



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:00 PM UTC

PDB ID : 5IE7 / pdb_00005ie7
Title : Crystal structure of a lactonase double mutant in complex with substrate b
Authors : Zheng, Y.Y.; Xu, Z.X.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2016-02-25
Resolution : 2.50 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

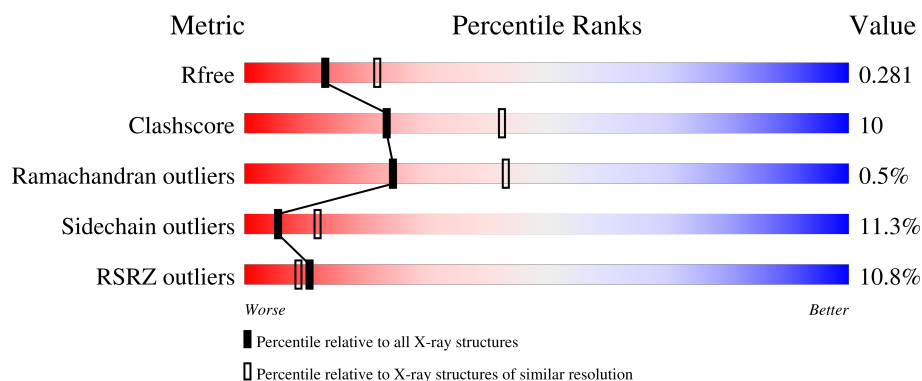
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	264	 80% 18% .
1	B	264	 78% 18% .
1	C	264	 26% 28% 17% 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5464 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.

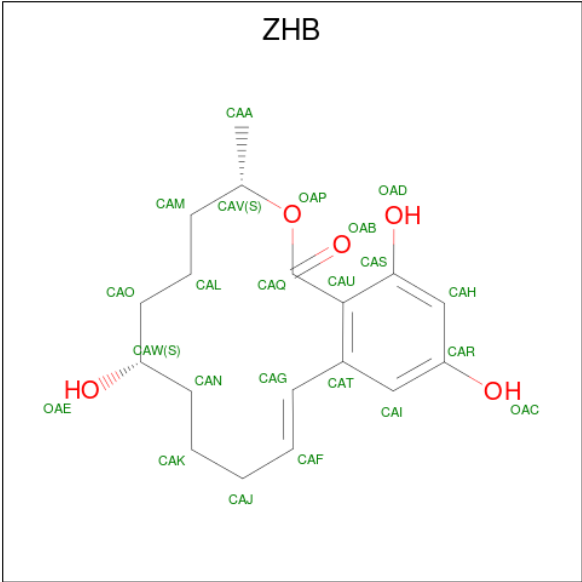
- Molecule 1 is a protein called Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2023	C 1283	N 343	O 386	S 11	0	0	0
1	B	264	Total 2023	C 1283	N 343	O 386	S 11	0	0	0
1	C	129	Total 988	C 632	N 160	O 191	S 5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	SER	engineered mutation	UNP Q8NKB0
A	153	HIS	VAL	engineered mutation	UNP Q8NKB0
B	102	ALA	SER	engineered mutation	UNP Q8NKB0
B	153	HIS	VAL	engineered mutation	UNP Q8NKB0
C	102	ALA	SER	engineered mutation	UNP Q8NKB0
C	153	HIS	VAL	engineered mutation	UNP Q8NKB0

- Molecule 2 is (3S,7S,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (CCD ID: ZHB) (formula: C₁₈H₂₄O₅).



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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	119	Total	O	0	0
			119	119		
3	C	112	Total	O	0	0
			112	112		

