



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:47 AM UTC

PDB ID : 9LZP / pdb\_00009lzp  
Title : Crystal structure of SARS-Cov-2 main protease P132H mutant in complex with Pomotrelvir  
Authors : Jiang, H.H.; Zhang, J.; Li, J.  
Deposited on : 2025-02-22  
Resolution : 1.97 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

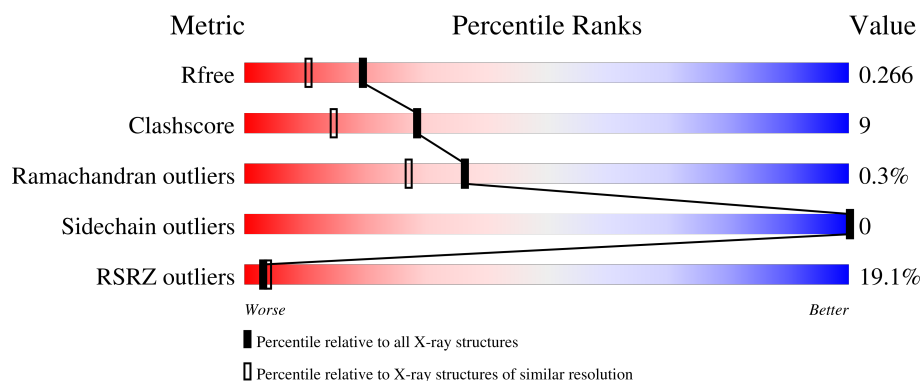
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>
1	B	296	<div> <div>30%</div> <div>82%</div> <div>18%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4745 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.

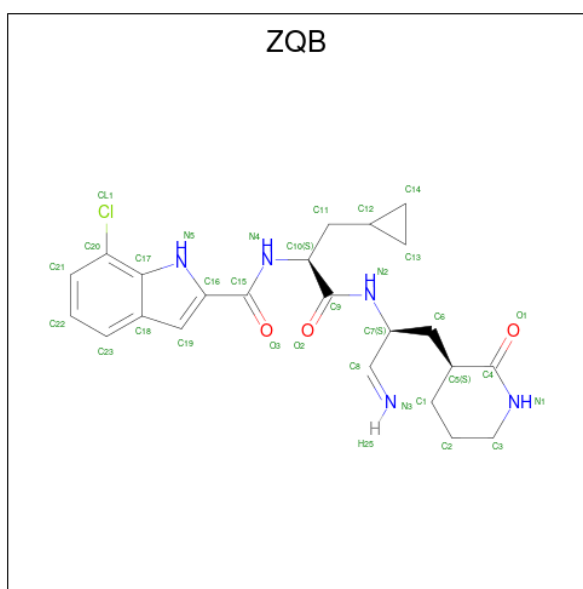
- Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2238	1418	379	420	21			
1	B	296	Total	C	N	O	S	0	0	0
			2255	1430	382	422	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	PRO	engineered mutation	UNP P0DTD1
B	132	HIS	PRO	engineered mutation	UNP P0DTD1

- Molecule 2 is Pomotrelvir bound form (CCD ID: ZQB) (formula:  $C_{23}H_{28}ClN_5O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			32	23	1	5	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			32	23	1	5	3		

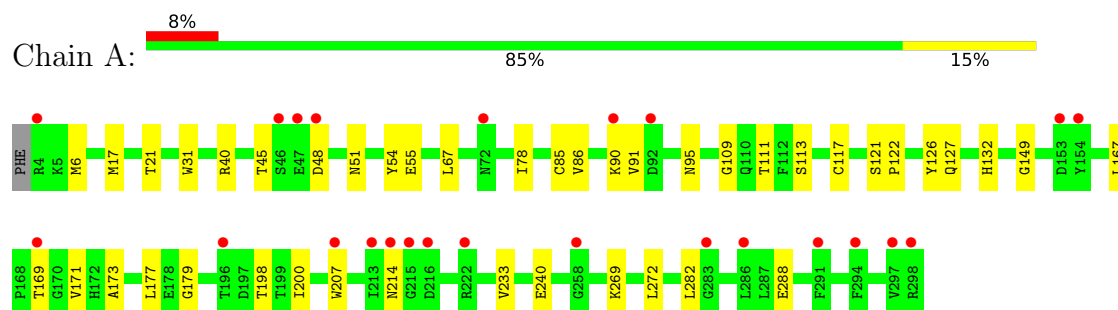
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	65	Total	O	0	0
			65	65		

