



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:03 am BST

PDB ID : 3WZM  
Title : ZEN lactonase mutant complex  
Authors : Ko, T.P.; Huang, C.H.; Liu, J.R.; Guo, R.T.  
Deposited on : 2014-10-01  
Resolution : 2.48 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

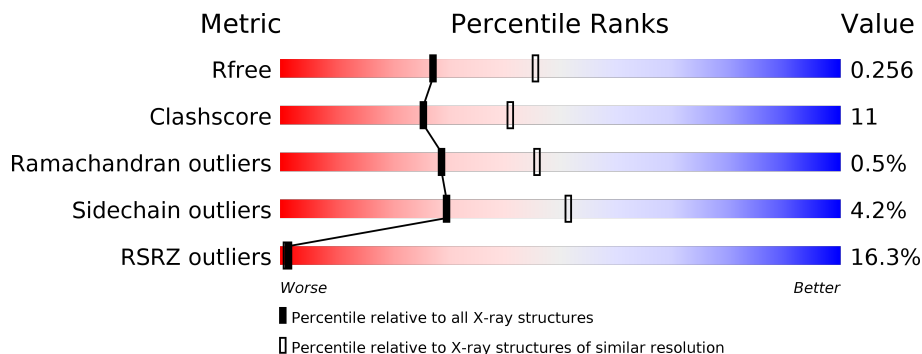
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	278	
1	B	278	
1	C	278	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6558 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 Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2021	1282	341	387	11	0	0	0
1	B	264	2021	1282	341	387	11	0	0	0
1	C	264	2021	1282	341	387	11	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

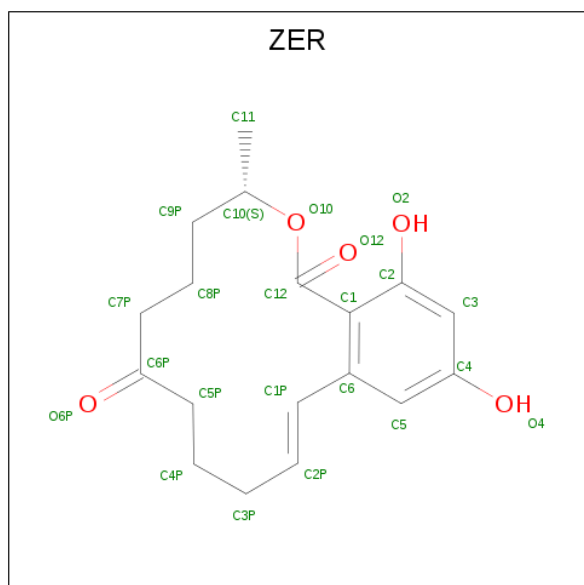
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
A	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
A	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
A	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
A	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0
B	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
B	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
B	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
B	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
B	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0
C	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
C	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
C	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
C	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
C	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0

- Molecule 2 is (3S,11E)-14,16-dihydroxy-3-methyl-3,4,5,6,9,10-hexahydro-1H-2-benzoxacyclo tetradecine-1,7(8H)-dione (three-letter code: ZER) (formula: C<sub>18</sub>H<sub>22</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		
2	C	1	Total	C	O	0	0
			23	18	5		


- Molecule 3 is water.

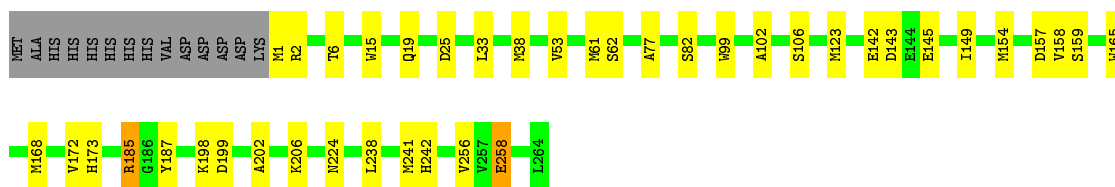
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		
3	B	162	Total	O	0	0
			162	162		
3	C	79	Total	O	0	0
			79	79		

### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

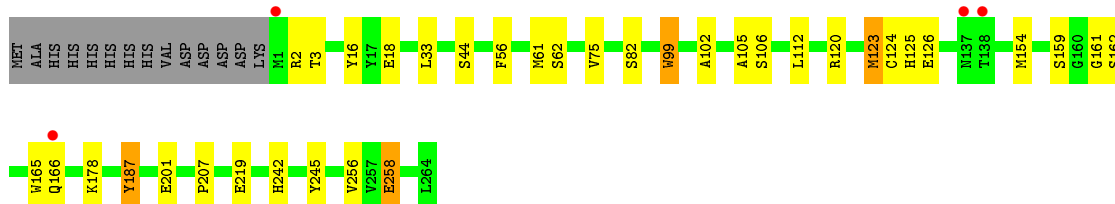
- Molecule 1: Zearalenone hydrolase

Chain A: 



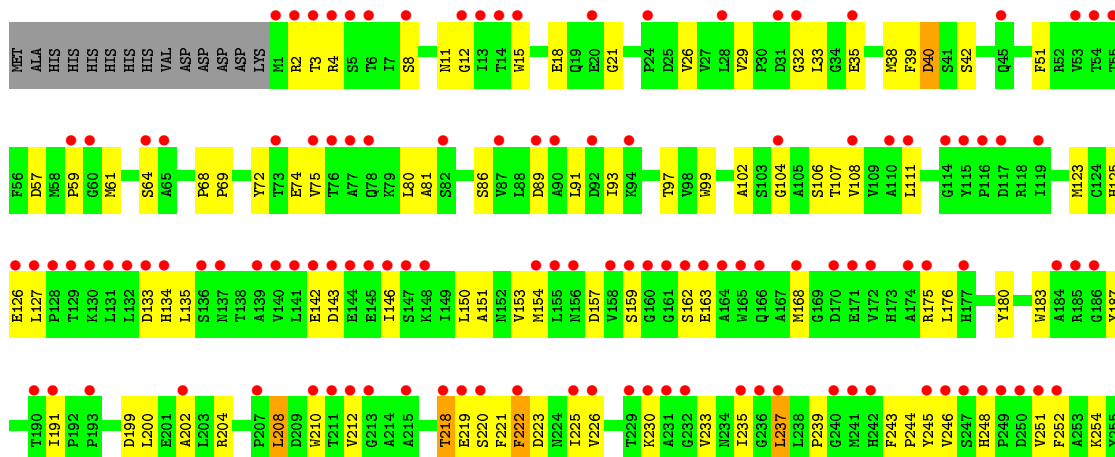
- Molecule 1: Zearalenone hydrolase

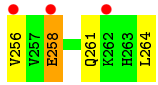
Chain B: 



