



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:07 PM UTC

PDB ID : 7PSG / pdb_00007psg
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

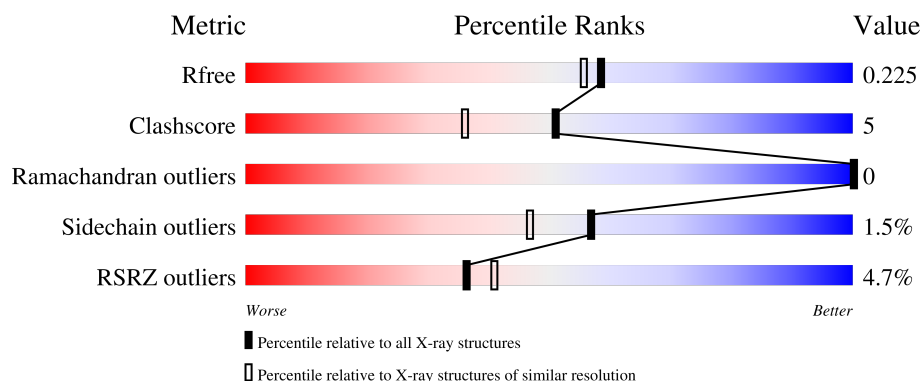
1 Overall quality at a glance

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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 ≥ 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	5% 78% 10% 11%
1	B	301	7% 79% 8% 11%
1	C	301	3% 79% 11% 10%
1	D	301	2% 75% 13% 11%

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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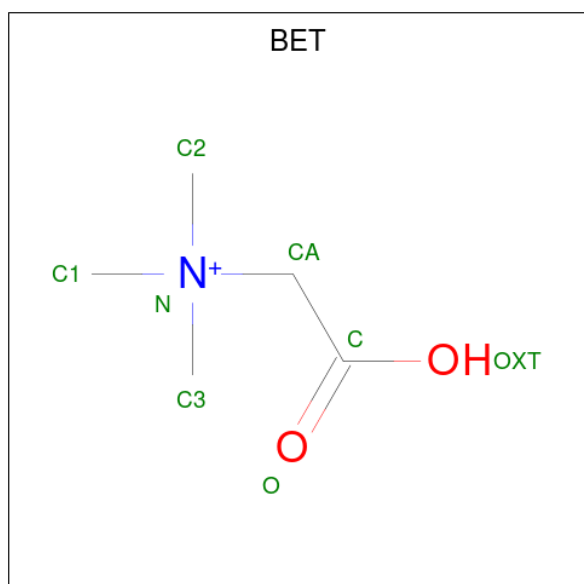
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP Q6D515
C	-9	SER	-	expression tag	UNP Q6D515
C	-8	SER	-	expression tag	UNP Q6D515
C	-7	HIS	-	expression tag	UNP Q6D515
C	-6	HIS	-	expression tag	UNP Q6D515
C	-5	HIS	-	expression tag	UNP Q6D515
C	-4	HIS	-	expression tag	UNP 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 (CCD ID: BET) (formula: $C_5H_{12}NO_2$) (labeled as "Ligand of Interest" by depositor).



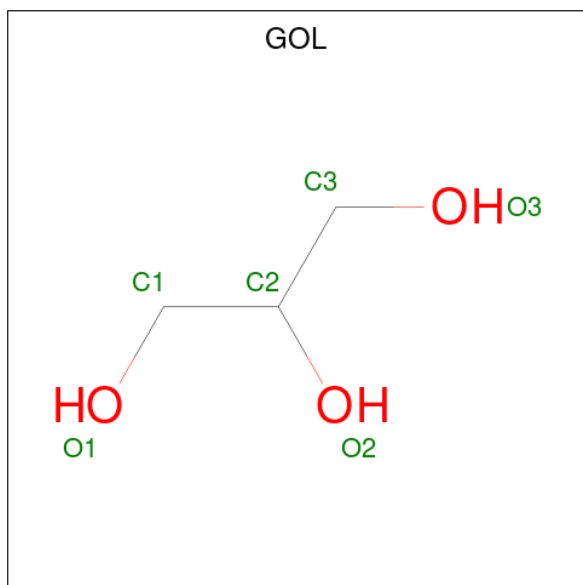
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			19	5	11	1	2		

