



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 03:18 AM JST

PDB ID : 8WFY  
Title : The Crystal Structure of SHP2 from Biortus.  
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Deposited on : 2023-09-20  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

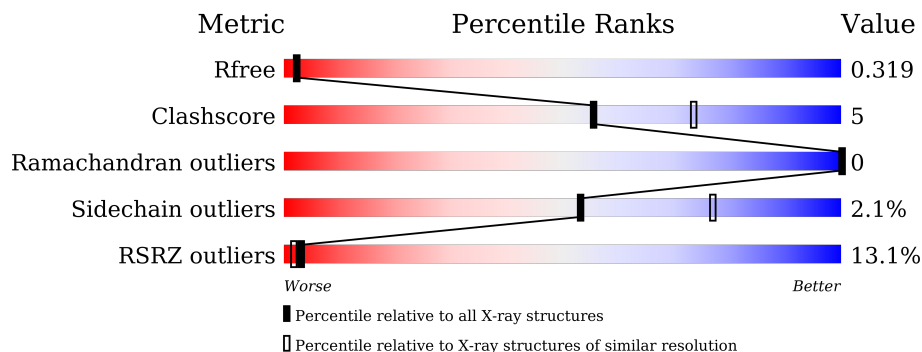
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	525	 14% 79% 13% 8%
1	B	525	 11% 82% 13% 6%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8400 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.

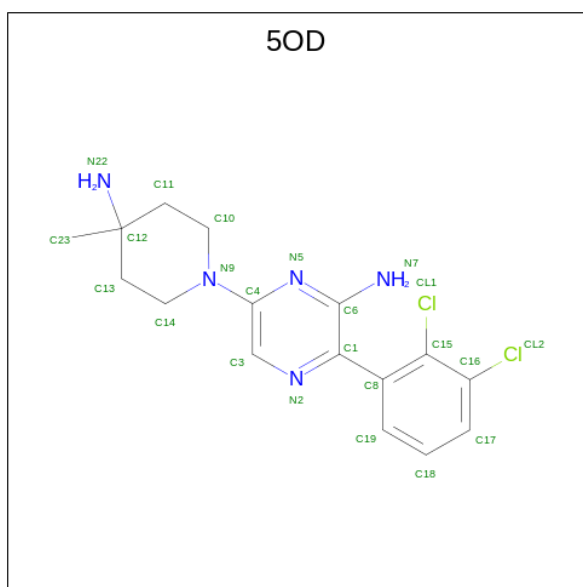
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3914	2460	699	736	19	0	1	0
1	B	496	4016	2530	713	754	19	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	THR	conflict	UNP Q06124
A	41	LEU	PHE	conflict	UNP Q06124
A	513	SER	PHE	conflict	UNP Q06124
B	2	LYS	THR	conflict	UNP Q06124
B	41	LEU	PHE	conflict	UNP Q06124
B	513	SER	PHE	conflict	UNP Q06124

- Molecule 2 is 6-(4-azanyl-4-methyl-piperidin-1-yl)-3-[2,3-bis(chloranyl)phenyl]pyrazin-2-amine (three-letter code: 5OD) (formula: C<sub>16</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	Cl			N
2	A	1	23	16	2	5	0	0
2	B	1	23	16	2	5	0	0

