



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 03:44 PM JST

PDB ID : 7E6V  
Title : The crystal structure of foot-and-mouth disease virus(FMDV) 2C protein 97-318aa  
Authors : Zhang, C.; Wojdyla, J.A.; Qin, B.; Wang, M.; Gao, X.; Cui, S.  
Deposited on : 2021-02-24  
Resolution : 1.83 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 : 4.02b-467  
Mogul : ?? (??), CSD ??CSD?? (????)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

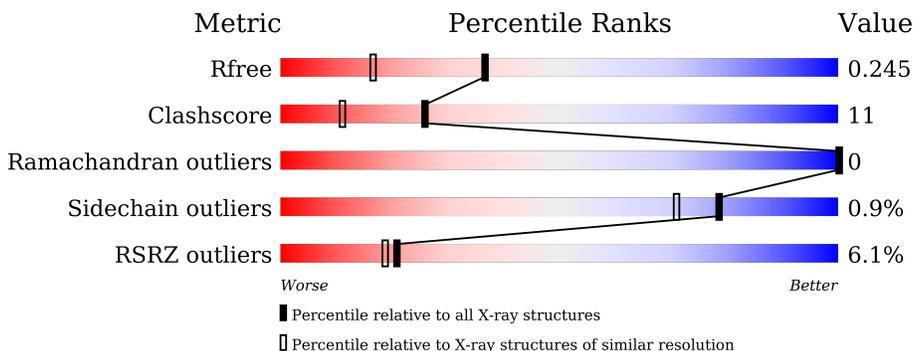
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	223	
1	B	223	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	401	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6599 atoms, of which 3066 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.

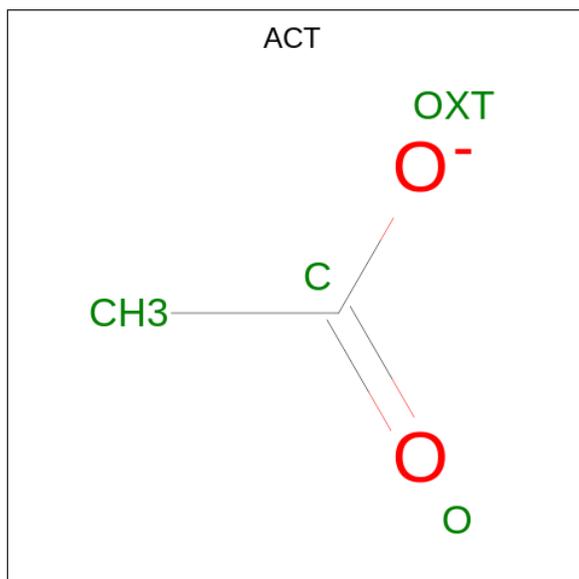
- Molecule 1 is a protein called Protein 2C.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	209	3218	1051	1569	279	309	3	7	0	1	0
1	B	196	3042	990	1491	262	288	3	8	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MSE	-	initiating methionine	UNP B8Y0J7
A	134	ALA	ARG	engineered mutation	UNP B8Y0J7
A	135	ALA	THR	engineered mutation	UNP B8Y0J7
B	96	MSE	-	initiating methionine	UNP B8Y0J7
B	134	ALA	ARG	engineered mutation	UNP B8Y0J7
B	135	ALA	THR	engineered mutation	UNP B8Y0J7

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		

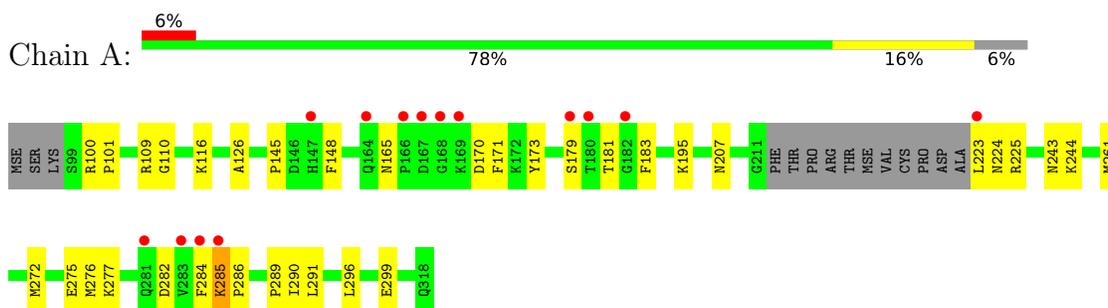
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	155	Total	O	0	0
			155	155		

