



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2022 – 02:48 pm BST

PDB ID : 7PSG  
Title : Structure of the ligand binding domain of the PacA (ECA2226) chemoreceptor of *Pectobacterium atrosepticum* SCRI1043 in complex with betaine.  
Authors : Gavira, J.A.; Matilla, M.A.; Velando, F.; Krell, T.  
Deposited on : 2021-09-23  
Resolution : 1.91 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

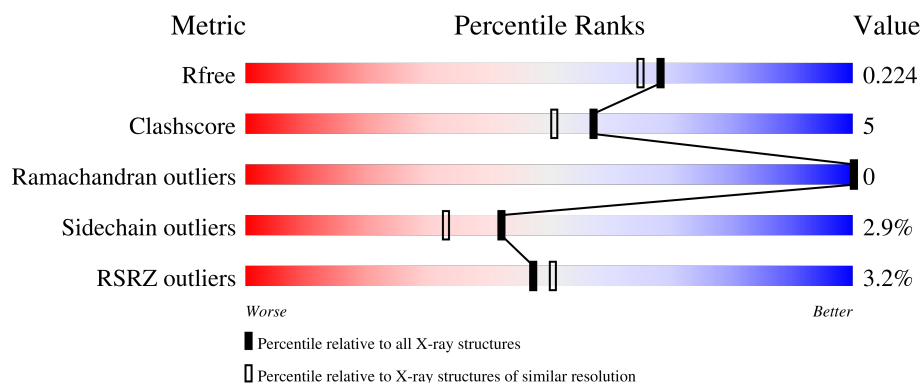
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

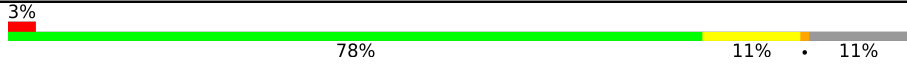



The reported resolution of this entry is 1.91 Å.

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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	301	
1	B	301	
1	C	301	
1	D	301	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17170 atoms, of which 8276 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 Methyl-accepting chemotaxis protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	H	N	O	S	0	10	0
			4213	1358	2080	353	417	5			
1	B	267	Total	C	H	N	O	S	0	4	0
			4136	1337	2038	349	407	5			
1	C	270	Total	C	H	N	O	S	0	1	0
			4111	1338	2006	353	409	5			
1	D	267	Total	C	H	N	O	S	0	6	0
			4183	1347	2076	349	406	5			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q6D515
A	-10	GLY	-	expression tag	UNP Q6D515
A	-9	SER	-	expression tag	UNP Q6D515
A	-8	SER	-	expression tag	UNP Q6D515
A	-7	HIS	-	expression tag	UNP Q6D515
A	-6	HIS	-	expression tag	UNP Q6D515
A	-5	HIS	-	expression tag	UNP Q6D515
A	-4	HIS	-	expression tag	UNP Q6D515
A	-3	HIS	-	expression tag	UNP Q6D515
A	-2	HIS	-	expression tag	UNP Q6D515
A	-1	SER	-	expression tag	UNP Q6D515
A	0	SER	-	expression tag	UNP Q6D515
A	1	GLY	-	expression tag	UNP Q6D515
A	2	LEU	-	expression tag	UNP Q6D515
A	3	VAL	-	expression tag	UNP Q6D515
A	4	PRO	-	expression tag	UNP Q6D515
A	5	ARG	-	expression tag	UNP Q6D515
A	6	GLY	-	expression tag	UNP Q6D515
A	7	SER	-	expression tag	UNP Q6D515
A	8	HIS	-	expression tag	UNP Q6D515
A	9	SER	-	expression tag	UNP Q6D515

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	TRP	-	expression tag	UNP Q6D515
A	11	GLN	-	expression tag	UNP Q6D515
A	12	SER	-	expression tag	UNP Q6D515
A	13	SER	-	expression tag	UNP Q6D515
A	14	SER	-	expression tag	UNP Q6D515
A	15	GLU	-	expression tag	UNP Q6D515
A	16	GLN	-	expression tag	UNP Q6D515
A	17	LYS	-	expression tag	UNP Q6D515
A	18	SER	-	expression tag	UNP Q6D515
A	19	LEU	-	expression tag	UNP Q6D515
B	-11	MET	-	initiating methionine	UNP Q6D515
B	-10	GLY	-	expression tag	UNP Q6D515
B	-9	SER	-	expression tag	UNP Q6D515
B	-8	SER	-	expression tag	UNP Q6D515
B	-7	HIS	-	expression tag	UNP Q6D515
B	-6	HIS	-	expression tag	UNP Q6D515
B	-5	HIS	-	expression tag	UNP Q6D515
B	-4	HIS	-	expression tag	UNP Q6D515
B	-3	HIS	-	expression tag	UNP Q6D515
B	-2	HIS	-	expression tag	UNP Q6D515
B	-1	SER	-	expression tag	UNP Q6D515
B	0	SER	-	expression tag	UNP Q6D515
B	1	GLY	-	expression tag	UNP Q6D515
B	2	LEU	-	expression tag	UNP Q6D515
B	3	VAL	-	expression tag	UNP Q6D515
B	4	PRO	-	expression tag	UNP Q6D515
B	5	ARG	-	expression tag	UNP Q6D515
B	6	GLY	-	expression tag	UNP Q6D515
B	7	SER	-	expression tag	UNP Q6D515
B	8	HIS	-	expression tag	UNP Q6D515
B	9	SER	-	expression tag	UNP Q6D515
B	10	TRP	-	expression tag	UNP Q6D515
B	11	GLN	-	expression tag	UNP Q6D515
B	12	SER	-	expression tag	UNP Q6D515
B	13	SER	-	expression tag	UNP Q6D515
B	14	SER	-	expression tag	UNP Q6D515
B	15	GLU	-	expression tag	UNP Q6D515
B	16	GLN	-	expression tag	UNP Q6D515
B	17	LYS	-	expression tag	UNP Q6D515
B	18	SER	-	expression tag	UNP Q6D515
B	19	LEU	-	expression tag	UNP Q6D515
C	-11	MET	-	initiating methionine	UNP Q6D515

