



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2021 – 04:06 pm BST

PDB ID : 7AWN
Title : Structure of the thermostabilized EAAT1 cryst mutant in complex with rubidium and barium and the allosteric inhibitor UCPH101
Authors : Canul-Tec, J.C.; Legrand, P.; Reyes, N.
Deposited on : 2020-11-08
Resolution : 3.92 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

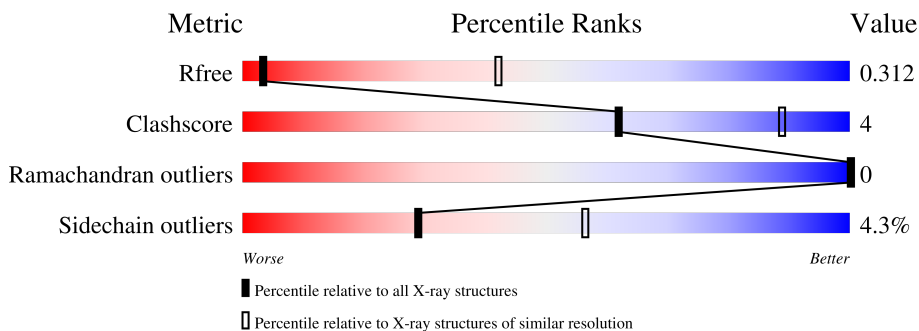
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	522	 63% 11% • 25%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3008 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Excitatory amino acid transporter 1,Neutral amino acid transporter B(0),Excitatory amino acid transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	2973	1962	477	517	17	0	0	0

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	ARG	engineered mutation	UNP P43003
A	44	PHE	TYR	engineered mutation	UNP P43003
A	46	ARG	PHE	engineered mutation	UNP P43003
A	50	LEU	PHE	engineered mutation	UNP P43003
A	51	LEU	VAL	engineered mutation	UNP P43003
A	56	LEU	THR	engineered mutation	UNP P43003
A	60	LEU	VAL	engineered mutation	UNP P43003
A	62	VAL	THR	engineered mutation	UNP P43003
A	63	VAL	ILE	engineered mutation	UNP P43003
A	67	LEU	THR	engineered mutation	UNP P43003
A	72	PRO	ARG	engineered mutation	UNP P43003
A	73	LEU	MET	engineered mutation	UNP P43003
A	75	PRO	TYR	engineered mutation	UNP P43003
A	82	ALA	SER	engineered mutation	UNP P43003
A	93	LYS	GLN	engineered mutation	UNP P43003
A	96	ILE	VAL	engineered mutation	UNP P43003
A	101	VAL	ILE	engineered mutation	UNP P43003
A	105	ILE	VAL	engineered mutation	UNP P43003
A	108	LEU	MET	engineered mutation	UNP P43003
A	110	SER	ALA	engineered mutation	UNP P43003
A	113	ALA	SER	engineered mutation	UNP P43003
A	118	ARG	LYS	engineered mutation	UNP P43003
A	119	LEU	MET	engineered mutation	UNP P43003
A	129	SER	THR	engineered mutation	UNP P43003
A	137	LEU	ILE	engineered mutation	UNP P43003
A	141	LEU	ILE	engineered mutation	UNP P43003