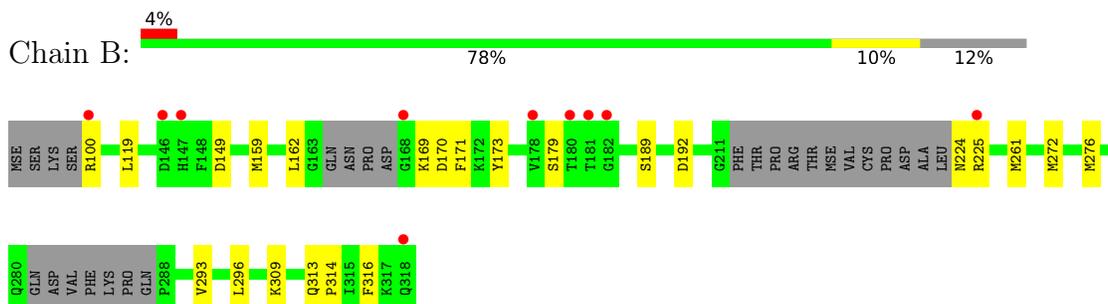
### 3 Residue-property plots [i](#)

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: Protein 2C



- Molecule 1: Protein 2C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.72Å 40.74Å 72.94Å 77.22° 84.38° 89.96°	Depositor
Resolution (Å)	38.48 – 1.83 38.48 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.6 (38.48-1.83) 97.0 (38.48-1.83)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.83Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.201 , 0.249 0.197 , 0.245	Depositor DCC
$R_{free}$ test set	1749 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.383	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% 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: ACT

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	0.44	0/1681	0.57	0/2268
1	B	0.41	0/1578	0.56	0/2122
All	All	0.42	0/3259	0.57	0/4390

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	1649	1569	1623	34	0
1	B	1551	1491	1531	32	0
2	A	4	3	3	0	0
2	B	4	3	3	2	0
3	A	170	0	0	15	3
3	B	155	0	0	21	1
All	All	3533	3066	3160	67	4

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 11.

