



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:32 AM BST

PDB ID : 5XO8
Title : Crystal structure of a novel ZEN lactonase mutant with ligand Z
Authors : Zheng, Y.Y.; Liu, W.T.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2017-05-27
Resolution : 1.88 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

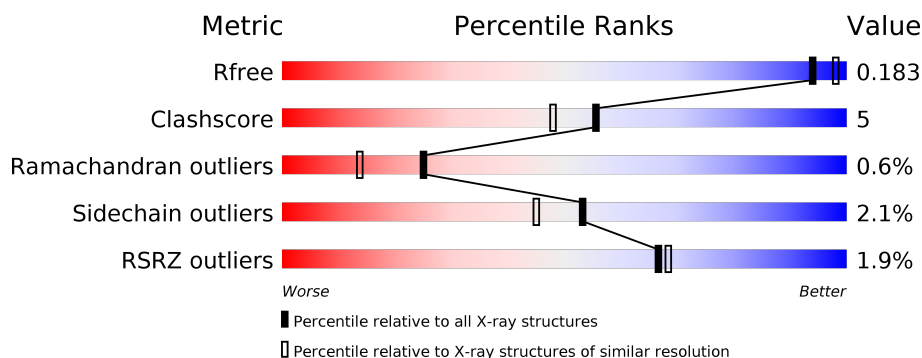
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 ≥ 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	266	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	266	<div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	266	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	266	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	E	266	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	F	266	<div> <div>8%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	266	
1	H	266	

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	ZER	A	301	-	-	X	-
2	ZER	B	301	-	-	X	-
2	ZER	G	301	-	-	X	-
2	ZER	H	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19224 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.

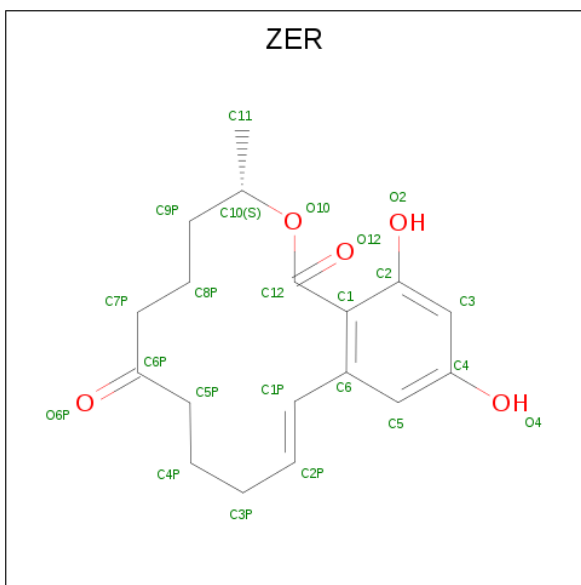
- Molecule 1 is a protein called Lactonase for protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	B	263	Total	C	N	O	S	0	1	0
			2063	1310	349	395	9			
1	C	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	D	264	Total	C	N	O	S	0	0	0
			2060	1309	348	394	9			
1	E	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	F	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	G	262	Total	C	N	O	S	0	0	0
			2045	1300	345	391	9			
1	H	263	Total	C	N	O	S	0	1	0
			2058	1307	348	394	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
B	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
C	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
D	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
E	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
F	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
G	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
H	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1

- 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: C₁₈H₂₂O₅).



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		
2	D	1	Total	C	O	0	0
			23	18	5		
2	E	1	Total	C	O	0	0
			23	18	5		
2	F	1	Total	C	O	0	0
			23	18	5		
2	G	1	Total	C	O	0	0
			23	18	5		
2	H	1	Total	C	O	0	0
			23	18	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	390	Total	O	0	0
			390	390		
3	C	324	Total	O	0	0
			324	324		
3	D	316	Total	O	0	0
			316	316		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	292	Total 292	O 292	0	0
3	F	209	Total 209	O 209	0	0
3	G	311	Total 311	O 311	0	0
3	H	355	Total 355	O 355	0	0

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: Lactonase for protein

Chain A: 

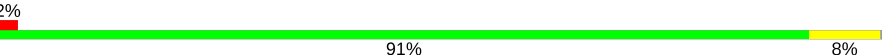


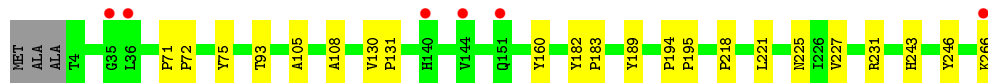
- Molecule 1: Lactonase for protein

Chain B: 




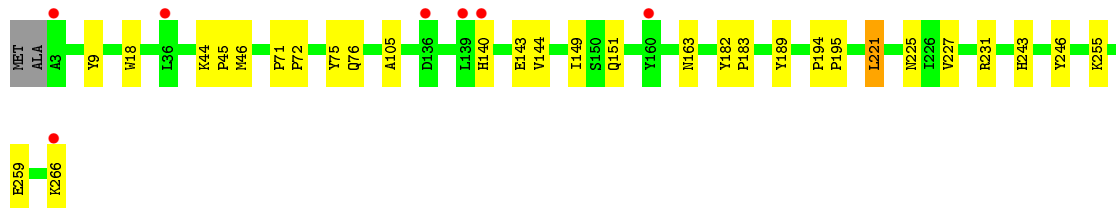
- Molecule 1: Lactonase for protein

Chain C: 



- Molecule 1: Lactonase for protein

Chain D: 



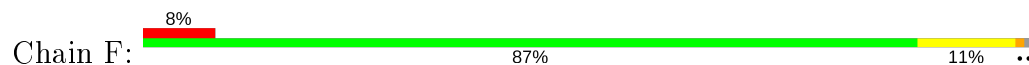
- Molecule 1: Lactonase for protein

Chain E: 

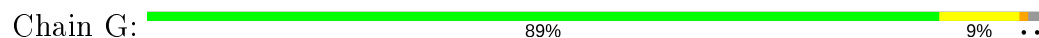




- Molecule 1: Lactonase for protein



- Molecule 1: Lactonase for protein



- Molecule 1: Lactonase for protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.47Å 95.20Å 101.66Å 90.21° 92.34° 91.48°	Depositor
Resolution (Å)	24.95 – 1.88 24.93 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.95-1.88) 97.7 (24.93-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.145 , 0.181 0.158 , 0.183	Depositor DCC
R_{free} test set	1999 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l 0.010 for -h,k,-l 0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19224	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	1.36	0/2114	0.79	0/2886
1	B	1.35	0/2122	0.78	0/2897
1	C	1.30	0/2114	0.76	0/2886
1	D	1.31	0/2119	0.77	0/2893
1	E	1.26	0/2114	0.77	0/2886
1	F	1.24	0/2114	0.82	0/2886
1	G	1.30	0/2104	0.78	0/2875
1	H	1.32	0/2117	0.77	0/2893
All	All	1.30	0/16918	0.78	0/23102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	1993	14	0
1	B	2063	0	1998	13	0
1	C	2055	0	1993	11	0
1	D	2060	0	1998	18	0
1	E	2055	0	1993	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2055	0	1993	23	0
1	G	2045	0	1980	15	0
1	H	2058	0	1990	9	0
2	A	23	0	21	13	0
2	B	23	0	20	9	0
2	C	23	0	21	6	0
2	D	23	0	21	5	0
2	E	23	0	21	3	0
2	F	23	0	21	8	0
2	G	23	0	21	11	0
2	H	23	0	20	10	0
3	A	397	0	0	2	0
3	B	390	0	0	5	1
3	C	324	0	0	1	0
3	D	316	0	0	2	1
3	E	292	0	0	4	1
3	F	209	0	0	4	0
3	G	311	0	0	6	0
3	H	355	0	0	1	1
All	All	19224	0	16104	166	2

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 5.