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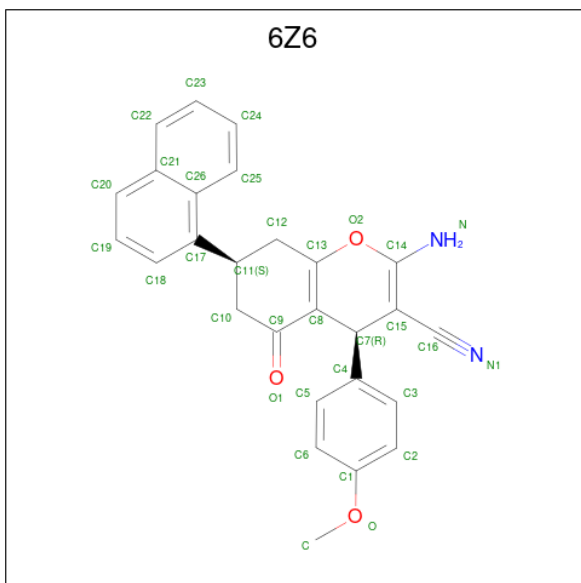
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	LEU	ILE	engineered mutation	UNP P43003
A	155	THR	ASN	engineered mutation	UNP Q15758
A	175	CYS	SER	engineered mutation	UNP Q15758
A	204	THR	ASN	engineered mutation	UNP Q15758
A	223	ILE	ALA	engineered mutation	UNP P43003
A	232	VAL	CYS	engineered mutation	UNP P43003
A	236	ALA	VAL	engineered mutation	UNP P43003
A	237	LEU	ILE	engineered mutation	UNP P43003
A	239	LYS	ASN	engineered mutation	UNP P43003
A	241	GLY	LYS	engineered mutation	UNP P43003
A	246	LEU	ALA	engineered mutation	UNP P43003
A	248	VAL	ARG	engineered mutation	UNP P43003
A	249	ASP	GLU	engineered mutation	UNP P43003
A	252	ASN	ASP	engineered mutation	UNP P43003
A	258	THR	ILE	engineered mutation	UNP P43003
A	260	LYS	ARG	engineered mutation	UNP P43003
A	264	ILE	VAL	engineered mutation	UNP P43003
A	271	LEU	VAL	engineered mutation	UNP P43003
A	287	LEU	MET	engineered mutation	UNP P43003
A	288	GLU	GLY	engineered mutation	UNP P43003
A	290	LEU	ILE	engineered mutation	UNP P43003
A	295	GLY	ALA	engineered mutation	UNP P43003
A	298	MET	THR	engineered mutation	UNP P43003
A	306	VAL	LEU	engineered mutation	UNP P43003
A	309	GLY	ALA	engineered mutation	UNP P43003
A	310	LEU	VAL	engineered mutation	UNP P43003
A	316	ILE	LEU	engineered mutation	UNP P43003
A	320	ILE	VAL	engineered mutation	UNP P43003
A	326	PHE	TRP	engineered mutation	UNP P43003
A	330	ALA	GLY	engineered mutation	UNP P43003
A	332	ILE	LEU	engineered mutation	UNP P43003
A	366	ILE	VAL	engineered mutation	UNP P43003
A	388	VAL	LEU	engineered mutation	UNP P43003
A	399	TYR	PHE	engineered mutation	UNP P43003
A	402	ASP	ASN	engineered mutation	UNP P43003
A	437	ALA	SER	engineered mutation	UNP P43003
A	454	LEU	PHE	engineered mutation	UNP P43003
A	458	PHE	LEU	engineered mutation	UNP P43003
A	461	MET	THR	engineered mutation	UNP P43003
A	462	VAL	THR	engineered mutation	UNP P43003
A	468	ALA	SER	engineered mutation	UNP P43003
A	480	LYS	HIS	engineered mutation	UNP P43003

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Chain	Residue	Modelled	Actual	Comment	Reference
A	483	GLU	LYS	engineered mutation	UNP P43003
A	484	LYS	ASN	engineered mutation	UNP P43003
A	485	GLN	ARG	engineered mutation	UNP P43003
A	487	ALA	VAL	engineered mutation	UNP P43003
A	489	LEU	MET	engineered mutation	UNP P43003

- Molecule 2 is 2-Amino-5,6,7,8-tetrahydro-4-(4-methoxyphenyl)-7-(naphthalen-1-yl)-5-oxo-4H-chromene-3-carbonitrile (three-letter code: 6Z6) (formula: C₂₇H₂₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	32	27	2	3	0	0