All (67) 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:225:ARG:NH1	3:B:501:HOH:O	1.89	0.99
1:A:243:ASN:ND2	3:A:1401:HOH:O	1.91	0.86
1:A:148:PHE:N	3:A:1403:HOH:O	2.06	0.85
1:B:224:ASN:N	3:B:505:HOH:O	2.09	0.85
1:A:183:PHE:N	3:A:1405:HOH:O	2.11	0.83
1:B:276[B]:MSE:HE1	1:B:296:LEU:HD22	1.60	0.83
1:A:195:LYS:O	3:A:1402:HOH:O	2.00	0.80
1:B:316:PHE:O	3:B:502:HOH:O	2.00	0.79
1:B:179:SER:O	3:B:504:HOH:O	2.02	0.77
1:A:289:PRO:HB2	1:A:291:LEU:HD11	1.68	0.76
1:A:282:ASP:OD2	1:A:285:LYS:HB2	1.86	0.74
1:B:192:ASP:N	3:B:503:HOH:O	2.02	0.71
1:B:189:SER:OG	3:B:503:HOH:O	2.07	0.71
1:A:299:GLU:OE2	3:A:1404:HOH:O	2.09	0.70
1:B:225:ARG:HD3	3:B:501:HOH:O	1.93	0.69
1:B:149:ASP:O	3:B:506:HOH:O	2.10	0.68
1:A:181:THR:O	3:A:1405:HOH:O	2.12	0.66
1:A:284:PHE:O	1:A:285:LYS:HD2	1.95	0.66
1:A:275:GLU:OE2	1:A:277:LYS:NZ	2.29	0.64
1:B:272[B]:MSE:SE	3:B:614:HOH:O	2.65	0.63
1:B:100:ARG:CD	3:B:507:HOH:O	2.46	0.63
1:B:276[A]:MSE:SE	3:B:508:HOH:O	2.66	0.63
1:B:170:ASP:OD1	1:B:171:PHE:N	2.33	0.61
1:B:100:ARG:NE	3:B:507:HOH:O	2.36	0.59
1:A:179:SER:OG	1:A:181:THR:O	2.11	0.58
1:A:243:ASN:OD1	3:A:1407:HOH:O	2.17	0.58
1:A:272:MSE:HE3	3:A:1522:HOH:O	2.03	0.57
1:A:116:LYS:HZ1	1:A:207:ASN:CG	2.07	0.57
1:A:165:ASN:ND2	3:A:1415:HOH:O	2.37	0.57
1:B:159:MSE:HE2	1:B:162:LEU:HD13	1.87	0.56
1:B:189:SER:O	3:B:503:HOH:O	2.17	0.56
1:B:100:ARG:CZ	3:B:507:HOH:O	2.55	0.55
1:A:244:LYS:HD2	3:A:1419:HOH:O	2.07	0.55
1:B:119:LEU:HD21	1:B:276[A]:MSE:HE2	1.87	0.54
1:B:276[B]:MSE:CE	1:B:296:LEU:HD22	2.35	0.54
1:B:192:ASP:CB	3:B:503:HOH:O	2.55	0.54
1:B:309:LYS:HE3	1:B:313:GLN:OE1	2.10	0.52
1:B:100:ARG:HD2	3:B:507:HOH:O	2.08	0.51
1:A:100:ARG:HB3	1:A:101:PRO:CD	2.42	0.49
2:B:401:ACT:H1	3:B:619:HOH:O	2.12	0.49
1:A:276[A]:MSE:HE1	1:A:296:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:OD1	1:A:171:PHE:N	2.46	0.47
1:A:261:MSE:H	1:A:261:MSE:SE	2.48	0.47
1:A:284:PHE:C	1:A:285:LYS:HD2	2.34	0.47
1:B:119:LEU:HD21	1:B:276[A]:MSE:CE	2.45	0.47
1:A:289:PRO:HB2	1:A:291:LEU:CD1	2.42	0.47
1:A:290:ILE:CD1	1:A:299:GLU:HG3	2.46	0.46
1:B:276[B]:MSE:HG3	3:B:508:HOH:O	2.14	0.46
1:A:223:LEU:HB2	3:A:1430:HOH:O	2.15	0.46
1:A:272:MSE:CE	3:A:1522:HOH:O	2.64	0.45
1:A:225:ARG:NH2	3:A:1406:HOH:O	2.16	0.45
1:B:261:MSE:SE	1:B:261:MSE:H	2.51	0.44
1:B:192:ASP:CG	3:B:503:HOH:O	2.56	0.43
1:B:313:GLN:O	2:B:401:ACT:H3	2.18	0.43
1:A:110:GLY:O	1:A:116:LYS:HE2	2.19	0.43
1:A:275:GLU:OE1	3:A:1408:HOH:O	2.21	0.42
1:B:169:LYS:HE3	1:B:173:TYR:HE2	1.84	0.42
1:A:145:PRO:HB2	1:A:173:TYR:CE2	2.54	0.42
1:A:126:ALA:O	1:A:261:MSE:HE2	2.19	0.42
1:A:276[A]:MSE:CE	1:A:296:LEU:HD22	2.51	0.41
1:B:276[B]:MSE:HE1	1:B:296:LEU:CD2	2.40	0.41
1:B:314:PRO:HB2	3:B:502:HOH:O	2.21	0.41
1:A:224:ASN:ND2	3:A:1430:HOH:O	2.54	0.40
1:A:100:ARG:HB3	1:A:101:PRO:HD2	2.03	0.40
1:A:291:LEU:HD12	1:A:291:LEU:N	2.36	0.40
1:B:159:MSE:CE	1:B:162:LEU:HD13	2.52	0.40
1:B:293:VAL:HG23	3:B:562:HOH:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1425:HOH:O	3:A:1498:HOH:O[1_565]	1.67	0.53
3:A:1427:HOH:O	3:A:1474:HOH:O[1_545]	1.82	0.38
3:B:576:HOH:O	3:B:616:HOH:O[1_545]	1.93	0.27
3:A:1561:HOH:O	3:A:1564:HOH:O[1_655]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/223 (92%)	199 (97%)	7 (3%)	0	100	100
1	B	190/223 (85%)	184 (97%)	6 (3%)	0	100	100
All	All	396/446 (89%)	383 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	183/187 (98%)	180 (98%)	3 (2%)	62	49
1	B	171/187 (91%)	171 (100%)	0	100	100
All	All	354/374 (95%)	351 (99%)	3 (1%)	78	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	285	LYS
1	A	286	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