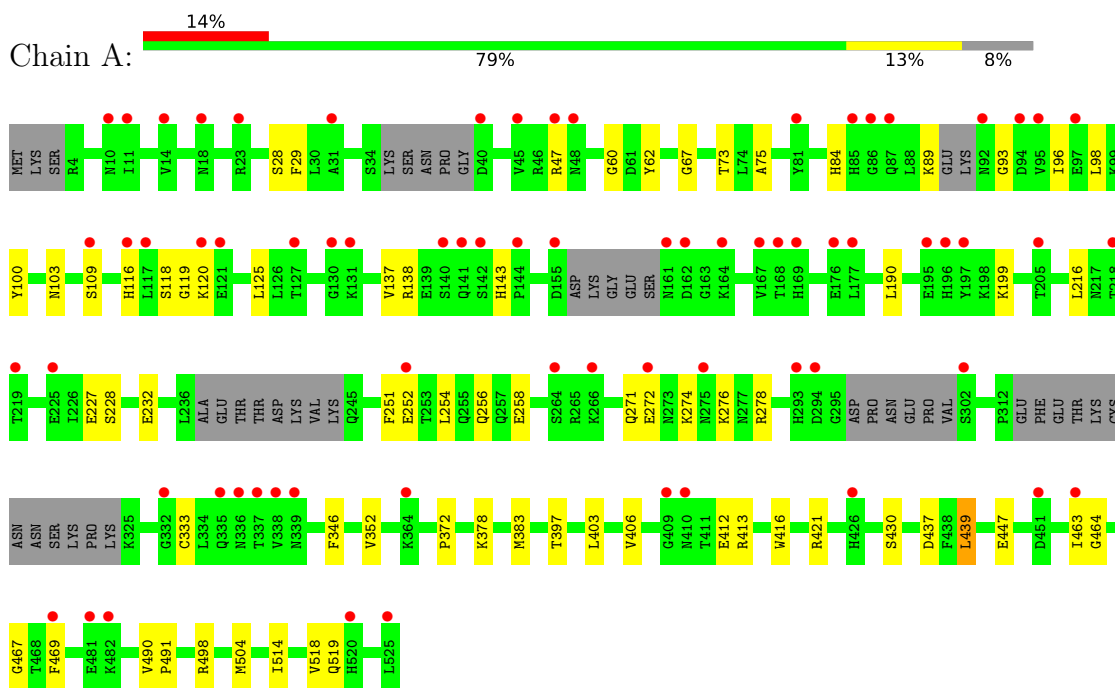
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	204	204	204	0	0
3	B	220	220	220	0	0

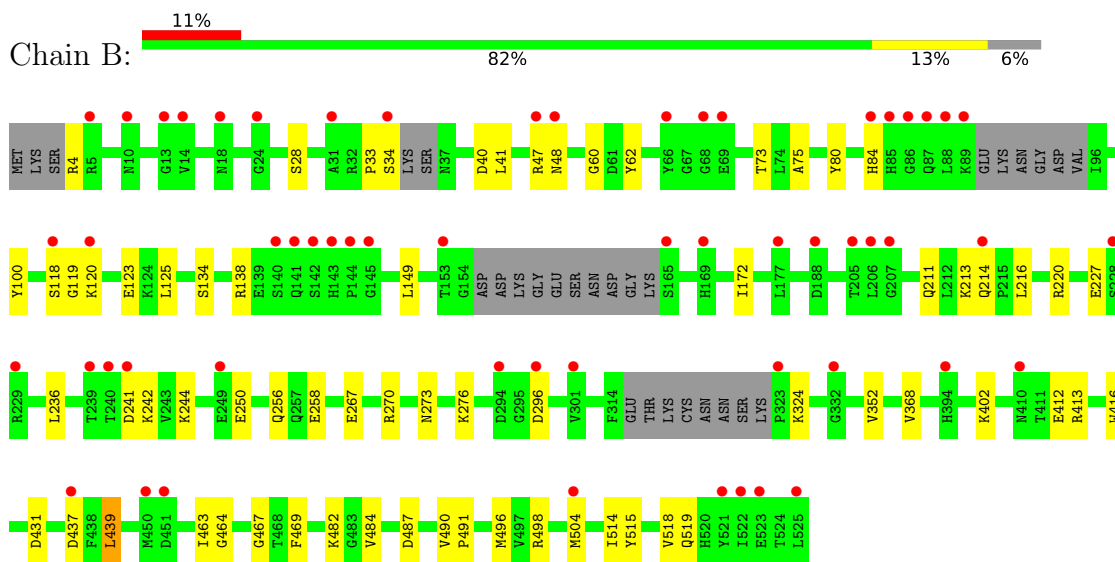
### 3 Residue-property plots [i](#)

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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.62Å 213.64Å 55.71Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	49.12 – 2.60 49.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.12-2.60) 98.7 (49.12-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.237 , 0.317 0.240 , 0.319	Depositor DCC
$R_{free}$ test set	1564 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5OD

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	0.66	0/3993	0.79	0/5381
1	B	0.65	0/4105	0.78	0/5539
All	All	0.66	0/8098	0.79	0/10920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3914	0	3853	43	0
1	B	4016	0	3967	38	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
3	A	204	0	0	5	0
3	B	220	0	0	6	0
All	All	8400	0	7820	81	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 5.

