



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 03:04 am BST

PDB ID : 3LPF
Title : Structure of E. coli beta-Glucuronidase bound with a novel, potent inhibitor
1-((6,7-dimethyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)-1-(2-hydroxyethyl)-3
-(3-methoxyphenyl)thiourea
Authors : Wallace, B.D.; Redinbo, M.R.
Deposited on : 2010-02-05
Resolution : 2.26 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

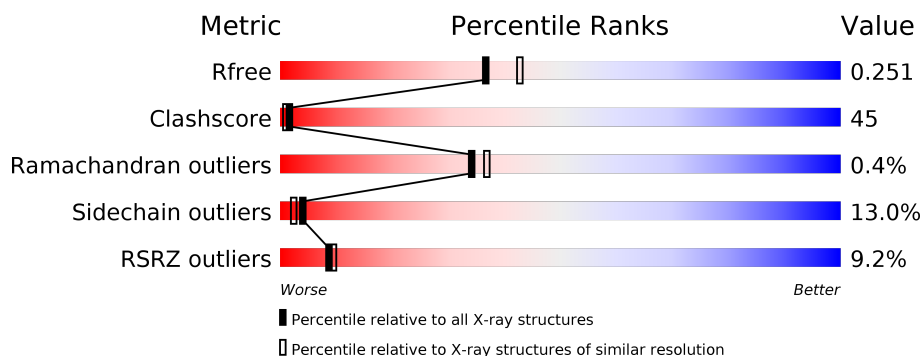
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	605	<div> <div>5%</div> <div>52%</div> <div>37%</div> <div>10%</div> </div>
1	B	605	<div> <div>12%</div> <div>41%</div> <div>47%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Z77	B	604	-	-	X	-

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.

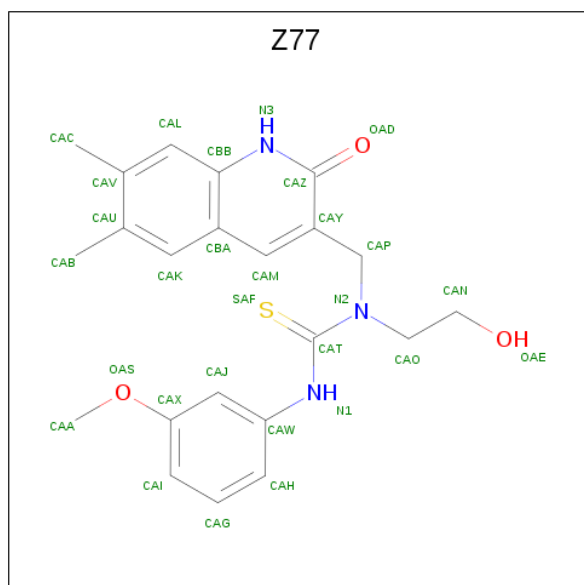
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total 4822	C 3060	N 833	O 907	S 9	Se 13	0	0	0
1	B	603	Total 4822	C 3060	N 833	O 907	S 9	Se 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is 1-[(6,7-dimethyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl]-1-(2-hydroxyethyl)-3-(3-methoxyphenyl)thiourea (three-letter code: *Z77*) (formula: C₂₂H₂₅N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 22	N 3	O 3	S 1	0	0
2	B	1	Total 29	C 22	N 3	O 3	S 1	0	0