All (166) 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)
2:H:301:ZER:C9P	2:H:301:ZER:C10	1.76	1.58
2:A:301:ZER:C9P	2:A:301:ZER:C8P	1.87	1.53
2:B:301:ZER:C9P	2:B:301:ZER:C10	1.84	1.52
2:G:301:ZER:C10	2:G:301:ZER:C9P	1.90	1.48
2:D:301:ZER:C10	2:D:301:ZER:O10	1.64	1.44
2:E:301:ZER:C10	2:E:301:ZER:O10	1.65	1.43
2:F:301:ZER:O10	2:F:301:ZER:C10	1.64	1.41
1:E:242:ASN:HB3	3:E:444:HOH:O	1.30	1.30
2:H:301:ZER:O10	2:H:301:ZER:C10	1.80	1.27
2:G:301:ZER:C10	2:G:301:ZER:O10	1.84	1.26
1:F:95:ASP:HB2	3:F:544:HOH:O	1.32	1.25
2:A:301:ZER:O10	2:A:301:ZER:C10	1.83	1.25
2:C:301:ZER:O10	2:C:301:ZER:C10	1.83	1.25
1:A:95:ASP:HB2	3:A:663:HOH:O	1.28	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ZER:O10	2:B:301:ZER:C10	1.89	1.20
1:F:146:PRO:HD3	1:F:187:TYR:OH	1.53	1.08
1:F:76:GLN:O	1:F:82:LYS:NZ	1.99	0.95
2:H:301:ZER:C9P	2:H:301:ZER:H1	2.03	0.83
1:H:242[B]:ASN:OD1	3:H:401:HOH:O	1.95	0.83
2:H:301:ZER:C10	2:H:301:ZER:C8P	2.58	0.82
2:G:301:ZER:H1	2:G:301:ZER:C9P	2.09	0.81
2:H:301:ZER:C11	2:H:301:ZER:C9P	2.58	0.80
2:B:301:ZER:C9P	2:B:301:ZER:H1	2.08	0.80
1:F:265:LEU:O	3:F:401:HOH:O	2.03	0.77
2:B:301:ZER:C11	2:B:301:ZER:C9P	2.63	0.76
1:F:146:PRO:HD3	1:F:187:TYR:HH	1.48	0.76
2:A:301:ZER:C12	2:A:301:ZER:C10	2.62	0.76
1:F:72:PRO:HA	1:F:75:TYR:CZ	2.22	0.75
2:A:301:ZER:C8P	2:A:301:ZER:C10	2.65	0.74
2:B:301:ZER:C8P	2:B:301:ZER:C10	2.66	0.74
1:F:72:PRO:HA	1:F:75:TYR:CE1	2.23	0.74
1:F:145:ASP:OD1	1:F:148:THR:OG1	2.05	0.73
1:F:81:ARG:NE	1:F:117:ASP:OD2	2.20	0.71
1:B:4:THR:HA	3:B:642:HOH:O	1.92	0.69
2:D:301:ZER:C10	2:D:301:ZER:C12	2.70	0.69
1:G:165:GLU:HG3	3:G:546:HOH:O	1.92	0.69
1:F:202:GLU:O	3:F:402:HOH:O	2.12	0.68
1:G:6:THR:CG2	3:G:532:HOH:O	2.42	0.67
2:D:301:ZER:O10	2:D:301:ZER:H1	1.85	0.67
1:B:165:GLU:HG3	3:B:626:HOH:O	1.95	0.66
1:D:255:LYS:NZ	1:D:259:GLU:OE2	2.19	0.65
2:G:301:ZER:C10	2:G:301:ZER:C8P	2.72	0.65
2:E:301:ZER:C10	2:E:301:ZER:C12	2.72	0.65
1:G:6:THR:HG22	3:G:532:HOH:O	1.96	0.65
1:B:196:SER:OG	3:B:401:HOH:O	2.01	0.64
2:G:301:ZER:C11	2:G:301:ZER:C9P	2.73	0.64
1:F:194:PRO:HB2	1:F:195:PRO:HD3	1.80	0.64
2:H:301:ZER:O10	2:H:301:ZER:H1	1.92	0.63
1:H:201:THR:HG23	1:H:232:GLU:OE2	1.99	0.63
2:E:301:ZER:H11	2:E:301:ZER:O10	1.97	0.62
1:F:146:PRO:CD	1:F:187:TYR:OH	2.39	0.62
1:A:194:PRO:HB2	1:A:195:PRO:HD3	1.81	0.61
1:F:160:TYR:CE2	2:F:301:ZER:H15	2.35	0.61
1:G:6:THR:HG21	3:G:471:HOH:O	1.99	0.61
1:E:182:TYR:HB2	1:E:183:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:TYR:CD2	2:F:301:ZER:H18	2.36	0.60
2:F:301:ZER:O10	2:F:301:ZER:H11	2.00	0.60
2:A:301:ZER:C11	2:A:301:ZER:C8P	2.80	0.60
2:B:301:ZER:C8P	2:B:301:ZER:H1	2.30	0.59
2:G:301:ZER:C8P	2:G:301:ZER:H1	2.33	0.59
1:E:121:ARG:HD3	3:E:497:HOH:O	2.00	0.59
2:H:301:ZER:C10	2:H:301:ZER:H22	2.32	0.58
1:F:182:TYR:HB2	1:F:183:PRO:HD3	1.85	0.58
2:C:301:ZER:C12	2:C:301:ZER:C10	2.81	0.58
2:D:301:ZER:H11	2:D:301:ZER:O10	2.03	0.58
2:H:301:ZER:O10	2:H:301:ZER:H11	2.05	0.57
2:G:301:ZER:H11	2:G:301:ZER:O10	2.05	0.57
1:D:144:VAL:HG23	1:D:149:ILE:HG13	1.88	0.56
1:A:160:TYR:CD2	2:A:301:ZER:H18	2.40	0.56
2:C:301:ZER:H11	2:C:301:ZER:O10	2.05	0.56
1:F:146:PRO:HB3	1:F:183:PRO:HB3	1.87	0.56
1:A:227:VAL:CG1	1:A:231:ARG:CZ	2.85	0.55
1:E:201:THR:HG23	1:E:232:GLU:OE2	2.07	0.54
2:H:301:ZER:C10	2:H:301:ZER:C12	2.81	0.54
1:G:118:TYR:N	1:G:119:PRO:CD	2.71	0.54
2:F:301:ZER:C12	2:F:301:ZER:C10	2.77	0.53
1:B:93:THR:HG21	3:B:593:HOH:O	2.07	0.53
1:B:227:VAL:CG1	1:B:231:ARG:NH2	2.72	0.53
1:B:242[B]:ASN:OD1	3:B:402:HOH:O	2.19	0.53
2:B:301:ZER:H11	2:B:301:ZER:O10	2.08	0.52
1:G:158:ARG:CZ	1:G:164:VAL:CG1	2.88	0.52
1:G:196:SER:OG	3:G:401:HOH:O	1.94	0.52
1:C:194:PRO:HB2	1:C:195:PRO:HD3	1.91	0.52
1:G:158:ARG:CZ	1:G:164:VAL:HG11	2.40	0.52
1:G:194:PRO:HB2	1:G:195:PRO:HD3	1.92	0.51
2:A:301:ZER:H3	2:A:301:ZER:H21	1.93	0.51
2:A:301:ZER:H11	2:A:301:ZER:O10	2.11	0.50
1:D:243:HIS:CD2	2:D:301:ZER:H4	2.46	0.50
1:B:87:ILE:HD12	1:B:110:THR:HG21	1.94	0.49
1:F:105:ALA:HB1	2:F:301:ZER:C12	2.41	0.49
1:D:227:VAL:CG1	1:D:231:ARG:CZ	2.90	0.49
1:H:105:ALA:HB1	2:H:301:ZER:C12	2.42	0.49
1:A:227:VAL:CG1	1:A:231:ARG:NH2	2.75	0.49
1:A:105:ALA:HB1	2:A:301:ZER:C12	2.43	0.49
1:D:72:PRO:HA	1:D:75:TYR:CZ	2.47	0.49
1:A:4:THR:N	3:A:409:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HB2	1:D:45:PRO:HD3	1.95	0.48
2:B:301:ZER:H1	2:B:301:ZER:H21	1.94	0.48
2:G:301:ZER:H1	2:G:301:ZER:H21	1.95	0.48
1:D:182:TYR:HB2	1:D:183:PRO:HD3	1.96	0.48
1:F:205:HIS:ND1	3:F:406:HOH:O	2.35	0.48
1:B:227:VAL:HG13	1:B:231:ARG:CZ	2.44	0.47
1:D:9:TYR:OH	3:D:401:HOH:O	2.19	0.47
1:A:182:TYR:HB2	1:A:183:PRO:HD3	1.96	0.47
2:A:301:ZER:H3	2:A:301:ZER:C8P	2.44	0.47
1:C:243:HIS:CD2	2:C:301:ZER:H6	2.48	0.47
1:B:227:VAL:CG1	1:B:231:ARG:CZ	2.92	0.47
1:F:139:LEU:HD23	1:F:140:HIS:NE2	2.29	0.47
1:D:140:HIS:HB3	1:D:143:GLU:OE1	2.15	0.47
2:G:301:ZER:O10	2:G:301:ZER:H1	2.03	0.46
1:F:160:TYR:CE2	2:F:301:ZER:C4P	2.98	0.46
1:G:182:TYR:HB2	1:G:183:PRO:HD3	1.96	0.46
1:D:72:PRO:HA	1:D:75:TYR:CE2	2.50	0.46
1:D:194:PRO:HB2	1:D:195:PRO:HD3	1.97	0.46
2:A:301:ZER:O12	2:A:301:ZER:O2	2.33	0.46
1:E:87:ILE:HD12	1:E:110:THR:HG21	1.98	0.46
1:C:108:ALA:HB1	1:C:130:VAL:HG22	1.97	0.46
1:D:76:GLN:NE2	3:D:405:HOH:O	2.41	0.45
1:B:194:PRO:HB2	1:B:195:PRO:HD3	1.97	0.45
1:C:72:PRO:HA	1:C:75:TYR:CZ	2.51	0.45
1:E:105:ALA:HA	1:E:131:PRO:HD3	1.97	0.45
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.82	0.45
1:H:87:ILE:HD12	1:H:110:THR:HG21	1.98	0.44
1:A:108:ALA:HB1	1:A:130:VAL:HG22	1.99	0.44
1:G:44:LYS:N	1:G:45:PRO:HD2	2.33	0.44
1:D:140:HIS:HD1	1:D:143:GLU:CD	2.21	0.44
1:C:105:ALA:HA	1:C:131:PRO:HD3	1.99	0.44
1:B:102:TRP:CD1	1:B:102:TRP:C	2.91	0.43
1:B:72:PRO:HA	1:B:75:TYR:CZ	2.53	0.43
2:C:301:ZER:O12	2:C:301:ZER:O2	2.26	0.43
1:A:204:LEU:HB3	1:A:234:ILE:HD11	2.00	0.43
1:H:182:TYR:HB2	1:H:183:PRO:HD3	2.00	0.43
1:E:97:LYS:HG3	3:E:564:HOH:O	2.19	0.43
1:B:255:LYS:HE2	1:B:259:GLU:OE2	2.19	0.43
1:D:9:TYR:HA	1:D:18:TRP:O	2.19	0.43
1:F:142:HIS:CD2	1:F:142:HIS:C	2.92	0.43
1:H:44:LYS:HB2	1:H:45:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ALA:HB2	1:D:243:HIS:CE1	2.54	0.42
1:F:145:ASP:OD1	1:F:148:THR:CB	2.67	0.42
2:F:301:ZER:H17	2:F:301:ZER:H1	2.01	0.42
1:G:202:GLU:HG2	3:G:538:HOH:O	2.19	0.42
1:G:144:VAL:HG23	1:G:149:ILE:HG13	2.02	0.42
1:A:160:TYR:CE2	2:A:301:ZER:H18	2.55	0.42
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.87	0.42
1:C:182:TYR:HB2	1:C:183:PRO:HD3	2.02	0.42
1:C:227:VAL:CG1	1:C:231:ARG:CZ	2.98	0.42
1:C:93:THR:HG22	3:C:539:HOH:O	2.19	0.42
2:G:301:ZER:O2	2:G:301:ZER:O12	2.36	0.42
1:E:151:GLN:NE2	3:E:404:HOH:O	2.42	0.41
1:D:221:LEU:HA	1:D:221:LEU:HD12	1.85	0.41
1:C:160:TYR:CD2	2:C:301:ZER:H18	2.55	0.41
1:D:227:VAL:HG13	1:D:231:ARG:CZ	2.50	0.41
1:H:118:TYR:N	1:H:119:PRO:CD	2.84	0.41
2:B:301:ZER:O2	2:B:301:ZER:O12	2.39	0.41
1:E:102:TRP:CD1	1:E:102:TRP:C	2.92	0.41
1:C:218:PRO:HD2	1:C:221:LEU:HD12	2.02	0.41
1:A:72:PRO:HA	1:A:75:TYR:CZ	2.56	0.41
1:E:194:PRO:HB2	1:E:195:PRO:HD3	2.02	0.41
1:H:9:TYR:HA	1:H:18:TRP:O	2.21	0.41
1:A:243:HIS:CD2	2:A:301:ZER:H6	2.56	0.41
1:E:118:TYR:N	1:E:119:PRO:CD	2.84	0.41
1:F:192:THR:O	1:F:196:SER:OG	2.39	0.41
1:G:105:ALA:HB1	2:G:301:ZER:C12	2.51	0.41
1:A:193:ILE:HB	1:A:194:PRO:HD3	2.03	0.40
1:G:108:ALA:HB1	1:G:130:VAL:HG22	2.03	0.40

All (2) 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:B:572:HOH:O	3:E:611:HOH:O[1_455]	2.11	0.09
3:D:466:HOH:O	3:H:559:HOH:O[1_464]	2.16	0.04

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	261/266 (98%)	254 (97%)	6 (2%)	1 (0%)	34	22
1	B	262/266 (98%)	254 (97%)	7 (3%)	1 (0%)	34	22
1	C	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	34	22
1	D	262/266 (98%)	254 (97%)	6 (2%)	2 (1%)	19	9
1	E	261/266 (98%)	254 (97%)	5 (2%)	2 (1%)	19	9
1	F	261/266 (98%)	250 (96%)	9 (3%)	2 (1%)	19	9
1	G	260/266 (98%)	252 (97%)	6 (2%)	2 (1%)	19	9
1	H	262/266 (98%)	254 (97%)	7 (3%)	1 (0%)	34	22
All	All	2090/2128 (98%)	2025 (97%)	53 (2%)	12 (1%)	25	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	147	ALA
1	D	163	ASN
1	G	163	ASN
1	A	189	TYR
1	D	189	TYR
1	E	189	TYR
1	H	189	TYR
1	B	189	TYR
1	C	189	TYR
1	E	163	ASN
1	F	189	TYR
1	G	189	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	223/224 (100%)	221 (99%)	2 (1%)	78	76
1	B	224/224 (100%)	220 (98%)	4 (2%)	59	52
1	C	223/224 (100%)	220 (99%)	3 (1%)	69	64
1	D	223/224 (100%)	217 (97%)	6 (3%)	44	34
1	E	223/224 (100%)	218 (98%)	5 (2%)	52	43
1	F	223/224 (100%)	216 (97%)	7 (3%)	40	29
1	G	222/224 (99%)	215 (97%)	7 (3%)	39	27
1	H	223/224 (100%)	220 (99%)	3 (1%)	69	64
All	All	1784/1792 (100%)	1747 (98%)	37 (2%)	53	45