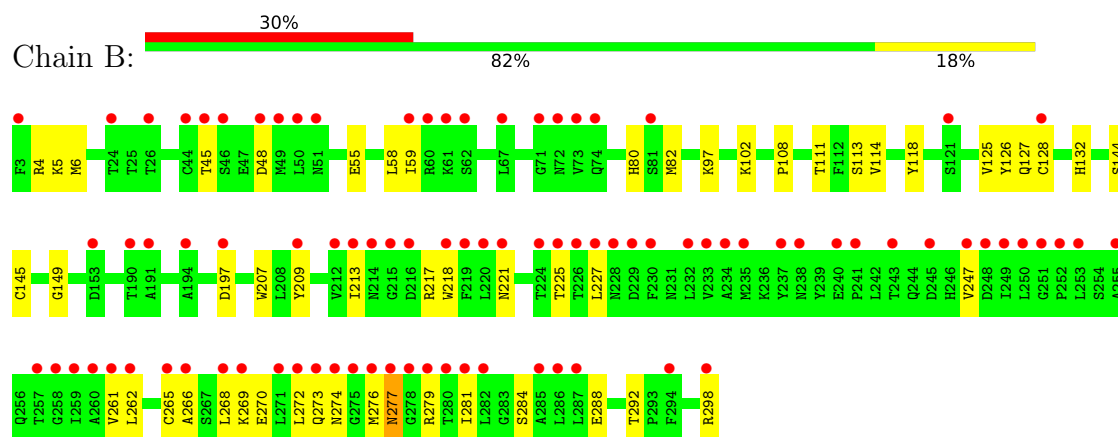
### 3 Residue-property plots

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: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.46Å 100.44Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.48 – 1.97 56.48 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.48-1.97) 99.9 (56.48-1.97)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.227 , 0.265 0.229 , 0.266	Depositor DCC
$R_{free}$ test set	2416 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.37	0/2288	0.61	0/3118
1	B	0.30	0/2306	0.52	0/3140
All	All	0.34	0/4594	0.57	0/6258

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2146	31	1
1	B	2255	0	2166	48	0
2	A	32	0	0	0	0
2	B	32	0	0	3	0
3	A	123	0	0	2	0
3	B	65	0	0	12	1
All	All	4745	0	4312	78	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 9.

