



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:12 pm BST

PDB ID : 5FI6
Title : Crystal structure of human GAC in complex with inhibitor UPGL_00011: 2-phenyl- {N}-[5-[[[(3 {S})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]p
yrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide
Authors : Huang, Q.; Cerione, R.
Deposited on : 2015-12-22
Resolution : 2.52 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 : 2.11
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) : 2.11

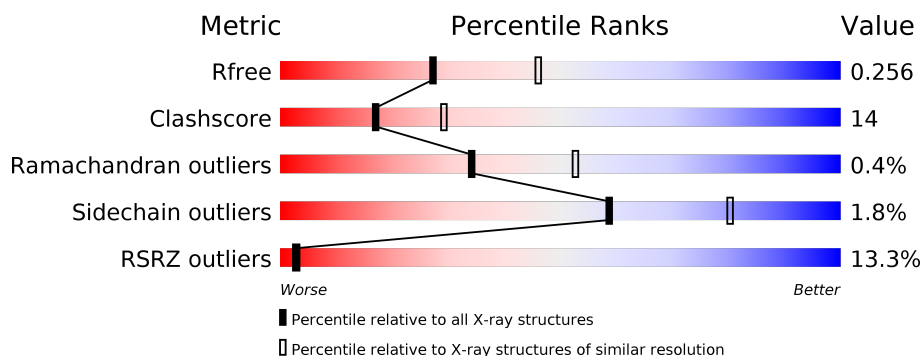
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	539	<div> <div>10%</div> <div> <div>56%</div> <div>18%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	539	<div> <div>9%</div> <div> <div>55%</div> <div>20%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	539	<div> <div>10%</div> <div> <div>58%</div> <div>17%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	539	<div> <div>12%</div> <div> <div>57%</div> <div>17%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13115 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	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	B	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	C	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	D	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			

There are 48 discrepancies between the modelled and reference sequences:

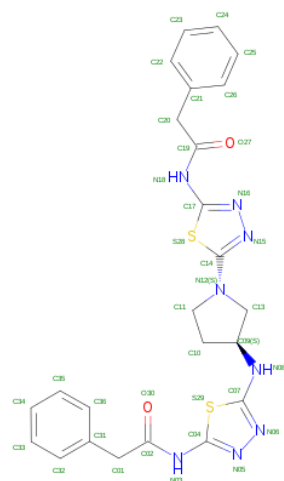
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	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	GLY	-	expression tag	UNP O94925
A	70	SER	-	expression tag	UNP O94925
B	59	MET	-	initiating methionine	UNP O94925
B	60	ARG	-	expression tag	UNP O94925
B	61	GLY	-	expression tag	UNP O94925
B	62	SER	-	expression tag	UNP O94925
B	63	HIS	-	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	GLY	-	expression tag	UNP O94925
B	70	SER	-	expression tag	UNP O94925
C	59	MET	-	initiating methionine	UNP O94925
C	60	ARG	-	expression tag	UNP O94925
C	61	GLY	-	expression tag	UNP O94925
C	62	SER	-	expression tag	UNP O94925
C	63	HIS	-	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	GLY	-	expression tag	UNP O94925
C	70	SER	-	expression tag	UNP O94925
D	59	MET	-	initiating methionine	UNP O94925
D	60	ARG	-	expression tag	UNP O94925
D	61	GLY	-	expression tag	UNP O94925
D	62	SER	-	expression tag	UNP O94925
D	63	HIS	-	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	GLY	-	expression tag	UNP O94925
D	70	SER	-	expression tag	UNP O94925

- Molecule 2 is 2-phenyl- {N}-[5-[(3 {S})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]pyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide (three-letter code: 5XY) (formula: C₂₄H₂₄N₈O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 24	N 8	O 2	S 2	0	0
2	C	1	Total 36	C 24	N 8	O 2	S 2	0	0

