



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 02:09 PM JST

PDB ID : 7E65  
Title : The crystal structure of peptidoglycan peptidase in complex with inhibitor 3  
Authors : Choi, Y.; Min, K.J.; Yoon, H.J.; Lee, H.H.  
Deposited on : 2021-02-21  
Resolution : 2.65 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.

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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 : 2.26  
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) : 2.26

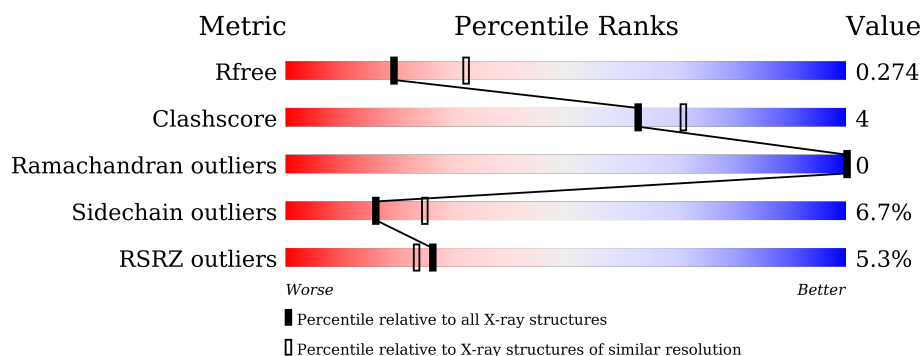
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	255	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	255	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4112 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 Peptidase M23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1997	1299	334	363	1			
1	B	255	Total	C	N	O	S	0	0	0
			1997	1299	334	363	1			

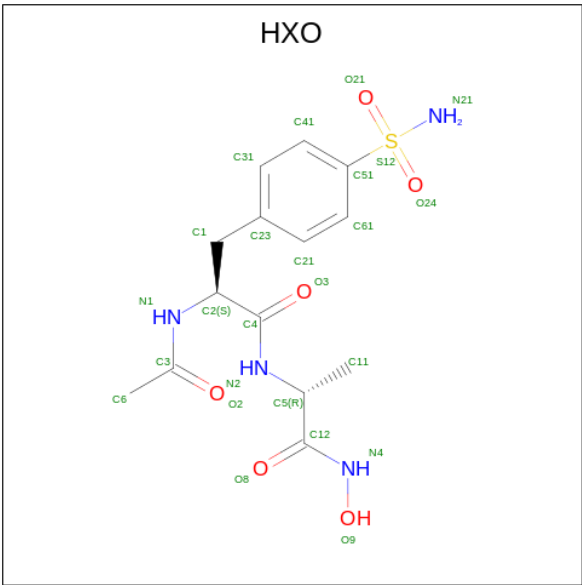
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A1J6PWI8
A	247	ALA	HIS	engineered mutation	UNP A0A1J6PWI8
A	274	LEU	-	expression tag	UNP A0A1J6PWI8
B	20	MET	-	initiating methionine	UNP A0A1J6PWI8
B	247	ALA	HIS	engineered mutation	UNP A0A1J6PWI8
B	274	LEU	-	expression tag	UNP A0A1J6PWI8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2S)-2-acetamido-N-[(2R)-1-(oxidanylamino)-1-oxidanylidene-propan-2-yl]-3-(4-sulfamoylphenyl)propanamide (three-letter code: HXO) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>4</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	14	4	6	1		