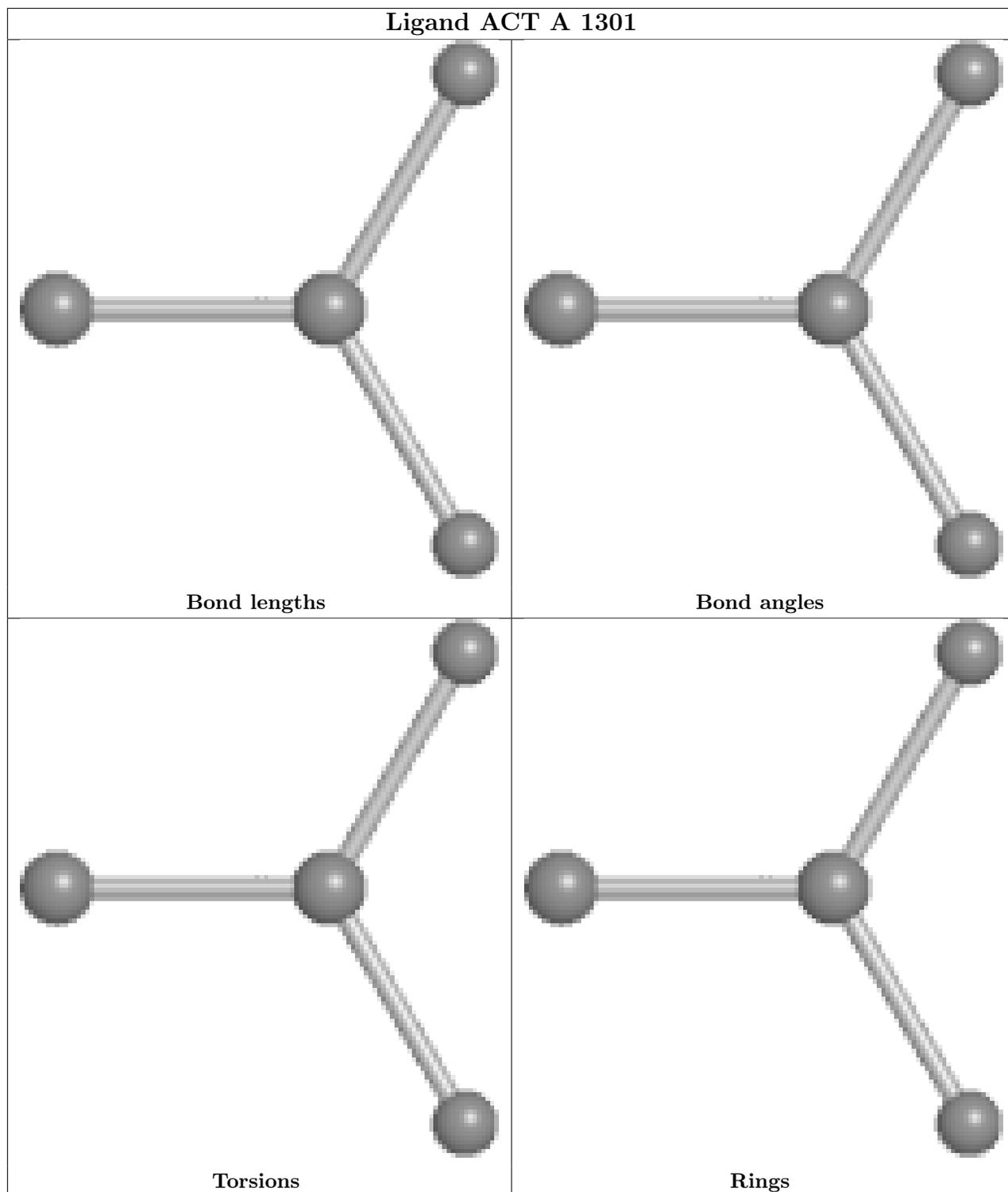
There are no chirality outliers.

