-C3-C2	-2.30	117.60	120.66
4	A	343	A6T	F1-C6-C3	2.25	120.67	117.58
4	A	343	A6T	C4-C2-CL11	2.23	124.32	119.97
4	B	343	A6T	O5-C3-C2	-2.23	117.70	120.66
3	B	342	NAG	O7-C7-C8	-2.23	117.92	122.06
4	B	343	A6T	F1-C6-C3	2.19	120.58	117.58
4	B	343	A6T	C29-C32-C34	2.17	124.39	120.11
4	A	343	A6T	C29-C32-C34	2.16	124.38	120.11
4	A	343	A6T	C30-C31-C28	2.09	61.61	59.80
4	B	343	A6T	CA-C24-N27	-2.06	105.26	109.52
3	A	342	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	343	A6T	C2-C3-O5-C8

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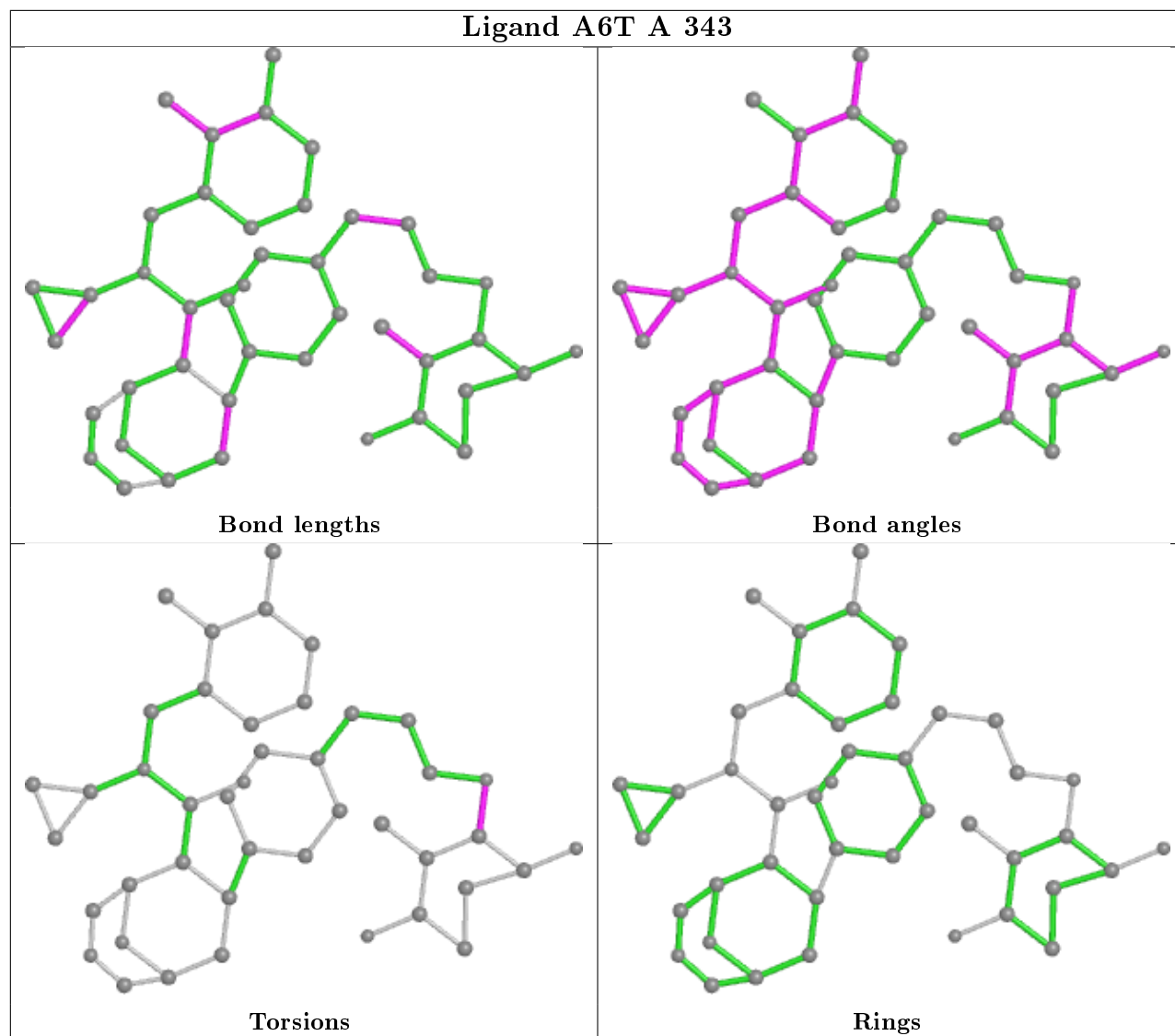
Mol	Chain	Res	Type	Atoms
3	A	342	NAG	C4-C5-C6-O6
3	A	342	NAG	O5-C5-C6-O6
3	A	342	NAG	O7-C7-N2-C2
3	A	342	NAG	C8-C7-N2-C2
4	B	343	A6T	C31-C28-N26-C22

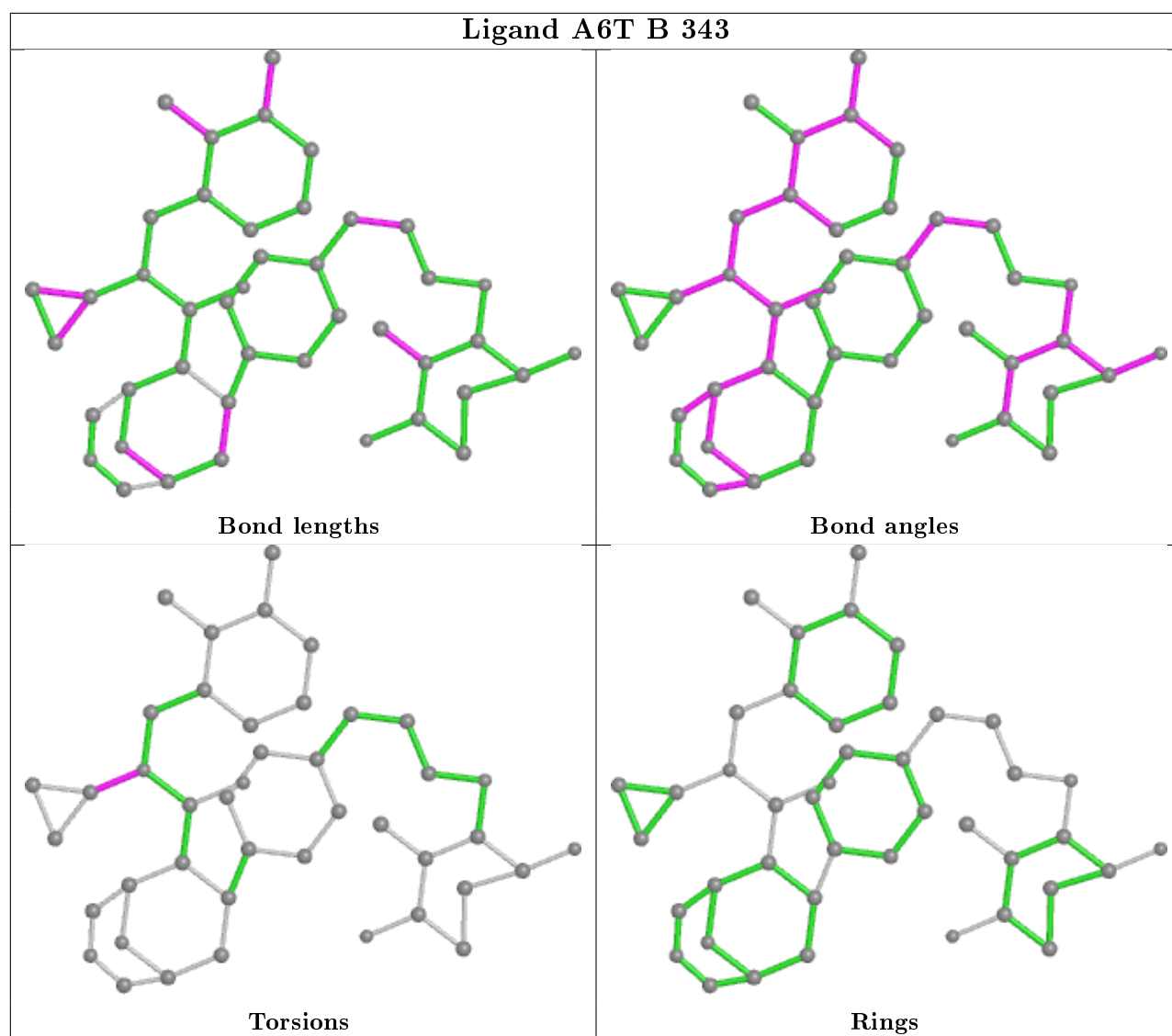
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	342	NAG	1	0
3	B	342	NAG	6	0
2	B	341	DMS	1	0
4	A	343	A6T	2	0
2	A	341	DMS	1	0
4	B	343	A6T	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	333/340 (97%)	0.38	32 (9%) 8 9	19, 33, 61, 74	0
1	B	336/340 (98%)	0.29	17 (5%) 28 31	20, 34, 56, 73	0
