



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 04:27 PM EST

PDB ID : 4G86  
Title : Crystal structure of the redox-active cofactor DBMIB bound to the full length circadian clock protein KaiA from *Synechococcus elongatus*  
Authors : Pattanayek, R.; Egli, M.  
Deposited on : 2012-07-21  
Resolution : 2.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

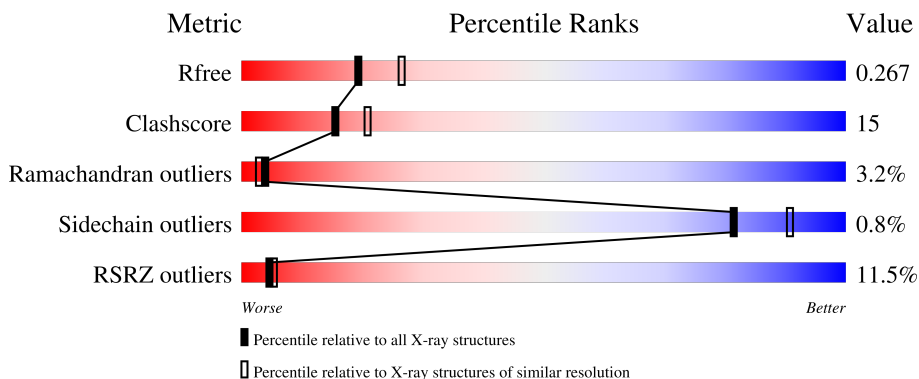
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 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	284	
1	B	284	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BNT	A	301	-	-	X	-
2	BNT	A	304	-	-	-	X
2	BNT	B	1301	-	-	X	X
2	BNT	B	1302	-	-	X	-
3	1PE	A	302	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4809 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.

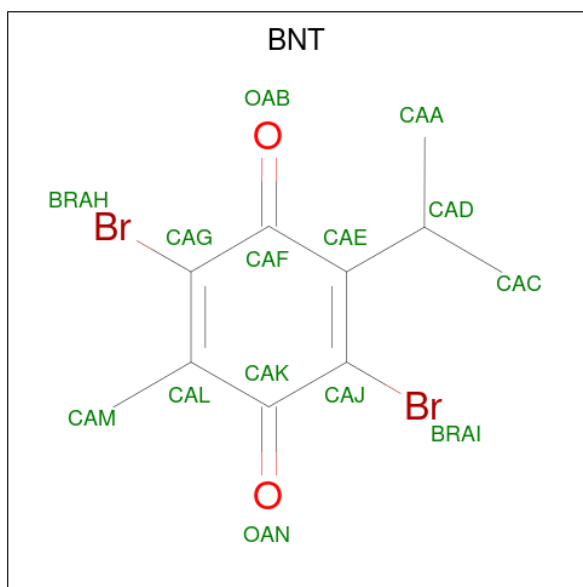
- Molecule 1 is a protein called Circadian clock protein kaiA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2271	1433	393	430	15	0	0	0
1	B	282	2271	1433	393	430	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP Q79PF6
B	1	VAL	-	expression tag	UNP Q79PF6

- Molecule 2 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (three-letter code: BNT) (formula: C<sub>10</sub>H<sub>10</sub>Br<sub>2</sub>O<sub>2</sub>).



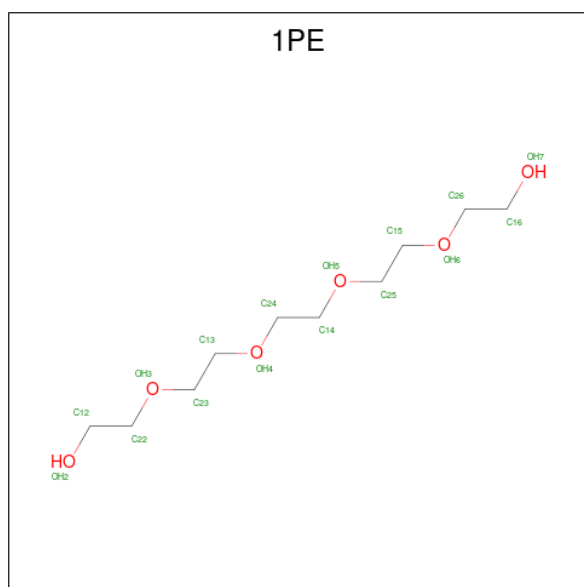
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
2	A	1	14	2	10	2	0	0

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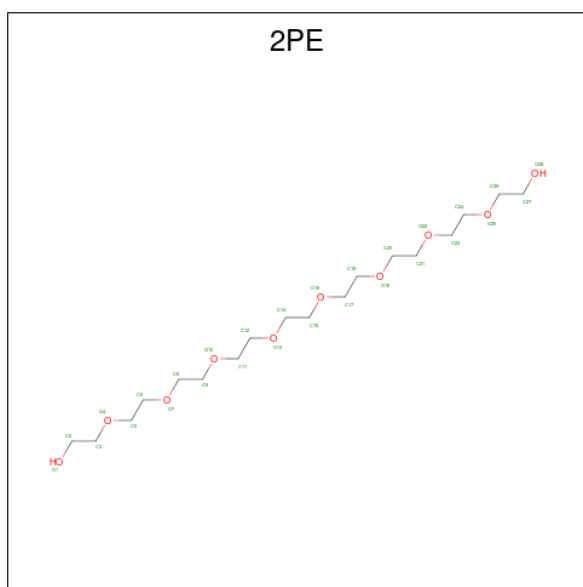
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
2	A	1	14	2	10	2	0	0
2	B	1	14	2	10	2	0	0
2	B	1	14	2	10	2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	10	6	4	0	0

- Molecule 4 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula:  $C_{18}H_{38}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	8	4		

- 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		
5	B	1	Total	C	O	0	0
			6	3	3		

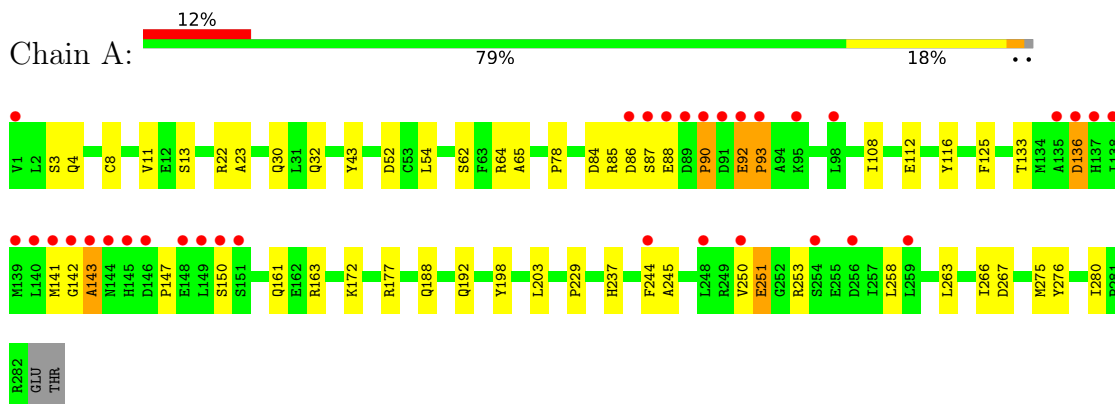
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	93	Total O 93 93	0	0
6	B	84	Total O 84 84	0	0