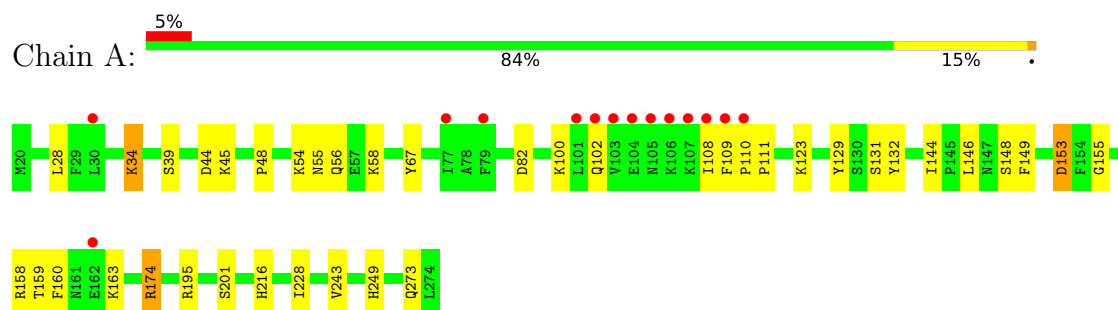
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	51	Total	O	0	0
			51	51		

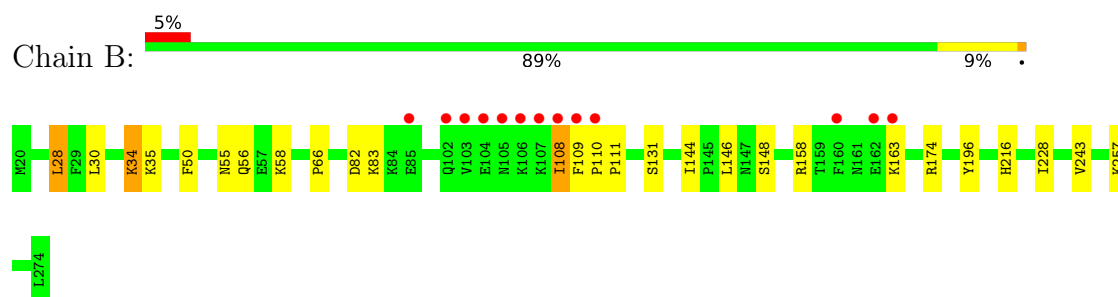
### 3 Residue-property plots [i](#)

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: Peptidase M23



#### • Molecule 1: Peptidase M23



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.44Å 91.04Å 100.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.58 – 2.65 45.52 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.0 (67.58-2.65) 93.1 (45.52-2.65)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.207 , 0.278 0.213 , 0.274	Depositor DCC
$R_{free}$ test set	728 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3816e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	0/2043	0.72	0/2752
1	B	0.54	0/2043	0.70	0/2752
All	All	0.54	0/4086	0.71	0/5504

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	1997	0	2020	21	0
1	B	1997	0	2020	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	4	0
4	A	40	0	0	2	0
4	B	51	0	0	2	0
All	All	4112	0	4040	35	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 4.