All (78) 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:102:LYS:NZ	3:B:401:HOH:O	1.80	1.13
1:B:276:MET:O	1:B:279:ARG:HD3	1.49	1.09
1:B:225:THR:HG21	1:B:269:LYS:HD3	1.61	0.82
1:A:78:ILE:HD11	1:A:90:LYS:HE3	1.69	0.75
1:B:197:ASP:OD1	3:B:403:HOH:O	2.06	0.73
1:B:298:ARG:O	3:B:402:HOH:O	2.06	0.72
1:A:169:THR:HG23	1:A:171:VAL:HG22	1.73	0.71
1:B:274:ASN:O	3:B:404:HOH:O	2.12	0.67
1:B:288:GLU:OE2	3:B:405:HOH:O	2.15	0.64
1:A:55:GLU:OE1	3:A:401:HOH:O	2.15	0.64
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.81	0.63
1:B:281:ILE:O	3:B:406:HOH:O	2.16	0.61
1:A:78:ILE:HD11	1:A:90:LYS:CE	2.31	0.60
1:B:58:LEU:HD22	1:B:82:MET:HE3	1.84	0.60
1:B:218:TRP:CE3	1:B:279:ARG:NH2	2.70	0.60
1:A:132:HIS:CD2	1:A:240:GLU:HG3	2.36	0.59
1:B:227:LEU:HD22	1:B:262:LEU:HD11	1.84	0.59
1:B:145:CYS:SG	2:B:301:ZQB:N2	2.75	0.59
1:B:247:VAL:HG13	1:B:261:VAL:HG21	1.85	0.58
1:A:126:TYR:CD1	1:B:4:ARG:HD2	2.38	0.58
1:B:277:ASN:OD1	1:B:279:ARG:NH1	2.34	0.58
1:A:198:THR:OG1	1:A:240:GLU:HG2	2.05	0.56
1:B:277:ASN:ND2	3:B:404:HOH:O	2.14	0.56
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.88	0.55
1:A:90:LYS:NZ	1:A:91:VAL:O	2.30	0.55
1:B:55:GLU:O	1:B:59:ILE:HG23	2.07	0.55
1:A:78:ILE:CG1	1:A:90:LYS:HD2	2.37	0.55
1:A:207:TRP:CZ2	1:A:282:LEU:HB2	2.44	0.53
1:B:277:ASN:HB2	1:B:279:ARG:HD3	1.92	0.52
1:B:277:ASN:HB2	1:B:279:ARG:CD	2.39	0.52
1:B:266:ALA:O	1:B:270:GLU:HG2	2.10	0.52
1:B:269:LYS:O	1:B:273:GLN:HG2	2.10	0.52
1:A:90:LYS:HD3	1:A:91:VAL:N	2.25	0.51
1:A:45:THR:H	1:A:48:ASP:HB2	1.75	0.51
1:B:247:VAL:HG22	1:B:261:VAL:HG21	1.91	0.51
1:A:269:LYS:NZ	3:A:412:HOH:O	2.41	0.50
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.47	0.49
1:B:207:TRP:CE2	1:B:288:GLU:HB2	2.48	0.49
1:B:221:ASN:HD21	1:B:266:ALA:HB1	1.78	0.48
1:A:233:VAL:HG21	1:A:269:LYS:HE3	1.94	0.48
1:A:17:MET:HG3	1:A:117:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:THR:HG23	1:B:292:THR:HG23	1.96	0.48
1:B:5:LYS:HG2	1:B:127:GLN:HB3	1.95	0.47
1:B:284:SER:N	3:B:406:HOH:O	2.48	0.47
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.49	0.47
1:A:113:SER:O	1:A:149:GLY:HA2	2.14	0.47
1:A:6:MET:HE3	1:A:6:MET:HB2	1.76	0.47
1:B:97:LYS:NZ	3:B:414:HOH:O	2.48	0.47
1:B:114:VAL:O	1:B:125:VAL:HA	2.16	0.46
1:A:21:THR:HB	1:A:67:LEU:HB3	1.97	0.46
1:A:132:HIS:NE2	1:A:240:GLU:HG3	2.32	0.45
1:B:218:TRP:HH2	1:B:276:MET:HA	1.81	0.45
1:B:262:LEU:HA	1:B:265:CYS:HB2	1.98	0.45
1:B:207:TRP:HZ2	3:B:406:HOH:O	2.00	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD13	1.77	0.44
1:A:207:TRP:CD2	1:A:288:GLU:HB3	2.52	0.44
1:B:45:THR:H	1:B:48:ASP:HB2	1.82	0.44
1:B:6:MET:HE3	1:B:6:MET:HB2	1.84	0.43
1:A:111:THR:HB	1:A:127:GLN:HE21	1.83	0.43
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.01	0.43
1:B:145:CYS:SG	2:B:301:ZQB:N3	2.92	0.43
1:B:127:GLN:HG2	3:B:441:HOH:O	2.18	0.43
1:B:268:LEU:O	1:B:272:LEU:HG	2.19	0.43
1:B:118:TYR:CE1	1:B:144:SER:HB3	2.54	0.42
1:B:218:TRP:HE3	1:B:279:ARG:HH21	1.66	0.42
1:B:58:LEU:HD11	1:B:80:HIS:HD2	1.83	0.42
1:B:217:ARG:HD2	3:B:432:HOH:O	2.20	0.42
1:A:167:LEU:HD21	1:A:173:ALA:HB2	2.01	0.42
1:B:108:PRO:HB3	1:B:132:HIS:HA	2.02	0.42
1:B:145:CYS:SG	2:B:301:ZQB:C8	3.08	0.42
1:B:225:THR:O	1:B:262:LEU:HD13	2.19	0.41
1:B:113:SER:O	1:B:149:GLY:HA2	2.21	0.41
1:B:126:TYR:HE1	1:B:128:CYS:SG	2.44	0.41
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.86	0.41
1:B:209:TYR:O	1:B:213:ILE:HG13	2.19	0.41
1:A:40:ARG:HG3	1:A:54:TYR:CE1	2.56	0.40
1:A:121:SER:HA	1:A:122:PRO:HD3	1.93	0.40
1:B:261:VAL:O	1:B:265:CYS:N	2.45	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)
1:A:51:ASN:OD1	3:B:401:HOH:O[2_454]	2.18	0.02

## 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	293/296 (99%)	286 (98%)	6 (2%)	1 (0%)	36	27
1	B	294/296 (99%)	288 (98%)	5 (2%)	1 (0%)	36	27
All	All	587/592 (99%)	574 (98%)	11 (2%)	2 (0%)	36	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	B	277	ASN