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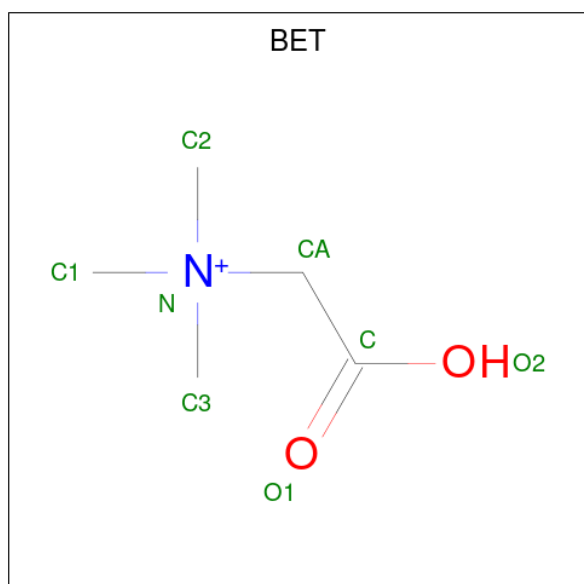
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP Q6D515
C	-9	SER	-	expression tag	UNP Q6D515
C	-8	SER	-	expression tag	UNP Q6D515
C	-7	HIS	-	expression tag	UNP Q6D515
C	-6	HIS	-	expression tag	UNP Q6D515
C	-5	HIS	-	expression tag	UNP Q6D515
C	-4	HIS	-	expression tag	UNP Q6D515
C	-3	HIS	-	expression tag	UNP Q6D515
C	-2	HIS	-	expression tag	UNP Q6D515
C	-1	SER	-	expression tag	UNP Q6D515
C	0	SER	-	expression tag	UNP Q6D515
C	1	GLY	-	expression tag	UNP Q6D515
C	2	LEU	-	expression tag	UNP Q6D515
C	3	VAL	-	expression tag	UNP Q6D515
C	4	PRO	-	expression tag	UNP Q6D515
C	5	ARG	-	expression tag	UNP Q6D515
C	6	GLY	-	expression tag	UNP Q6D515
C	7	SER	-	expression tag	UNP Q6D515
C	8	HIS	-	expression tag	UNP Q6D515
C	9	SER	-	expression tag	UNP Q6D515
C	10	TRP	-	expression tag	UNP Q6D515
C	11	GLN	-	expression tag	UNP Q6D515
C	12	SER	-	expression tag	UNP Q6D515
C	13	SER	-	expression tag	UNP Q6D515
C	14	SER	-	expression tag	UNP Q6D515
C	15	GLU	-	expression tag	UNP Q6D515
C	16	GLN	-	expression tag	UNP Q6D515
C	17	LYS	-	expression tag	UNP Q6D515
C	18	SER	-	expression tag	UNP Q6D515
C	19	LEU	-	expression tag	UNP Q6D515
D	-11	MET	-	initiating methionine	UNP Q6D515
D	-10	GLY	-	expression tag	UNP Q6D515
D	-9	SER	-	expression tag	UNP Q6D515
D	-8	SER	-	expression tag	UNP Q6D515
D	-7	HIS	-	expression tag	UNP Q6D515
D	-6	HIS	-	expression tag	UNP Q6D515
D	-5	HIS	-	expression tag	UNP Q6D515
D	-4	HIS	-	expression tag	UNP Q6D515
D	-3	HIS	-	expression tag	UNP Q6D515
D	-2	HIS	-	expression tag	UNP Q6D515
D	-1	SER	-	expression tag	UNP Q6D515
D	0	SER	-	expression tag	UNP Q6D515

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP Q6D515
D	2	LEU	-	expression tag	UNP Q6D515
D	3	VAL	-	expression tag	UNP Q6D515
D	4	PRO	-	expression tag	UNP Q6D515
D	5	ARG	-	expression tag	UNP Q6D515
D	6	GLY	-	expression tag	UNP Q6D515
D	7	SER	-	expression tag	UNP Q6D515
D	8	HIS	-	expression tag	UNP Q6D515
D	9	SER	-	expression tag	UNP Q6D515
D	10	TRP	-	expression tag	UNP Q6D515
D	11	GLN	-	expression tag	UNP Q6D515
D	12	SER	-	expression tag	UNP Q6D515
D	13	SER	-	expression tag	UNP Q6D515
D	14	SER	-	expression tag	UNP Q6D515
D	15	GLU	-	expression tag	UNP Q6D515
D	16	GLN	-	expression tag	UNP Q6D515
D	17	LYS	-	expression tag	UNP Q6D515
D	18	SER	-	expression tag	UNP Q6D515
D	19	LEU	-	expression tag	UNP Q6D515

- Molecule 2 is TRIMETHYL GLYCINE (three-letter code: BET) (formula:  $C_5H_{12}NO_2$ ) (labeled as "Ligand of Interest" by depositor).



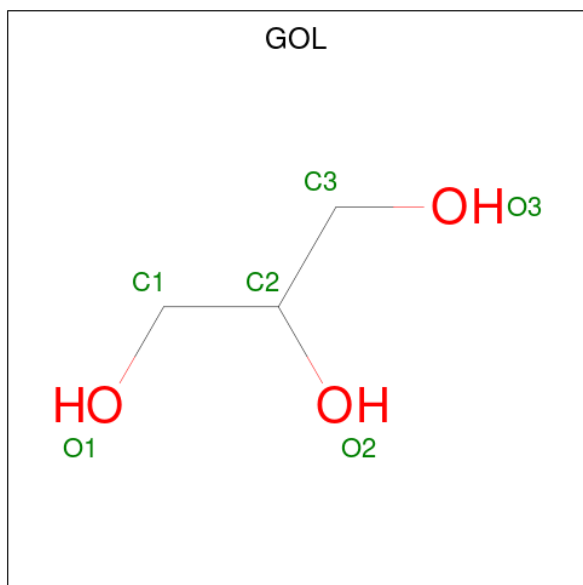
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			19	5	11	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			19	5	11	1	2		
2	C	1	Total	C	H	N	O	0	0
			19	5	11	1	2		
2	D	1	Total	C	H	N	O	0	0
			19	5	11	1	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	88	Total	O	0	0
			88	88		

