



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2022 – 08:07 AM EST

PDB ID : 7SBN
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 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 : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

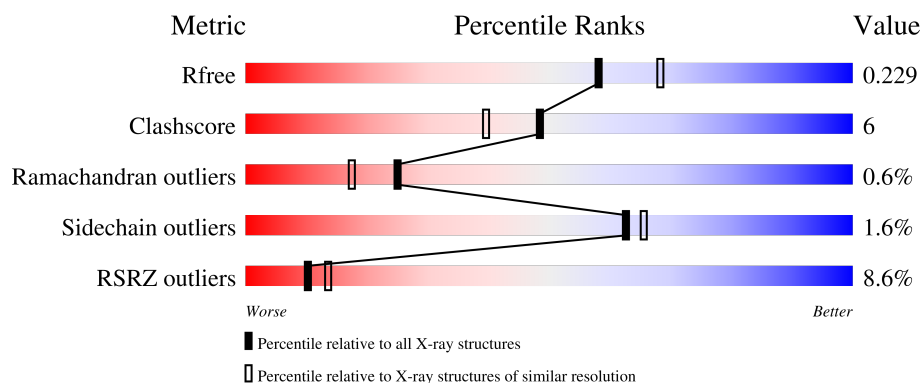
1 Overall quality at a glance

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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	539	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>10%</div> <div>24%</div> </div> </div>
1	B	539	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>25%</div> </div> </div>
1	C	539	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>24%</div> </div> </div>
1	D	539	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>10%</div> <div>25%</div> </div> </div>

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:

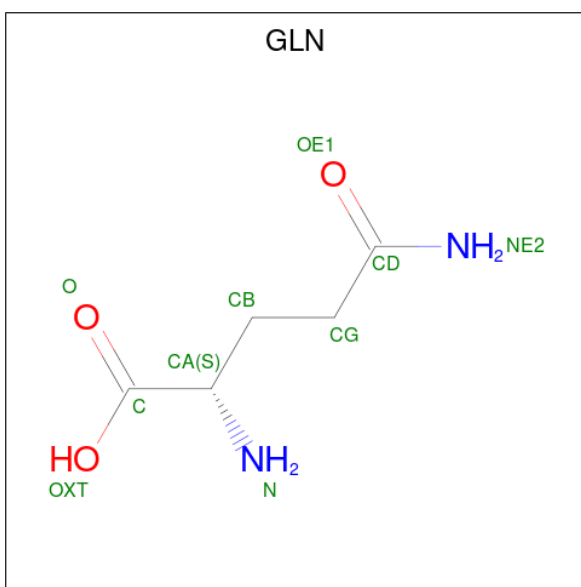
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	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

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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 (three-letter code: 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		

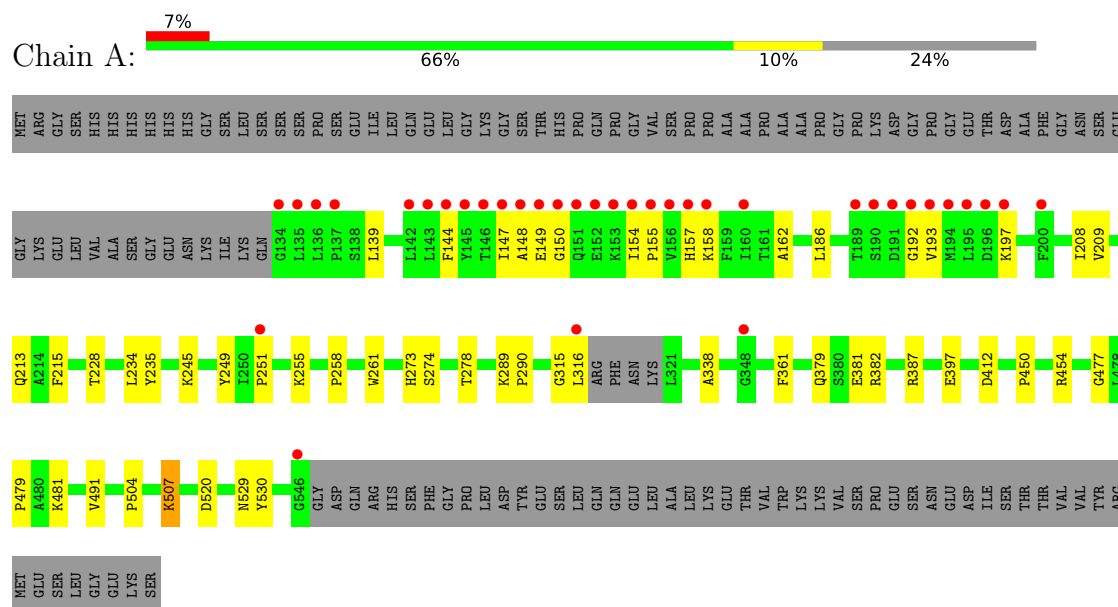
- Molecule 3 is water.

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		

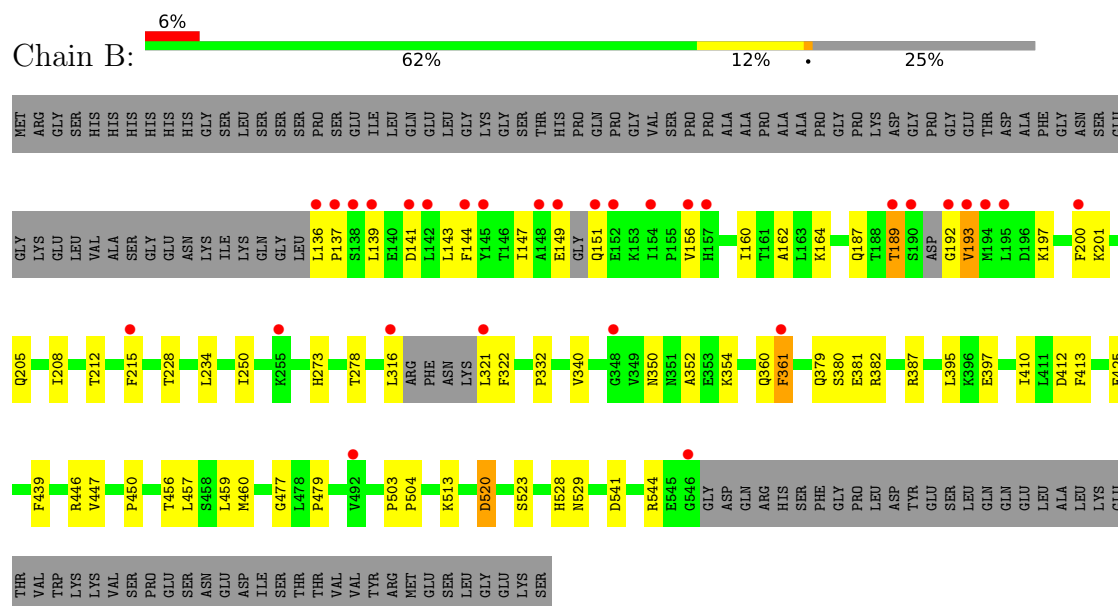
3 Residue-property plots

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.

