



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:58 PM UTC

PDB ID : 3WZM / pdb_00003wzm
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

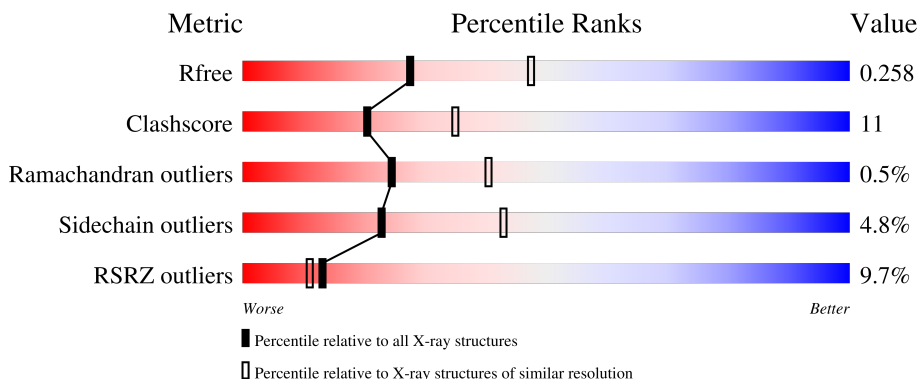
1 Overall quality at a glance

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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 76% 18% • 5%
1	B	278	 79% 14% • 5%
1	C	278	 27% 57% 36% • 5%

2 Entry composition

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
1	A	264	Total	C	N	O	S	0	0	0
			2021	1282	341	387	11			
1	B	264	Total	C	N	O	S	0	0	0
			2021	1282	341	387	11			
1	C	264	Total	C	N	O	S	0	0	0
			2021	1282	341	387	11			

There are 45 discrepancies between the modelled and reference sequences:

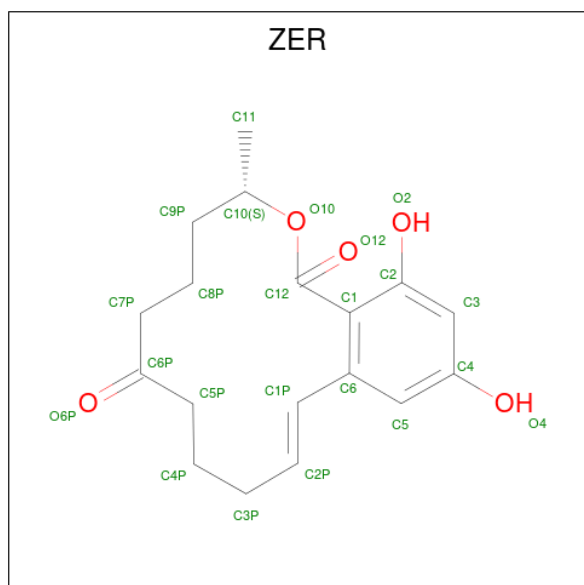
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8NKB0
A	-12	ALA	-	expression tag	UNP Q8NKB0
A	-11	HIS	-	expression tag	UNP Q8NKB0
A	-10	HIS	-	expression tag	UNP Q8NKB0
A	-9	HIS	-	expression tag	UNP Q8NKB0
A	-8	HIS	-	expression tag	UNP Q8NKB0
A	-7	HIS	-	expression tag	UNP 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

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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-benzoxacyclopentadecene-1,7(8H)-dione (CCD ID: ZER) (formula: $C_{18}H_{22}O_5$).



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		

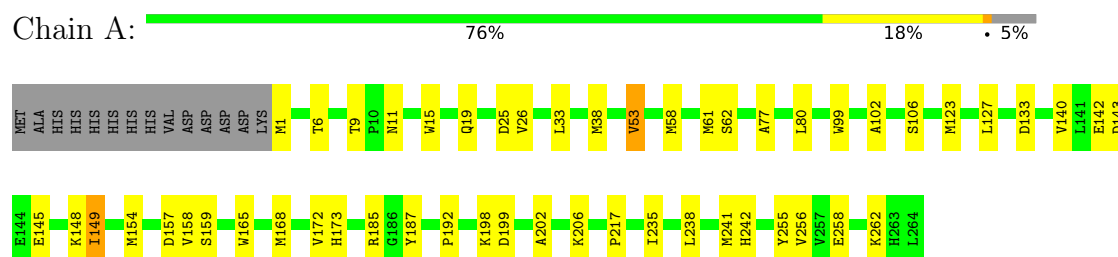
- Molecule 3 is water.

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		

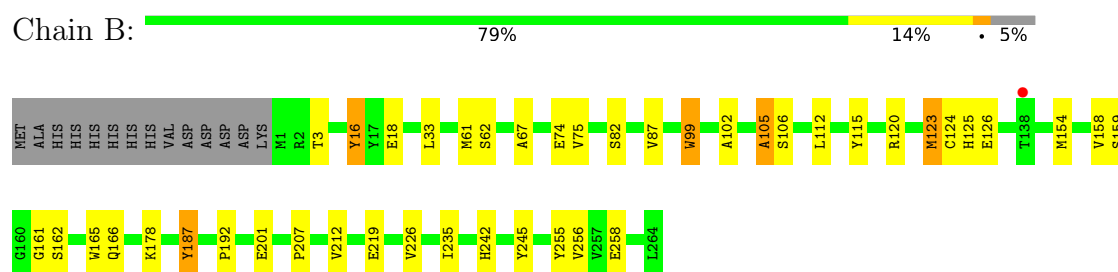
3 Residue-property plots [i](#)

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.

