



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2020 – 11:13 AM EDT

PDB ID : 6UMD
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-09
Resolution : 2.70 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 : 2.14.6
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) : 2.14.6

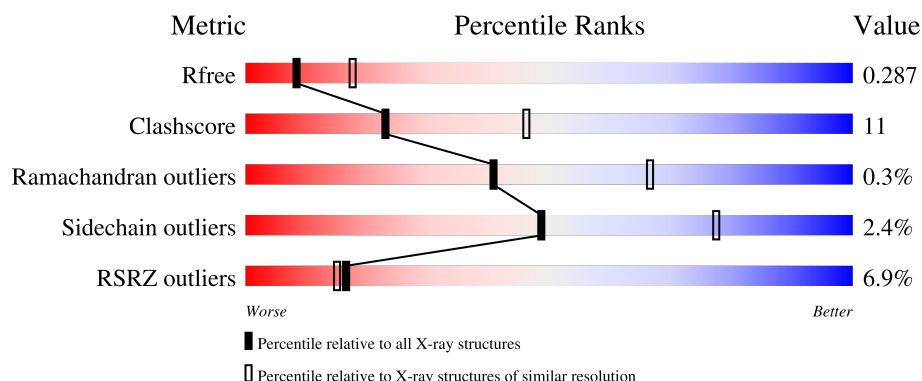
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	527	 5% 57% 17% 24%
1	B	527	 6% 57% 18% 22%
1	C	527	 7% 56% 20% 22%
1	D	527	 4% 58% 18% 22%

2 Entry composition [i](#)

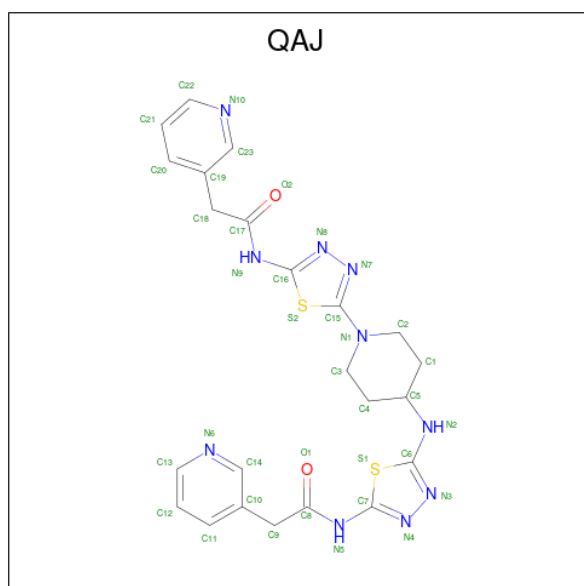
There are 3 unique types of molecules in this entry. The entry contains 12842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	1	0	0
			3146	2005	531	582	28			
1	B	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			
1	C	410	Total	C	N	O	S	1	0	0
			3196	2038	540	590	28			
1	D	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			

- Molecule 2 is 2-(pyridin-3-yl)-N-(5-{4-[(5-{[(pyridin-3-yl)acetyl]amino}-1,3,4-thiadiazol-2-yl)amino]piperidin-1-yl}-1,3,4-thiadiazol-2-yl)acetamide (three-letter code: QAJ) (formula: C₂₃H₂₄N₁₀O₂S₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