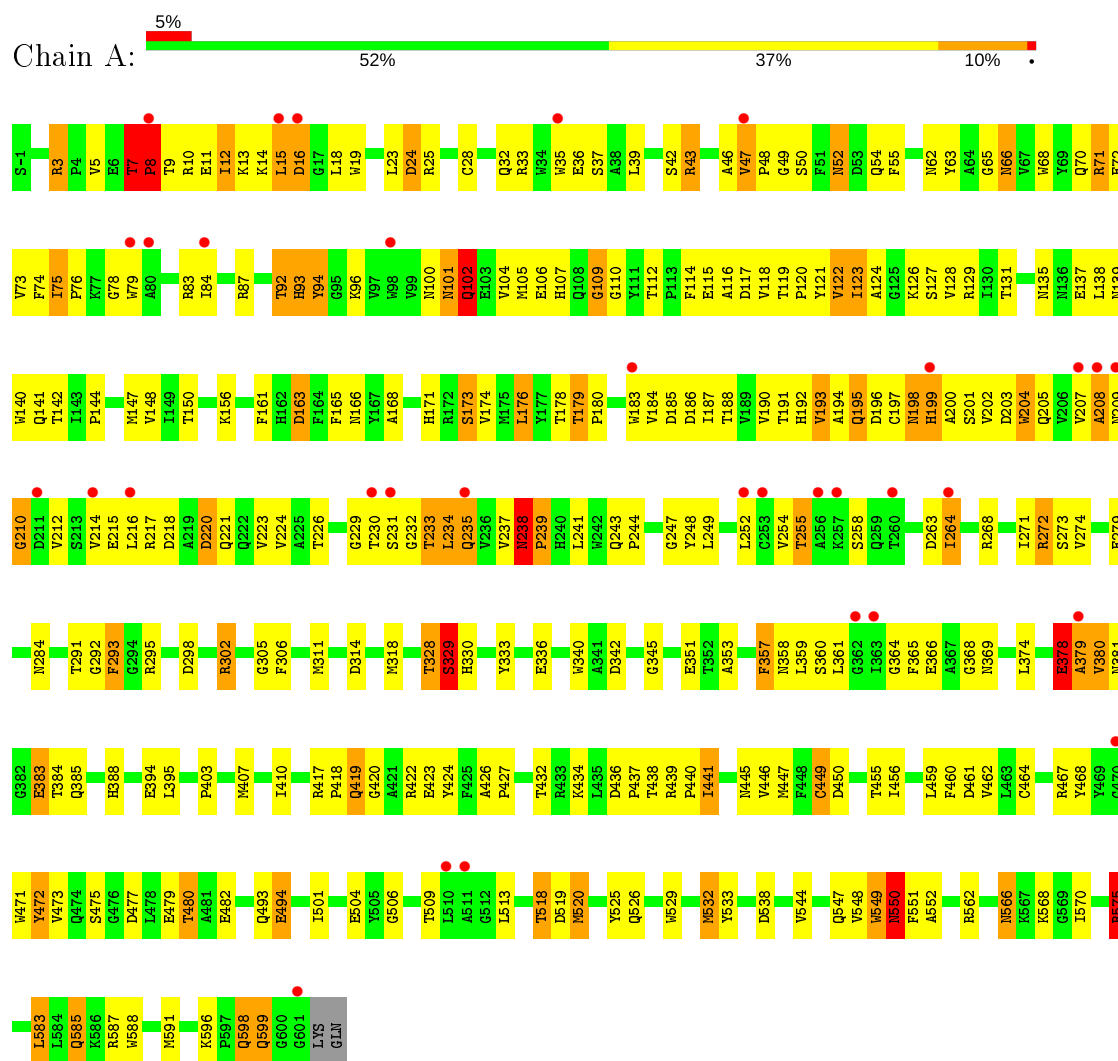
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	269	Total 269	O 269	0	0
3	B	129	Total 129	O 129	0	0

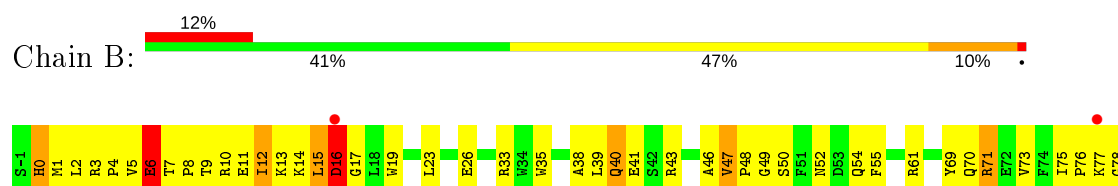
3 Residue-property plots

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: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