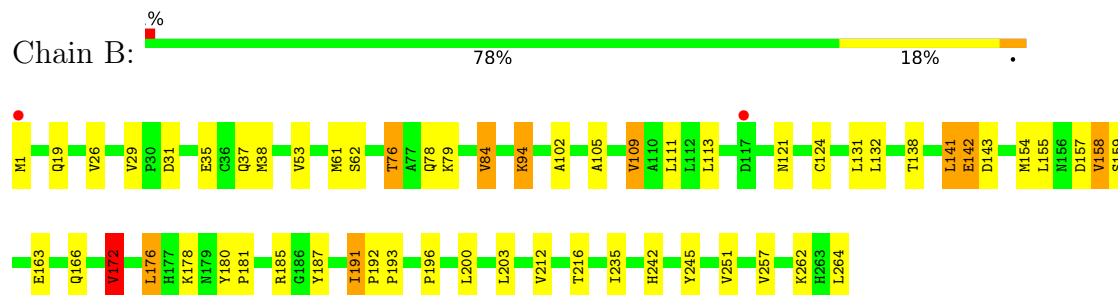
3 Residue-property plots

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

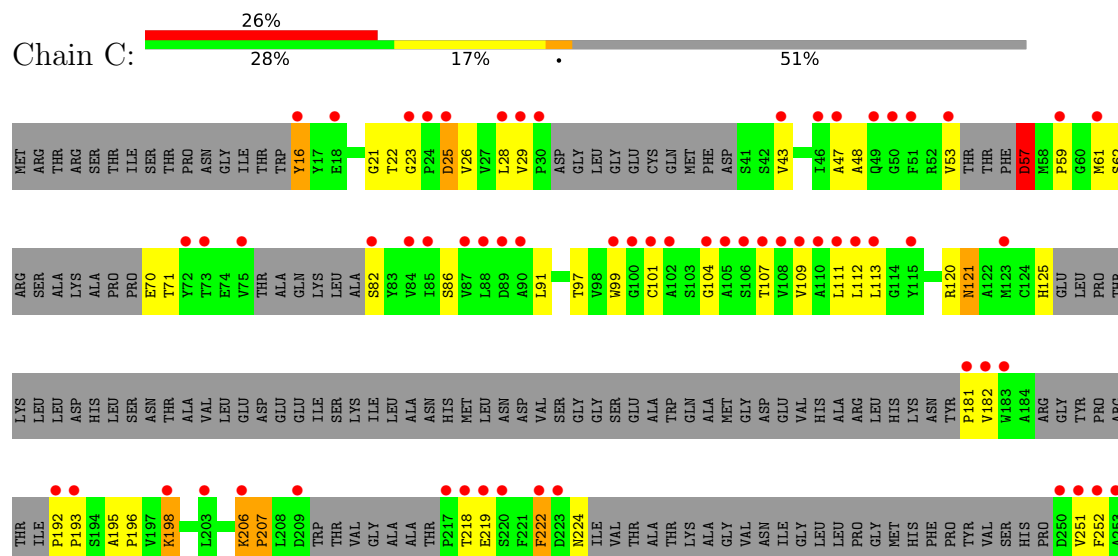
• Molecule 1: Zearalenone hydrolase



• Molecule 1: Zearalenone hydrolase



• Molecule 1: Zearalenone hydrolase



K254	Y255	V256	V257	E258	T259	T260	Q261	K262	H263	L264
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.41 Å 86.41 Å 470.45 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.50) 99.6 (25.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.50 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.217 , 0.289 (Not available) , 0.281	Depositor DCC
R_{free} test set	1870 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5464	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZHB

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	0.76	0/2075	0.96	2/2834 (0.1%)
1	B	0.74	0/2075	1.00	2/2834 (0.1%)
1	C	0.67	0/1006	0.90	2/1361 (0.1%)
All	All	0.73	0/5156	0.97	6/7029 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	VAL	N-CA-CB	-7.15	102.87	112.16
1	B	29	VAL	N-CA-C	6.27	114.03	108.63
1	C	23	GLY	CA-C-N	6.07	126.39	119.83
1	C	23	GLY	C-N-CA	6.07	126.39	119.83
1	B	172	VAL	N-CA-CB	5.48	118.80	110.58
1	A	13	ILE	CB-CA-C	-5.41	103.36	110.98

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	ASP	Peptide
1	C	181	PRO	Peptide
1	C	48	ALA	Peptide
1	C	57	ASP	Peptide