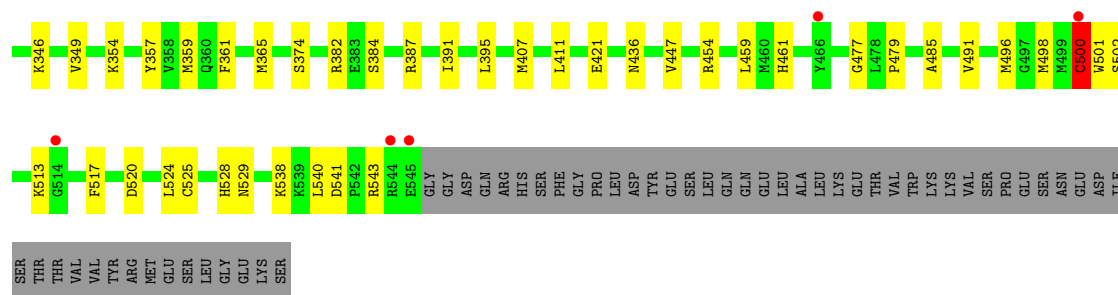
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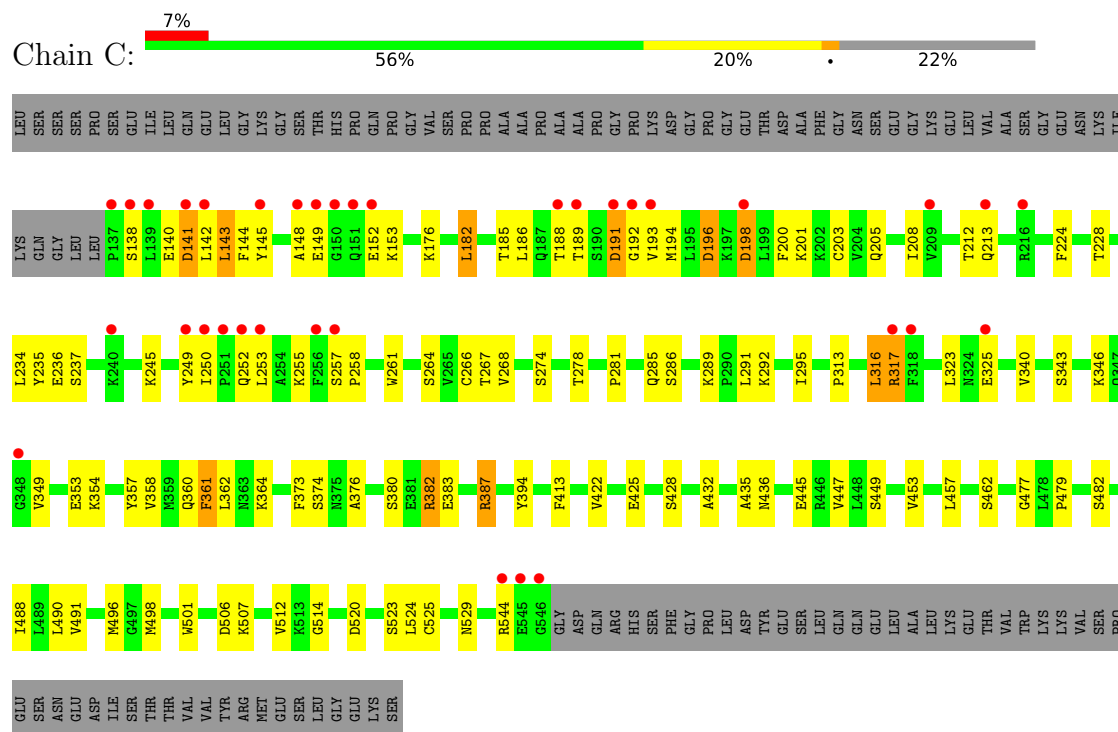
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

- Molecule 3 is water.