L583	E494	R422	V355	I271	V211	H47	W79
R587	R497	E423	G366	R272	V212	V148	
R588	Q498	Y424	F357	S273	S213	I149	R83
	F425	F425	N358	V274	V214	T150	
M591	P499	A426	L359	K277	L216	E151	L86
I501	I501	P427	S360		R217	E152	R87
I502			L361		N153	F88	
T503	T432		G362	F281	G154	D89	
E504	R433		I363	L282	D218	A90	
				L283	D220	V91	
V507	R439		E366	N284	Q221	Q158	
D508	P440		A367	H285	Q222	H93	
D509	I441		G368	K286	V224	X94	
T509	T442		N369	F287	A225	G95	
L510	C443		K370	F288	T226	K96	
	V444		E377	Y289	G227	V97	
	N445		K372	F290	Q228	W98	
	V446		E373	T291	Q229	W99	
T518	M447		L374	G292	Y167	N100	
D619	F448		Y375	F293	A168	H101	
M520	C449		S376	G294	S231	Q102	
M521	D450		E378	R295	T233	E103	
S522			E377		T234	M105	
E523	D454		A379	D298	L234	E106	
	T455		V380		Q235	M175	
Q526	I456		N381	R302	V236	L176	
	S457		G382	G303	V237	L177	
D631	D458		E383	K304	N238	T178	
M532	L459		T384	G305	P239	T179	
Y533	F460		Q385	F306	H240	P180	
H534	D461		Q386	L241	L241	M181	
R535	V462		A387	V311	V242	T182	
V536	L463		H388	V312	Q243	M183	
F537	C464		L389	H313	P244	V184	
D638	L465		Q390	D314	D185	V118	
R539	N466		A391	H315	D186	T119	
	R467		I392	E315	E246	P120	
	Y468		K393	G322	G247	Y121	
A542	Y469		E394	A323	Y248	T188	
V543	G470		L395	N324	Y250	V190	
G545	W471		I396	S325	E251	I123	
E546	Y472		A397		L252	T191	
Q547	V473		R398	T328	C253	V193	
V548	Q474		D399	S329	V254	A194	
R549	S475		K400	R330	T255	Q195	
R550	G476		N401	V331	A256	D196	
F551	D477		H402	P332	K257	C197	
A552	L478		P403	V333	S258	H199	
D553	E479				Q259	N198	
F554	T480		V406	E336	T260	N135	
	A481		M407	A341	E261	M136	
	E482		W408		D262	E137	
	E486		S409	D263	V202	L138	
	K487		I410	G345	D203	N139	
	E488		A411	I346	W204	W140	
	L489		N412		Q205	Q141	
	L490		D415	D350	V206	T142	
	Q493		T352	E351	V207	I143	
					M209	P144	
					G210	G146	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.06Å 77.41Å 126.15Å 90.00° 124.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.26 48.11 – 2.26	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.26) 94.4 (48.11-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.249 0.214 , 0.251	Depositor DCC
R_{free} test set	2982 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: Z77

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	0.60	0/4939	1.05	41/6700 (0.6%)
1	B	0.54	2/4939 (0.0%)	0.98	35/6700 (0.5%)
All	All	0.57	2/9878 (0.0%)	1.02	76/13400 (0.6%)

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	6
1	B	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	PRO	N-CD	-7.47	1.37	1.47
1	B	144	PRO	N-CD	6.81	1.57	1.47

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	TRP	CB-CA-C	17.72	145.84	110.40
1	A	329	SER	CB-CA-C	14.82	138.26	110.10
1	A	379	ALA	N-CA-C	11.13	141.06	111.00
1	A	208	ALA	CB-CA-C	-10.96	93.66	110.10
1	B	549	TRP	N-CA-C	-10.54	82.55	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	GLN	Peptide
1	A	238	ASN	Peptide
1	A	329	SER	Peptide
1	A	364	GLY	Peptide
1	A	92	THR	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	4822	0	4593	356	1
1	B	4822	0	4593	489	1
2	A	29	0	25	6	0
2	B	29	0	25	10	0
3	A	269	0	0	38	0
3	B	129	0	0	34	0
All	All	10100	0	9236	845	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 45.