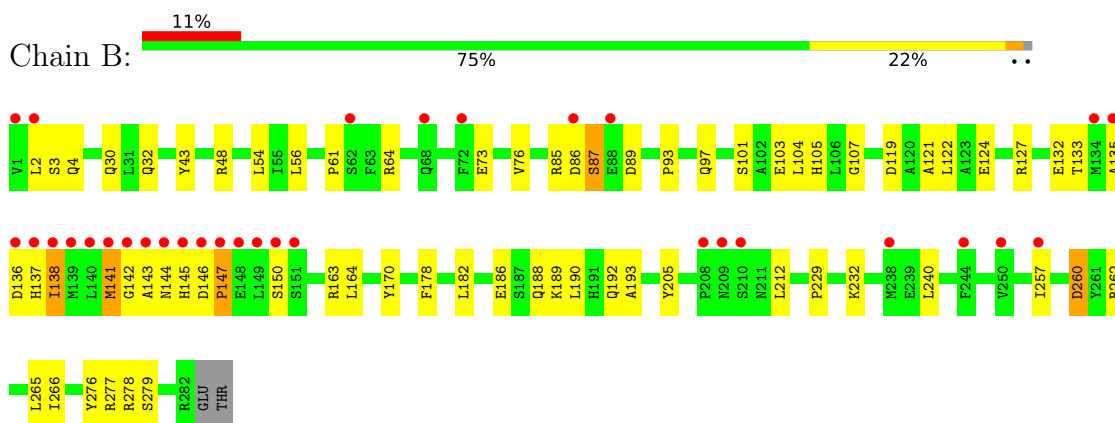
### 3 Residue-property plots

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 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: Circadian clock protein kaiA



- Molecule 1: Circadian clock protein kaiA





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.25Å 126.35Å 56.38Å 90.00° 114.36° 90.00°	Depositor
Resolution (Å)	47.58 – 2.39 47.58 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.58-2.39) 93.3 (47.58-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069), CNS	Depositor
R, $R_{free}$	0.219 , 0.265 0.221 , 0.267	Depositor DCC
$R_{free}$ test set	1202 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: GOL, BNT, 1PE, 2PE

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	0.27	0/2314	0.48	0/3138
1	B	0.29	0/2314	0.49	0/3138
All	All	0.28	0/4628	0.48	0/6276

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

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	2271	0	2242	59	0
1	B	2271	0	2242	76	0
2	A	28	0	20	20	0
2	B	28	0	20	19	0
3	A	10	0	13	10	0
4	A	12	0	15	4	0
5	B	12	0	16	2	0
6	A	93	0	0	1	0
6	B	84	0	0	1	0
All	All	4809	0	4568	136	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 15.

