



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 11:48 PM UTC

PDB ID : 7SBN / pdb_00007sbn
Title : Human glutaminase C (Y466W) with L-Gln, closed conformation
Authors : Nguyen, T.-T.T.; Cerione, R.A.
Deposited on : 2021-09-25
Resolution : 2.14 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 : **FAILED**
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

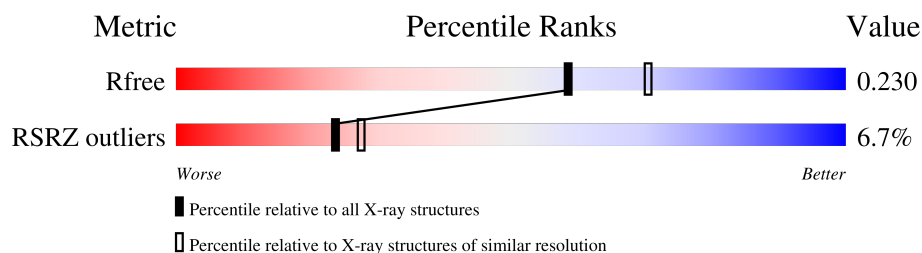
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13069 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 Isoform 3 of Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	2	0	0
			3182	2030	535	589	28			
1	B	405	Total	C	N	O	S	2	0	0
			3158	2016	531	583	28			
1	C	407	Total	C	N	O	S	2	0	0
			3175	2026	534	587	28			
1	D	406	Total	C	N	O	S	2	0	0
			3173	2026	535	584	28			

There are 52 discrepancies between the modelled and reference sequences:

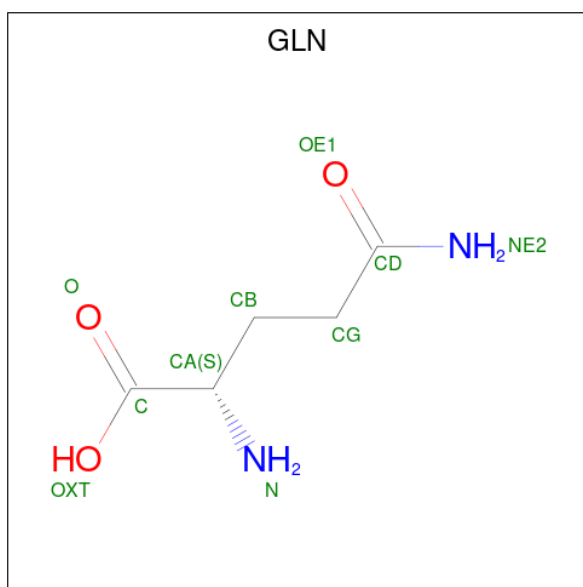
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	GLY	-	expression tag	UNP O94925
A	71	SER	-	expression tag	UNP O94925
A	466	TRP	TYR	engineered mutation	UNP O94925
B	60	MET	-	initiating methionine	UNP O94925
B	61	ARG	-	expression tag	UNP O94925
B	62	GLY	-	expression tag	UNP O94925
B	63	SER	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	68	HIS	-	expression tag	UNP O94925
B	69	HIS	-	expression tag	UNP O94925
B	70	GLY	-	expression tag	UNP O94925
B	71	SER	-	expression tag	UNP O94925
B	466	TRP	TYR	engineered mutation	UNP O94925
C	60	MET	-	initiating methionine	UNP O94925
C	61	ARG	-	expression tag	UNP O94925
C	62	GLY	-	expression tag	UNP O94925
C	63	SER	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	GLY	-	expression tag	UNP O94925
C	71	SER	-	expression tag	UNP O94925
C	466	TRP	TYR	engineered mutation	UNP O94925
D	60	MET	-	initiating methionine	UNP O94925
D	61	ARG	-	expression tag	UNP O94925
D	62	GLY	-	expression tag	UNP O94925
D	63	SER	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	GLY	-	expression tag	UNP O94925
D	71	SER	-	expression tag	UNP O94925
D	466	TRP	TYR	engineered mutation	UNP O94925