The worst 5 of 845 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:548:VAL:HG12	1:B:549:TRP:O	1.23	1.32
1:A:598:GLN:CG	1:A:598:GLN:O	1.82	1.18
1:A:15:LEU:HD12	1:A:173:SER:CB	1.79	1.11
1:A:7:THR:HB	1:A:8:PRO:HD3	1.33	1.11
1:A:15:LEU:CD1	1:A:173:SER:HB3	1.80	1.09

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:366:GLU:OE2	1:B:474:GLN:N[2_555]	2.05	0.15

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	601/605 (99%)	579 (96%)	20 (3%)	2 (0%)	41	46
1	B	601/605 (99%)	556 (92%)	42 (7%)	3 (0%)	29	29
All	All	1202/1210 (99%)	1135 (94%)	62 (5%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	239	PRO
1	B	143	ILE
1	B	370	LYS
1	B	144	PRO

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	509/500 (102%)	450 (88%)	59 (12%)	5	3
1	B	509/500 (102%)	436 (86%)	73 (14%)	3	2
All	All	1018/1000 (102%)	886 (87%)	132 (13%)	4	2

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	HIS
1	B	130	ILE
1	B	513	LEU
1	B	6	GLU
1	B	47	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	B	52	ASN
1	B	474	GLN
1	A	550	ASN
1	A	585	GLN

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	Z77	A	604	-	31,31,31	1.63	7 (22%)	41,43,43	1.97	9 (21%)
2	Z77	B	604	-	31,31,31	1.65	4 (12%)	41,43,43	1.52	8 (19%)

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	Z77	A	604	-	-	2/17/17/17	0/3/3/3
2	Z77	B	604	-	-	2/17/17/17	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	Z77	CAZ-N3	4.81	1.41	1.33
2	B	604	Z77	CAZ-N3	4.22	1.40	1.33
2	B	604	Z77	CAT-SAF	3.95	1.74	1.67
2	B	604	Z77	CAW-N1	-3.90	1.33	1.41
2	A	604	Z77	CBB-N3	3.19	1.40	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	Z77	N1-CAT-N2	6.30	122.98	115.11
2	A	604	Z77	SAF-CAT-N2	-5.84	116.20	124.42
2	B	604	Z77	CAP-CAY-CAZ	4.12	125.61	118.95
2	B	604	Z77	CAY-CAZ-N3	-3.89	119.54	125.25
2	A	604	Z77	CAY-CAZ-N3	-3.87	119.58	125.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