All (35) 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:A:195:ARG:NH2	3:A:302:H XO:O21	2.20	0.75
1:A:100:LYS:HA	1:A:159:THR:HB	1.75	0.69
1:A:174:ARG:NE	4:A:401:HOH:O	2.22	0.63
1:B:108:ILE:O	1:B:108:ILE:HG13	1.99	0.61
1:B:28:LEU:HD11	1:B:30:LEU:HD23	1.85	0.59
1:A:129:TYR:OH	3:A:302:H XO:N21	2.37	0.57
1:B:55:ASN:ND2	1:B:58:LYS:HG2	2.21	0.56
1:A:54:LYS:NZ	1:A:273:GLN:O	2.40	0.53
1:A:216:HIS:CE1	1:A:243:VAL:HG13	2.45	0.52
1:B:34:LYS:HE2	1:B:56:GLN:O	2.10	0.51
1:A:34:LYS:HE2	1:A:56:GLN:O	2.11	0.51
1:A:216:HIS:CD2	1:A:243:VAL:HG11	2.47	0.50
1:A:149:PHE:CD1	1:B:50:PHE:HA	2.45	0.50
1:B:28:LEU:HD11	1:B:30:LEU:CD2	2.41	0.50
1:B:216:HIS:CD2	1:B:243:VAL:HG11	2.47	0.50
1:A:55:ASN:ND2	1:A:58:LYS:HG2	2.27	0.50
1:B:216:HIS:CE1	1:B:243:VAL:HG13	2.48	0.49
1:B:66:PRO:HB3	1:B:257:LYS:HE3	1.96	0.47
1:B:196:TYR:HB3	4:B:422:HOH:O	2.16	0.46
1:A:153:ASP:HB3	4:A:432:HOH:O	2.16	0.44
1:B:110:PRO:HB2	1:B:111:PRO:HD2	2.00	0.43
1:A:82:ASP:OD1	1:A:82:ASP:N	2.52	0.42
1:A:67:TYR:OH	1:A:155:GLY:O	2.21	0.41
1:A:249:HIS:CE1	3:A:302:H XO:O8	2.73	0.41
1:B:66:PRO:HB3	1:B:257:LYS:CE	2.50	0.41
1:B:109:PHE:HA	1:B:110:PRO:HD3	1.80	0.41
1:B:144:ILE:CG2	1:B:146:LEU:O	2.69	0.41
1:A:110:PRO:HB2	1:A:111:PRO:HD2	2.02	0.41
1:A:195:ARG:HD3	1:A:201:SER:OG	2.20	0.41
1:A:249:HIS:ND1	3:A:302:H XO:O8	2.54	0.41
1:A:144:ILE:CG2	1:A:146:LEU:O	2.69	0.41
1:A:149:PHE:H	1:A:149:PHE:HD1	1.66	0.40
1:B:35:LYS:NZ	4:B:404:HOH:O	2.47	0.40
1:A:48:PRO:HB2	1:A:132:TYR:CE2	2.56	0.40
1:A:34:LYS:NZ	1:A:56:GLN:O	2.54	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	253/255 (99%)	241 (95%)	12 (5%)	0	100	100
1	B	253/255 (99%)	241 (95%)	12 (5%)	0	100	100
All	All	506/510 (99%)	482 (95%)	24 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/215 (98%)	193 (92%)	17 (8%)	11	17
1	B	210/215 (98%)	199 (95%)	11 (5%)	23	36
All	All	420/430 (98%)	392 (93%)	28 (7%)	16	25

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

Mol	Chain	Res	Type
1	A	28	LEU
1	A	34	LYS
1	A	39	SER
1	A	44	ASP
1	A	45	LYS
1	A	102	GLN
1	A	108	ILE
1	A	109	PHE

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Mol	Chain	Res	Type
1	A	123	LYS
1	A	131	SER
1	A	148	SER
1	A	153	ASP
1	A	158	ARG
1	A	160	PHE
1	A	163	LYS
1	A	174	ARG
1	A	228	ILE
1	B	28	LEU
1	B	34	LYS
1	B	82	ASP
1	B	83	LYS
1	B	108	ILE
1	B	131	SER
1	B	148	SER
1	B	158	ARG
1	B	163	LYS
1	B	174	ARG
1	B	228	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
3	HXO	A	302	2	25,25,25	4.39	10 (40%)	34,35,35	2.34	13 (38%)

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
3	HXO	A	302	2	-	5/28/28/28	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	HXO	O24-S12	12.06	1.66	1.43
3	A	302	HXO	O21-S12	12.05	1.66	1.43
3	A	302	HXO	C12-N4	9.44	1.46	1.33
3	A	302	HXO	C4-N2	5.56	1.46	1.34
3	A	302	HXO	S12-N21	5.03	1.70	1.60
3	A	302	HXO	C3-N1	3.54	1.46	1.34
3	A	302	HXO	C51-S12	3.41	1.82	1.77
3	A	302	HXO	O2-C3	-2.39	1.17	1.23
3	A	302	HXO	O8-C12	-2.15	1.19	1.23
3	A	302	HXO	O3-C4	-2.11	1.19	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	HXO	O24-S12-O21	-6.33	108.35	118.76
3	A	302	HXO	O21-S12-C51	5.69	113.70	107.35
3	A	302	HXO	C11-C5-N2	-3.97	102.92	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	HXO	C41-C51-S12	3.80	125.24	119.73
3	A	302	HXO	C61-C51-S12	-3.66	114.43	119.73
3	A	302	HXO	C6-C3-N1	3.53	122.08	116.10
3	A	302	HXO	C1-C23-C21	-3.52	113.92	120.91
3	A	302	HXO	O8-C12-N4	-2.32	120.27	123.27
3	A	302	HXO	O21-S12-N21	2.24	110.69	107.36
3	A	302	HXO	C2-C4-N2	2.18	121.48	116.70
3	A	302	HXO	O3-C4-N2	-2.13	118.99	122.93
3	A	302	HXO	O2-C3-C6	-2.10	118.15	122.06
3	A	302	HXO	C1-C23-C31	2.10	125.07	120.91