All (136) 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:137:HIS:CA	1:B:138:ILE:HG22	1.08	1.53
1:B:137:HIS:HA	1:B:138:ILE:CG2	1.07	1.51
1:B:143:ALA:N	1:B:144:ASN:HA	1.57	1.17
1:B:141:MET:SD	1:B:144:ASN:HB2	1.96	1.04
1:B:137:HIS:HA	1:B:138:ILE:CB	1.80	1.02
1:A:64:ARG:HB2	2:A:301:BNT:BRAI	2.17	0.98
1:B:137:HIS:CB	1:B:138:ILE:HG22	1.94	0.97
1:A:64:ARG:HB2	2:A:301:BNT:HAC2	1.43	0.96
1:A:64:ARG:N	2:A:301:BNT:BRAI	2.56	0.93
1:B:132:GLU:HG3	1:B:137:HIS:NE2	1.89	0.88
1:A:64:ARG:HE	2:A:301:BNT:HAC1	1.36	0.87
1:B:137:HIS:N	1:B:138:ILE:HG22	1.90	0.87
2:A:304:BNT:HAC2	1:B:277:ARG:HH12	1.39	0.86
1:A:64:ARG:HB2	2:A:301:BNT:CAC	2.05	0.85
1:B:141:MET:CE	1:B:144:ASN:O	2.26	0.84
1:B:143:ALA:N	1:B:144:ASN:CA	2.41	0.81
1:B:141:MET:SD	1:B:144:ASN:CB	2.68	0.80
1:B:64:ARG:HB2	2:B:1302:BNT:HAM1	1.62	0.80
1:A:112:GLU:HB2	2:B:1301:BNT:HAM3	1.64	0.79
1:B:61:PRO:HA	2:B:1302:BNT:HAC1	1.64	0.79
1:A:64:ARG:NE	2:A:301:BNT:HAC1	2.01	0.76
3:A:302:1PE:H262	2:B:1301:BNT:CAK	2.15	0.75
1:A:64:ARG:CB	2:A:301:BNT:BRAI	2.92	0.72
1:B:136:ASP:O	1:B:138:ILE:CG2	2.39	0.71
1:B:142:GLY:C	1:B:144:ASN:HA	2.11	0.71
2:A:301:BNT:BRAI	2:A:301:BNT:HAC2	2.45	0.70
2:B:1302:BNT:BRAI	2:B:1302:BNT:HAA3	2.47	0.69
1:B:141:MET:HE1	1:B:144:ASN:O	1.92	0.69
1:B:137:HIS:CA	1:B:138:ILE:CG2	1.99	0.67
1:B:186:GLU:HG3	2:B:1301:BNT:BRAI	2.50	0.67
1:B:48:ARG:NH2	1:B:73:GLU:O	2.25	0.67
1:A:65:ALA:N	2:A:301:BNT:BRAI	2.82	0.66
1:B:141:MET:SD	1:B:144:ASN:CG	2.74	0.66
1:B:143:ALA:H	1:B:144:ASN:HA	1.59	0.66
1:B:279:SER:HB3	5:B:1304:GOL:H32	1.75	0.66
1:A:112:GLU:HB3	3:A:302:1PE:H241	1.77	0.65
1:B:278:ARG:HH12	5:B:1303:GOL:H31	1.60	0.65
1:A:112:GLU:HA	3:A:302:1PE:H151	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1302:BNT:BRAI	2:B:1302:BNT:HAC2	2.53	0.63
1:A:64:ARG:CB	2:A:301:BNT:HAC2	2.24	0.63
1:A:64:ARG:CB	2:A:301:BNT:CAC	2.77	0.63
1:B:137:HIS:CB	1:B:138:ILE:CG2	2.64	0.62
1:B:141:MET:SD	1:B:144:ASN:ND2	2.72	0.62
1:A:22:ARG:NE	4:A:303:2PE:H51	2.16	0.61
1:A:161:GLN:NE2	6:A:459:HOH:O	2.32	0.61
1:B:136:ASP:O	1:B:138:ILE:HG21	2.00	0.61
1:A:64:ARG:CA	2:A:301:BNT:BRAI	3.03	0.61
1:A:112:GLU:O	3:A:302:1PE:H261	2.02	0.60
1:A:22:ARG:CZ	4:A:303:2PE:H51	2.33	0.59
1:A:263:LEU:HD11	1:B:262:ARG:CZ	2.32	0.58
1:A:198:TYR:OH	1:A:237:HIS:ND1	2.23	0.58
1:A:23:ALA:O	3:A:302:1PE:H161	2.04	0.57
1:A:229:PRO:HD3	2:A:304:BNT:HAC1	1.86	0.57
1:B:193:ALA:HB2	2:B:1301:BNT:BRAH	2.60	0.57
1:A:275:MET:SD	6:B:1462:HOH:O	2.58	0.56
3:A:302:1PE:H262	2:B:1301:BNT:CAL	2.35	0.56
1:A:147:PRO:HG2	1:A:150:SER:HB2	1.87	0.56
1:A:172:LYS:HE2	1:B:2:LEU:HD23	1.88	0.56
1:B:141:MET:HA	1:B:141:MET:HE2	1.88	0.55
1:A:251:GLU:HB3	1:A:253:ARG:HG3	1.89	0.55
2:A:301:BNT:BRAI	2:A:301:BNT:HAA3	2.62	0.55
3:A:302:1PE:H152	2:B:1301:BNT:HAM1	1.90	0.53
1:A:64:ARG:CD	2:A:301:BNT:HAC1	2.39	0.53
1:B:182:LEU:HD13	2:B:1301:BNT:HAC2	1.90	0.53
1:A:92:GLU:HB2	1:A:93:PRO:HD3	1.91	0.53
1:B:137:HIS:HB3	1:B:138:ILE:CG2	2.37	0.52
1:B:124:GLU:OE1	1:B:127:ARG:NH2	2.31	0.52
1:B:76:VAL:HG21	1:B:133:THR:HG21	1.93	0.51
1:B:141:MET:CE	1:B:141:MET:N	2.73	0.51
1:A:85:ARG:C	1:A:87:SER:H	2.14	0.50
1:B:260:ASP:OD1	1:B:260:ASP:N	2.44	0.50
1:B:133:THR:OG1	1:B:136:ASP:HB3	2.11	0.50
1:A:22:ARG:NH2	4:A:303:2PE:H51	2.27	0.49
1:B:4:GLN:OE1	1:B:30:GLN:NE2	2.44	0.49
1:B:141:MET:N	1:B:141:MET:HE3	2.28	0.49
1:B:141:MET:HE2	1:B:144:ASN:O	2.13	0.49
1:A:8:CYS:HB3	1:A:54:LEU:HD23	1.95	0.48
1:A:203:LEU:HG	1:A:244:PHE:HZ	1.77	0.48
1:A:133:THR:OG1	1:A:136:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:NH1	1:B:119:ASP:OD2	2.37	0.48
1:A:280:ILE:HD12	1:B:170:TYR:CE1	2.49	0.48
1:A:52:ASP:CG	1:A:163:ARG:HH22	2.18	0.47
1:B:144:ASN:H	1:B:145:HIS:CD2	2.33	0.47
1:A:78:PRO:HG3	1:A:125:PHE:CG	2.49	0.47
1:B:85:ARG:O	1:B:87:SER:N	2.46	0.47
1:B:54:LEU:HD22	1:B:56:LEU:HD21	1.97	0.47
1:A:276:TYR:HB3	1:B:276:TYR:HB3	1.97	0.47
1:B:103:GLU:OE2	1:B:105:HIS:NE2	2.34	0.46
1:A:22:ARG:HG3	3:A:302:1PE:H252	1.96	0.46
1:B:136:ASP:C	1:B:138:ILE:HG22	2.34	0.46
1:A:116:TYR:HE2	2:B:1301:BNT:HAA2	1.81	0.46
1:A:245:ALA:HB2	1:A:258:LEU:HD11	1.97	0.46
1:A:64:ARG:CB	2:A:301:BNT:HAC1	2.45	0.46
1:A:112:GLU:CA	3:A:302:1PE:H151	2.45	0.46
1:B:205:TYR:HA	1:B:212:LEU:HD13	1.98	0.46
1:A:4:GLN:OE1	1:A:30:GLN:NE2	2.48	0.45
1:A:172:LYS:HG2	1:B:164:LEU:O	2.16	0.45
1:B:141:MET:HA	1:B:142:GLY:HA3	1.66	0.45
1:B:64:ARG:CB	2:B:1302:BNT:HAM1	2.41	0.45
1:B:144:ASN:OD1	1:B:145:HIS:CE1	2.70	0.44
1:A:3:SER:OG	1:A:163:ARG:HB3	2.18	0.44
3:A:302:1PE:H152	2:B:1301:BNT:CAM	2.47	0.44
1:B:122:LEU:HD13	1:B:164:LEU:HD13	2.00	0.44
1:B:64:ARG:HB2	2:B:1302:BNT:CAM	2.40	0.44
1:B:186:GLU:HB3	2:B:1301:BNT:HAC1	2.00	0.43
1:B:64:ARG:HD3	1:B:85:ARG:NH1	2.34	0.43
1:B:147:PRO:O	1:B:150:SER:N	2.41	0.43
1:B:141:MET:SD	1:B:144:ASN:O	2.76	0.43
1:B:189:LYS:HD2	2:B:1301:BNT:HAM2	2.00	0.43
1:B:141:MET:CE	1:B:141:MET:CA	2.97	0.43
1:B:190:LEU:HB2	2:B:1301:BNT:HAC3	2.01	0.42
1:A:32:GLN:HG2	1:A:43:TYR:CZ	2.54	0.42
1:A:142:GLY:N	1:A:143:ALA:HB2	2.34	0.42
1:B:188:GLN:NE2	1:B:192:GLN:OE1	2.53	0.42
1:B:93:PRO:HG3	1:B:107:GLY:N	2.34	0.42
1:B:240:LEU:HD13	1:B:240:LEU:HA	1.93	0.42
1:A:64:ARG:HD3	2:A:301:BNT:CAE	2.50	0.42
1:A:11:VAL:HG22	1:A:13:SER:H	1.85	0.42
1:B:97:GLN:NE2	1:B:101:SER:HA	2.34	0.42
1:B:229:PRO:HD2	1:B:232:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HD13	1:B:265:LEU:HD23	2.02	0.42
1:A:52:ASP:OD2	1:A:163:ARG:NH2	2.48	0.41
1:B:32:GLN:HG2	1:B:43:TYR:CZ	2.55	0.41
1:B:178:PHE:O	1:B:182:LEU:HG	2.20	0.41
1:A:84:ASP:HB3	1:A:90:PRO:O	2.21	0.41
1:A:263:LEU:HD11	1:B:262:ARG:NH1	2.35	0.41
1:B:141:MET:HE2	1:B:141:MET:CA	2.50	0.41
1:B:3:SER:OG	1:B:163:ARG:HD2	2.19	0.41
1:A:62:SER:C	2:A:301:BNT:BRAI	3.13	0.41
1:A:188:GLN:NE2	1:A:192:GLN:OE1	2.52	0.41
1:A:85:ARG:O	1:A:87:SER:N	2.54	0.41
1:B:189:LYS:HB3	2:B:1301:BNT:CAG	2.51	0.41
1:A:22:ARG:CZ	4:A:303:2PE:H22	2.51	0.40
2:A:301:BNT:BRAI	2:A:301:BNT:CAC	3.20	0.40
1:B:104:LEU:HD13	1:B:121:ALA:HA	2.04	0.40
1:A:92:GLU:OE2	1:A:108:ILE:HG12	2.22	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	280/284 (99%)	259 (92%)	12 (4%)	9 (3%)	4	3
1	B	280/284 (99%)	257 (92%)	14 (5%)	9 (3%)	4	3
All	All	560/568 (99%)	516 (92%)	26 (5%)	18 (3%)	4	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	B	138	ILE

Continued on next page...