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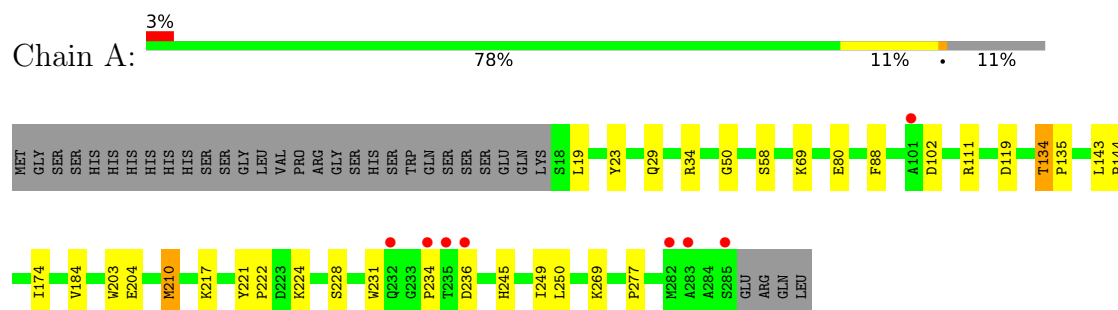
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	120	Total 120	O 120	0	0
4	D	100	Total 100	O 100	0	0



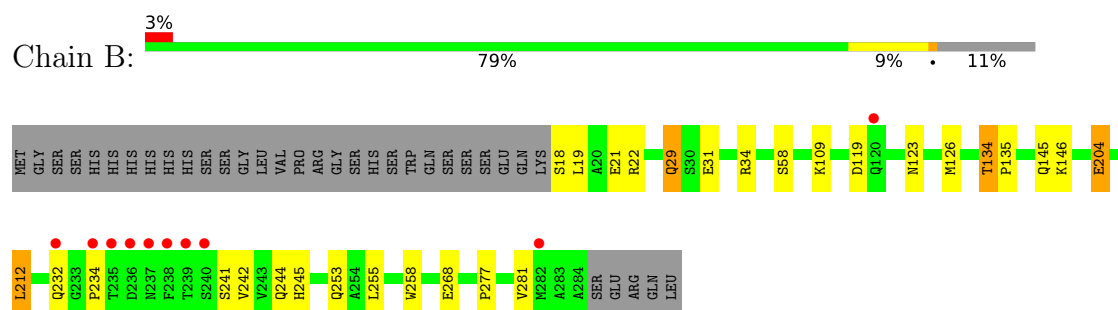
### 3 Residue-property plots [i](#)

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.

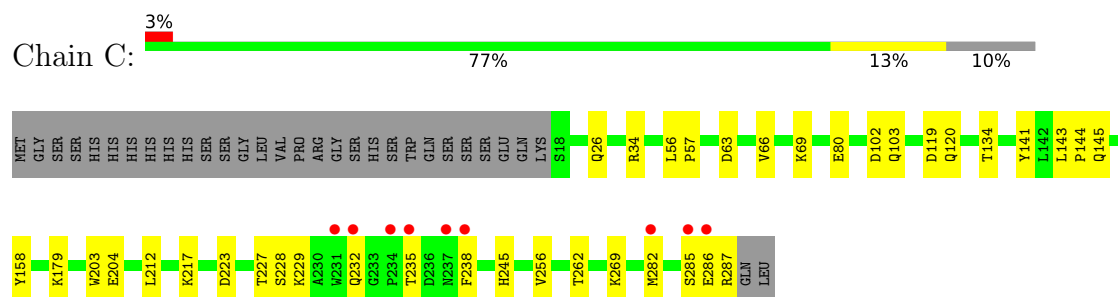
- Molecule 1: Methyl-accepting chemotaxis protein



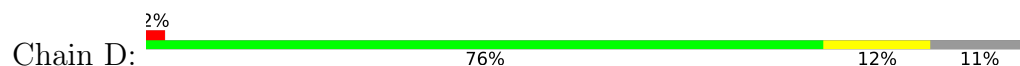
- Molecule 1: Methyl-accepting chemotaxis protein

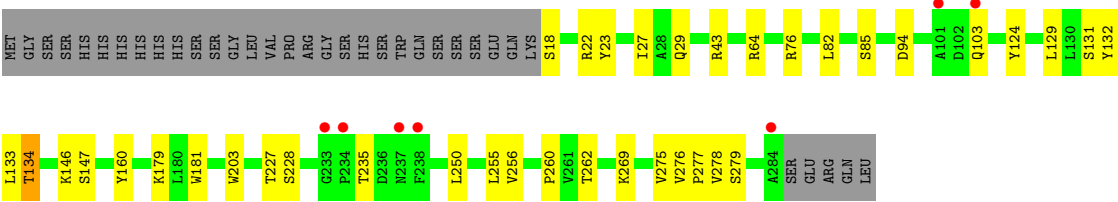


- Molecule 1: Methyl-accepting chemotaxis protein



- Molecule 1: Methyl-accepting chemotaxis protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.78Å 83.44Å 94.91Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	39.99 – 1.91 61.45 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.99-1.91) 98.2 (61.45-1.91)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.19-4092	Depositor
R, $R_{free}$	0.185 , 0.227 0.183 , 0.224	Depositor DCC
$R_{free}$ test set	4628 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtrriage
Anisotropy	0.423	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: BET, GOL

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	0.51	0/2213	0.72	1/3016 (0.0%)
1	B	0.57	0/2160	0.77	3/2944 (0.1%)
1	C	0.53	0/2157	0.76	0/2939
1	D	0.51	0/2174	0.73	0/2963
All	All	0.53	0/8704	0.75	4/11862 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204[A]	GLU	C-N-CA	-7.63	106.28	122.30
1	B	204[B]	GLU	C-N-CA	-7.63	106.28	122.30
1	B	126	MET	CG-SD-CE	5.44	108.90	100.20
1	A	210	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLN	Sidechain

## CLOSE-CONTACTS INFOmissingINFO

## 5.2 Torsion angles ⓘ

## 5.2.1 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	276/301 (92%)	270 (98%)	6 (2%)	0	100	100
1	B	269/301 (89%)	264 (98%)	5 (2%)	0	100	100
1	C	269/301 (89%)	264 (98%)	5 (2%)	0	100	100
1	D	271/301 (90%)	265 (98%)	6 (2%)	0	100	100
All	All	1085/1204 (90%)	1063 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