There are no chirality outliers.

All (5) torsion outliers are listed below:

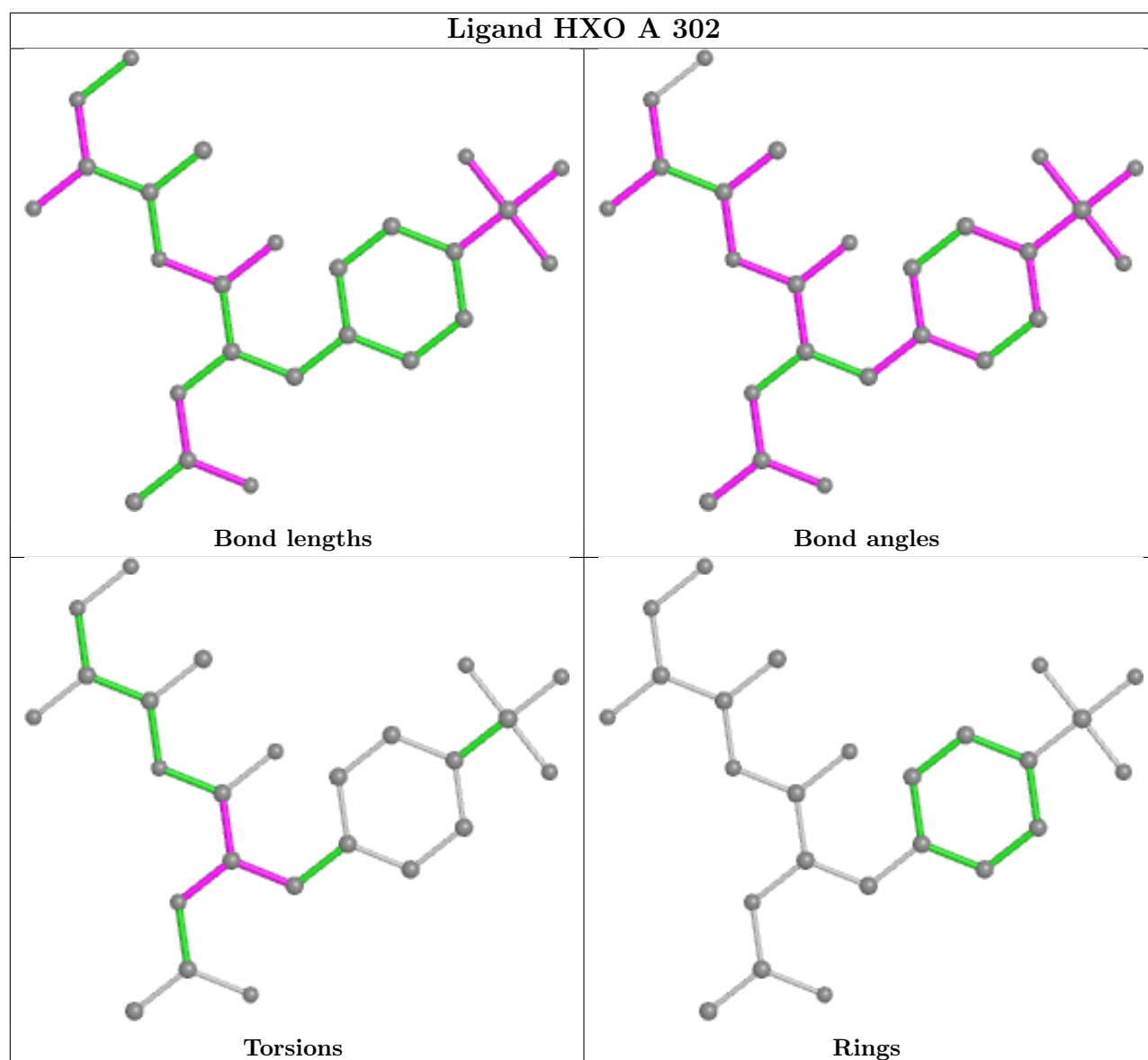
Mol	Chain	Res	Type	Atoms
3	A	302	HXO	C23-C1-C2-N1
3	A	302	HXO	C23-C1-C2-C4
3	A	302	HXO	C1-C2-C4-O3
3	A	302	HXO	C1-C2-C4-N2
3	A	302	HXO	C4-C2-N1-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	HXO	4	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	255/255 (100%)	0.16	14 (5%) 25 21	22, 37, 92, 137	0
1	B	255/255 (100%)	0.15	13 (5%) 28 25	22, 38, 90, 149	0
All	All	510/510 (100%)	0.16	27 (5%) 26 23	22, 38, 92, 149	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	VAL	10.8
1	A	103	VAL	9.0
1	B	109	PHE	7.7
1	B	105	ASN	6.5
1	B	107	LYS	6.1
1	A	108	ILE	5.9
1	B	106	LYS	5.5
1	A	102	GLN	4.8
1	B	160	PHE	4.8
1	B	108	ILE	4.4
1	B	104	GLU	4.2
1	A	104	GLU	3.9
1	A	109	PHE	3.3
1	A	107	LYS	3.1
1	A	106	LYS	3.0
1	A	105	ASN	2.9
1	A	162	GLU	2.9
1	B	102	GLN	2.6
1	B	162	GLU	2.5
1	A	110	PRO	2.5
1	B	163	LYS	2.4
1	A	101	LEU	2.3
1	A	30	LEU	2.3
1	A	77	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	110	PRO	2.2
1	B	85	GLU	2.0
1	A	79	PHE	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](#)