- Molecule 2 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	2	3		
2	B	1	Total	C	N	O	0	0
			10	5	2	3		
2	C	1	Total	C	N	O	0	0
			10	5	2	3		
2	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	74	Total	O	0	0
			74	74		
3	C	81	Total	O	0	0
			81	81		
3	D	62	Total	O	0	0
			62	62		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.06Å 140.15Å 177.23Å 90.00° 95.37° 90.00°	Depositor
Resolution (Å)	47.79 – 2.14 47.79 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.79-2.14) 98.4 (47.79-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.188 , 0.229 0.190 , 0.230	Depositor DCC
R_{free} test set	1999 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13069	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

4 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	GLN	B	601	-	8,9,9	0.74	0	8,11,11	0.63	0
2	GLN	C	601	-	8,9,9	0.73	0	8,11,11	0.55	0
2	GLN	D	601	-	8,9,9	0.80	0	8,11,11	0.85	1 (12%)
2	GLN	A	601	-	8,9,9	0.74	0	8,11,11	0.99	1 (12%)

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	GLN	B	601	-	-	3/9/9/9	-
2	GLN	C	601	-	-	6/9/9/9	-
2	GLN	D	601	-	-	0/9/9/9	-
2	GLN	A	601	-	-	0/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GLN	OXT-C-O	-2.77	117.80	124.08
2	D	601	GLN	OXT-C-O	-2.32	118.82	124.08

There are no chirality outliers.

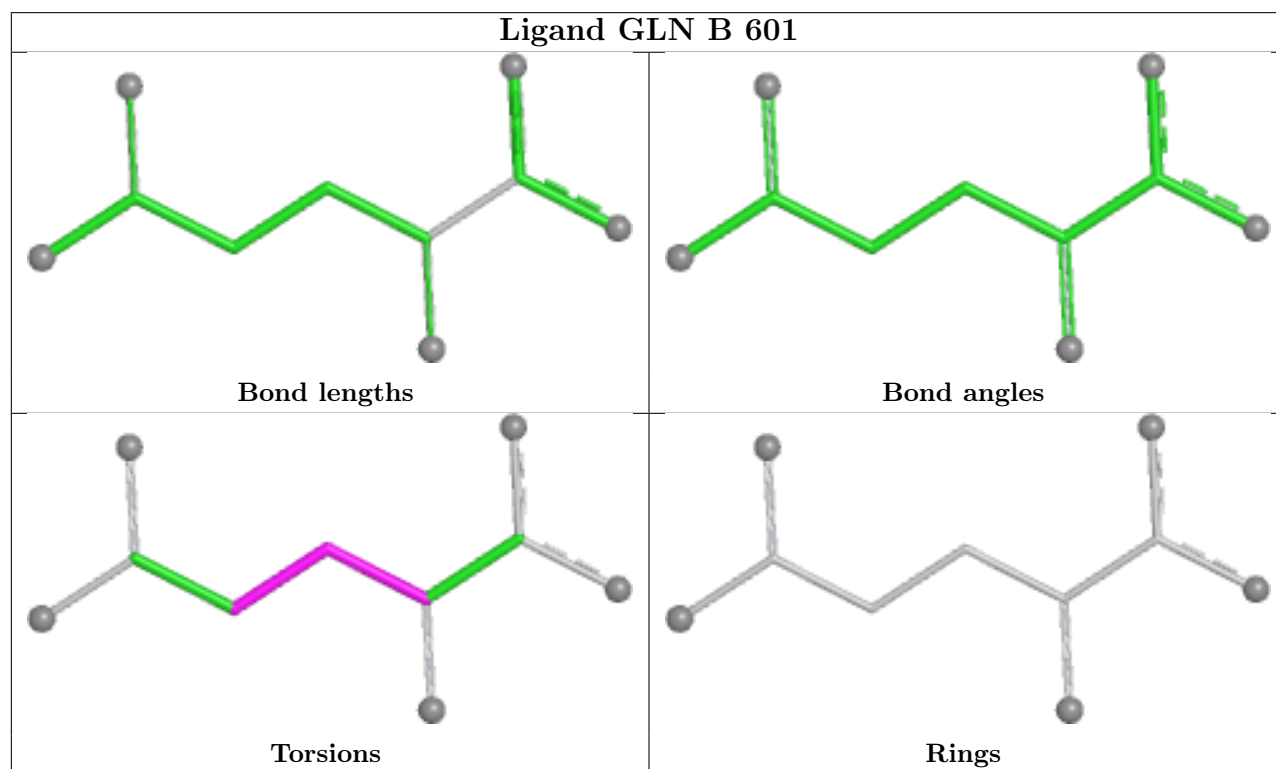
All (9) torsion outliers are listed below:

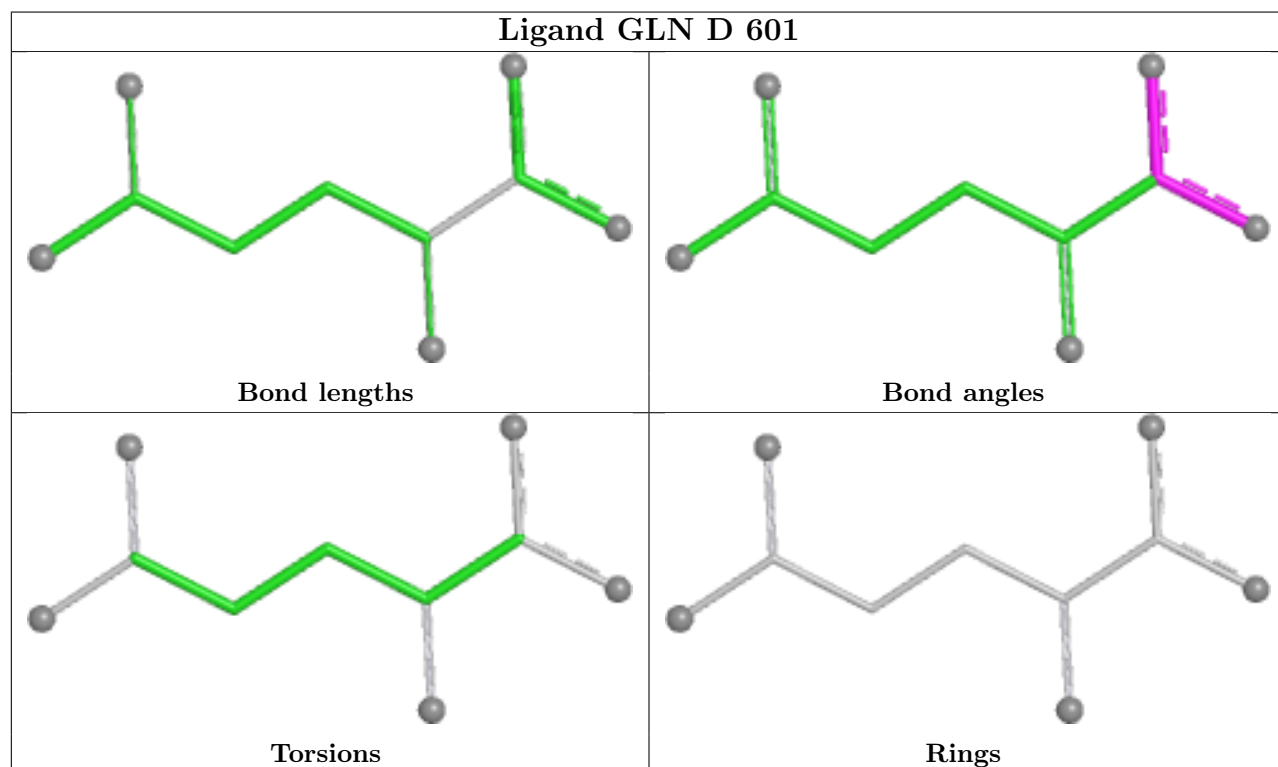
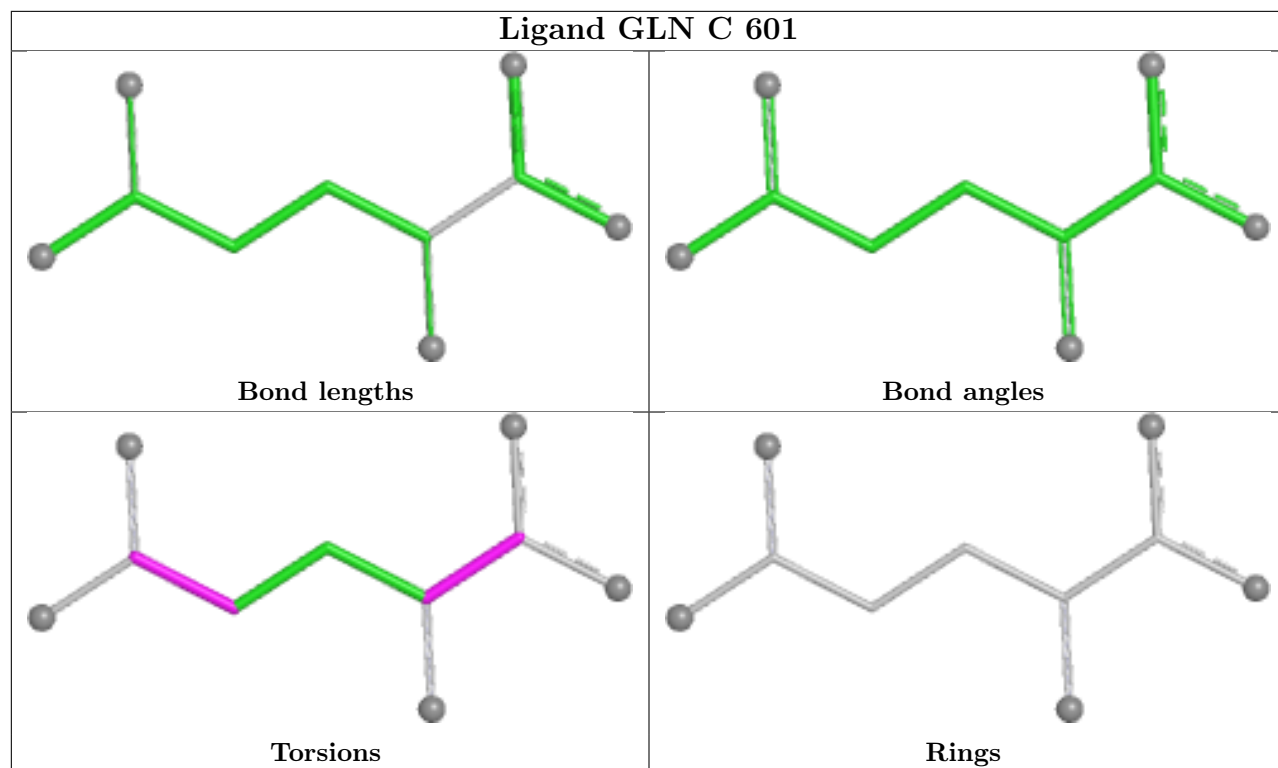
Mol	Chain	Res	Type	Atoms
2	B	601	GLN	C-CA-CB-CG
2	C	601	GLN	O-C-CA-N
2	C	601	GLN	OXT-C-CA-N
2	C	601	GLN	O-C-CA-CB
2	C	601	GLN	OXT-C-CA-CB
2	B	601	GLN	N-CA-CB-CG
2	B	601	GLN	CA-CB-CG-CD
2	C	601	GLN	NE2-CD-CG-CB
2	C	601	GLN	OE1-CD-CG-CB