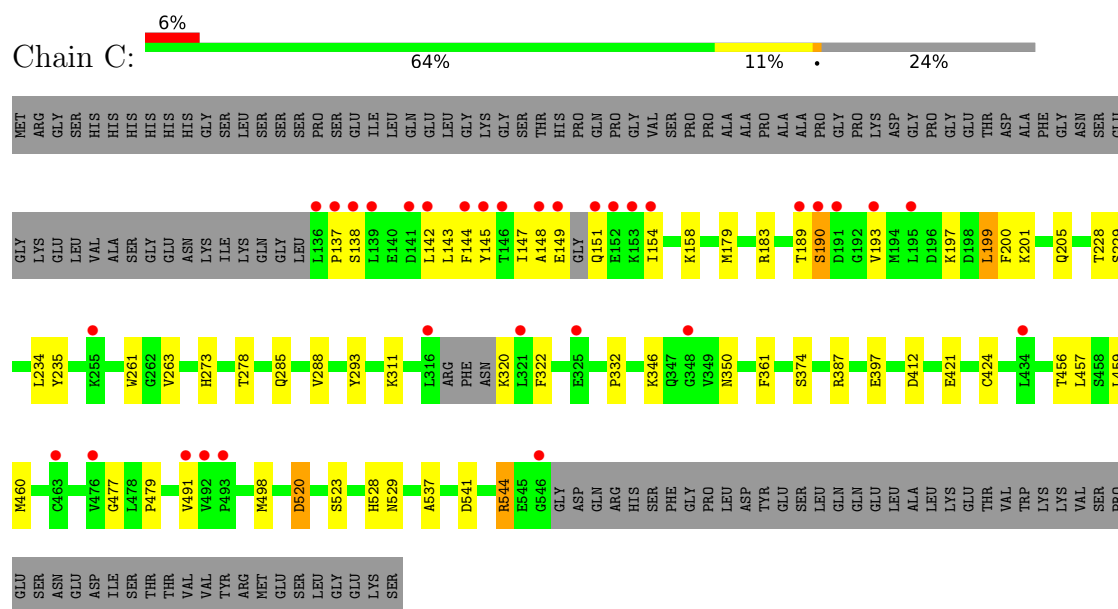
- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



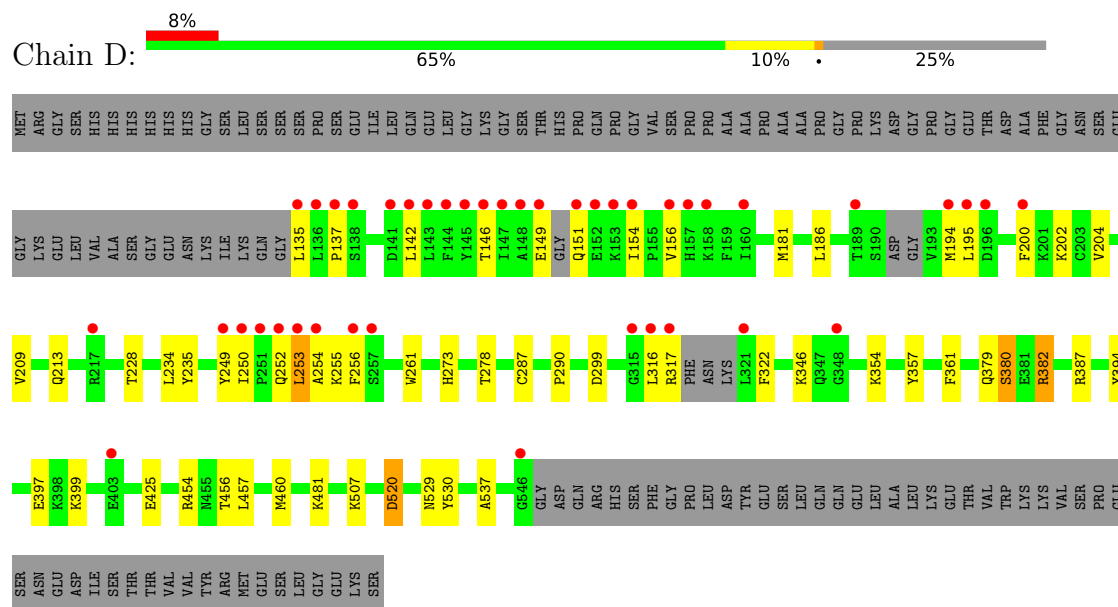
- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



4 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 0.188 , 0.229	Depositor DCC
R_{free} test set	1999 reflections (1.49%)	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 , 41.6	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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/3253	0.56	0/4393
1	B	0.40	0/3227	0.56	0/4355
1	C	0.40	0/3245	0.56	0/4380
1	D	0.38	0/3242	0.55	0/4375
All	All	0.40	0/12967	0.56	0/17503

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	254	ALA	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	A	3182	0	3159	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3158	0	3136	49	0
1	C	3175	0	3154	43	0
1	D	3173	0	3157	43	0
2	A	10	0	7	0	0
2	B	10	0	7	1	0
2	C	10	0	7	0	0
2	D	10	0	7	0	0
3	A	124	0	0	1	0
3	B	74	0	0	1	0
3	C	81	0	0	2	0
3	D	62	0	0	0	0
All	All	13069	0	12634	152	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 6.