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	2023	0	1989	26	0
1	B	2023	0	1989	42	0
1	C	988	0	959	33	0
2	A	23	0	0	1	0
2	B	23	0	0	2	0
3	A	153	0	0	0	0
3	B	119	0	0	4	0
3	C	112	0	0	5	0
All	All	5464	0	4937	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (102) 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:212:VAL:HG13	3:B:411:HOH:O	1.70	0.92
1:B:76:THR:HG22	1:B:79:LYS:H	1.33	0.92
1:A:38:MET:HE3	1:A:245:TYR:HE2	1.37	0.90
1:B:38:MET:HE3	1:B:245:TYR:HE2	1.36	0.88
1:A:38:MET:CE	1:A:245:TYR:HE2	1.87	0.88
1:B:38:MET:CE	1:B:245:TYR:HE2	1.85	0.88
1:C:16:TYR:O	1:C:57:ASP:HB3	1.77	0.84
1:B:212:VAL:CG1	3:B:411:HOH:O	2.23	0.84
1:B:109:VAL:HG22	1:B:196:PRO:HG2	1.57	0.83
1:C:182:VAL:O	1:C:182:VAL:HG13	1.83	0.78
1:B:38:MET:HE3	1:B:245:TYR:CE2	2.18	0.78
1:A:38:MET:HE3	1:A:245:TYR:CE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:CG2	1:B:79:LYS:H	2.01	0.73
1:A:67:ALA:HB1	1:A:71:THR:HG21	1.69	0.73
1:C:255:TYR:OH	3:C:301:HOH:O	2.06	0.72
1:B:172:VAL:HG23	1:B:176:LEU:HD22	1.76	0.68
1:A:31:ASP:OD2	1:A:38:MET:HE1	1.94	0.67
1:B:31:ASP:OD2	1:B:38:MET:HE1	1.97	0.64
1:B:76:THR:HG23	1:B:78:GLN:H	1.63	0.64
1:A:134:HIS:CE1	1:A:135:LEU:HD13	2.33	0.64
1:C:101:CYS:HA	1:C:125:HIS:HB2	1.82	0.62
1:C:57:ASP:N	1:C:57:ASP:OD1	2.34	0.60
1:C:97:THR:HG1	1:C:120:ARG:HE	1.49	0.59
1:C:222:PHE:C	1:C:222:PHE:CD1	2.83	0.57
1:C:206:LYS:HD3	1:C:207:PRO:HD2	1.88	0.56
1:A:59:PRO:HB2	1:A:71:THR:HG23	1.87	0.56
1:B:109:VAL:HG22	1:B:196:PRO:CG	2.32	0.56
1:C:252:PHE:O	1:C:256:VAL:HG23	2.06	0.56
1:A:38:MET:CE	1:A:245:TYR:CE2	2.79	0.55
1:B:155:LEU:HD13	1:B:166:GLN:HG2	1.87	0.55
1:C:182:VAL:O	1:C:182:VAL:CG1	2.55	0.55
1:B:158:VAL:HG13	1:B:242:HIS:HD2	1.72	0.54
1:C:251:VAL:HG23	3:C:342:HOH:O	2.07	0.53
1:A:81:ALA:HB1	1:A:111:LEU:HD13	1.90	0.52
2:B:301:ZHB:OAP	2:B:301:ZHB:CAG	2.56	0.51
1:B:94:LYS:HD3	1:B:94:LYS:H	1.75	0.51
1:B:94:LYS:HD3	1:B:94:LYS:N	2.25	0.51
1:A:102:ALA:HB1	2:A:300:ZHB:CAQ	2.40	0.50
1:B:155:LEU:CD1	1:B:166:GLN:HG2	2.42	0.50
1:C:120:ARG:HD3	3:C:330:HOH:O	2.11	0.50
1:B:38:MET:CE	1:B:245:TYR:CE2	2.78	0.50
1:A:31:ASP:OD2	1:A:38:MET:CE	2.61	0.49
1:B:143:ASP:OD1	1:B:185:ARG:NH1	2.38	0.48
1:B:84:VAL:CG2	1:B:111:LEU:HD11	2.43	0.48
1:B:84:VAL:HG21	1:B:111:LEU:HD11	1.95	0.48
1:C:29:VAL:HG11	1:C:107:THR:HG21	1.96	0.48
1:B:109:VAL:CG2	1:B:196:PRO:HG2	2.36	0.48
1:C:224:ASN:HA	3:C:350:HOH:O	2.13	0.47
1:A:37:GLN:HG2	1:A:172:VAL:CG2	2.44	0.47
1:B:154:MET:O	1:B:159:SER:HB3	2.14	0.47
1:C:192:PRO:HB2	1:C:193:PRO:HD3	1.96	0.47
1:C:255:TYR:O	1:C:259:THR:OG1	2.33	0.47
1:C:70:GLU:O	1:C:71:THR:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:HG1	1:C:120:ARG:NE	2.11	0.46
1:C:97:THR:OG1	1:C:260:THR:HG23	2.15	0.46
1:B:31:ASP:OD2	1:B:38:MET:CE	2.64	0.46
1:C:120:ARG:HG2	1:C:121:ASN:HD22	1.81	0.46
1:B:138:THR:HA	1:B:141:LEU:HD22	1.98	0.46
1:A:59:PRO:CB	1:A:71:THR:HG23	2.46	0.45
1:B:94:LYS:N	1:B:94:LYS:CD	2.80	0.45
1:B:105:ALA:HB1	1:B:124:CYS:HB2	1.99	0.45
1:A:138:THR:HA	1:A:141:LEU:HD22	1.98	0.45
1:A:134:HIS:ND1	1:A:135:LEU:HD13	2.31	0.44
1:A:154:MET:O	1:A:159:SER:HB3	2.17	0.44
1:B:158:VAL:HG13	1:B:242:HIS:CD2	2.51	0.44
1:C:112:LEU:O	1:C:206:LYS:NZ	2.51	0.44
1:A:250:ASP:OD2	1:A:254:LYS:HE2	2.15	0.44
1:B:76:THR:HG23	1:B:78:GLN:N	2.29	0.44
1:C:195:ALA:O	1:C:198:LYS:HE2	2.18	0.43
1:B:142:GLU:O	1:B:143:ASP:C	2.61	0.43
1:B:19:GLN:HA	1:B:53:VAL:O	2.18	0.43
1:C:28:LEU:HD22	1:C:252:PHE:HZ	1.83	0.43
1:A:3:THR:O	1:A:18:GLU:HA	2.18	0.43
1:C:26:VAL:O	1:C:53:VAL:HA	2.17	0.43
1:B:180:TYR:N	1:B:181:PRO:CD	2.82	0.43
1:B:61:MET:O	1:B:62:SER:C	2.60	0.43
1:C:21:GLY:CA	1:C:47:ALA:HB1	2.49	0.43
1:B:26:VAL:O	1:B:53:VAL:HA	2.19	0.43
1:B:178:LYS:O	1:B:181:PRO:HD2	2.19	0.43
1:C:192:PRO:HD2	3:C:307:HOH:O	2.18	0.42
1:A:99:TRP:CD1	1:A:99:TRP:C	2.97	0.42
1:A:146:ILE:CG2	1:A:150:LEU:HD22	2.49	0.42
1:A:105:ALA:HB1	1:A:124:CYS:HB2	2.01	0.42
1:B:94:LYS:HG2	3:B:413:HOH:O	2.19	0.42
1:C:61:MET:O	1:C:62:SER:C	2.63	0.42
1:C:222:PHE:CD1	1:C:222:PHE:O	2.72	0.42
1:B:35:GLU:OE2	1:B:37:GLN:HB3	2.20	0.42
1:A:26:VAL:O	1:A:53:VAL:HA	2.19	0.41
1:B:102:ALA:HB1	2:B:301:ZHB:CAQ	2.50	0.41
1:B:180:TYR:HB2	1:B:181:PRO:HD3	2.02	0.41
1:C:104:GLY:O	1:C:107:THR:HB	2.21	0.41
1:B:187:TYR:CD2	1:B:191:ILE:HD13	2.54	0.41
1:C:109:VAL:CG1	1:C:196:PRO:HG2	2.50	0.41
1:A:178:LYS:O	1:A:181:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ASP:O	1:C:120:ARG:NH2	2.54	0.41
1:B:192:PRO:HB2	1:B:193:PRO:HD3	2.02	0.41
1:C:59:PRO:HB2	1:C:71:THR:CG2	2.50	0.41
1:A:192:PRO:HB2	1:A:193:PRO:HD3	2.02	0.41
1:B:216:THR:HB	3:B:411:HOH:O	2.20	0.40
1:A:61:MET:O	1:A:62:SER:C	2.64	0.40
1:C:70:GLU:O	1:C:70:GLU:HG2	2.20	0.40
1:A:221:PHE:O	1:A:222:PHE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	247 (94%)	14 (5%)	1 (0%)	30	49
1	B	262/264 (99%)	249 (95%)	13 (5%)	0	100	100
1	C	111/264 (42%)	98 (88%)	11 (10%)	2 (2%)	6	12
All	All	635/792 (80%)	594 (94%)	38 (6%)	3 (0%)	24	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	PRO
1	A	161	GLY
1	C	43	VAL