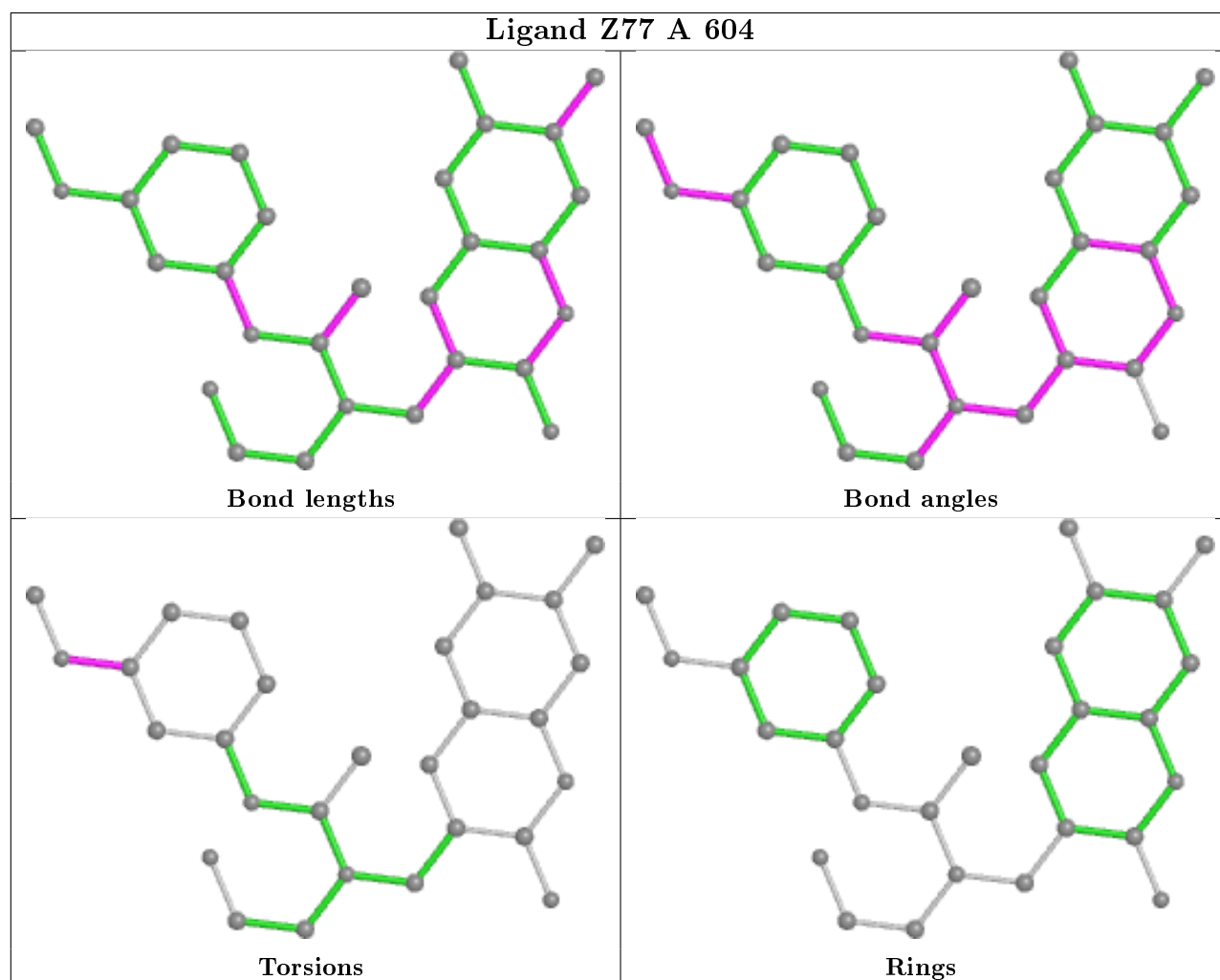
Mol	Chain	Res	Type	Atoms
2	B	604	Z77	CAI-CAX-OAS-CAA
2	B	604	Z77	CAJ-CAX-OAS-CAA
2	A	604	Z77	CAJ-CAX-OAS-CAA
2	A	604	Z77	CAI-CAX-OAS-CAA