- Molecule 3 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
3	A	2	2	2	0	0

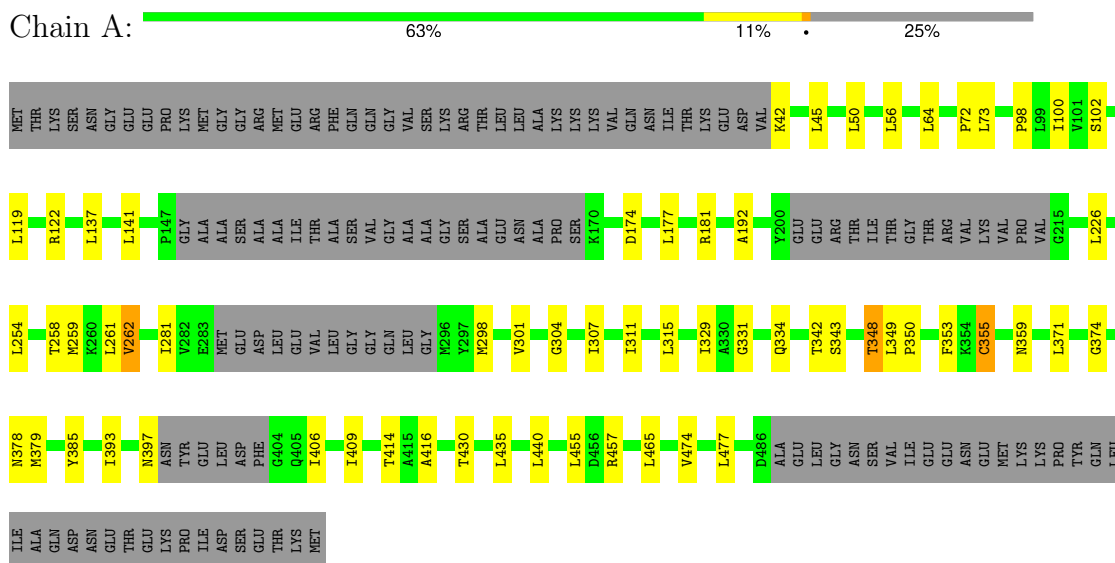
- Molecule 4 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Rb		
4	A	1	1	1	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. 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. 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: Excitatory amino acid transporter 1,Neutral amino acid transporter B(0),Excitatory amino acid transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	124.24Å 124.24Å 91.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.85 – 3.92 46.34 – 3.92	Depositor EDS
% Data completeness (in resolution range)	80.8 (21.85-3.92) 81.1 (46.34-3.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.88Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.230 , 0.279 0.275 , 0.312	Depositor DCC
R_{free} test set	294 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	168.0	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.118 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	3008	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: 6Z6, BA, RB

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	0.44	0/3019	0.61	0/4099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts 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	A	2973	0	3184	27	0
2	A	32	0	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
All	All	3008	0	3184	27	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 4.

The worst 5 of 27 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:SER:HB2	1:A:457:ARG:HD3	1.76	0.68
1:A:262:VAL:HG21	1:A:350:PRO:HB2	1.77	0.66
1:A:72:PRO:HD2	1:A:73:LEU:HD22	1.84	0.60
1:A:393:ILE:HD13	1:A:435:LEU:HD21	1.83	0.60
1:A:141:LEU:HD11	1:A:304:GLY:HA3	1.83	0.59

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	381/522 (73%)	361 (95%)	20 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/431 (75%)	310 (96%)	14 (4%)	29 56

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	VAL
1	A	281	ILE

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Mol	Chain	Res	Type
1	A	474	VAL
1	A	353	PHE
1	A	355	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	6Z6	A	601	-	36,36,36	1.43	6 (16%)	51,52,52	1.54	7 (13%)

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	6Z6	A	601	-	-	5/10/44/44	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	6Z6	C17-C26	3.50	1.49	1.43
2	A	601	6Z6	C14-N	2.65	1.36	1.33
2	A	601	6Z6	C9-C8	2.46	1.50	1.45
2	A	601	6Z6	C10-C9	2.31	1.54	1.50
2	A	601	6Z6	C2-C1	2.06	1.42	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	6Z6	C4-C7-C15	-4.70	105.28	111.48
2	A	601	6Z6	C11-C17-C26	4.64	125.51	120.67
2	A	601	6Z6	C18-C17-C11	-3.38	117.06	120.55
2	A	601	6Z6	O2-C13-C8	2.93	124.64	122.69
2	A	601	6Z6	O2-C13-C12	-2.52	108.20	112.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

