



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 02:38 PM EDT

PDB ID : 8UUR / pdb\_00008uur  
Title : Structure of Serratia proteamaculans antifeeding prophage mini-fibre (AfpX13)  
Authors : Young, P.G.; Hurst, M.R.H.  
Deposited on : 2023-11-01  
Resolution : 2.50 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 Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

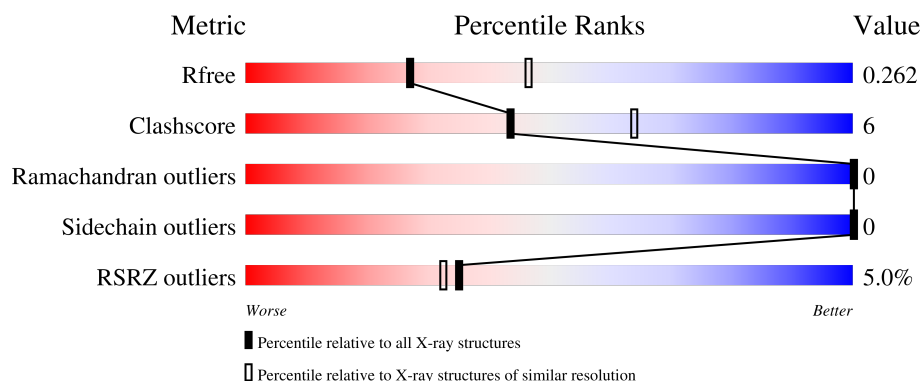
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


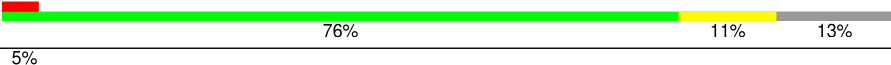
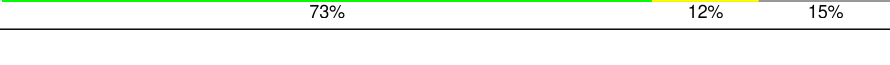
The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	278	
1	B	278	
1	C	278	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5383 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 AfpX13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1731	1084	295	342	10			
1	B	242	Total	C	N	O	S	0	0	0
			1727	1081	294	342	10			
1	C	236	Total	C	N	O	S	0	0	0
			1702	1069	290	333	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2R2Q2I2
A	2	ALA	-	expression tag	UNP A0A2R2Q2I2
B	1	GLY	-	expression tag	UNP A0A2R2Q2I2
B	2	ALA	-	expression tag	UNP A0A2R2Q2I2
C	1	GLY	-	expression tag	UNP A0A2R2Q2I2
C	2	ALA	-	expression tag	UNP A0A2R2Q2I2

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	66	Total 66	O 66	0	0
3	C	82	Total 82	O 82	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.56Å 68.41Å 132.76Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	45.47 – 2.50 45.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.47-2.50) 99.5 (45.47-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.217 , 0.264 0.218 , 0.262	Depositor DCC
$R_{free}$ test set	1860 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.038 for 1/2*h+3/2*k,1/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: CD

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	0/1758	0.58	0/2383
1	B	0.40	0/1754	0.64	0/2379
1	C	0.37	0/1725	0.64	0/2330
All	All	0.38	0/5237	0.62	0/7092

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	1731	0	1707	27	0
1	B	1727	0	1696	24	0
1	C	1702	0	1687	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	72	0	0	0	0
3	B	66	0	0	1	0
3	C	82	0	0	2	0
All	All	5383	0	5090	61	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 6.