All (81) 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:109:SER:HB3	1:A:256:GLN:HG3	1.74	0.68
1:A:397:THR:OG1	1:A:421:ARG:NH1	2.30	0.65
1:A:73:THR:HG21	3:A:754:HOH:O	1.98	0.63
1:B:484:VAL:HG13	3:B:767:HOH:O	1.98	0.63
1:B:227:GLU:HA	1:B:519:GLN:OE1	2.00	0.62
1:A:227:GLU:HA	1:A:519:GLN:OE1	2.00	0.61
1:B:236:LEU:HD21	1:B:242:LYS:HA	1.82	0.61
1:B:368[A]:VAL:HG11	3:B:902:HOH:O	2.01	0.60
1:B:211:GLN:HG3	1:B:213:LYS:HG3	1.83	0.60
1:B:28:SER:HA	1:B:100:TYR:O	2.02	0.59
1:A:28:SER:HA	1:A:100:TYR:O	2.02	0.58
1:B:439:LEU:HG	1:B:469:PHE:CE2	2.39	0.58
1:A:467:GLY:HA3	1:A:504:MET:O	2.04	0.57
1:B:467:GLY:HA3	1:B:504:MET:O	2.04	0.57
1:B:34:SER:N	1:B:40:ASP:O	2.38	0.56
1:A:29:PHE:CG	1:A:98:LEU:HD22	2.41	0.56
1:B:47:ARG:NH1	1:B:48:ASN:OD1	2.40	0.55
1:B:236:LEU:CD2	1:B:242:LYS:HA	2.37	0.55
1:A:89:LYS:C	1:A:96:ILE:HG12	2.26	0.55
1:A:89:LYS:HG2	1:A:93:GLY:HA2	1.88	0.54
1:A:372:PRO:HG3	1:A:378:LYS:HB2	1.91	0.53
1:B:80:TYR:O	1:B:84:HIS:HB2	2.09	0.52
1:A:406:VAL:HG21	3:A:759:HOH:O	2.09	0.52
1:A:228:SER:O	1:A:232:GLU:HG3	2.09	0.51
1:A:47:ARG:O	1:A:47:ARG:HD2	2.10	0.51
1:B:463:ILE:O	1:B:504:MET:O	2.28	0.51
1:A:89:LYS:CG	1:A:93:GLY:HA2	2.40	0.51
1:B:73:THR:HG21	3:B:711:HOH:O	2.11	0.50
1:B:273:ASN:HA	1:B:276:LYS:HD3	1.93	0.50
1:A:463:ILE:O	1:A:504:MET:O	2.29	0.50
1:A:498:ARG:HG2	1:A:504:MET:H	1.76	0.50
1:B:498:ARG:HG2	1:B:504:MET:H	1.77	0.50
1:A:271:GLN:HA	1:A:274:LYS:HE2	1.93	0.49
1:B:250:GLU:OE2	1:B:515:TYR:OH	2.22	0.49
1:A:73:THR:HG22	1:A:75:ALA:N	2.28	0.48
1:A:439:LEU:HG	1:A:469:PHE:CE2	2.49	0.48
1:A:125:LEU:HB3	1:A:216:LEU:HD21	1.95	0.48
1:B:256:GLN:HG2	3:B:795:HOH:O	2.14	0.48
1:B:73:THR:HG22	1:B:75:ALA:N	2.28	0.48
1:B:60:GLY:O	1:B:464:GLY:HA3	2.15	0.47
1:B:125:LEU:HB3	1:B:216:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG11	1:A:190:LEU:HD23	1.96	0.47
1:B:402:LYS:HE2	1:B:412:GLU:HG2	1.95	0.47
1:A:352:VAL:HA	1:A:416:TRP:O	2.14	0.47
1:B:73:THR:HG23	1:B:258:GLU:CD	2.36	0.46
1:A:278:ARG:NH2	1:A:333:CYS:O	2.48	0.46