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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 (CCD ID: 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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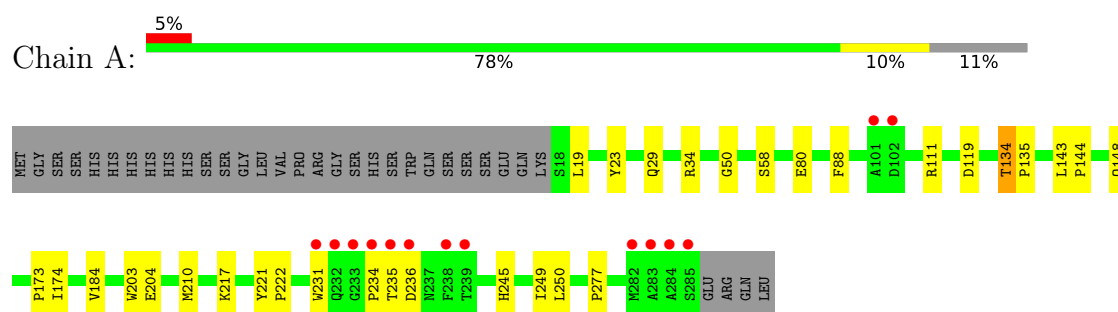
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	120	Total 120	O 120	0	0
4	D	100	Total 100	O 100	0	0

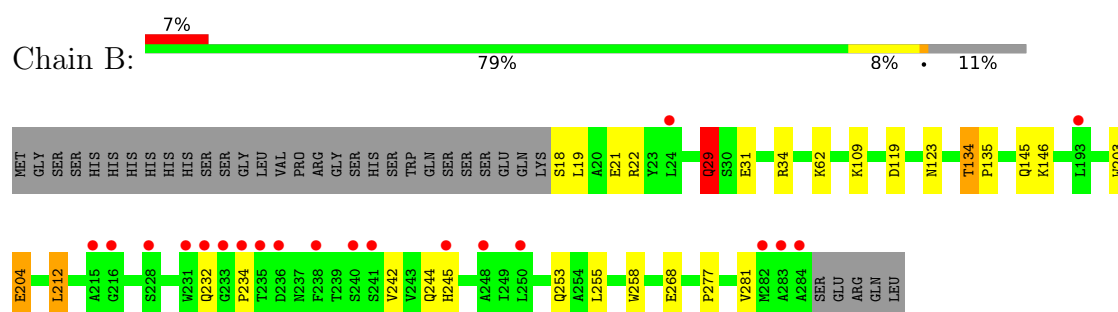
3 Residue-property plots

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.

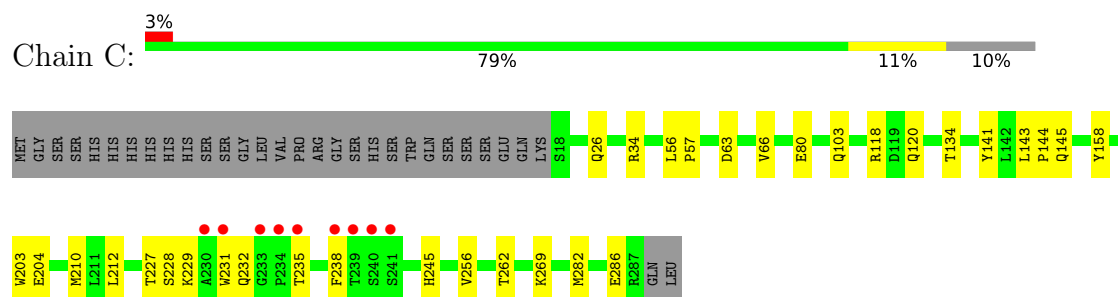
- Molecule 1: Methyl-accepting chemotaxis protein



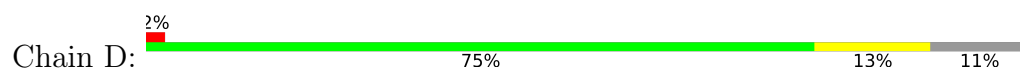
- Molecule 1: Methyl-accepting chemotaxis protein