All (152) 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:D:252:GLN:HG3	1:D:380:SER:HB2	1.43	0.99
1:B:139:LEU:CD2	1:B:212:THR:HG21	2.04	0.87
1:B:139:LEU:HD21	1:B:212:THR:HG21	1.56	0.87
1:C:457:LEU:HD23	1:C:460:MET:HE1	1.58	0.84
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.62	0.80
1:D:457:LEU:HD23	1:D:460:MET:HE3	1.63	0.80
1:C:456:THR:HG22	1:C:460:MET:HE2	1.64	0.79
1:C:228:THR:HG23	1:C:273:HIS:CE1	2.19	0.78
1:D:228:THR:HG23	1:D:273:HIS:CE1	2.20	0.77
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.69	0.75
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.67	0.75
1:B:228:THR:HG23	1:B:273:HIS:CE1	2.27	0.70
1:B:456:THR:HG22	1:B:460:MET:HE2	1.76	0.67
1:A:228:THR:HG23	1:A:273:HIS:CE1	2.30	0.67
1:C:544:ARG:NH2	3:C:701:HOH:O	2.27	0.66
1:B:141:ASP:OD2	1:B:197:LYS:NZ	2.25	0.63
1:A:251:PRO:O	1:A:255:LYS:HG3	2.00	0.61
1:B:529:ASN:OD1	1:D:529:ASN:ND2	2.30	0.61
1:A:382:ARG:NH1	3:A:701:HOH:O	2.30	0.60
1:B:321:LEU:HG	1:B:322:PHE:H	1.67	0.60
1:C:456:THR:HG22	1:C:460:MET:CE	2.30	0.60
1:C:137:PRO:HG2	1:C:142:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LYS:HE2	3:C:745:HOH:O	2.00	0.60
1:C:143:LEU:HD12	1:C:200:PHE:HZ	1.68	0.58
1:A:397:GLU:HG3	1:B:387:ARG:HB2	1.85	0.58
1:A:148:ALA:O	1:A:150:GLY:N	2.37	0.58
1:C:397:GLU:HG3	1:D:387:ARG:HB2	1.85	0.58
1:C:148:ALA:HB2	1:C:154:ILE:HG12	1.84	0.58
1:A:387:ARG:HB2	1:B:397:GLU:HG3	1.86	0.58
1:C:147:ILE:O	1:C:158:LYS:NZ	2.28	0.58
1:B:136:LEU:HG	1:B:137:PRO:HD3	1.85	0.58
1:C:541:ASP:HB3	1:C:544:ARG:HG2	1.85	0.57
1:A:507:LYS:H	1:A:507:LYS:HE2	1.67	0.57
1:B:321:LEU:HG	1:B:322:PHE:N	2.20	0.56
1:B:197:LYS:HZ2	1:B:197:LYS:HB3	1.71	0.55
1:B:456:THR:HG22	1:B:460:MET:CE	2.36	0.55
1:A:209:VAL:O	1:A:213:GLN:HG3	2.06	0.55
1:D:317:ARG:HH12	1:D:322:PHE:H	1.55	0.55
1:B:350:ASN:HD21	1:B:352:ALA:HB3	1.72	0.55
1:A:379:GLN:O	1:A:382:ARG:HG2	2.08	0.53
1:D:249:TYR:CE1	1:D:250:ILE:HG23	2.44	0.53
1:D:253:LEU:C	1:D:255:LYS:H	2.13	0.52
1:D:457:LEU:HD23	1:D:460:MET:CE	2.36	0.52
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.73	0.52
1:C:144:PHE:CE2	1:C:197:LYS:HG2	2.44	0.52
1:A:154:ILE:HG23	1:A:158:LYS:HD3	1.90	0.52
1:A:507:LYS:H	1:A:507:LYS:CE	2.22	0.51
1:B:457:LEU:HD23	1:B:460:MET:HE1	1.92	0.51
1:D:252:GLN:HG3	1:D:380:SER:CB	2.29	0.51
1:A:274:SER:HB3	1:A:278:THR:HG21	1.92	0.51
1:A:450:PRO:HG2	1:C:537:ALA:HB2	1.91	0.51
1:C:320:LYS:HG3	1:D:394:TYR:OH	2.10	0.51
1:D:456:THR:HG22	1:D:460:MET:CE	2.41	0.51
1:D:290:PRO:HD3	1:D:481:LYS:HG2	1.94	0.50
1:C:320:LYS:HB3	1:C:322:PHE:CE1	2.47	0.50
1:D:149:GLU:O	1:D:151:GLN:HB3	2.10	0.50
1:D:142:LEU:O	1:D:146:THR:HG23	2.12	0.50
1:C:387:ARG:N	1:D:397:GLU:HG3	2.27	0.50
1:C:457:LEU:HD23	1:C:460:MET:CE	2.35	0.50
1:B:381:GLU:OE2	2:B:601:GLN:N	2.45	0.50
1:C:148:ALA:HB2	1:C:154:ILE:CG1	2.42	0.49
1:A:530:TYR:CE1	1:C:479:PRO:HG3	2.47	0.49
1:B:192:GLY:O	1:B:193:VAL:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.93	0.49
1:C:320:LYS:O	1:C:322:PHE:N	2.39	0.49
1:A:454:ARG:HD2	1:C:528:HIS:CD2	2.48	0.49
1:D:278:THR:O	1:D:425:GLU:HG3	2.12	0.49
1:B:450:PRO:HG2	1:D:537:ALA:HB2	1.94	0.48
1:B:541:ASP:OD2	1:B:544:ARG:NH1	2.47	0.47
1:C:179:MET:O	1:C:183:ARG:HG2	2.13	0.47
1:B:477:GLY:O	1:B:529:ASN:HB2	2.14	0.47
1:D:209:VAL:O	1:D:213:GLN:HG3	2.14	0.47
1:B:197:LYS:NZ	1:B:197:LYS:HB3	2.29	0.47
1:B:529:ASN:CG	1:D:529:ASN:HD21	2.18	0.47
1:D:149:GLU:HB2	1:D:151:GLN:NE2	2.29	0.47
1:D:181:MET:HE1	1:D:202:LYS:HE2	1.97	0.47
1:B:144:PHE:CE2	1:B:197:LYS:HG2	2.50	0.47
1:B:340:VAL:HG23	1:B:395:LEU:HD13	1.96	0.47
1:B:479:PRO:HG3	1:D:530:TYR:CE1	2.50	0.47
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.75	0.47
1:B:139:LEU:HD22	1:B:208:ILE:HG13	1.98	0.47
1:D:252:GLN:CG	1:D:380:SER:HB2	2.31	0.47
1:B:316:LEU:HD22	1:B:321:LEU:HB2	1.97	0.46
1:D:253:LEU:O	1:D:256:PHE:CD1	2.68	0.46
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.80	0.46
1:B:361:PHE:HE1	1:B:447:VAL:HG12	1.79	0.46
1:D:154:ILE:O	1:D:195:LEU:HB2	2.14	0.46
1:B:379:GLN:O	1:B:382:ARG:HG2	2.16	0.46
1:A:249:TYR:OH	1:A:381:GLU:OE1	2.21	0.46
1:D:346:LYS:HB3	1:D:354:LYS:HG2	1.97	0.46
1:A:258:PRO:HB3	1:A:504:PRO:HG3	1.97	0.45
1:D:253:LEU:C	1:D:255:LYS:N	2.68	0.45
1:D:507:LYS:HE2	1:D:507:LYS:H	1.82	0.45
1:D:317:ARG:NH1	1:D:322:PHE:H	2.13	0.45
1:C:477:GLY:O	1:C:529:ASN:HB2	2.16	0.45
1:A:289:LYS:HE3	1:A:338:ALA:CB	2.47	0.45
1:A:290:PRO:HD3	1:A:481:LYS:HG2	1.98	0.45
1:B:139:LEU:HD23	1:B:139:LEU:O	2.17	0.45
1:C:235:TYR:CE1	1:C:261:TRP:CD1	3.05	0.45
1:B:439:PHE:CE2	1:B:446:ARG:HB2	2.52	0.44
1:D:456:THR:HG22	1:D:460:MET:HE1	1.99	0.44
1:C:479:PRO:HD2	1:C:491:VAL:O	2.17	0.44
1:C:149:GLU:O	1:C:151:GLN:HB2	2.17	0.44
1:B:143:LEU:HD11	1:B:147:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLU:O	1:B:151:GLN:HB3	2.18	0.44
1:B:156:VAL:HG12	1:B:193:VAL:HG22	1.99	0.44
1:A:315:GLY:O	1:A:316:LEU:HD12	2.18	0.44
1:A:477:GLY:O	1:A:529:ASN:HB2	2.17	0.43
1:C:374:SER:HB2	1:C:421:GLU:OE2	2.18	0.43
1:A:235:TYR:CE1	1:A:261:TRP:CD1	3.06	0.43
1:B:201:LYS:O	1:B:205:GLN:HB2	2.18	0.43
1:A:147:ILE:O	1:A:158:LYS:HE2	2.18	0.43
1:A:186:LEU:HD23	1:A:193:VAL:HG12	2.00	0.43
1:B:160:ILE:HG22	1:B:164:LYS:HD2	2.00	0.43
1:D:235:TYR:CE1	1:D:261:TRP:CD1	3.06	0.43
1:C:143:LEU:HD12	1:C:200:PHE:CZ	2.50	0.43
1:A:479:PRO:HD2	1:A:491:VAL:O	2.19	0.43
1:B:513:LYS:HG3	3:B:736:HOH:O	2.18	0.43
1:C:145:TYR:CE1	1:C:197:LYS:HE3	2.54	0.43
1:C:285:GLN:O	1:C:288:VAL:HG12	2.18	0.43
1:B:410:ILE:HD13	1:B:410:ILE:HA	1.90	0.43
1:D:194:MET:O	1:D:195:LEU:HD12	2.19	0.43
1:C:350:ASN:HD22	1:C:350:ASN:H	1.66	0.42
1:A:139:LEU:HD23	1:A:208:ILE:HG13	2.01	0.42
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.65	0.42
1:D:156:VAL:HG21	1:D:186:LEU:HD21	2.01	0.42
1:B:503:PRO:N	1:B:504:PRO:HD2	2.34	0.42
1:C:293:TYR:CD1	1:C:332:PRO:HG3	2.55	0.42
1:D:299:ASP:OD2	1:D:357:TYR:OH	2.34	0.42
1:D:200:PHE:O	1:D:204:VAL:HG22	2.20	0.42
1:A:155:PRO:HB2	1:A:157:HIS:CD2	2.55	0.41
1:B:250:ILE:CG2	1:B:380:SER:HB3	2.49	0.41
1:C:138:SER:O	1:C:142:LEU:HG	2.19	0.41
1:C:201:LYS:O	1:C:205:GLN:HB3	2.20	0.41
1:B:332:PRO:HD2	1:B:459:LEU:HD13	2.02	0.41
1:B:144:PHE:HB2	1:B:200:PHE:CD2	2.55	0.41
1:B:528:HIS:CD2	1:D:454:ARG:HD2	2.56	0.41
1:D:287:CYS:O	1:D:290:PRO:HD2	2.20	0.41
1:B:139:LEU:HD22	1:B:208:ILE:CG1	2.50	0.41
1:C:332:PRO:HD2	1:C:459:LEU:HD13	2.02	0.41
1:C:350:ASN:H	1:C:350:ASN:ND2	2.19	0.41
1:B:354:LYS:HB3	1:B:413:PHE:CE2	2.56	0.41
1:D:379:GLN:OE1	1:D:382:ARG:HD3	2.21	0.41
1:D:507:LYS:H	1:D:507:LYS:CE	2.34	0.41
1:B:278:THR:O	1:B:425:GLU:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:THR:HA	1:C:424:CYS:HB2	2.03	0.40
1:C:346:LYS:HA	1:C:346:LYS:HD2	1.86	0.40
1:C:197:LYS:H	1:C:197:LYS:HG3	1.76	0.40
1:D:135:LEU:O	1:D:137:PRO:HD3	2.22	0.40
1:A:144:PHE:CE2	1:A:197:LYS:HG2	2.57	0.40
1:C:263:VAL:HG13	1:C:498:MET:CE	2.52	0.40
1:B:187:GLN:C	1:B:189:THR:H	2.24	0.40

