



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 18, 2022 – 12:08 PM JST

PDB ID : 7E7E  
Title : The co-crystal structure of ACE2 with Fab  
Authors : Xiao, J.Y.; Zhang, Y.  
Deposited on : 2021-02-26  
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
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) : 2.25

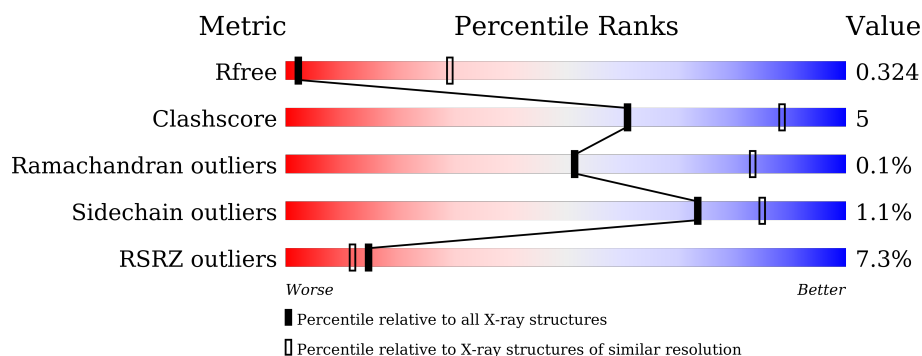
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	606	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	606	<div> <div>9%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	C	228	<div> <div>11%</div> <div>75%</div> <div>16%</div> <div>9%</div> </div>
2	H	228	<div> <div>6%</div> <div>75%</div> <div>16%</div> <div>9%</div> </div>
3	D	214	<div> <div>15%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
3	L	214	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

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
4	ZN	B	701	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16055 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4798	3071	796	902	29			
1	B	592	Total	C	N	O	S	0	0	0
			4828	3089	800	910	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
B	616	HIS	-	expression tag	UNP Q9BYF1
B	617	HIS	-	expression tag	UNP Q9BYF1
B	618	HIS	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1
B	622	HIS	-	expression tag	UNP Q9BYF1
B	623	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called h11B11-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1585	1001	267	309	8			
2	C	208	Total	C	N	O	S	0	0	0
			1584	1001	267	308	8			

- Molecule 3 is a protein called h11B11-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1629	1021	274	328	6			
3	D	210	Total	C	N	O	S	0	0	0
			1629	1021	274	328	6			

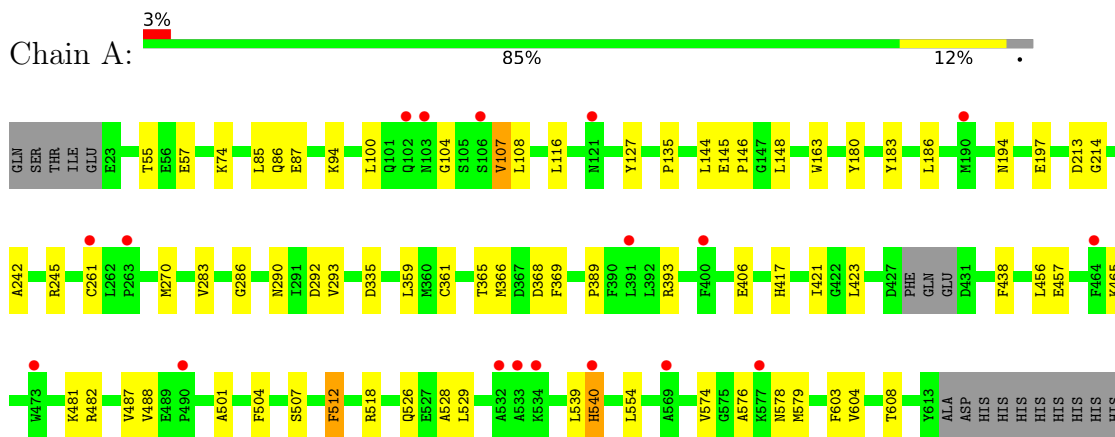
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