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Mol	Chain	Res	Type
1	A	90	PRO
1	A	92	GLU
1	A	136	ASP
1	A	143	ALA
1	B	86	ASP
1	B	87	SER
1	B	135	ALA
1	A	93	PRO
1	A	141	MET
1	A	86	ASP
1	B	141	MET
1	A	250	VAL
1	B	89	ASP
1	B	147	PRO
1	B	146	ASP
1	B	266	ILE

### 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	250/252 (99%)	248 (99%)	2 (1%)	81	91
1	B	250/252 (99%)	248 (99%)	2 (1%)	81	91
All	All	500/504 (99%)	496 (99%)	4 (1%)	81	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	267	ASP
1	B	257	ILE
1	B	260	ASP

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

Mol	Chain	Res	Type
1	A	30	GLN
1	B	145	HIS
1	B	271	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](#)

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
5	GOL	B	1303	-	5,5,5	0.35	0	5,5,5	0.33	0
2	BNT	A	301	-	13,14,14	1.32	2 (15%)	15,21,21	1.34	1 (6%)
2	BNT	A	304	-	13,14,14	1.33	2 (15%)	15,21,21	1.90	5 (33%)
2	BNT	B	1301	-	13,14,14	1.32	3 (23%)	15,21,21	1.52	3 (20%)
4	2PE	A	303	-	11,11,27	0.66	0	10,10,26	1.44	0
2	BNT	B	1302	-	13,14,14	1.38	2 (15%)	15,21,21	1.50	2 (13%)
3	1PE	A	302	-	9,9,15	0.71	0	8,8,14	1.49	1 (12%)
5	GOL	B	1304	-	5,5,5	0.37	0	5,5,5	0.36	0

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
5	GOL	B	1303	-	-	2/4/4/4	-
2	BNT	A	301	-	-	0/4/28/28	0/1/1/1
2	BNT	A	304	-	-	0/4/28/28	0/1/1/1
2	BNT	B	1301	-	-	0/4/28/28	0/1/1/1
4	2PE	A	303	-	-	3/9/9/25	-
2	BNT	B	1302	-	-	0/4/28/28	0/1/1/1
3	1PE	A	302	-	-	4/7/7/13	-
5	GOL	B	1304	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	BNT	BRAI-CAJ	2.98	1.94	1.88
2	A	304	BNT	BRAI-CAJ	2.80	1.94	1.88
2	B	1302	BNT	BRAH-CAG	2.79	1.94	1.88
2	A	301	BNT	BRAI-CAJ	2.76	1.94	1.88
2	A	304	BNT	BRAH-CAG	2.76	1.94	1.88
2	A	301	BNT	BRAH-CAG	2.73	1.94	1.88
2	B	1301	BNT	BRAI-CAJ	2.71	1.94	1.88
2	B	1301	BNT	BRAH-CAG	2.56	1.93	1.88
2	B	1301	BNT	CAD-CAE	-2.11	1.49	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	304	BNT	BRAH-CAG-CAL	-3.75	119.39	122.47
2	B	1302	BNT	CAM-CAL-CAG	-3.59	119.17	123.02
2	A	304	BNT	CAM-CAL-CAG	-3.03	119.78	123.02
2	A	304	BNT	CAD-CAE-CAJ	-3.01	117.86	123.86
2	A	301	BNT	CAM-CAL-CAG	-3.01	119.80	123.02
2	B	1301	BNT	CAM-CAL-CAG	-2.62	120.21	123.02
2	B	1302	BNT	BRAH-CAG-CAL	-2.44	120.47	122.47
2	B	1301	BNT	BRAH-CAG-CAL	-2.35	120.54	122.47
2	A	304	BNT	BRAH-CAG-CAF	2.14	120.18	116.28
2	B	1301	BNT	CAD-CAE-CAJ	-2.11	119.66	123.86
3	A	302	1PE	OH6-C26-C16	2.08	119.20	110.07
2	A	304	BNT	OAB-CAF-CAG	-2.06	118.91	123.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

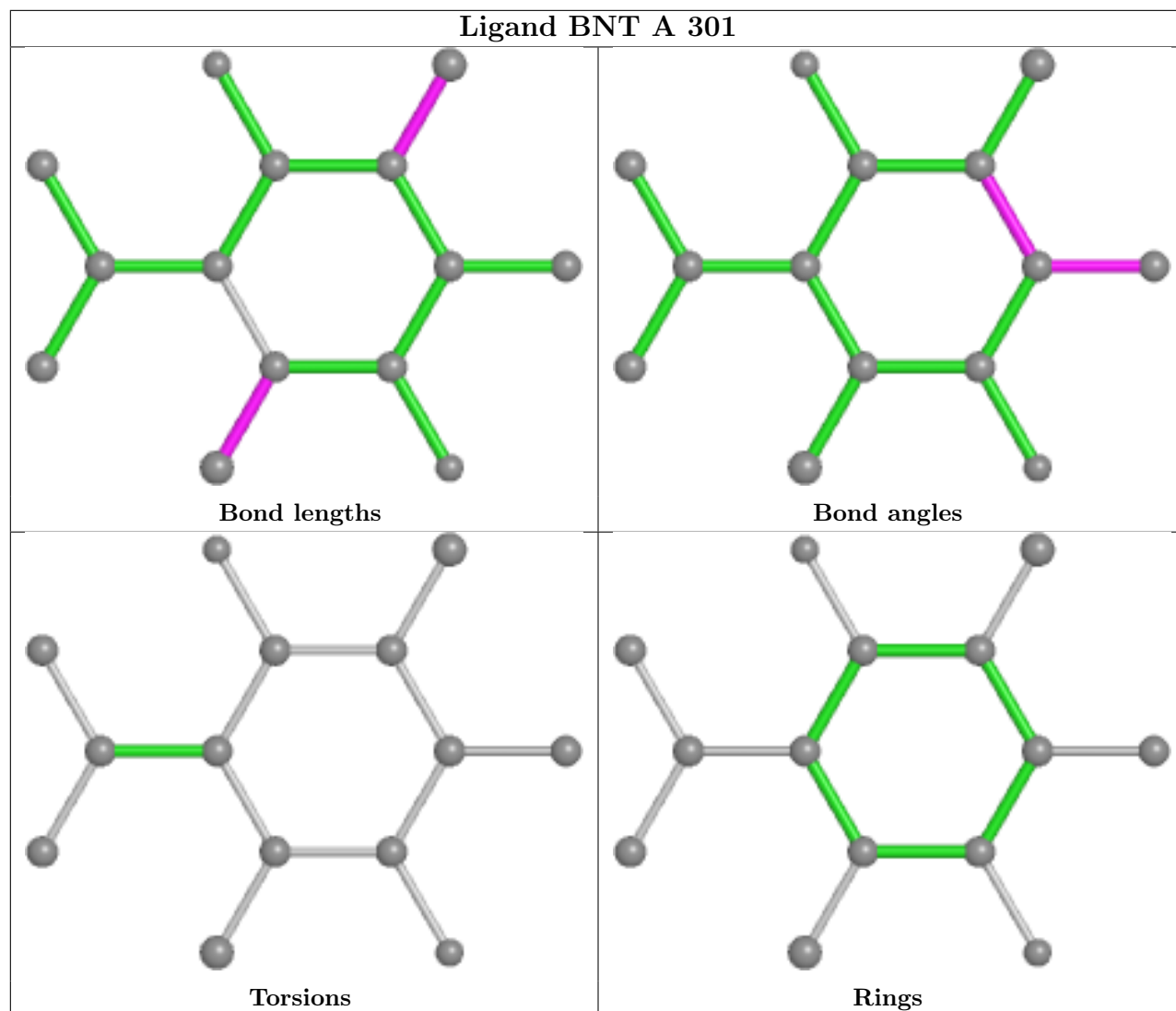
Mol	Chain	Res	Type	Atoms
5	B	1303	GOL	O1-C1-C2-C3
4	A	303	2PE	O7-C8-C9-O10
3	A	302	1PE	OH6-C15-C25-OH5
3	A	302	1PE	OH5-C14-C24-OH4
5	B	1304	GOL	O1-C1-C2-C3
5	B	1304	GOL	C1-C2-C3-O3
5	B	1303	GOL	O1-C1-C2-O2
5	B	1304	GOL	O1-C1-C2-O2
4	A	303	2PE	O1-C2-C3-O4
3	A	302	1PE	C15-C25-OH5-C14
5	B	1304	GOL	O2-C2-C3-O3
3	A	302	1PE	C25-C15-OH6-C26
4	A	303	2PE	O4-C5-C6-O7