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	405/539 (75%)	391 (96%)	12 (3%)	2 (0%)	29	22
1	B	397/539 (74%)	385 (97%)	10 (2%)	2 (0%)	29	22
1	C	401/539 (74%)	384 (96%)	14 (4%)	3 (1%)	22	14
1	D	398/539 (74%)	381 (96%)	15 (4%)	2 (0%)	29	22
All	All	1601/2156 (74%)	1541 (96%)	51 (3%)	9 (1%)	25	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	THR
1	B	193	VAL
1	C	189	THR
1	D	253	LEU
1	A	149	GLU
1	D	316	LEU
1	A	192	GLY
1	C	190	SER

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Mol	Chain	Res	Type
1	C	193	VAL

5.3.2 Protein sidechains ⓘ

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	353/462 (76%)	349 (99%)	4 (1%)	73	76
1	B	351/462 (76%)	346 (99%)	5 (1%)	67	70
1	C	353/462 (76%)	345 (98%)	8 (2%)	50	51
1	D	353/462 (76%)	348 (99%)	5 (1%)	67	70
All	All	1410/1848 (76%)	1388 (98%)	22 (2%)	62	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
1	A	361	PHE
1	A	412	ASP
1	A	507	LYS
1	B	360	GLN
1	B	361	PHE
1	B	412	ASP
1	B	520	ASP
1	B	523	SER
1	C	190	SER
1	C	199	LEU
1	C	229	SER
1	C	361	PHE
1	C	412	ASP
1	C	520	ASP
1	C	523	SER
1	C	544	ARG
1	D	361	PHE
1	D	380	SER
1	D	382	ARG

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Mol	Chain	Res	Type
1	D	399	LYS
1	D	520	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	350	ASN
1	C	350	ASN
1	C	360	GLN
1	D	252	GLN

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](#)

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	C	601	-	5,9,9	0.37	0	5,11,11	0.23	0
2	GLN	A	601	-	5,9,9	0.21	0	5,11,11	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLN	B	601	-	5,9,9	0.47	0	5,11,11	0.42	0
2	GLN	D	601	-	5,9,9	0.39	0	5,11,11	0.15	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
2	GLN	C	601	-	-	2/5/9/9	-
2	GLN	A	601	-	-	0/5/9/9	-
2	GLN	B	601	-	-	3/5/9/9	-
2	GLN	D	601	-	-	0/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GLN	C-CA-CB-CG
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

