



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:46 pm BST

PDB ID : 5OIZ
Title : Penicillin-Binding Protein 2X (PBP2X) from *Streptococcus pneumoniae* in complex with oxacillin
Authors : Bernardo-Garcia, N.; Hermoso, J.A.
Deposited on : 2017-07-20
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	:	2.11
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

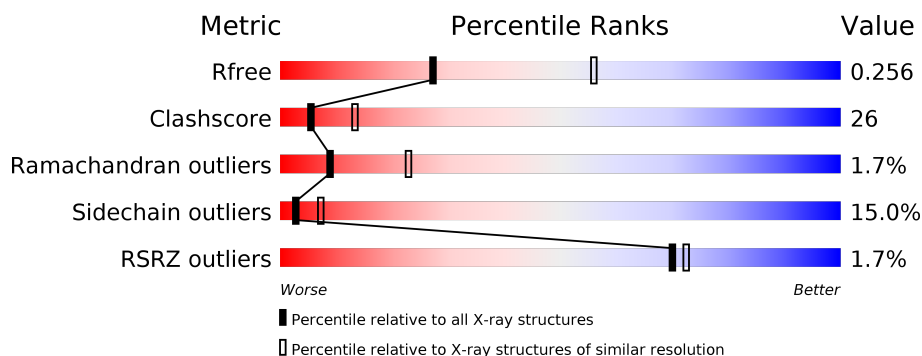
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	702	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>9%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

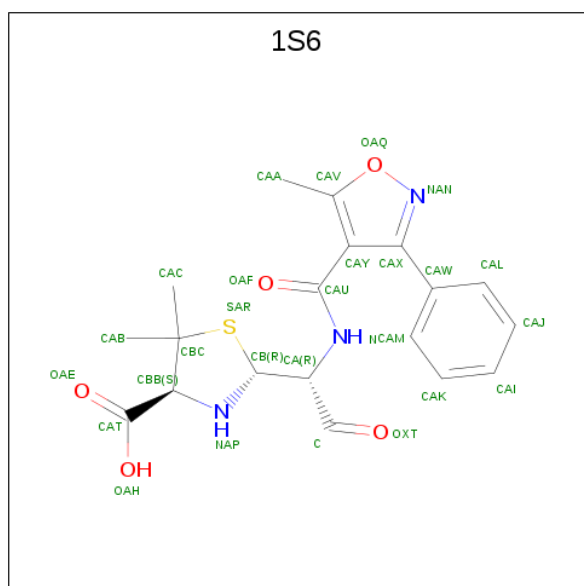
There are 3 unique types of molecules in this entry. The entry contains 5122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	651	4994	3131	831	1009	23	0	0	0

- Molecule 2 is (2R,4S)-5,5-dimethyl-2-[(1R)-1-{[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbon yl]amino}-2-oxoethyl]-1,3-thiazolidine-4-carboxylic acid (three-letter code: 1S6) (formula: C₁₉H₂₁N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	28	19	3	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:

290

49% 34% 9% 7%

GLY THR GLY THR ARG PHE GLY THR ASP LEU ALA LYS GLU LYS VAL HIS GLN THR THR ARG W71 W72 P73 P76 W79 W80 D81 D87 D88 D89 W94 W95 W96 W97 W98 W99 D100 D101 GLU ASN ALN TTR LYS SER ALA THR GLY LYS ILE LEU Y113 Y114 E115 K116 K117 Q118 E220 S221 S222 L223 N224 S225 I226 T230 D231 G232 ILE E233 E234 TYR E235 G236 G237 L238 G239 VAL G240 G241 G242 G243 G244 G245 G246 G247 G248 G249 G250 G251 G252 G253 G254 G255 G256 G257 G258 G259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 T290 D375 D376 D377 D378 D379 D380 D381 D382 D383 D384 D385 D386 D387 D388 D389 D390 D391 D392 D393 D394 D395 D396 D397 D398 D399 D400 D401 D402 D403 D404 D405 D406 D407 D408 D409 D410 D411 D412 D413 D414 D415 D416 D417 D418 D419 D420 D421 D422 D423 D424 D425 D426 D427 D428 D429 D430 D431 D432 D433 D434 D435 D436 D437 D438 D439 D440 D441 D442 D443 D444 D445 D446 D447 D448 D449 D450 D451 D452 D453 D454 D455 D456 D457 D458 D459 D460 D461 D462 D463 D464 D465 D466 D467 D468 D469 D470 D471 D472 D473 D474 D475 D476 D477 D478 D479 D480 D481 D482 D483 D484 D485 D486 D487 D488 D489 D490 D491 D492 D493 D494 D495 D496 D497 D498 D499 D500 D501 D502 D503 D504 D505 D506 D507 D508 D509 D510 D511 D512 D513 D514 D515 D516 D517 D518 D519 D520 D521 D522 D523 D524 D525 D526 D527 D528 D529 D530 D531 D532 D533 D534 D535 D536 D537 D538 D539 D540 D541 D542 D543 D544 D545 D546 D547 D548 D549 D550 D551 D552 D553 D554 D555 D556 D557 D558 D559 D560 D561 D562 D563 D564 D565 D566 D567 D568 D569 D570 D571 D572 D573 D574 D575 D576 D577 D578 D579 D580 D581 D582 D583 D584 D585 D586 D587 D588 D589 D590 D591 D592 D593 D594 D595 D596 D597 D598 D599 D600 D601 D602 D603 D604 D605 D606 D607 D608 D609 D610 D611 D612 D613 D614 D615 D616 D617 D618 D619 D620 D621 D622 D623 D624 D625 D626 D627 D628 D629 D630 D631 D632 D633 D634 D635 D636 D637 D638 D639 D640 D641 D642 D643 D644 D645 D646 D647 D648 D649 D650 D651 D652 D653 D654 D655 D656 D657 D658 D659 D660 D661 D662 D663 D664 D665 D666 D667 D668 D669 D670 D671 D672 D673 D674 D675 D676 D677 D678 D679 D680 D681 D682 D683 D684 D685 D686 D687 D688 D689 D690 D691 D692 D693 D694 D695 D696 D697 D698 D699 D700 D701 D702 D703 D704 D705 D706 D707 D708 D709 D710 D711 D712 D713 D714 D715 D716 D717 D718 D719 D720 D721 D722 D723 D724 D725 D726 D727 D728 D729 D730 D731 D732 D733 D734 D735 D736 D737 D738 D739 D740 D741 D742 D743 D744 D745 D746 D747 D748 D749 D750

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.42Å 100.42Å 189.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 2.70 48.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-2.70) 100.0 (48.54-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.217 , 0.281 0.207 , 0.256	Depositor DCC
R_{free} test set	1601 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5122	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1S6

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	1.40	21/5081 (0.4%)	1.28	18/6883 (0.3%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	694	GLU	CD-OE1	7.58	1.33	1.25
1	A	596	SER	CB-OG	7.40	1.51	1.42
1	A	595	TYR	CE1-CZ	6.94	1.47	1.38
1	A	367	ALA	CA-C	6.55	1.70	1.52
1	A	415	TYR	CG-CD2	6.33	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	426	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	A	89	GLU	CB-CA-C	-6.86	96.69	110.40
1	A	260	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	440	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	349	ASP	CB-CG-OD1	6.22	123.90	118.30

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	4994	0	4907	259	9
2	A	28	0	19	2	0
3	A	100	0	0	6	1
All	All	5122	0	4926	259	10

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 26.

The worst 5 of 259 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:491:ALA:C	1:A:632:GLN:NE2	1.69	1.40
1:A:491:ALA:CB	1:A:632:GLN:OE1	1.78	1.31
1:A:491:ALA:CA	1:A:632:GLN:OE1	1.80	1.27
1:A:491:ALA:HB3	1:A:632:GLN:OE1	1.30	1.25
1:A:175:VAL:N	1:A:176:LYS:HZ2	1.43	1.15

The worst 5 of 10 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)
3:A:963:HOH:O	3:A:976:HOH:O[6_665]	0.11	2.09
1:A:365:LYS:CE	1:A:367:ALA:C[5_554]	1.25	0.95
1:A:365:LYS:CE	1:A:367:ALA:O[5_554]	1.42	0.78
1:A:365:LYS:CE	1:A:367:ALA:CA[5_554]	1.48	0.72
1:A:365:LYS:CD	1:A:367:ALA:O[5_554]	1.62	0.58

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	645/702 (92%)	567 (88%)	67 (10%)	11 (2%)	9 23

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LYS
1	A	396	SER
1	A	620	LEU
1	A	633	GLN
1	A	739	LYS

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	548/590 (93%)	466 (85%)	82 (15%)	3 7

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	THR
1	A	505	LYS
1	A	719	GLU
1	A	387	THR
1	A	456	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	ASN
1	A	444	ASN
1	A	679	ASN
1	A	394	HIS
1	A	659	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	1S6	A	801	1	20,30,30	2.24	6 (30%)	23,44,44	1.45	5 (21%)