All	All	669/680 (98%)	0.33	49 (7%) 15 16	19, 33, 58, 74	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	PHE	4.4
1	A	225	VAL	4.1
1	A	5	ASN	4.1
1	A	307	PRO	3.9
1	B	293	LYS	3.8
1	B	82	ARG	3.8
1	B	294	LYS	3.7
1	B	292	SER	3.6
1	A	215	LEU	3.6
1	B	128	VAL	3.5
1	B	253	PHE	3.4
1	B	295	LEU	3.4
1	B	290	TYR	3.3
1	A	211	GLY	3.2
1	A	4	GLY	3.1
1	A	166	SER	3.1
1	A	172	LEU	3.0
1	A	213	SER	2.9
1	A	252	LEU	2.9
1	A	229	ALA	2.8
1	A	127[A]	VAL	2.8
1	A	60	TYR	2.7
1	A	201	TRP	2.5
1	A	212	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	2.5
1	B	218	GLU	2.5
1	A	308	PRO	2.4
1	A	249	LYS	2.4
1	A	7	THR	2.4
1	A	130	MET	2.4
1	A	244	GLU	2.3
1	B	252	LEU	2.3
1	A	219	ASP	2.3
1	B	213	SER	2.3
1	A	184	GLN	2.3
1	B	212	SER	2.3
1	B	37	PHE	2.2
1	A	320	ILE	2.2
1	B	219	ASP	2.2
1	A	187	GLU	2.2
1	A	188	GLY	2.2
1	B	53	ARG	2.2
1	A	218	GLU	2.1
1	A	183	PRO	2.1
1	A	39	THR	2.1
1	A	293	LYS	2.1
1	B	227	THR	2.1
1	A	340	ARG	2.0
1	B	66	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

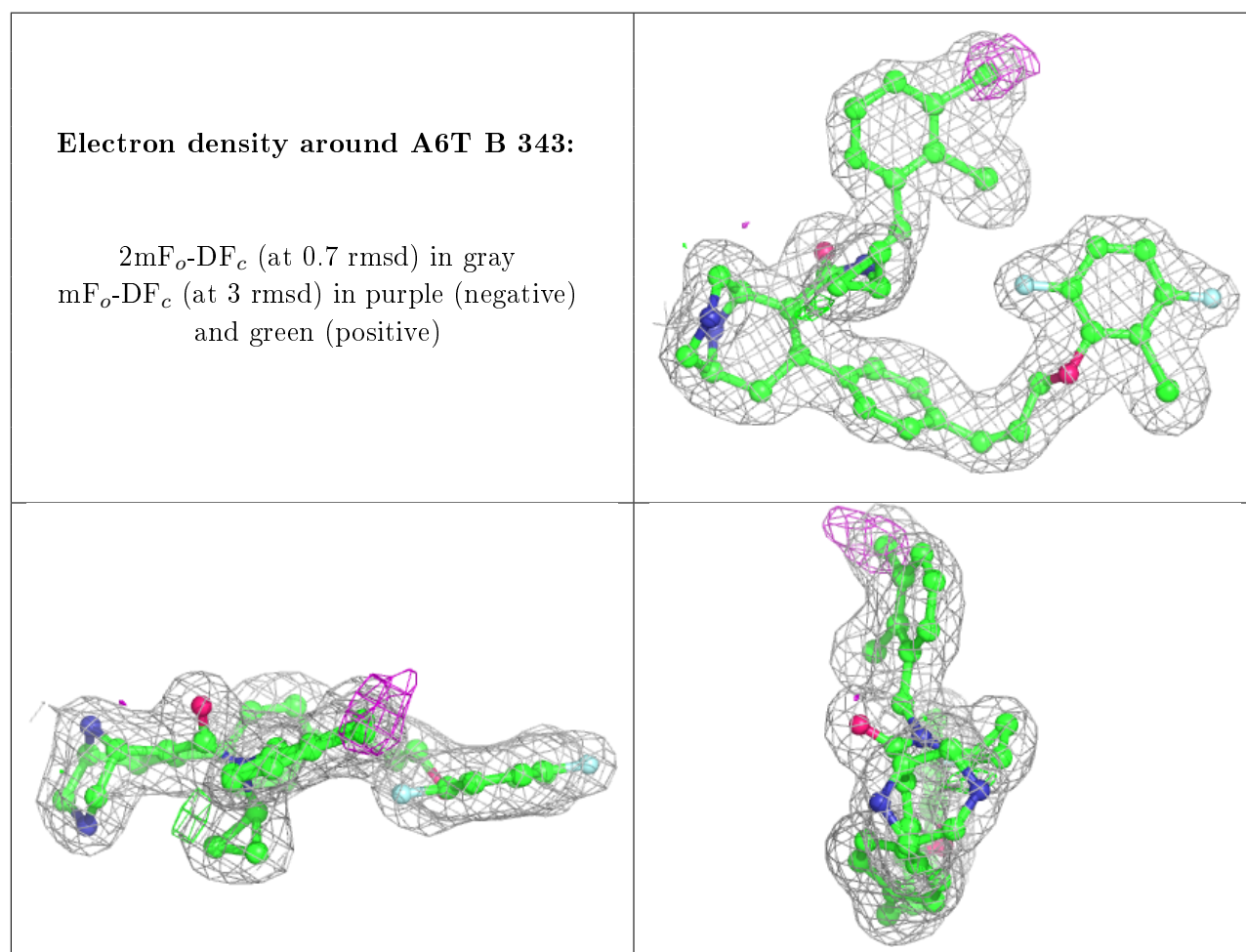
There are no monosaccharides in this entry.

