



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:44 AM UTC

PDB ID : 7PR6 / pdb_00007pr6
Title : Crystal structure of E. coli beta-glucuronidase in complex with covalent inhibitor ME727
Authors : Wu, L.; Armstrong, Z.; Davies, G.J.
Deposited on : 2021-09-20
Resolution : 1.99 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

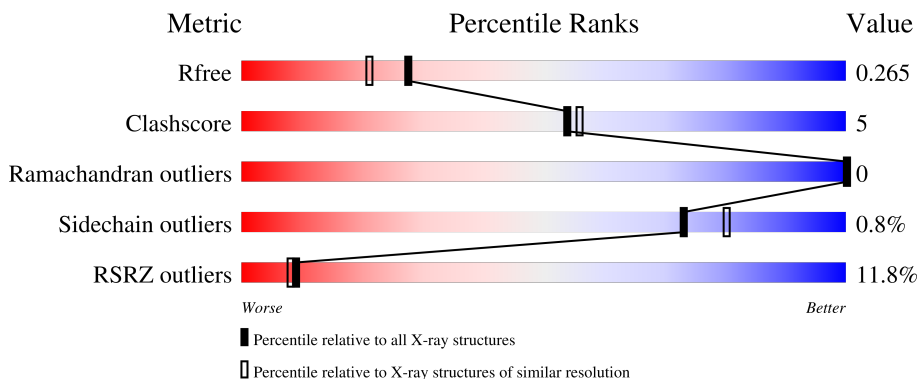
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	601	 4% 84% 15%
1	BBB	601	 20% 87% 11%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 19287 atoms, of which 9218 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-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	599	9440	3059	4625	831	902	23	134	1	0
1	BBB	592	9332	3024	4573	821	892	22	134	0	0

There are 38 discrepancies between the modelled and reference sequences:

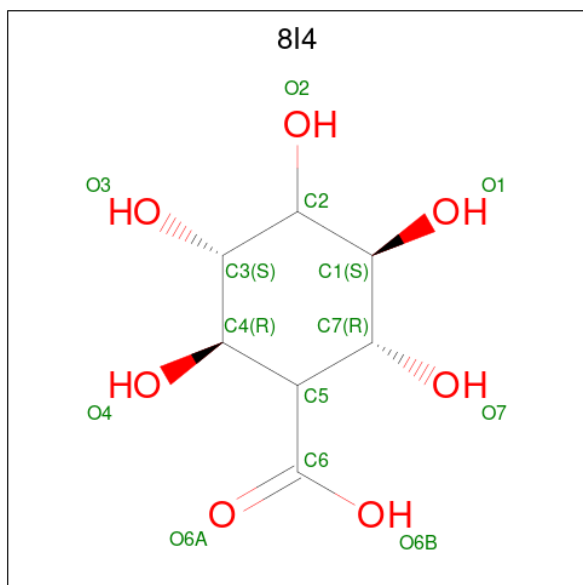
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	SER	-	expression tag	UNP P05804
AAA	0	HIS	-	expression tag	UNP P05804
AAA	1	MET	-	expression tag	UNP P05804
AAA	2	LEU	-	expression tag	UNP P05804
AAA	3	ARG	-	expression tag	UNP P05804
AAA	4	PRO	-	expression tag	UNP P05804
AAA	5	VAL	-	expression tag	UNP P05804
AAA	6	GLU	-	expression tag	UNP P05804
AAA	7	THR	-	expression tag	UNP P05804
AAA	8	PRO	-	expression tag	UNP P05804
AAA	9	THR	-	expression tag	UNP P05804
AAA	10	ARG	-	expression tag	UNP P05804
AAA	11	GLU	-	expression tag	UNP P05804
AAA	12	ILE	-	expression tag	UNP P05804
AAA	13	LYS	-	expression tag	UNP P05804
AAA	14	LYS	-	expression tag	UNP P05804
AAA	15	LEU	-	expression tag	UNP P05804
AAA	16	ASP	-	expression tag	UNP P05804
AAA	17	GLY	-	expression tag	UNP P05804
BBB	-1	SER	-	expression tag	UNP P05804
BBB	0	HIS	-	expression tag	UNP P05804
BBB	1	MET	-	expression tag	UNP P05804
BBB	2	LEU	-	expression tag	UNP P05804
BBB	3	ARG	-	expression tag	UNP P05804
BBB	4	PRO	-	expression tag	UNP P05804