## 5.2.2 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	231/251 (92%)	221 (96%)	10 (4%)	29	18
1	B	224/251 (89%)	219 (98%)	5 (2%)	52	45
1	C	224/251 (89%)	216 (96%)	8 (4%)	35	24
1	D	226/251 (90%)	220 (97%)	6 (3%)	44	36
All	All	905/1004 (90%)	876 (97%)	29 (3%)	42	29

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	102	ASP
1	A	119[A]	ASP
1	A	119[B]	ASP
1	A	134	THR
1	A	224	LYS
1	A	228	SER
1	A	236[A]	ASP
1	A	236[B]	ASP
1	A	269	LYS
1	B	58	SER
1	B	134	THR
1	B	212	LEU
1	B	232	GLN
1	B	241	SER
1	C	69	LYS
1	C	102	ASP
1	C	119	ASP
1	C	134	THR
1	C	217	LYS
1	C	223	ASP
1	C	285	SER
1	C	287	ARG
1	D	43	ARG
1	D	103[A]	GLN
1	D	103[B]	GLN
1	D	134	THR
1	D	235	THR
1	D	279	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	GLN
1	B	195	GLN
1	C	25	GLN
1	C	245	HIS
1	D	29	GLN

### 5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.4 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

8 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	$\# Z  > 2$
2	BET	D	301	-	4,7,7	1.78	1 (25%)	7,10,10	0.88	0
2	BET	C	301	-	4,7,7	1.68	1 (25%)	7,10,10	0.94	0
3	GOL	C	302	-	5,5,5	1.03	1 (20%)	5,5,5	1.15	1 (20%)
2	BET	B	301	-	4,7,7	1.61	0	7,10,10	0.82	0
3	GOL	B	302	-	5,5,5	0.98	0	5,5,5	1.19	1 (20%)
2	BET	A	301	-	4,7,7	1.48	0	7,10,10	0.77	0
3	GOL	A	302	-	5,5,5	1.06	0	5,5,5	1.06	1 (20%)
3	GOL	D	302	-	5,5,5	0.96	0	5,5,5	1.33	1 (20%)

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	BET	D	301	-	-	3/3/5/5	-
2	BET	C	301	-	-	0/3/5/5	-
3	GOL	C	302	-	-	2/4/4/4	-
2	BET	B	301	-	-	0/3/5/5	-
3	GOL	B	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BET	A	301	-	-	0/3/5/5	-
3	GOL	A	302	-	-	0/4/4/4	-
3	GOL	D	302	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	BET	CA-N	-2.53	1.45	1.52
2	C	301	BET	CA-N	-2.08	1.46	1.52
3	C	302	GOL	C1-C2	2.04	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	GOL	C3-C2-C1	-2.49	102.03	111.70
3	B	302	GOL	C3-C2-C1	-2.17	103.27	111.70
3	C	302	GOL	C3-C2-C1	-2.08	103.62	111.70
3	A	302	GOL	C3-C2-C1	-2.07	103.66	111.70

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	D	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-O2
2	D	301	BET	C-CA-N-C3
3	B	302	GOL	O1-C1-C2-C3
2	D	301	BET	C-CA-N-C1
2	D	301	BET	C-CA-N-C2
3	B	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
3	D	302	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	BET	1	0