### 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	242/255 (95%)	242 (100%)	0	100	100
1	B	244/255 (96%)	244 (100%)	0	100	100
All	All	486/510 (95%)	486 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	127	GLN
1	B	164	HIS
1	B	221	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	ZQB	A	301	1	33,35,35	3.12	11 (33%)	43,49,49	5.18	13 (30%)
2	ZQB	B	301	-	33,35,35	3.11	13 (39%)	43,49,49	5.45	15 (34%)

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	ZQB	A	301	1	-	1/24/39/39	0/4/4/4
2	ZQB	B	301	-	-	1/24/39/39	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ZQB	C4-N1	8.88	1.48	1.33
2	A	301	ZQB	O1-C4	8.64	1.40	1.23
2	B	301	ZQB	C4-N1	8.50	1.47	1.33
2	B	301	ZQB	O1-C4	8.07	1.38	1.23
2	B	301	ZQB	C9-N2	6.69	1.48	1.34
2	B	301	ZQB	C15-N4	6.62	1.48	1.34
2	A	301	ZQB	C15-N4	5.87	1.46	1.34
2	A	301	ZQB	C9-N2	5.42	1.45	1.34
2	A	301	ZQB	C16-N5	-4.54	1.32	1.38
2	B	301	ZQB	C16-N5	-3.76	1.33	1.38
2	A	301	ZQB	C5-C4	3.74	1.55	1.50
2	A	301	ZQB	C18-C17	-3.56	1.37	1.41
2	B	301	ZQB	C20-CL1	2.76	1.80	1.73
2	B	301	ZQB	C14-C13	-2.72	1.39	1.48
2	B	301	ZQB	C18-C17	-2.60	1.38	1.41
2	A	301	ZQB	O2-C9	-2.55	1.18	1.23
2	B	301	ZQB	O2-C9	-2.53	1.18	1.23
2	B	301	ZQB	C16-C15	2.53	1.54	1.48
2	A	301	ZQB	C14-C13	-2.45	1.40	1.48
2	A	301	ZQB	C20-CL1	2.33	1.79	1.73
2	B	301	ZQB	C5-C4	2.32	1.54	1.50
2	A	301	ZQB	O3-C15	-2.27	1.19	1.23
2	B	301	ZQB	O3-C15	-2.08	1.19	1.23
2	B	301	ZQB	C17-C20	2.02	1.43	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ZQB	C11-C12-C14	21.91	150.18	119.71
2	A	301	ZQB	C11-C12-C13	21.72	149.92	119.71
2	B	301	ZQB	C11-C12-C13	21.69	149.87	119.71
2	A	301	ZQB	C11-C12-C14	21.62	149.78	119.71
2	A	301	ZQB	O1-C4-N1	-8.21	111.29	122.41
2	B	301	ZQB	O1-C4-N1	-8.10	111.43	122.41
2	B	301	ZQB	O1-C4-C5	-7.76	109.86	122.72
2	A	301	ZQB	O1-C4-C5	-6.49	111.97	122.72
2	B	301	ZQB	C3-N1-C4	-6.15	109.13	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ZQB	C8-C7-N2	4.99	119.56	110.37
2	B	301	ZQB	C6-C7-C8	-4.98	103.38	110.99
2	A	301	ZQB	C3-N1-C4	-4.92	112.46	125.79
2	B	301	ZQB	C6-C7-N2	-4.40	104.04	110.69
2	B	301	ZQB	C12-C11-C10	-4.27	108.77	114.52
2	B	301	ZQB	C10-C9-N2	3.62	124.34	116.63
2	A	301	ZQB	C18-C17-N5	3.05	110.29	107.84
2	B	301	ZQB	O3-C15-C16	-3.04	117.17	121.09
2	A	301	ZQB	C6-C7-N2	-3.04	106.10	110.69
2	A	301	ZQB	C17-C20-CL1	-2.96	115.92	119.28
2	A	301	ZQB	C21-C20-CL1	2.86	124.05	118.42
2	B	301	ZQB	C16-C15-N4	2.75	120.53	116.86
2	A	301	ZQB	C9-C10-N4	-2.29	104.91	111.11
2	A	301	ZQB	O2-C9-N2	-2.27	118.90	122.96
2	A	301	ZQB	C8-C7-N2	-2.21	106.31	110.37
2	B	301	ZQB	C18-C19-C16	-2.18	105.46	107.41
2	B	301	ZQB	O2-C9-N2	-2.16	119.09	122.96
2	A	301	ZQB	C17-C18-C19	-2.13	105.12	106.51
2	B	301	ZQB	C1-C2-C3	2.02	114.84	110.55