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	5	VAL	-	expression tag	UNP P05804
BBB	6	GLU	-	expression tag	UNP P05804
BBB	7	THR	-	expression tag	UNP P05804
BBB	8	PRO	-	expression tag	UNP P05804
BBB	9	THR	-	expression tag	UNP P05804
BBB	10	ARG	-	expression tag	UNP P05804
BBB	11	GLU	-	expression tag	UNP P05804
BBB	12	ILE	-	expression tag	UNP P05804
BBB	13	LYS	-	expression tag	UNP P05804
BBB	14	LYS	-	expression tag	UNP P05804
BBB	15	LEU	-	expression tag	UNP P05804
BBB	16	ASP	-	expression tag	UNP P05804
BBB	17	GLY	-	expression tag	UNP P05804

- Molecule 2 is (2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid (CCD ID: 8I4) (formula: C₇H₁₂O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	AAA	1	Total	C	H	O	4	0
			23	7	10	6		
2	BBB	1	Total	C	H	O	4	0
			23	7	10	6		

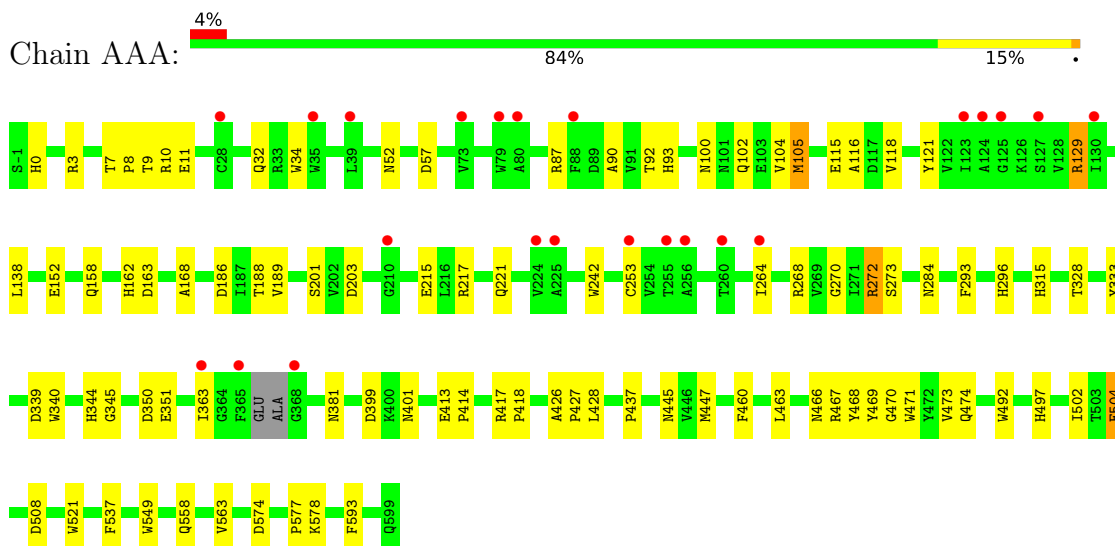
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	321	Total 321	O 321	0	0
3	BBB	148	Total 148	O 148	0	0