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	246	TYR
1	B	4	THR
1	B	151	GLN
1	B	225	ASN
1	B	246	TYR
1	C	225	ASN
1	C	246	TYR
1	C	266	LYS
1	D	46	MET
1	D	151	GLN
1	D	221	LEU
1	D	225	ASN
1	D	246	TYR
1	D	266	LYS
1	E	139	LEU
1	E	184	ARG
1	E	202	GLU
1	E	225	ASN
1	E	246	TYR
1	F	13	LYS
1	F	73	GLU
1	F	82	LYS

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Mol	Chain	Res	Type
1	F	196	SER
1	F	225	ASN
1	F	236	ILE
1	F	246	TYR
1	G	5	ARG
1	G	6	THR
1	G	13	LYS
1	G	202	GLU
1	G	221	LEU
1	G	225	ASN
1	G	246	TYR
1	H	46	MET
1	H	225	ASN
1	H	246	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	D	76	GLN
1	F	142	HIS
1	G	134	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	ZER	B	301	-	24,24,24	5.67	9 (37%)	32,32,32	3.51	12 (37%)
2	ZER	F	301	-	24,24,24	2.71	6 (25%)	32,32,32	2.74	7 (21%)
2	ZER	D	301	-	24,24,24	2.62	7 (29%)	32,32,32	2.77	8 (25%)
2	ZER	C	301	-	24,24,24	4.61	6 (25%)	32,32,32	2.17	11 (34%)
2	ZER	A	301	-	24,24,24	5.10	9 (37%)	32,32,32	2.64	13 (40%)
2	ZER	G	301	-	24,24,24	5.30	8 (33%)	32,32,32	3.98	11 (34%)
2	ZER	E	301	-	24,24,24	2.87	9 (37%)	32,32,32	3.89	11 (34%)
2	ZER	H	301	-	24,24,24	4.63	8 (33%)	32,32,32	3.51	7 (21%)

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	B	301	-	-	9/22/22/22	0/1/2/2
2	ZER	F	301	-	-	8/22/22/22	0/1/2/2
2	ZER	D	301	-	-	12/22/22/22	0/1/2/2
2	ZER	C	301	-	-	8/22/22/22	0/1/2/2
2	ZER	A	301	-	-	9/22/22/22	0/1/2/2
2	ZER	G	301	-	-	8/22/22/22	0/1/2/2
2	ZER	E	301	-	-	7/22/22/22	0/1/2/2
2	ZER	H	301	-	-	7/22/22/22	0/1/2/2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ZER	O10-C10	24.93	1.89	1.47
2	G	301	ZER	O10-C10	21.89	1.84	1.47
2	A	301	ZER	O10-C10	21.23	1.83	1.47
2	C	301	ZER	O10-C10	21.05	1.83	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	ZER	O10-C10	19.43	1.80	1.47
2	G	301	ZER	C9P-C10	11.00	1.90	1.52
2	E	301	ZER	O10-C10	10.65	1.65	1.47
2	F	301	ZER	O10-C10	10.22	1.64	1.47
2	D	301	ZER	O10-C10	9.89	1.64	1.47
2	B	301	ZER	C9P-C10	9.29	1.84	1.52
2	A	301	ZER	C8P-C9P	8.21	1.87	1.52
2	H	301	ZER	C9P-C10	6.84	1.76	1.52
2	A	301	ZER	C8P-C7P	5.02	1.70	1.52
2	H	301	ZER	C5P-C6P	-4.83	1.38	1.50
2	A	301	ZER	C9P-C10	-4.53	1.36	1.52
2	G	301	ZER	C8P-C7P	4.17	1.67	1.52
2	E	301	ZER	C9P-C10	4.15	1.66	1.52
2	G	301	ZER	C4P-C5P	4.06	1.67	1.52
2	F	301	ZER	C5P-C6P	-3.82	1.41	1.50
2	F	301	ZER	C9P-C10	3.80	1.65	1.52
2	C	301	ZER	C8P-C7P	3.75	1.66	1.52
2	A	301	ZER	O6P-C6P	3.61	1.27	1.21
2	D	301	ZER	C8P-C7P	3.54	1.65	1.52
2	E	301	ZER	C6-C1P	-3.52	1.41	1.47
2	H	301	ZER	C3-C4	-3.50	1.34	1.39
2	A	301	ZER	C11-C10	3.48	1.64	1.51
2	E	301	ZER	C1P-C2P	3.44	1.42	1.31
2	D	301	ZER	C8P-C9P	3.31	1.66	1.52
2	D	301	ZER	C1-C12	-3.25	1.42	1.50
2	A	301	ZER	C5P-C6P	-3.16	1.43	1.50
2	G	301	ZER	C1P-C2P	3.15	1.41	1.31
2	H	301	ZER	C8P-C7P	3.12	1.63	1.52
2	C	301	ZER	C1-C12	-3.05	1.43	1.50
2	F	301	ZER	C1P-C2P	3.01	1.41	1.31
2	B	301	ZER	O6P-C6P	2.94	1.26	1.21
2	D	301	ZER	C1P-C2P	2.93	1.40	1.31
2	C	301	ZER	C5P-C6P	-2.88	1.43	1.50
2	E	301	ZER	C1-C12	-2.78	1.44	1.50
2	E	301	ZER	C5P-C6P	-2.78	1.43	1.50
2	G	301	ZER	O6P-C6P	2.77	1.26	1.21
2	B	301	ZER	C5P-C6P	-2.76	1.44	1.50
2	G	301	ZER	C6-C1P	-2.65	1.43	1.47
2	F	301	ZER	C7P-C6P	-2.63	1.44	1.50
2	C	301	ZER	C1P-C2P	2.63	1.40	1.31
2	B	301	ZER	C4P-C5P	2.60	1.61	1.52
2	H	301	ZER	C1-C2	-2.52	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ZER	C1P-C2P	2.52	1.39	1.31
2	C	301	ZER	O6P-C6P	2.50	1.26	1.21
2	G	301	ZER	C1-C12	-2.50	1.44	1.50
2	D	301	ZER	O6P-C6P	2.36	1.25	1.21
2	H	301	ZER	C7P-C6P	-2.35	1.45	1.50
2	A	301	ZER	C4P-C5P	2.30	1.60	1.52
2	D	301	ZER	C4P-C5P	2.24	1.60	1.52
2	F	301	ZER	C6-C1P	-2.24	1.43	1.47
2	E	301	ZER	C1-C6	2.23	1.45	1.42
2	B	301	ZER	C1-C12	-2.21	1.45	1.50
2	B	301	ZER	C1P-C2P	2.20	1.38	1.31
2	B	301	ZER	O4-C4	-2.20	1.31	1.37
2	E	301	ZER	O2-C2	2.10	1.40	1.36
2	H	301	ZER	C1P-C2P	2.08	1.38	1.31
2	B	301	ZER	C3-C2	-2.08	1.36	1.38
2	E	301	ZER	O6P-C6P	2.02	1.25	1.21

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	ZER	O10-C10-C9P	14.55	137.18	106.85
2	G	301	ZER	O10-C10-C9P	14.13	136.29	106.85
2	B	301	ZER	O10-C10-C9P	14.08	136.19	106.85
2	G	301	ZER	C10-O10-C12	12.53	139.40	117.61
2	E	301	ZER	C3P-C2P-C1P	12.47	148.95	125.45
2	E	301	ZER	C6-C1P-C2P	12.28	152.02	125.52
2	F	301	ZER	C10-O10-C12	10.68	136.18	117.61
2	B	301	ZER	C10-O10-C12	9.49	134.11	117.61
2	D	301	ZER	O10-C10-C9P	8.12	123.77	106.85
2	A	301	ZER	O10-C10-C9P	7.90	123.32	106.85
2	F	301	ZER	O10-C10-C9P	7.42	122.32	106.85
2	E	301	ZER	C10-O10-C12	7.07	129.89	117.61
2	E	301	ZER	O10-C10-C9P	6.69	120.79	106.85
2	H	301	ZER	C10-O10-C12	6.42	128.76	117.61
2	H	301	ZER	C9P-C8P-C7P	6.37	130.66	113.36
2	H	301	ZER	C5P-C4P-C3P	-6.25	102.09	113.23
2	D	301	ZER	C9P-C8P-C7P	6.23	130.27	113.36
2	C	301	ZER	O10-C10-C9P	6.20	119.76	106.85
2	D	301	ZER	C10-O10-C12	5.82	127.73	117.61
2	G	301	ZER	C7P-C6P-C5P	5.75	127.89	116.98
2	D	301	ZER	C11-C10-C9P	-5.32	99.62	113.97
2	D	301	ZER	O10-C10-C11	5.12	119.63	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	ZER	C5P-C4P-C3P	-5.08	104.17	113.23
2	G	301	ZER	C8P-C7P-C6P	-5.03	101.67	114.60
2	A	301	ZER	C5P-C4P-C3P	-5.00	104.31	113.23
2	G	301	ZER	C9P-C8P-C7P	4.75	126.25	113.36
2	E	301	ZER	O10-C12-O12	-4.74	115.80	123.53
2	B	301	ZER	C8P-C7P-C6P	-4.51	103.00	114.60
2	A	301	ZER	C9P-C8P-C7P	4.46	125.46	113.36
2	C	301	ZER	C6-C5-C4	4.23	125.43	120.94
2	C	301	ZER	C5P-C4P-C3P	-4.20	105.74	113.23
2	A	301	ZER	C2-C3-C4	-4.18	115.92	119.70
2	A	301	ZER	C11-C10-C9P	-4.16	102.74	113.97
2	A	301	ZER	C10-O10-C12	-4.06	110.54	117.61
2	B	301	ZER	C9P-C8P-C7P	4.06	124.37	113.36
2	G	301	ZER	C6-C1P-C2P	3.71	133.53	125.52
2	H	301	ZER	C11-C10-C9P	-3.57	104.32	113.97
2	H	301	ZER	C8P-C9P-C10	-3.57	100.43	115.34
2	F	301	ZER	C9P-C8P-C7P	3.28	122.27	113.36
2	C	301	ZER	C11-C10-C9P	-3.13	105.53	113.97
2	A	301	ZER	C3-C2-C1	3.11	124.55	120.93
2	C	301	ZER	C5-C6-C1	-3.07	116.04	119.99
2	A	301	ZER	C5-C6-C1	-3.06	116.06	119.99
2	E	301	ZER	O10-C12-C1	3.05	121.10	113.33
2	B	301	ZER	C6-C1P-C2P	3.01	132.01	125.52
2	D	301	ZER	C8P-C9P-C10	-2.99	102.85	115.34
2	G	301	ZER	C5P-C4P-C3P	-2.93	108.01	113.23
2	B	301	ZER	C11-C10-C9P	-2.90	106.15	113.97
2	C	301	ZER	C6-C1P-C2P	2.86	131.69	125.52
2	C	301	ZER	C8P-C7P-C6P	-2.84	107.30	114.60
2	G	301	ZER	O6P-C6P-C5P	-2.80	114.04	121.44
2	D	301	ZER	C6-C1P-C2P	2.79	131.53	125.52
2	A	301	ZER	C3P-C2P-C1P	2.74	130.61	125.45
2	E	301	ZER	C9P-C8P-C7P	2.74	120.79	113.36
2	C	301	ZER	O10-C12-C1	2.67	120.12	113.33
2	C	301	ZER	C3-C2-C1	2.65	124.02	120.93
2	A	301	ZER	C6-C1P-C2P	2.65	131.23	125.52
2	G	301	ZER	C8P-C9P-C10	-2.60	104.47	115.34
2	B	301	ZER	C7P-C6P-C5P	2.53	121.79	116.98
2	C	301	ZER	C10-O10-C12	2.51	121.97	117.61
2	B	301	ZER	O10-C12-O12	-2.50	119.45	123.53
2	C	301	ZER	O2-C2-C1	-2.43	116.59	121.14
2	B	301	ZER	C6-C1-C2	-2.40	116.58	118.91
2	F	301	ZER	C6-C1P-C2P	2.38	130.65	125.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	ZER	O10-C10-C11	2.33	113.27	107.93
2	B	301	ZER	C8P-C9P-C10	-2.31	105.69	115.34
2	G	301	ZER	C11-C10-C9P	-2.31	107.74	113.97
2	E	301	ZER	C8P-C7P-C6P	2.28	120.45	114.60
2	F	301	ZER	C4P-C3P-C2P	-2.25	99.56	112.43
2	H	301	ZER	C3-C2-C1	2.24	123.54	120.93
2	A	301	ZER	O2-C2-C1	-2.24	116.96	121.14
2	E	301	ZER	C8P-C9P-C10	-2.20	106.14	115.34
2	B	301	ZER	C4P-C3P-C2P	2.19	125.00	112.43
2	E	301	ZER	C4P-C5P-C6P	-2.16	109.03	114.60
2	D	301	ZER	C5P-C4P-C3P	-2.12	109.45	113.23
2	A	301	ZER	O10-C10-C11	2.10	112.74	107.93
2	A	301	ZER	C6-C5-C4	2.10	123.17	120.94
2	B	301	ZER	C6-C5-C4	2.02	123.08	120.94
2	G	301	ZER	C3P-C2P-C1P	-2.00	121.68	125.45
2	F	301	ZER	C8P-C9P-C10	-2.00	106.98	115.34