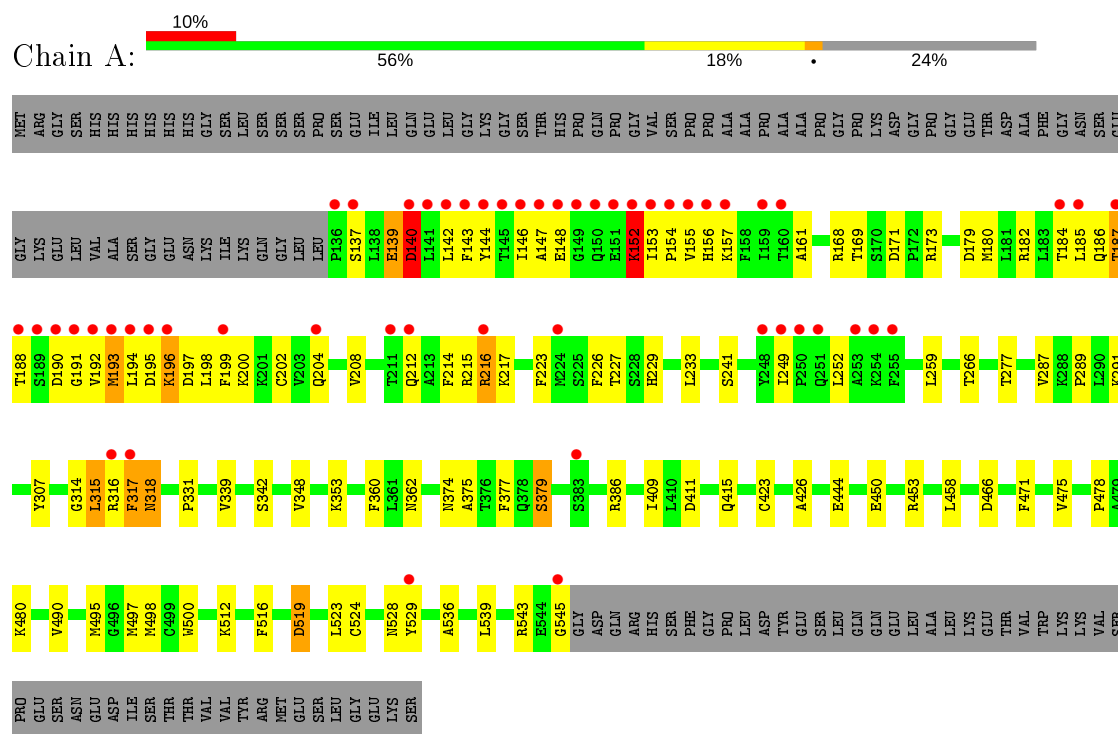
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	56	Total O 56 56	0	0
3	C	77	Total O 77 77	0	0
3	D	59	Total O 59 59	0	0

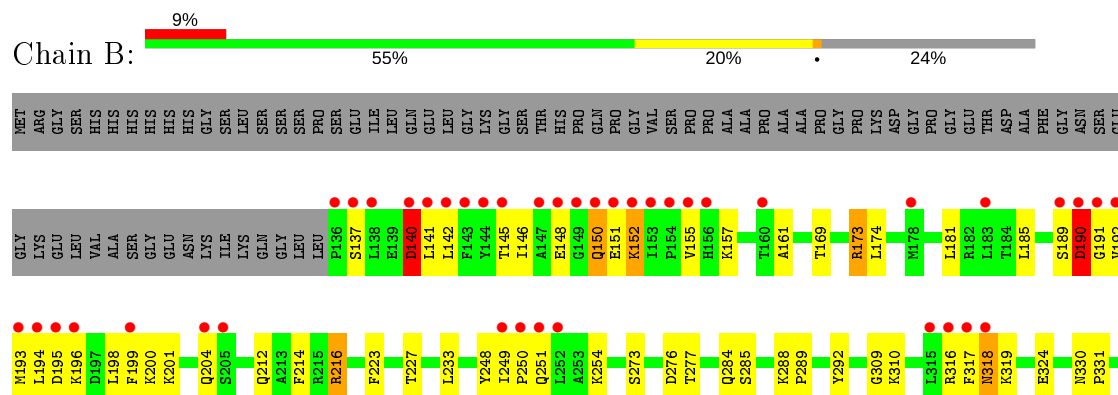
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Glutaminase kidney isoform, mitochondrial