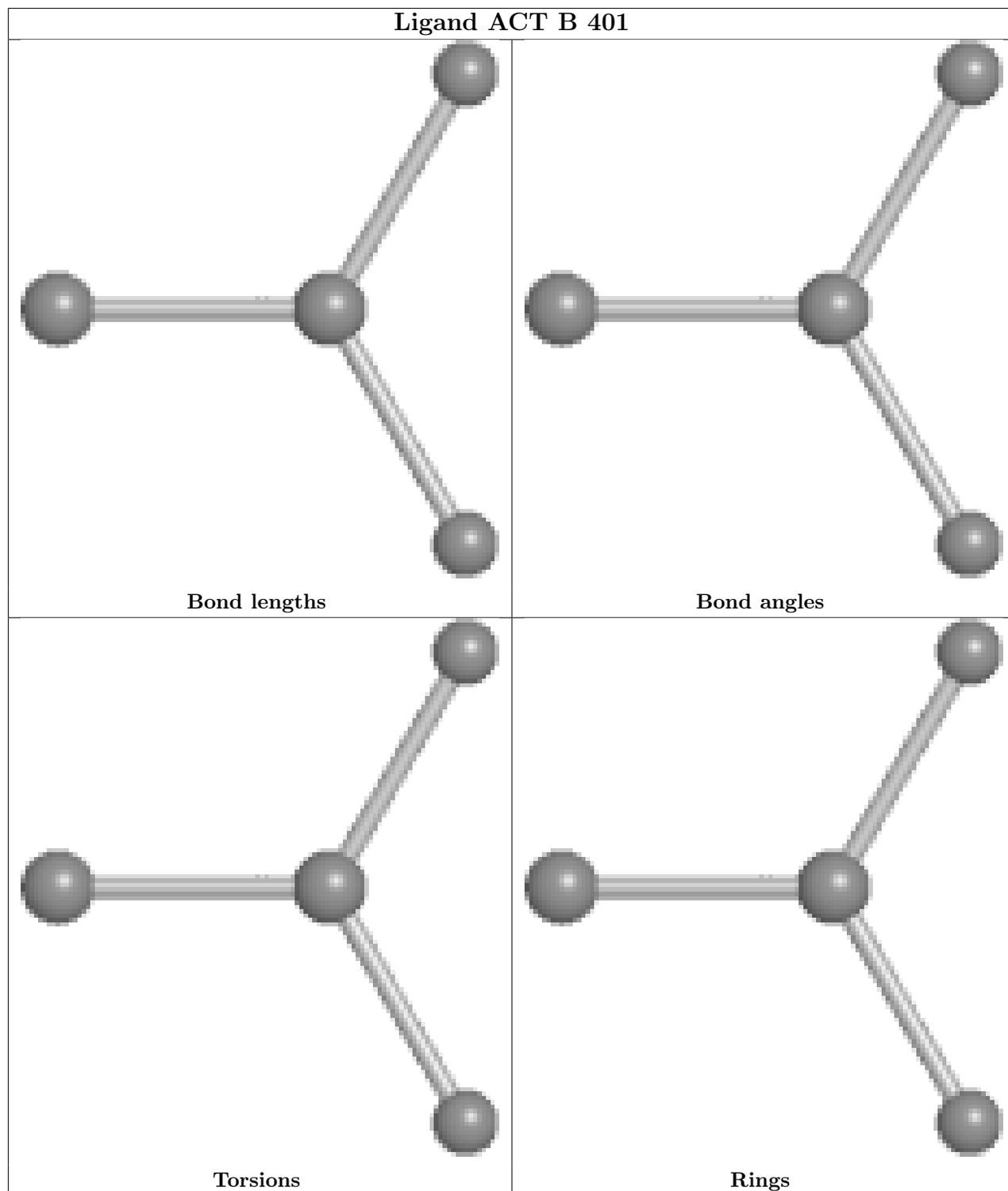
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	203/223 (91%)	0.39	14 (6%) 16 15	13, 27, 68, 85	0
1	B	190/223 (85%)	0.14	10 (5%) 26 24	14, 27, 62, 83	0
All	All	393/446 (88%)	0.27	24 (6%) 21 19	13, 27, 65, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	12.2
1	A	166	PRO	6.1
1	A	167	ASP	5.5
1	B	180	THR	4.5
1	A	283	VAL	4.2
1	A	223	LEU	3.6
1	B	181	THR	3.6
1	B	318	GLN	3.6
1	A	182	GLY	3.6
1	A	164	GLN	3.4
1	A	180	THR	3.4
1	A	281	GLN	3.3
1	A	169	LYS	2.9
1	A	147	HIS	2.9
1	A	168	GLY	2.8
1	B	178	VAL	2.7
1	B	182	GLY	2.6
1	B	146	ASP	2.5
1	B	225	ARG	2.5
1	B	100	ARG	2.4
1	A	285	LYS	2.4
1	B	168	GLY	2.2
1	B	147	HIS	2.1
1	A	179	SER	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](#)