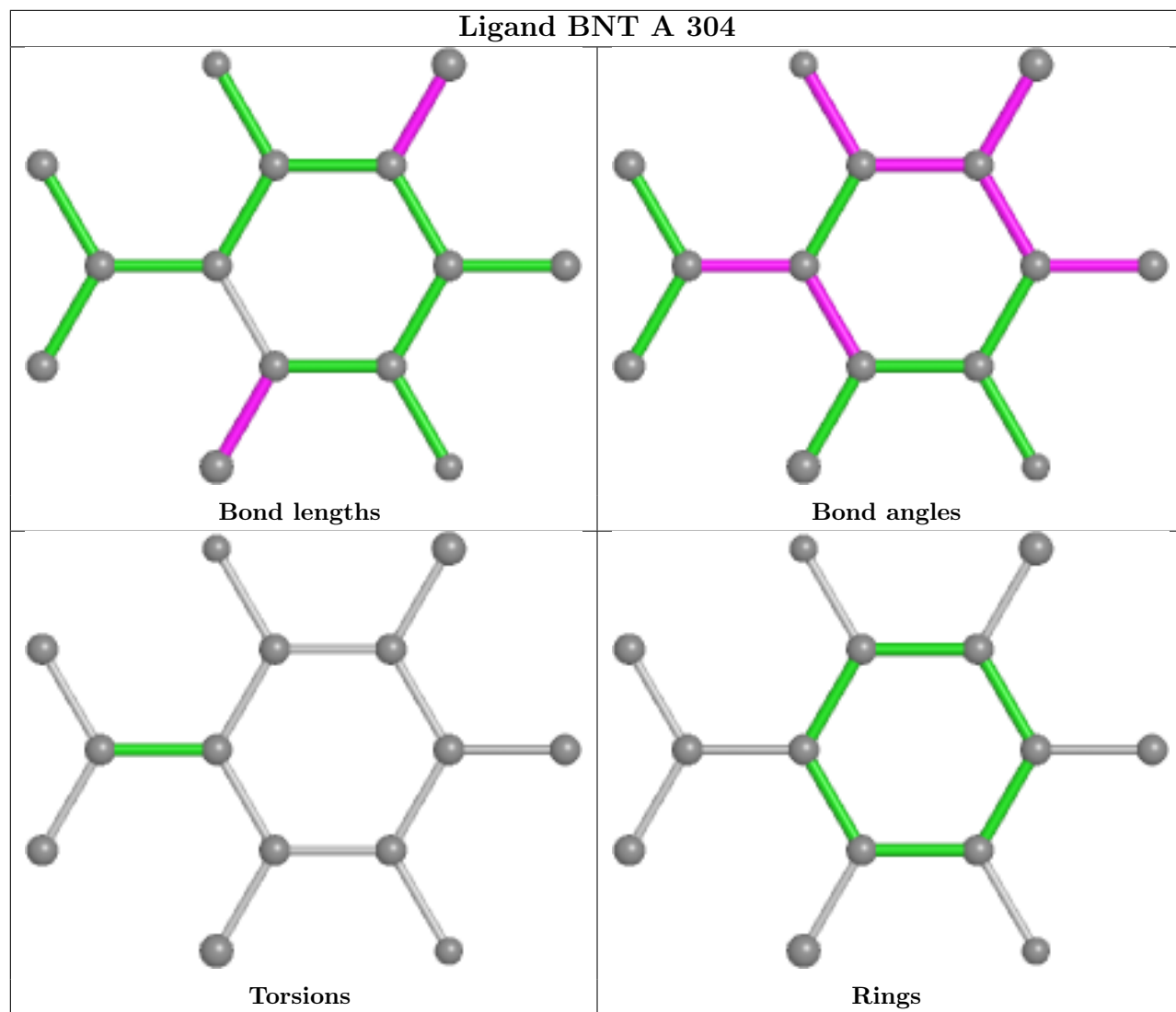
There are no ring outliers.

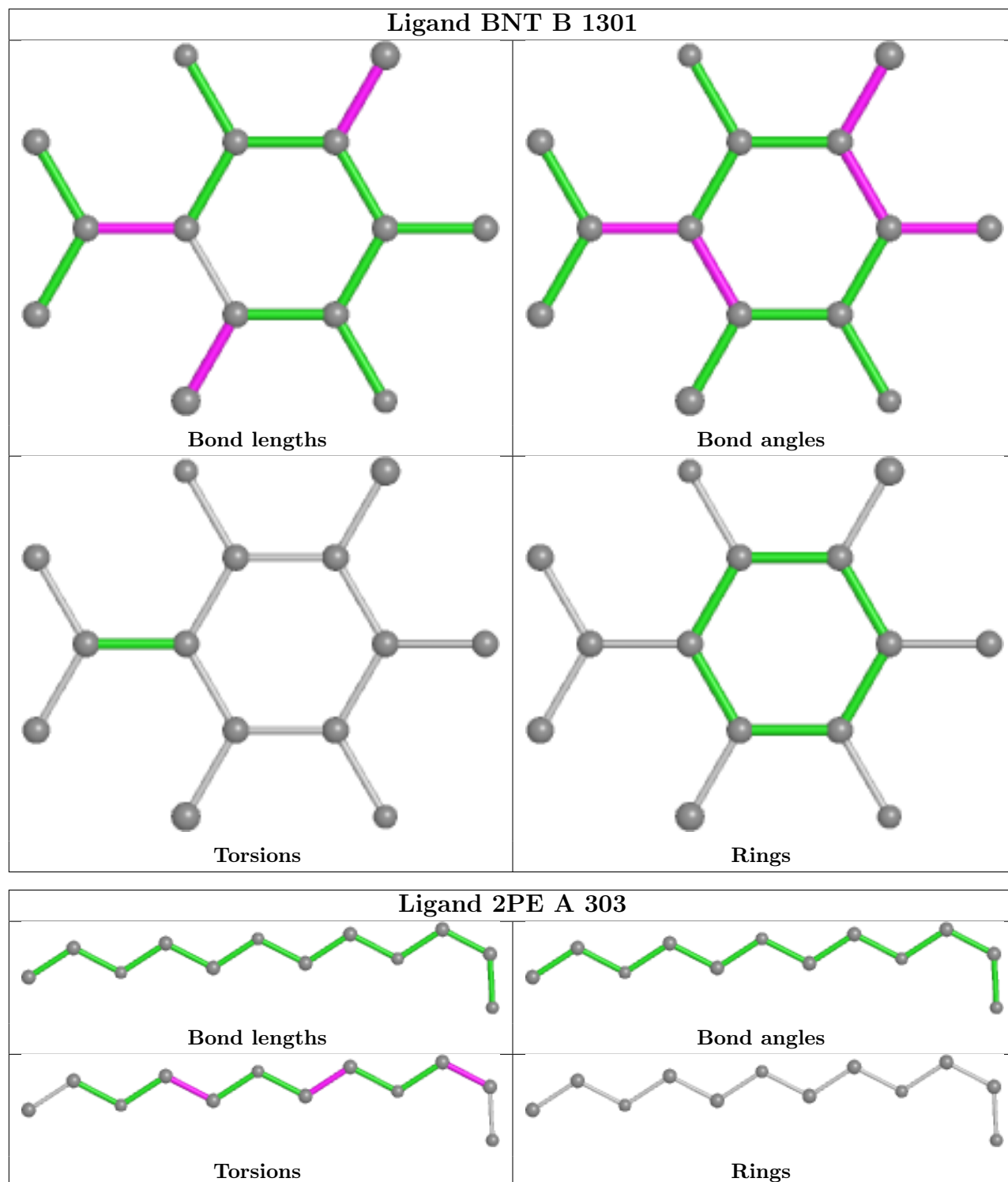
8 monomers are involved in 51 short contacts:

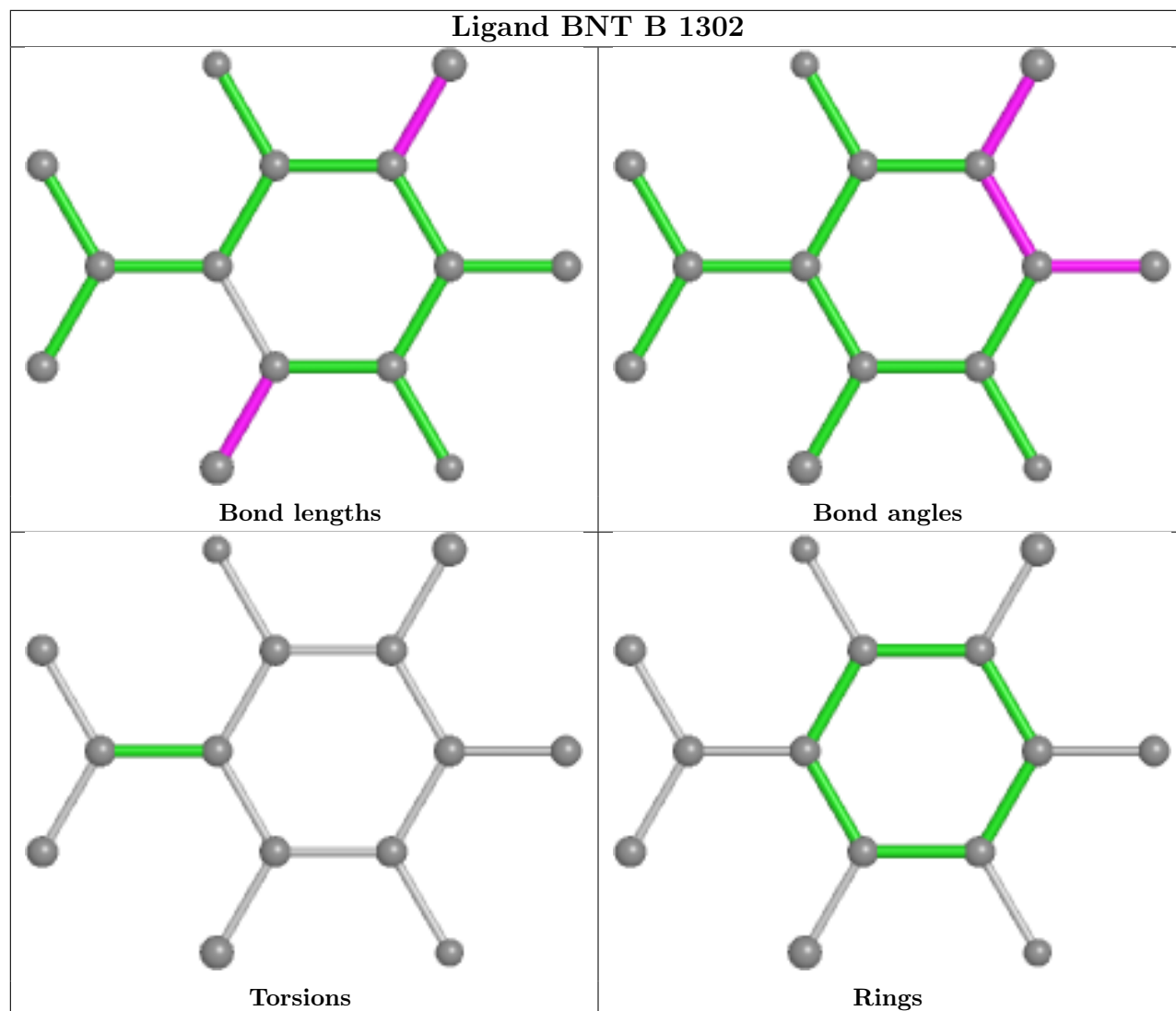
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1303	GOL	1	0
2	A	301	BNT	18	0
2	A	304	BNT	2	0
2	B	1301	BNT	13	0
4	A	303	2PE	4	0
2	B	1302	BNT	6	0
3	A	302	1PE	10	0
5	B	1304	GOL	1	0

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	282/284 (99%)	0.80	33 (11%) 4   5	23, 36, 64, 75	0
1	B	282/284 (99%)	0.71	32 (11%) 5   5	22, 40, 69, 77	0
All	All	564/568 (99%)	0.76	65 (11%) 4   5	22, 38, 68, 77	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	ASN	10.6
1	B	141	MET	8.1
1	A	145	HIS	7.8
1	B	142	GLY	7.7
1	A	89	ASP	7.7
1	A	135	ALA	7.7
1	B	143	ALA	7.6
1	B	139	MET	7.0
1	A	87	SER	6.9
1	A	88	GLU	6.6
1	B	209	ASN	6.5
1	A	146	ASP	6.3
1	B	140	LEU	6.2
1	A	142	GLY	6.0
1	A	93	PRO	5.9
1	A	1	VAL	5.8
1	A	254	SER	5.7
1	A	90	PRO	5.6
1	B	145	HIS	5.6
1	A	141	MET	5.5
1	B	136	ASP	5.4
1	A	148	GLU	5.2
1	A	244	PHE	5.2
1	B	86	ASP	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	144	ASN	4.8
1	A	136	ASP	4.8
1	A	91	ASP	4.7
1	B	134	MET	4.5
1	A	137	HIS	4.4
1	A	149	LEU	4.3
1	A	92	GLU	4.2
1	A	143	ALA	4.1
1	B	135	ALA	4.1
1	B	146	ASP	4.0
1	B	72	PHE	3.8
1	B	148	GLU	3.8
1	A	86	ASP	3.7
1	A	138	ILE	3.6
1	A	140	LEU	3.4
1	A	248	LEU	3.2
1	B	257	ILE	3.1
1	A	139	MET	3.1
1	B	137	HIS	3.1
1	A	150	SER	3.1
1	A	256	ASP	3.0
1	B	1	VAL	3.0
1	B	68	GLN	3.0
1	B	2	LEU	2.9
1	A	95	LYS	2.7
1	B	147	PRO	2.6
1	B	138	ILE	2.6
1	A	151	SER	2.5
1	B	250	VAL	2.5
1	B	150	SER	2.5
1	B	88	GLU	2.5
1	B	149	LEU	2.4
1	A	259	LEU	2.4
1	B	62	SER	2.4
1	B	238	MET	2.4
1	B	210	SER	2.4
1	A	250	VAL	2.3
1	B	151	SER	2.3
1	B	244	PHE	2.2
1	B	208	PRO	2.1
1	A	98	LEU	2.1