- Molecule 1: Zearalenone hydrolase

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.84Å 86.84Å 471.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.48 19.95 – 2.48	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.95-2.48) 95.5 (19.95-2.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.30 (at 2.50Å)	Xtrriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.204 , 0.268 0.200 , 0.256	Depositor DCC
$R_{free}$ test set	1848 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtrriage
Anisotropy	0.573	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: ZER

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	0.99	2/2072 (0.1%)	0.87	3/2829 (0.1%)
1	B	0.96	2/2072 (0.1%)	0.86	1/2829 (0.0%)
1	C	0.73	0/2072	0.72	0/2829
All	All	0.90	4/6216 (0.1%)	0.82	4/8487 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLU	CG-CD	5.79	1.60	1.51
1	B	258	GLU	CG-CD	5.74	1.60	1.51
1	A	82	SER	CB-OG	-5.70	1.34	1.42
1	B	258	GLU	CD-OE2	5.07	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	185	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	2	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	B	2	ARG	NE-CZ-NH1	-6.23	117.19	120.30

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	2021	0	1991	31	0
1	B	2021	0	1991	16	0
1	C	2021	0	1991	79	0
2	A	23	0	20	2	0
2	B	23	0	20	3	0
2	C	23	0	20	2	0
3	A	185	0	0	3	1
3	B	162	0	0	2	0
3	C	79	0	0	9	1
All	All	6558	0	6033	129	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 (129) 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:123:MET:HE1	1:B:256:VAL:HA	1.23	1.07
1:A:38:MET:HG2	1:A:168:MET:HE1	1.45	0.98
1:C:40:ASP:HB3	3:C:436:HOH:O	1.67	0.95
1:C:125:HIS:CD2	1:C:126:GLU:HG3	2.02	0.93
1:A:158:VAL:HA	1:A:241:MET:HE2	1.53	0.89
1:C:123:MET:HE1	1:C:256:VAL:HA	1.60	0.84
1:A:145:GLU:O	1:A:149:ILE:HG12	1.81	0.79
1:A:38:MET:HG2	1:A:168:MET:CE	2.12	0.79
1:B:201:GLU:O	3:B:562:HOH:O	2.01	0.78
1:C:57:ASP:HB2	1:C:64:SER:OG	1.86	0.75
1:C:208:LEU:HG	1:C:233:VAL:HG11	1.69	0.75
1:C:134:HIS:HD2	1:C:135:LEU:HG	1.52	0.74
1:A:123:MET:HE1	1:A:256:VAL:HA	1.74	0.70
1:A:123:MET:HE1	1:A:256:VAL:HG22	1.72	0.70
1:A:199:ASP:HB2	3:C:429:HOH:O	1.92	0.69
1:C:35:GLU:CD	1:C:175:ARG:HH21	1.95	0.69
1:A:143:ASP:OD1	1:A:185:ARG:NH2	2.25	0.69
1:C:150:LEU:O	1:C:154:MET:HG2	1.91	0.69
1:A:1:MET:HE3	3:A:595:HOH:O	1.92	0.68
1:A:123:MET:CE	1:A:256:VAL:HA	2.23	0.68
1:C:261:GLN:HA	1:C:264:LEU:HG	1.75	0.67
1:C:200:LEU:HD13	1:C:230:LYS:HB3	1.75	0.67
1:C:226:VAL:HG12	1:C:226:VAL:O	1.95	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:MET:O	1:C:159:SER:HB3	1.95	0.66
1:A:38:MET:CG	1:A:168:MET:HE1	2.25	0.63
1:C:163:GLU:OE2	3:C:415:HOH:O	2.16	0.61
1:C:151:ALA:HB2	1:C:180:TYR:CE2	2.36	0.61
1:A:25:ASP:OD2	3:A:637:HOH:O	2.16	0.60
1:C:212:VAL:O	1:C:237:LEU:HB2	2.00	0.60
1:C:99:TRP:CH2	1:C:125:HIS:HB2	2.36	0.60
1:C:91:LEU:HB3	1:C:93:ILE:HD12	1.84	0.59
1:A:33:LEU:HG	2:A:300:ZER:H2	1.84	0.59
1:B:120:ARG:NH2	3:B:436:HOH:O	2.26	0.58
1:A:168:MET:CE	1:A:172:VAL:HG11	2.34	0.58
1:C:29:VAL:N	1:C:99:TRP:O	2.28	0.58
1:B:99:TRP:C	1:B:99:TRP:CD1	2.77	0.57
1:C:21:GLY:HA3	1:C:51:PHE:O	2.05	0.56
1:C:38:MET:HB3	1:C:246:VAL:CG2	2.35	0.56
1:C:107:THR:O	1:C:111:LEU:HG	2.06	0.56
1:C:99:TRP:CE2	1:C:252:PHE:HE1	2.23	0.56
1:C:239:PRO:HG2	1:C:251:VAL:HG11	1.88	0.55
1:C:38:MET:HG2	1:C:168:MET:CE	2.35	0.55
1:C:208:LEU:HG	1:C:233:VAL:CG1	2.35	0.55
1:C:134:HIS:CD2	1:C:135:LEU:HG	2.39	0.54
1:C:226:VAL:CG1	1:C:226:VAL:O	2.54	0.54
1:C:39:PHE:O	1:C:42:SER:N	2.40	0.54
1:C:123:MET:CE	1:C:256:VAL:HA	2.36	0.54
1:C:239:PRO:HG3	3:C:445:HOH:O	2.07	0.53
1:C:11:ASN:O	1:C:68:PRO:HG3	2.09	0.53
1:C:254:LYS:O	1:C:258:GLU:HB2	2.08	0.52
1:A:158:VAL:HA	1:A:241:MET:CE	2.33	0.52
1:A:168:MET:HE2	1:A:172:VAL:HG11	1.91	0.52