1:A:103:ASN:ND2	3:A:708:HOH:O	2.37	0.46
1:B:120:LYS:HA	1:B:123:GLU:CB	2.47	0.45
1:B:352:VAL:HA	1:B:416:TRP:O	2.17	0.45
1:A:73:THR:HG23	1:A:258:GLU:CD	2.37	0.44
1:A:67:GLY:HA3	1:A:89:LYS:HD2	1.99	0.44
1:B:324:LYS:HB3	3:B:801:HOH:O	2.18	0.44
1:B:514:ILE:O	1:B:518:VAL:HG23	2.17	0.44
1:B:119:GLY:HA2	1:B:138:ARG:CZ	2.48	0.43
1:A:346:PHE:CD1	1:A:383:MET:HE1	2.53	0.43
1:A:60:GLY:O	1:A:464:GLY:HA3	2.18	0.43
1:A:190:LEU:HD13	3:A:829:HOH:O	2.17	0.43
1:A:272:GLU:O	1:A:276:LYS:HE3	2.18	0.43
1:B:241:ASP:OD2	1:B:244:LYS:HB3	2.19	0.43
1:A:403:LEU:O	1:A:412:GLU:HA	2.18	0.43
1:A:346:PHE:HB2	1:A:383:MET:HE2	2.00	0.42
1:A:119:GLY:HA2	1:A:138:ARG:CZ	2.50	0.42
1:A:490:VAL:N	1:A:491:PRO:HD2	2.35	0.42
1:B:4:ARG:NH1	1:B:256:GLN:OE1	2.53	0.42
1:A:383:MET:CE	1:A:403:LEU:HD11	2.49	0.42
1:A:190:LEU:HD12	1:A:190:LEU:N	2.35	0.42
1:B:267:GLU:HA	1:B:270:ARG:HG3	2.02	0.41
1:B:490:VAL:N	1:B:491:PRO:HD2	2.34	0.41
1:A:252:GLU:O	1:A:256:GLN:HG2	2.20	0.41
1:B:220:ARG:HD2	1:B:487:ASP:HB3	2.03	0.41
1:A:120:LYS:HE3	3:A:870:HOH:O	2.20	0.41
1:A:73:THR:HG22	1:A:75:ALA:H	1.85	0.41
1:B:73:THR:HG22	1:B:75:ALA:H	1.85	0.41
1:B:33:PRO:HA	1:B:41:LEU:HD23	2.02	0.41
1:B:482:LYS:HE3	3:B:863:HOH:O	2.20	0.41
1:A:514:ILE:O	1:A:518:VAL:HG23	2.21	0.41
1:A:199:LYS:HD3	1:A:199:LYS:HA	1.89	0.40
1:B:134:SER:HA	1:B:214:GLN:O	2.21	0.40
1:B:149:LEU:HB2	1:B:172:ILE:HD11	2.02	0.40
1:A:383:MET:HE2	1:A:403:LEU:HD11	2.02	0.40
1:A:251:PHE:O	1:A:254:LEU:HB3	2.21	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	471/525 (90%)	451 (96%)	20 (4%)	0	100	100
1	B	488/525 (93%)	464 (95%)	24 (5%)	0	100	100
All	All	959/1050 (91%)	915 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	430/467 (92%)	420 (98%)	10 (2%)	50	75
1	B	443/467 (95%)	435 (98%)	8 (2%)	59	80
All	All	873/934 (94%)	855 (98%)	18 (2%)	53	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	TYR
1	A	84	HIS
1	A	116	HIS
1	A	118	SER
1	A	143	HIS
1	A	413	ARG
1	A	430	SER
1	A	437	ASP