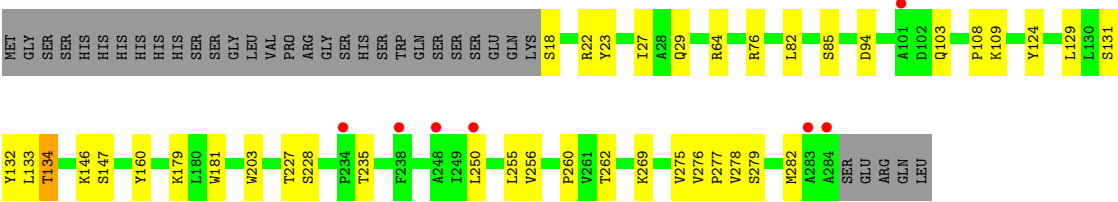


- Molecule 1: Methyl-accepting chemotaxis protein



- 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, α , β , γ	80.78Å 83.44Å 94.91Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	39.99 – 1.91 39.99 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.99-1.91) 98.2 (39.99-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
R, R_{free}	0.185 , 0.227 0.184 , 0.225	Depositor DCC
R_{free} test set	4628 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.47	0/2213	0.69	0/3016
1	B	0.53	0/2160	0.79	7/2944 (0.2%)
1	C	0.51	0/2157	0.73	2/2939 (0.1%)
1	D	0.47	0/2174	0.70	0/2963
All	All	0.50	0/8704	0.73	9/11862 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204[A]	GLU	CA-C-N	-7.83	106.28	121.78
1	B	204[A]	GLU	C-N-CA	-7.83	106.28	121.78
1	B	204[B]	GLU	CA-C-N	-7.83	106.28	121.78
1	B	204[B]	GLU	C-N-CA	-7.83	106.28	121.78
1	B	204[A]	GLU	N-CA-C	-5.94	103.19	111.39
1	B	204[B]	GLU	N-CA-C	-5.94	103.19	111.39
1	B	29	GLN	CG-CD-NE2	-5.48	108.18	116.40
1	C	118	ARG	CA-C-N	5.08	129.98	120.95
1	C	118	ARG	C-N-CA	5.08	129.98	120.95

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 [i](#)

5.2.1 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	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 [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	231/251 (92%)	225 (97%)	6 (3%)	40	24
1	B	224/251 (89%)	220 (98%)	4 (2%)	51	39
1	C	224/251 (89%)	223 (100%)	1 (0%)	84	83
1	D	226/251 (90%)	221 (98%)	5 (2%)	45	32
All	All	905/1004 (90%)	889 (98%)	16 (2%)	57	39

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119[A]	ASP
1	A	119[B]	ASP
1	A	134	THR
1	A	235	THR
1	A	236[A]	ASP
1	A	236[B]	ASP
1	B	62	LYS
1	B	134	THR
1	B	212	LEU
1	B	232	GLN
1	C	134	THR
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	106	GLN
1	B	48	ASN
1	B	106	GLN
1	B	137	GLN
1	B	226	GLN
1	C	25	GLN
1	C	48	ASN
1	C	245	HIS
1	D	26	GLN
1	D	29	GLN
1	D	48	ASN
1	D	106	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 oligosaccharides 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	C	301	-	7,7,7	1.47	1 (14%)	10,10,10	1.15	2 (20%)
3	GOL	A	302	-	5,5,5	1.11	0	5,5,5	1.14	1 (20%)
2	BET	A	301	-	7,7,7	1.40	0	10,10,10	1.01	0
3	GOL	B	302	-	5,5,5	1.02	0	5,5,5	1.27	1 (20%)
2	BET	B	301	-	7,7,7	1.35	0	10,10,10	0.93	0
3	GOL	D	302	-	5,5,5	1.01	0	5,5,5	1.42	1 (20%)
2	BET	D	301	-	7,7,7	1.50	1 (14%)	10,10,10	1.12	1 (10%)
3	GOL	C	302	-	5,5,5	1.10	1 (20%)	5,5,5	1.23	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	C	301	-	-	0/5/5/5	-
3	GOL	A	302	-	-	0/4/4/4	-
2	BET	A	301	-	-	0/5/5/5	-
3	GOL	B	302	-	-	2/4/4/4	-
2	BET	B	301	-	-	0/5/5/5	-

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	BET	CA-N	-2.68	1.45	1.50
3	C	302	GOL	C1-C2	2.19	1.60	1.51
2	C	301	BET	CA-N	-2.04	1.46	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	GOL	C3-C2-C1	-2.66	102.03	111.80
2	D	301	BET	C1-N-CA	-2.37	104.02	109.92
3	B	302	GOL	C3-C2-C1	-2.33	103.27	111.80
3	C	302	GOL	C3-C2-C1	-2.23	103.62	111.80
3	A	302	GOL	C3-C2-C1	-2.22	103.66	111.80
2	C	301	BET	C3-N-CA	-2.12	104.62	109.92
2	C	301	BET	OXT-C-O	-2.05	118.06	123.33

There are no chirality outliers.

All (13) torsion outliers are listed below:

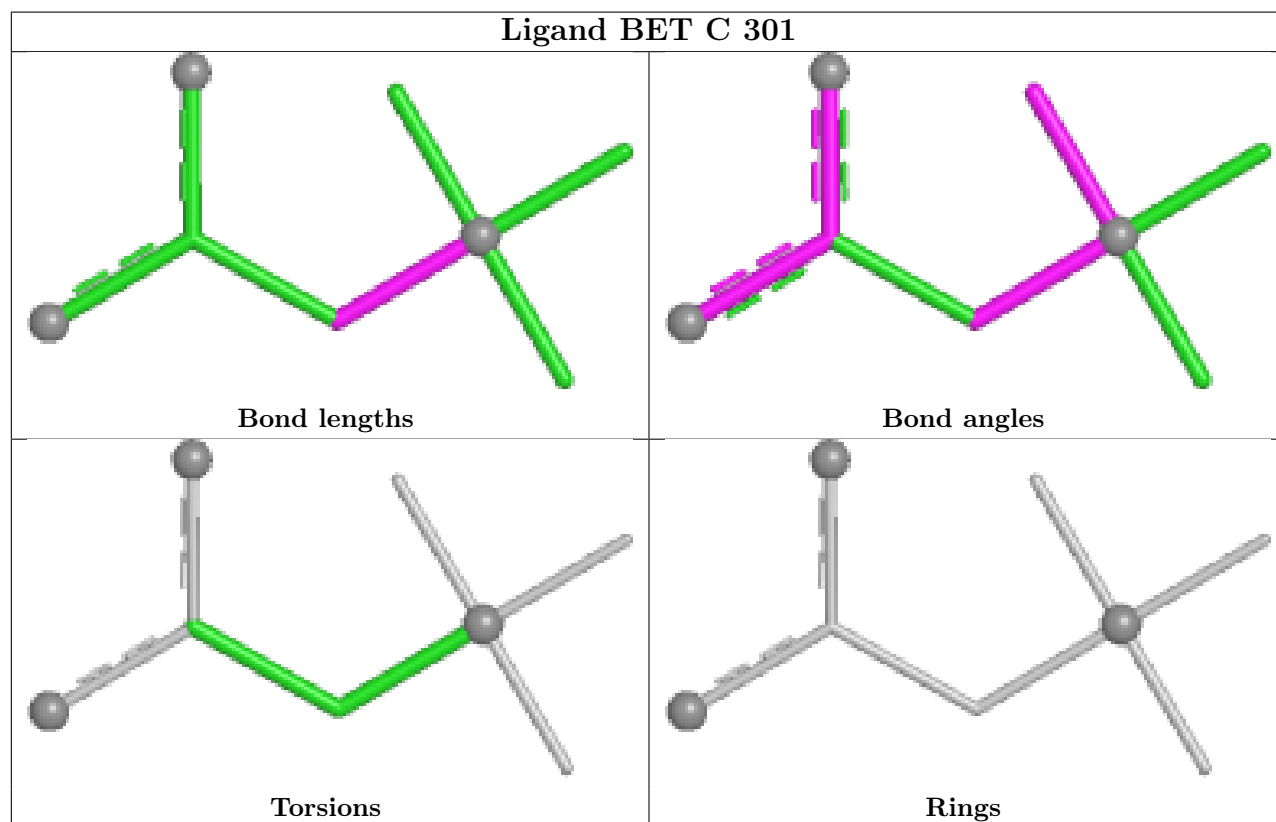
Mol	Chain	Res	Type	Atoms
3	C	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	D	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-O2
2	D	301	BET	C-CA-N-C1
3	B	302	GOL	O1-C1-C2-C3
2	D	301	BET	C-CA-N-C3
2	D	301	BET	O-C-CA-N
2	D	301	BET	C-CA-N-C2
3	B	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
3	D	302	GOL	O2-C2-C3-O3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