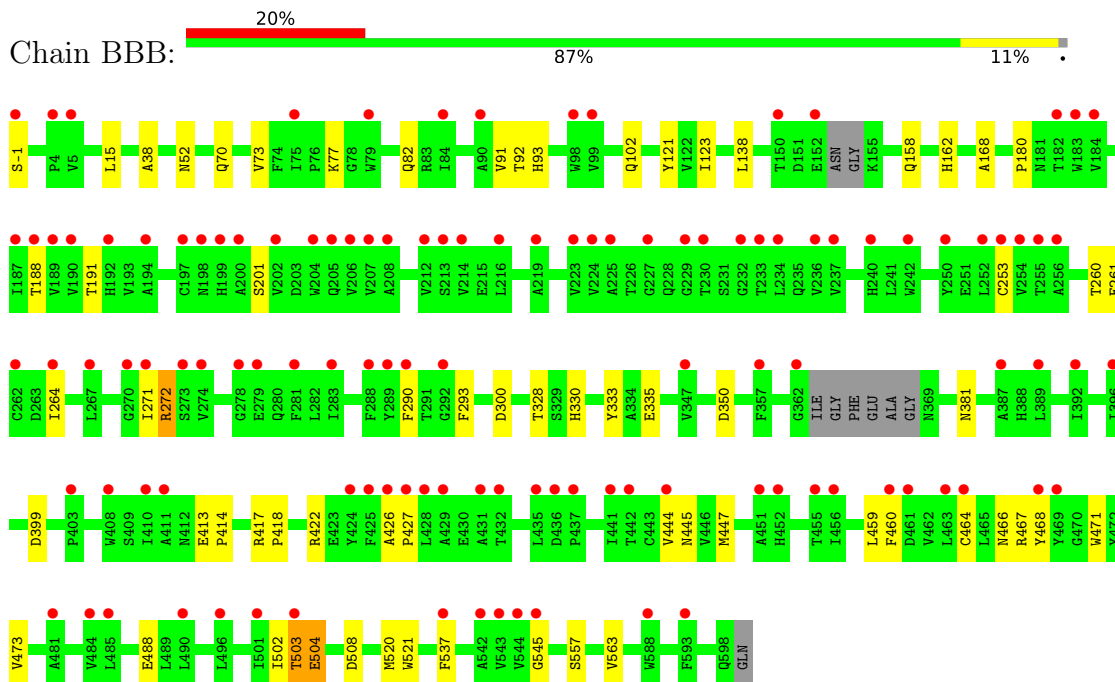
3 Residue-property plots i

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: Beta-glucuronidase



- Molecule 1: Beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.80Å 76.58Å 125.74Å 90.00° 125.01° 90.00°	Depositor
Resolution (Å)	47.80 – 1.99 47.80 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.80-1.99) 92.9 (47.80-1.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.263 0.226 , 0.265	Depositor DCC
R_{free} test set	4333 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19287	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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:
8I4

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	1.16	10/4944 (0.2%)	1.39	19/6725 (0.3%)
1	BBB	1.11	4/4886 (0.1%)	1.36	9/6647 (0.1%)
All	All	1.13	14/9830 (0.1%)	1.38	28/13372 (0.2%)

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	AAA	0	2
1	BBB	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	504	GLU	CD-OE2	10.43	1.45	1.25
1	AAA	504	GLU	CD-OE2	7.16	1.39	1.25
1	AAA	437	PRO	C-O	-6.91	1.15	1.24
1	AAA	296	HIS	CE1-NE2	6.38	1.39	1.32
1	AAA	351	GLU	C-O	6.37	1.31	1.23

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	503	THR	CB-CA-C	7.27	123.10	110.01
1	BBB	563	VAL	CA-C-O	-6.48	116.99	122.63
1	AAA	129	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	AAA	563	VAL	CA-C-O	-6.25	117.20	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	188	THR	CA-CB-OG1	-6.01	100.58	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	105	MET	Mainchain
1	AAA	293	PHE	Peptide
1	BBB	293	PHE	Peptide

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	4815	4625	4603	49	0
1	BBB	4759	4573	4551	43	0
2	AAA	13	10	0	0	0
2	BBB	13	10	0	1	0
3	AAA	321	0	0	3	0
3	BBB	148	0	0	2	1
All	All	10069	9218	9154	91	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 91 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:AAA:7:THR:HG21	1:AAA:264:ILE:O	1.55	1.05
1:AAA:272:ARG:HA	1:AAA:284:ASN:HD21	1.43	0.81
1:AAA:104:VAL:HG21	1:AAA:118:VAL:HG12	1.63	0.80
1:BBB:467:ARG:NH2	1:BBB:488:GLU:OE1	2.22	0.73
1:AAA:426:ALA:HB3	1:AAA:427:PRO:HD3	1.72	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BBB:838:HOH:O	3:BBB:838:HOH:O[2_556]	1.30	0.90

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	596/601 (99%)	570 (96%)	26 (4%)	0	100	100
1	BBB	586/601 (98%)	561 (96%)	25 (4%)	0	100	100
All	All	1182/1202 (98%)	1131 (96%)	51 (4%)	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	511/511 (100%)	508 (99%)	3 (1%)	78	85
1	BBB	506/511 (99%)	501 (99%)	5 (1%)	68	75
All	All	1017/1022 (100%)	1009 (99%)	8 (1%)	73	80

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	557	SER
1	BBB	468	TYR
1	BBB	201	SER