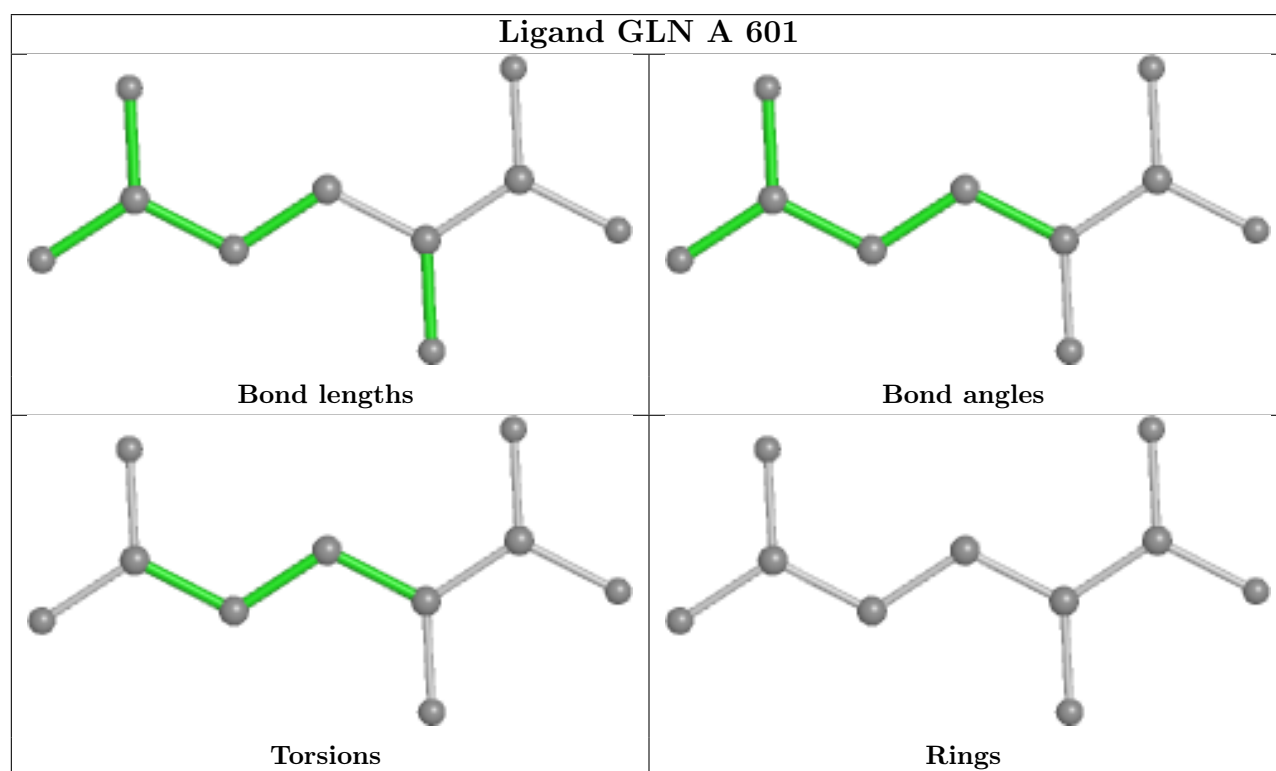
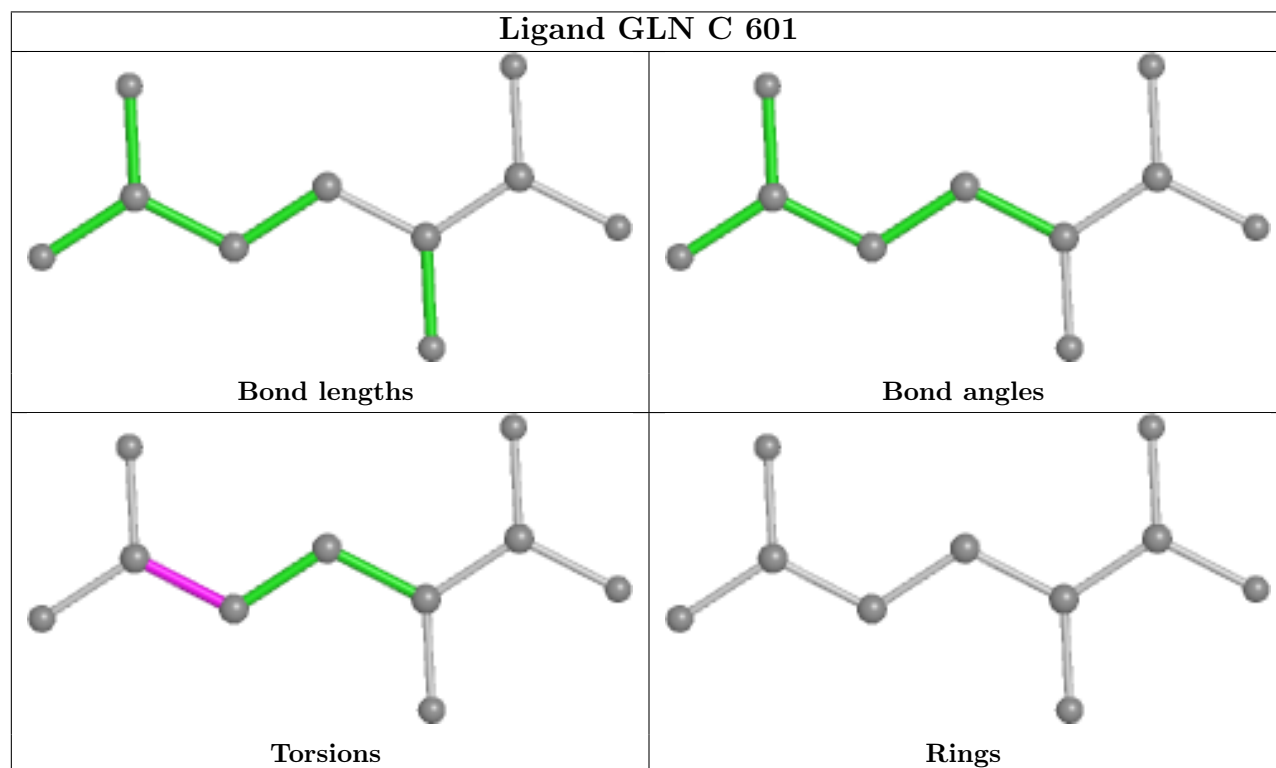
There are no ring outliers.