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZQB	C10-C11-C12-C14
2	B	301	ZQB	C10-C11-C12-C13

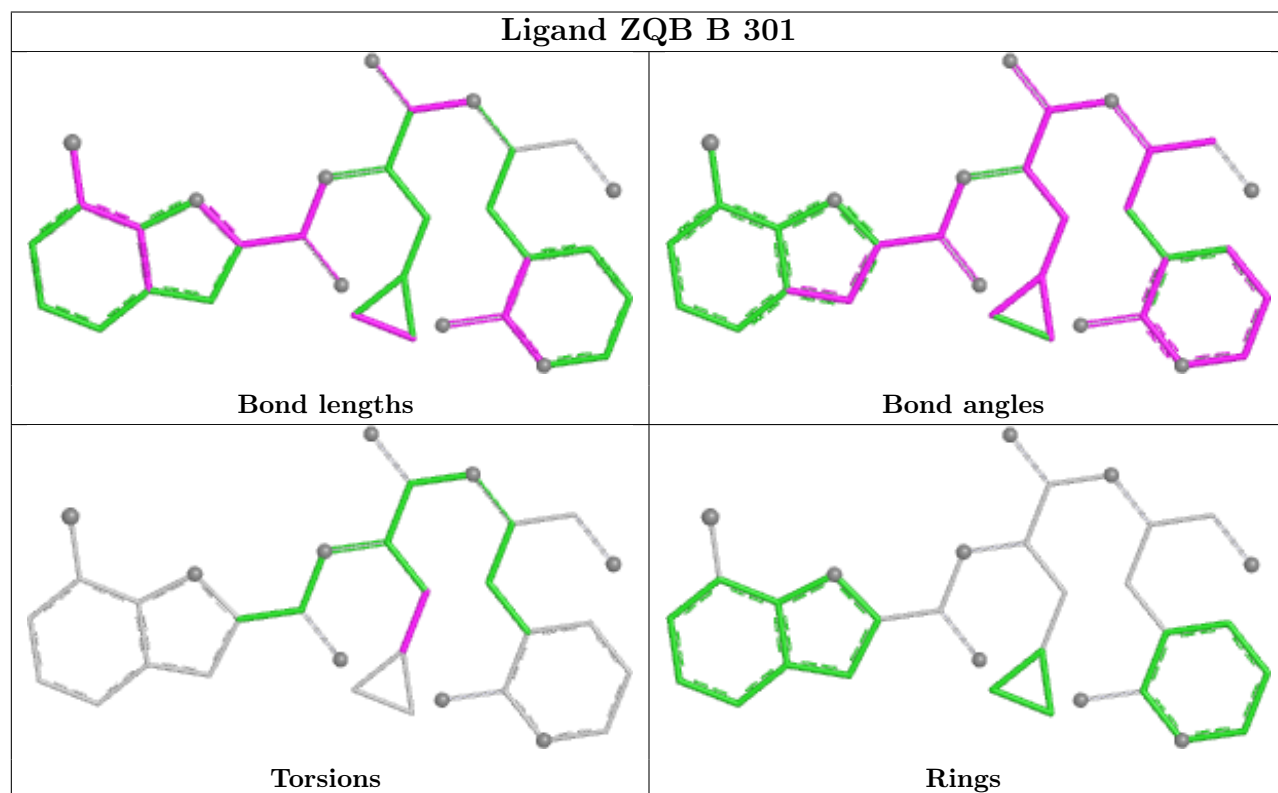
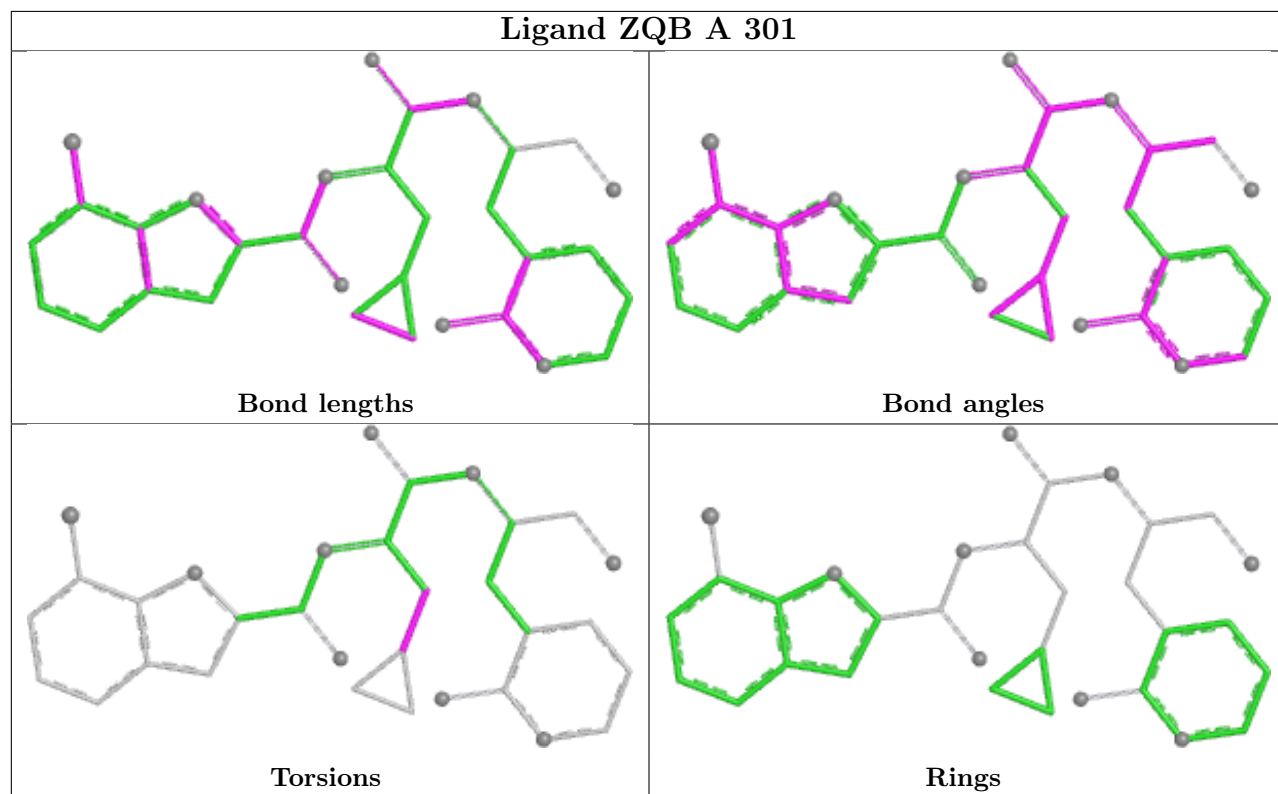
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ZQB	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	295/296 (99%)	0.59	24 (8%) 18 25	13, 22, 36, 46	0
1	B	296/296 (100%)	1.34	89 (30%) 1 1	14, 30, 53, 65	0
All	All	591/592 (99%)	0.97	113 (19%) 3 4	13, 25, 49, 65	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	ASN	5.3
1	B	275	GLY	5.1
1	B	261	VAL	5.1
1	B	282	LEU	4.7
1	B	278	GLY	4.6
1	B	272	LEU	4.5
1	B	225	THR	4.4
1	B	230	PHE	4.2
1	A	154	TYR	4.1
1	B	224	THR	4.0
1	B	226	THR	4.0
1	B	50	LEU	4.0
1	B	232	LEU	3.9
1	B	276	MET	3.9
1	B	191	ALA	3.8
1	B	279	ARG	3.8
1	B	229	ASP	3.8
1	B	227	LEU	3.8
1	B	251	GLY	3.7
1	A	72	ASN	3.7
1	B	271	LEU	3.6
1	B	258	GLY	3.6
1	B	24	THR	3.6
1	B	59	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	235	MET	3.5
1	B	259	ILE	3.5
1	B	213	ILE	3.5
1	B	233	VAL	3.5
1	B	265	CYS	3.4
1	B	153	ASP	3.4
1	B	60	ARG	3.4
1	B	277	ASN	3.3
1	B	255	ALA	3.3
1	A	153	ASP	3.3
1	B	218	TRP	3.3
1	B	72	ASN	3.2
1	B	212	VAL	3.2
1	B	253	LEU	3.2
1	B	237	TYR	3.1
1	B	247	VAL	3.1
1	B	215	GLY	3.1
1	B	262	LEU	3.0
1	B	266	ALA	3.0