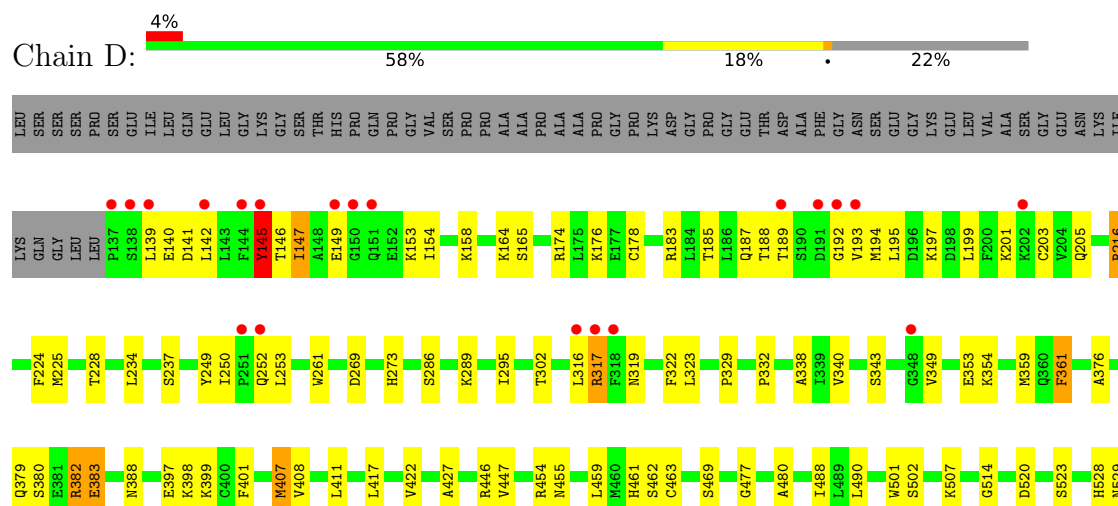
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	10	Total	O	0	0
			10	10		
3	C	11	Total	O	0	0
			11	11		
3	D	14	Total	O	0	0
			14	14		



- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



YS-60	LS-40	ES-45	GLY	GLY	ASP	GLN	ARG	HIS	SER	PHE	GLY	PRO	LEU	ASP	TYR	GLU	SER	LEU	GLN	GLN	GLY	THR	VAL	TRP	THR	LYS	LYS	VAL	VAL	ASN	PRO	GLU	ILE	SER	THR	THR	VAL	VAL	TYR	ARG	MET	GLU	GLY	LEU	GLY	GLU	LYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.48Å 139.16Å 178.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.23 – 2.70 20.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.23-2.70) 98.7 (20.23-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.71Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.228 , 0.288 0.228 , 0.287	Depositor DCC
R_{free} test set	1586 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	1.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12842	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3565e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: QAJ

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	0.62	6/3216 (0.2%)	0.91	14/4339 (0.3%)
1	B	0.56	1/3264 (0.0%)	0.86	15/4406 (0.3%)
1	C	0.58	2/3268 (0.1%)	0.88	16/4411 (0.4%)
1	D	0.57	1/3264 (0.0%)	0.84	12/4406 (0.3%)
All	All	0.58	10/13012 (0.1%)	0.87	57/17562 (0.3%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	CYS	CB-SG	-7.32	1.69	1.82
1	C	191	ASP	CA-CB	6.76	1.68	1.53
1	B	500	CYS	CB-SG	-5.93	1.72	1.81
1	A	197	LYS	CE-NZ	5.68	1.63	1.49
1	A	500	CYS	CB-SG	-5.66	1.72	1.81

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	LEU	CB-CG-CD2	-15.37	84.87	111.00
1	B	186	LEU	CA-CB-CG	14.95	149.69	115.30
1	C	191	ASP	CB-CG-OD1	12.38	129.45	118.30
1	D	398	LYS	CD-CE-NZ	-11.27	85.78	111.70
1	B	142	LEU	CB-CA-C	-10.22	90.77	110.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	LEU	Peptide
1	A	317	ARG	Peptide
1	B	316	LEU	Peptide
1	B	317	ARG	Peptide
1	C	316	LEU	Peptide

5.2 Too-close contacts

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	3146	0	3115	67	1
1	B	3192	0	3171	78	1
1	C	3196	0	3174	77	0
1	D	3192	0	3171	76	0
2	B	37	0	0	0	0
2	D	37	0	0	0	0
3	A	7	0	0	2	0
3	B	10	0	0	0	0
3	C	11	0	0	2	0
3	D	14	0	0	1	0
All	All	12842	0	12631	290	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 11.