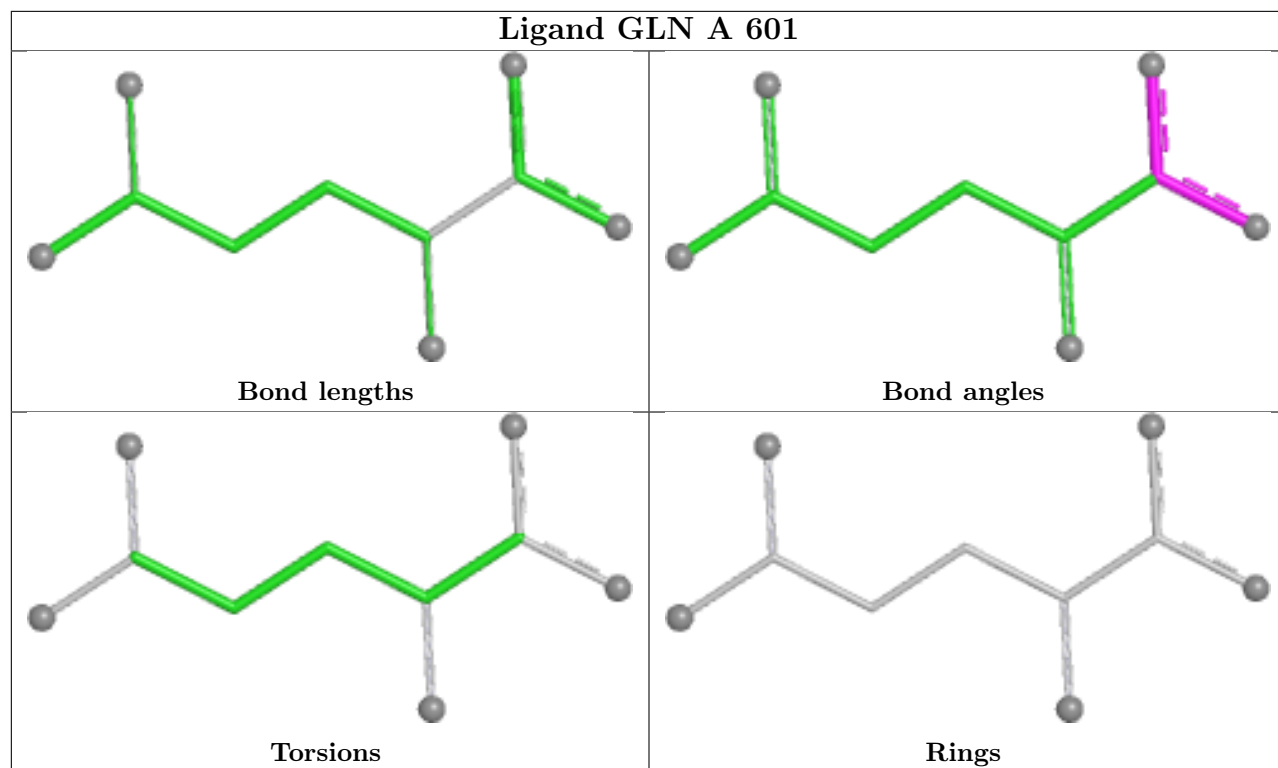
There are no ring outliers.