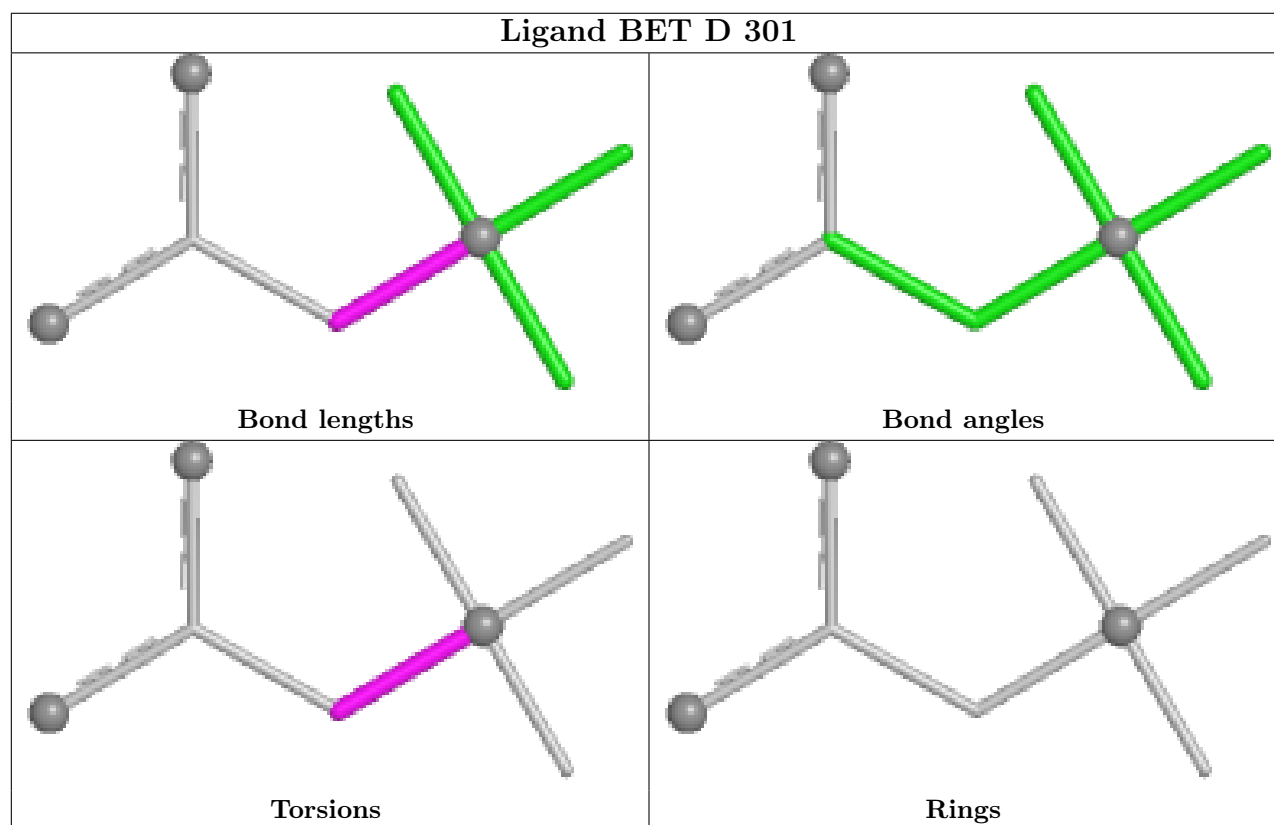
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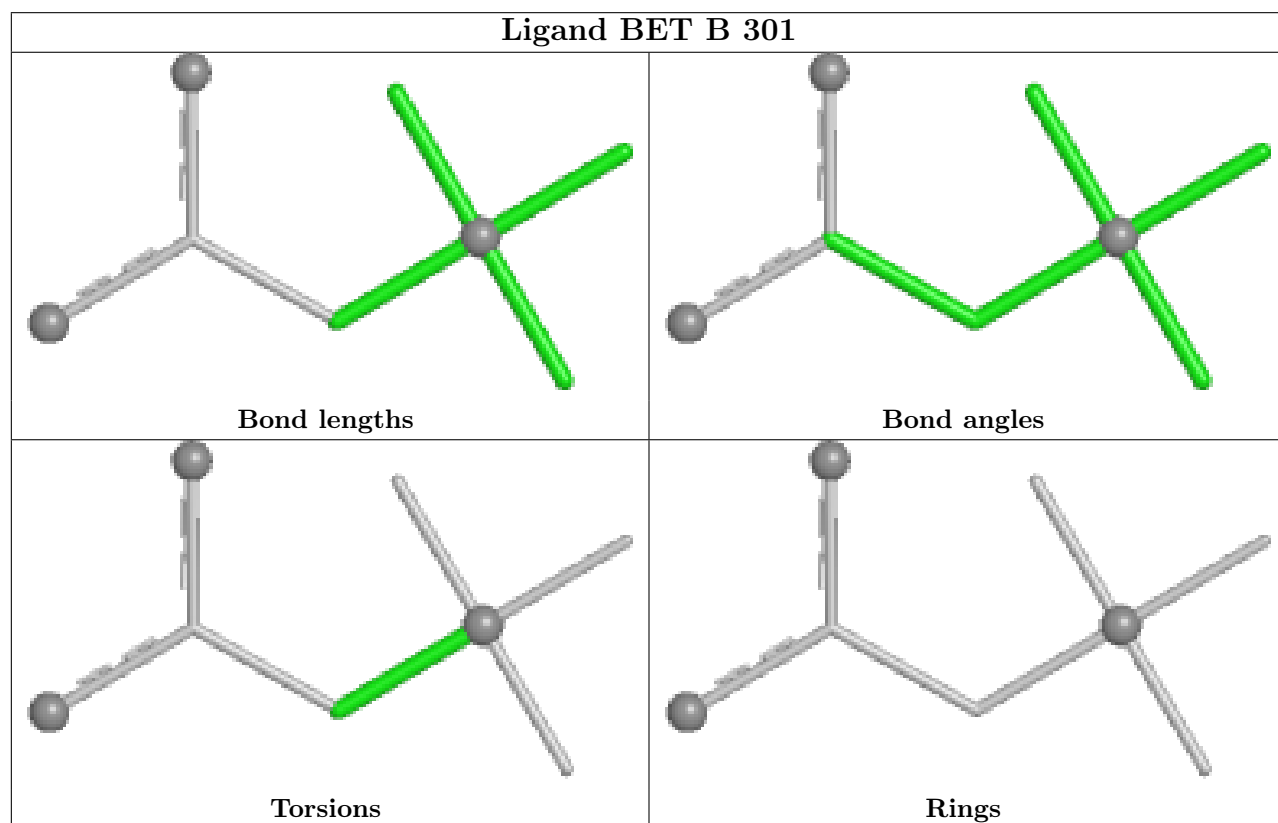
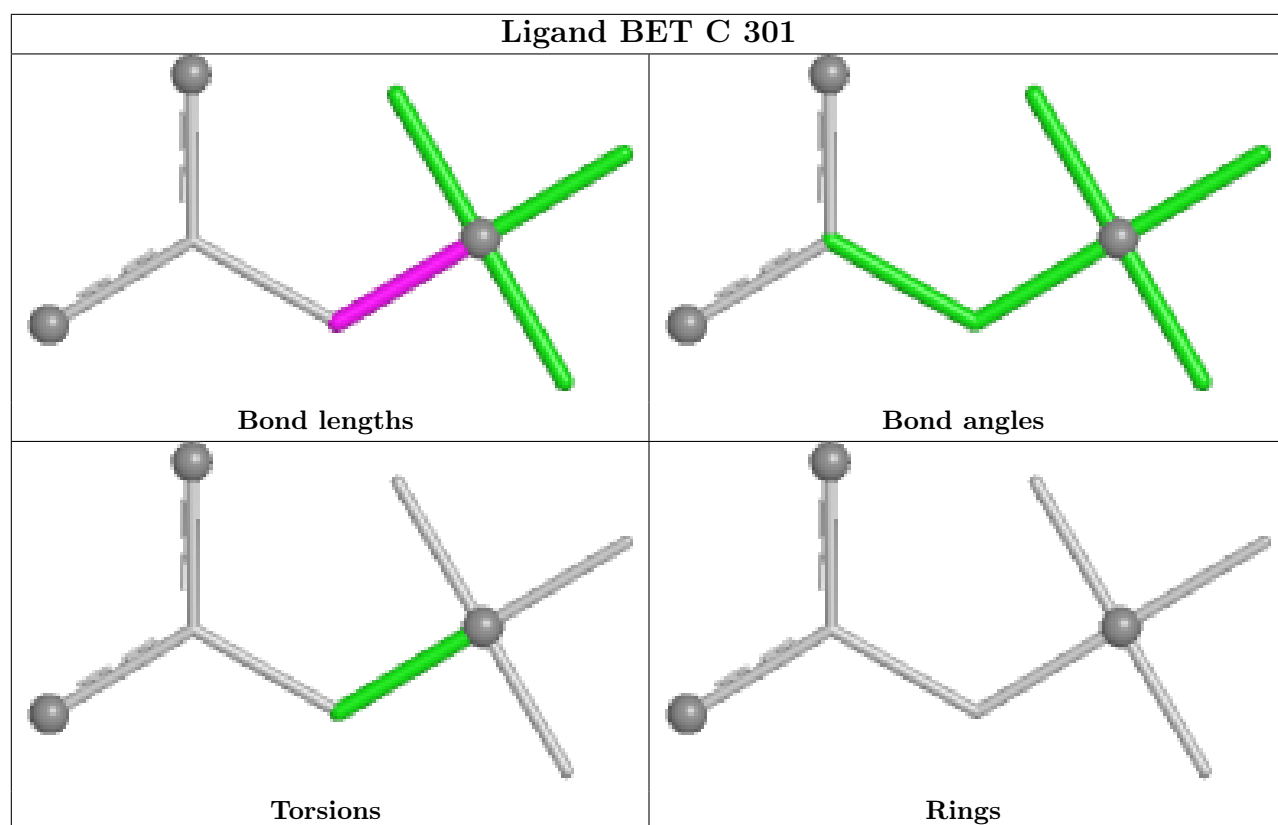


