



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:05 am BST

PDB ID : 5OJ1
Title : Penicillin Binding Protein 2x (PBP2x) from S.pneumoniae in complex with Oxacillin and a tetrasaccharide
Authors : Bernardo-Garcia, N.; Hermoso, J.A.
Deposited on : 2017-07-20
Resolution : 2.85 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

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

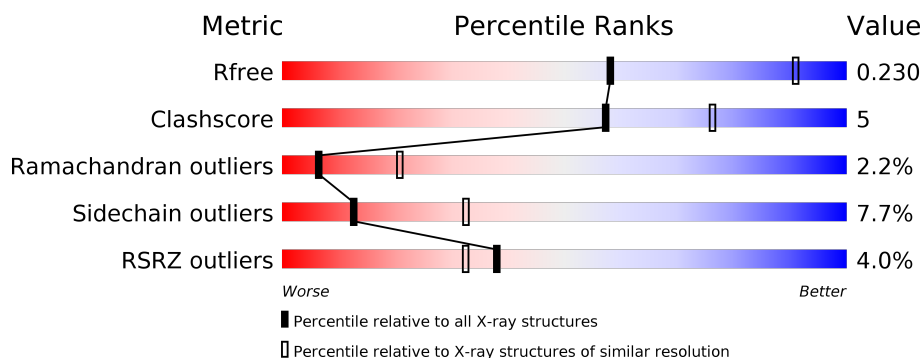
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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.

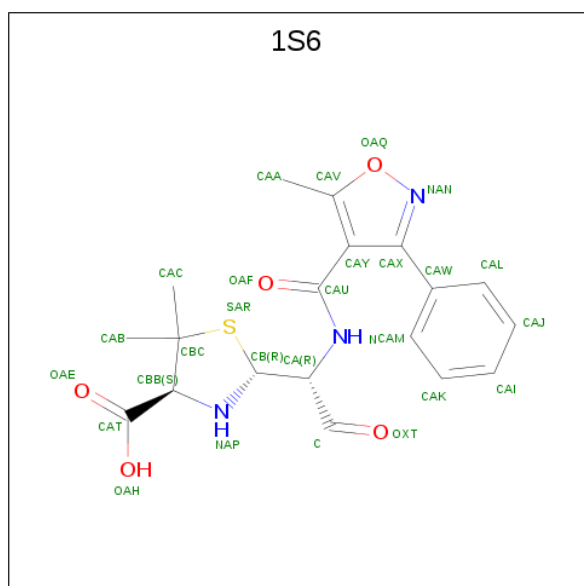
Mol	Chain	Length	Quality of chain
1	A	702	<div> <div>4%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div>

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
1	A	675	Total	C	N	O	S	0	2	0
			5197	3265	862	1047	23			

- 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
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

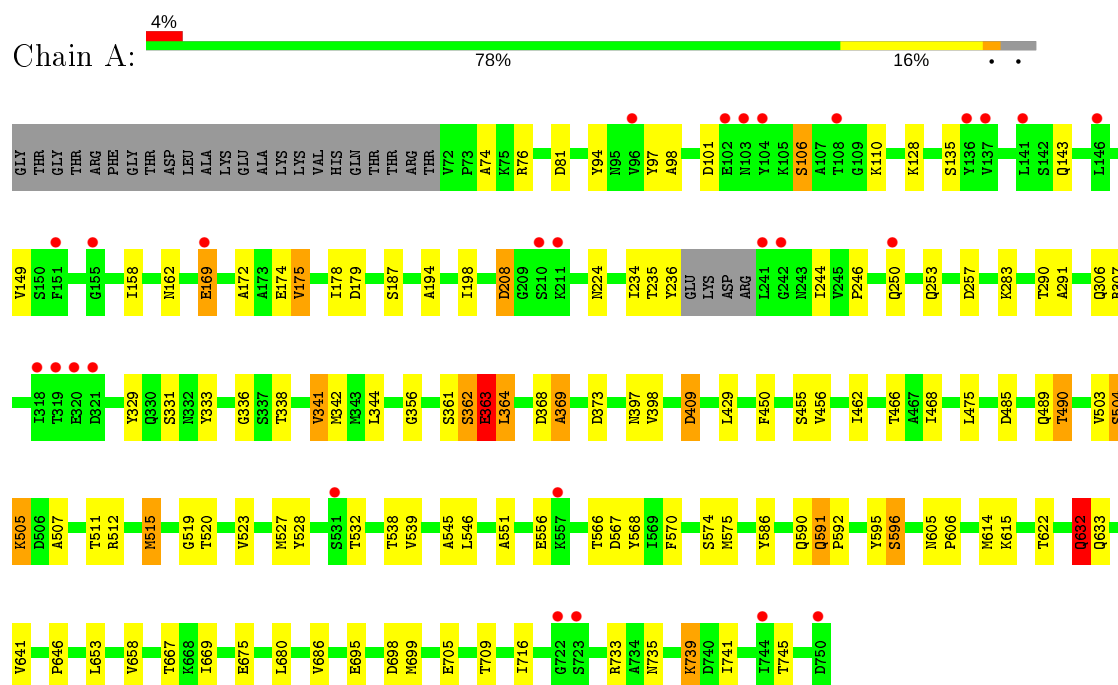
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