1:C:239:PRO:CG	1:C:251:VAL:HG11	2.39	0.52
1:A:102:ALA:HB2	1:A:242:HIS:NE2	2.25	0.52
1:C:237:LEU:CD1	1:C:237:LEU:N	2.73	0.51
1:A:77:ALA:HB2	1:A:106:SER:HB3	1.93	0.51
1:B:33:LEU:HG	2:B:300:ZER:H2	1.92	0.51
2:A:300:ZER:O10	2:A:300:ZER:H11	2.11	0.51
1:C:15:TRP:CH2	1:C:59:PRO:HG3	2.46	0.51
1:C:69:PRO:HA	1:C:72:TYR:CZ	2.46	0.51
1:C:12:GLY:HA3	1:C:68:PRO:HD3	1.94	0.50
1:C:237:LEU:HD22	3:C:412:HOH:O	2.12	0.50
1:C:239:PRO:HB2	1:C:248:HIS:ND1	2.27	0.50
1:C:163:GLU:CD	3:C:415:HOH:O	2.50	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:SER:HB3	3:C:453:HOH:O	2.12	0.50
1:C:210:TRP:O	1:C:235:ILE:HA	2.12	0.49
1:C:159:SER:HA	1:C:243:PHE:HD2	1.77	0.49
1:B:154:MET:O	1:B:159:SER:HB3	2.13	0.48
1:C:38:MET:HG2	1:C:168:MET:HE3	1.96	0.48
1:B:125:HIS:CD2	1:B:126:GLU:HG3	2.48	0.48
1:C:91:LEU:CB	1:C:93:ILE:HD12	2.44	0.48
1:A:157:ASP:O	1:A:241:MET:HE1	2.14	0.47
1:B:154:MET:HE3	2:B:300:ZER:H6	1.96	0.47
1:C:2:ARG:HH12	1:C:40:ASP:HA	1.79	0.47
1:C:248:HIS:HB3	1:C:251:VAL:CG2	2.45	0.47
1:C:264:LEU:O	3:C:463:HOH:O	2.20	0.47
1:A:154:MET:O	1:A:159:SER:HB3	2.13	0.47
1:C:102:ALA:HA	1:C:126:GLU:O	2.14	0.47
1:A:102:ALA:HB2	1:A:242:HIS:CE1	2.50	0.47
1:B:112:LEU:HD11	1:B:207:PRO:HD2	1.98	0.46
1:A:19:GLN:HA	1:A:53:VAL:O	2.15	0.46
1:A:168:MET:HE3	1:A:172:VAL:HG11	1.98	0.46
1:C:135:LEU:HD22	1:C:183:TRP:HH2	1.81	0.46
1:C:33:LEU:HD13	1:C:176:LEU:HD22	1.98	0.45
1:C:3:THR:O	1:C:18:GLU:HA	2.16	0.45
1:C:212:VAL:HG23	1:C:235:ILE:HD11	1.98	0.45
1:C:81:ALA:HB1	1:C:111:LEU:HD23	1.98	0.45
1:C:221:PHE:HZ	2:C:300:ZER:H13	1.82	0.45
1:C:32:GLY:O	1:C:61:MET:HE2	2.17	0.44
1:B:3:THR:O	1:B:18:GLU:HA	2.17	0.44
1:C:99:TRP:HE3	1:C:123:MET:HB2	1.83	0.44
1:C:80:LEU:HD11	1:C:187:TYR:CE1	2.52	0.44
1:C:26:VAL:HG22	1:C:97:THR:HB	2.00	0.44
1:C:204:ARG:NH2	1:C:230:LYS:O	2.46	0.44
1:B:102:ALA:HB2	1:B:242:HIS:CE1	2.53	0.44
1:B:154:MET:HB3	1:B:165:TRP:CZ2	2.52	0.43
1:C:38:MET:HG2	1:C:168:MET:HE1	1.99	0.43
1:C:86:SER:O	1:C:89:ASP:HB2	2.19	0.43
1:C:218:THR:O	1:C:222:PHE:HB3	2.19	0.43
1:C:212:VAL:O	1:C:237:LEU:CB	2.66	0.43
1:B:61:MET:O	1:B:62:SER:C	2.55	0.43
1:C:244:PRO:HD2	1:C:245:TYR:CD2	2.53	0.43
1:C:91:LEU:HB3	1:C:93:ILE:CD1	2.46	0.43
1:C:125:HIS:NE2	1:C:126:GLU:HG3	2.31	0.43
1:C:143:ASP:HA	1:C:146:ILE:HD12	2.01	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:VAL:HG13	1:C:157:ASP:HB2	2.01	0.42
1:C:4:ARG:HB2	3:C:419:HOH:O	2.19	0.42
1:A:99:TRP:C	1:A:99:TRP:CD1	2.92	0.42
1:B:105:ALA:HB1	1:B:124:CYS:HB2	2.02	0.42
2:B:300:ZER:H12	2:B:300:ZER:H10	1.84	0.42
1:C:159:SER:HA	1:C:243:PHE:CD2	2.55	0.42
2:C:300:ZER:H17	2:C:300:ZER:H22	1.88	0.41
1:A:61:MET:O	1:A:62:SER:C	2.58	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.88	0.41
1:B:75:VAL:HG21	1:B:187:TYR:CE2	2.55	0.41
1:C:108:VAL:HA	1:C:111:LEU:HD12	2.01	0.41
1:C:142:GLU:O	1:C:146:ILE:HG13	2.20	0.41
1:C:199:ASP:O	1:C:202:ALA:HB3	2.21	0.41
1:C:208:LEU:O	1:C:233:VAL:HG13	2.21	0.41
1:A:202:ALA:O	1:A:206:LYS:HE2	2.21	0.41
1:C:222:PHE:O	1:C:226:VAL:HG23	2.21	0.41
1:A:6:THR:HA	1:A:15:TRP:O	2.21	0.40
1:C:222:PHE:HA	1:C:225:ILE:HD12	2.03	0.40
1:C:75:VAL:HG12	1:C:191:ILE:HD11	2.03	0.40
1:A:123:MET:HE3	1:A:256:VAL:HA	2.02	0.40
1:B:16:TYR:OH	1:B:18:GLU:OE2	2.24	0.40
1:C:104:GLY:O	1:C:108:VAL:HG22	2.21	0.40
1:A:165:TRP:NE1	1:A:173:HIS:HE1	2.20	0.40
1:A:198:LYS:HE2	3:A:673:HOH:O	2.21	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)
3:A:668:HOH:O	3:C:430:HOH:O[8_555]	1.94	0.26

## 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	262/278 (94%)	251 (96%)	10 (4%)	1 (0%)	34	52
1	B	262/278 (94%)	250 (95%)	10 (4%)	2 (1%)	19	33
1	C	262/278 (94%)	229 (87%)	32 (12%)	1 (0%)	34	52
All	All	786/834 (94%)	730 (93%)	52 (7%)	4 (0%)	29	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ASP
1	A	187	TYR
1	B	161	GLY
1	B	187	TYR