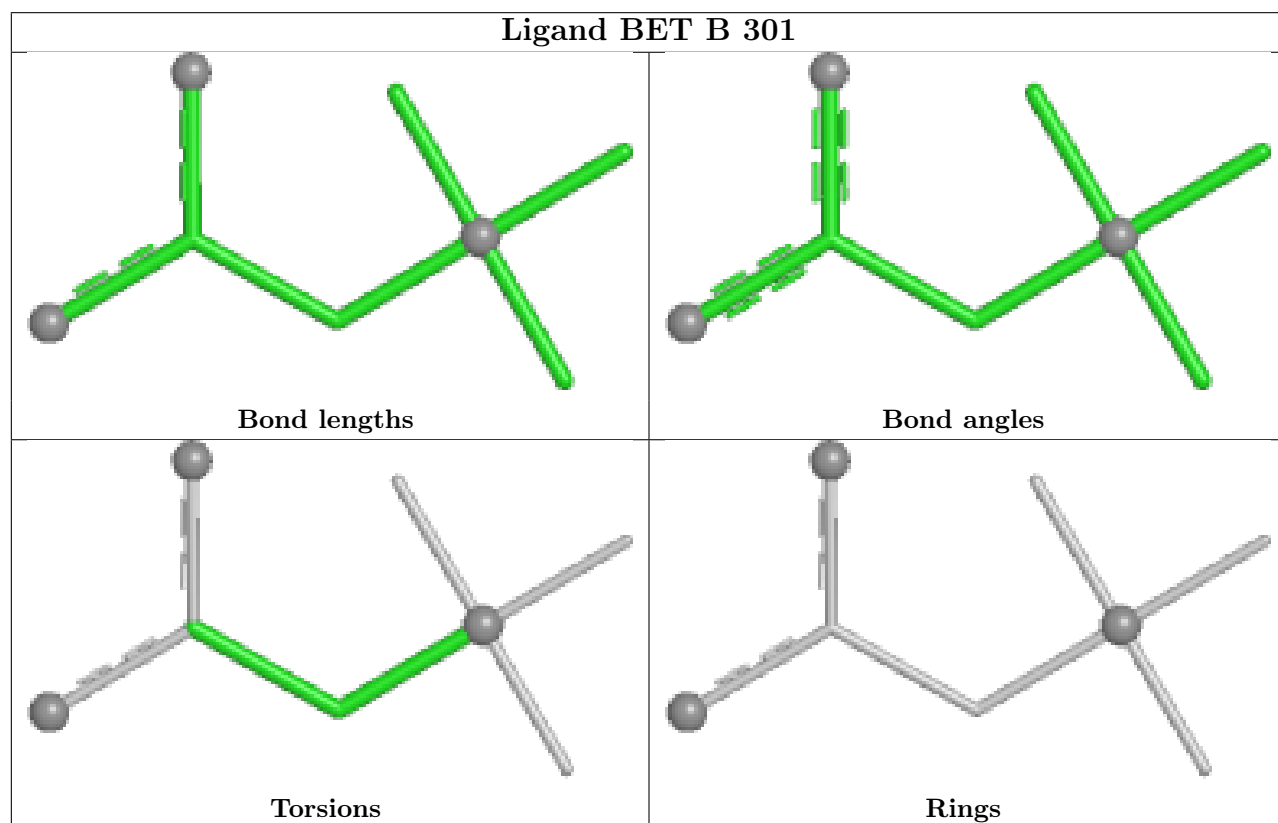
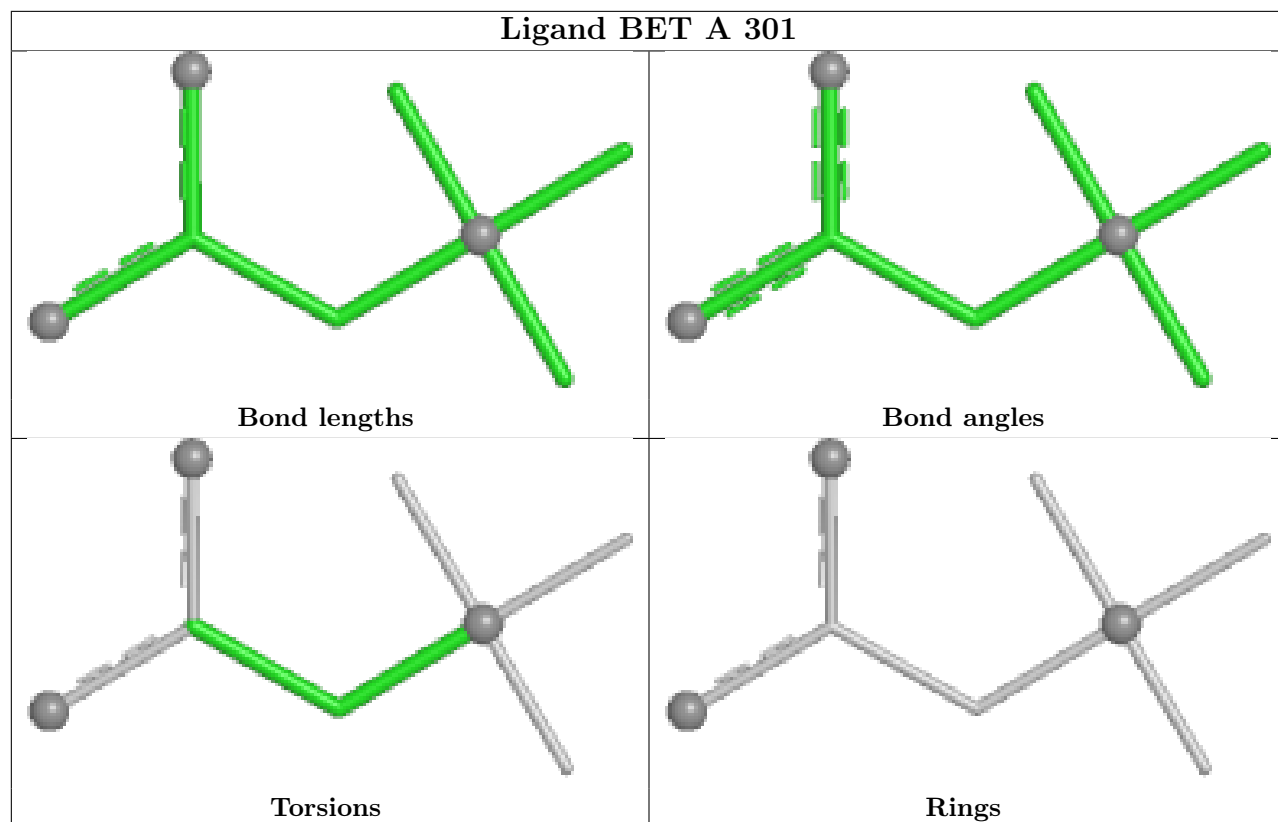
There are no ring outliers.