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.







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	409/539 (75%)	-0.09	28 (6%)	23	27	18, 30, 71, 137	1 (0%)
1	B	405/539 (75%)	0.10	25 (6%)	26	30	24, 35, 71, 106	1 (0%)
1	C	407/539 (75%)	0.11	24 (5%)	28	32	21, 35, 72, 125	1 (0%)
1	D	406/539 (75%)	0.25	32 (7%)	18	21	24, 38, 83, 128	1 (0%)
All	All	1627/2156 (75%)	0.09	109 (6%)	24	27	18, 35, 76, 137	4 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	LEU	12.1
1	C	316	LEU	8.2
1	C	189	THR	8.1
1	B	316	LEU	8.0
1	A	136	LEU	7.6
1	A	316	LEU	7.3
1	D	135	LEU	7.3
1	D	316	LEU	7.1
1	C	136	LEU	7.0
1	B	321	LEU	6.9
1	D	136	LEU	6.9
1	B	189	THR	6.7
1	C	321	LEU	6.4
1	D	321	LEU	6.4
1	B	192	GLY	6.3
1	D	254	ALA	6.3
1	B	136	LEU	6.2
1	A	546	GLY	6.0
1	D	193	VAL	5.6
1	A	135	LEU	5.5
1	C	546	GLY	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	546	GLY	5.0
1	A	315	GLY	5.0
1	D	315	GLY	4.9
1	A	321	LEU	4.9
1	C	192	GLY	4.7
1	D	137	PRO	4.7
1	B	546	GLY	4.6
1	B	190	SER	4.5
1	D	255	LYS	4.5
1	D	252	GLN	4.4
1	D	250	ILE	4.3
1	A	137	PRO	4.1
1	B	137	PRO	4.1
1	B	151	GLN	4.1
1	C	193	VAL	4.0
1	D	317	ARG	4.0
1	C	315	GLY	3.8
1	C	320	LYS	3.8
1	D	148	ALA	3.8
1	B	348	GLY	3.7
1	C	191	ASP	3.6
1	C	148	ALA	3.6
1	C	137	PRO	3.6
1	B	361	PHE	3.5
1	B	193	VAL	3.4
1	D	256	PHE	3.4
1	C	151	GLN	3.3
1	D	145	TYR	3.2
1	C	544	ARG	3.2
1	D	189	THR	3.2
1	B	325	GLU	3.1
1	D	190	SER	3.1
1	D	195	LEU	3.1
1	B	322	PHE	3.0
1	D	251	PRO	3.0
1	A	191	ASP	3.0
1	B	538	LYS	3.0
1	A	190	SER	3.0
1	D	314	SER	3.0
1	A	348	GLY	3.0
1	A	144	PHE	2.9
1	C	538	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	2.8
1	A	192	GLY	2.8
1	D	348	GLY	2.8
1	D	139	LEU	2.8
1	A	150	GLY	2.7
1	C	348	GLY	2.7
1	D	540	LEU	2.7
1	D	194	MET	2.7
1	C	142	LEU	2.7
1	C	325	GLU	2.7
1	A	537	ALA	2.6
1	D	152	GLU	2.6
1	A	148	ALA	2.6
1	B	139	LEU	2.6
1	B	507	LYS	2.5
1	D	149	GLU	2.5
1	D	249	TYR	2.5
1	C	322	PHE	2.5
1	A	189	THR	2.5
1	C	190	SER	2.5
1	B	315	GLY	2.5
1	C	360	GLN	2.4
1	A	145	TYR	2.4
1	B	225	MET	2.4
1	C	145	TYR	2.4
1	B	144	PHE	2.3
1	D	325	GLU	2.3
1	C	149	GLU	2.2
1	D	142	LEU	2.2
1	D	538	LYS	2.2
1	A	152	GLU	2.1
1	B	147	ILE	2.1
1	A	193	VAL	2.1
1	A	146	THR	2.1
1	A	200	PHE	2.1
1	A	540	LEU	2.1
1	B	142	LEU	2.1
1	B	145	TYR	2.1
1	A	536	PHE	2.1
1	A	538	LYS	2.1
1	B	255	LYS	2.1
1	B	149	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	GLN	2.1
1	C	188	THR	2.1
1	A	188	THR	2.0
1	A	251	PRO	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

