



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2022 – 01:16 pm BST

PDB ID : 7PFN
Title : Crystal Structure of a Class D Carbapenemase_K73ALY Complexed with Imipenem
Authors : Zhou, Q.; He, Y.; Jin, Y.
Deposited on : 2021-08-11
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

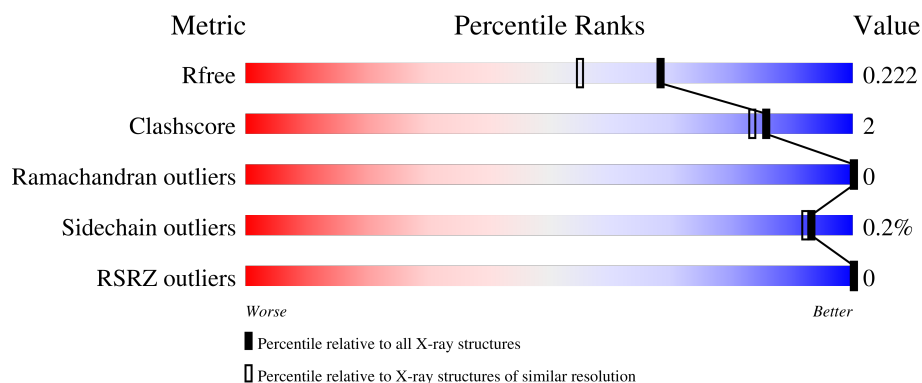
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	AAA	260	 88% 5% 7%
1	BBB	260	 89% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8456 atoms, of which 4021 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	243	Total	C	H	N	O	S	45	4	0
			3999	1284	1987	354	365	9			
1	BBB	242	Total	C	H	N	O	S	45	1	0
			3938	1267	1950	349	364	8			

There are 34 discrepancies between the modelled and reference sequences:

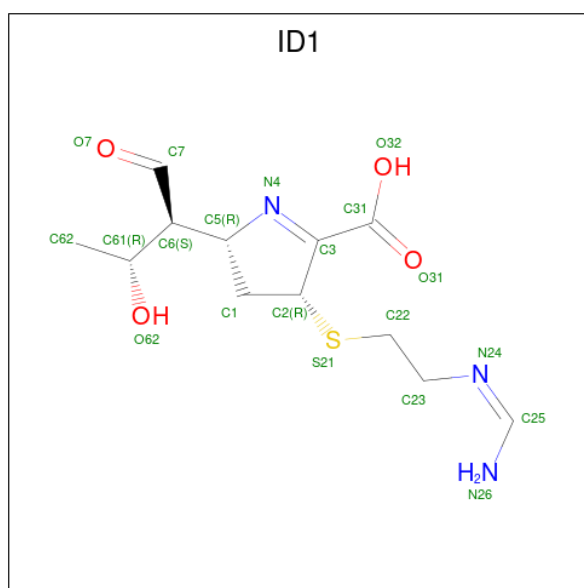
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP A0A482LRD5
AAA	7	HIS	-	expression tag	UNP A0A482LRD5
AAA	8	HIS	-	expression tag	UNP A0A482LRD5
AAA	9	HIS	-	expression tag	UNP A0A482LRD5
AAA	10	HIS	-	expression tag	UNP A0A482LRD5
AAA	11	HIS	-	expression tag	UNP A0A482LRD5
AAA	12	HIS	-	expression tag	UNP A0A482LRD5
AAA	13	SER	-	expression tag	UNP A0A482LRD5
AAA	14	ALA	-	expression tag	UNP A0A482LRD5
AAA	15	GLY	-	expression tag	UNP A0A482LRD5
AAA	16	GLU	-	expression tag	UNP A0A482LRD5
AAA	17	ASN	-	expression tag	UNP A0A482LRD5
AAA	18	LEU	-	expression tag	UNP A0A482LRD5
AAA	19	TYR	-	expression tag	UNP A0A482LRD5
AAA	20	PHE	-	expression tag	UNP A0A482LRD5
AAA	21	GLN	-	expression tag	UNP A0A482LRD5
AAA	22	GLY	-	expression tag	UNP A0A482LRD5
BBB	6	MET	-	initiating methionine	UNP A0A482LRD5
BBB	7	HIS	-	expression tag	UNP A0A482LRD5
BBB	8	HIS	-	expression tag	UNP A0A482LRD5
BBB	9	HIS	-	expression tag	UNP A0A482LRD5
BBB	10	HIS	-	expression tag	UNP A0A482LRD5
BBB	11	HIS	-	expression tag	UNP A0A482LRD5
BBB	12	HIS	-	expression tag	UNP A0A482LRD5
BBB	13	SER	-	expression tag	UNP A0A482LRD5