### 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	220/233 (94%)	217 (99%)	3 (1%)	67	84
1	B	220/233 (94%)	208 (94%)	12 (6%)	21	39
1	C	220/233 (94%)	207 (94%)	13 (6%)	19	35
All	All	660/699 (94%)	632 (96%)	28 (4%)	30	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	GLU
1	A	224	ASN
1	A	258	GLU
1	B	44	SER
1	B	56	PHE
1	B	82	SER
1	B	99	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	106	SER
1	B	123	MET
1	B	162	SER
1	B	166	GLN
1	B	178	LYS
1	B	219	GLU
1	B	245	TYR
1	B	258	GLU
1	C	8	SER
1	C	74	GLU
1	C	106	SER
1	C	127	LEU
1	C	133	ASP
1	C	208	LEU
1	C	218	THR
1	C	219	GLU
1	C	220	SER
1	C	222	PHE
1	C	223	ASP
1	C	237	LEU
1	C	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	B	261	GLN
1	B	263	HIS
1	C	134	HIS
1	C	166	GLN
1	C	261	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	ZER	A	300	-	24,24,24	1.31	3 (12%)	32,32,32	2.16	10 (31%)
2	ZER	C	300	-	24,24,24	1.36	2 (8%)	32,32,32	1.69	9 (28%)
2	ZER	B	300	-	24,24,24	1.18	2 (8%)	32,32,32	2.14	10 (31%)

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	ZER	A	300	-	-	10/22/22/22	0/1/2/2
2	ZER	C	300	-	-	11/22/22/22	0/1/2/2
2	ZER	B	300	-	-	10/22/22/22	0/1/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	ZER	O10-C12	4.42	1.43	1.34
2	C	300	ZER	C6-C1P	3.73	1.53	1.47
2	A	300	ZER	C6-C1P	3.71	1.53	1.47
2	B	300	ZER	O10-C12	3.50	1.41	1.34
2	A	300	ZER	O10-C12	3.23	1.41	1.34
2	B	300	ZER	C6-C1P	3.07	1.52	1.47
2	A	300	ZER	C1-C6	-2.03	1.39	1.42



All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ZER	C11-C10-C9P	-5.85	98.19	113.97
2	A	300	ZER	C4P-C5P-C6P	-5.09	101.53	114.60
2	A	300	ZER	C7P-C6P-C5P	4.90	126.28	116.98
2	A	300	ZER	C11-C10-C9P	-4.78	101.06	113.97
2	B	300	ZER	C7P-C6P-C5P	4.56	125.63	116.98
2	B	300	ZER	C4P-C5P-C6P	-4.30	103.54	114.60
2	B	300	ZER	O10-C10-C11	3.66	116.29	107.93
2	C	300	ZER	C11-C10-C9P	-3.64	104.15	113.97
2	A	300	ZER	C5P-C4P-C3P	-3.50	107.00	113.23
2	C	300	ZER	C4P-C5P-C6P	-3.39	105.88	114.60
2	B	300	ZER	C5P-C4P-C3P	-3.33	107.30	113.23
2	A	300	ZER	O10-C10-C11	3.27	115.41	107.93
2	C	300	ZER	O10-C10-C11	3.18	115.19	107.93
2	C	300	ZER	C5P-C4P-C3P	-3.18	107.56	113.23
2	A	300	ZER	C9P-C8P-C7P	-3.14	104.83	113.36
2	A	300	ZER	C6-C1-C2	2.99	121.81	118.91
2	C	300	ZER	C7P-C6P-C5P	2.93	122.55	116.98
2	B	300	ZER	C10-O10-C12	2.91	122.67	117.61
2	B	300	ZER	C9P-C8P-C7P	-2.72	105.98	113.36
2	C	300	ZER	C6-C1P-C2P	-2.64	119.82	125.52
2	A	300	ZER	C2-C3-C4	-2.50	117.44	119.70
2	A	300	ZER	O6P-C6P-C5P	-2.48	114.87	121.44
2	C	300	ZER	C6-C1-C2	2.47	121.31	118.91
2	C	300	ZER	C9P-C8P-C7P	-2.42	106.79	113.36
2	B	300	ZER	C6-C1P-C2P	-2.33	120.49	125.52
2	B	300	ZER	C6-C1-C2	2.30	121.14	118.91
2	A	300	ZER	C6-C1P-C2P	-2.14	120.91	125.52
2	B	300	ZER	O6P-C6P-C5P	-2.09	115.90	121.44
2	C	300	ZER	C10-O10-C12	2.05	121.17	117.61

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	ZER	C11-C10-O10-C12
2	A	300	ZER	C5P-C6P-C7P-C8P
2	A	300	ZER	O6P-C6P-C7P-C8P
2	C	300	ZER	C11-C10-O10-C12
2	C	300	ZER	C5P-C6P-C7P-C8P
2	C	300	ZER	O6P-C6P-C7P-C8P
2	B	300	ZER	C11-C10-O10-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	300	ZER	C5P-C6P-C7P-C8P
2	B	300	ZER	O6P-C6P-C7P-C8P
2	B	300	ZER	C1-C12-O10-C10
2	A	300	ZER	C1-C12-O10-C10
2	C	300	ZER	C1-C12-O10-C10
2	A	300	ZER	C3P-C4P-C5P-C6P
2	C	300	ZER	C3P-C4P-C5P-C6P
2	B	300	ZER	C3P-C4P-C5P-C6P
2	A	300	ZER	C2P-C3P-C4P-C5P
2	B	300	ZER	C2P-C3P-C4P-C5P
2	C	300	ZER	O12-C12-O10-C10
2	A	300	ZER	C6P-C7P-C8P-C9P
2	A	300	ZER	O12-C12-O10-C10
2	C	300	ZER	C2P-C3P-C4P-C5P
2	C	300	ZER	C6P-C7P-C8P-C9P
2	B	300	ZER	O12-C12-O10-C10
2	C	300	ZER	C6-C1-C12-O12
2	A	300	ZER	C6-C1-C12-O12
2	B	300	ZER	C6P-C7P-C8P-C9P
2	A	300	ZER	C6-C1-C12-O10
2	C	300	ZER	C6-C1-C12-O10
2	C	300	ZER	C2-C1-C12-O10
2	B	300	ZER	C6-C1-C12-O10
2	B	300	ZER	C6-C1-C12-O12