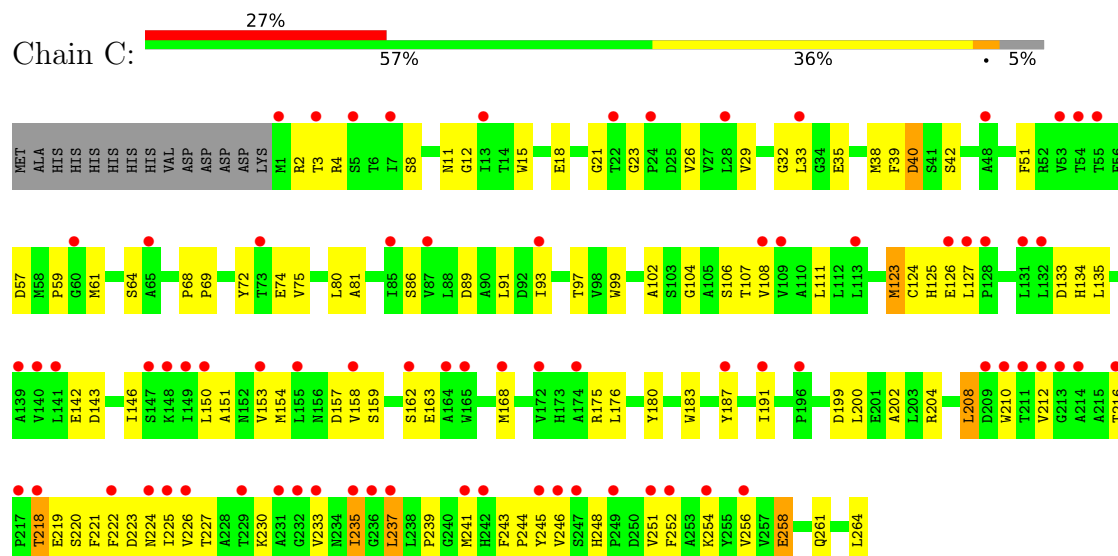
• Molecule 1: Zearalenone hydrolase



• Molecule 1: Zearalenone hydrolase



• Molecule 1: Zearalenone hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 95.2 (19.95-2.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.30 (at 2.50Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.268 0.200 , 0.258	Depositor DCC
R_{free} test set	1848 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.20	3/2072 (0.1%)	1.16	6/2829 (0.2%)
1	B	1.17	2/2072 (0.1%)	1.16	8/2829 (0.3%)
1	C	0.99	1/2072 (0.0%)	1.15	6/2829 (0.2%)
All	All	1.12	6/6216 (0.1%)	1.16	20/8487 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	ILE	CA-CB	7.55	1.63	1.54
1	B	192	PRO	CA-C	5.64	1.57	1.52
1	A	140	VAL	CA-CB	5.57	1.61	1.54
1	B	226	VAL	CA-CB	5.09	1.60	1.54
1	A	217	PRO	N-CA	5.04	1.53	1.47
1	A	26	VAL	C-O	5.02	1.29	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ALA	CA-C-N	-7.62	112.53	120.38
1	B	67	ALA	C-N-CA	-7.62	112.53	120.38
1	C	158	VAL	N-CA-C	7.14	119.45	111.88
1	A	11	ASN	N-CA-C	-6.61	104.79	112.92
1	C	23	GLY	CA-C-N	6.41	126.44	119.90
1	C	23	GLY	C-N-CA	6.41	126.44	119.90
1	A	9	THR	CA-C-N	-6.30	111.96	119.84
1	A	9	THR	C-N-CA	-6.30	111.96	119.84
1	B	158	VAL	N-CA-C	6.13	119.05	113.10
1	C	227	THR	CB-CA-C	5.98	116.88	109.16
1	B	115	TYR	CA-C-N	5.69	125.54	119.28
1	B	115	TYR	C-N-CA	5.69	125.54	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ALA	N-CA-C	-5.58	105.11	111.14
1	C	224	ASN	CA-C-N	5.43	128.19	120.53
1	C	224	ASN	C-N-CA	5.43	128.19	120.53
1	B	212	VAL	N-CA-C	-5.39	100.08	108.81
1	A	149	ILE	CB-CA-C	-5.17	105.34	111.81
1	A	192	PRO	N-CA-C	5.14	116.97	110.70
1	B	16	TYR	N-CA-C	-5.04	101.50	109.96
1	A	133	ASP	N-CA-C	5.01	116.74	111.28