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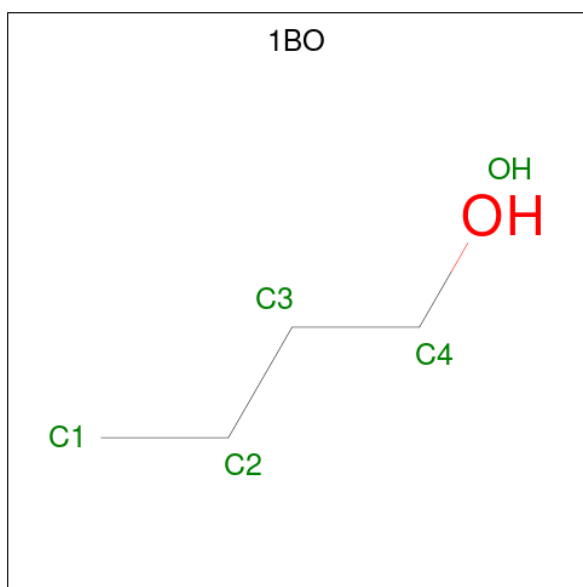
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	14	ALA	-	expression tag	UNP A0A482LRD5
BBB	15	GLY	-	expression tag	UNP A0A482LRD5
BBB	16	GLU	-	expression tag	UNP A0A482LRD5
BBB	17	ASN	-	expression tag	UNP A0A482LRD5
BBB	18	LEU	-	expression tag	UNP A0A482LRD5
BBB	19	TYR	-	expression tag	UNP A0A482LRD5
BBB	20	PHE	-	expression tag	UNP A0A482LRD5
BBB	21	GLN	-	expression tag	UNP A0A482LRD5
BBB	22	GLY	-	expression tag	UNP A0A482LRD5

- Molecule 2 is Imipenem (three-letter code: ID1) (formula: C₁₂H₁₉N₃O₄S) (labeled as "Ligand of Interest" by depositor).



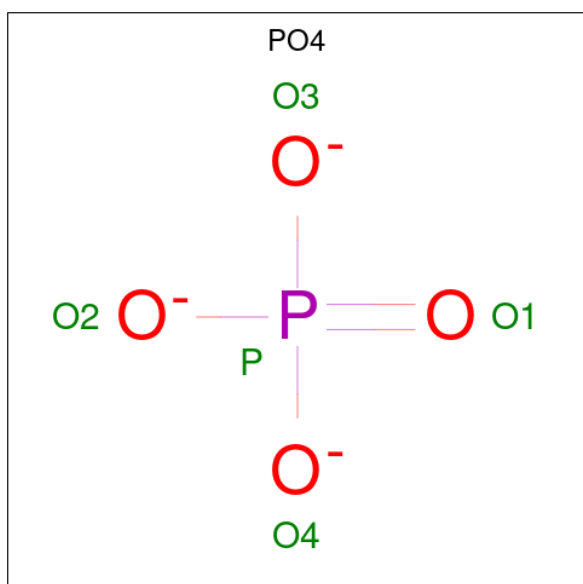
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	BBB	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		

- Molecule 3 is 1-BUTANOL (three-letter code: 1BO) (formula: C₄H₁₀O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
3	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
3	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
3	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
3	BBB	1	Total	C	H	O	0	0
			15	4	10	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	173	Total	O	0	0
			173	173		
5	BBB	192	Total	O	0	0
			192	192		

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: Beta-lactamase

Chain AAA: 



- Molecule 1: Beta-lactamase

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	44.80Å 105.00Å 124.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.37 – 1.80 62.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.37-1.80) 100.0 (62.37-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.214 0.190 , 0.222	Depositor DCC
R_{free} test set	2744 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.642	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 1BO, ALY, ID1

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	AAA	0.72	0/2060	0.80	1/2783 (0.0%)
1	BBB	0.70	0/2027	0.83	0/2740
All	All	0.71	0/4087	0.81	1/5523 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	206	ARG	NE-CZ-NH1	6.78	123.69	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	AAA	2012	1987	1983	9	0
1	BBB	1988	1950	1943	7	0
2	AAA	20	17	0	0	0
2	BBB	20	17	0	1	0
3	AAA	15	30	30	3	0
3	BBB	10	20	20	3	0
4	AAA	5	0	0	0	0
5	AAA	173	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BBB	192	0	0	3	0
All	All	4435	4021	3976	18	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 2.