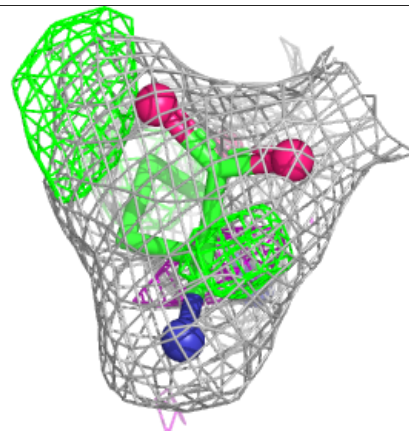
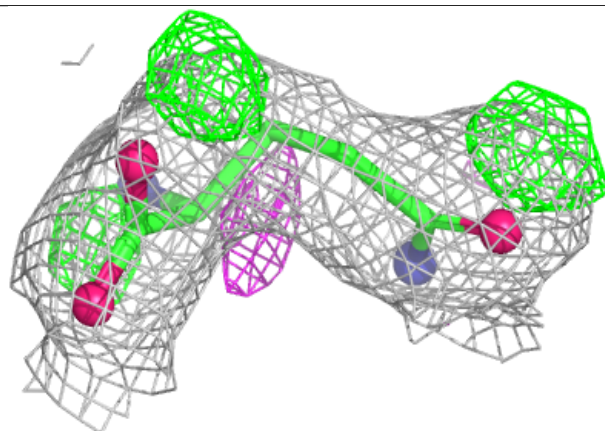
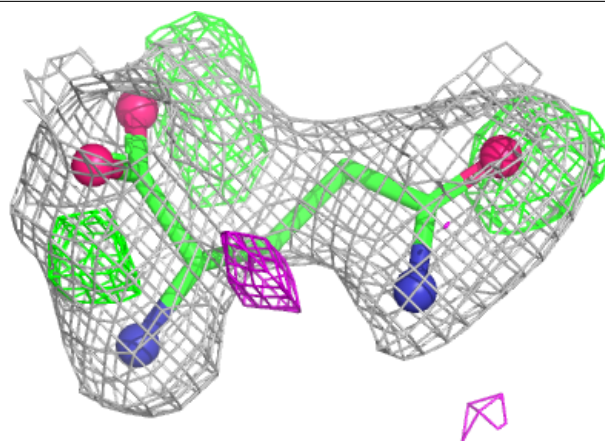
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLN	C	601	10/10	0.82	0.19	44,53,60,64	0
2	GLN	B	601	10/10	0.94	0.09	27,38,43,45	0
2	GLN	A	601	10/10	0.95	0.08	25,35,41,43	0
2	GLN	D	601	10/10	0.95	0.08	30,40,44,45	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.