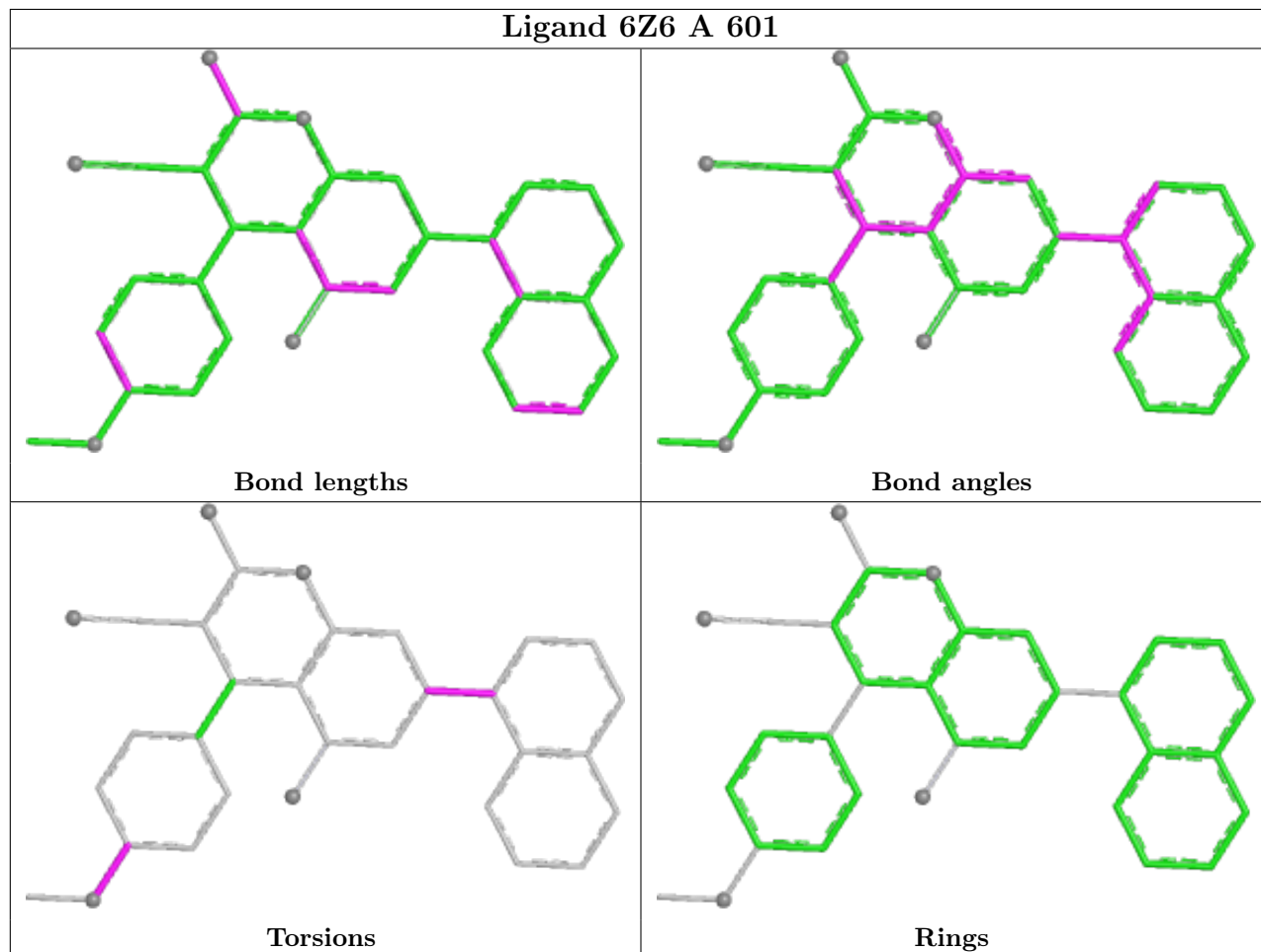
Mol	Chain	Res	Type	Atoms
2	A	601	6Z6	C6-C1-O-C
2	A	601	6Z6	C2-C1-O-C
2	A	601	6Z6	C12-C11-C17-C18
2	A	601	6Z6	C12-C11-C17-C26
2	A	601	6Z6	C10-C11-C17-C18