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	2021	0	1991	35	0
1	B	2021	0	1991	19	0
1	C	2021	0	1991	79	0
2	A	23	0	20	2	0
2	B	23	0	20	4	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	136	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 (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:123:MET:HE1	1:B:256:VAL:HA	1.25	1.12
1:C:123:MET:HE1	1:C:256:VAL:HA	1.42	1.00
1:A:123:MET:HE1	1:A:256:VAL:HA	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:MET:HE2	1:A:172:VAL:HG11	1.50	0.91
1:A:38:MET:HG2	1:A:168:MET:HE3	1.57	0.86
1:A:158:VAL:HA	1:A:241:MET:HE2	1.61	0.80
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:35:GLU:CD	1:C:175:ARG:HH21	1.95	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:199:ASP:HB2	3:C:429:HOH:O	1.92	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:B:154:MET:HE1	2:B:300:ZER:H19	1.76	0.67
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:O	1:C:226:VAL:HG12	1.95	0.67
1:C:154:MET:O	1:C:159:SER:HB3	1.95	0.66
1:A:123:MET:CE	1:A:256:VAL:HA	2.23	0.65
1:B:99:TRP:C	1:B:99:TRP:CD1	2.77	0.61
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:124:CYS:HG	1:C:210:TRP:CD1	2.20	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:158:VAL:HA	1:A:241:MET:CE	2.33	0.58
1:C:29:VAL:N	1:C:99:TRP:O	2.28	0.58
1:C:38:MET:HG2	1:C:168:MET:HE3	1.87	0.57
1:A:157:ASP:O	1:A:241:MET:HE1	2.05	0.57
1:C:21:GLY:HA3	1:C:51:PHE:O	2.05	0.56
1:A:168:MET:HE2	1:A:172:VAL:CG1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:GLU:CD	3:C:415:HOH:O	2.50	0.55
1:C:208:LEU:HG	1:C:233:VAL:CG1	2.35	0.55
1:C:39:PHE:O	1:C:42:SER:N	2.40	0.54
1:C:134:HIS:CD2	1:C:135:LEU:HG	2.39	0.54
1:C:226:VAL:O	1:C:226:VAL:CG1	2.54	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:A:123:MET:HE1	1:A:256:VAL:CA	2.28	0.53
1:B:154:MET:HE1	2:B:300:ZER:C7P	2.39	0.53
1:C:254:LYS:O	1:C:258:GLU:HB2	2.08	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:N	1:C:237:LEU:CD1	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:H11	2:A:300:ZER:O10	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:A:38:MET:HG2	1:A:168:MET:HE1	1.94	0.50
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:216:THR:HA	1:C:241:MET:HE3	1.93	0.50
1:C:162:SER:HB3	3:C:453:HOH:O	2.12	0.50
1:A:38:MET:HE2	1:A:168:MET:HE1	1.94	0.49
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:A:123:MET:HE1	1:A:256:VAL:HG22	1.95	0.48
1:B:16:TYR:OH	1:B:18:GLU:OE2	2.24	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:B:61:MET:O	1:B:62:SER:C	2.55	0.48
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:A:99:TRP:CD1	1:A:99:TRP:C	2.92	0.47
1:A:102:ALA:HB2	1:A:242:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ALA:HA	1:C:126:GLU:O	2.14	0.47
1:A:61:MET:O	1:A:62:SER:C	2.58	0.46
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:123:MET:HE3	1:A:255:TYR:CE2	2.50	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:B:123:MET:HE2	1:B:255:TYR:CE2	2.51	0.45
1:C:3:THR:O	1:C:18:GLU:HA	2.16	0.45
1:C:32:GLY:O	1:C:61:MET:HE2	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:B:3:THR:O	1:B:18:GLU:HA	2.17	0.44
1:C:26:VAL:HG22	1:C:97:THR:HB	2.00	0.44
1:C:80:LEU:HD11	1:C:187:TYR:CE1	2.52	0.44
1:C:99:TRP:HE3	1:C:123:MET:HB2	1.83	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:A:127:LEU:C	1:A:127:LEU:HD23	2.42	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:C:91:LEU:HB3	1:C:93:ILE:CD1	2.46	0.43
1:C:244:PRO:HD2	1:C:245:TYR:CD2	2.53	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
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:B:105:ALA:HB1	1:B:124:CYS:HB2	2.02	0.42
2:B:300:ZER:H10	2:B:300:ZER:H12	1.84	0.42
1:C:159:SER:HA	1:C:243:PHE:CD2	2.55	0.42
1:B:123:MET:HE1	1:B:256:VAL:CA	2.19	0.41
2:C:300:ZER:H22	2:C:300:ZER:H17	1.88	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:102:ALA:HB2	1:A:242:HIS:HE2	1.84	0.40
1:C:75:VAL:HG12	1:C:191:ILE:HD11	2.03	0.40
1:C:222:PHE:HA	1:C:225:ILE:HD12	2.03	0.40
1:A:58:MET:HE3	1:A:80:LEU:HD22	2.04	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%)	30	46
1	B	262/278 (94%)	250 (95%)	10 (4%)	2 (1%)	16	28
1	C	262/278 (94%)	229 (87%)	32 (12%)	1 (0%)	30	46
All	All	786/834 (94%)	730 (93%)	52 (7%)	4 (0%)	24	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ASP
1	A	187	TYR

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Mol	Chain	Res	Type
1	B	161	GLY
1	B	187	TYR

5.3.2 Protein sidechains ⓘ

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%)	214 (97%)	6 (3%)	39	64
1	B	220/233 (94%)	207 (94%)	13 (6%)	18	34
1	C	220/233 (94%)	207 (94%)	13 (6%)	18	34
All	All	660/699 (94%)	628 (95%)	32 (5%)	23	43