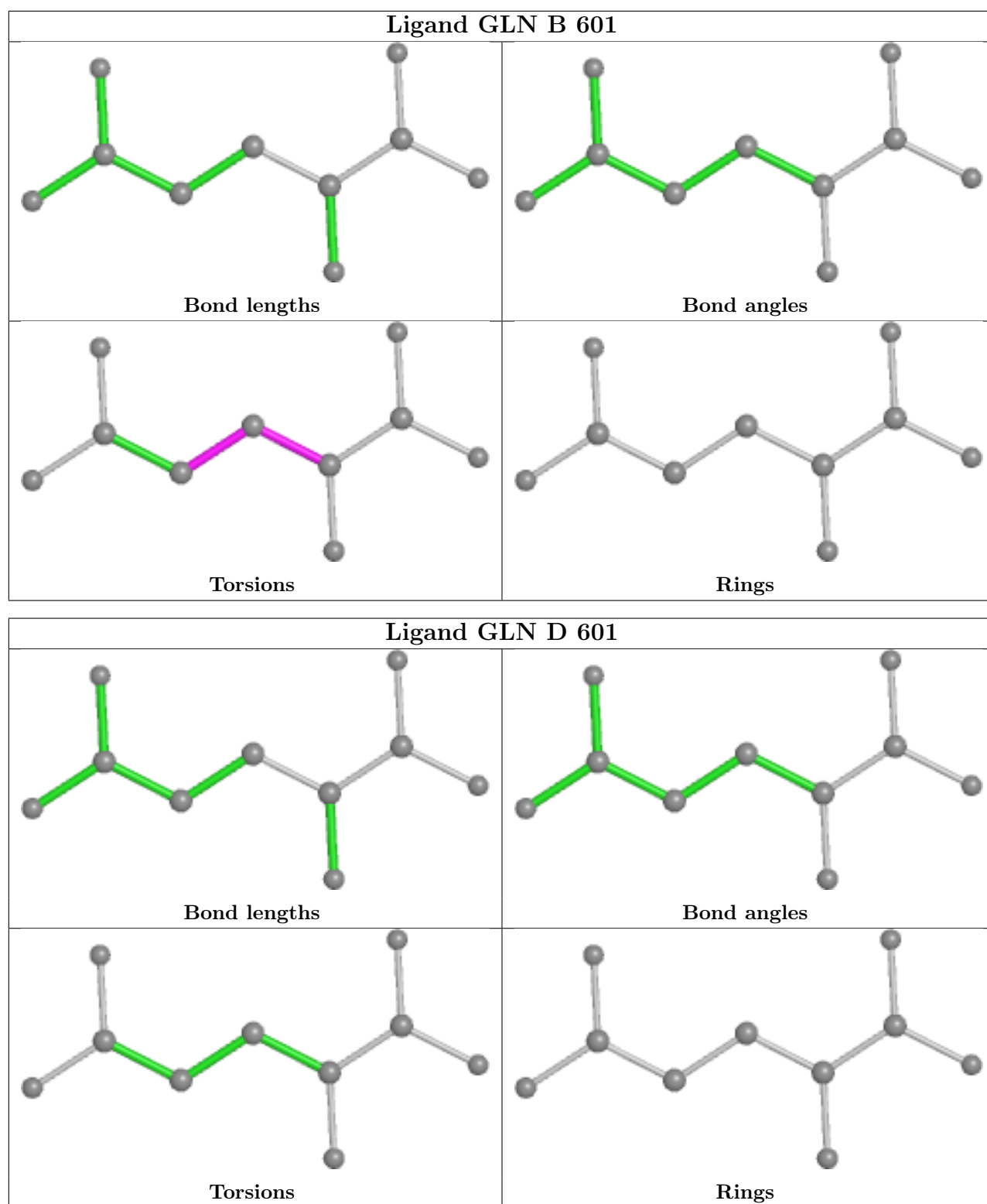
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GLN	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 ⓘ

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	409/539 (75%)	0.40	36 (8%)	10 13	18, 30, 71, 137	1 (0%)
1	B	405/539 (75%)	0.37	30 (7%)	14 18	24, 35, 71, 106	1 (0%)
1	C	407/539 (75%)	0.45	32 (7%)	12 16	21, 35, 72, 125	1 (0%)
1	D	406/539 (75%)	0.44	42 (10%)	6 8	24, 38, 83, 128	1 (0%)
All	All	1627/2156 (75%)	0.42	140 (8%)	10 13	18, 35, 76, 137	4 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	LEU	10.1
1	A	136	LEU	8.1
1	C	136	LEU	6.8
1	D	136	LEU	6.7
1	D	156	VAL	6.3
1	C	191	ASP	6.1
1	D	145	TYR	6.0
1	D	148	ALA	6.0
1	D	135	LEU	5.9
1	B	136	LEU	5.8
1	A	191	ASP	5.6
1	B	142	LEU	5.6
1	D	152	GLU	5.6
1	A	144	PHE	5.5
1	B	546	GLY	5.2
1	C	142	LEU	5.2
1	A	190	SER	5.1
1	D	321	LEU	5.1
1	D	153	LYS	5.1
1	D	142	LEU	5.1
1	D	137	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	138	SER	4.9
1	D	252	GLN	4.8
1	B	316	LEU	4.6
1	B	144	PHE	4.5
1	C	151	GLN	4.5
1	A	145	TYR	4.3
1	D	149	GLU	4.3
1	D	546	GLY	4.2
1	D	144	PHE	4.2
1	A	150	GLY	4.2
1	C	321	LEU	4.2
1	C	148	ALA	4.2
1	A	154	ILE	4.2
1	A	189	THR	4.1
1	A	148	ALA	4.1
1	B	137	PRO	4.1
1	D	251	PRO	4.0
1	B	193	VAL	4.0
1	D	250	ILE	4.0
1	A	135	LEU	4.0
1	B	348	GLY	4.0
1	B	151	GLN	3.9
1	D	154	ILE	3.9
1	D	316	LEU	3.8
1	C	137	PRO	3.7
1	B	148	ALA	3.7
1	A	192	GLY	3.6
1	D	200	PHE	3.6
1	D	256	PHE	3.6
1	D	195	LEU	3.6
1	A	151	GLN	3.6
1	A	137	PRO	3.5
1	A	546	GLY	3.5
1	A	134	GLY	3.4
1	B	195	LEU	3.4
1	A	156	VAL	3.4
1	C	144	PHE	3.4
1	C	145	TYR	3.4
1	A	160	ILE	3.3
1	B	192	GLY	3.3
1	D	146	THR	3.3
1	D	249	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	200	PHE	3.3
1	A	195	LEU	3.3
1	C	193	VAL	3.3
1	A	149	GLU	3.2
1	B	139	LEU	3.2
1	B	145	TYR	3.2
1	A	152	GLU	3.2
1	A	142	LEU	3.2
1	B	156	VAL	3.2
1	B	255	LYS	3.1
1	D	194	MET	3.1
1	B	149	GLU	3.1
1	D	151	GLN	3.1
1	C	195	LEU	3.0
1	C	348	GLY	3.0
1	D	189	THR	3.0
1	A	251	PRO	3.0
1	B	157	HIS	2.9
1	C	476	VAL	2.9
1	C	154	ILE	2.9
1	D	196	ASP	2.9
1	C	546	GLY	2.9
1	A	146	THR	2.9
1	C	189	THR	2.9
1	C	149	GLU	2.9
1	A	143	LEU	2.8
1	C	152	GLU	2.8
1	C	190	SER	2.8
1	C	153	LYS	2.7
1	C	138	SER	2.7
1	B	189	THR	2.7
1	C	492	VAL	2.7
1	B	200	PHE	2.7
1	D	348	GLY	2.7
1	A	193	VAL	2.6
1	A	197	LYS	2.6
1	D	147	ILE	2.6
1	D	157	HIS	2.6
1	A	153	LYS	2.6
1	C	255	LYS	2.6
1	D	257	SER	2.6
1	D	317	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	143	LEU	2.5
1	A	348	GLY	2.5
1	A	157	HIS	2.5
1	A	194	MET	2.4
1	A	316	LEU	2.4
1	B	152	GLU	2.4
1	C	139	LEU	2.4
1	C	434	LEU	2.4
1	C	491	VAL	2.4
1	C	146	THR	2.4
1	B	321	LEU	2.3
1	B	492	VAL	2.3
1	D	138	SER	2.3
1	D	315	GLY	2.3
1	D	254	ALA	2.2
1	B	190	SER	2.2
1	D	217	ARG	2.2
1	B	154	ILE	2.2
1	C	325	GLU	2.1
1	D	403	GLU	2.1
1	B	215	PHE	2.1
1	C	141	ASP	2.1
1	C	316	LEU	2.1
1	D	158	LYS	2.1
1	B	361	PHE	2.1
1	C	493	PRO	2.1
1	B	194	MET	2.1
1	C	463	CYS	2.1
1	A	196	ASP	2.0
1	D	160	ILE	2.0
1	A	158	LYS	2.0
1	B	141	ASP	2.0
1	D	141	ASP	2.0
1	A	155	PRO	2.0
1	A	147	ILE	2.0