- Molecule 1: 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	50.69 Å 139.03 Å 176.78 Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	47.30 – 2.52 47.43 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.30-2.52) 97.4 (47.43-2.52)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.253 0.211 , 0.256	Depositor DCC
R_{free} test set	1996 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13115	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5XY

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	0.51	3/3266 (0.1%)	0.69	4/4408 (0.1%)
1	B	0.50	3/3266 (0.1%)	0.65	3/4408 (0.1%)
1	C	0.47	0/3266	0.62	1/4408 (0.0%)
1	D	0.57	6/3266 (0.2%)	0.65	4/4408 (0.1%)
All	All	0.51	12/13064 (0.1%)	0.65	12/17632 (0.1%)

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	1
1	C	0	2
1	D	0	1
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	316	ARG	CZ-NH1	-8.69	1.21	1.33
1	D	316	ARG	NE-CZ	-8.68	1.21	1.33
1	B	196	LYS	CD-CE	-7.38	1.32	1.51
1	D	316	ARG	CZ-NH2	-7.04	1.23	1.33
1	A	196	LYS	CD-CE	-6.71	1.34	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	CB-CG-OD1	9.44	126.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	MET	CG-SD-CE	7.77	112.63	100.20
1	A	193	MET	CB-CG-SD	7.55	135.05	112.40
1	C	196	LYS	CD-CE-NZ	-6.72	96.25	111.70
1	B	140	ASP	CB-CG-OD1	6.09	123.78	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
1	C	315	LEU	Peptide
1	C	316	ARG	Peptide
1	D	140	ASP	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	3194	0	3167	104	0
1	B	3194	0	3167	90	0
1	C	3194	0	3167	82	0
1	D	3194	0	3167	97	0
2	A	36	0	0	2	0
2	C	36	0	0	2	0
3	A	75	0	0	9	0
3	B	56	0	0	5	0
3	C	77	0	0	5	0
3	D	59	0	0	4	0
All	All	13115	0	12668	356	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 14.

The worst 5 of 356 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:152:LYS:NZ	1:A:193:MET:HB3	1.52	1.24
1:C:249:ILE:CG2	1:C:252:LEU:HD12	1.71	1.19
1:A:152:LYS:NZ	1:A:193:MET:CB	2.14	1.10
1:D:195:ASP:H	1:D:198:LEU:HD21	1.16	1.09
1:A:152:LYS:HZ3	1:A:193:MET:CB	1.65	1.08

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	408/539 (76%)	390 (96%)	14 (3%)	4 (1%)	15	27
1	B	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	47	67
1	C	408/539 (76%)	390 (96%)	18 (4%)	0	100	100
1	D	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	47	67
All	All	1632/2156 (76%)	1550 (95%)	76 (5%)	6 (0%)	34	53

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	A	318	ASN
1	B	190	ASP
1	A	315	LEU
1	D	196	LYS

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	353/462 (76%)	345 (98%)	8 (2%)	50	74
1	B	353/462 (76%)	346 (98%)	7 (2%)	55	78
1	C	353/462 (76%)	350 (99%)	3 (1%)	81	92
1	D	353/462 (76%)	346 (98%)	7 (2%)	55	78
All	All	1412/1848 (76%)	1387 (98%)	25 (2%)	59	80

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	THR
1	B	318	ASN
1	D	519	ASP
1	B	216	ARG
1	B	360	PHE

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	150	GLN
1	D	528	ASN
1	B	240	GLN
1	A	528	ASN
1	D	515	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	5XY	C	601	-	31,40,40	3.83	9 (29%)	34,54,54	1.37	4 (11%)
2	5XY	A	601	-	31,40,40	3.73	9 (29%)	34,54,54	1.42	4 (11%)