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	142	GLU
1	A	148	LYS
1	A	235	ILE
1	A	258	GLU
1	A	262	LYS
1	B	74	GLU
1	B	82	SER
1	B	87	VAL
1	B	99	TRP
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	235	ILE
1	B	245	TYR
1	B	258	GLU
1	C	8	SER

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Mol	Chain	Res	Type
1	C	74	GLU
1	C	106	SER
1	C	123	MET
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	223	ASP
1	C	237	LEU
1	C	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	152	ASN
1	A	156	ASN
1	A	261	GLN
1	B	263	HIS
1	C	95	HIS
1	C	134	HIS
1	C	152	ASN
1	C	166	GLN
1	C	261	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	300	-	24,24,24	1.34	2 (8%)	32,32,32	1.68	8 (25%)
2	ZER	B	300	-	24,24,24	1.17	2 (8%)	32,32,32	2.14	10 (31%)
2	ZER	A	300	-	24,24,24	1.31	3 (12%)	32,32,32	2.15	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	C	300	-	-	11/22/22/22	0/1/2/2
2	ZER	B	300	-	-	9/22/22/22	0/1/2/2
2	ZER	A	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	4.39	1.43	1.34
2	C	300	ZER	C6-C1P	3.66	1.53	1.47
2	A	300	ZER	C6-C1P	3.63	1.53	1.47
2	B	300	ZER	O10-C12	3.47	1.41	1.34
2	A	300	ZER	O10-C12	3.21	1.41	1.34
2	B	300	ZER	C6-C1P	3.01	1.52	1.47
2	A	300	ZER	C1-C6	-2.06	1.39	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ZER	C11-C10-C9P	-6.06	98.19	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	ZER	C4P-C5P-C6P	-5.15	101.53	114.59
2	A	300	ZER	C11-C10-C9P	-4.96	101.06	113.90
2	A	300	ZER	C7P-C6P-C5P	4.93	126.28	116.95
2	B	300	ZER	C7P-C6P-C5P	4.59	125.63	116.95
2	B	300	ZER	C4P-C5P-C6P	-4.36	103.54	114.59
2	C	300	ZER	C11-C10-C9P	-3.77	104.15	113.90
2	B	300	ZER	O10-C10-C11	3.72	116.29	107.96
2	C	300	ZER	C4P-C5P-C6P	-3.44	105.88	114.59
2	A	300	ZER	O10-C10-C11	3.33	115.41	107.96
2	C	300	ZER	O10-C10-C11	3.23	115.19	107.96
2	A	300	ZER	C9P-C8P-C7P	-3.17	104.83	113.26
2	A	300	ZER	C6-C1-C2	3.03	121.81	118.73
2	C	300	ZER	C7P-C6P-C5P	2.96	122.55	116.95
2	A	300	ZER	C5P-C4P-C3P	-2.91	107.00	113.35
2	B	300	ZER	C5P-C4P-C3P	-2.77	107.30	113.35
2	B	300	ZER	C9P-C8P-C7P	-2.73	105.98	113.26
2	C	300	ZER	C6-C1P-C2P	-2.72	119.82	125.55
2	B	300	ZER	C10-O10-C12	2.69	122.67	117.67
2	C	300	ZER	C5P-C4P-C3P	-2.65	107.56	113.35
2	C	300	ZER	C6-C1-C2	2.54	121.31	118.73
2	A	300	ZER	O6P-C6P-C5P	-2.49	114.87	121.40
2	C	300	ZER	C9P-C8P-C7P	-2.43	106.79	113.26
2	A	300	ZER	C2-C3-C4	-2.42	117.44	119.67
2	B	300	ZER	C6-C1P-C2P	-2.40	120.49	125.55
2	B	300	ZER	C6-C1-C2	2.38	121.14	118.73
2	A	300	ZER	C6-C1P-C2P	-2.20	120.91	125.55
2	B	300	ZER	O6P-C6P-C5P	-2.10	115.90	121.40

There are no chirality outliers.

All (30) 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	B	300	ZER	C11-C10-O10-C12
2	B	300	ZER	C5P-C6P-C7P-C8P
2	B	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	C1-C12-O10-C10