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Mol	Chain	Res	Type
1	BBB	-1	SER
1	BBB	272	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	8I4	BBB	601	-	13,13,14	0.97	1 (7%)	18,19,21	2.02	5 (27%)
2	8I4	AAA	601	-	13,13,14	1.41	3 (23%)	18,19,21	1.16	1 (5%)

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	8I4	BBB	601	-	-	2/4/24/28	0/1/1/1
2	8I4	AAA	601	-	-	2/4/24/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	601	8I4	O4-C4	2.70	1.49	1.43
2	AAA	601	8I4	O6B-C6	-2.38	1.23	1.30
2	AAA	601	8I4	C2-C3	2.28	1.56	1.52
2	AAA	601	8I4	O6A-C6	2.14	1.28	1.22

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	601	8I4	C7-C1-C2	4.74	117.00	111.50
2	BBB	601	8I4	O6A-C6-C5	-3.59	113.68	122.84
2	BBB	601	8I4	C2-C3-C4	3.24	116.56	110.86
2	BBB	601	8I4	C5-C4-C3	-3.05	106.07	110.58
2	BBB	601	8I4	O6B-C6-C5	2.57	121.31	113.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	8I4	C4-C5-C6-O6B
2	AAA	601	8I4	C4-C5-C6-O6A
2	BBB	601	8I4	C4-C5-C6-O6B
2	BBB	601	8I4	C4-C5-C6-O6A

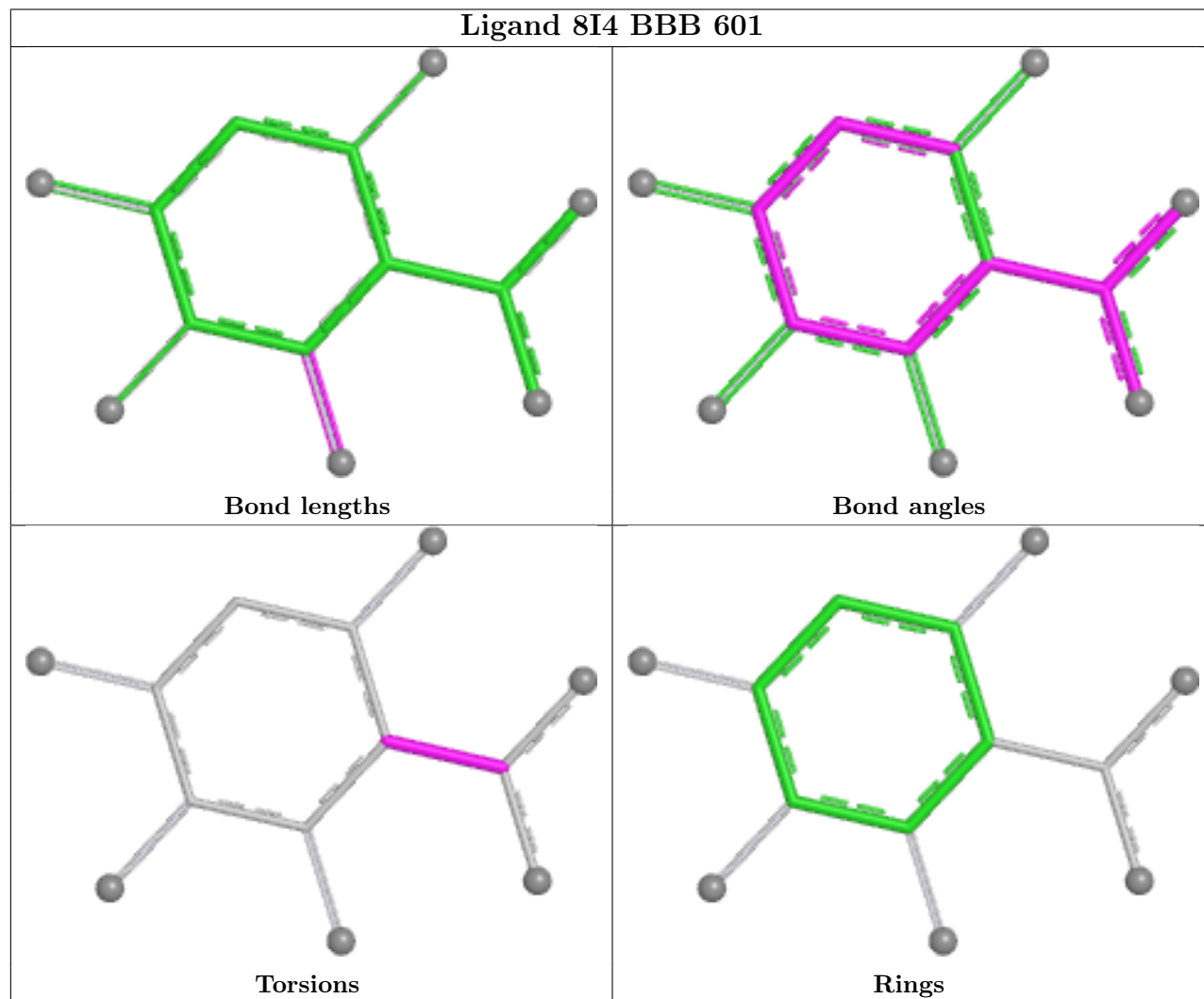
There are no ring outliers.