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	5XY	C	601	-	-	3/14/33/33	0/5/5/5
2	5XY	A	601	-	-	1/14/33/33	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	5XY	C13-N12	12.45	1.62	1.46
2	A	601	5XY	C13-N12	12.07	1.62	1.46
2	A	601	5XY	C11-N12	-10.00	1.31	1.47
2	C	601	5XY	C13-C09	-9.88	1.34	1.53
2	C	601	5XY	C11-N12	-9.73	1.32	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	5XY	C11-N12-C13	-4.15	100.82	111.55
2	C	601	5XY	C17-N18-C19	-3.02	121.38	129.54
2	C	601	5XY	C01-C02-N03	2.90	120.76	114.77
2	C	601	5XY	C20-C19-N18	2.86	120.69	114.77
2	A	601	5XY	C04-N03-C02	-2.74	122.15	129.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

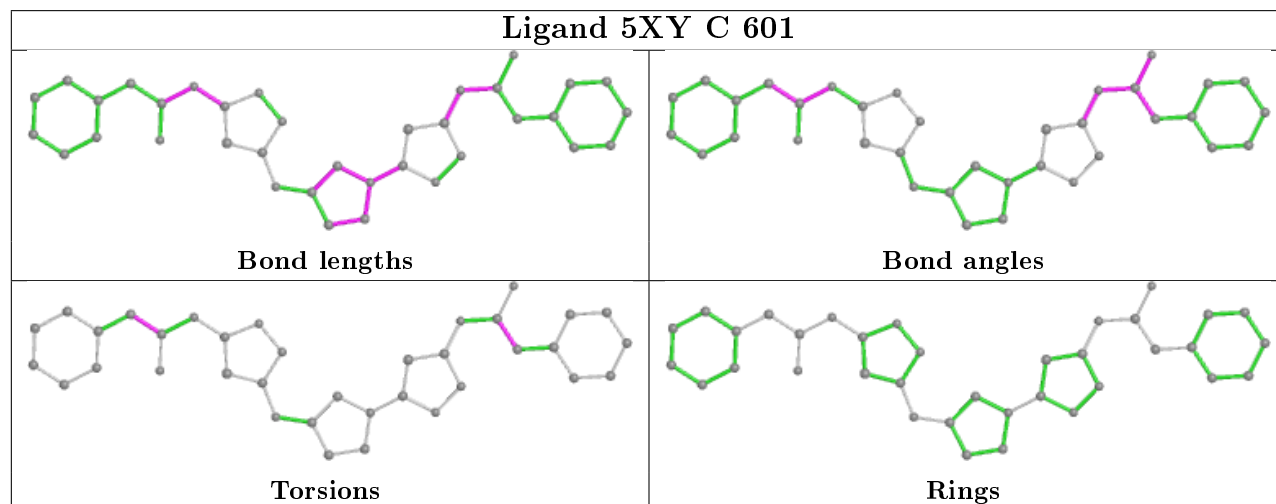
Mol	Chain	Res	Type	Atoms
2	A	601	5XY	C13-C09-N08-C07
2	C	601	5XY	O27-C19-C20-C21
2	C	601	5XY	N18-C19-C20-C21
2	C	601	5XY	C31-C01-C02-O30