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

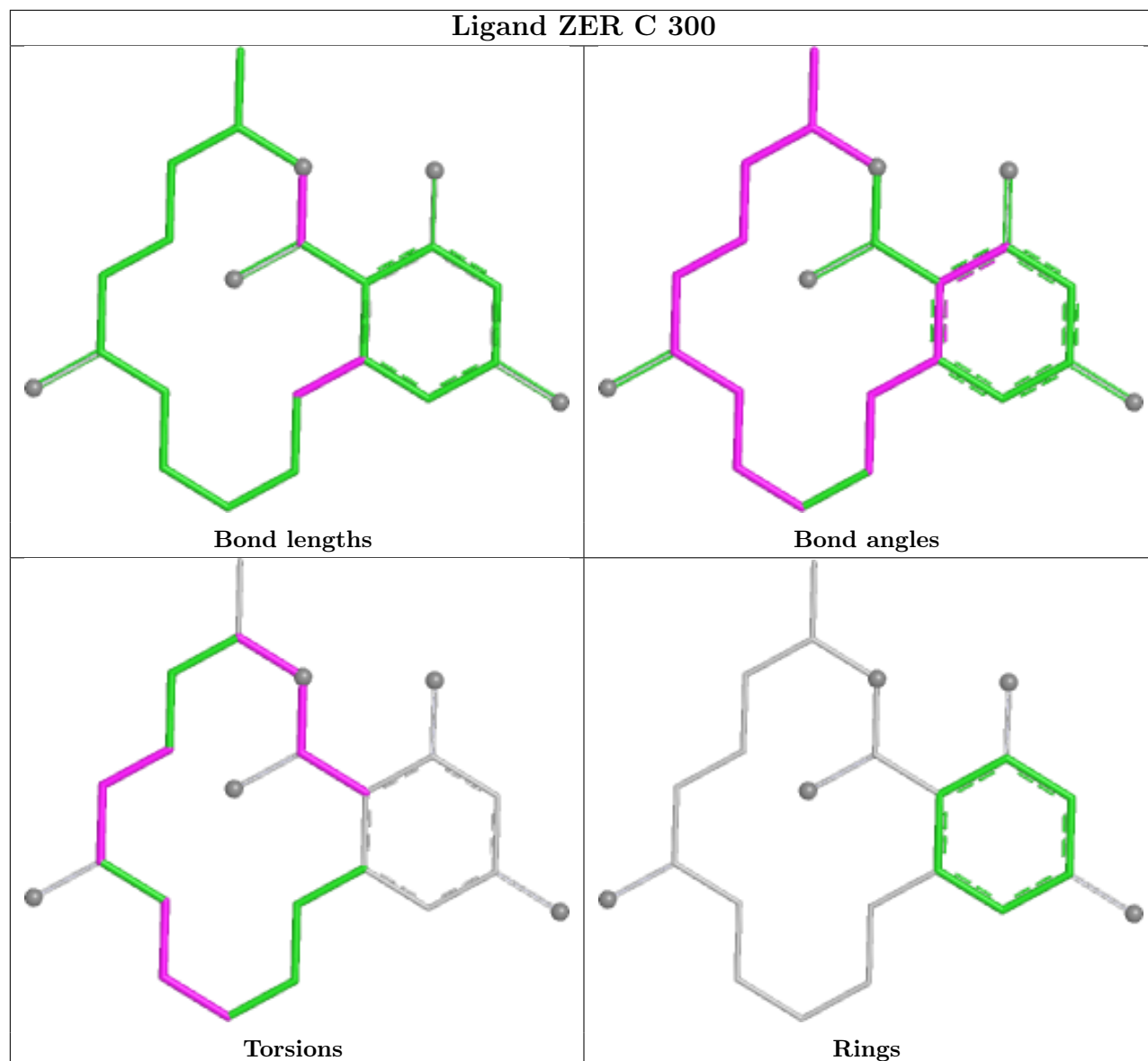
There are no ring outliers.

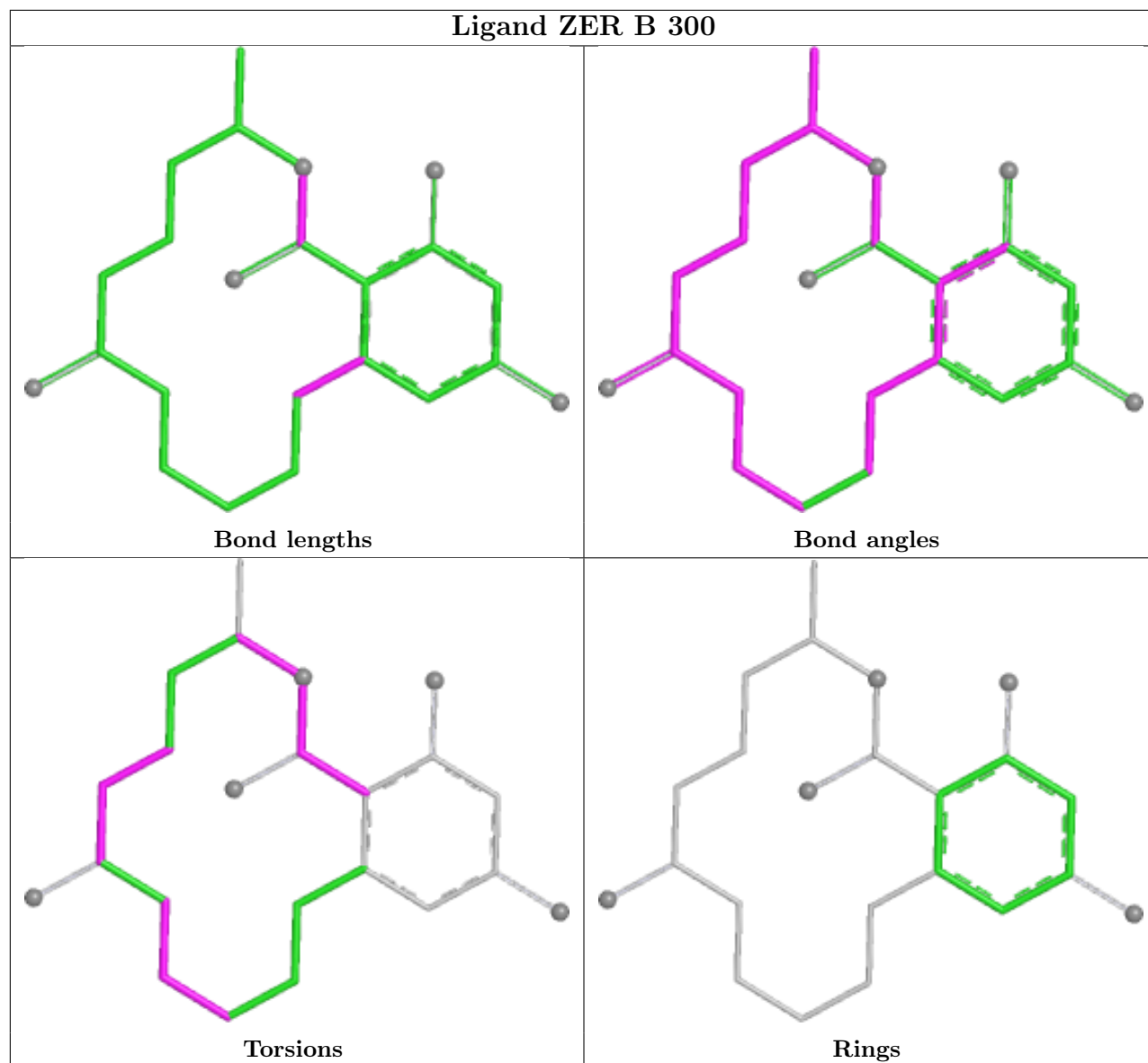
3 monomers are involved in 8 short contacts:

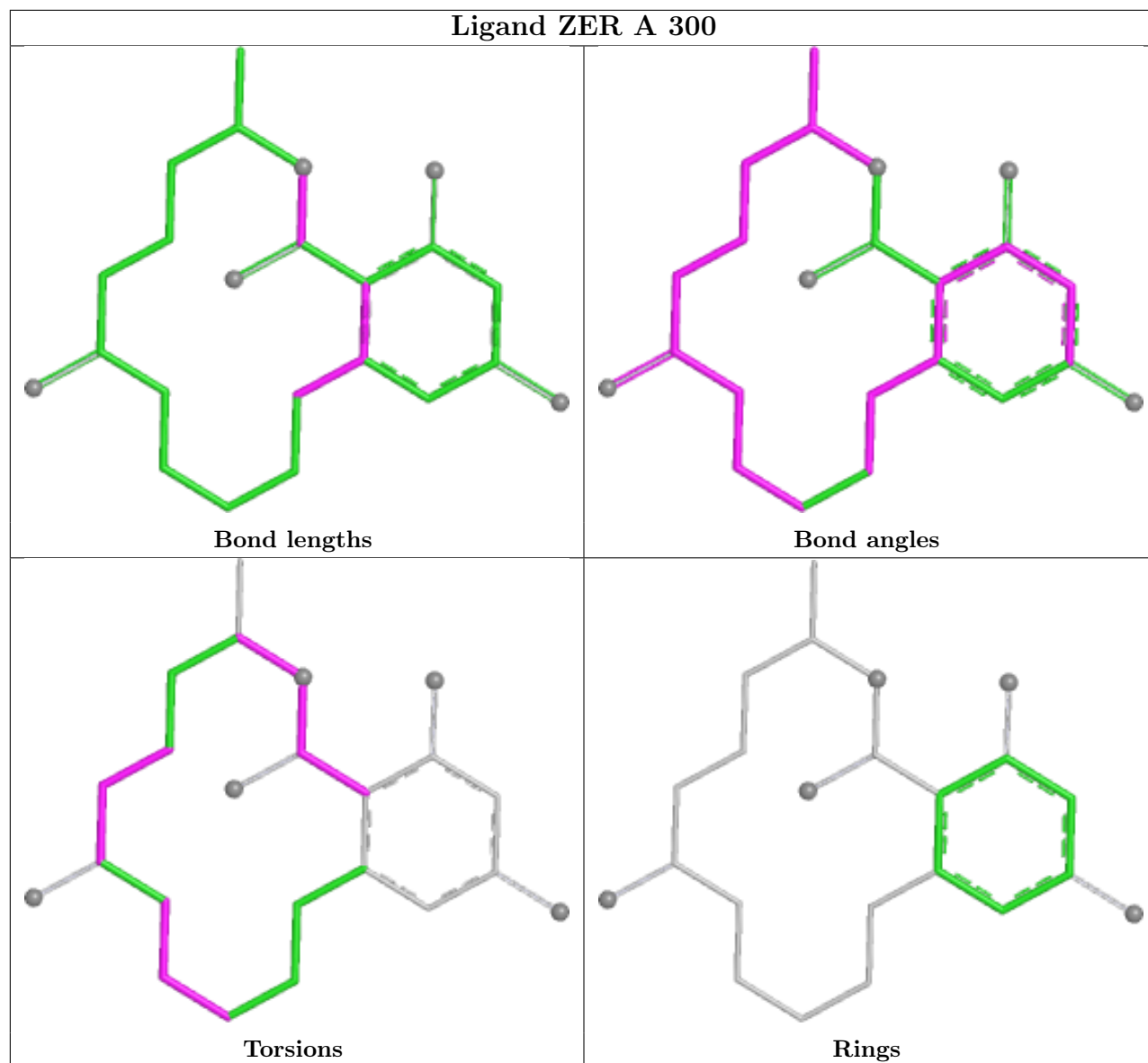
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	ZER	2	0
2	B	300	ZER	4	0
2	A	300	ZER	2	0