1	B	249	ILE	3.0
1	A	298	ARG	2.9
1	B	49	MET	2.9
1	B	240	GLU	2.9
1	B	51	ASN	2.9
1	A	4	ARG	2.9
1	B	197	ASP	2.8
1	B	273	GLN	2.8
1	B	257	THR	2.8
1	A	92	ASP	2.8
1	B	245	ASP	2.8
1	A	222	ARG	2.7
1	B	48	ASP	2.7
1	A	207	TRP	2.7
1	A	48	ASP	2.7
1	B	280	THR	2.7
1	B	269	LYS	2.7
1	B	128	CYS	2.6
1	B	3	PHE	2.6
1	B	252	PRO	2.6
1	B	268	LEU	2.6
1	B	286	LEU	2.6
1	B	44	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	221	ASN	2.6
1	B	234	ALA	2.6
1	B	238	ASN	2.5
1	A	283	GLY	2.5
1	B	214	ASN	2.5
1	A	297	VAL	2.5
1	A	46	SER	2.5
1	B	281	ILE	2.5
1	B	294	PHE	2.4
1	B	62	SER	2.4
1	B	248	ASP	2.4
1	B	250	LEU	2.4
1	B	73	VAL	2.4
1	B	121	SER	2.4
1	B	209	TYR	2.4
1	B	285	ALA	2.4
1	A	47	GLU	2.4
1	B	298	ARG	2.3
1	B	228	ASN	2.3
1	A	90	LYS	2.3
1	A	294	PHE	2.2
1	A	214	ASN	2.2
1	A	216	ASP	2.2
1	B	216	ASP	2.2
1	B	260	ALA	2.2
1	B	219	PHE	2.2
1	B	45	THR	2.2
1	B	190	THR	2.2
1	B	220	LEU	2.2
1	A	215	GLY	2.2
1	A	291	PHE	2.2
1	B	67	LEU	2.1
1	B	194	ALA	2.1
1	B	74	GLN	2.1
1	B	81	SER	2.1
1	A	169	THR	2.1
1	A	196	THR	2.1
1	B	243	THR	2.1
1	B	241	PRO	2.1
1	A	286	LEU	2.1
1	B	287	LEU	2.1
1	A	213	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	46	SER	2.0
1	B	71	GLY	2.0
1	B	61	LYS	2.0
1	A	258	GLY	2.0
1	B	26	THR	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](#)