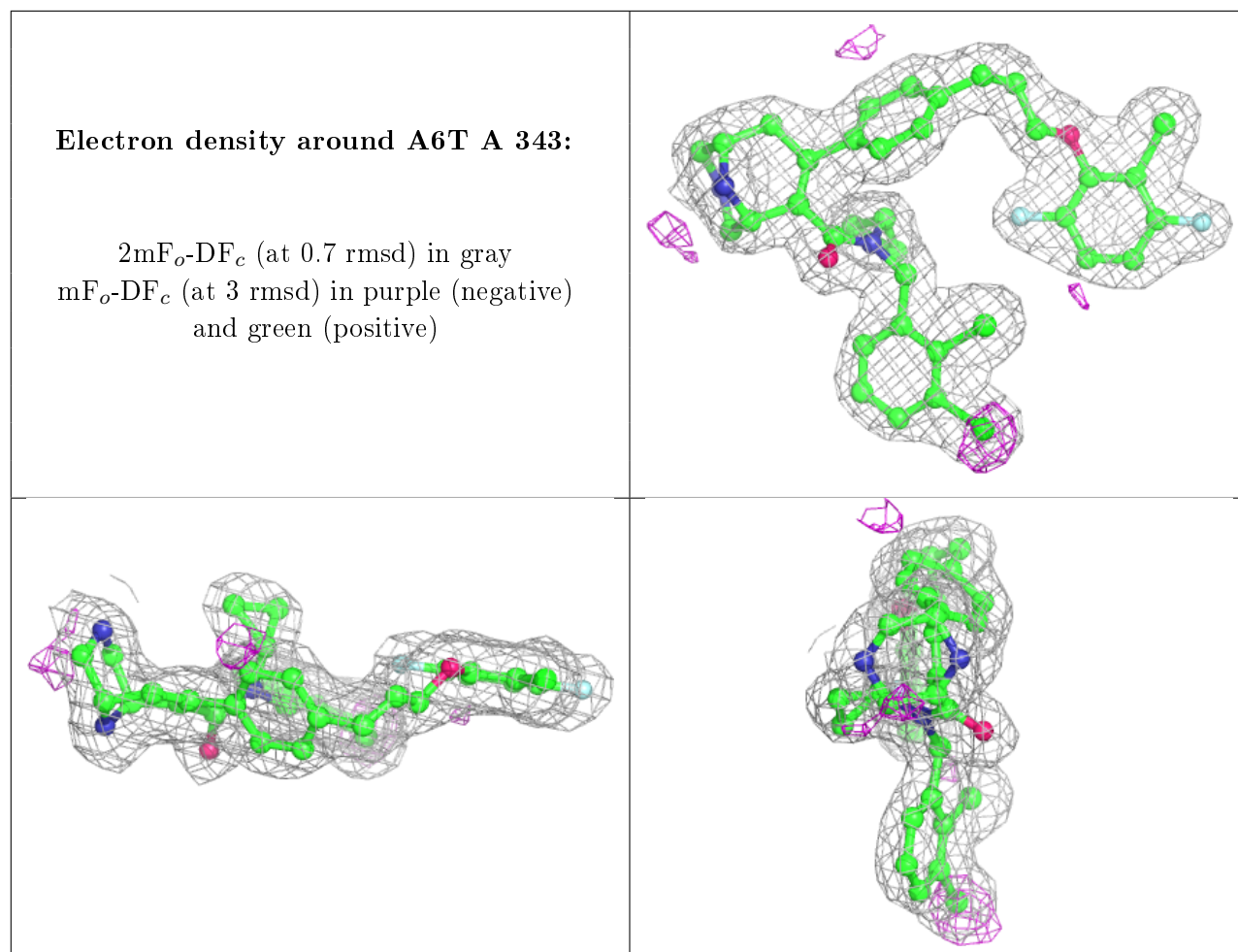
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	A	342	14/15	0.73	0.22	50,56,58,59	0
3	NAG	B	342	14/15	0.76	0.26	67,70,72,72	0
4	A6T	B	343	43/43	0.93	0.13	23,29,35,37	0
2	DMS	A	341	4/4	0.94	0.15	32,38,39,41	0
4	A6T	A	343	43/43	0.94	0.11	22,28,33,36	0
2	DMS	B	341	4/4	0.98	0.10	33,34,35,36	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.