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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

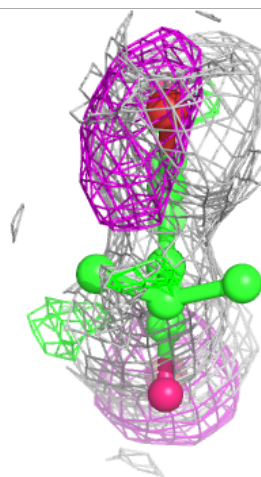
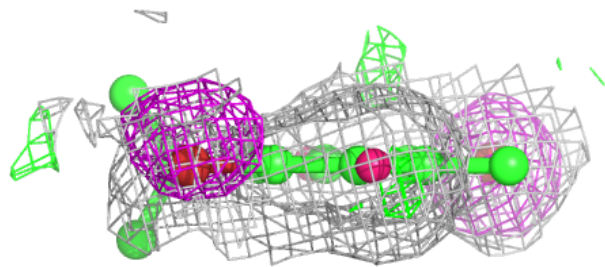
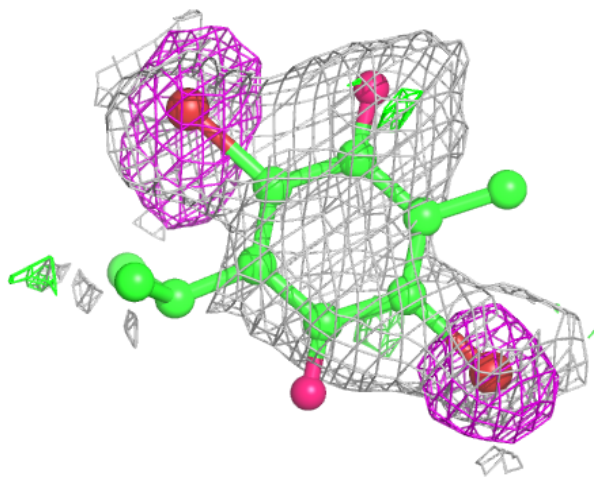
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	BNT	A	301	14/14	0.56	0.39	45,62,69,75	14
2	BNT	B	1301	14/14	0.58	0.57	24,43,59,60	14
2	BNT	A	304	14/14	0.59	0.46	41,47,55,56	14
2	BNT	B	1302	14/14	0.65	0.40	51,58,68,68	14
4	2PE	A	303	12/28	0.78	0.27	46,52,56,57	0
5	GOL	B	1304	6/6	0.83	0.19	39,41,43,44	0
3	1PE	A	302	10/16	0.87	0.27	34,39,42,48	0
5	GOL	B	1303	6/6	0.96	0.14	31,33,37,47	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.

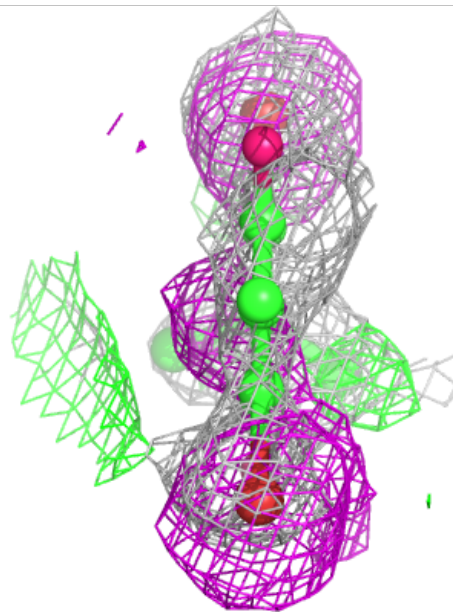
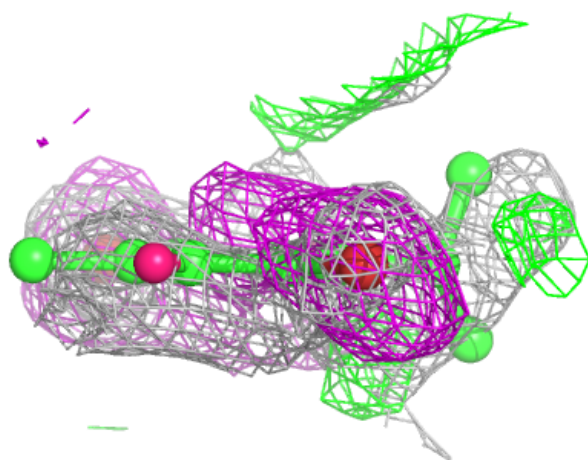
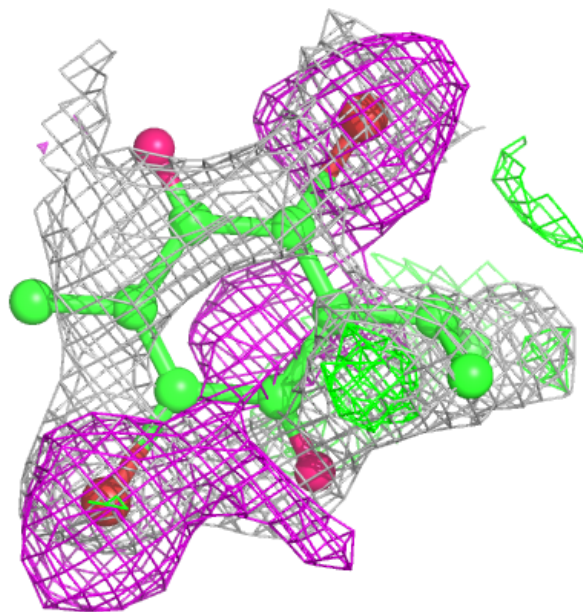
**Electron density around BNT A 301:**