The worst 5 of 18 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:BBB:301:ID1:N26	5:BBB:401:HOH:O	2.21	0.73
1:BBB:250:ARG:HH12	3:BBB:302:1BO:H22	1.70	0.56
1:AAA:231:ASN:HD22	3:AAA:303:1BO:H41	1.73	0.54
1:AAA:231:ASN:HD22	3:AAA:303:1BO:C3	2.26	0.48
1:BBB:250:ARG:HH12	3:BBB:302:1BO:C2	2.26	0.48

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	AAA	244/260 (94%)	239 (98%)	5 (2%)	0	100	100
1	BBB	240/260 (92%)	235 (98%)	5 (2%)	0	100	100
All	All	484/520 (93%)	474 (98%)	10 (2%)	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	AAA	214/225 (95%)	214 (100%)	0	100	100
1	BBB	211/225 (94%)	210 (100%)	1 (0%)	88	87
All	All	425/450 (94%)	424 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	163	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	ALY	BBB	73	1	10,11,12	0.43	0	7,12,14	0.62	0
1	ALY	AAA	73	1	10,11,12	0.47	0	7,12,14	0.44	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
1	ALY	BBB	73	1	-	0/9/10/12	-
1	ALY	AAA	73	1	-	0/9/10/12	-

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 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	$\# Z > 2$
3	1BO	AAA	303	-	4,4,4	0.29	0	3,3,3	0.35	0
3	1BO	AAA	302	-	4,4,4	0.30	0	3,3,3	0.27	0
3	1BO	AAA	304	-	4,4,4	0.20	0	3,3,3	0.10	0
2	ID1	BBB	301	1	15,20,20	0.84	1 (6%)	10,26,26	2.31	2 (20%)
3	1BO	BBB	303	-	4,4,4	0.34	0	3,3,3	0.31	0
2	ID1	AAA	301	1	15,20,20	1.28	2 (13%)	10,26,26	1.11	1 (10%)
3	1BO	BBB	302	-	4,4,4	0.52	0	3,3,3	0.50	0
4	PO4	AAA	305	-	4,4,4	0.65	0	6,6,6	0.65	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
3	1BO	AAA	303	-	-	1/2/2/2	-
3	1BO	AAA	302	-	-	2/2/2/2	-
3	1BO	AAA	304	-	-	1/2/2/2	-
2	ID1	BBB	301	1	-	2/17/32/32	0/1/1/1
3	1BO	BBB	303	-	-	0/2/2/2	-
2	ID1	AAA	301	1	-	3/17/32/32	0/1/1/1
3	1BO	BBB	302	-	-	1/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301	ID1	O32-C31	-3.07	1.21	1.30
2	AAA	301	ID1	C2-S21	3.04	1.86	1.83
2	BBB	301	ID1	O32-C31	-2.52	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	301	ID1	C22-C23-N24	-6.03	106.12	110.78
2	BBB	301	ID1	C23-N24-C25	3.46	121.55	117.22
2	AAA	301	ID1	C6-C5-N4	-2.29	107.60	112.00