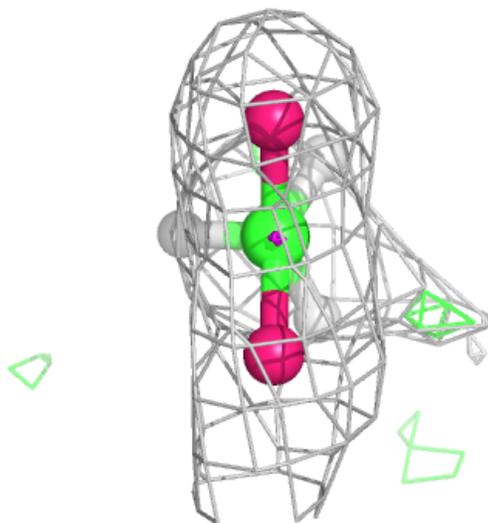
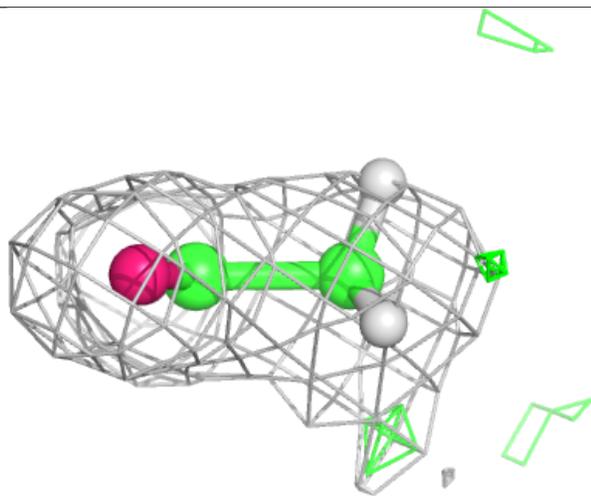
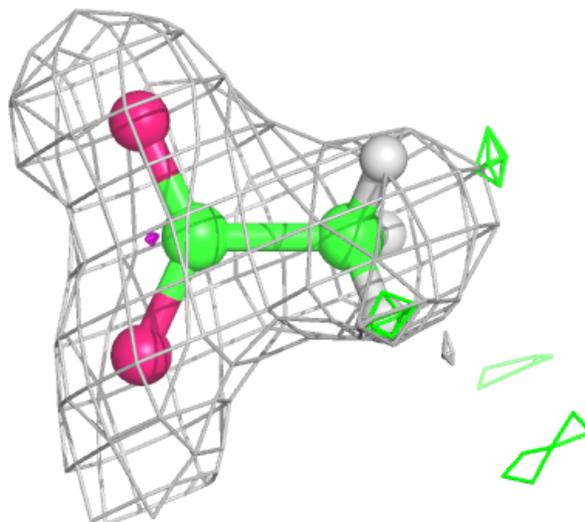
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