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	1S6	A	801	1	-	0/8/37/37	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1S6	CAY-CAX	7.72	1.50	1.41
2	A	801	1S6	CAX-NAN	3.23	1.39	1.33
2	A	801	1S6	CBB-NAP	2.66	1.50	1.46
2	A	801	1S6	CBC-SAR	-2.50	1.80	1.85
2	A	801	1S6	OAF-CAU	2.42	1.28	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1S6	OAF-CAU-N	3.05	128.06	122.45
2	A	801	1S6	CA-N-CAU	2.85	126.71	122.26
2	A	801	1S6	OXT-C-CA	-2.78	117.09	124.83
2	A	801	1S6	CB-CA-N	-2.64	104.22	109.98
2	A	801	1S6	CBB-CBC-SAR	2.53	108.81	103.81

There are no chirality outliers.

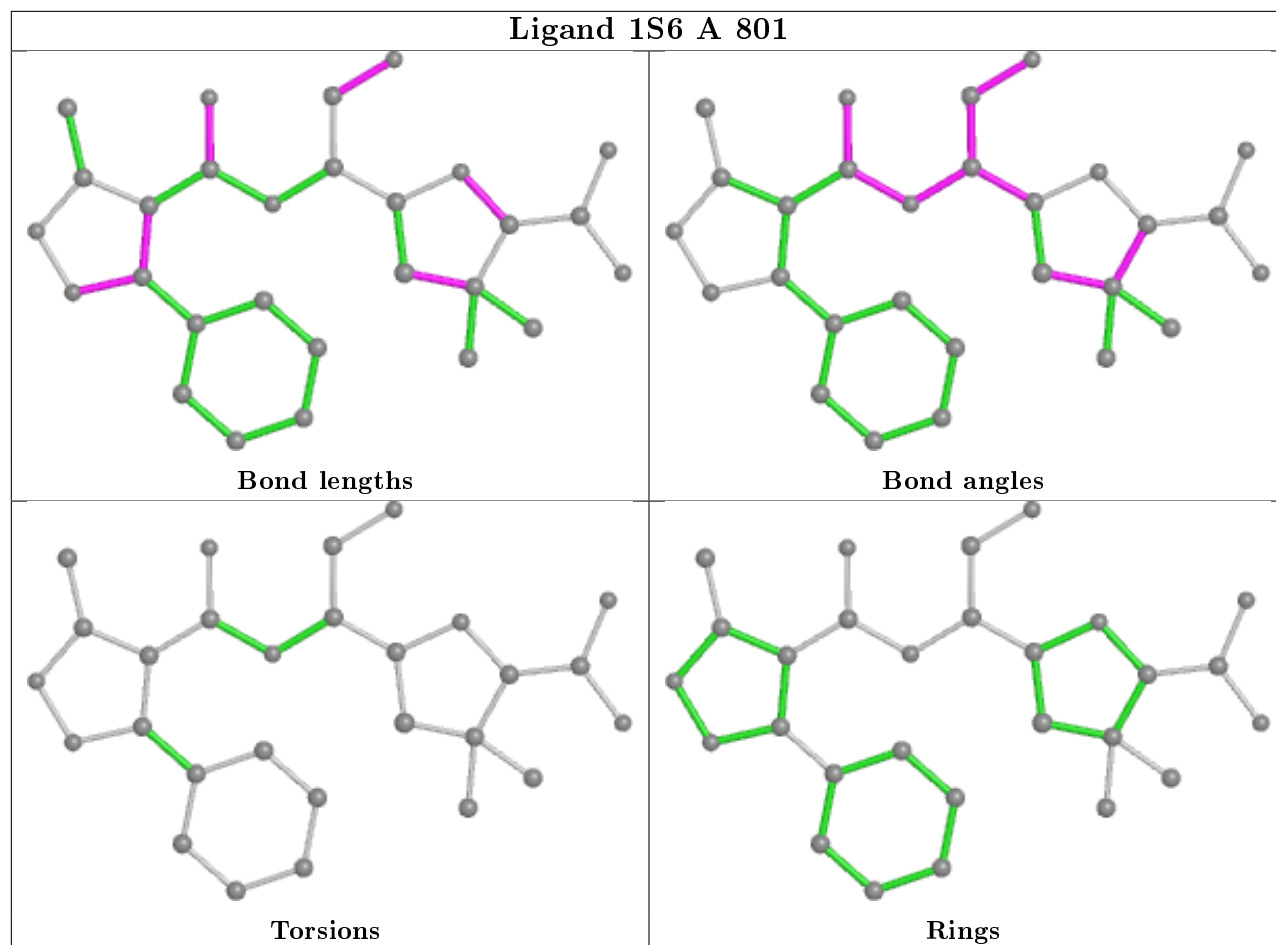
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	1S6	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	651/702 (92%)	-0.13	11 (1%) 70 72	52, 62, 74, 84	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	3.3
1	A	716	ILE	2.9
1	A	560	GLY	2.8
1	A	319	THR	2.7
1	A	251	VAL	2.6

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.