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

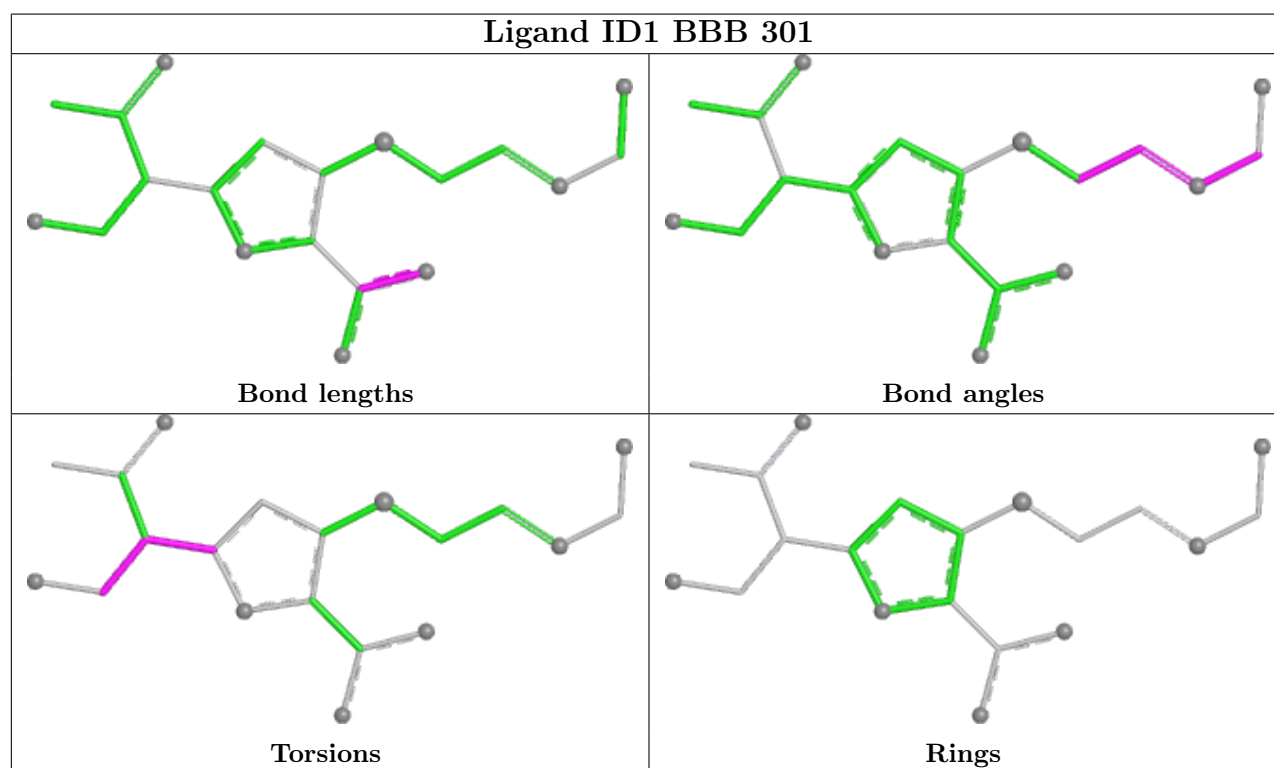
Mol	Chain	Res	Type	Atoms
2	AAA	301	ID1	C3-C2-S21-C22
2	AAA	301	ID1	C1-C5-C6-C7
2	AAA	301	ID1	S21-C22-C23-N24
2	BBB	301	ID1	C61-C6-C7-O7
2	BBB	301	ID1	C1-C5-C6-C7