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Mol	Chain	Res	Type
1	A	439	LEU
1	A	447	GLU
1	B	62	TYR
1	B	118	SER
1	B	296	ASP
1	B	413	ARG
1	B	431	ASP
1	B	437	ASP
1	B	439	LEU
1	B	496	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	HIS
1	B	245	GLN
1	B	335	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](#)

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	5OD	B	601	-	23,25,25	0.50	0	28,37,37	0.82	1 (3%)
2	5OD	A	601	-	23,25,25	0.42	0	28,37,37	0.85	1 (3%)

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	5OD	B	601	-	-	0/8/20/20	0/3/3/3
2	5OD	A	601	-	-	0/8/20/20	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	601	5OD	C8-C1-C6	2.32	125.21	122.34
2	B	601	5OD	C8-C1-C6	2.09	124.92	122.34

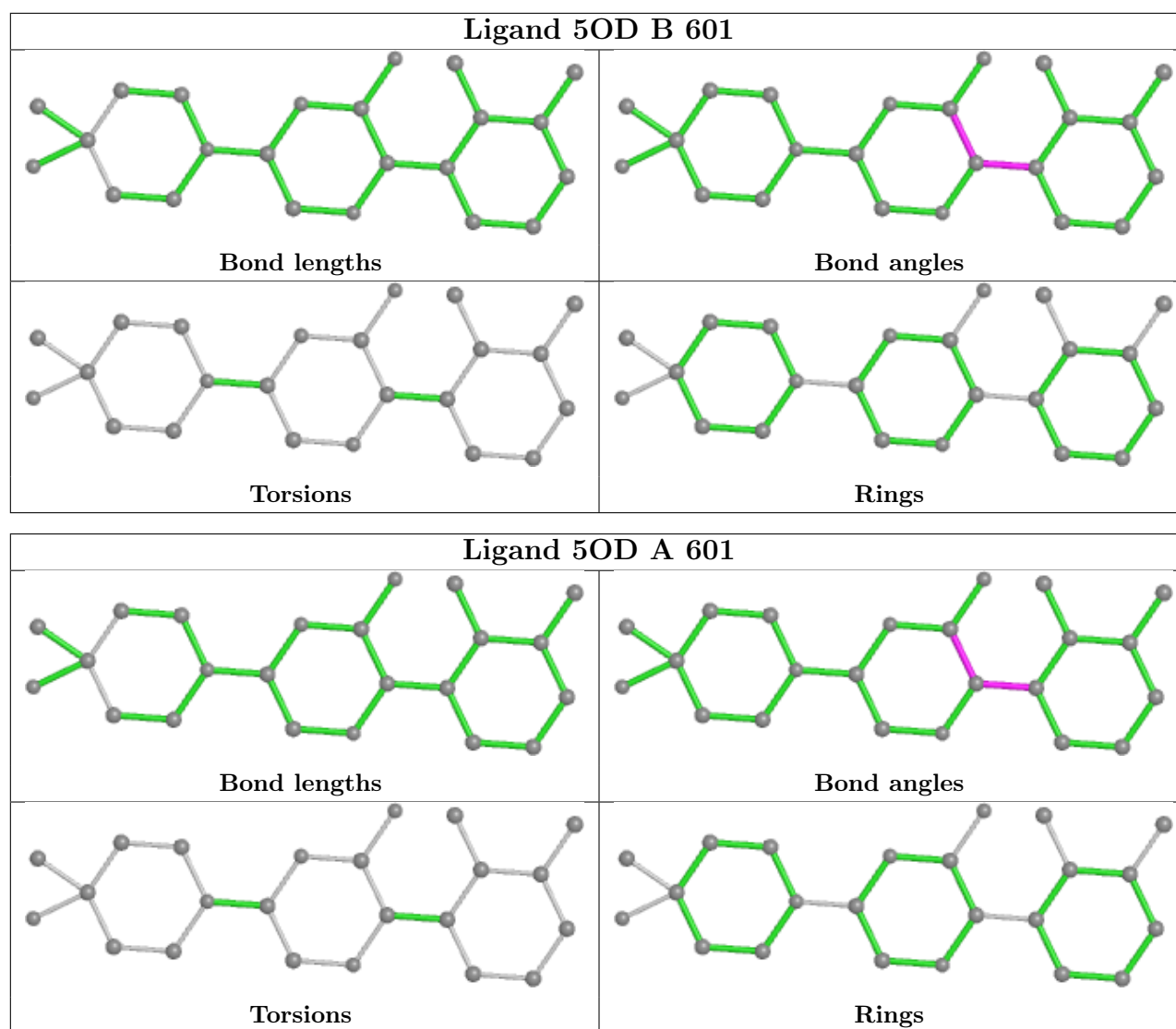
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	484/525 (92%)	0.96	71 (14%) <b>2</b> <b>1</b>	15, 37, 66, 103	0
1	B	496/525 (94%)	0.81	57 (11%) <b>4</b> <b>3</b>	14, 34, 62, 88	0
All	All	980/1050 (93%)	0.88	128 (13%) <b>3</b> <b>2</b>	14, 35, 64, 103	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	HIS	8.1
1	A	85	HIS	6.2
1	B	86	GLY	5.6
1	A	86	GLY	5.3
1	B	240	THR	4.8
1	B	142	SER	4.7
1	A	140	SER	4.6
1	A	161	ASN	4.4
1	B	140	SER	4.4
1	A	14	VAL	4.3
1	A	164	LYS	4.3
1	A	95	VAL	3.9
1	B	120	LYS	3.8
1	B	48	ASN	3.8
1	A	120	LYS	3.8
1	B	522	ILE	3.7
1	B	14	VAL	3.6
1	B	301	VAL	3.6
1	A	205	THR	3.5
1	A	481	GLU	3.5
1	A	177	LEU	3.4
1	B	394	HIS	3.4
1	B	207	GLY	3.4
1	A	294	ASP	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	141	GLN	3.3
1	A	162	ASP	3.3
1	A	117	LEU	3.3
1	A	525	LEU	3.3
1	A	142	SER	3.3
1	A	31	ALA	3.2
1	B	47	ARG	3.2