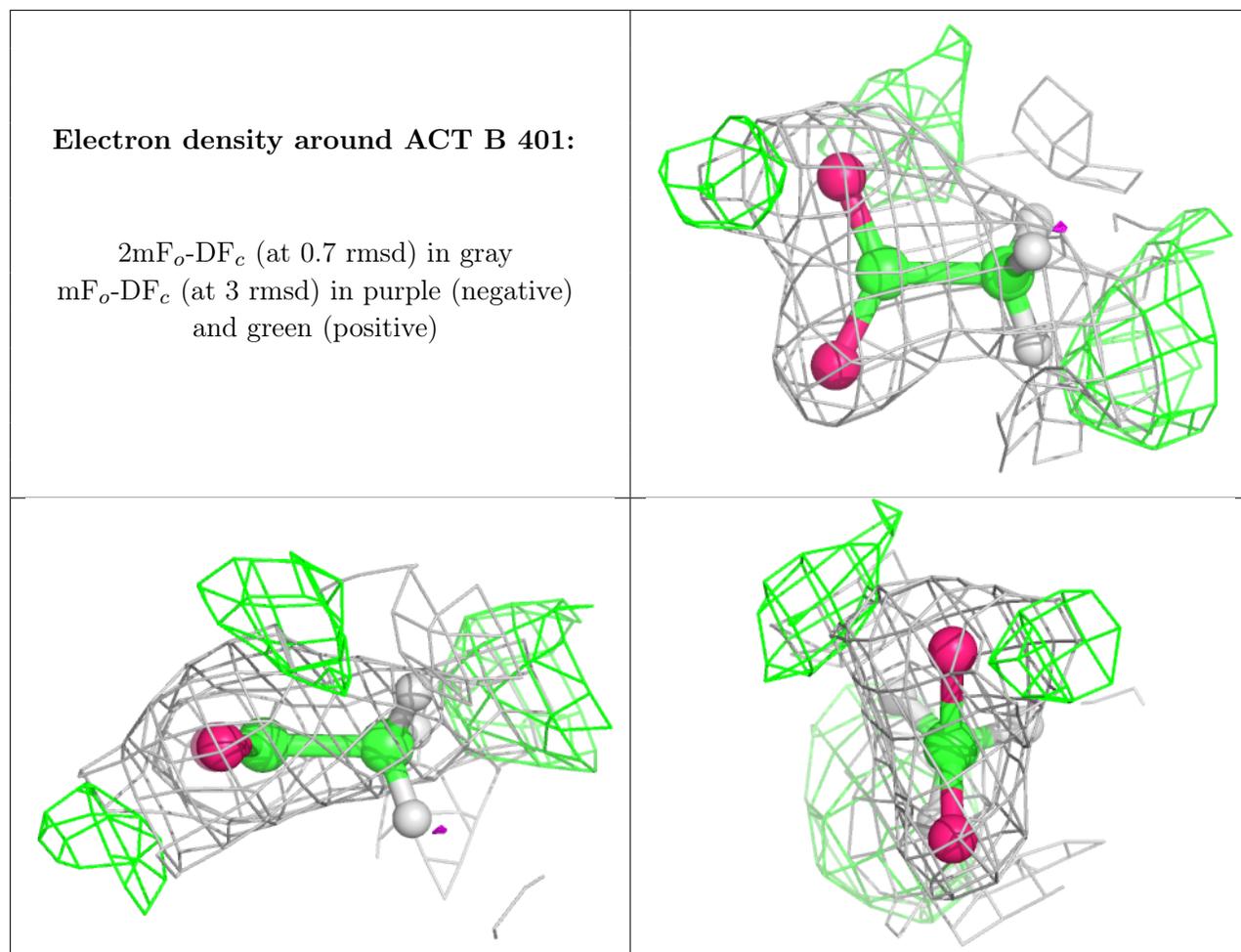
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	A	1301	4/4	0.85	0.13	30,34,36,36	0
2	ACT	B	401	4/4	0.88	0.17	33,40,40,42	0

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 ACT A 1301:**

$2mF_o-DF_c$  (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.