



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:53 am BST

PDB ID : 5A93  
Title : 293K Joint X-ray Neutron with Cefotaxime: EXPLORING THE MECHANISM OF BETA-LACTAM RING PROTONATION IN THE CLASS A BETA-LACTAMASE ACYLATION MECHANISM USING NEUTRON AND X-RAY CRYSTALLOGRAPHY  
Authors : Vandavasi, V.G.; Weiss, K.L.; Cooper, J.B.; Erskine, P.T.; Tomanicek, S.J.; Ostermann, A.; Schrader, T.E.; Ginell, S.L.; Coates, L.  
Deposited on : 2015-07-17  
Resolution : 1.60 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 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 : 2.11  
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) : 2.11

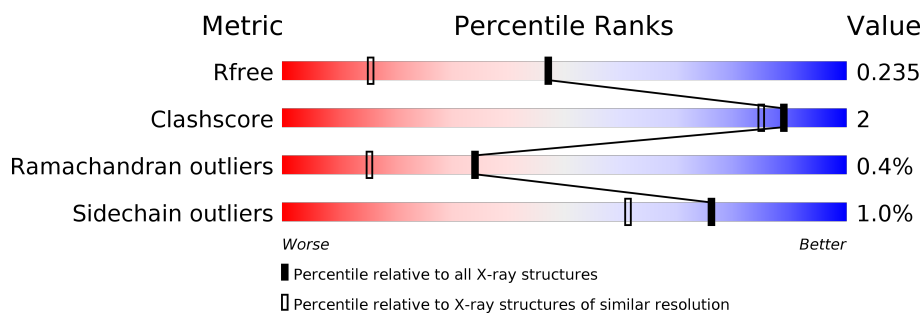
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*NEUTRON DIFFRACTION, X-RAY DIFFRACTION*

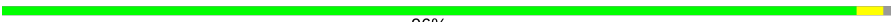
The reported resolution of this entry is 1.60 Å.

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 on 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	262	 96% ..

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	CEF	A	1291	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4452 atoms, of which 0 are hydrogens and 2109 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.

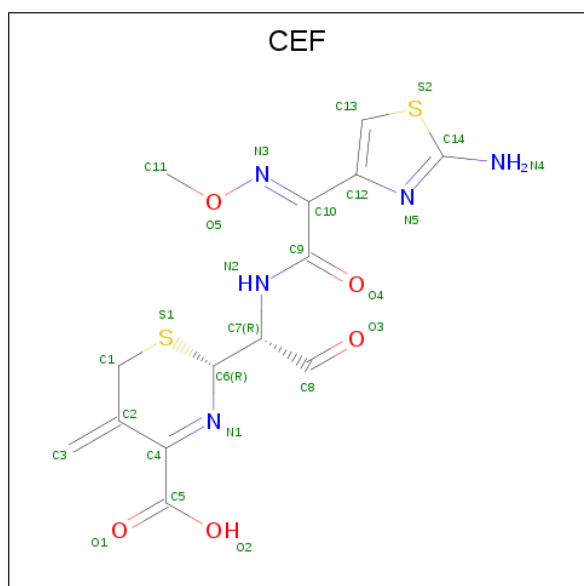
- Molecule 1 is a protein called BETA-LACTAMASE CTX-M-97.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	260	Total	C	D	N	O	S	0	21	0
			4163	1284	2109	359	404	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	GLU	engineered mutation	UNP E1ANH6
A	274	ASN	SER	conflict	UNP E1ANH6
A	276	ASN	ARG	conflict	UNP E1ANH6

- Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (three-letter code: CEF) (formula:  $C_{14}H_{15}N_5O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total	O	0	0
			238	238		

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

These plots are drawn for all protein, RNA and DNA 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. 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. 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: BETA-LACTAMASE CTX-M-97

Chain A:  96%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.31Å 73.31Å 98.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.50 – 1.60 14.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.50-1.60) 72.2 (14.72-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.133 , 0.156 0.221 , 0.235	Depositor DCC
$R_{free}$ test set	574 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.06 , -80.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.115 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: CEF, SO4

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	0/2152	0.76	1/2920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	275	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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	4163	0	2088	5	0
2	A	26	0	0	1	0
3	A	25	0	0	2	0
4	A	238	0	0	6	1
All	All	4452	0	2088	8	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 2.