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	ZER	O12-C12-O10-C10
2	B	301	ZER	C1-C12-O10-C10
2	F	301	ZER	O12-C12-O10-C10
2	F	301	ZER	C1-C12-O10-C10
2	D	301	ZER	O12-C12-O10-C10
2	D	301	ZER	C1-C12-O10-C10
2	D	301	ZER	C9P-C10-O10-C12
2	D	301	ZER	O10-C10-C9P-C8P
2	D	301	ZER	C7P-C8P-C9P-C10
2	C	301	ZER	C1-C12-O10-C10
2	C	301	ZER	C11-C10-O10-C12
2	A	301	ZER	C1-C12-O10-C10
2	A	301	ZER	C11-C10-O10-C12
2	G	301	ZER	O12-C12-O10-C10
2	G	301	ZER	C1-C12-O10-C10
2	E	301	ZER	O12-C12-O10-C10
2	E	301	ZER	C1-C12-O10-C10
2	E	301	ZER	C9P-C10-O10-C12
2	E	301	ZER	C6-C1P-C2P-C3P
2	H	301	ZER	O12-C12-O10-C10
2	H	301	ZER	C1-C12-O10-C10

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Mol	Chain	Res	Type	Atoms
2	C	301	ZER	O12-C12-O10-C10
2	H	301	ZER	C6P-C7P-C8P-C9P
2	A	301	ZER	O12-C12-O10-C10
2	F	301	ZER	C6P-C7P-C8P-C9P
2	H	301	ZER	C9P-C10-O10-C12
2	D	301	ZER	C11-C10-C9P-C8P
2	H	301	ZER	O10-C10-C9P-C8P
2	E	301	ZER	C3P-C4P-C5P-C6P
2	D	301	ZER	C2P-C3P-C4P-C5P
2	C	301	ZER	C2P-C3P-C4P-C5P
2	F	301	ZER	C9P-C10-O10-C12
2	B	301	ZER	C2P-C3P-C4P-C5P
2	F	301	ZER	C2P-C3P-C4P-C5P
2	A	301	ZER	C2P-C3P-C4P-C5P
2	E	301	ZER	C1P-C2P-C3P-C4P
2	G	301	ZER	C2P-C3P-C4P-C5P
2	F	301	ZER	O10-C10-C9P-C8P
2	E	301	ZER	O10-C10-C9P-C8P
2	A	301	ZER	C3P-C4P-C5P-C6P
2	A	301	ZER	C6P-C7P-C8P-C9P
2	B	301	ZER	C11-C10-C9P-C8P
2	B	301	ZER	C3P-C4P-C5P-C6P
2	B	301	ZER	C5P-C6P-C7P-C8P
2	C	301	ZER	C11-C10-C9P-C8P
2	C	301	ZER	C6P-C7P-C8P-C9P
2	H	301	ZER	C7P-C8P-C9P-C10
2	B	301	ZER	C9P-C10-O10-C12
2	H	301	ZER	C2P-C3P-C4P-C5P
2	D	301	ZER	C6P-C7P-C8P-C9P
2	D	301	ZER	C5P-C6P-C7P-C8P
2	G	301	ZER	C11-C10-C9P-C8P
2	C	301	ZER	O10-C10-C9P-C8P
2	A	301	ZER	C7P-C8P-C9P-C10
2	D	301	ZER	O6P-C6P-C7P-C8P
2	D	301	ZER	C1P-C2P-C3P-C4P
2	D	301	ZER	C3P-C4P-C5P-C6P
2	F	301	ZER	C5P-C6P-C7P-C8P
2	A	301	ZER	C5P-C6P-C7P-C8P
2	G	301	ZER	C7P-C8P-C9P-C10
2	G	301	ZER	C5P-C6P-C7P-C8P
2	B	301	ZER	O6P-C6P-C7P-C8P
2	F	301	ZER	O6P-C6P-C7P-C8P

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Mol	Chain	Res	Type	Atoms
2	B	301	ZER	C7P-C8P-C9P-C10
2	G	301	ZER	C3P-C4P-C5P-C6P
2	C	301	ZER	O6P-C6P-C7P-C8P
2	A	301	ZER	O6P-C6P-C7P-C8P
2	G	301	ZER	O6P-C6P-C7P-C8P

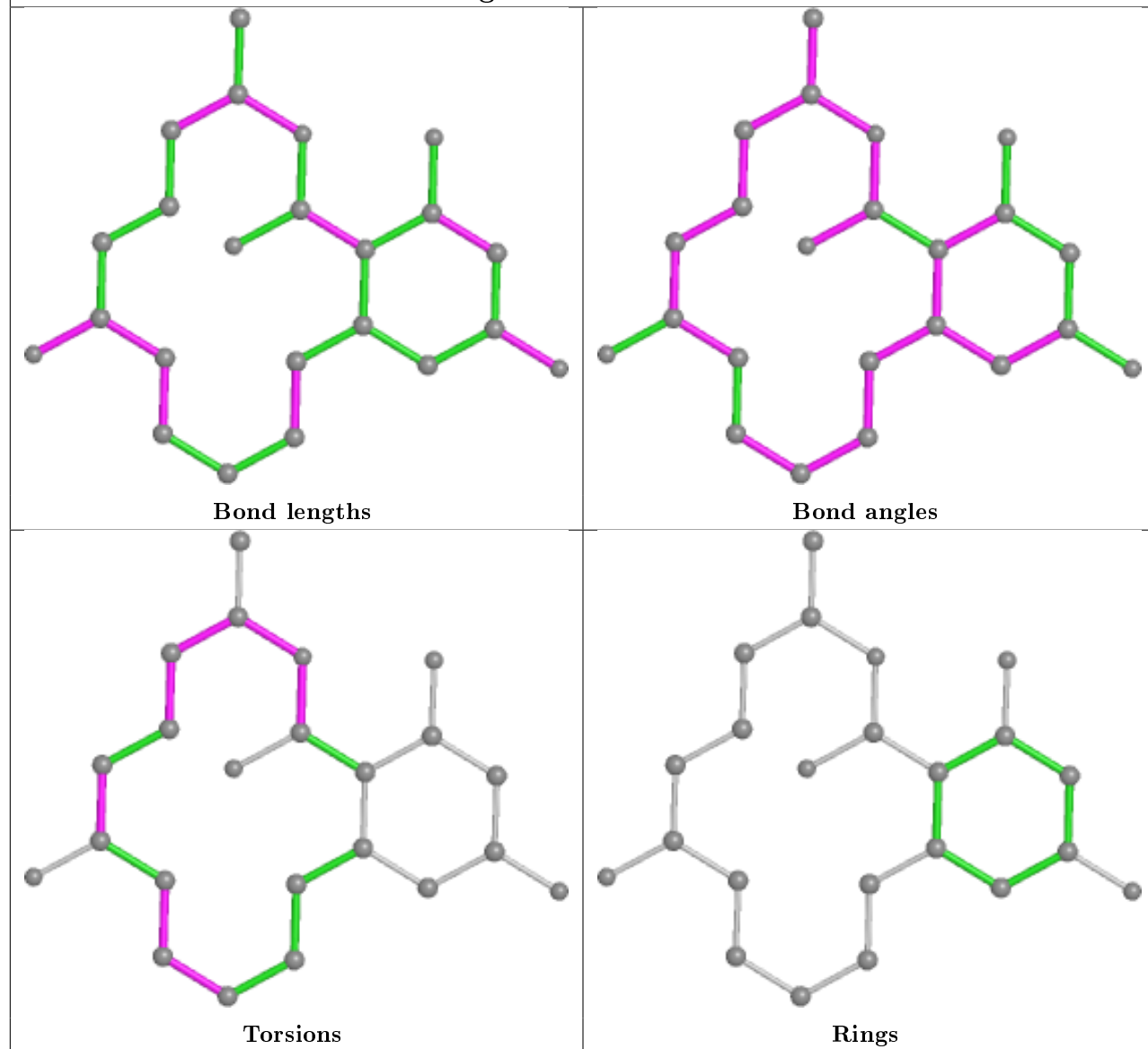
There are no ring outliers.

8 monomers are involved in 65 short contacts:

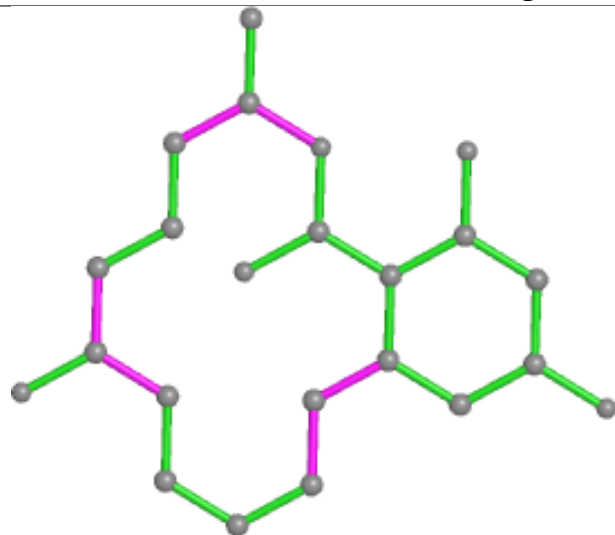
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ZER	9	0
2	F	301	ZER	8	0
2	D	301	ZER	5	0
2	C	301	ZER	6	0
2	A	301	ZER	13	0
2	G	301	ZER	11	0
2	E	301	ZER	3	0
2	H	301	ZER	10	0

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.