1	A	92	ASN	3.2
1	A	40	ASP	3.2
1	B	239	THR	3.2
1	B	165	SER	3.1
1	B	10	ASN	3.1
1	B	84	HIS	3.1
1	B	205	THR	3.0
1	A	225	GLU	3.0
1	A	48	ASN	3.0
1	A	336	ASN	2.9
1	A	155	ASP	2.9
1	B	145	GLY	2.8
1	A	410	ASN	2.8
1	A	81	TYR	2.7
1	A	332	GLY	2.7
1	B	249	GLU	2.7
1	A	338	VAL	2.7
1	A	116	HIS	2.7
1	A	264	SER	2.6
1	A	169	HIS	2.6
1	A	339	ASN	2.6
1	B	241	ASP	2.6
1	B	66	TYR	2.6
1	A	168	THR	2.6
1	A	426	HIS	2.6
1	B	206	LEU	2.6
1	A	337	THR	2.6
1	B	294	ASP	2.5
1	A	87	GLN	2.5
1	B	228	SER	2.5
1	B	332	GLY	2.5
1	A	266	LYS	2.5
1	B	525	LEU	2.5
1	B	144	PRO	2.4
1	A	482	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	47	ARG	2.4
1	A	219	THR	2.4
1	A	18	ASN	2.4
1	A	94	ASP	2.4
1	B	504	MET	2.4
1	A	121	GLU	2.4
1	A	109	SER	2.4
1	A	252	GLU	2.4
1	A	293	HIS	2.4
1	B	5	ARG	2.4
1	A	520	HIS	2.3
1	B	143	HIS	2.3
1	B	24	GLY	2.3
1	A	463	ILE	2.3
1	A	23	ARG	2.3
1	B	188	ASP	2.3
1	B	34	SER	2.3
1	A	167	VAL	2.3
1	A	144	PRO	2.3
1	B	87	GLN	2.3
1	B	450	MET	2.3
1	B	153	THR	2.3
1	A	11	ILE	2.3
1	A	127	THR	2.2
1	A	451	ASP	2.2
1	B	451	ASP	2.2
1	A	10	ASN	2.2
1	B	31	ALA	2.2
1	A	176	GLU	2.2
1	A	130	GLY	2.2
1	B	177	LEU	2.2
1	A	335	GLN	2.2
1	B	89	LYS	2.2
1	B	521	TYR	2.2
1	A	131	LYS	2.2
1	A	302	SER	2.2
1	B	437	ASP	2.1
1	B	68	GLY	2.1
1	A	469	PHE	2.1
1	A	197	TYR	2.1
1	B	18	ASN	2.1
1	A	364	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLU	2.1
1	A	195	GLU	2.1
1	B	296	ASP	2.1
1	B	523	GLU	2.1
1	A	196	HIS	2.1
1	B	169	HIS	2.1
1	A	218	THR	2.1
1	A	272	GLU	2.1
1	B	118	SER	2.1
1	A	45	VAL	2.0
1	B	229	ARG	2.0
1	A	275	ASN	2.0
1	B	69	GLU	2.0
1	B	410	ASN	2.0
1	A	409	GLY	2.0
1	B	323	PRO	2.0
1	B	214	GLN	2.0
1	B	13	GLY	2.0
1	B	141	GLN	2.0
1	B	88	LEU	2.0