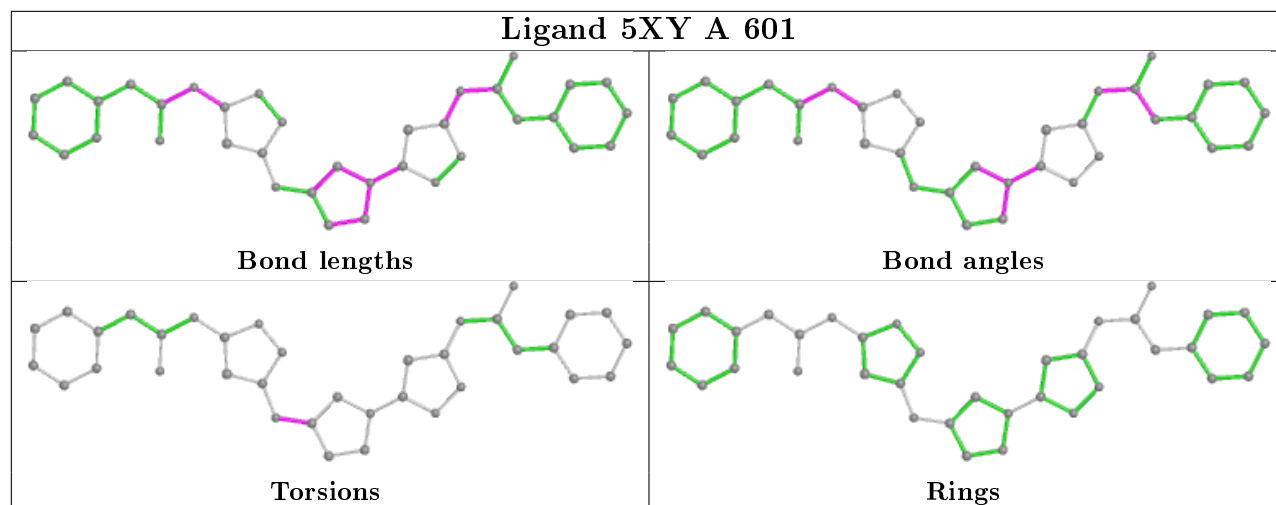
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	5XY	2	0
2	A	601	5XY	2	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	A	410/539 (76%)	0.92	52 (12%) 3 3	30, 44, 79, 114	0
1	B	410/539 (76%)	0.80	47 (11%) 4 5	33, 48, 80, 98	0
1	C	410/539 (76%)	0.87	54 (13%) 3 3	31, 44, 80, 95	0
1	D	410/539 (76%)	0.99	65 (15%) 1 1	34, 47, 87, 111	0
All	All	1640/2156 (76%)	0.90	218 (13%) 3 3	30, 46, 81, 114	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	PHE	12.7
1	A	188	THR	12.3
1	A	190	ASP	9.3
1	D	188	THR	8.9
1	D	194	LEU	8.4

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](#)