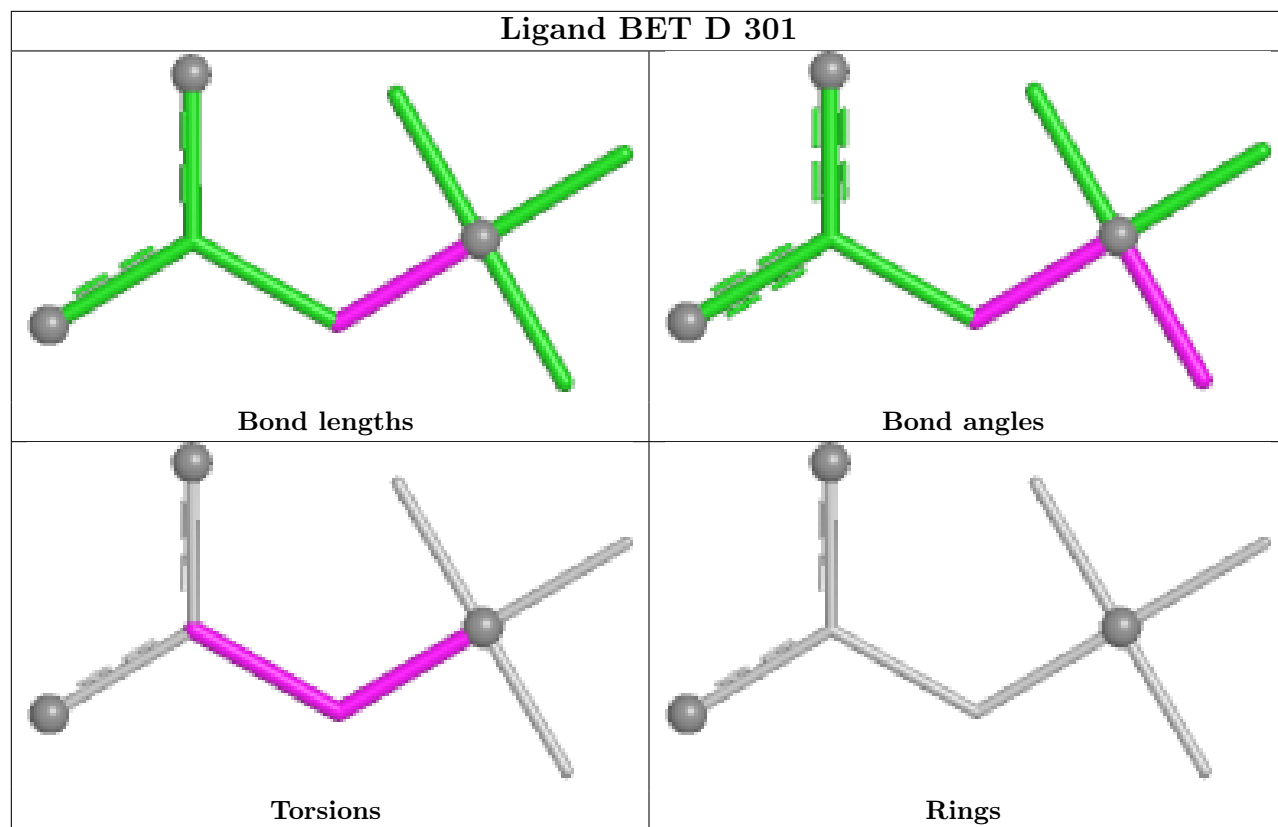
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	BET	1	0
2	A	301	BET	1	0
2	B	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, 95th 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 ²)	Q<0.9
1	A	268/301 (89%)	0.30	14 (5%)	33 37	31, 53, 85, 113	10 (3%)
1	B	267/301 (88%)	0.49	20 (7%)	20 24	31, 56, 101, 121	4 (1%)
1	C	270/301 (89%)	0.28	9 (3%)	49 54	33, 51, 93, 123	1 (0%)
1	D	267/301 (88%)	0.32	7 (2%)	57 63	26, 53, 96, 118	6 (2%)
All	All	1072/1204 (89%)	0.35	50 (4%)	36 41	26, 54, 97, 123	21 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	238	PHE	6.1
1	C	234	PRO	5.9
1	A	234	PRO	5.6
1	D	284	ALA	5.4
1	C	231	TRP	5.0
1	A	283	ALA	4.9
1	D	234	PRO	4.8
1	B	284	ALA	4.5
1	B	234	PRO	4.3
1	A	101	ALA	3.5
1	A	284	ALA	3.4
1	B	235	THR	3.4
1	B	283	ALA	3.2
1	B	245[A]	HIS	3.1
1	B	248	ALA	3.1
1	B	241	SER	2.9
1	A	232[A]	GLN	2.9
1	A	282	MET	2.8
1	B	215	ALA	2.7
1	B	240	SER	2.7
1	B	231	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASP	2.7
1	C	235	THR	2.7
1	C	240	SER	2.7
1	C	239	THR	2.6
1	B	24	LEU	2.6
1	C	233	GLY	2.6
1	A	235	THR	2.6
1	C	230	ALA	2.6
1	A	285	SER	2.6
1	A	233	GLY	2.5
1	B	282	MET	2.5
1	D	250	LEU	2.5
1	B	216	GLY	2.5
1	D	283	ALA	2.5
1	B	233	GLY	2.4
1	C	241	SER	2.4
1	A	239	THR	2.4
1	D	101	ALA	2.4
1	B	228	SER	2.4
1	B	238	PHE	2.3
1	A	231	TRP	2.2
1	D	248	ALA	2.2
1	D	238	PHE	2.2
1	A	238	PHE	2.1
1	B	232	GLN	2.1
1	A	102	ASP	2.1
1	A	236[A]	ASP	2.1
1	B	193	LEU	2.1
1	B	250	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