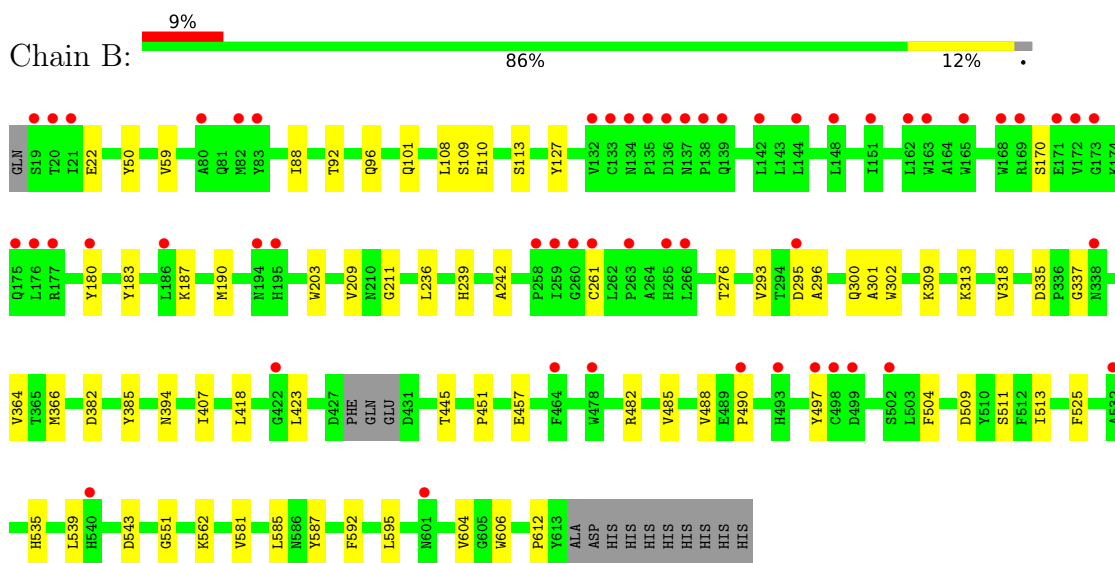
### 3 Residue-property plots

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.

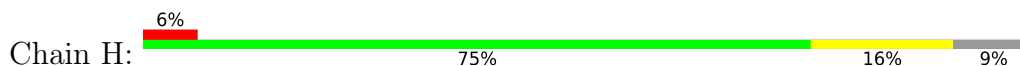
- Molecule 1: Processed angiotensin-converting enzyme 2

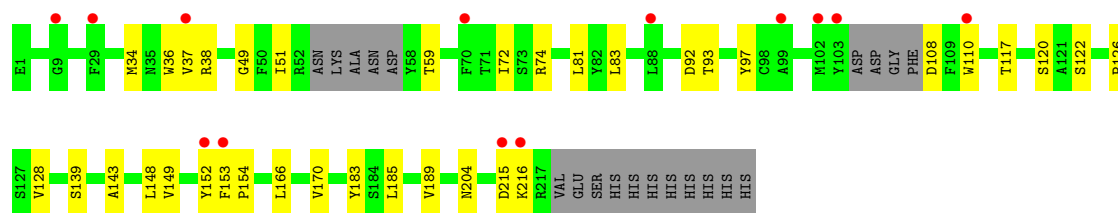


- Molecule 1: Processed angiotensin-converting enzyme 2

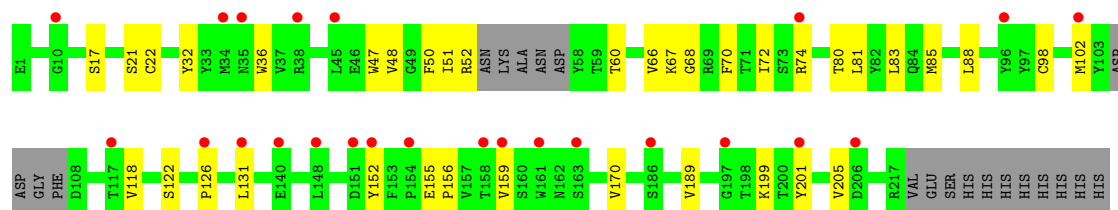
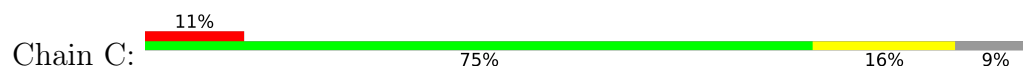


- Molecule 2: h11B11-Fab

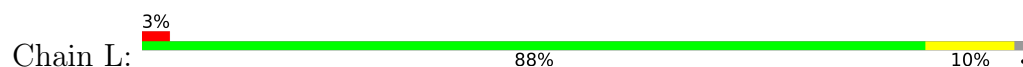




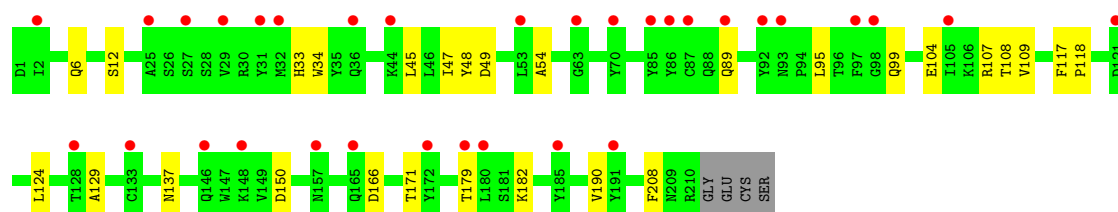
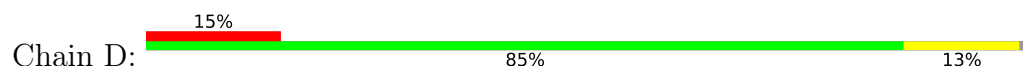
● Molecule 2: h11B11-Fab