All (8) 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)
2:A:1291:CEF:N4	4:A:2200:HOH:O	2.22	0.71
3:A:1293:SO4:O2	4:A:2234:HOH:O	2.16	0.63
1:A:146[B]:ASP:OD1	4:A:2104:HOH:O	2.18	0.62
1:A:259:LEU:HD11	1:A:290:PHE:CE2	2.37	0.54
1:A:259:LEU:HD11	1:A:290:PHE:HE2	1.66	0.50
1:A:218[A]:SER:OG	4:A:2185:HOH:O	2.23	0.49
3:A:1296:SO4:O2	4:A:2194:HOH:O	2.23	0.49
1:A:288:HIS:ND1	4:A:2231:HOH:O	2.40	0.46

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)
4:A:2028:HOH:O	4:A:2184:HOH:O[3_455]	2.11	0.09

## 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	279/262 (106%)	274 (98%)	4 (1%)	1 (0%)	34 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	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	229/209 (110%)	226 (99%)	3 (1%)	69 50

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

Mol	Chain	Res	Type
1	A	88	LYS
1	A	130[A]	SER
1	A	130[B]	SER

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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
3	SO4	A	1295	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	A	1292	-	4,4,4	0.26	0	6,6,6	0.52	0
3	SO4	A	1294	-	4,4,4	0.35	0	6,6,6	0.37	0
3	SO4	A	1293	-	4,4,4	0.44	0	6,6,6	0.88	0
2	CEF	A	1291	1	17,27,27	7.18	9 (52%)	11,37,37	4.17	8 (72%)
3	SO4	A	1296	-	4,4,4	0.19	0	6,6,6	0.11	0

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	CEF	A	1291	1	1/1/7/9	5/11/38/38	0/1/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1291	CEF	C4-N1	21.21	1.51	1.28
2	A	1291	CEF	C5-C4	-11.72	1.34	1.52
2	A	1291	CEF	C1-S1	-9.45	1.60	1.82
2	A	1291	CEF	C10-N3	8.98	1.43	1.29
2	A	1291	CEF	C4-C2	6.73	1.69	1.46
2	A	1291	CEF	C3-C2	5.43	1.44	1.32
2	A	1291	CEF	C7-N2	-4.23	1.40	1.46
2	A	1291	CEF	C9-N2	3.80	1.41	1.34
2	A	1291	CEF	C14-N4	2.70	1.43	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1291	CEF	C1-S1-C6	7.07	108.34	94.47
2	A	1291	CEF	C12-C13-S2	-6.39	103.94	111.79
2	A	1291	CEF	O4-C9-C10	5.42	126.59	120.35
2	A	1291	CEF	O5-N3-C10	-4.93	105.85	111.28
2	A	1291	CEF	O3-C8-C7	-4.07	113.49	124.83
2	A	1291	CEF	C7-N2-C9	-3.11	117.40	122.26
2	A	1291	CEF	C2-C1-S1	3.08	118.00	111.65
2	A	1291	CEF	O4-C9-N2	-2.12	119.37	123.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1291	CEF	C6

All (5) torsion outliers are listed below:

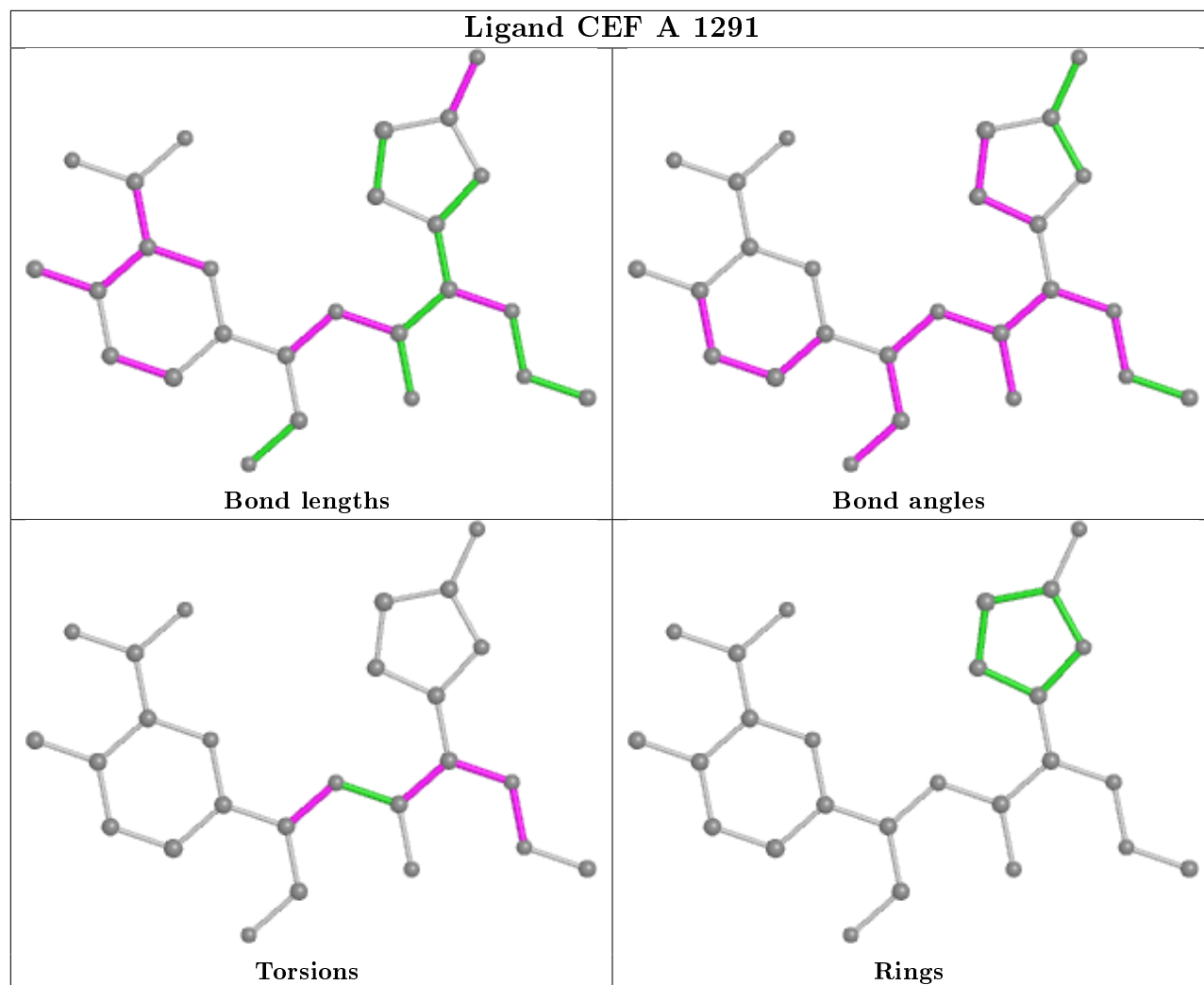
Mol	Chain	Res	Type	Atoms
2	A	1291	CEF	C12-C10-C9-N2
2	A	1291	CEF	C9-C10-N3-O5
2	A	1291	CEF	C10-N3-O5-C11
2	A	1291	CEF	C12-C10-C9-O4
2	A	1291	CEF	C8-C7-N2-C9