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 [i](#)

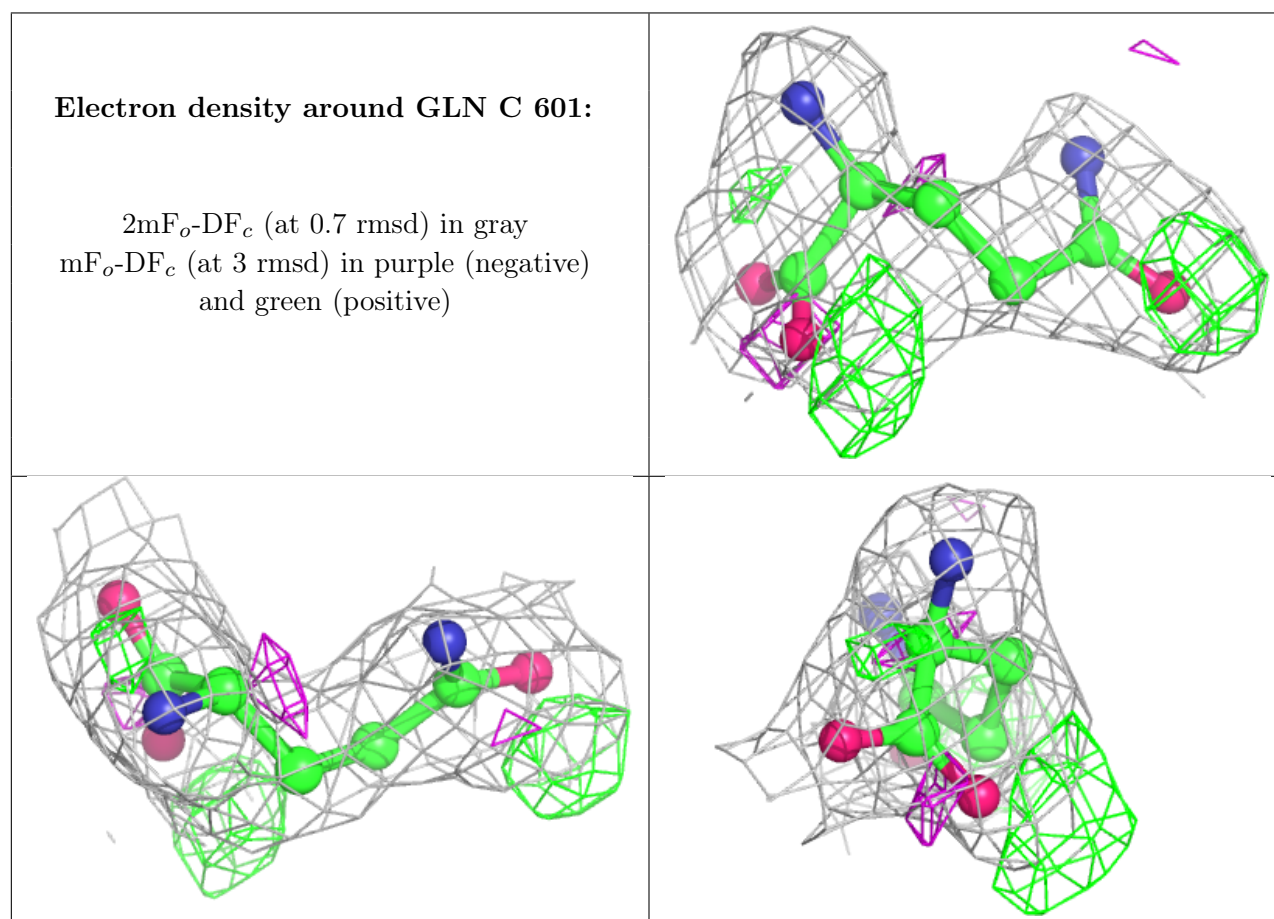
There are no monosaccharides in this entry.

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.

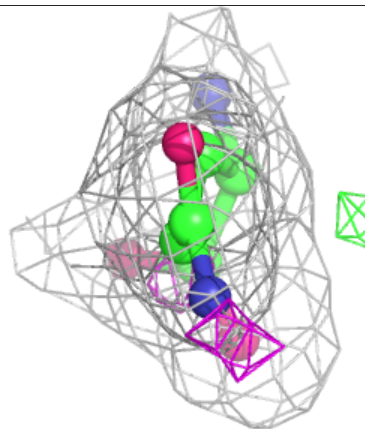
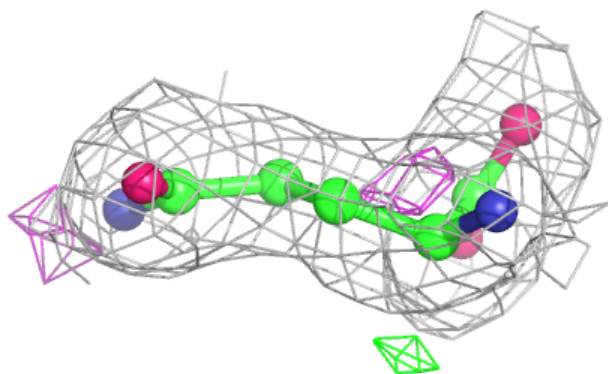
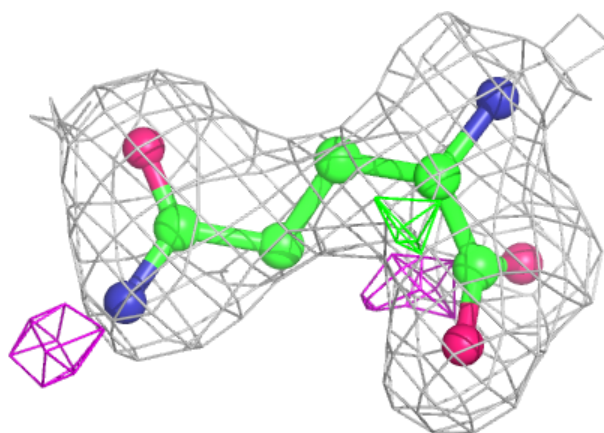
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLN	C	601	10/10	0.86	0.23	44,53,60,64	0
2	GLN	B	601	10/10	0.95	0.11	27,38,43,45	0
2	GLN	A	601	10/10	0.95	0.14	25,35,41,43	0
2	GLN	D	601	10/10	0.95	0.13	30,40,44,45	0

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.