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



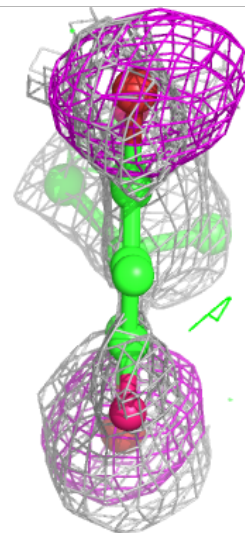
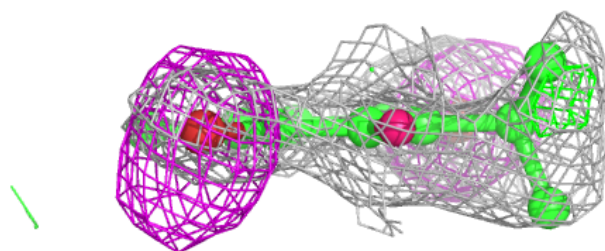
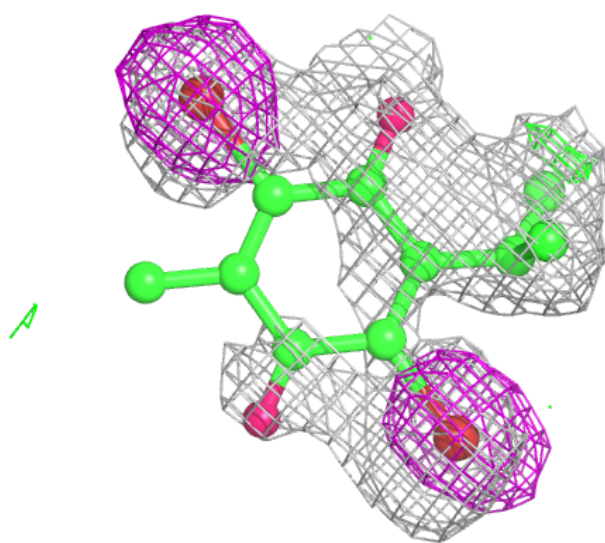
**Electron density around BNT B 1301:**

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



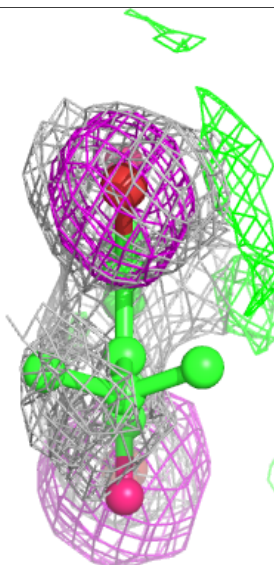
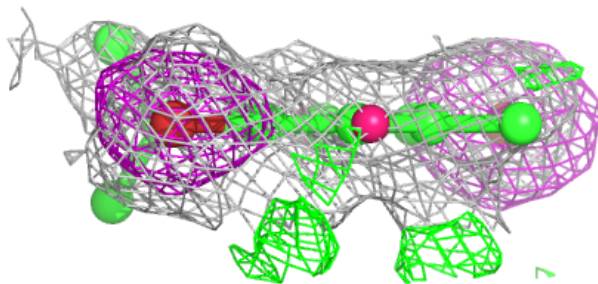
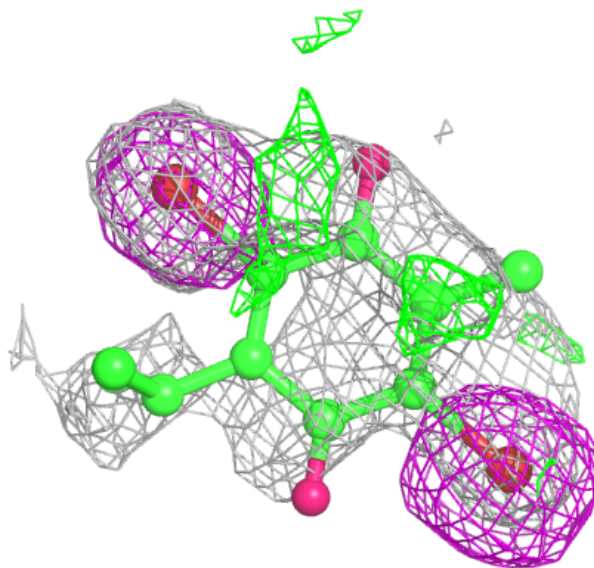
**Electron density around BNT A 304:**

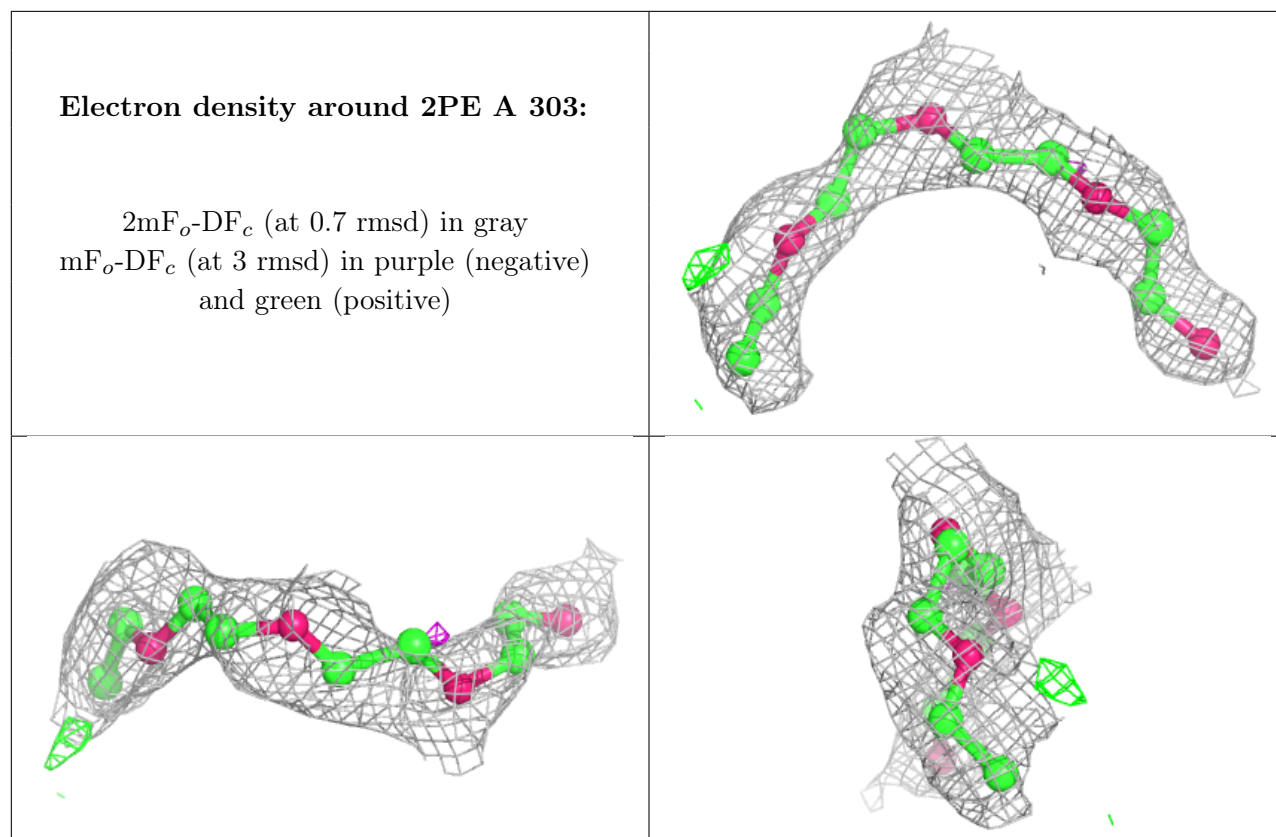
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BNT B 1302:**

$2mF_o-DF_c$  (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.