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

Ligand ZER C 300







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, 95th 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 ²)	Q<0.9
1	A	264/278 (94%)	-0.54	0 100 100	22, 36, 58, 73	0
1	B	264/278 (94%)	-0.48	1 (0%) 88 87	24, 39, 61, 83	0
1	C	264/278 (94%)	1.58	76 (28%) 1 1	68, 88, 128, 153	0
All	All	792/834 (94%)	0.19	77 (9%) 13 11	22, 46, 112, 153	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	TRP	7.4
1	C	235	ILE	4.9
1	C	127	LEU	4.8
1	C	226	VAL	4.0
1	C	212	VAL	3.9
1	C	225	ILE	3.8
1	C	245	TYR	3.8
1	C	149	ILE	3.7
1	C	164	ALA	3.4
1	C	140	VAL	3.4
1	C	24	PRO	3.4
1	C	13	ILE	3.3
1	C	222	PHE	3.2
1	C	108	VAL	3.1
1	C	251	VAL	3.1
1	C	155	LEU	3.1
1	C	211	THR	3.1
1	C	28	LEU	3.1
1	B	138	THR	3.0
1	C	1	MET	3.0
1	C	126	GLU	2.9
1	C	87	VAL	2.9
1	C	233	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	210	TRP	2.8
1	C	3	THR	2.8
1	C	53	VAL	2.8
1	C	249	PRO	2.8
1	C	236	GLY	2.7
1	C	147	SER	2.7
1	C	214	ALA	2.7
1	C	7	ILE	2.7
1	C	128	PRO	2.7
1	C	109	VAL	2.7
1	C	60	GLY	2.6
1	C	85	ILE	2.6
1	C	150	LEU	2.6
1	C	252	PHE	2.6
1	C	246	VAL	2.6
1	C	231	ALA	2.6
1	C	254	LYS	2.6
1	C	174	ALA	2.5
1	C	191	ILE	2.5
1	C	158	VAL	2.5
1	C	247	SER	2.5
1	C	139	ALA	2.5
1	C	213	GLY	2.5
1	C	162	SER	2.4
1	C	132	LEU	2.4
1	C	218	THR	2.4
1	C	33	LEU	2.4
1	C	229	THR	2.3
1	C	148	LYS	2.3
1	C	22	THR	2.3
1	C	5	SER	2.3
1	C	237	LEU	2.3
1	C	187	TYR	2.3
1	C	256	VAL	2.3
1	C	54	THR	2.3
1	C	113	LEU	2.3
1	C	242	HIS	2.3
1	C	93	ILE	2.2
1	C	131	LEU	2.2
1	C	141	LEU	2.2
1	C	224	ASN	2.2
1	C	232	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	172	VAL	2.1
1	C	168	MET	2.1
1	C	55	THR	2.1
1	C	73	THR	2.1
1	C	216	THR	2.1
1	C	217	PRO	2.1
1	C	65	ALA	2.1
1	C	209	ASP	2.1
1	C	196	PRO	2.1
1	C	241	MET	2.1
1	C	48	ALA	2.0
1	C	153	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

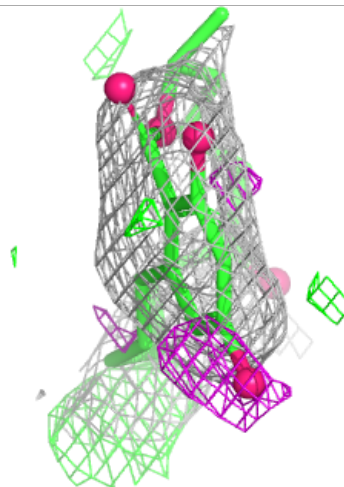
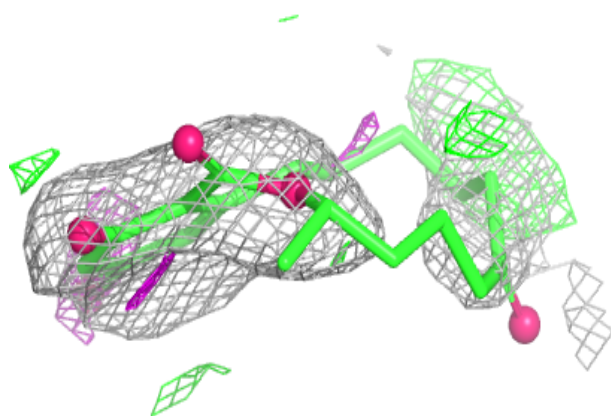
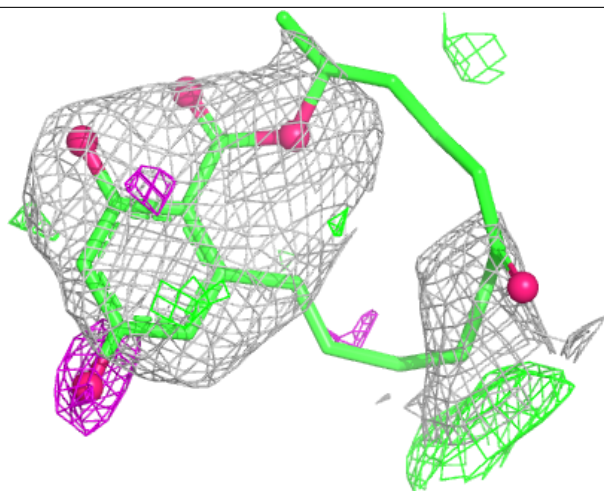
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZER	C	300	23/23	0.57	0.17	77,86,100,106	0
2	ZER	B	300	23/23	0.92	0.13	57,64,74,78	0
2	ZER	A	300	23/23	0.93	0.13	55,64,74,78	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.