All (61) 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:258:LEU:HD23	1:A:260:LYS:HE3	1.76	0.67
1:A:194:HIS:CE1	1:B:263:ILE:HD12	2.31	0.66
1:C:141:GLY:O	1:C:143:GLY:N	2.32	0.62
1:A:155:GLN:HG3	1:A:164:ASN:HB3	1.81	0.62
1:B:74:VAL:HG12	1:B:95:LEU:HD13	1.82	0.62
1:A:115:LYS:NZ	1:B:126:ALA:O	2.24	0.62
1:A:133:ALA:HB2	1:A:139:VAL:HG23	1.83	0.60
1:C:125:THR:HG22	1:C:126:ALA:H	1.65	0.60
1:B:171:MET:HE3	1:C:171:MET:HG3	1.85	0.57
1:A:119:SER:HB3	1:B:141:GLY:HA2	1.85	0.57
1:C:125:THR:HG22	1:C:126:ALA:N	2.23	0.54
1:A:171:MET:HE3	1:B:163:LEU:HD13	1.89	0.54
1:B:171:MET:HE3	1:C:171:MET:CG	2.38	0.54
1:A:171:MET:HA	1:A:171:MET:HE2	1.90	0.53
1:C:74:VAL:HG12	1:C:95:LEU:HD13	1.90	0.52
1:B:228:ILE:HD11	1:C:262:LEU:HD21	1.90	0.52
1:B:133:ALA:HB2	1:B:139:VAL:HG23	1.91	0.52
1:C:248:LYS:NZ	3:C:406:HOH:O	2.39	0.51
1:A:171:MET:HE1	1:B:167:ALA:HB3	1.93	0.51
1:C:184:ASP:O	1:C:205:ARG:NH1	2.40	0.50
1:B:215:GLY:HA2	1:B:223:ASP:OD1	2.12	0.50
1:A:161:VAL:HG12	1:C:154:LEU:HD12	1.95	0.49
1:A:65:ASP:OD2	1:C:46:LYS:NZ	2.42	0.49
1:B:53:SER:O	1:B:55:PRO:HD3	2.11	0.49
1:B:155:GLN:HG3	1:B:164:ASN:HB3	1.95	0.47
1:B:75:GLY:HA2	1:B:80:GLN:NE2	2.31	0.46
1:A:88:THR:HG23	1:A:96:GLU:HB2	1.97	0.46
1:C:212:MET:HB3	1:C:239:ALA:HB2	1.98	0.46
1:A:228:ILE:HB	1:A:241:MET:HB2	1.96	0.46
1:A:168:TRP:CE3	1:C:175:LEU:HA	2.51	0.46
1:B:165:ASN:ND2	3:B:407:HOH:O	2.48	0.46
1:C:38:ALA:HB1	3:C:461:HOH:O	2.15	0.45
1:C:171:MET:HA	1:C:171:MET:HE2	1.98	0.45
1:A:126:ALA:HA	1:C:102:ALA:HA	1.98	0.45
1:A:88:THR:CG2	1:A:96:GLU:HB2	2.48	0.44
1:A:227:ILE:HD11	1:A:239:ALA:CB	2.47	0.43
1:B:180:PHE:CD1	1:B:276:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:HG13	1:C:144:VAL:HG12	1.99	0.43
1:A:254:SER:HA	1:A:273:THR:HG22	2.01	0.43
1:A:197:GLY:HA3	1:A:244:TRP:O	2.18	0.43
1:C:182:VAL:HG22	1:C:189:VAL:HB	2.01	0.43
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.63	0.43
1:B:218:LYS:HB2	1:B:256:LYS:HB2	2.00	0.42
1:B:171:MET:HE1	1:C:167:ALA:HB1	2.00	0.42
1:A:43:ASP:OD1	1:A:43:ASP:N	2.52	0.42
1:C:180:PHE:CZ	1:C:250:ALA:HA	2.55	0.42
1:B:41:GLN:HG3	1:C:78:GLU:OE1	2.20	0.42
1:A:78:GLU:OE1	1:C:41:GLN:HG3	2.19	0.42
1:A:193:ASN:OD1	1:A:198:CYS:HB3	2.20	0.42
1:A:48:ARG:NH2	1:A:56:LEU:HD23	2.35	0.41
1:C:106:VAL:HG13	1:C:115:LYS:HD2	2.02	0.41
1:C:48:ARG:HA	1:C:48:ARG:HD2	1.91	0.41
1:B:261:ASN:OD1	1:B:261:ASN:C	2.63	0.41
1:C:57:GLN:HG3	1:C:58:THR:N	2.36	0.41
1:A:257:TYR:CE1	1:A:270:GLY:HA3	2.54	0.41
1:B:43:ASP:OD1	1:B:44:ALA:N	2.54	0.41
1:B:135:ASP:HB3	1:C:156:VAL:HG22	2.01	0.41
1:A:228:ILE:HD11	1:B:262:LEU:HD21	2.02	0.40
1:C:45:LEU:HA	1:C:45:LEU:HD23	1.91	0.40
1:C:172:MET:HE3	1:C:172:MET:HB3	1.83	0.40
1:A:55:PRO:HB2	1:A:60:PHE:CE2	2.56	0.40