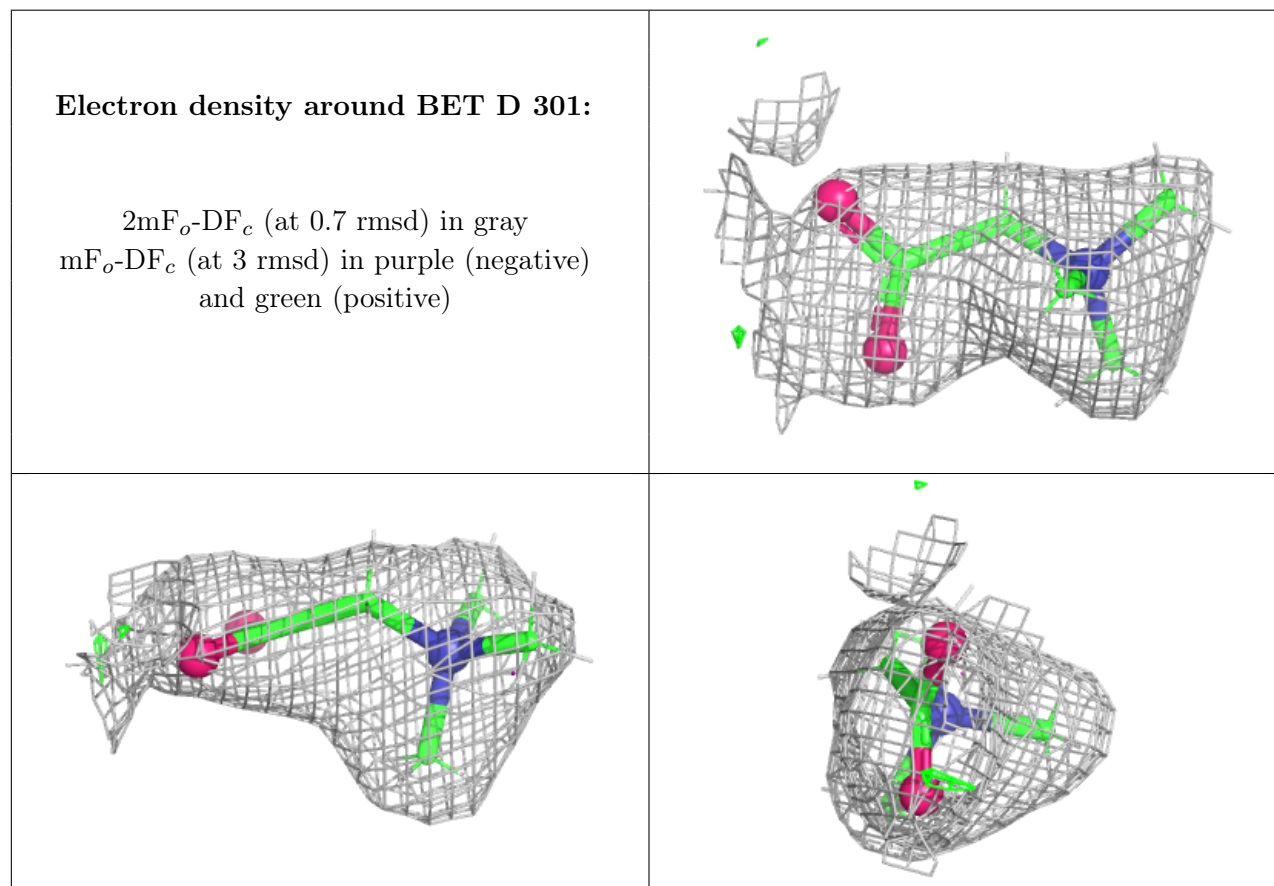
There are no oligosaccharides in this entry.

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, 95th 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.