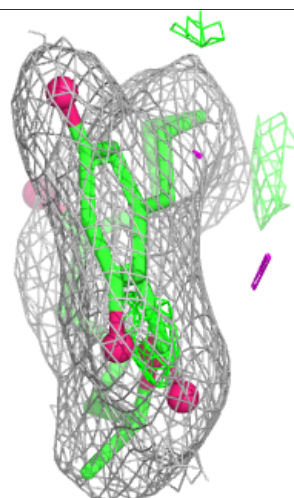
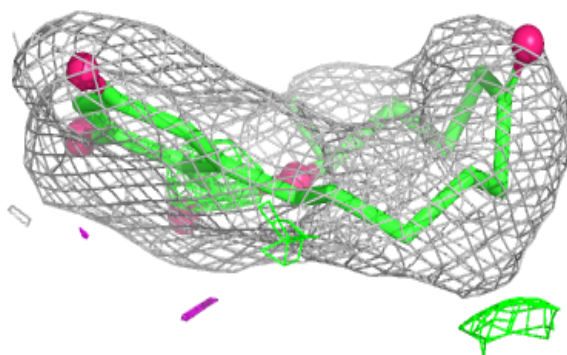
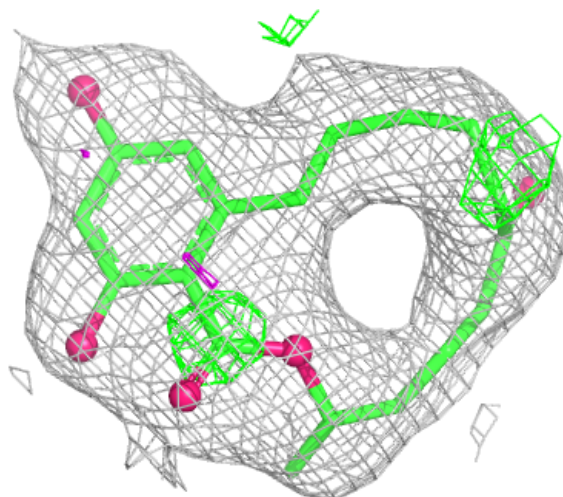
Electron density around ZER C 300:

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



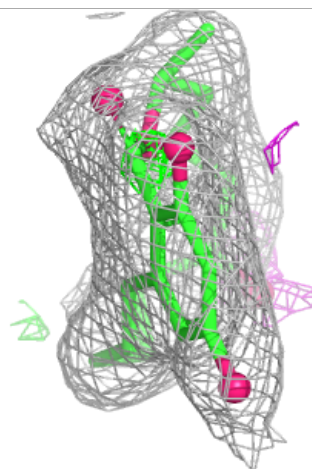
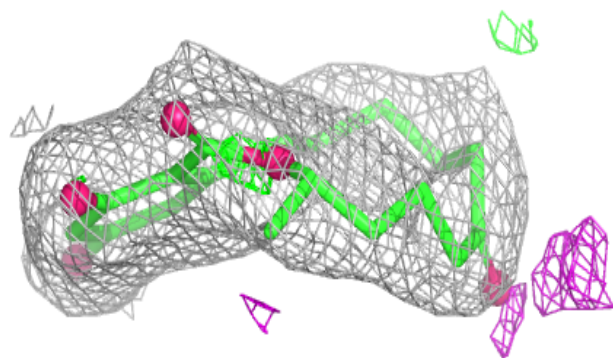
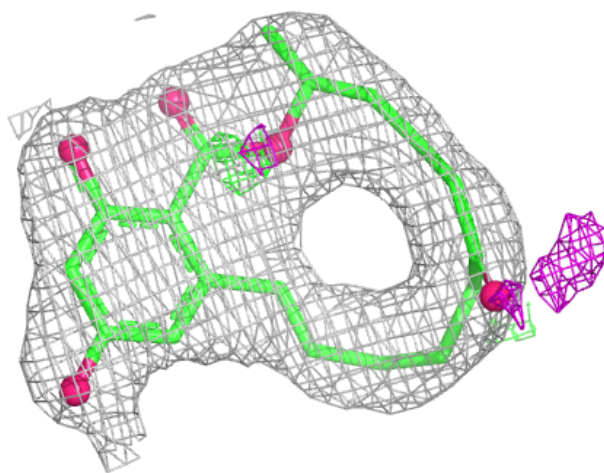
Electron density around ZER B 300:

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



Electron density around 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.