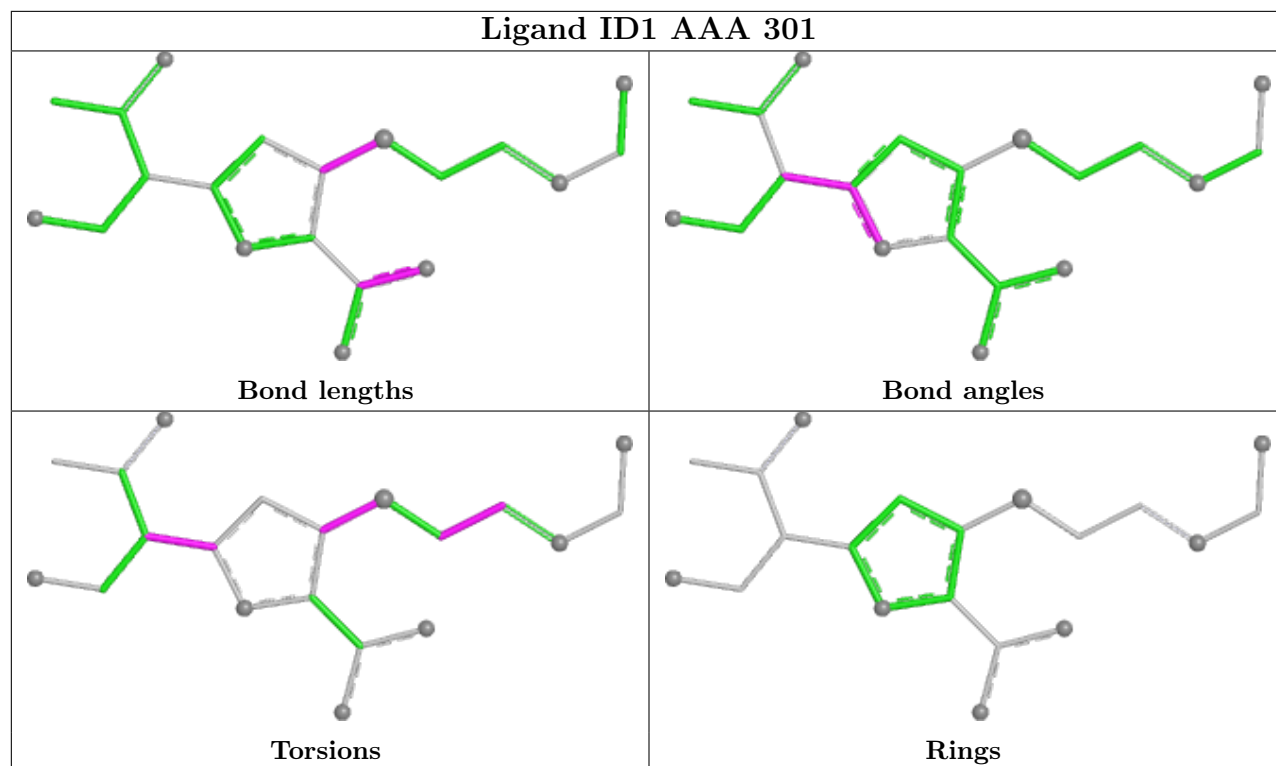
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	303	1BO	3	0
2	BBB	301	ID1	1	0
3	BBB	302	1BO	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	242/260 (93%)	-0.47	0 100 100	16, 23, 47, 76	2 (0%)
1	BBB	241/260 (92%)	-0.39	0 100 100	15, 24, 44, 62	1 (0%)
All	All	483/520 (92%)	-0.43	0 100 100	15, 24, 46, 76	3 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	ALY	AAA	73	12/13	0.98	0.08	17,19,22,23	0
1	ALY	BBB	73	12/13	0.98	0.07	15,19,24,24	0

6.3 Carbohydrates [i](#)

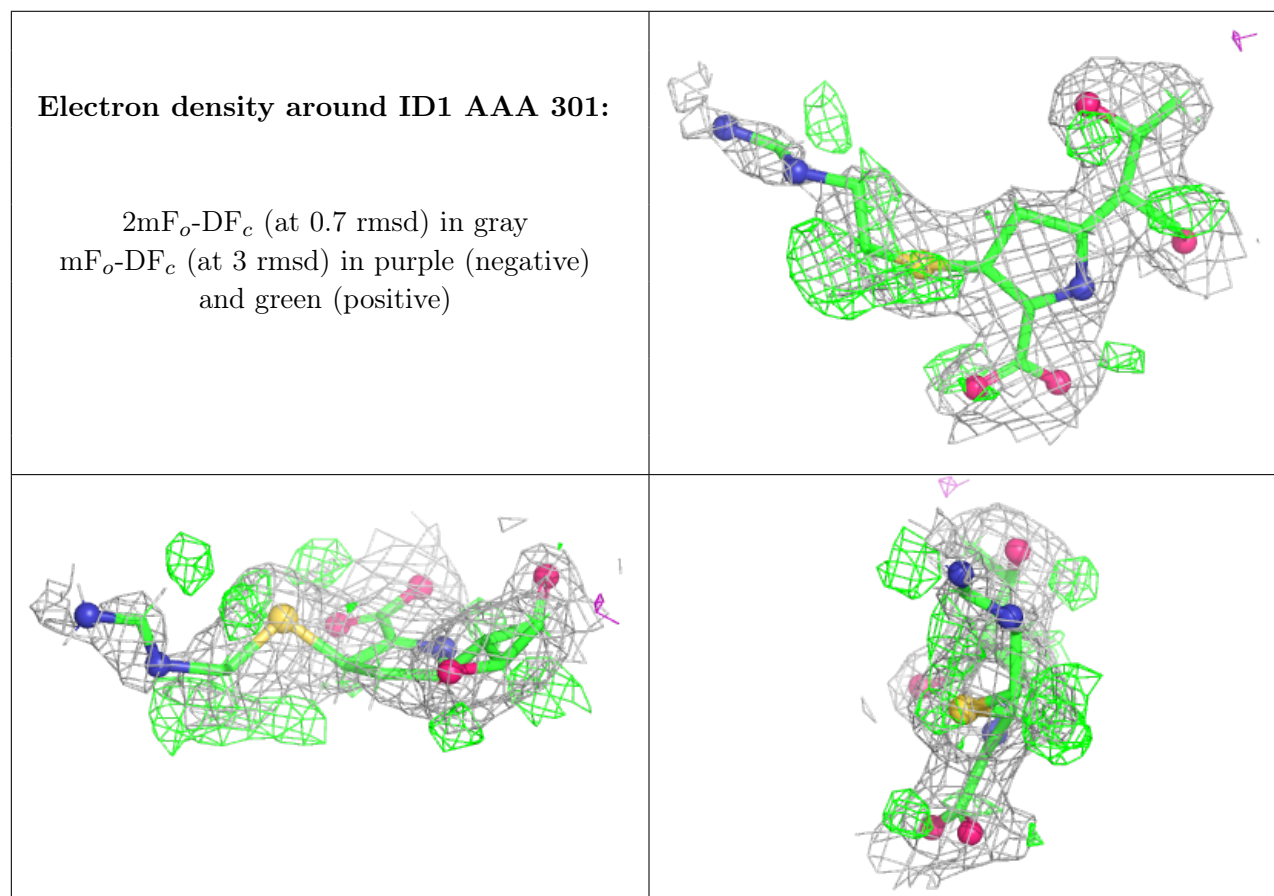
There are no monosaccharides in this entry.