● Molecule 3: h11B11-Fab



● Molecule 3: h11B11-Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.78Å 115.46Å 224.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.80 49.84 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.84-3.80) 99.1 (49.84-3.80)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.276 , 0.327 0.274 , 0.324	Depositor DCC
$R_{free}$ test set	1284 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.0	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 102.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	16055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/4933	0.49	1/6701 (0.0%)
1	B	0.27	0/4963	0.47	0/6742
2	C	0.29	0/1621	0.56	0/2204
2	H	0.28	0/1622	0.57	0/2205
3	D	0.27	0/1666	0.53	0/2262
3	L	0.28	0/1666	0.54	0/2262
All	All	0.27	0/16471	0.51	1/22376 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	LEU	CA-CB-CG	5.17	127.19	115.30

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	4798	0	4585	42	0
1	B	4828	0	4614	35	0
2	C	1584	0	1540	22	0
2	H	1585	0	1545	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1629	0	1589	15	0
3	L	1629	0	1591	12	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	16055	0	15464	142	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 5.

The worst 5 of 142 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)
3:D:6:GLN:NE2	3:D:99:GLN:O	2.19	0.74
1:A:261:CYS:HB2	1:A:488:VAL:HG13	1.70	0.73
3:L:33:HIS:ND1	3:L:48:TYR:O	2.22	0.72
1:B:261:CYS:HB2	1:B:488:VAL:HG13	1.75	0.67
1:A:438:PHE:HD2	1:A:540:HIS:HE1	1.42	0.67

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	584/606 (96%)	568 (97%)	16 (3%)	0	100	100
1	B	588/606 (97%)	569 (97%)	17 (3%)	2 (0%)	41	74
2	C	202/228 (89%)	199 (98%)	3 (2%)	0	100	100
2	H	202/228 (89%)	195 (96%)	7 (4%)	0	100	100
3	D	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	L	208/214 (97%)	203 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1992/2096 (95%)	1935 (97%)	55 (3%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	ALA
1	B	364	VAL

### 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	519/536 (97%)	515 (99%)	4 (1%)	81 89
1	B	523/536 (98%)	519 (99%)	4 (1%)	81 89
2	C	177/196 (90%)	175 (99%)	2 (1%)	73 85
2	H	178/196 (91%)	176 (99%)	2 (1%)	73 85
3	D	187/190 (98%)	183 (98%)	4 (2%)	53 74
3	L	187/190 (98%)	184 (98%)	3 (2%)	62 79
All	All	1771/1844 (96%)	1752 (99%)	19 (1%)	73 85

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	122	SER
3	D	108	THR
3	D	109	VAL
3	D	107	ARG
3	L	155	SER

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

Mol	Chain	Res	Type
1	B	101	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	588/606 (97%)	0.22	18 (3%)	49	40	72, 103, 159, 221	0
1	B	592/606 (97%)	0.46	54 (9%)	9	7	80, 113, 174, 263	0
2	C	208/228 (91%)	0.76	24 (11%)	4	5	81, 119, 198, 283	0
2	H	208/228 (91%)	0.46	13 (6%)	20	15	85, 114, 161, 211	0
3	D	210/214 (98%)	0.83	32 (15%)	2	2	86, 126, 161, 204	0
3	L	210/214 (98%)	0.37	7 (3%)	46	38	101, 124, 171, 230	0
All	All	2016/2096 (96%)	0.45	148 (7%)	15	12	72, 114, 171, 283	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	498	CYS	6.1
1	B	499	ASP	5.9
2	H	103	TYR	5.5
1	B	136	ASP	5.4
1	B	261	CYS	4.5