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	220/220 (100%)	200 (91%)	20 (9%)	9	19
1	B	220/220 (100%)	197 (90%)	23 (10%)	6	14
1	C	109/220 (50%)	90 (83%)	19 (17%)	2	3
All	All	549/660 (83%)	487 (89%)	62 (11%)	5	12

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	111	LEU
1	A	113	LEU
1	A	132	LEU
1	A	135	LEU
1	A	141	LEU
1	A	142	GLU
1	A	145	GLU
1	A	148	LYS
1	A	150	LEU
1	A	163	GLU
1	A	166	GLN
1	A	182	VAL
1	A	197	VAL
1	A	200	LEU
1	A	203	LEU
1	A	235	ILE
1	A	238	LEU
1	A	257	VAL
1	A	262	LYS
1	B	1	MET
1	B	76	THR
1	B	84	VAL
1	B	94	LYS
1	B	109	VAL
1	B	113	LEU
1	B	121	ASN
1	B	131	LEU
1	B	132	LEU
1	B	141	LEU

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Mol	Chain	Res	Type
1	B	142	GLU
1	B	158	VAL
1	B	163	GLU
1	B	172	VAL
1	B	176	LEU
1	B	191	ILE
1	B	200	LEU
1	B	203	LEU
1	B	235	ILE
1	B	251	VAL
1	B	257	VAL
1	B	262	LYS
1	B	264	LEU
1	C	16	TYR
1	C	22	THR
1	C	25	ASP
1	C	57	ASP
1	C	82	SER
1	C	86	SER
1	C	91	LEU
1	C	99	TRP
1	C	111	LEU
1	C	113	LEU
1	C	121	ASN
1	C	198	LYS
1	C	206	LYS
1	C	218	THR
1	C	219	GLU
1	C	222	PHE
1	C	254	LYS
1	C	259	THR
1	C	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	134	HIS
1	A	156	ASN
1	A	166	GLN
1	A	177	HIS
1	A	263	HIS

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Mol	Chain	Res	Type
1	B	121	ASN
1	B	137	ASN
1	B	177	HIS
1	B	261	GLN
1	B	263	HIS
1	C	121	ASN
1	C	125	HIS