The worst 5 of 290 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:B:541:ASP:OD1	1:B:543:ARG:NH1	1.70	1.23
1:B:143:LEU:HD11	1:B:212:THR:HG22	1.31	1.08
1:D:407:MET:HE2	1:D:411:LEU:HD23	1.10	1.06
1:D:141:ASP:OD1	1:D:197:LYS:HE3	1.55	1.05
1:D:407:MET:CE	1:D:411:LEU:HD23	1.87	1.04

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)
1:A:307:ARG:NH2	1:B:259:ASP:OD1[1_655]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	399/527 (76%)	374 (94%)	24 (6%)	1 (0%)	41	66
1	B	407/527 (77%)	388 (95%)	17 (4%)	2 (0%)	29	54
1	C	408/527 (77%)	390 (96%)	17 (4%)	1 (0%)	47	73
1	D	407/527 (77%)	386 (95%)	20 (5%)	1 (0%)	47	73
All	All	1621/2108 (77%)	1538 (95%)	78 (5%)	5 (0%)	41	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	SER
1	B	188	THR
1	C	141	ASP
1	D	145	TYR
1	B	151	GLN

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	349/452 (77%)	342 (98%)	7 (2%)	55	81
1	B	354/452 (78%)	346 (98%)	8 (2%)	50	78
1	C	354/452 (78%)	345 (98%)	9 (2%)	47	76
1	D	354/452 (78%)	344 (97%)	10 (3%)	43	73
All	All	1411/1808 (78%)	1377 (98%)	34 (2%)	49	77

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	GLU
1	C	361	PHE
1	D	407	MET
1	C	237	SER
1	A	500	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	529	ASN
1	D	510	ASN
1	C	285	GLN
1	B	461	HIS
1	D	319	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](#)

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	QAJ	D	601	-	32,41,41	0.89	1 (3%)	35,55,55	1.65	9 (25%)
2	QAJ	B	601	-	32,41,41	0.86	0	35,55,55	2.64	8 (22%)

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	QAJ	D	601	-	-	6/16/34/34	1/5/5/5
2	QAJ	B	601	-	-	5/16/34/34	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	QAJ	C15-N1	2.48	1.36	1.32

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAJ	C6-N2-C5	-10.21	105.22	124.26
2	B	601	QAJ	C4-C5-N2	4.70	117.92	110.60
2	B	601	QAJ	C3-C4-C5	-4.35	102.87	110.50
2	B	601	QAJ	C2-C1-C5	-4.20	103.13	110.50
2	D	601	QAJ	C7-N5-C8	-3.98	118.79	129.54

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

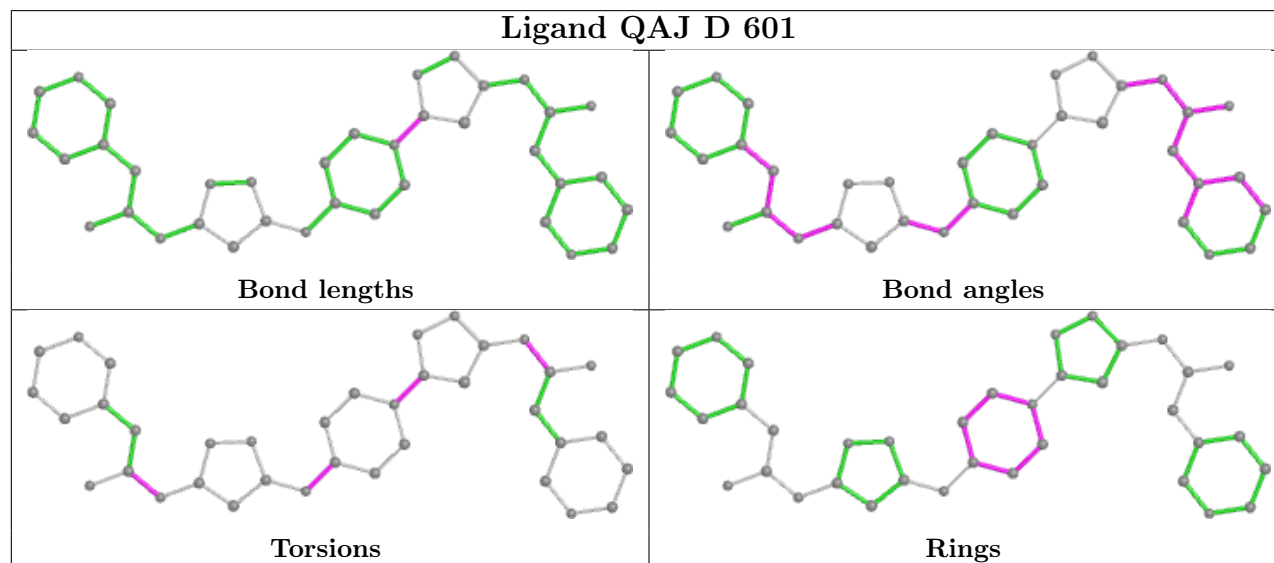
Mol	Chain	Res	Type	Atoms
2	D	601	QAJ	S2-C15-N1-C2
2	D	601	QAJ	C1-C5-N2-C6
2	D	601	QAJ	O1-C8-N5-C7
2	D	601	QAJ	O2-C17-N9-C16
2	B	601	QAJ	S2-C15-N1-C2