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1293	SO4	1	0
2	A	1291	CEF	1	0
3	A	1296	SO4	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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

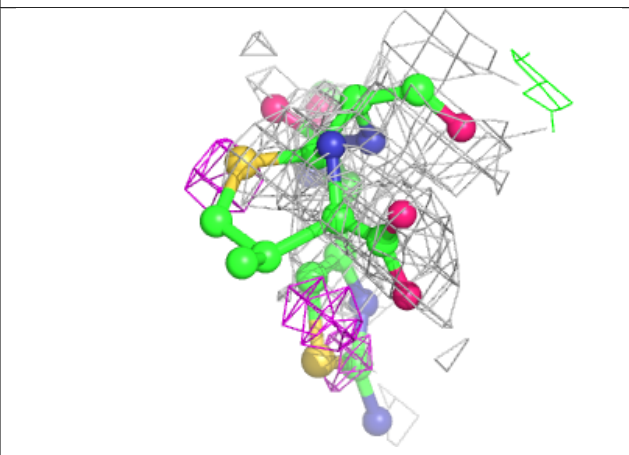
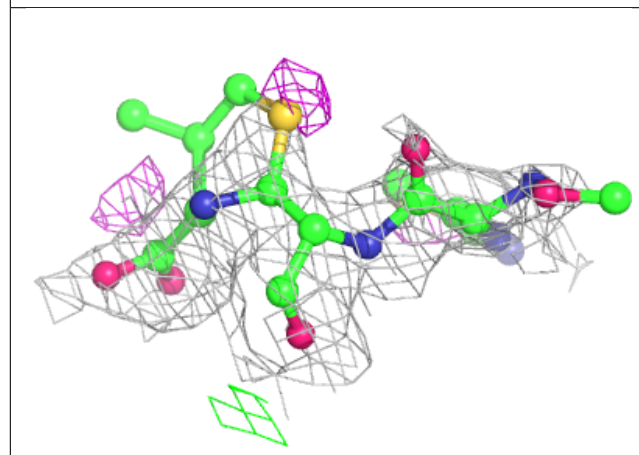
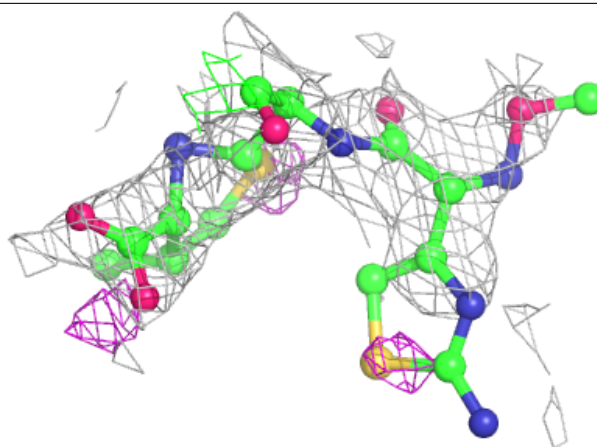
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 CEF A 1291:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.