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 ⓘ

2 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	ZHB	B	301	-	24,24,24	1.43	3 (12%)	32,32,32	1.30	5 (15%)
2	ZHB	A	300	-	24,24,24	1.45	4 (16%)	32,32,32	1.67	6 (18%)

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	ZHB	B	301	-	-	8/22/22/22	1/2/2/2
2	ZHB	A	300	-	-	7/22/22/22	1/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZHB	CAT-CAG	-4.16	1.40	1.47
2	A	300	ZHB	CAU-CAQ	-4.15	1.40	1.50
2	B	301	ZHB	CAU-CAQ	-4.08	1.41	1.50
2	B	301	ZHB	CAT-CAG	-3.78	1.41	1.47
2	A	300	ZHB	CAG-CAF	2.63	1.39	1.31
2	B	301	ZHB	CAG-CAF	2.61	1.39	1.31
2	A	300	ZHB	CAJ-CAF	-2.13	1.38	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	ZHB	CAK-CAN-CAW	-4.07	103.47	114.68
2	A	300	ZHB	CAT-CAG-CAF	-3.91	117.29	125.55
2	A	300	ZHB	CAA-CAV-CAM	-3.66	104.42	113.90
2	B	301	ZHB	CAV-OAP-CAQ	3.48	124.15	117.67
2	A	300	ZHB	CAL-CAO-CAW	-3.20	105.86	114.68
2	B	301	ZHB	CAK-CAN-CAW	-2.45	107.93	114.68
2	B	301	ZHB	CAJ-CAF-CAG	-2.41	120.14	125.48
2	B	301	ZHB	CAA-CAV-CAM	-2.31	107.92	113.90
2	B	301	ZHB	OAP-CAV-CAA	2.22	112.94	107.96
2	A	300	ZHB	CAI-CAT-CAG	-2.10	115.27	120.66
2	A	300	ZHB	CAN-CAK-CAJ	-2.08	109.96	114.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	ZHB	CAA-CAV-OAP-CAQ
2	A	300	ZHB	CAK-CAN-CAW-CAO
2	B	301	ZHB	CAL-CAO-CAW-CAN
2	B	301	ZHB	CAL-CAM-CAV-CAA
2	B	301	ZHB	CAL-CAM-CAV-OAP
2	B	301	ZHB	CAA-CAV-OAP-CAQ
2	A	300	ZHB	CAK-CAN-CAW-OAE

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Mol	Chain	Res	Type	Atoms
2	B	301	ZHB	CAL-CAO-CAW-OAE
2	B	301	ZHB	CAU-CAQ-OAP-CAV
2	B	301	ZHB	OAB-CAQ-OAP-CAV
2	A	300	ZHB	CAG-CAF-CAJ-CAK
2	A	300	ZHB	CAL-CAO-CAW-OAE
2	A	300	ZHB	CAU-CAQ-OAP-CAV
2	B	301	ZHB	CAM-CAL-CAO-CAW
2	A	300	ZHB	OAP-CAQ-CAU-CAT