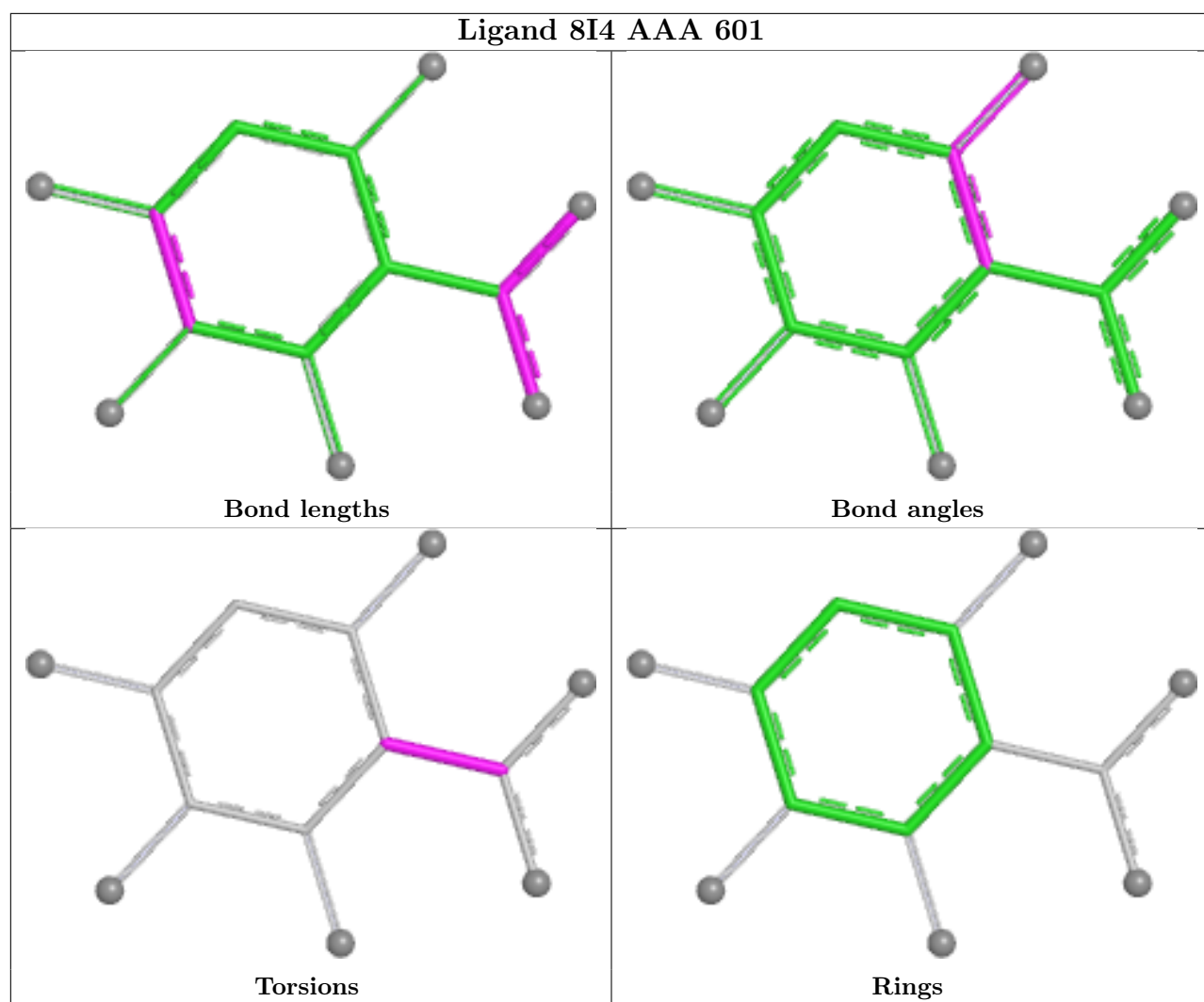
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	601	8I4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	599/601 (99%)	0.42	23 (3%) 44 43	20, 40, 68, 95	1 (0%)
1	BBB	592/601 (98%)	1.18	118 (19%) 3 2	33, 58, 85, 118	0
All	All	1191/1202 (99%)	0.80	141 (11%) 9 8	20, 49, 81, 118	1 (0%)