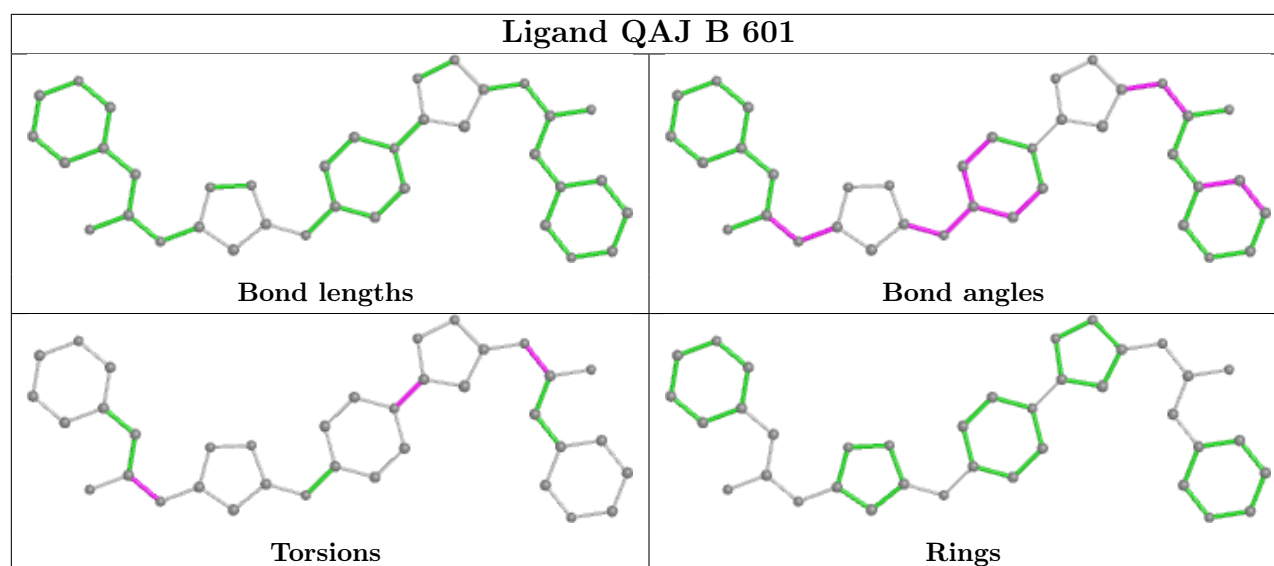
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	QAJ	C1-C2-C3-C4-C5-N1