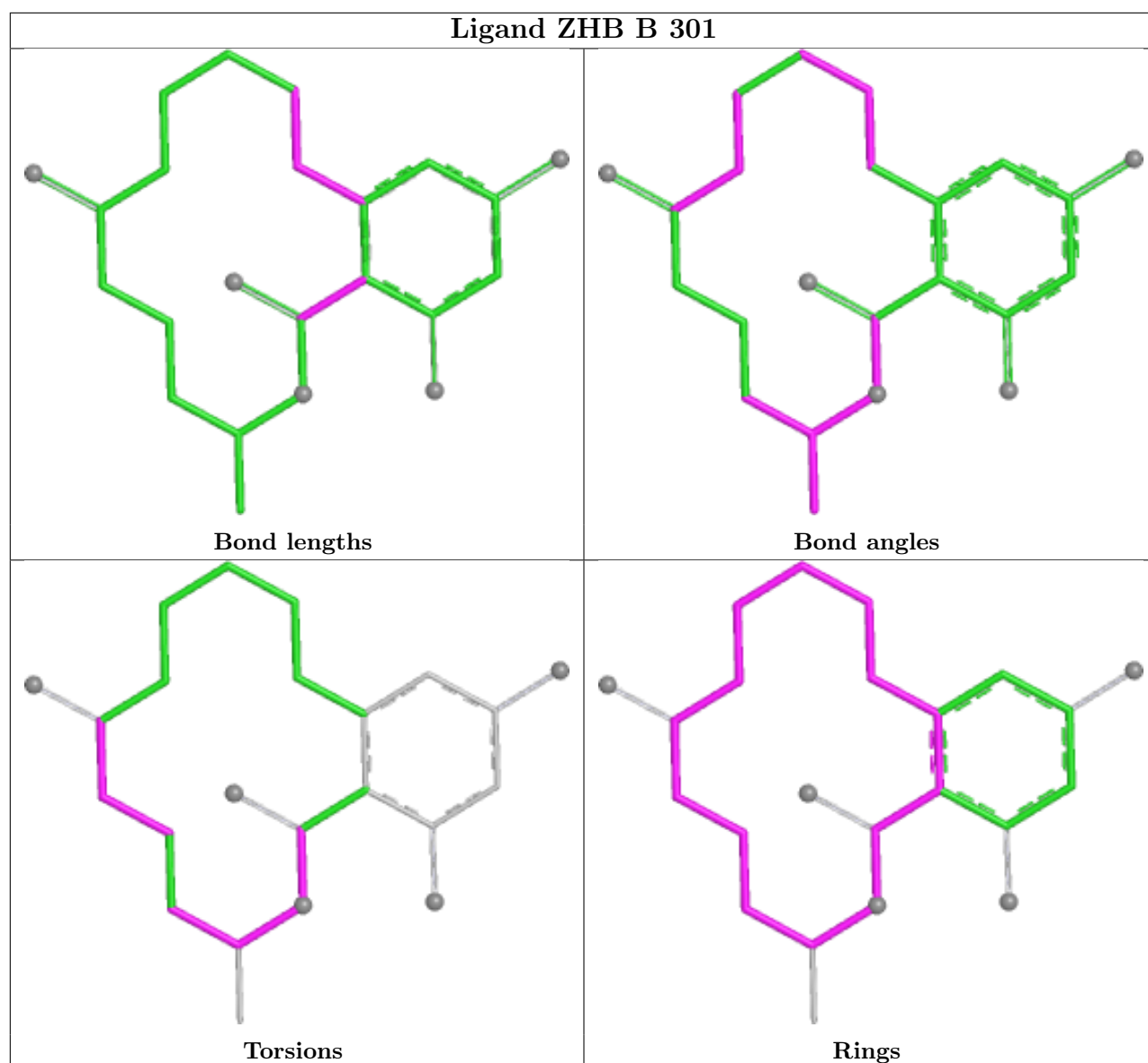
All (2) ring outliers are listed below:

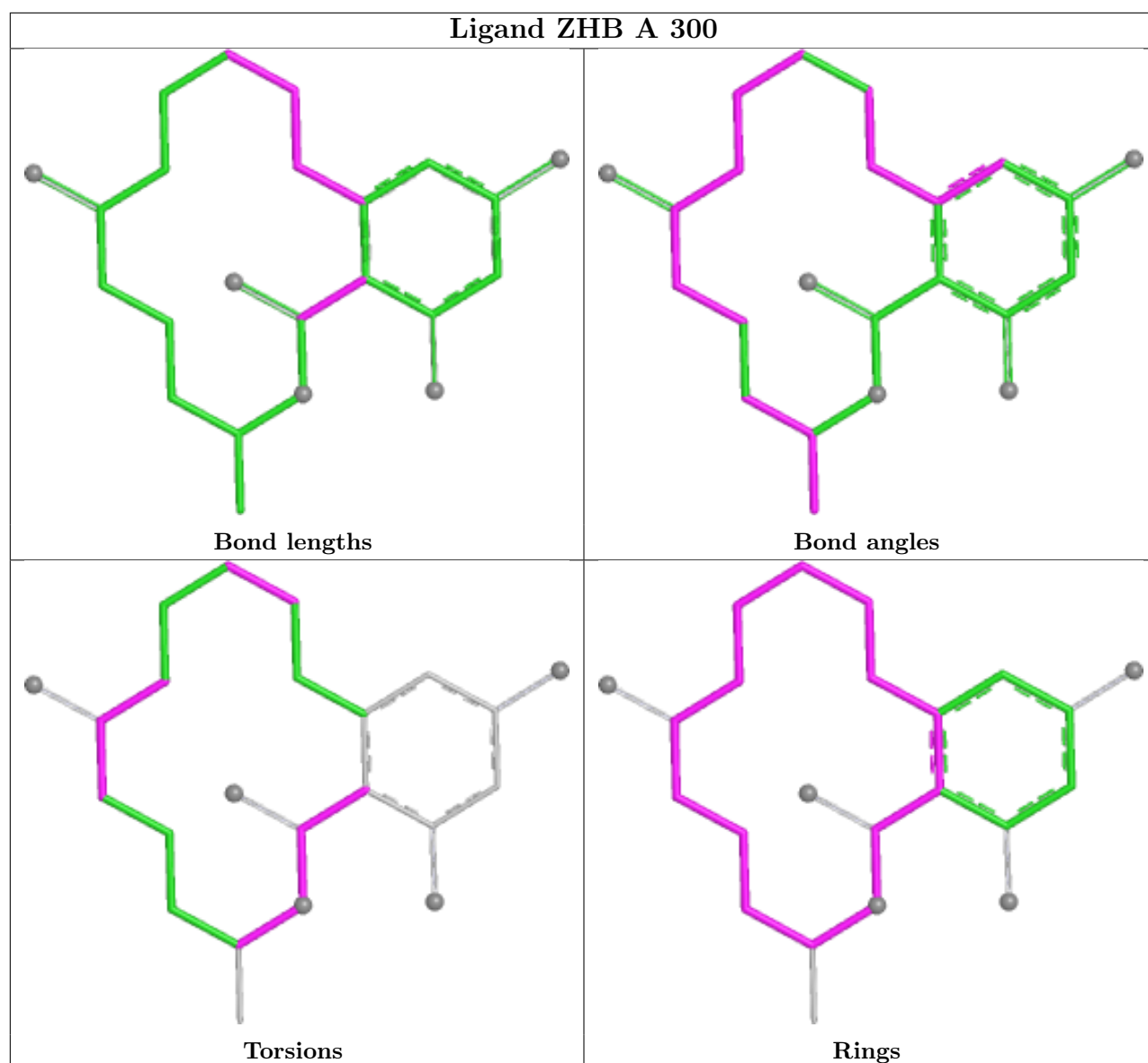
Mol	Chain	Res	Type	Atoms
2	A	300	ZHB	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C
2	B	301	ZHB	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ZHB	2	0
2	A	300	ZHB	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	264/264 (100%)	-0.17	1 (0%) 88 86	15, 23, 42, 62	0
1	B	264/264 (100%)	0.05	2 (0%) 82 80	17, 26, 43, 68	0
1	C	129/264 (48%)	2.29	68 (52%) 0 0	49, 70, 90, 102	0
All	All	657/792 (82%)	0.40	71 (10%) 11 9	15, 26, 79, 102	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	7.7
1	C	24	PRO	5.9
1	C	111	LEU	5.3
1	C	43	VAL	4.9
1	C	108	VAL	4.7
1	C	113	LEU	4.6
1	C	30	PRO	4.4
1	C	222	PHE	4.4
1	C	53	VAL	4.2
1	C	84	VAL	4.2
1	C	51	PHE	4.1
1	C	82	SER	4.0
1	C	47	ALA	4.0
1	C	102	ALA	4.0
1	C	250	ASP	3.9
1	C	112	LEU	3.9
1	C	181	PRO	3.9
1	C	85	ILE	3.8
1	C	29	VAL	3.8
1	C	254	LYS	3.7
1	C	61	MET	3.7
1	C	123	MET	3.7
1	C	46	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	90	ALA	3.5
1	C	251	VAL	3.3
1	C	253	ALA	3.3
1	C	75	VAL	3.2
1	C	109	VAL	3.1
1	C	107	THR	3.1
1	C	218	THR	3.0
1	C	72	TYR	3.0
1	C	209	ASP	3.0
1	C	259	THR	2.9
1	C	192	PRO	2.8
1	C	115	TYR	2.8
1	C	59	PRO	2.8
1	C	99	TRP	2.8
1	C	110	ALA	2.8
1	C	217	PRO	2.7
1	C	203	LEU	2.6
1	C	257	VAL	2.6
1	C	264	LEU	2.6
1	C	193	PRO	2.5
1	C	206	LYS	2.5
1	C	87	VAL	2.5
1	C	105	ALA	2.5
1	C	220	SER	2.5
1	C	260	THR	2.5
1	C	16	TYR	2.5
1	C	183	TRP	2.5
1	C	252	PHE	2.4
1	C	182	VAL	2.4
1	C	18	GLU	2.4
1	C	101	CYS	2.4
1	C	223	ASP	2.3
1	B	1	MET	2.3
1	C	219	GLU	2.3
1	C	100	GLY	2.3
1	C	73	THR	2.2
1	C	23	GLY	2.2
1	C	104	GLY	2.2
1	C	106	SER	2.2
1	B	117	ASP	2.2
1	C	25	ASP	2.2
1	C	89	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLY	2.2
1	C	198	LYS	2.2
1	A	1	MET	2.1
1	C	255	TYR	2.1
1	C	88	LEU	2.0
1	C	49	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

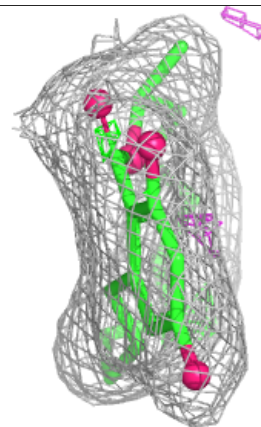
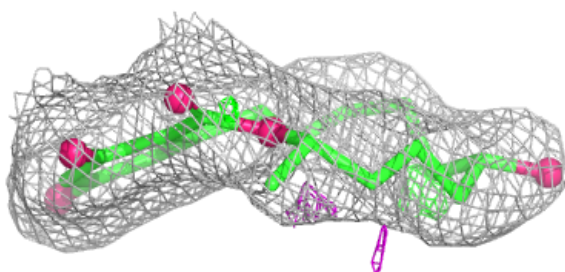
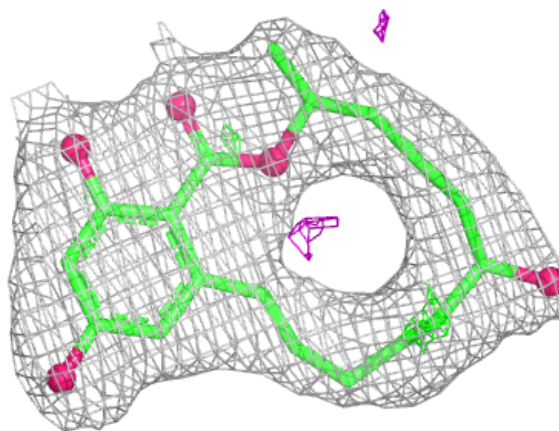
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