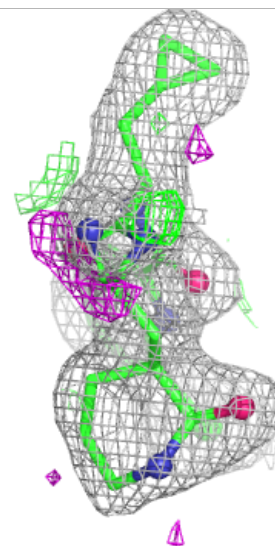
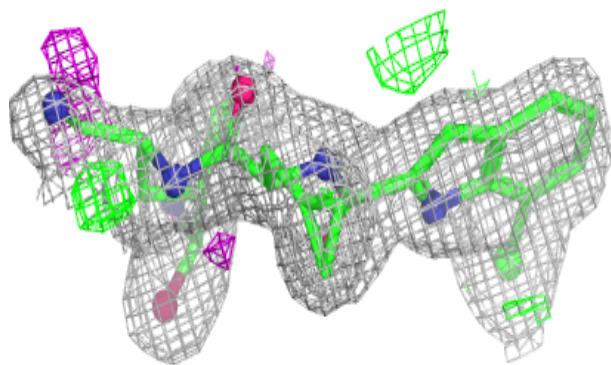
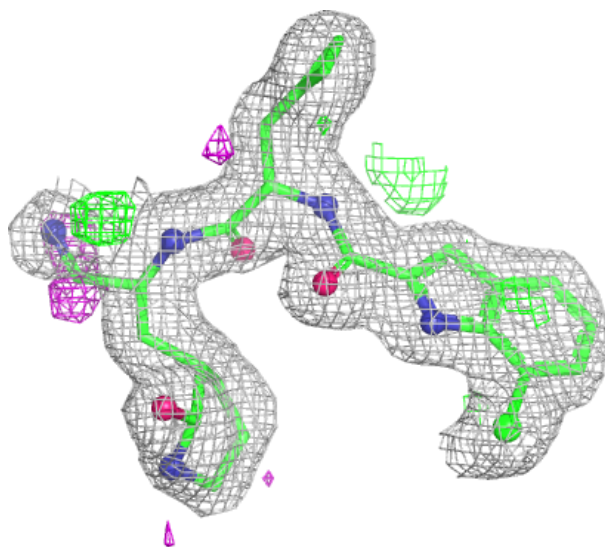
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