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	365	PHE	5.4
1	BBB	435	LEU	4.8
1	BBB	428	LEU	4.3
1	BBB	227	GLY	4.1
1	BBB	256	ALA	4.0

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](#)

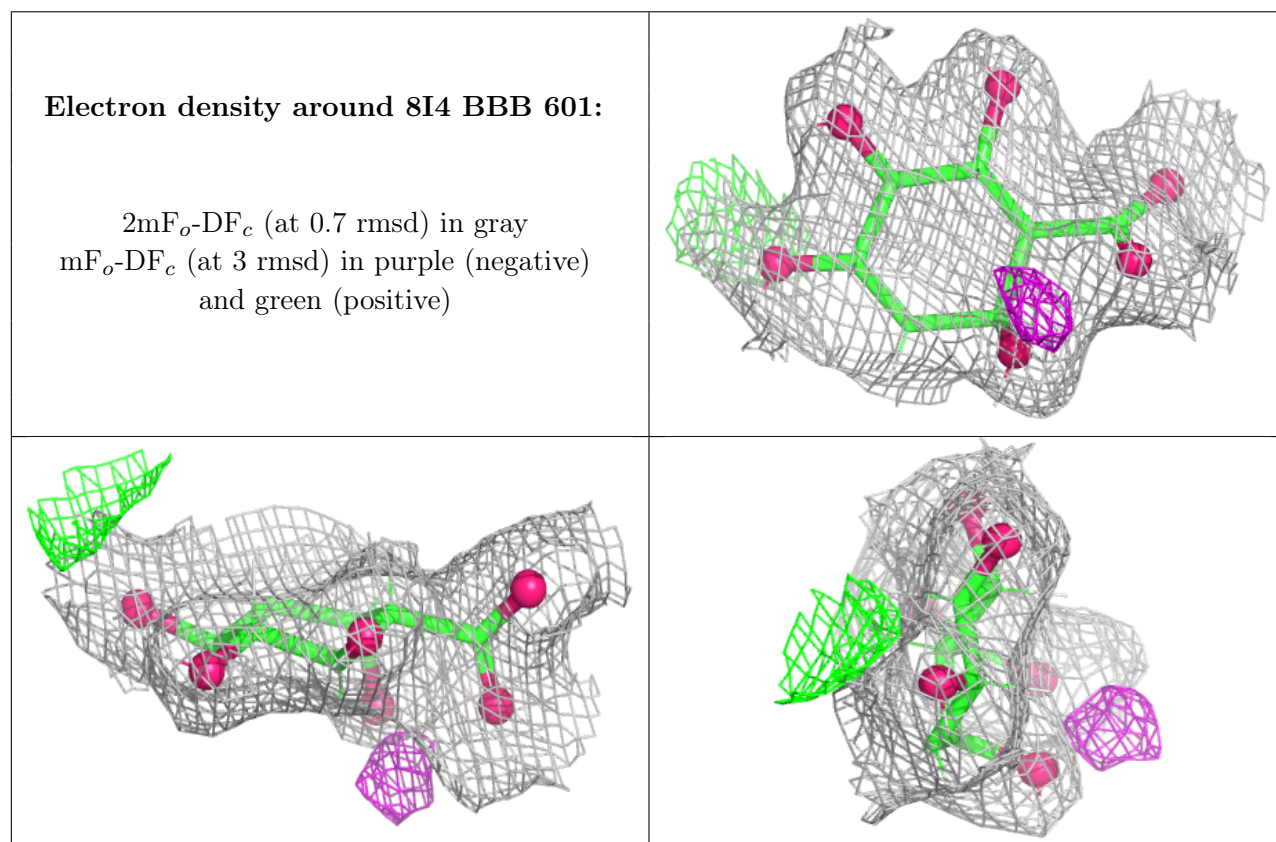
There are no oligosaccharides in this entry.