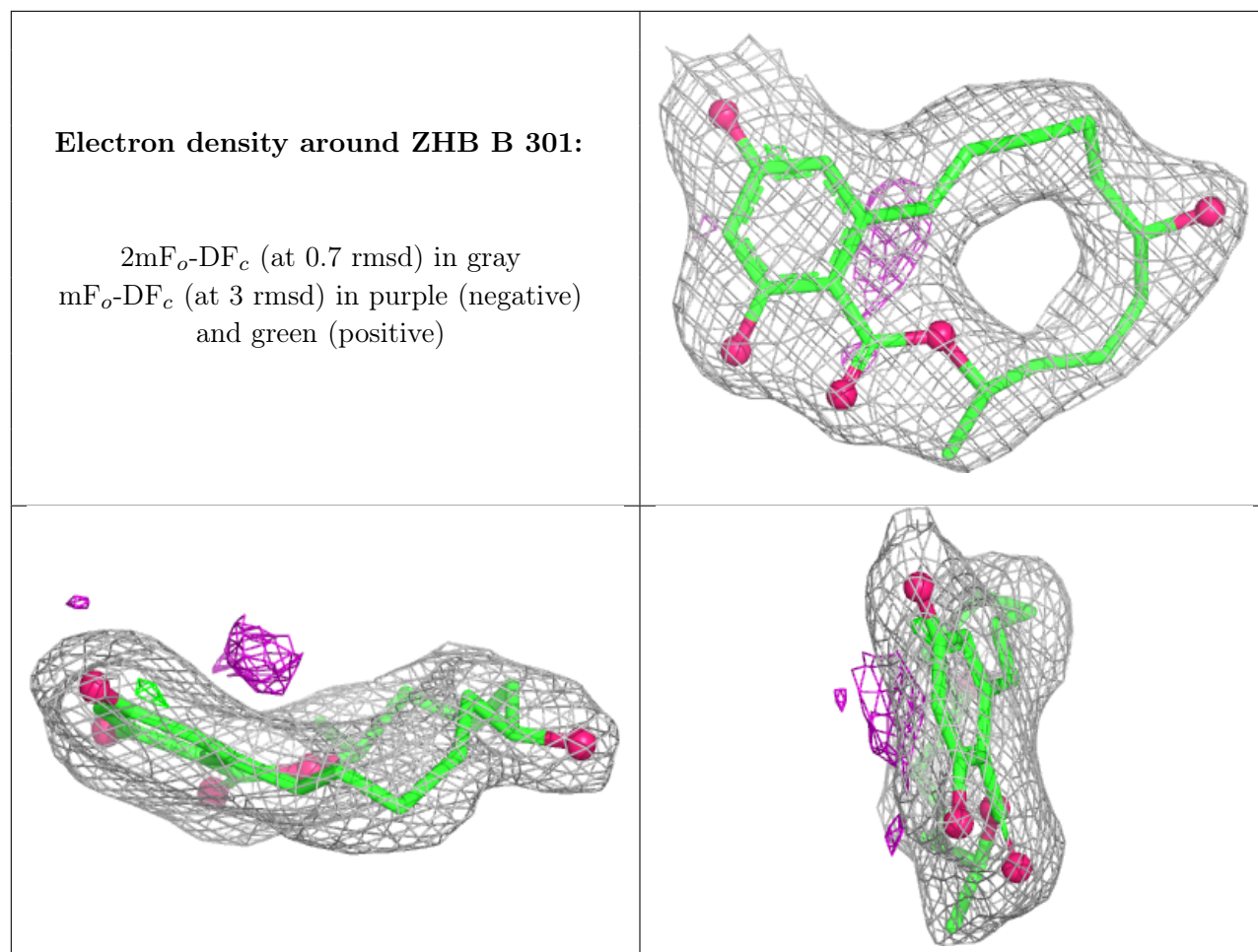
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZHB	A	300	23/23	0.93	0.15	29,42,52,54	0
2	ZHB	B	301	23/23	0.94	0.13	30,39,54,57	0

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 ZHB 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 ⓘ

There are no such residues in this entry.