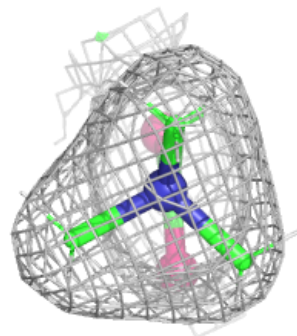
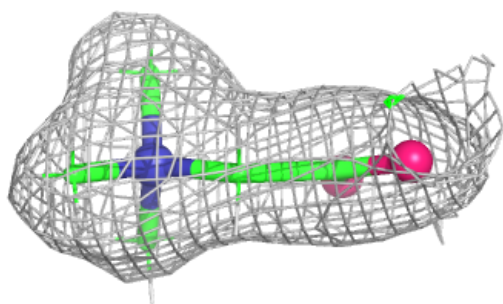
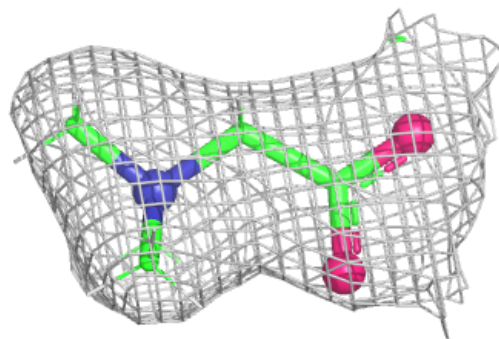
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	302	6/6	0.86	0.13	52,65,79,84	0
3	GOL	B	302	6/6	0.86	0.14	61,75,82,90	0
3	GOL	C	302	6/6	0.89	0.12	54,70,78,89	0
3	GOL	D	302	6/6	0.92	0.10	49,66,76,85	0
2	BET	D	301	8/8	0.93	0.10	45,55,61,64	0
2	BET	B	301	8/8	0.94	0.10	40,51,66,68	0
2	BET	C	301	8/8	0.95	0.08	41,49,58,58	0
2	BET	A	301	8/8	0.95	0.08	41,49,55,55	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.

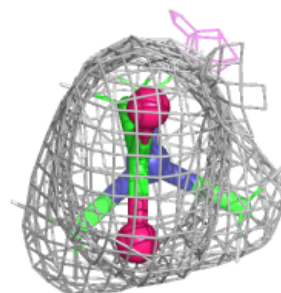
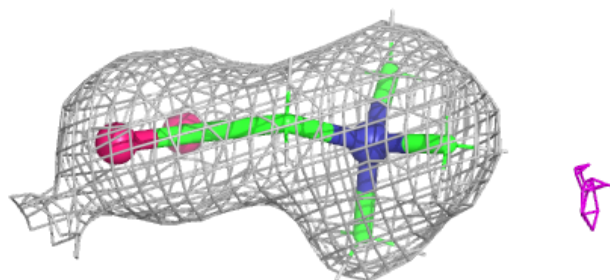
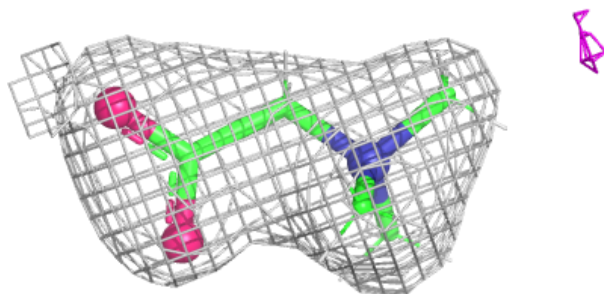


Electron density around BET B 301:

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

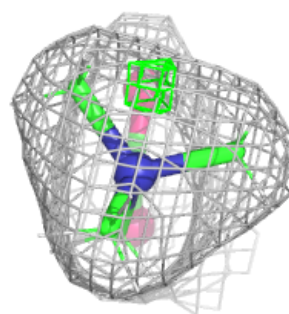
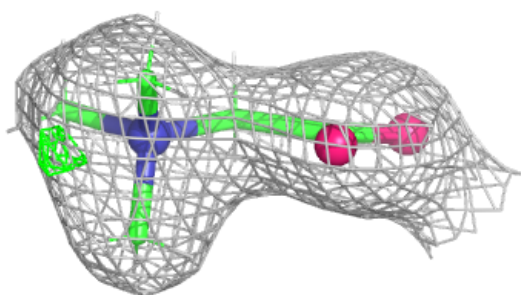
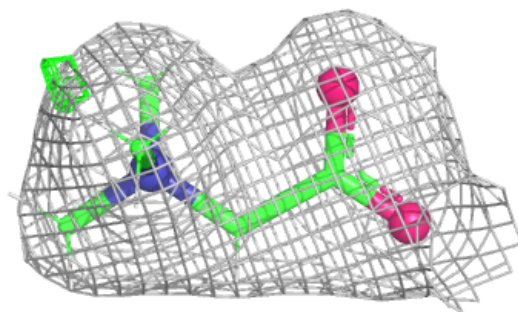
**Electron density around BET C 301:**

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



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 ⓘ

There are no such residues in this entry.