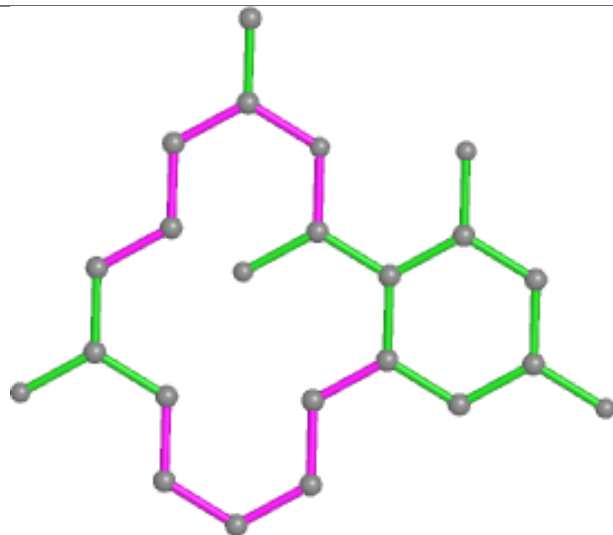
Ligand ZER B 301



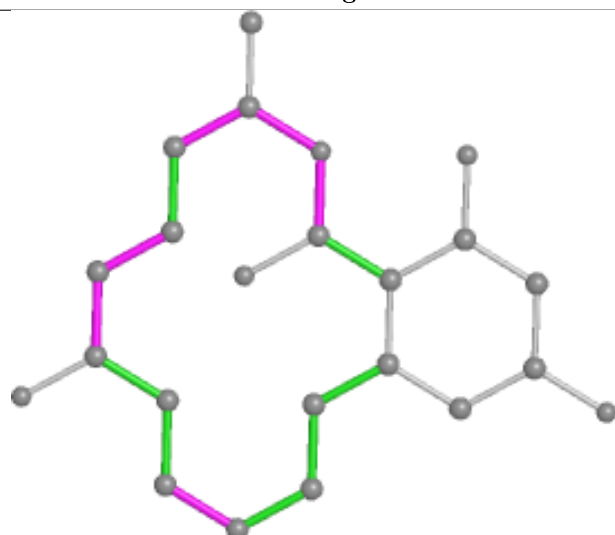
Ligand ZER F 301



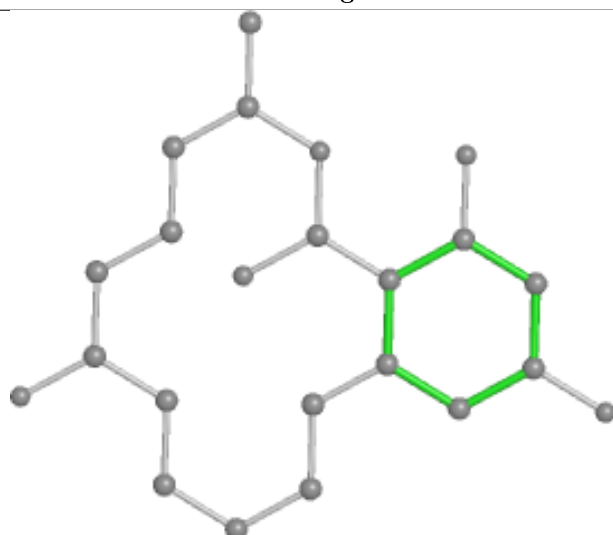
Bond lengths



Bond angles

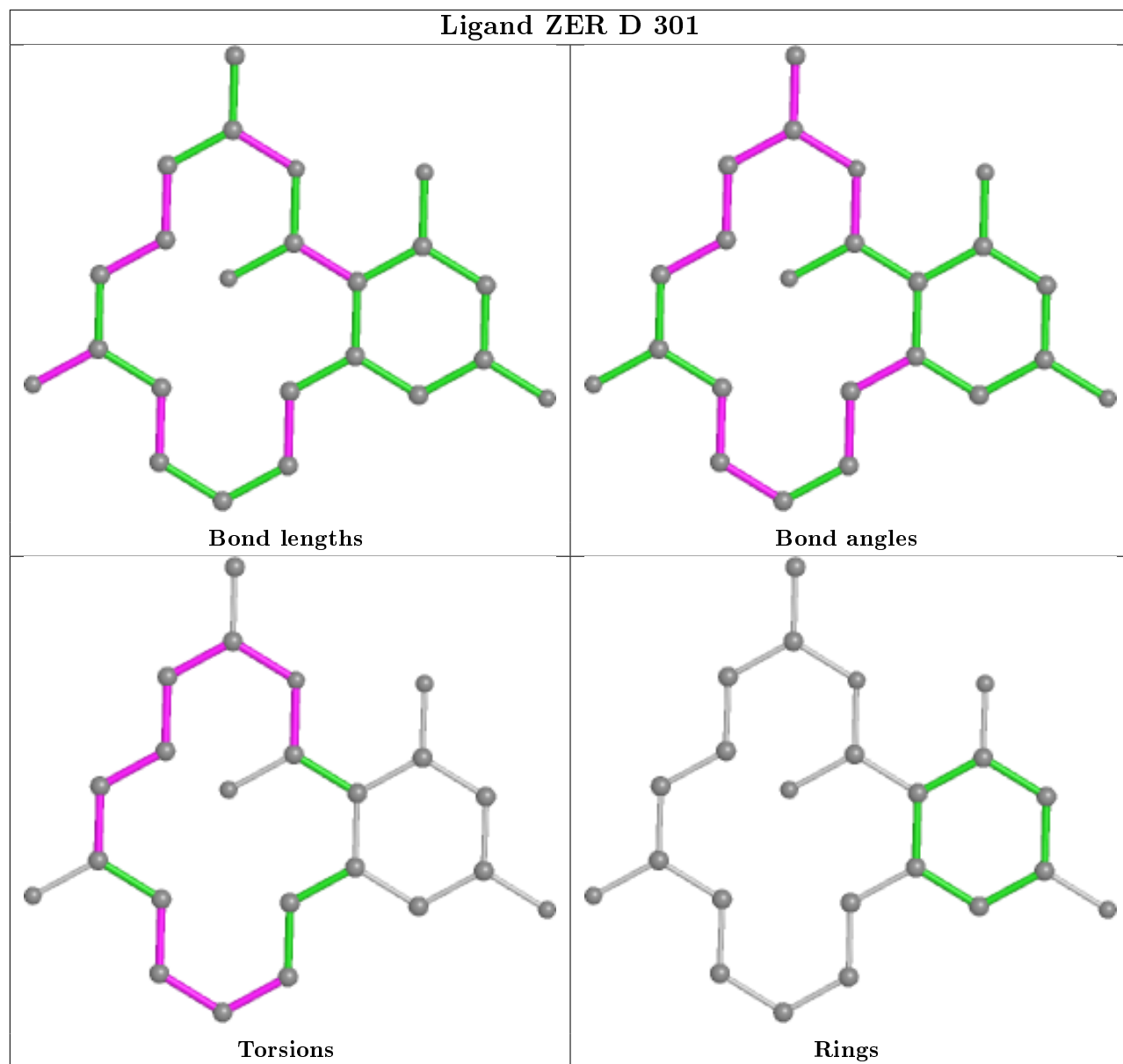


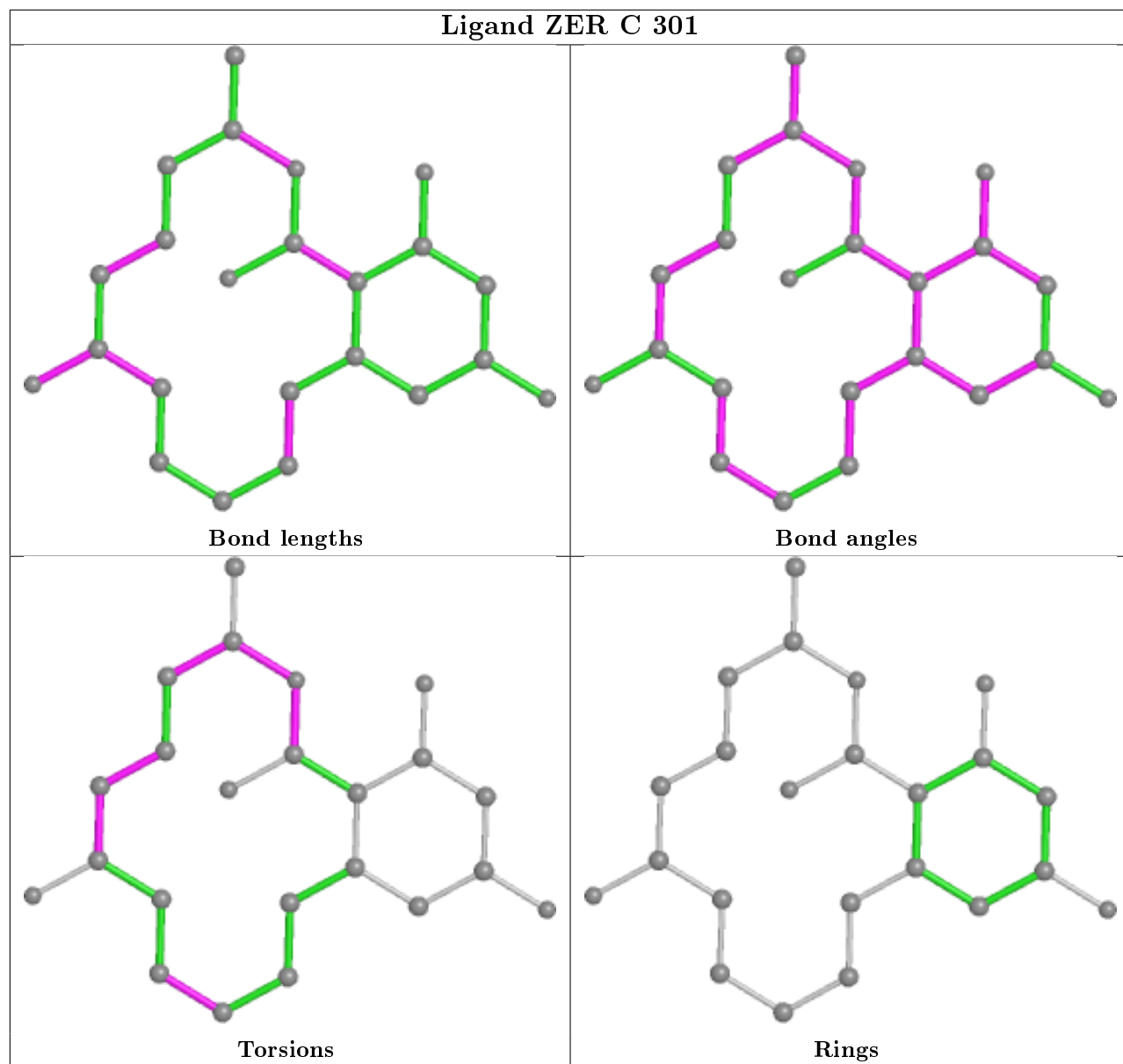
Torsions

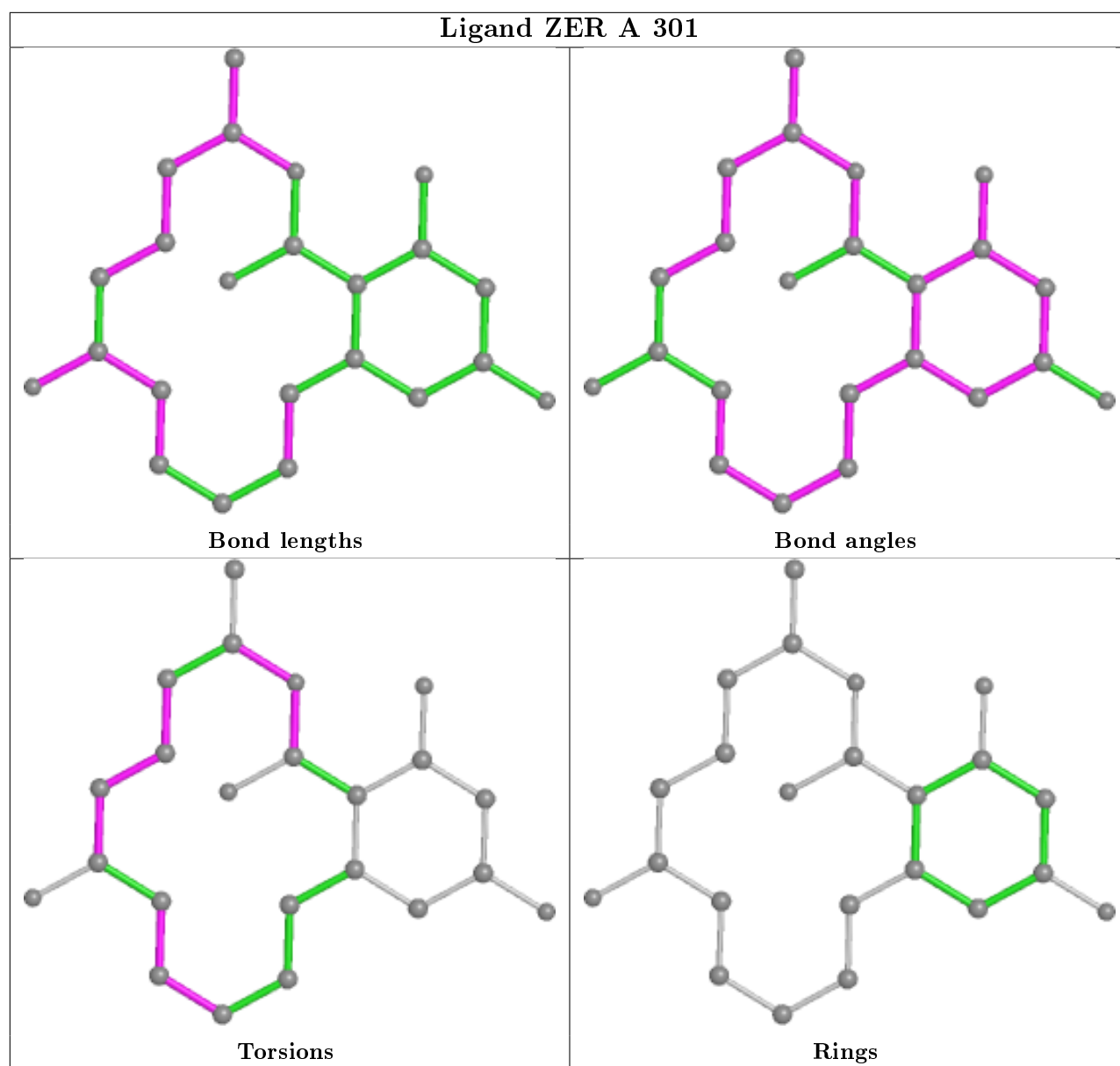


Rings

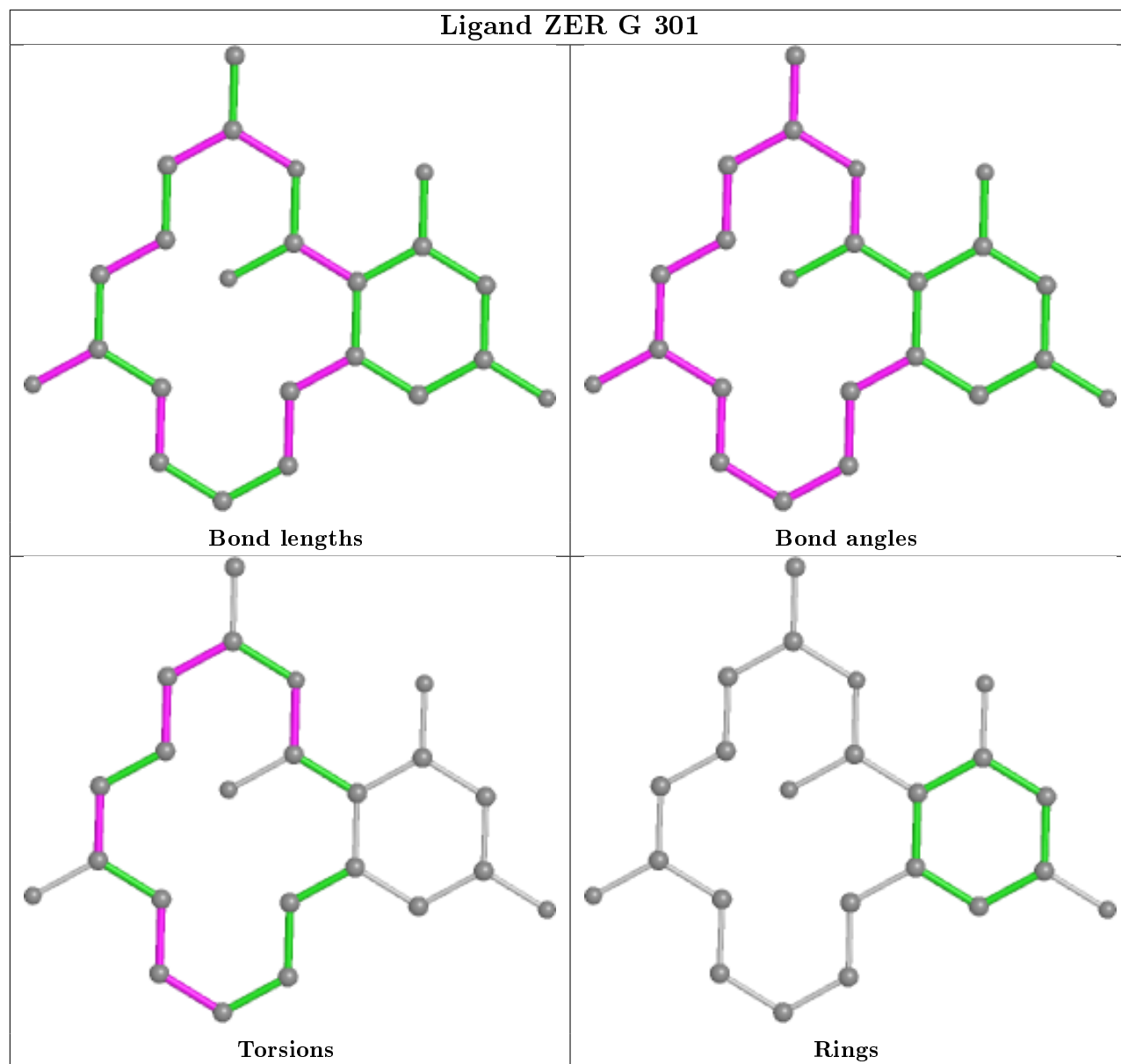
Ligand ZER D 301



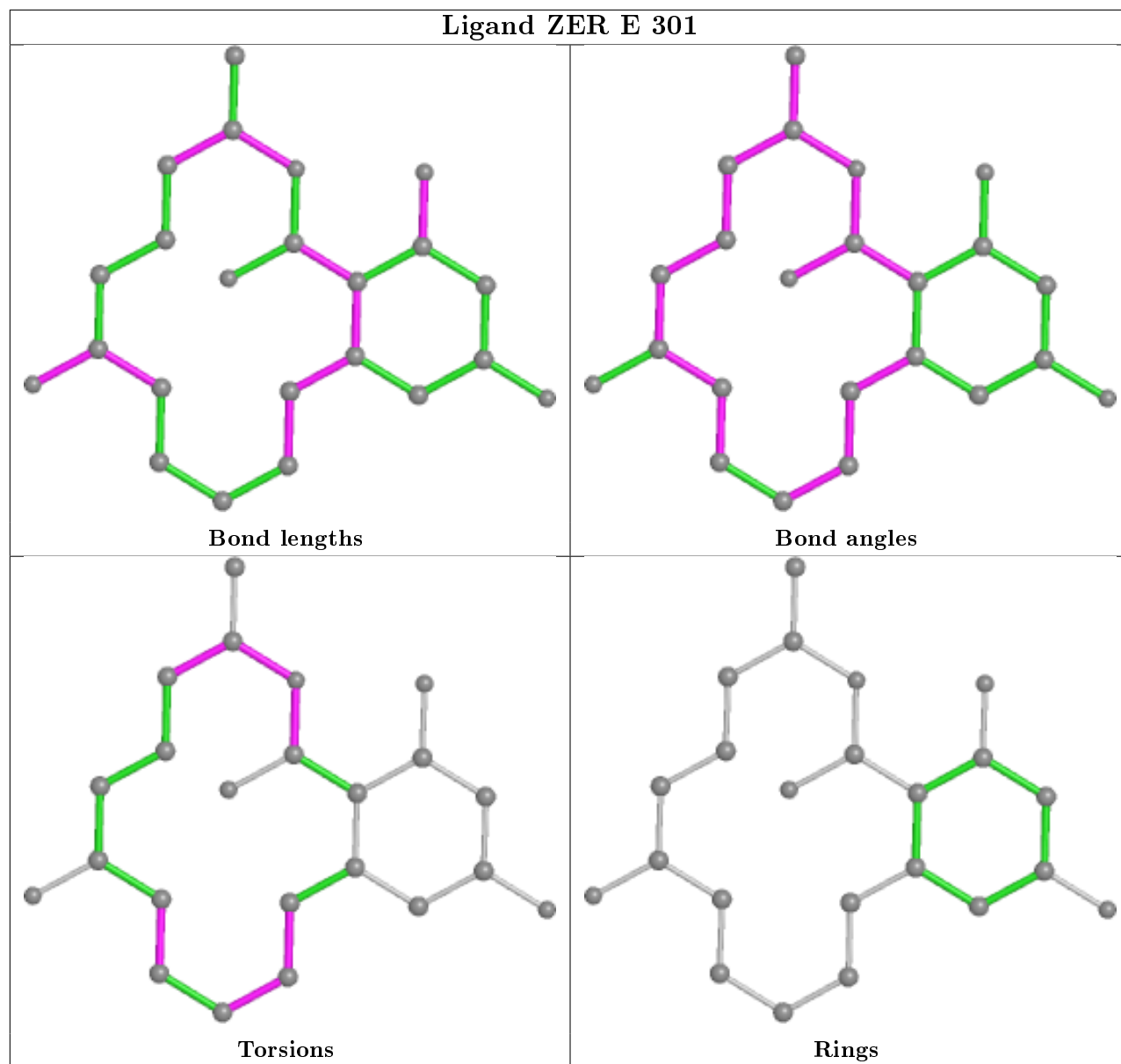


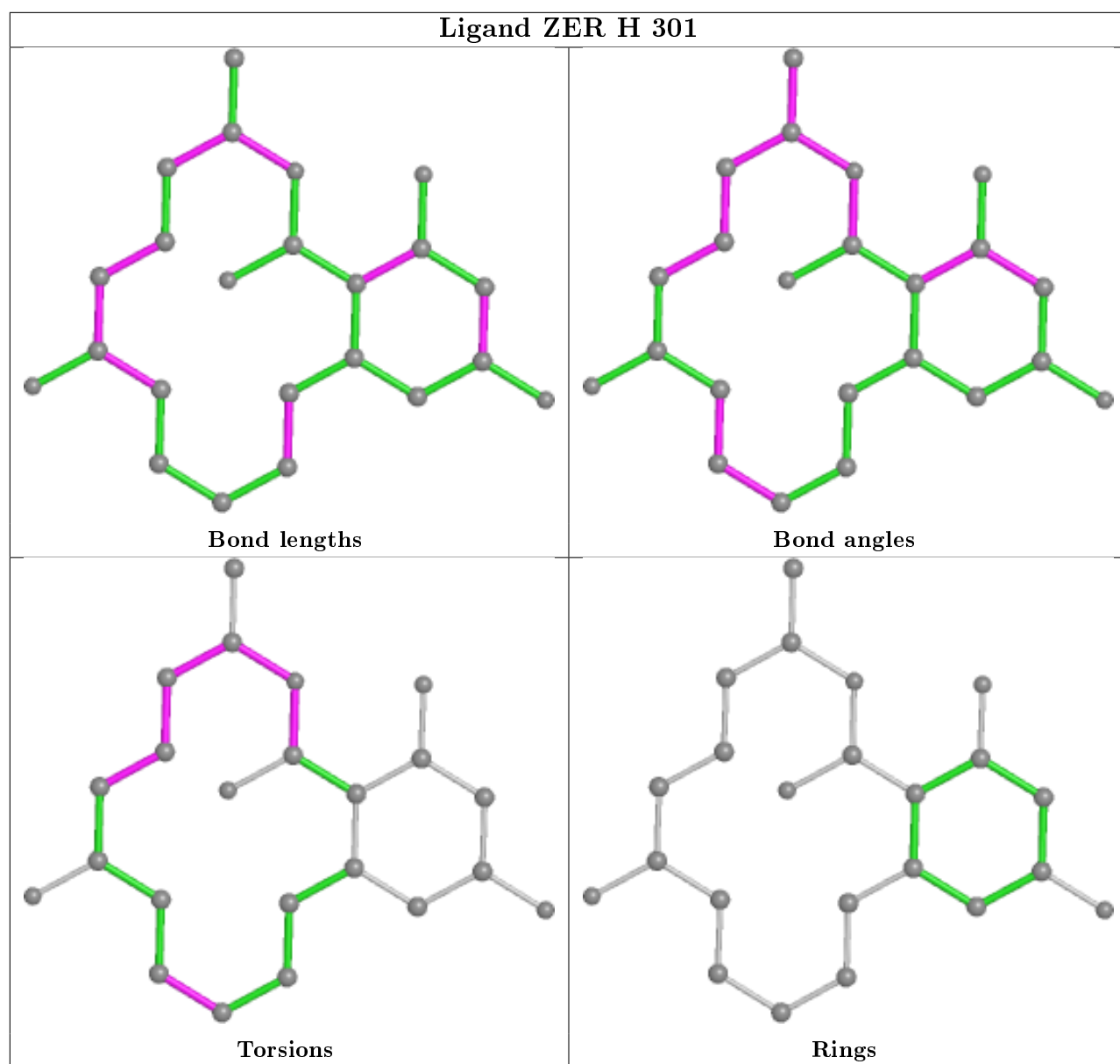


Ligand ZER G 301



Ligand ZER E 301





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	263/266 (98%)	-0.39	1 (0%) 92 93	14, 20, 32, 49	0
1	B	263/266 (98%)	-0.39	0 100 100	14, 21, 33, 48	0
1	C	263/266 (98%)	-0.24	6 (2%) 60 62	15, 24, 41, 73	0
1	D	264/266 (99%)	-0.12	7 (2%) 54 56	16, 24, 43, 62	0
1	E	263/266 (98%)	-0.02	3 (1%) 80 82	19, 27, 43, 57	0
1	F	263/266 (98%)	0.42	21 (7%) 12 13	19, 33, 59, 71	0