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

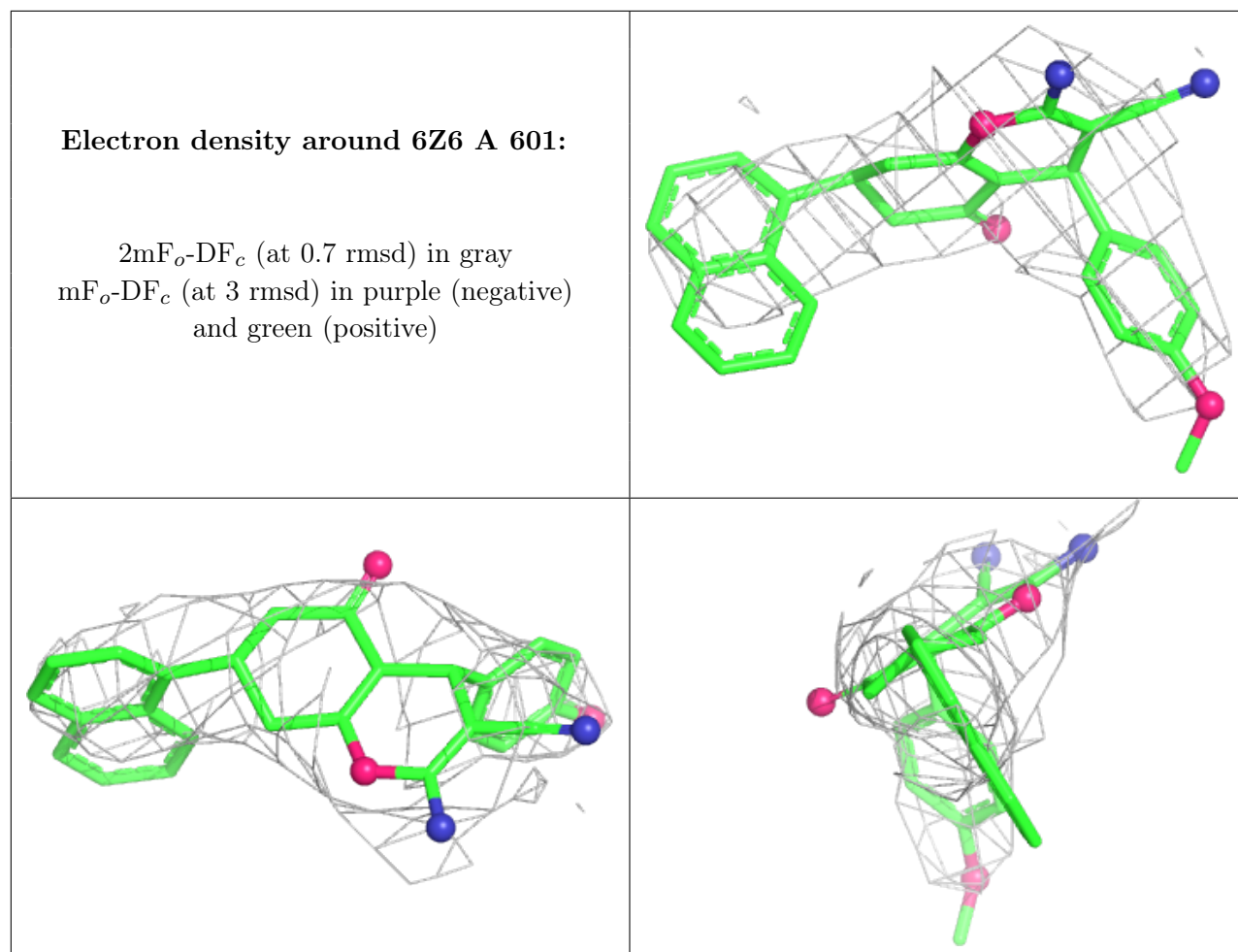
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.