## 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](#)

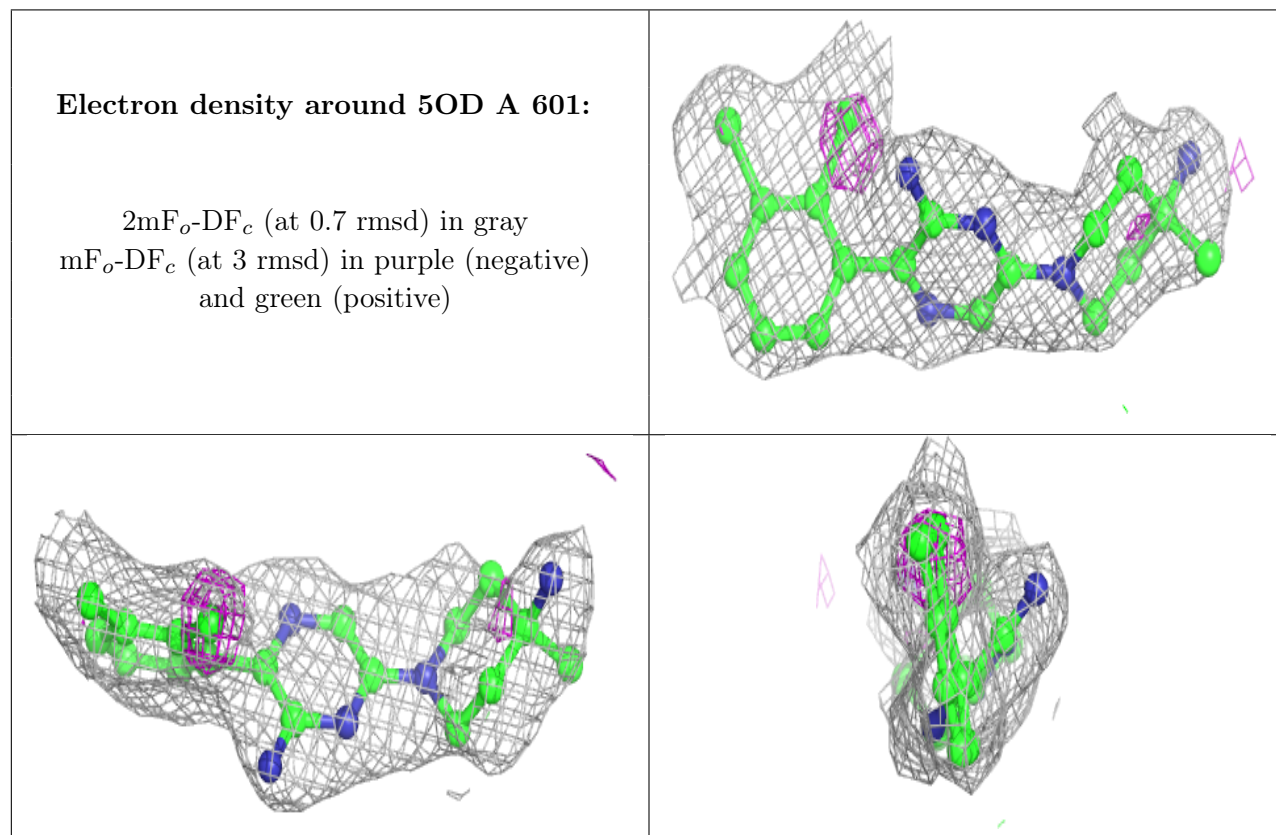
There are no monosaccharides in this entry.