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	240/278 (86%)	235 (98%)	5 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	240/278 (86%)	233 (97%)	7 (3%)	0	100	100
1	C	226/278 (81%)	218 (96%)	8 (4%)	0	100	100
All	All	706/834 (85%)	686 (97%)	20 (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	179/215 (83%)	179 (100%)	0	100	100
1	B	178/215 (83%)	178 (100%)	0	100	100
1	C	177/215 (82%)	177 (100%)	0	100	100
All	All	534/645 (83%)	534 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

### 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	242/278 (87%)	0.35	11 (4%) 39 36	25, 38, 63, 74	0
1	B	242/278 (87%)	0.38	11 (4%) 39 36	25, 38, 63, 78	0
1	C	236/278 (84%)	0.39	14 (5%) 29 27	27, 39, 63, 72	0
All	All	720/834 (86%)	0.37	36 (5%) 35 32	25, 38, 63, 78	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	ALA	4.5
1	C	141	GLY	4.4
1	C	118	ALA	4.1
1	B	150	ALA	4.0
1	C	121	GLY	3.4
1	C	120	LYS	3.4
1	B	141	GLY	3.3
1	B	131	VAL	3.0
1	C	140	ALA	3.0
1	C	54	ILE	2.9
1	C	143	GLY	2.9
1	B	142	THR	2.8
1	B	91	LEU	2.8
1	A	118	ALA	2.8
1	A	140	ALA	2.7
1	B	140	ALA	2.7
1	C	139	VAL	2.6
1	A	120	LYS	2.5
1	B	119	SER	2.5
1	A	79	GLY	2.5
1	C	38	ALA	2.5
1	A	142	THR	2.5
1	A	92	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	165	ASN	2.4
1	C	79	GLY	2.3
1	A	151	SER	2.3
1	A	38	ALA	2.2
1	A	150	ALA	2.2
1	B	109	LYS	2.2
1	A	121	GLY	2.2
1	C	234	GLY	2.2
1	B	118	ALA	2.2
1	C	269	SER	2.1
1	A	200	ALA	2.0
1	C	132	GLN	2.0
1	B	120	LYS	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](#)

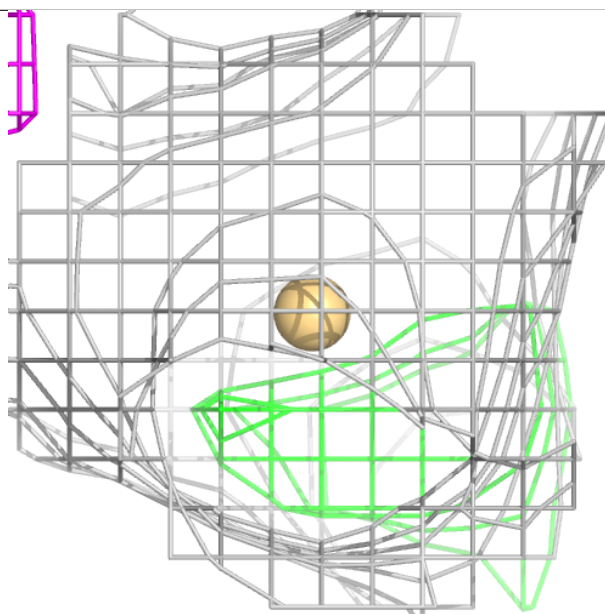
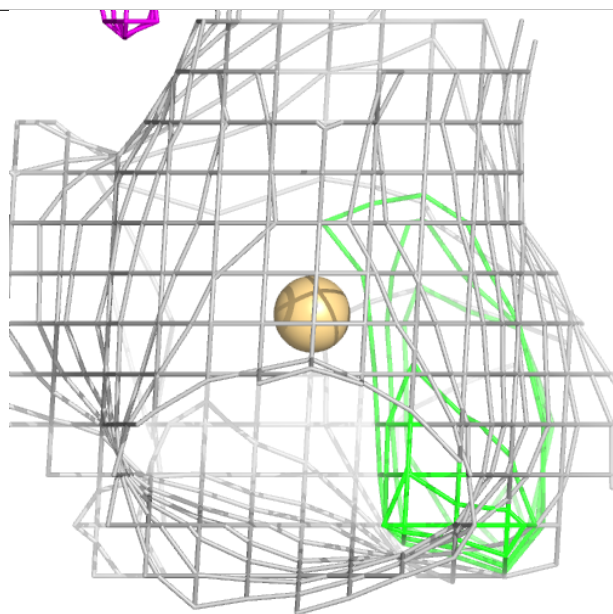
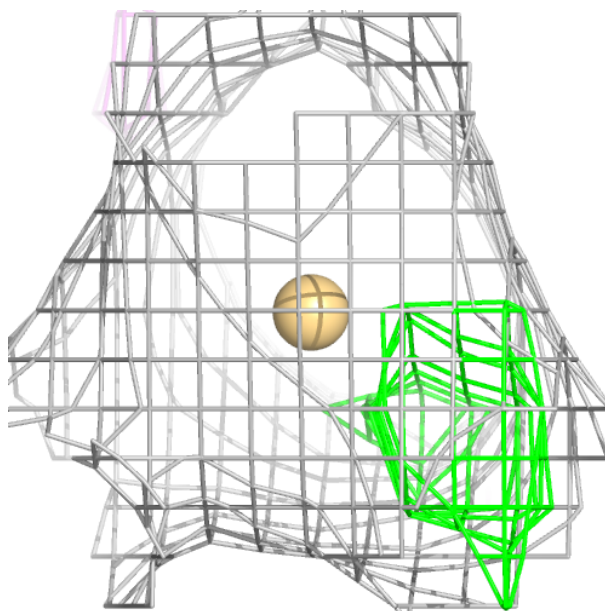
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CD	A	301	1/1	0.99	0.04	35,35,35,35	0
2	CD	B	301	1/1	1.00	0.04	34,34,34,34	0
2	CD	C	301	1/1	1.00	0.04	37,37,37,37	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.