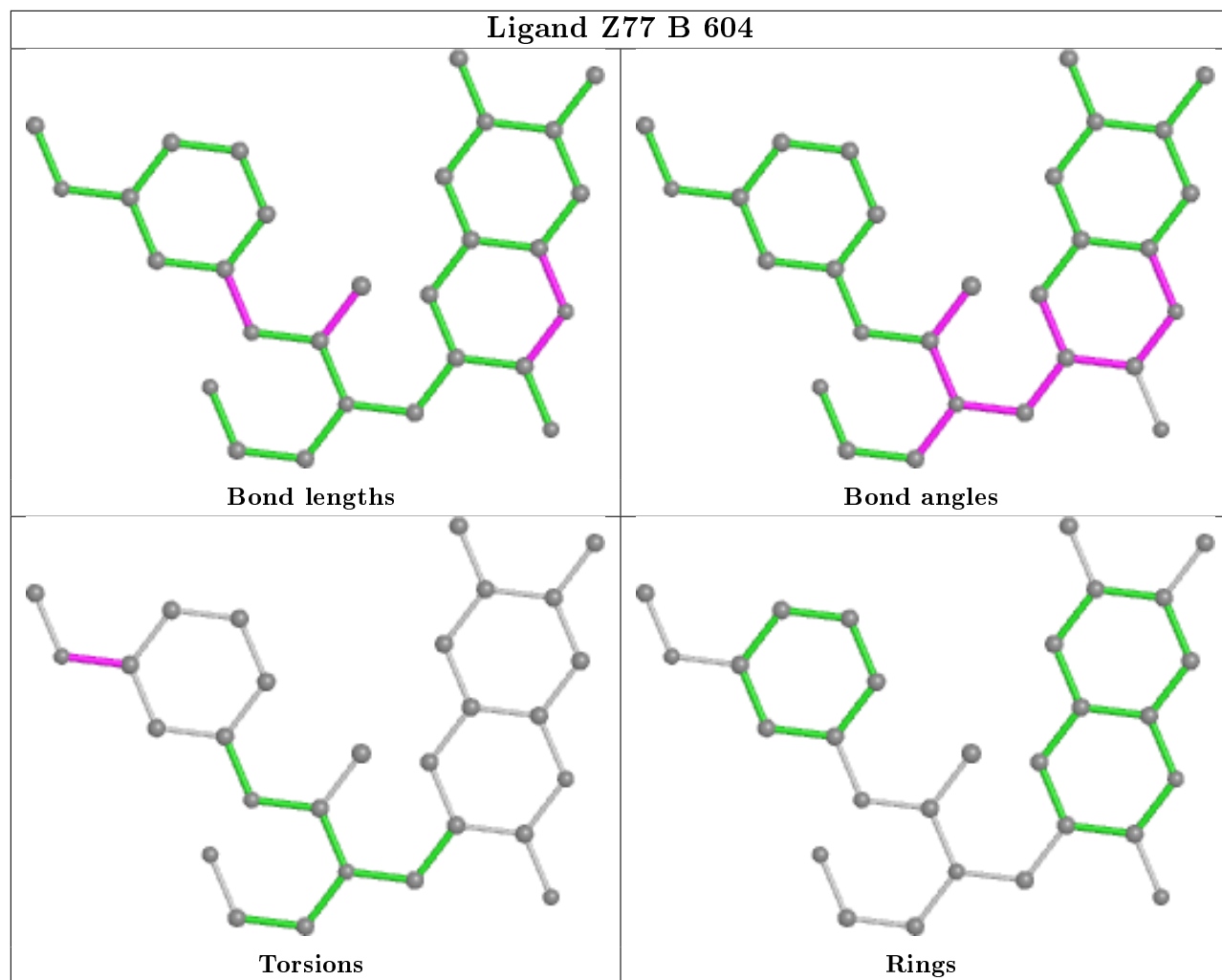
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	Z77	6	0
2	B	604	Z77	10	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	590/605 (97%)	0.29	33 (5%)	24 26	21, 47, 105, 138	0
1	B	590/605 (97%)	0.77	75 (12%)	3 3	29, 85, 166, 230	0
All	All	1180/1210 (97%)	0.53	108 (9%)	9 9	21, 66, 142, 230	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	GLY	8.6
1	B	204	TRP	7.9
1	B	231	SER	7.4
1	B	208	ALA	7.1
1	B	209	ASN	6.9

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](#)