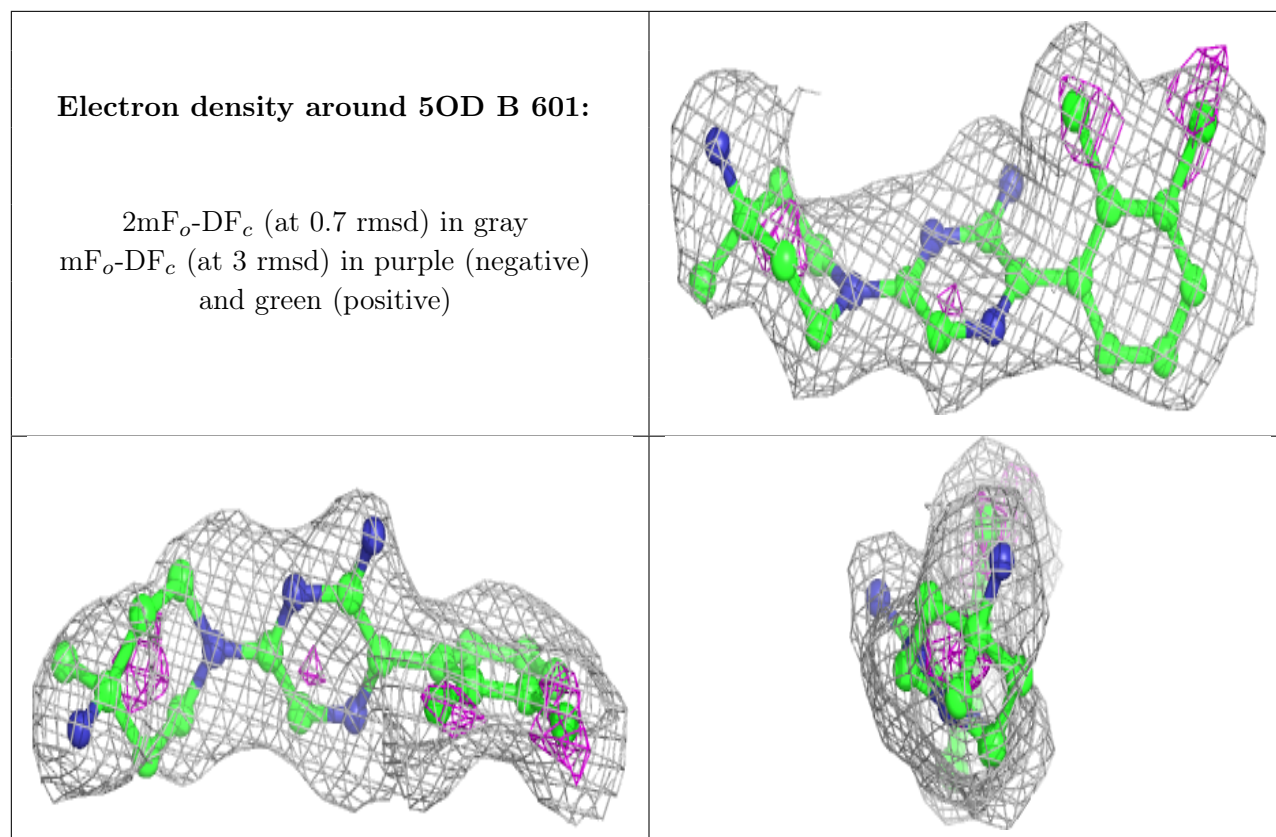
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	5OD	A	601	23/23	0.90	0.20	30,32,36,43	0
2	5OD	B	601	23/23	0.91	0.19	23,25,28,33	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.