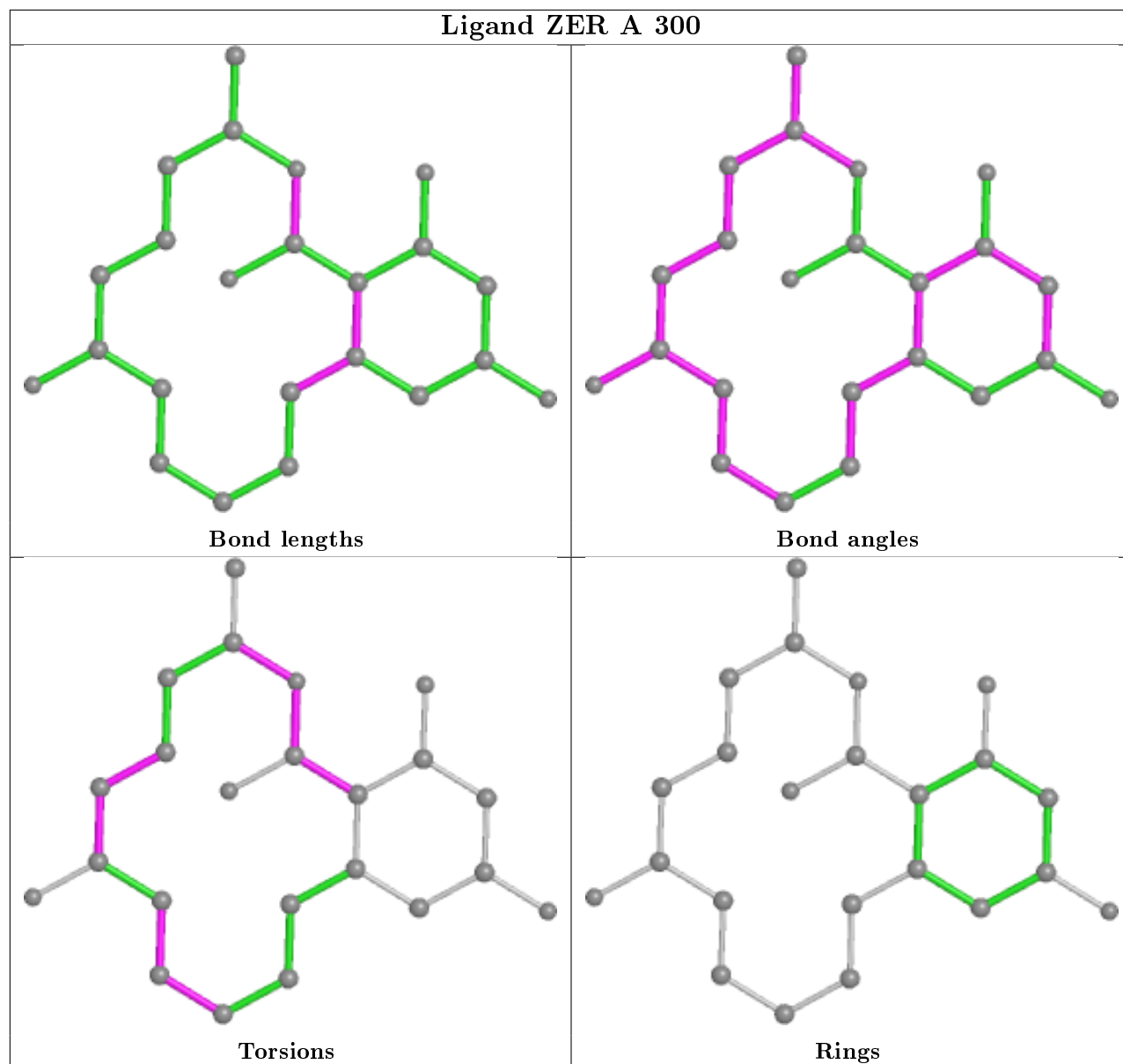
There are no ring outliers.

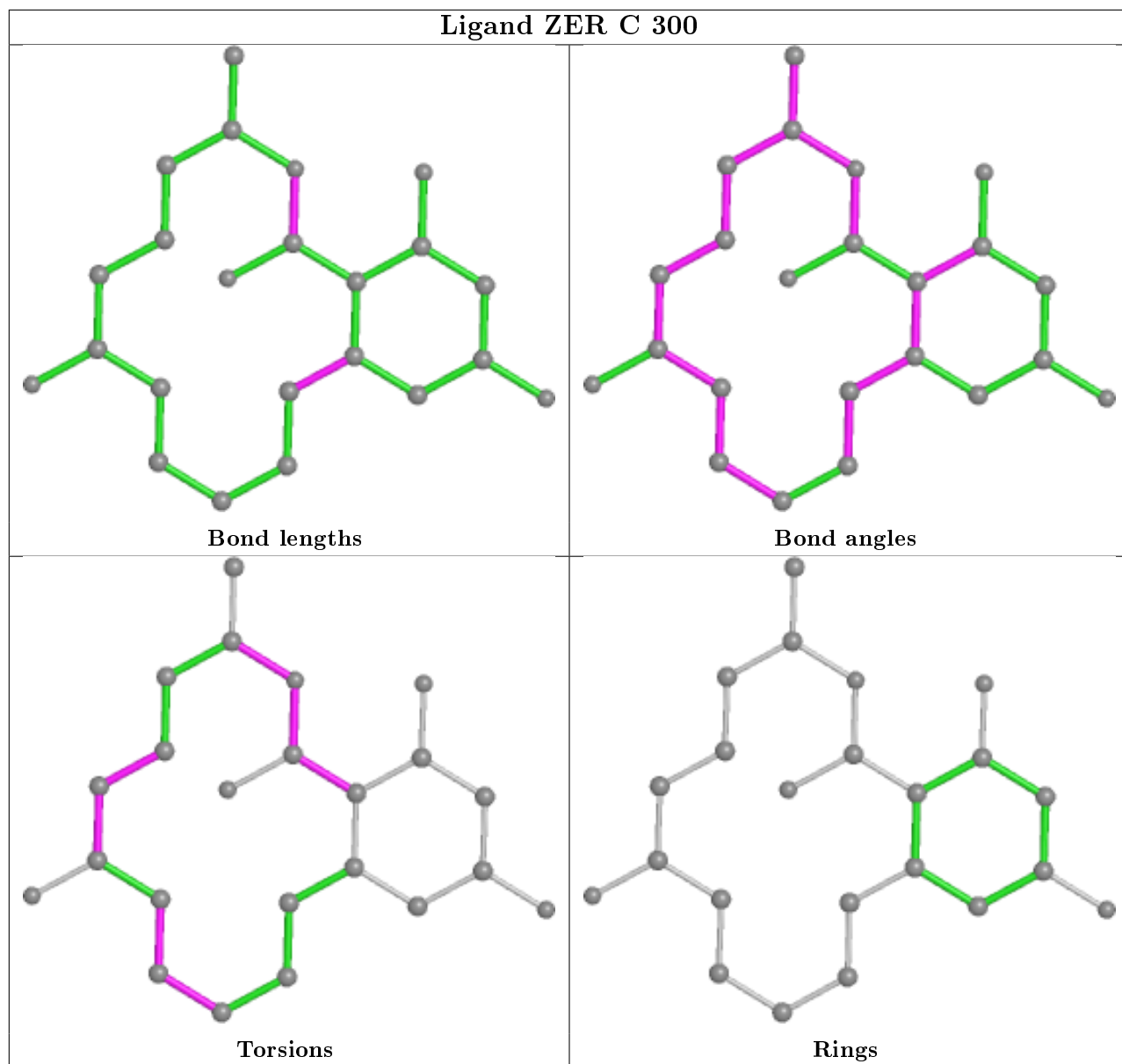
3 monomers are involved in 7 short contacts:

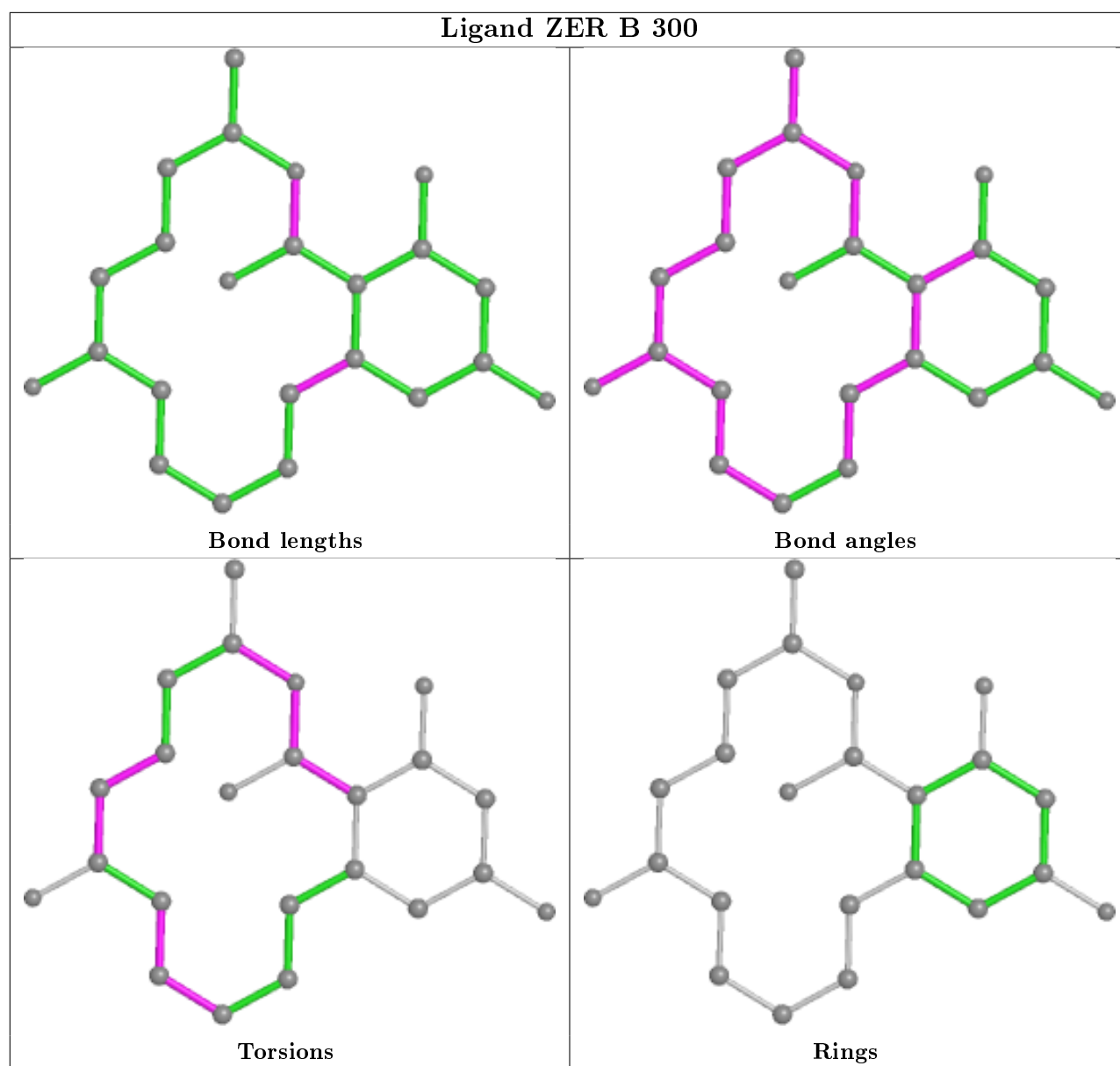
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ZER	2	0
2	C	300	ZER	2	0
2	B	300	ZER	3	0