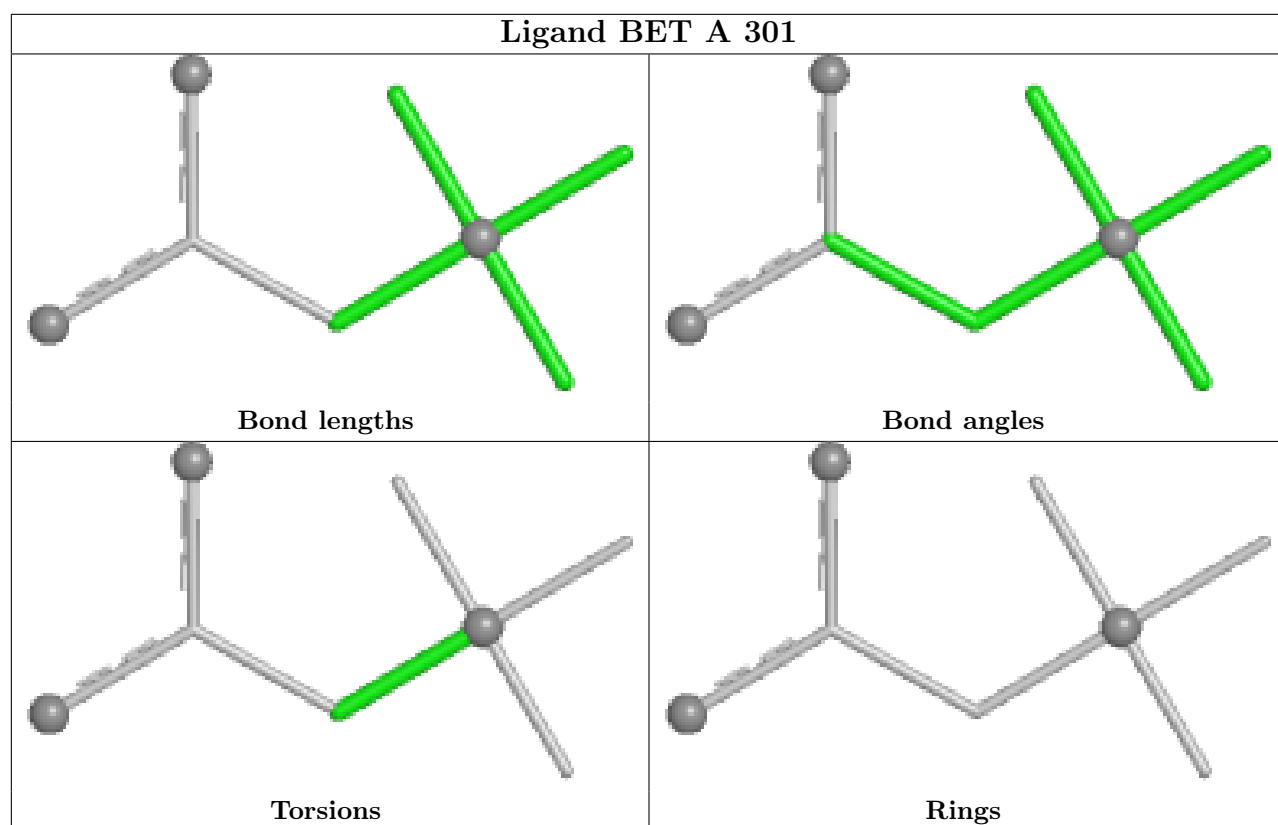
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	BET	1	0
2	A	301	BET	1	0

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.







## 5.6 Other polymers [i](#)

There are no such residues in this entry.

## 5.7 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	268/301 (89%)	-0.02	8 (2%) 50 53	36, 49, 80, 107	0
1	B	267/301 (88%)	0.15	10 (3%) 41 44	35, 51, 94, 109	0
1	C	270/301 (89%)	0.03	9 (3%) 46 49	33, 46, 86, 113	0
1	D	267/301 (88%)	0.02	7 (2%) 56 59	34, 49, 89, 109	0
All	All	1072/1204 (89%)	0.05	34 (3%) 47 50	33, 49, 88, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	234	PRO	7.1
1	C	238	PHE	7.0
1	A	234	PRO	6.3
1	C	234	PRO	6.0
1	A	285	SER	4.9
1	A	282	MET	4.7
1	B	234	PRO	4.6
1	B	282	MET	4.5
1	B	236	ASP	4.5
1	C	235	THR	3.9
1	A	101	ALA	3.8
1	C	286	GLU	3.8
1	B	237	ASN	3.7
1	B	232	GLN	3.5
1	A	236[A]	ASP	3.5
1	A	283	ALA	3.2
1	D	101	ALA	3.0
1	D	238	PHE	2.7
1	B	239	THR	2.6
1	D	237	ASN	2.5
1	D	103[A]	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	240	SER	2.4
1	C	232	GLN	2.3
1	C	237	ASN	2.3
1	B	120	GLN	2.3
1	B	235	THR	2.3
1	A	232[A]	GLN	2.2
1	C	282	MET	2.2
1	C	231	TRP	2.2
1	D	284	ALA	2.2
1	C	285	SER	2.1
1	A	235	THR	2.1
1	B	238	PHE	2.1
1	D	233	GLY	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.