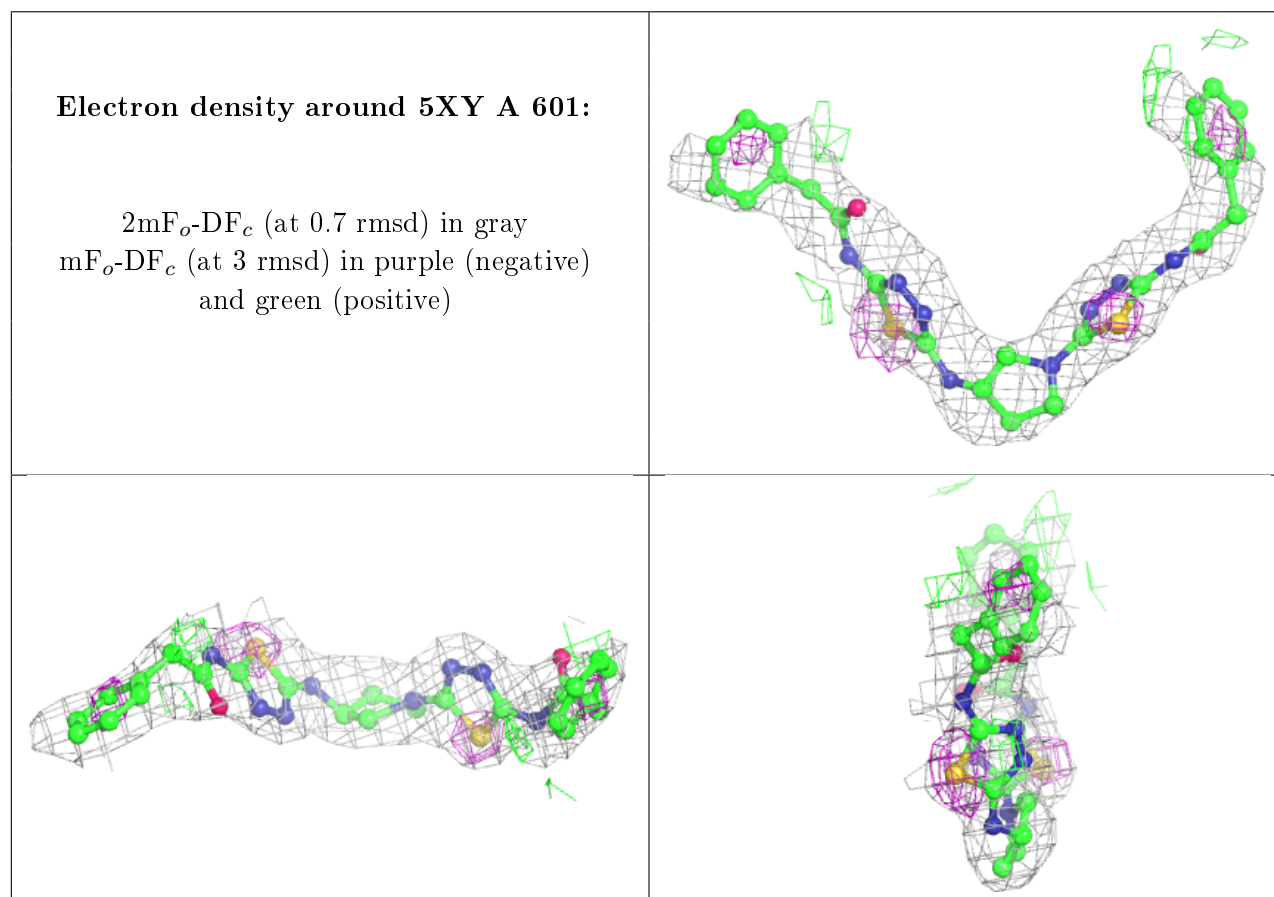
There are no carbohydrates in this entry.

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.

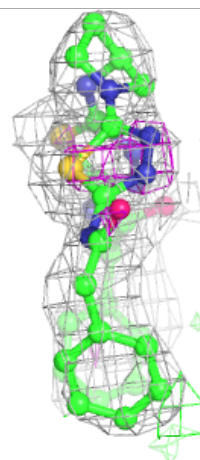
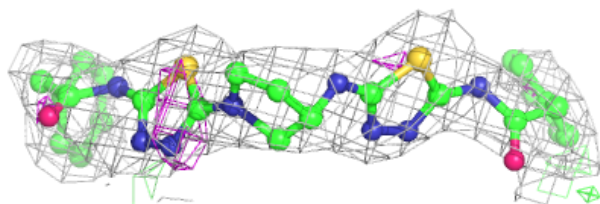
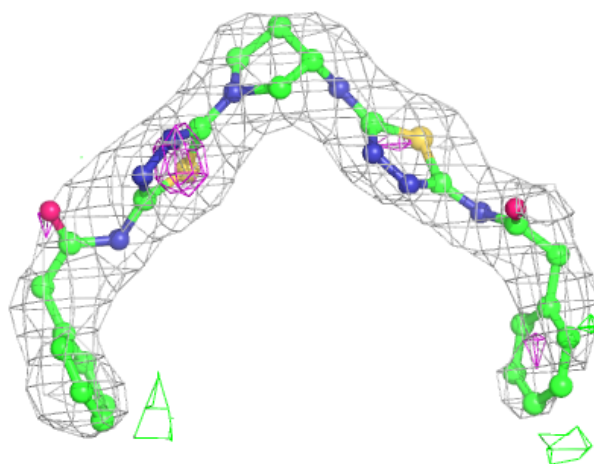
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	5XY	A	601	36/36	0.87	0.26	48,65,82,85	0
2	5XY	C	601	36/36	0.89	0.23	52,67,83,84	0

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 5XY 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.