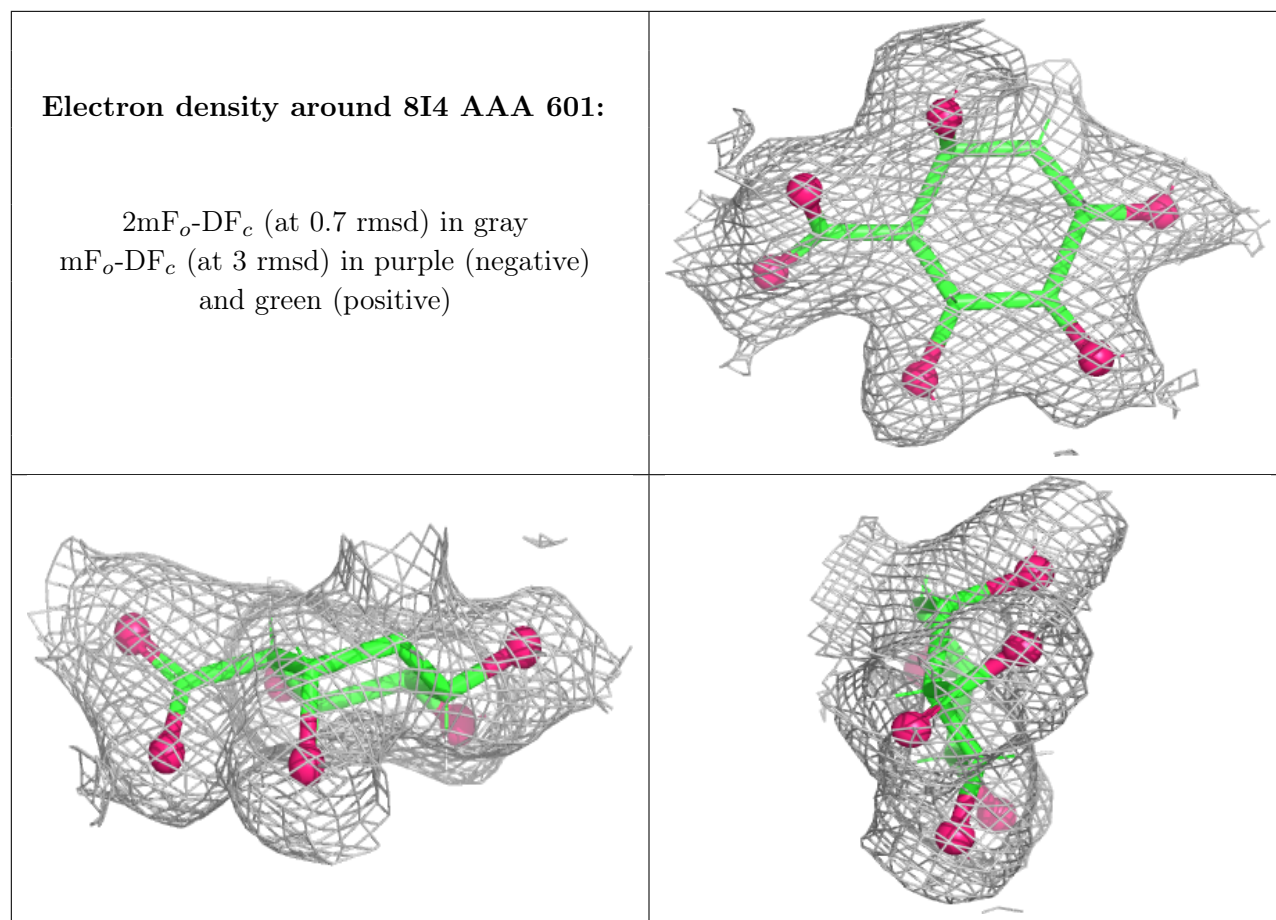
6.4 Ligands [i](#)

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, 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
2	8I4	BBB	601	13/14	0.90	0.07	40,42,44,46	4
2	8I4	AAA	601	13/14	0.97	0.04	25,28,29,32	4

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.