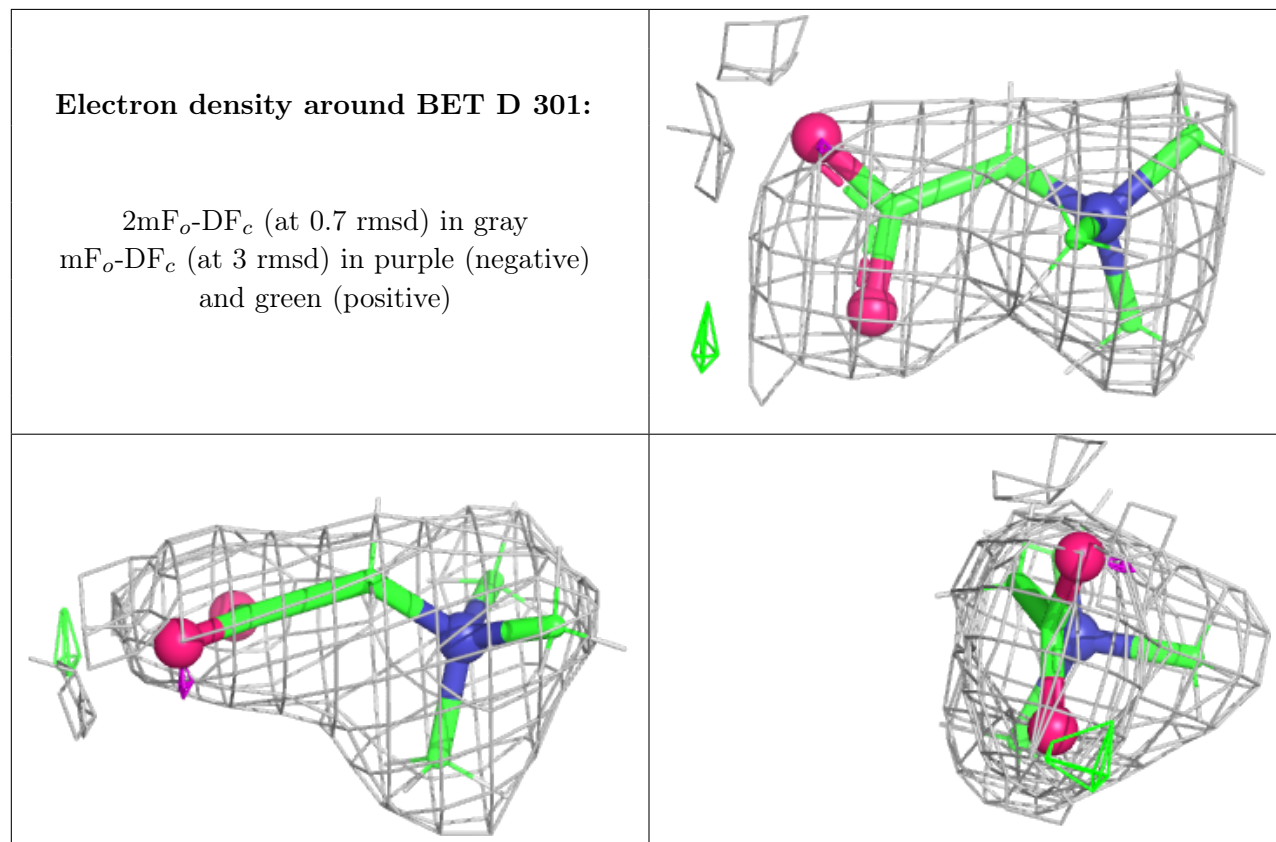
## 6.4 Ligands [i](#)

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
3	GOL	C	302	6/6	0.79	0.13	54,70,78,89	0
3	GOL	B	302	6/6	0.82	0.14	61,75,82,90	0
3	GOL	D	302	6/6	0.90	0.15	49,66,76,85	0
3	GOL	A	302	6/6	0.91	0.10	52,65,79,84	0
2	BET	D	301	8/8	0.93	0.13	45,55,61,64	0
2	BET	B	301	8/8	0.96	0.12	40,51,66,68	0
2	BET	A	301	8/8	0.96	0.10	41,49,55,55	0
2	BET	C	301	8/8	0.97	0.14	41,49,58,58	0

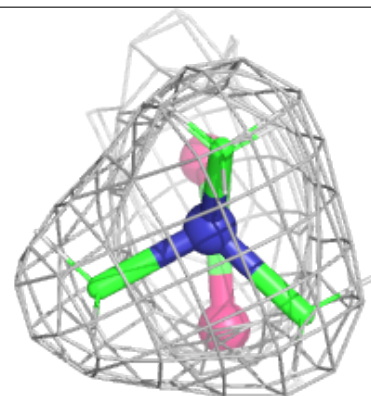
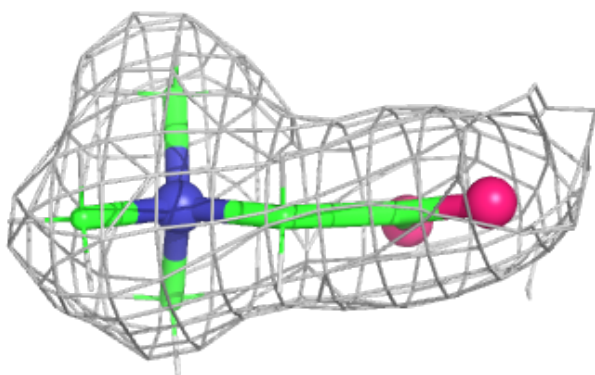
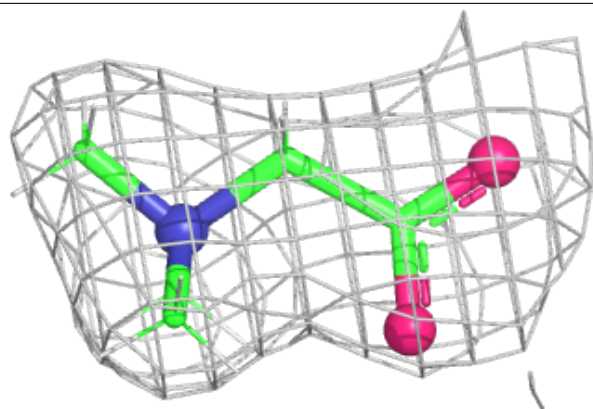
The following is a graphical depiction of the model fit to experimental electron density of all

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.