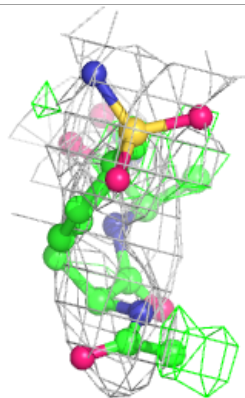
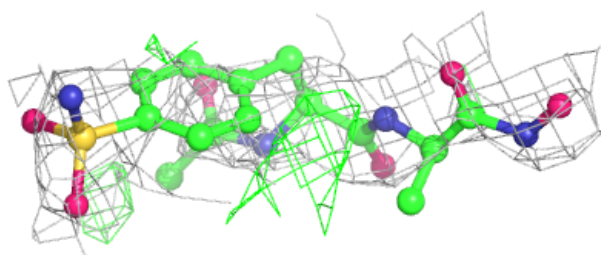
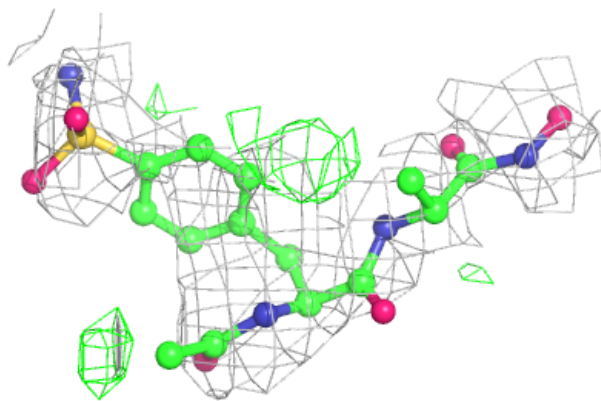
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HXO	A	302	25/25	0.85	0.26	62,98,111,117	0
2	ZN	B	300	1/1	0.99	0.09	42,42,42,42	0
2	ZN	A	301	1/1	0.99	0.10	48,48,48,48	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 HXO A 302:**