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 [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	A	403/527 (76%)	0.27	28 (6%) 16 15	38, 56, 113, 164	0
1	B	409/527 (77%)	0.25	30 (7%) 15 13	39, 56, 119, 186	0
1	C	410/527 (77%)	0.40	35 (8%) 10 9	42, 57, 126, 195	0
1	D	409/527 (77%)	0.22	20 (4%) 29 28	38, 55, 110, 166	0
All	All	1631/2108 (77%)	0.29	113 (6%) 16 15	38, 56, 116, 195	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	SER	14.2
1	B	192	GLY	9.8
1	C	150	GLY	9.5
1	C	546	GLY	9.1
1	D	145	TYR	7.7

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](#)

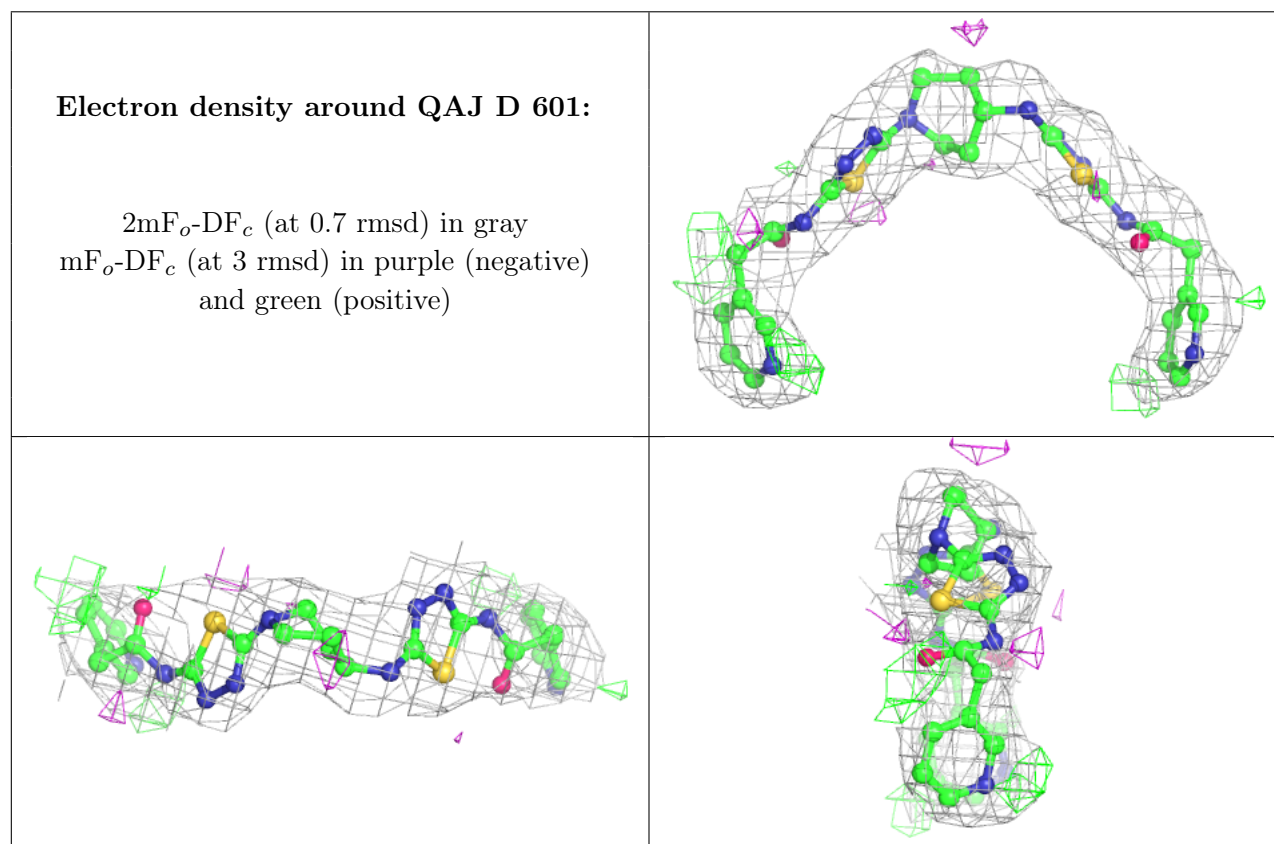
There are no monosaccharides in this entry.