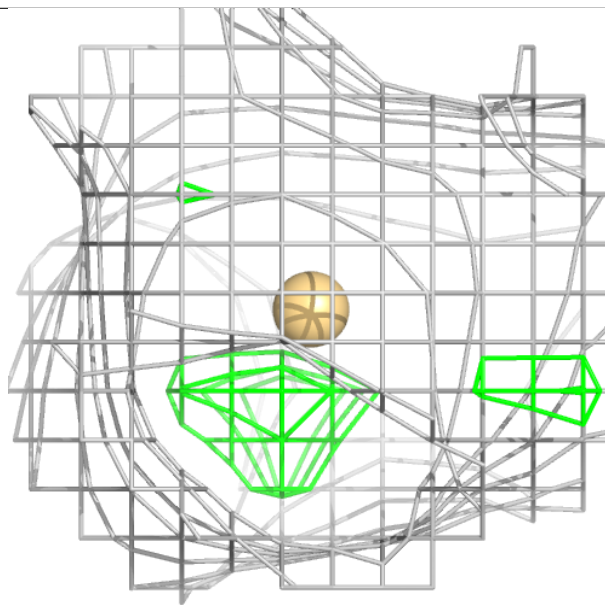
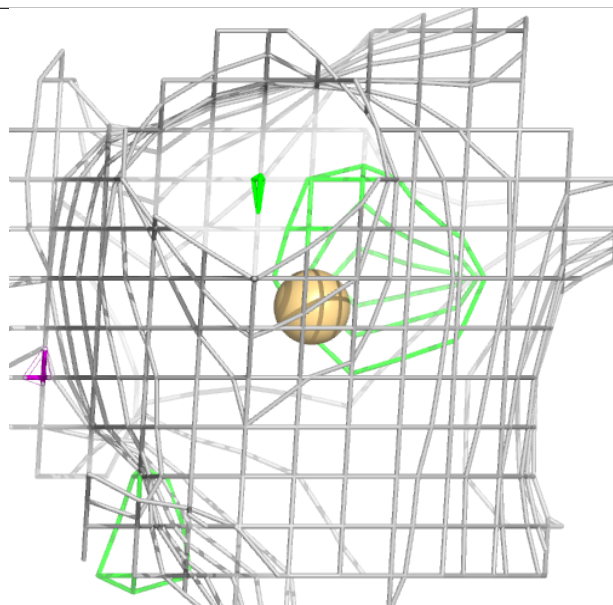
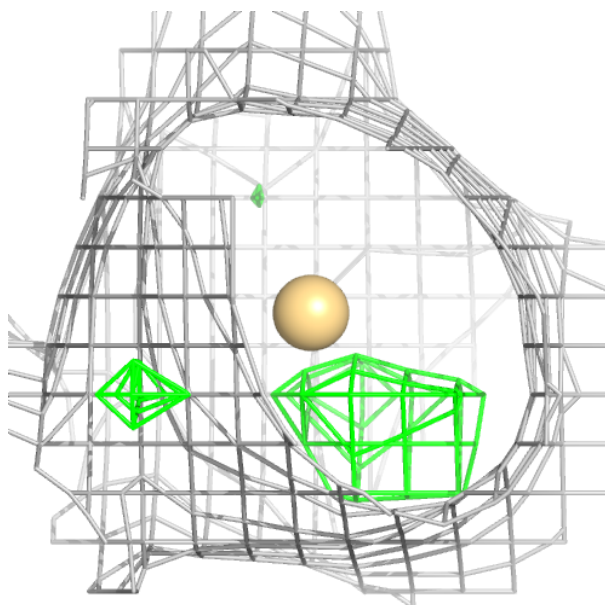
**Electron density around CD A 301:**