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	264/278 (94%)	-0.47	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	22, 36, 58, 73	0
1	B	264/278 (94%)	-0.44	4 (1%) <span style="border: 1px solid blue; padding: 2px;">73</span> <span style="border: 1px solid blue; padding: 2px;">75</span>	24, 39, 61, 83	0
1	C	264/278 (94%)	2.17	125 (47%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	68, 88, 128, 153	0
All	All	792/834 (94%)	0.42	129 (16%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	22, 46, 112, 153	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	GLU	11.1
1	C	155	LEU	10.2
1	C	165	TRP	10.1
1	C	24	PRO	7.5
1	C	174	ALA	7.3
1	C	164	ALA	6.6
1	C	241	MET	6.1
1	C	3	THR	6.0
1	C	170	ASP	5.9
1	C	235	ILE	5.9
1	C	158	VAL	5.8
1	C	147	SER	5.7
1	C	142	GLU	5.6
1	C	230	LYS	5.5
1	C	171	GLU	5.5
1	C	13	ILE	5.3
1	C	60	GLY	5.1
1	C	127	LEU	4.9
1	C	219	GLU	4.8
1	C	226	VAL	4.8
1	C	136	SER	4.8
1	C	1	MET	4.7
1	C	65	ALA	4.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	237	LEU	4.6
1	C	251	VAL	4.6
1	C	156	ASN	4.6
1	C	231	ALA	4.4
1	C	222	PHE	4.3
1	C	144	GLU	4.2
1	C	6	THR	4.2
1	C	87	VAL	4.1
1	C	92	ASP	4.1
1	C	232	GLY	4.0
1	C	128	PRO	4.0
1	C	108	VAL	4.0
1	C	64	SER	4.0
1	C	137	ASN	3.9
1	C	252	PHE	3.9
1	C	114	GLY	3.9
1	C	168	MET	3.8
1	C	212	VAL	3.8
1	C	249	PRO	3.8
1	C	191	ILE	3.7
1	C	141	LEU	3.7
1	C	115	TYR	3.7
1	C	148	LYS	3.7
1	C	193	PRO	3.7
1	C	229	THR	3.7
1	C	160	GLY	3.6
1	C	8	SER	3.6
1	C	213	GLY	3.6
1	C	5	SER	3.5
1	C	14	THR	3.5
1	C	116	PRO	3.5
1	C	53	VAL	3.4
1	C	73	THR	3.4
1	C	185	ARG	3.4
1	C	202	ALA	3.3
1	C	117	ASP	3.3
1	C	90	ALA	3.3
1	C	162	SER	3.3
1	C	166	GLN	3.3
1	C	262	LYS	3.2
1	C	140	VAL	3.2
1	C	236	GLY	3.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	146	ILE	3.1
1	C	28	LEU	3.1
1	C	131	LEU	3.1
1	C	210	TRP	3.1
1	C	143	ASP	3.1
1	C	12	GLY	3.1
1	C	159	SER	3.1
1	C	211	THR	3.0
1	C	242	HIS	3.0
1	C	89	ASP	2.9
1	C	163	GLU	2.9
1	C	133	ASP	2.9
1	C	75	VAL	2.9
1	C	177	HIS	2.9
1	C	256	VAL	2.9
1	C	20	GLU	2.8
1	B	137	ASN	2.8
1	C	132	LEU	2.8
1	C	129	THR	2.8
1	C	161	GLY	2.8
1	C	126	GLU	2.8
1	C	54	THR	2.8
1	C	139	ALA	2.7
1	B	1	MET	2.7
1	C	77	ALA	2.7
1	C	186	GLY	2.6
1	C	190	THR	2.6
1	C	4	ARG	2.6
1	C	154	MET	2.6
1	C	82	SER	2.6
1	C	76	THR	2.6
1	C	59	PRO	2.5
1	C	215	ALA	2.5
1	C	258	GLU	2.5
1	C	32	GLY	2.5
1	C	220	SER	2.5
1	C	130	LYS	2.4
1	C	248	HIS	2.4
1	B	138	THR	2.4
1	C	2	ARG	2.4
1	C	240	GLY	2.3
1	C	250	ASP	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	119	ILE	2.3
1	C	111	LEU	2.3
1	C	110	ALA	2.3
1	C	218	THR	2.2
1	C	245	TYR	2.2
1	C	15	TRP	2.2
1	C	247	SER	2.2
1	C	104	GLY	2.2
1	C	45	GLN	2.2
1	C	172	VAL	2.2
1	C	31	ASP	2.2
1	C	55	THR	2.1
1	C	78	GLN	2.1
1	C	225	ILE	2.1
1	C	94	LYS	2.1
1	C	184	ALA	2.1
1	C	134	HIS	2.1
1	C	246	VAL	2.0
1	C	35	GLU	2.0
1	C	175	ARG	2.0
1	C	207	PRO	2.0
1	B	166	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

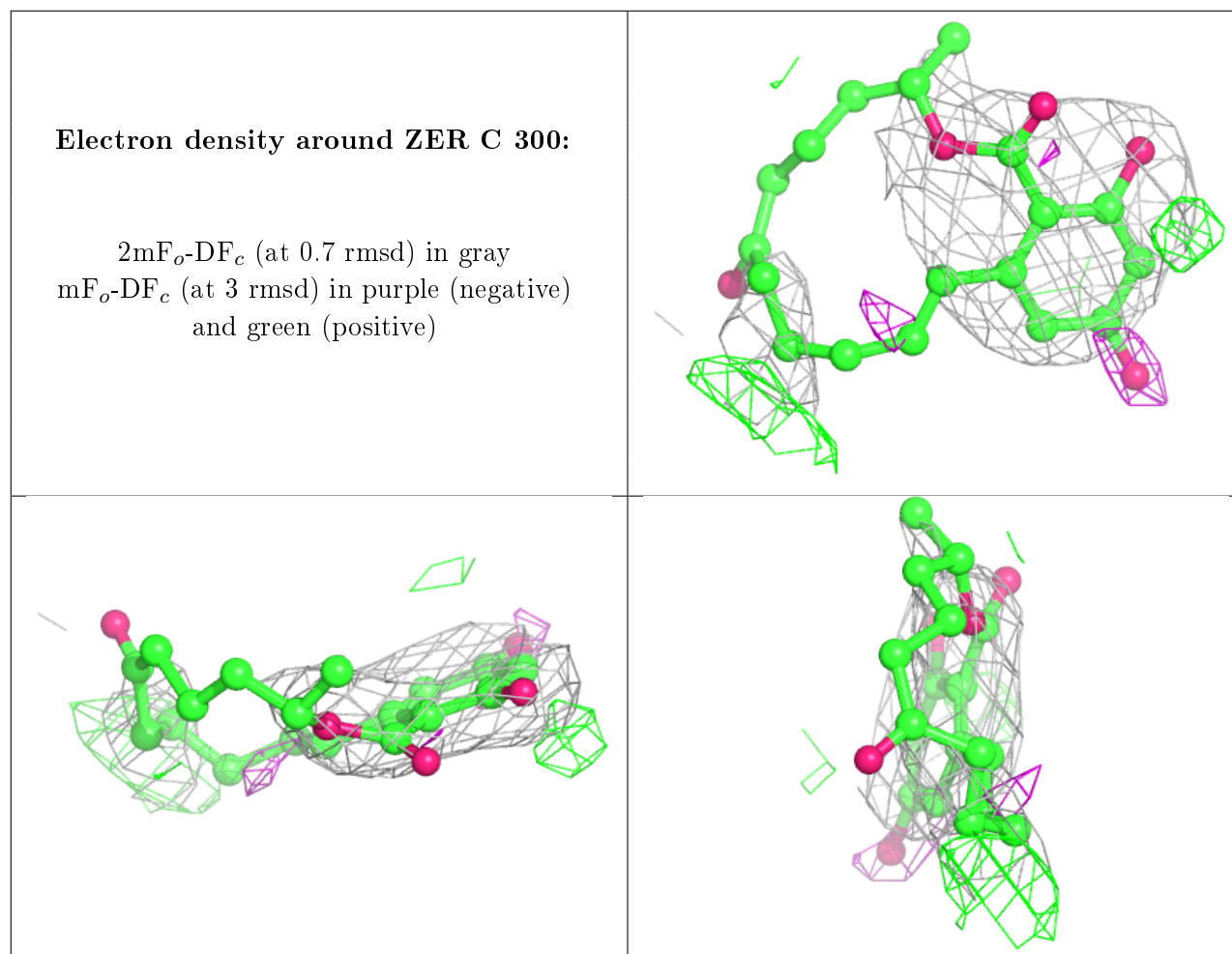
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZER	C	300	23/23	0.75	0.35	77,86,100,106	0

*Continued on next page...*

Continued from previous page...