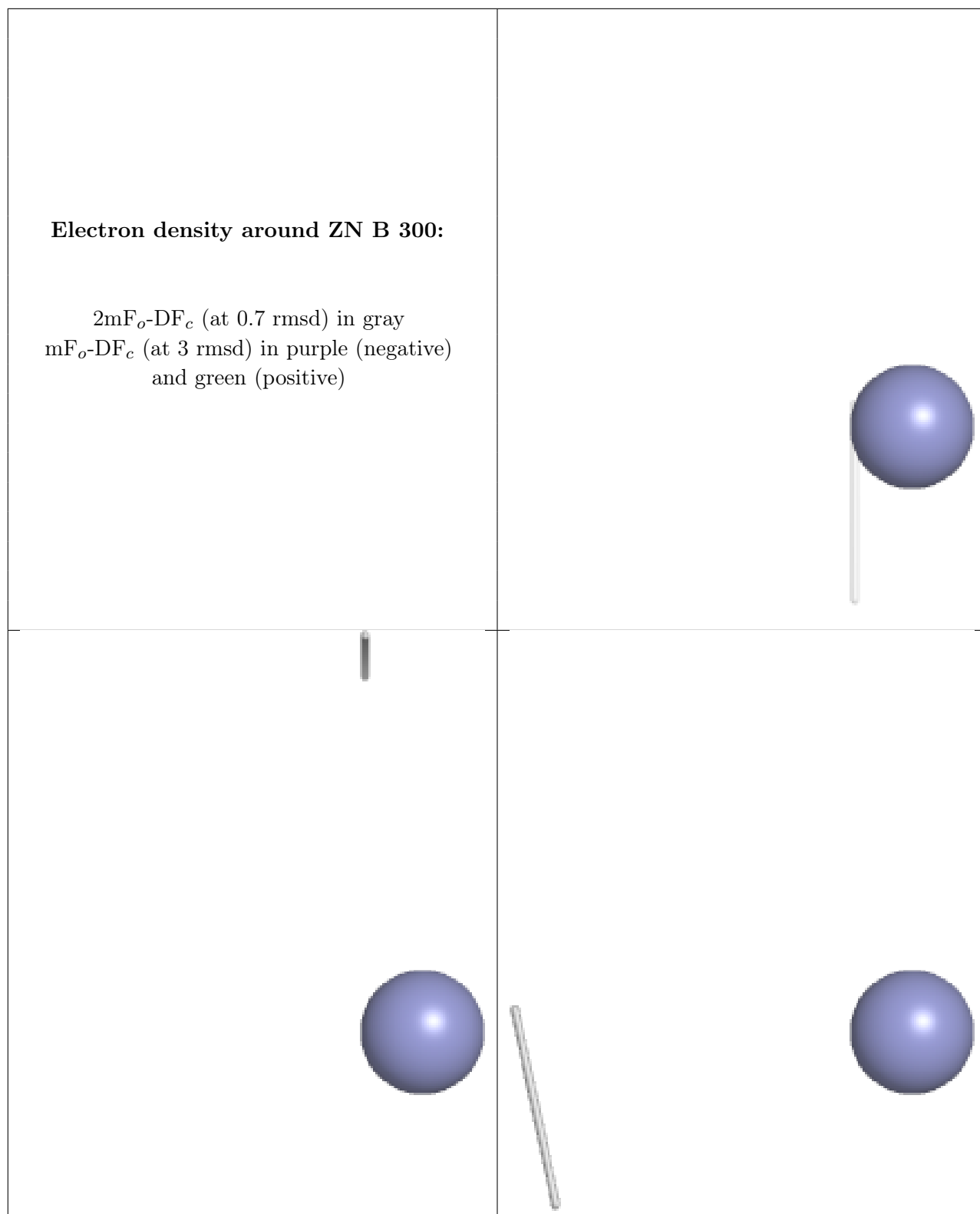
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