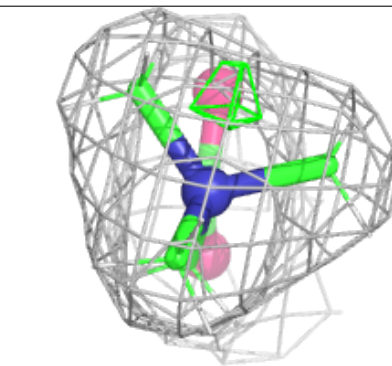
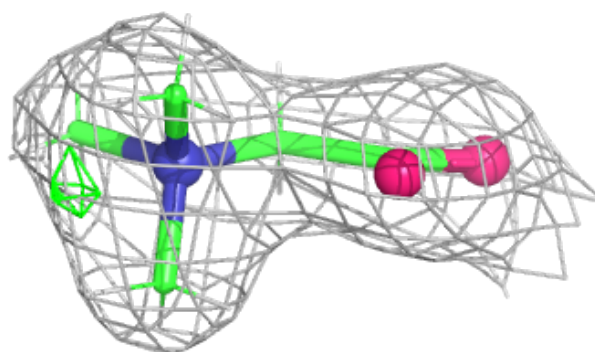
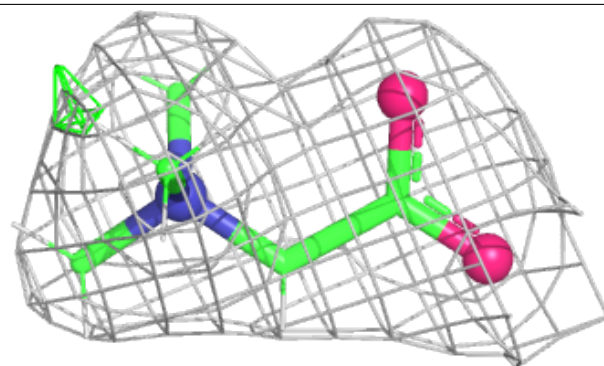


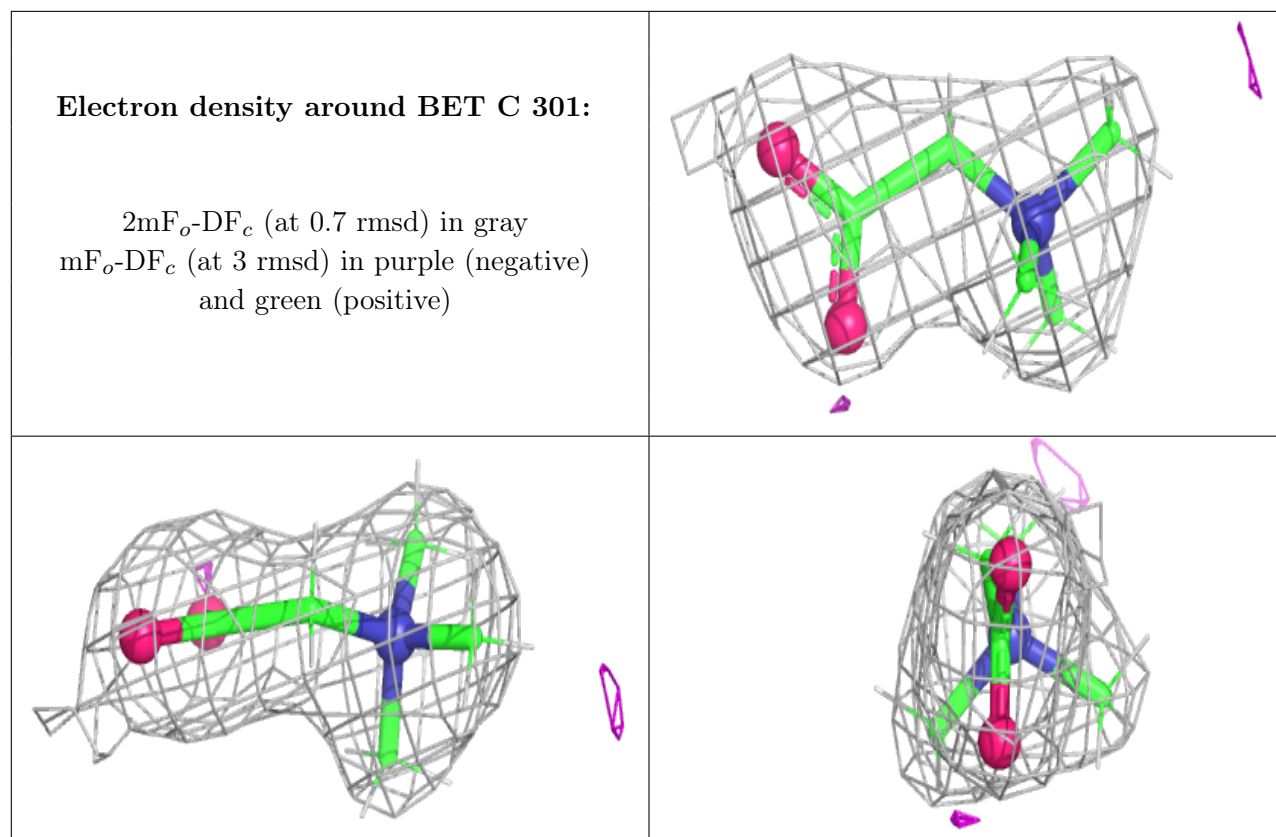
**Electron density around BET B 301:**

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

**Electron density around BET 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.