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, 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.

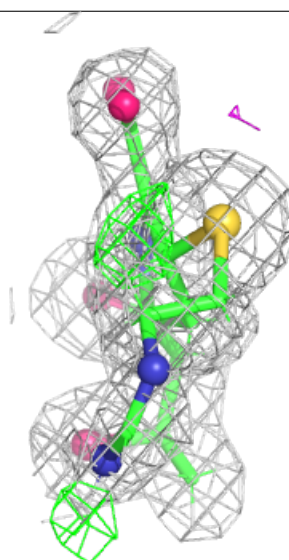
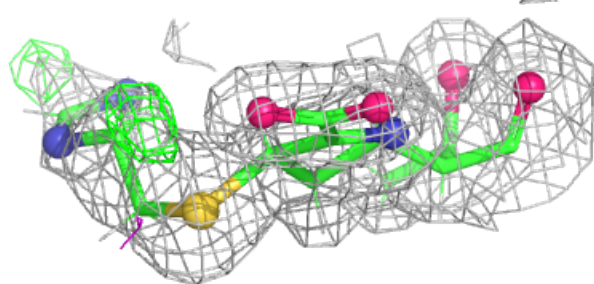
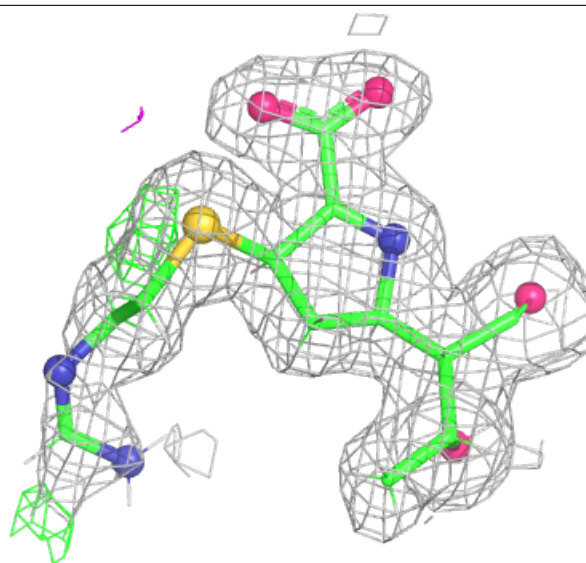
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1BO	BBB	302	5/5	0.80	0.14	28,34,37,38	0
3	1BO	BBB	303	5/5	0.80	0.16	44,46,47,47	0
3	1BO	AAA	303	5/5	0.81	0.16	28,34,42,42	0
3	1BO	AAA	302	5/5	0.82	0.16	42,46,46,47	0
2	ID1	AAA	301	20/20	0.88	0.13	28,40,45,46	24
3	1BO	AAA	304	5/5	0.95	0.10	42,45,47,48	0
4	PO4	AAA	305	5/5	0.96	0.10	32,36,40,46	5
2	ID1	BBB	301	20/20	0.97	0.11	18,23,48,48	7

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 ID1 BBB 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.