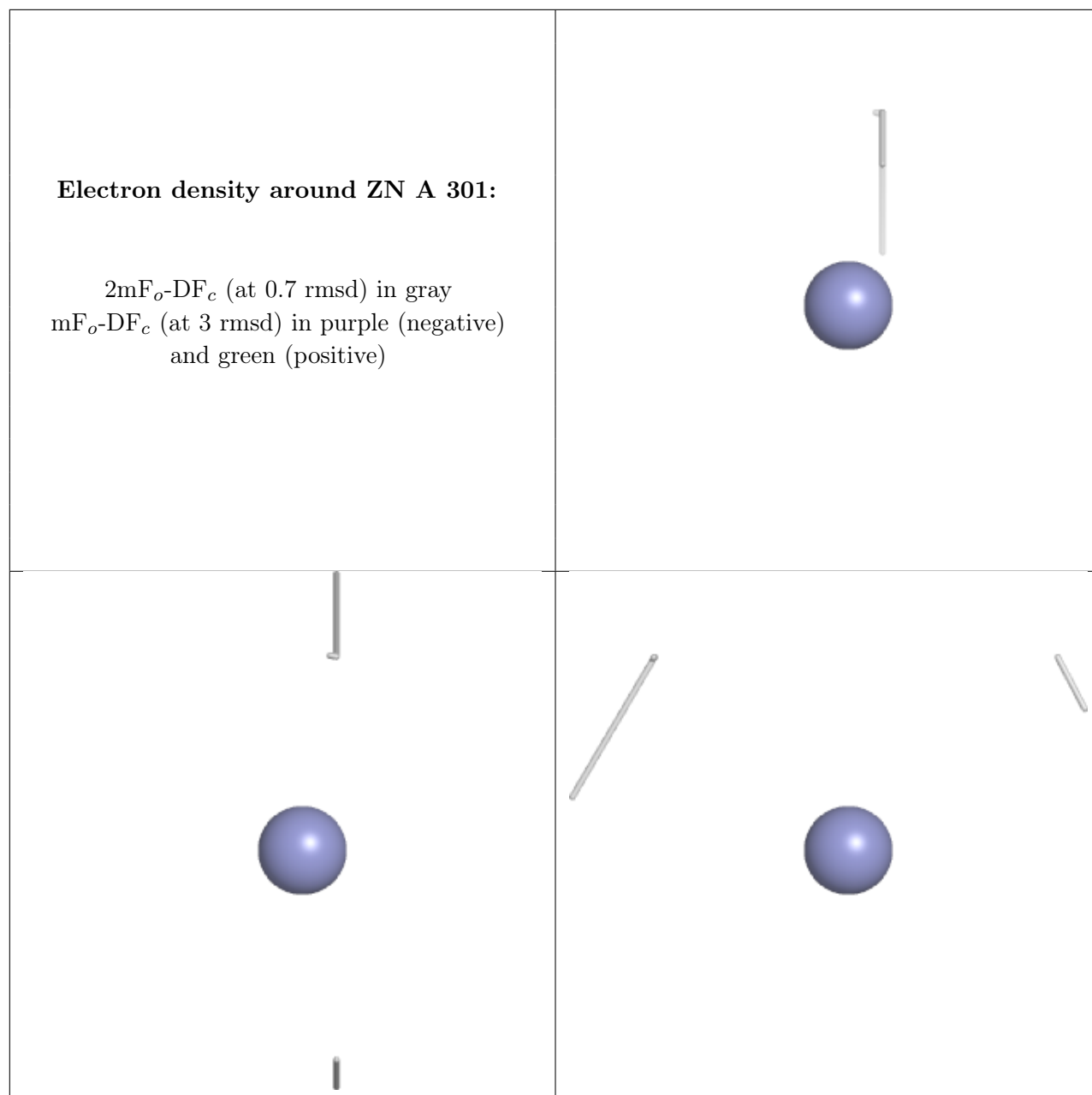




**Electron density around ZN B 300:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.