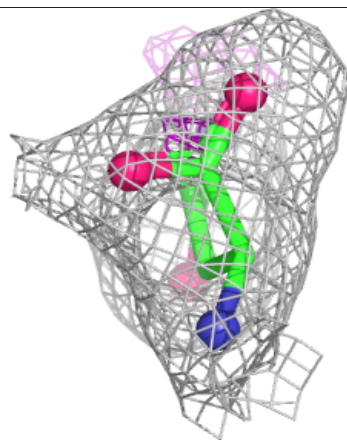
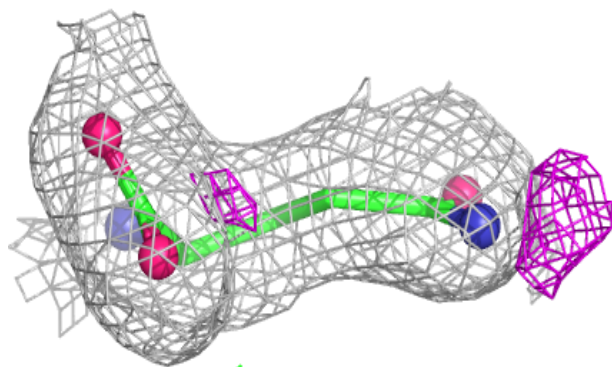
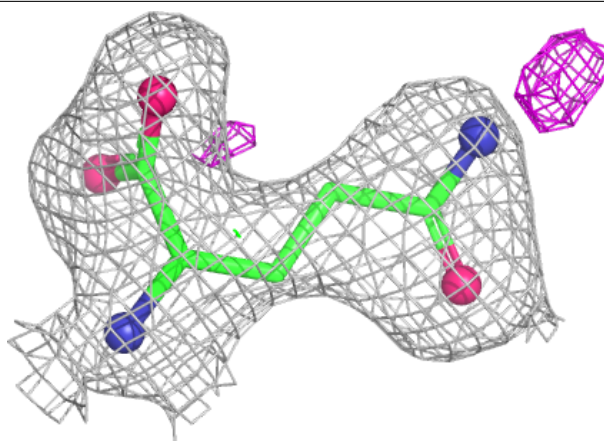
Electron density around GLN C 601:

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



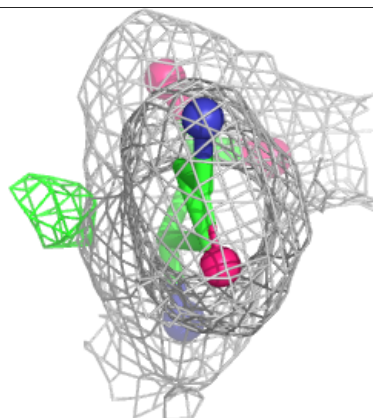
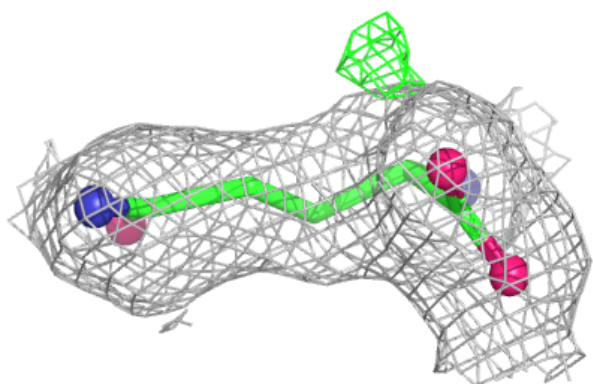
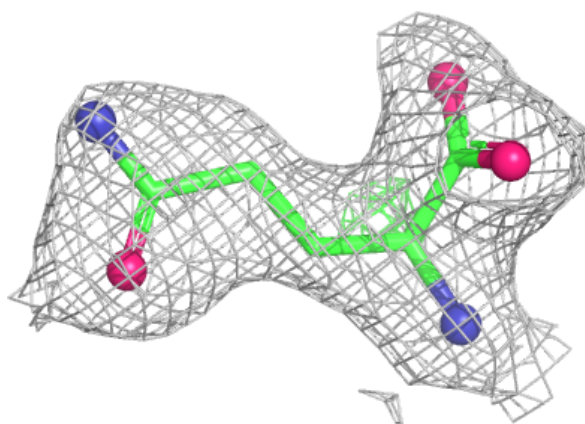
Electron density around GLN B 601:

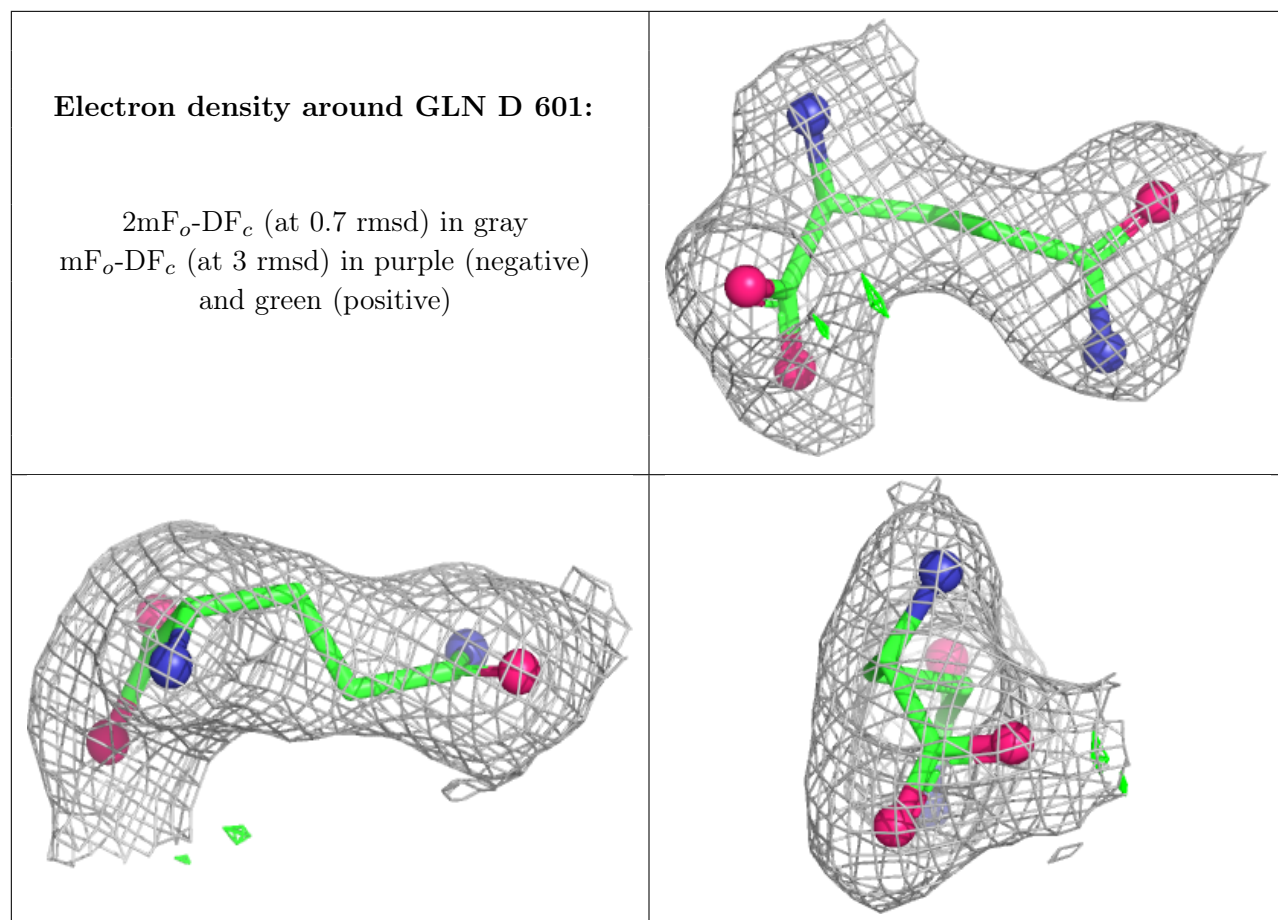
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GLN A 601:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.