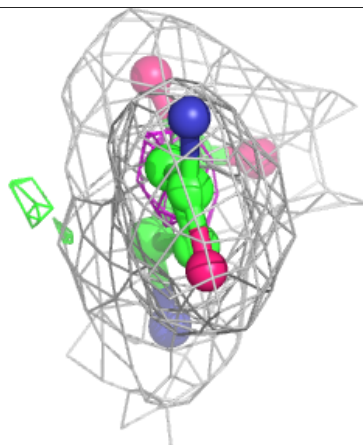
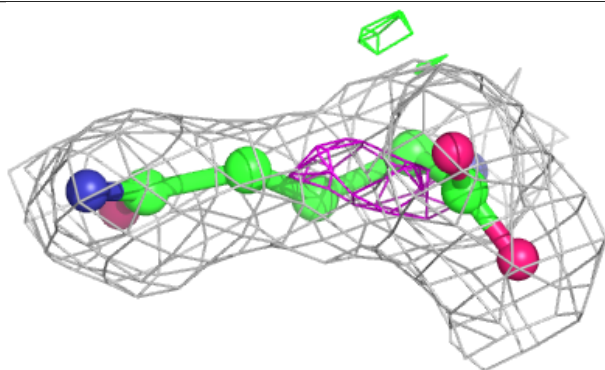
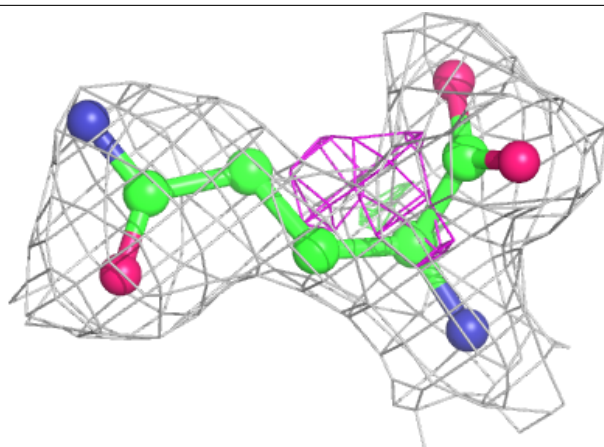
Electron density around GLN B 601:

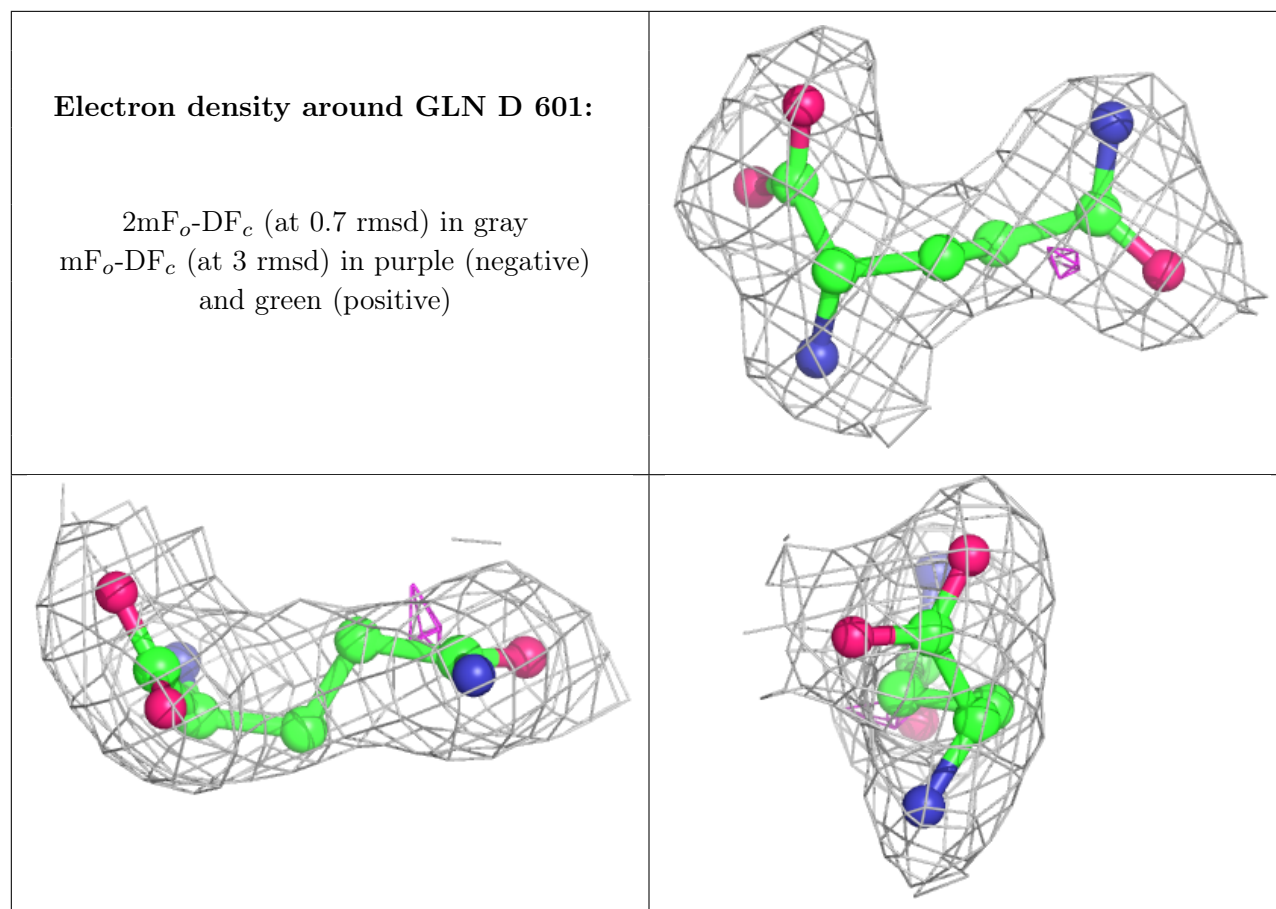
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.