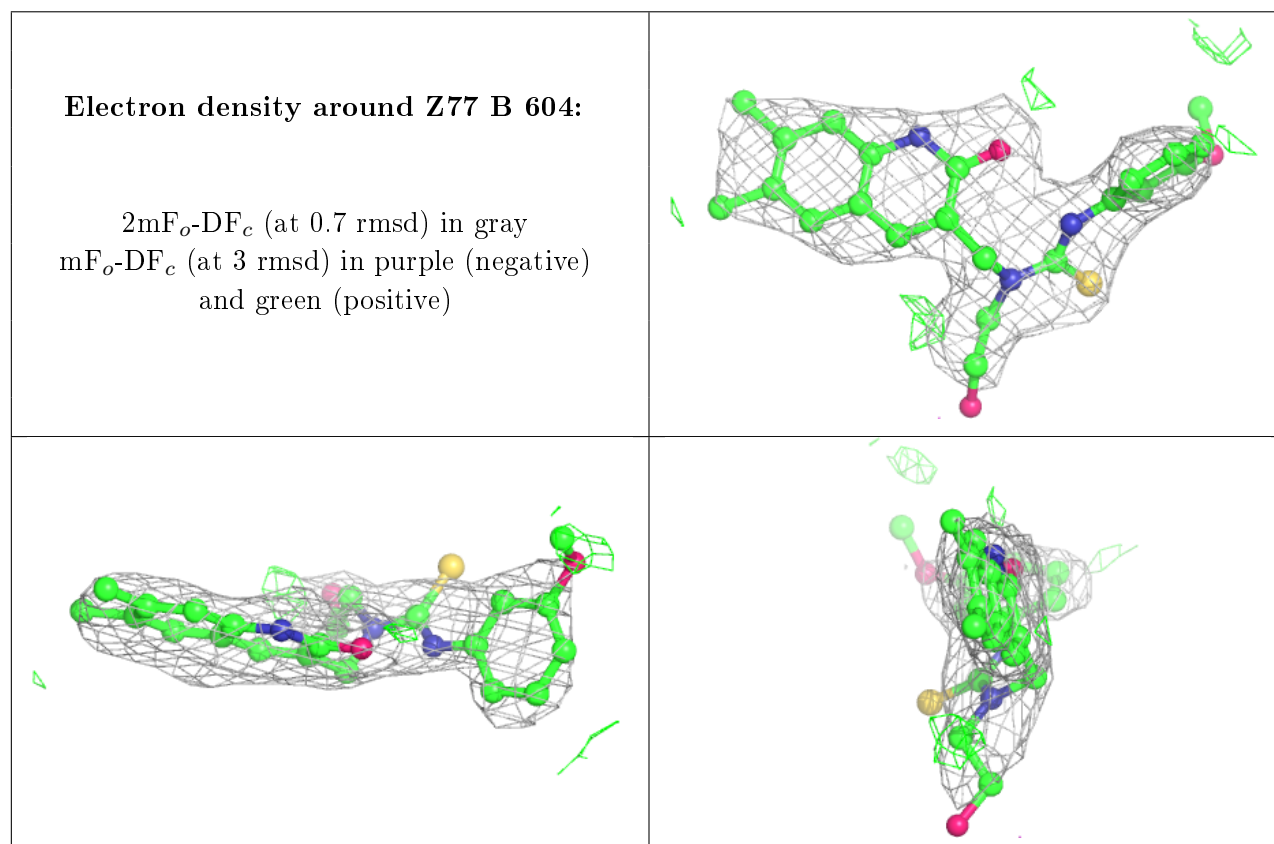
There are no carbohydrates in this entry.

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.

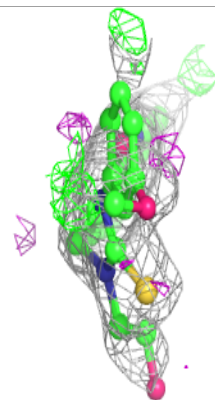
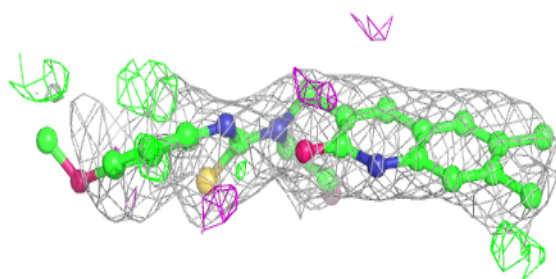
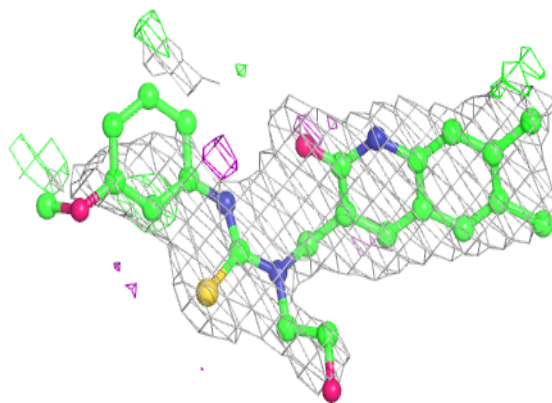
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	Z77	B	604	29/29	0.85	0.21	63,75,94,123	5
2	Z77	A	604	29/29	0.91	0.17	48,65,106,111	2

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 Z77 A 604:

$2mF_o-DF_c$ (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.