1	G	262/266 (98%)	-0.20	1 (0%) 92 93	18, 26, 37, 50	0
1	H	263/266 (98%)	-0.27	1 (0%) 92 93	16, 23, 35, 56	0
All	All	2104/2128 (98%)	-0.15	40 (1%) 66 68	14, 24, 43, 73	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	148	THR	5.4
1	F	139	LEU	4.8
1	F	72	PRO	3.9
1	F	36	LEU	3.7
1	F	140	HIS	3.4
1	D	3	ALA	3.4
1	F	32	ILE	3.3
1	C	266	LYS	3.2
1	F	16	ILE	3.2
1	F	136	ASP	3.2
1	H	3	ALA	3.1
1	F	31	LEU	3.0
1	D	139	LEU	2.8
1	E	139	LEU	2.8
1	F	151	GLN	2.8
1	F	143	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	33	PRO	2.8
1	F	75	TYR	2.7
1	F	146	PRO	2.6
1	D	36	LEU	2.6
1	F	73	GLU	2.5
1	C	36	LEU	2.5
1	F	97	LYS	2.5
1	E	32	ILE	2.4
1	E	140	HIS	2.4
1	F	144	VAL	2.4
1	D	266	LYS	2.3
1	C	144	VAL	2.3
1	D	140	HIS	2.3
1	C	35	GLY	2.3
1	F	14	ASP	2.3
1	D	160	TYR	2.2
1	C	140	HIS	2.2
1	D	136	ASP	2.2
1	F	164	VAL	2.1
1	F	141	ILE	2.1
1	G	32	ILE	2.1
1	C	151	GLN	2.1
1	A	4	THR	2.0
1	F	145	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