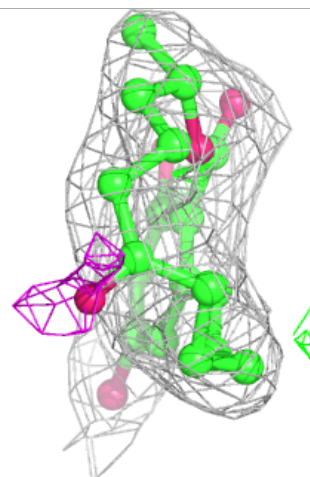
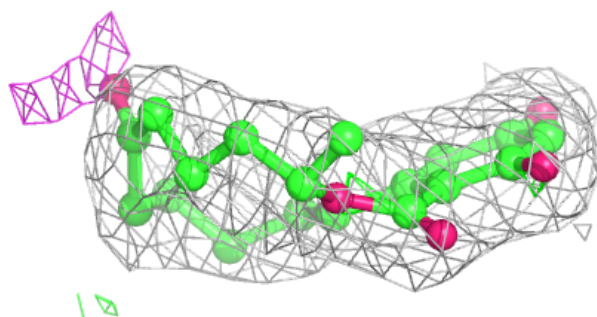
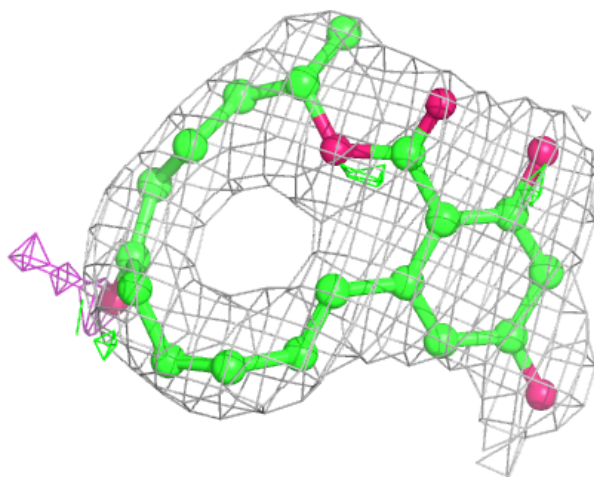
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZER	A	300	23/23	0.92	0.26	55,64,74,78	0
2	ZER	B	300	23/23	0.95	0.24	57,64,74,78	0

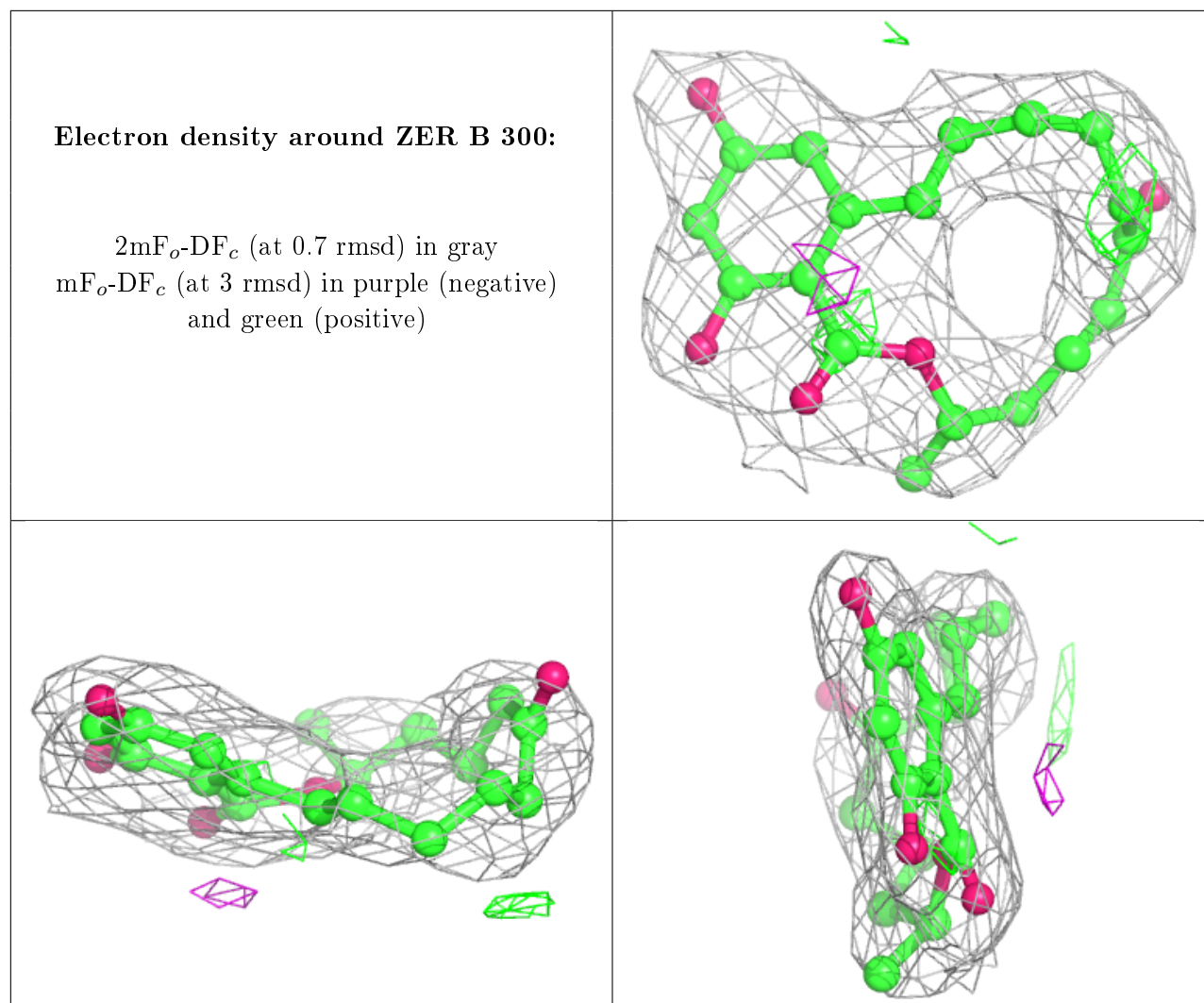
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around ZER A 300:**

$2mF_o-DF_c$  (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.