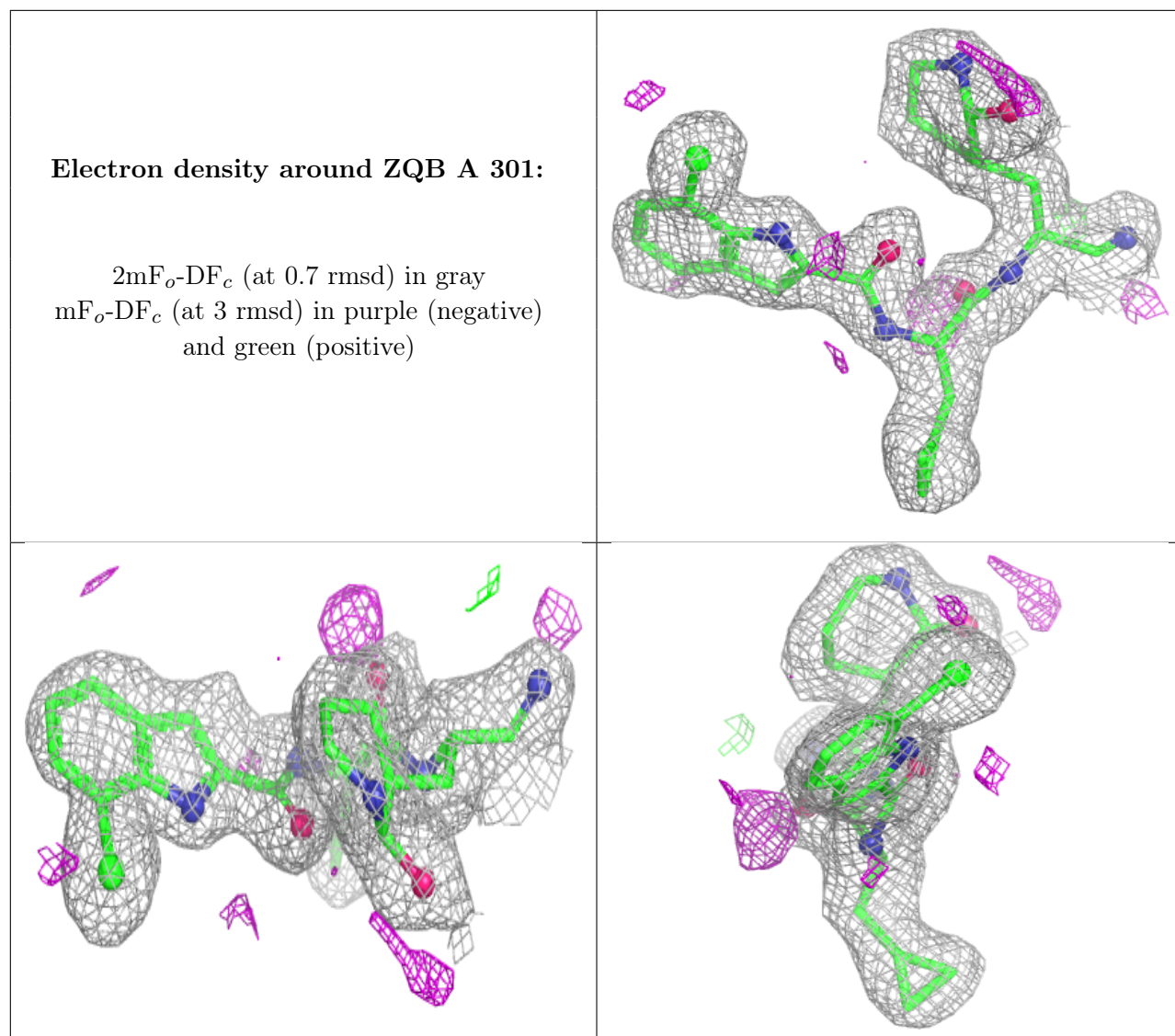
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZQB	B	301	32/32	0.89	0.12	21,31,40,42	0
2	ZQB	A	301	32/32	0.94	0.09	16,22,33,35	0

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 ZQB 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.