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



**Electron density around CD B 301:**

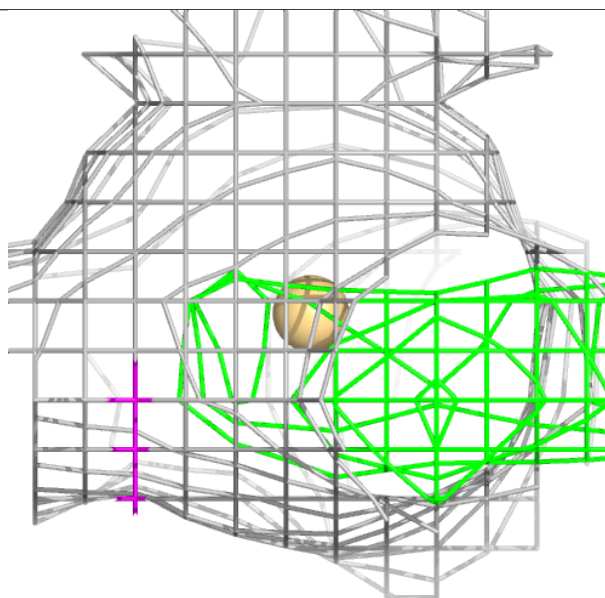
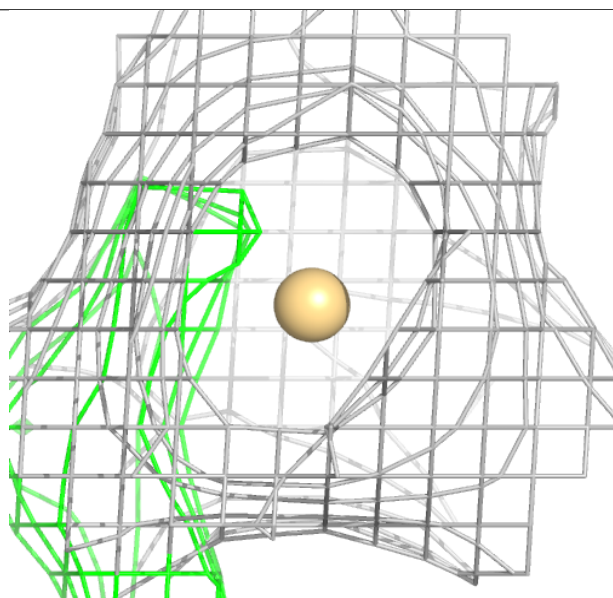
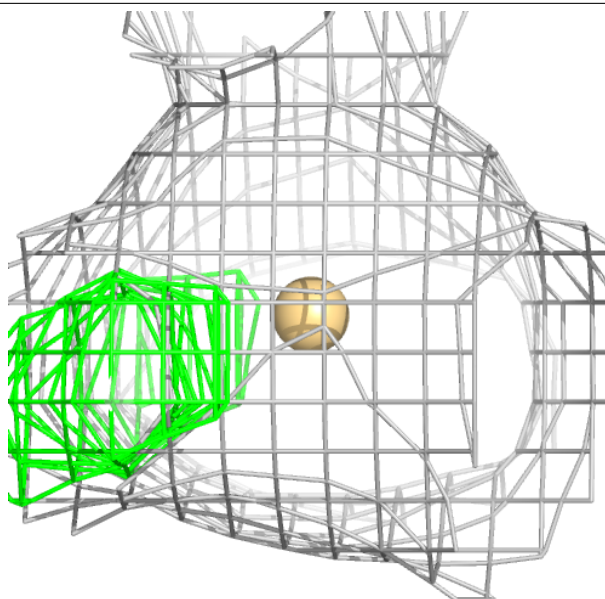
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CD C 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 ⓘ

There are no such residues in this entry.