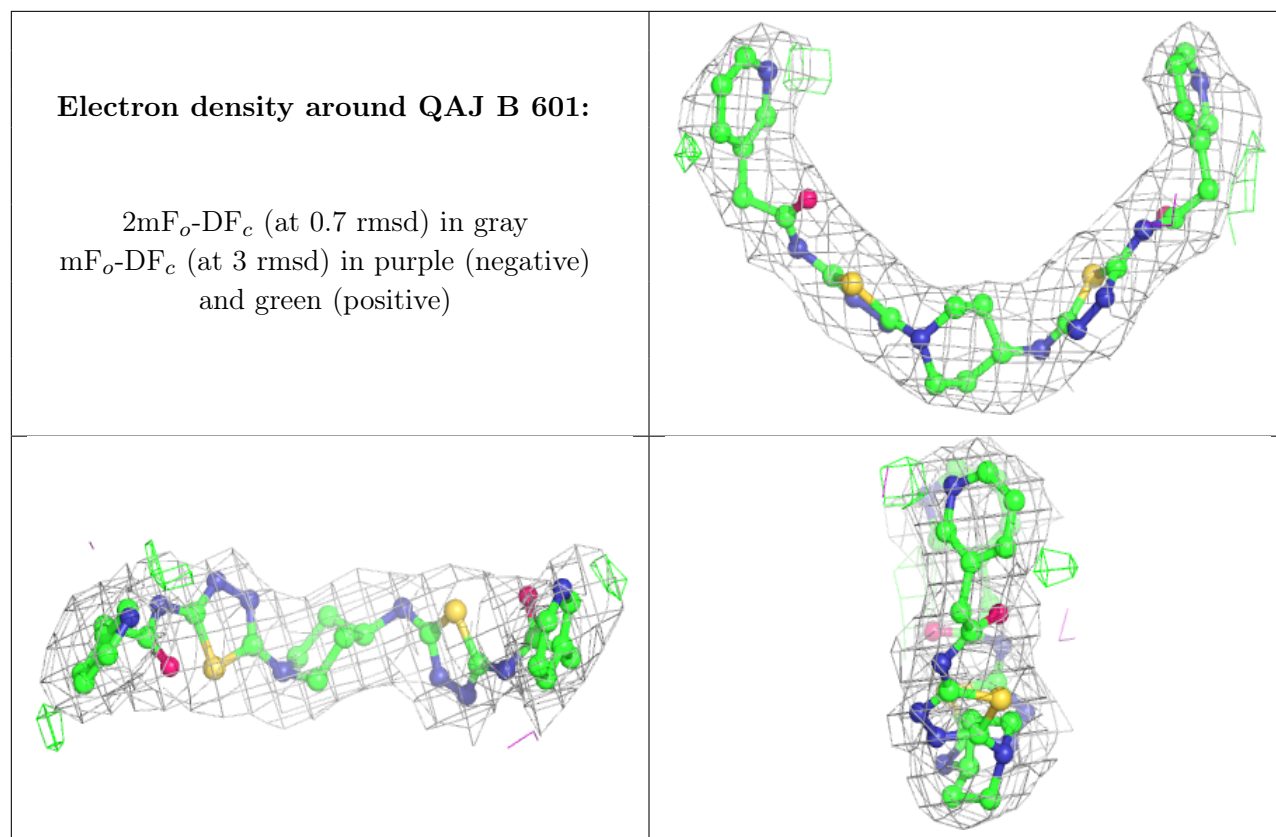
6.4 Ligands [i](#)

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	QAJ	D	601	37/37	0.91	0.15	39,62,79,83	0
2	QAJ	B	601	37/37	0.93	0.14	52,67,87,89	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.