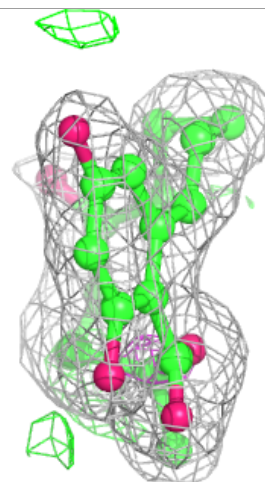
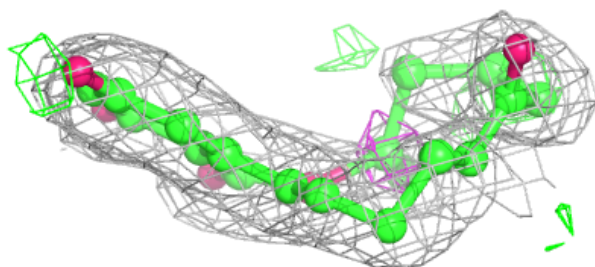
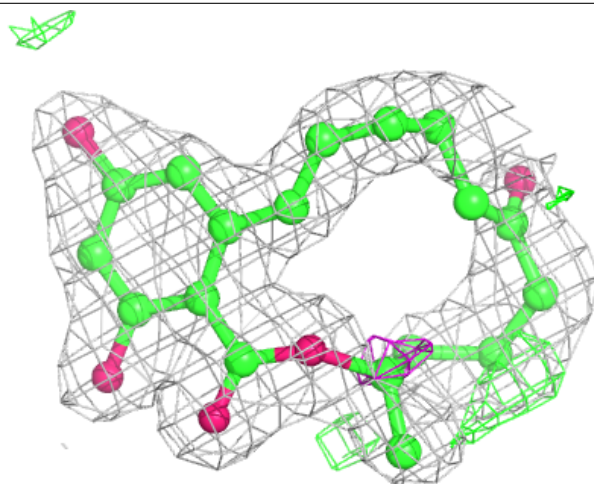
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZER	F	301	23/23	0.89	0.21	30,37,63,70	0
2	ZER	G	301	23/23	0.91	0.15	19,23,43,48	0
2	ZER	A	301	23/23	0.92	0.16	15,22,33,36	0
2	ZER	E	301	23/23	0.92	0.20	24,27,52,56	0
2	ZER	B	301	23/23	0.94	0.17	16,22,52,61	0
2	ZER	D	301	23/23	0.94	0.17	17,26,50,56	0
2	ZER	C	301	23/23	0.94	0.18	19,26,45,47	0
2	ZER	H	301	23/23	0.95	0.13	16,20,35,37	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.

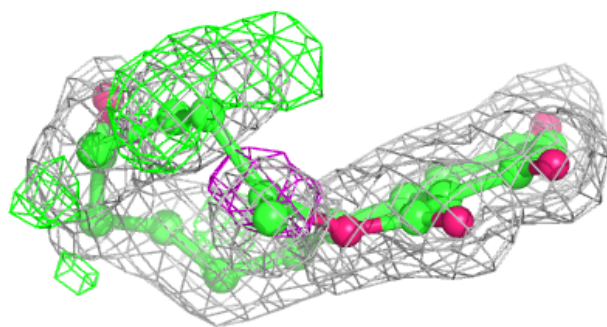
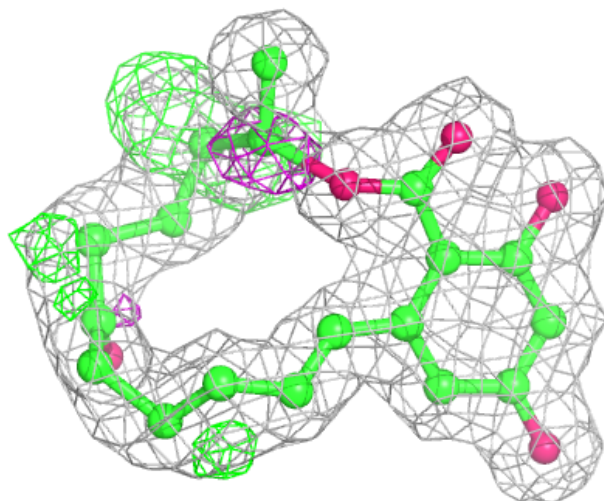
Electron density around ZER F 301:

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



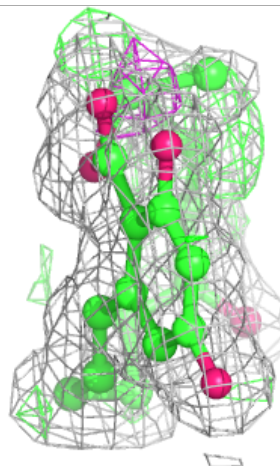
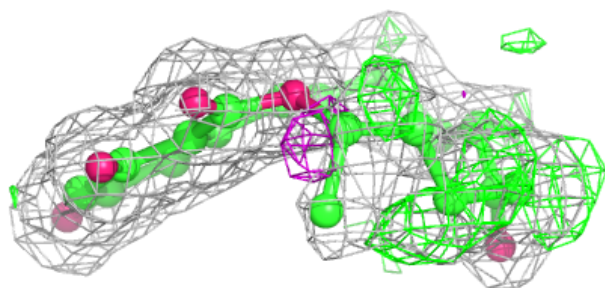
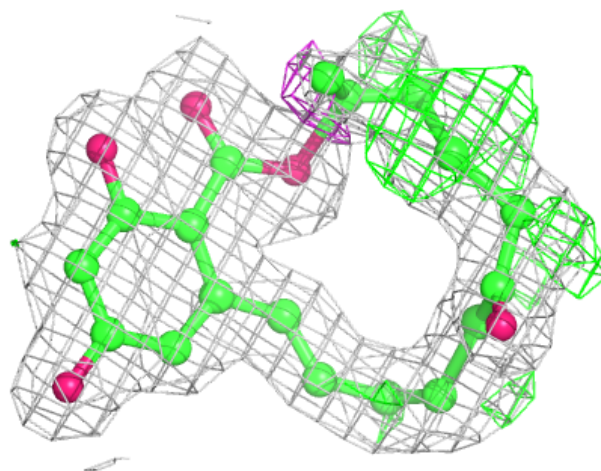
Electron density around ZER G 301:

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



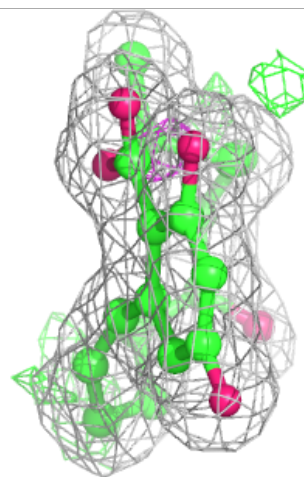
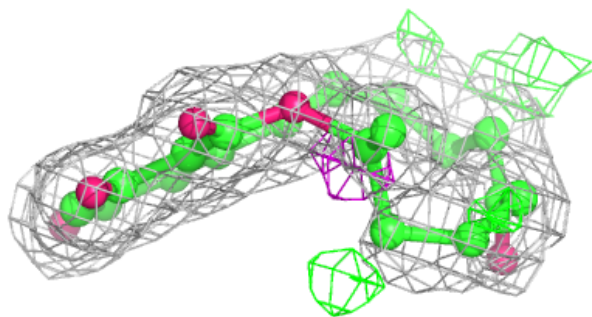
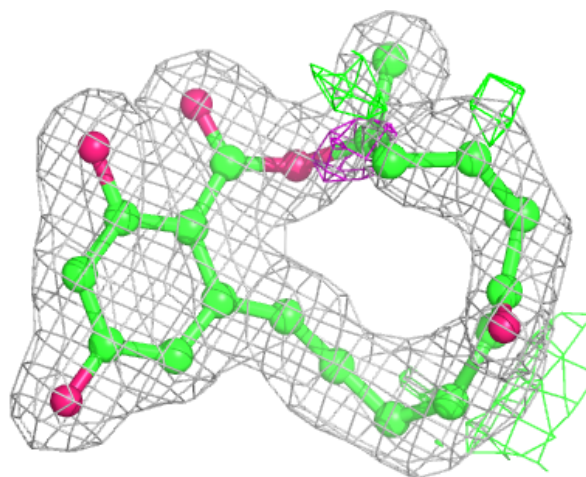
Electron density around ZER A 301:

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and green (positive)



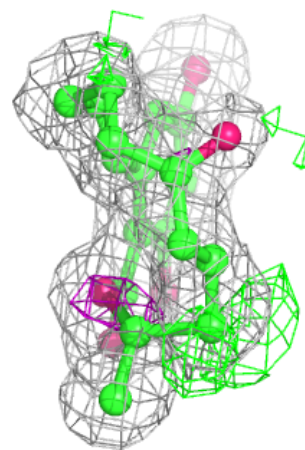
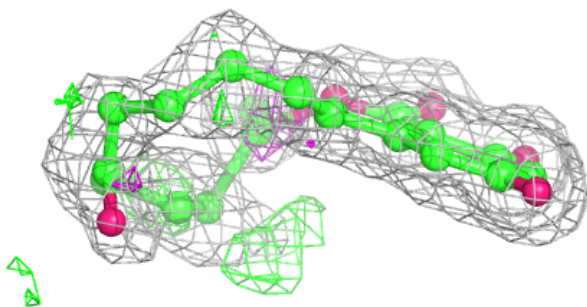
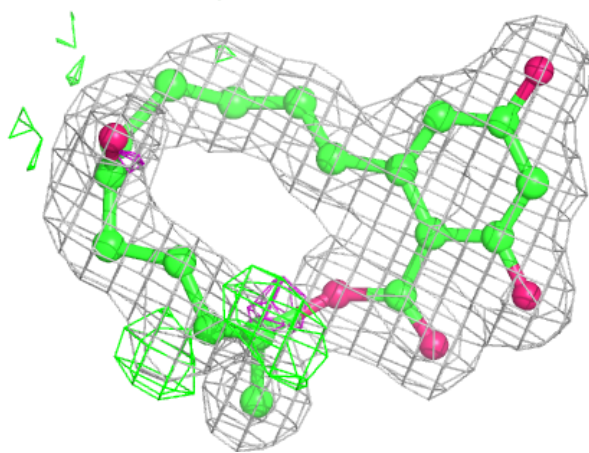
Electron density around ZER E 301:

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



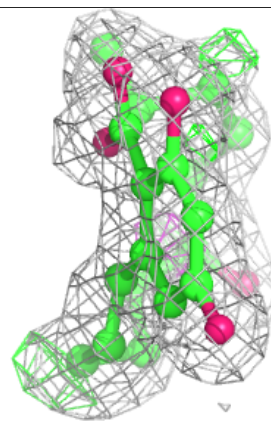
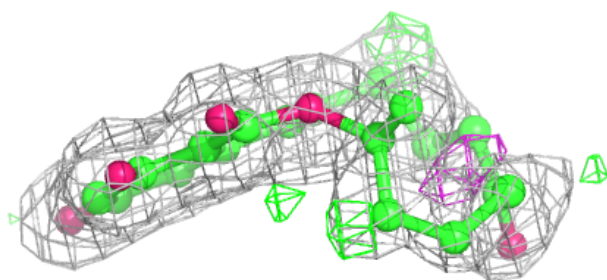
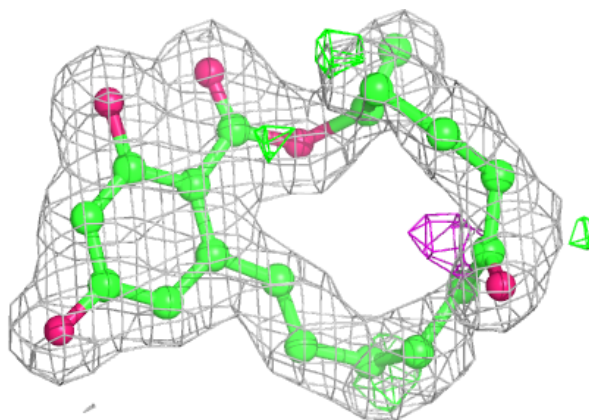
Electron density around ZER B 301:

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



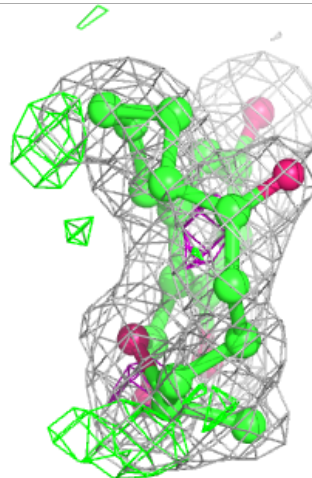
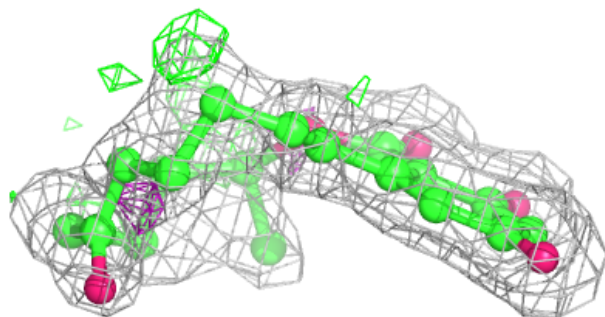
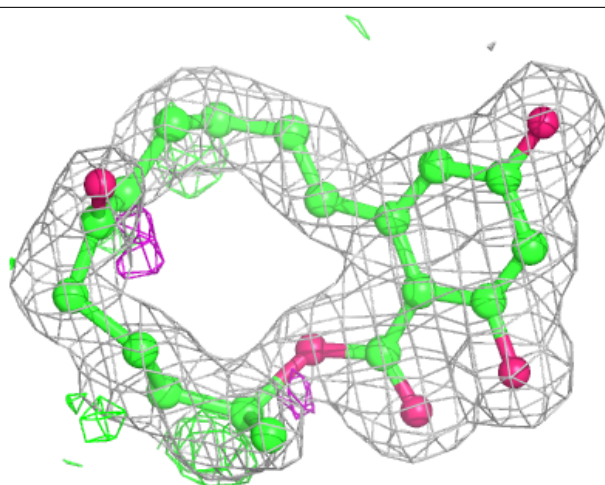
Electron density around ZER D 301:

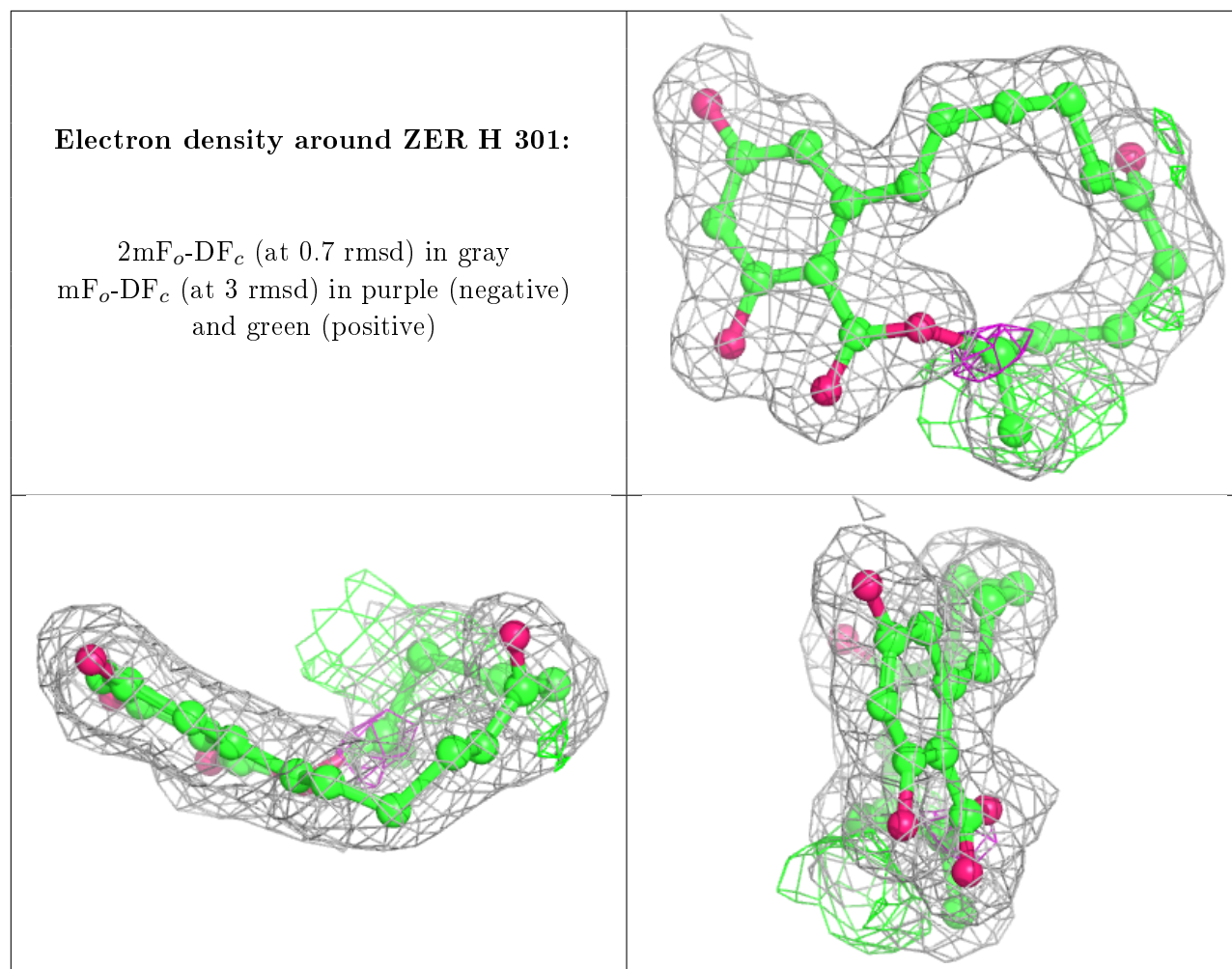
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZER C 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.