### 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

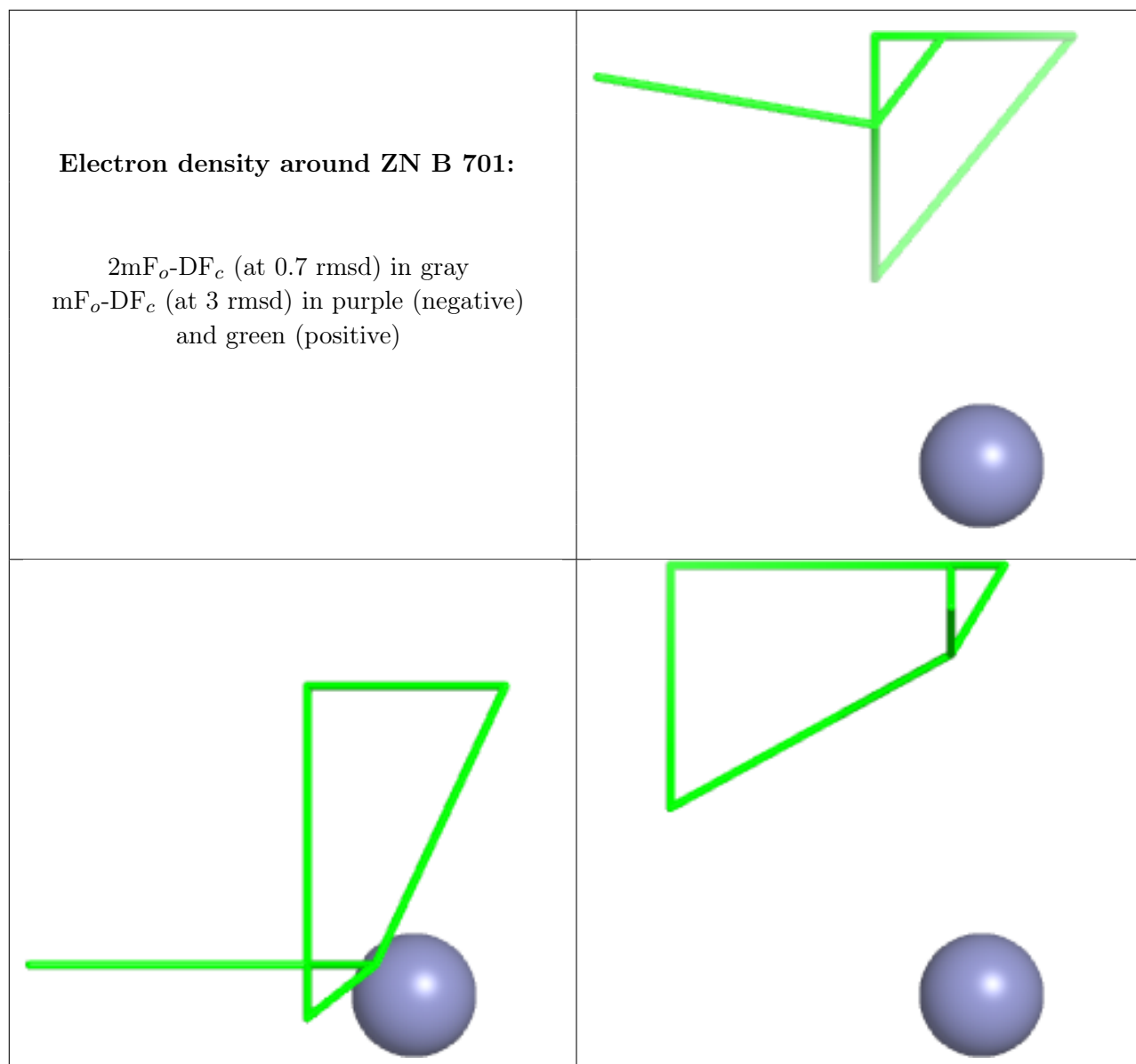
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	ZN	B	701	1/1	0.74	0.53	191,191,191,191	0
4	ZN	A	701	1/1	0.91	0.25	105,105,105,105	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.

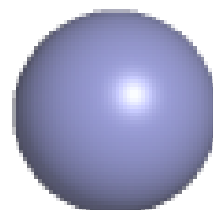
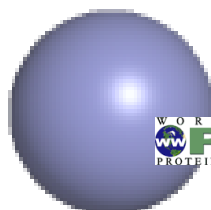
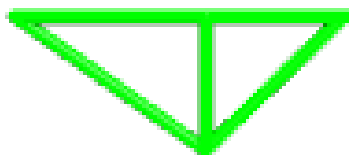
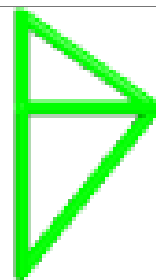
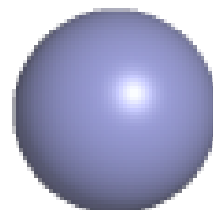
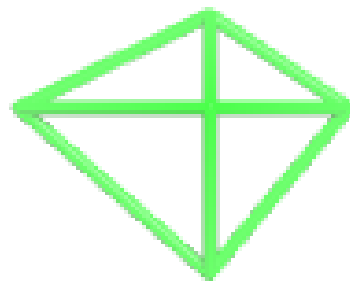
**Electron density around ZN B 701:**

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



**Electron density around ZN A 701:**

$2mF_o-DF_c$  (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.