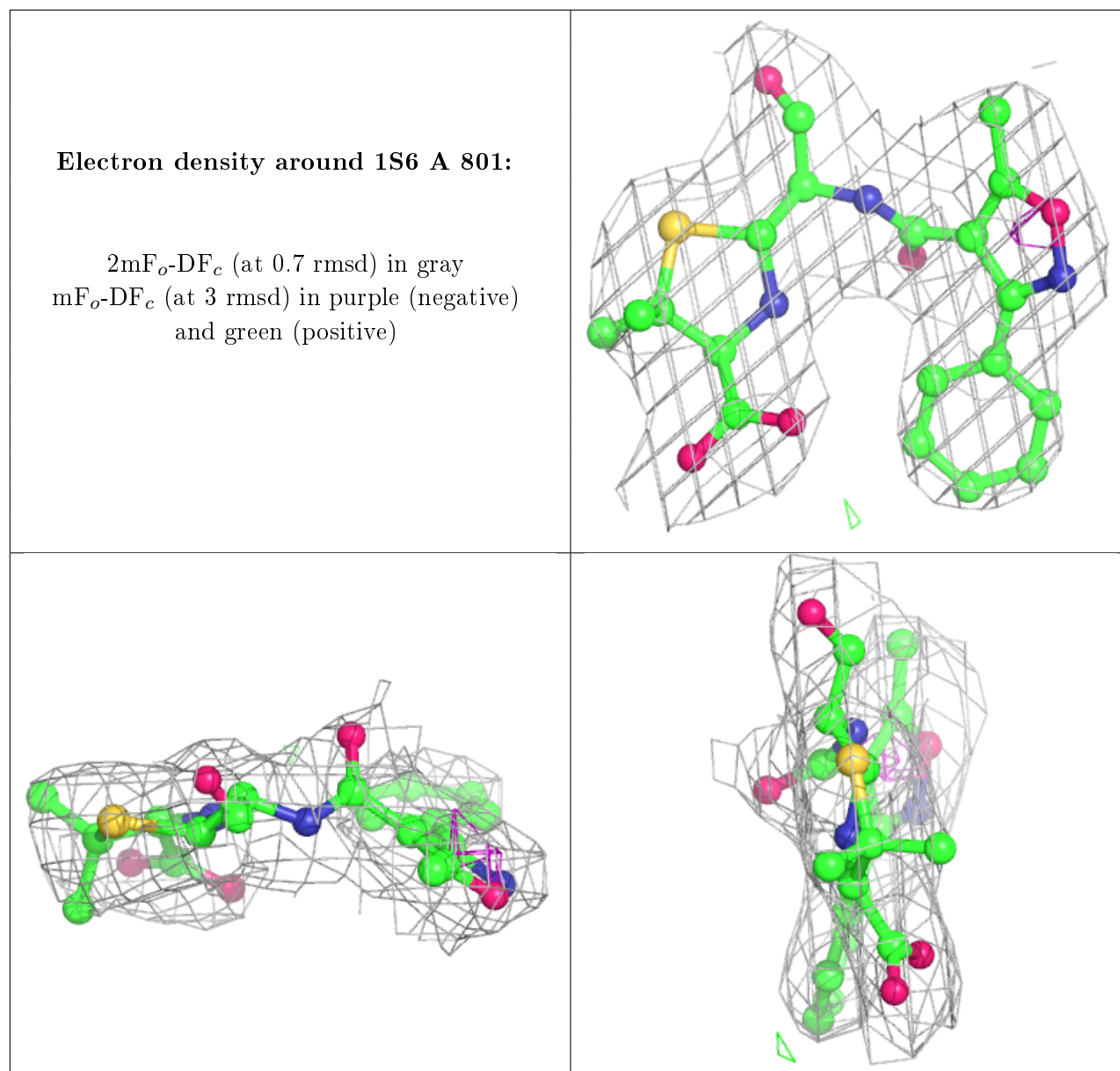
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	1S6	A	801	28/28	0.93	0.20	57,65,69,75	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 ⓘ

There are no such residues in this entry.