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: Penicillin-binding protein 2X



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.84Å 100.84Å 189.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.33 – 2.85 48.72 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.33-2.85) 100.0 (48.72-2.85)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.167 , 0.229 0.171 , 0.230	Depositor DCC
R_{free} test set	1303 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: NA, 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	0.70	0/5289	0.85	5/7167 (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	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	409	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	485	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	512	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	515	MET	CA-CB-CG	5.41	122.50	113.30
1	A	485	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLN	Peptide
1	A	363	GLU	Peptide
1	A	528	TYR	Peptide
1	A	532	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	5197	0	5118	51	0
2	A	28	0	19	1	0
3	A	1	0	0	0	0
4	A	41	0	0	0	0
All	All	5267	0	5137	51	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 (51) 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:234:ILE:HG21	1:A:250:GLN:HA	1.52	0.89
1:A:466:THR:HG21	1:A:475:LEU:HB2	1.75	0.69
1:A:716:ILE:HD12	1:A:741:ILE:HD11	1.81	0.63
1:A:361:SER:HB2	1:A:363:GLU:HG2	1.83	0.60
1:A:194:ALA:HB3	1:A:198:ILE:HD13	1.84	0.59
1:A:362:SER:HA	1:A:398:VAL:HG21	1.85	0.59
1:A:97:TYR:HB3	1:A:179:ASP:O	2.05	0.56
1:A:94:TYR:HB2	1:A:158:ILE:HG23	1.87	0.56
1:A:329:TYR:CE1	1:A:429:LEU:HD23	2.42	0.54
1:A:566:THR:OG1	1:A:592:PRO:O	2.24	0.54
1:A:333:TYR:OH	1:A:586:TYR:OH	2.21	0.54
1:A:306:GLN:O	1:A:307:ARG:NH1	2.39	0.53
1:A:368:ASP:O	1:A:369:ALA:HB2	2.09	0.52
1:A:98:ALA:HA	1:A:178:ILE:HG22	1.92	0.51
1:A:98:ALA:HB3	1:A:149:VAL:HG22	1.93	0.50
1:A:705:GLU:O	1:A:709:THR:HG23	2.14	0.48
1:A:695:GLU:HB3	1:A:735:ASN:HA	1.96	0.46
1:A:158:ILE:HD11	1:A:162:ASN:HB3	1.96	0.46
1:A:646:PRO:HA	1:A:669:ILE:HD11	1.97	0.46
1:A:641:VAL:HG13	1:A:669:ILE:HB	1.97	0.46
1:A:641:VAL:HG22	1:A:669:ILE:HG21	1.97	0.46
1:A:545:ALA:HB3	1:A:575:MET:HB2	1.97	0.45
1:A:450:PHE:HD1	2:A:801:1S6:H6	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:CG2	1:A:468:ILE:HD13	2.47	0.45
1:A:632:GLN:OE1	1:A:633:GLN:N	2.35	0.45
1:A:76:ARG:NH2	1:A:224:ASN:OD1	2.49	0.45
1:A:675:GLU:N	1:A:675:GLU:OE2	2.50	0.45
1:A:336:GLY:HA3	1:A:551:ALA:HB2	1.98	0.44
1:A:605:ASN:N	1:A:606:PRO:HD2	2.33	0.44
1:A:504:SER:O	1:A:505:LYS:CB	2.64	0.44
1:A:158:ILE:HD11	1:A:162:ASN:CB	2.47	0.44
1:A:344:LEU:HD23	1:A:511:THR:HG23	2.00	0.44
1:A:373:ASP:OD1	1:A:398:VAL:HG22	2.18	0.44
1:A:503:VAL:HG13	1:A:507:ALA:HB3	1.99	0.43
1:A:490:THR:HB	1:A:632:GLN:HG2	2.00	0.43
1:A:680:LEU:HD22	1:A:686:VAL:HG21	2.00	0.43
1:A:590:GLN:HG2	1:A:591:GLN:NE2	2.34	0.43
1:A:169:GLU:HA	1:A:172:ALA:HB3	2.01	0.42
1:A:208:ASP:OD1	1:A:208:ASP:N	2.52	0.42
1:A:595:TYR:CG	1:A:596:SER:N	2.86	0.42
1:A:519:GLY:O	1:A:527:MET:HB3	2.19	0.42
1:A:234:ILE:O	1:A:234:ILE:HG22	2.18	0.42
1:A:538:THR:OG1	1:A:539:VAL:N	2.52	0.42
1:A:545:ALA:O	1:A:574:SER:HA	2.20	0.42
1:A:632:GLN:CD	1:A:632:GLN:N	2.74	0.41
1:A:290:THR:HG22	1:A:291:ALA:N	2.36	0.41
1:A:234:ILE:HD11	1:A:253:GLN:HB3	2.01	0.41
1:A:568:TYR:HB2	1:A:570[B]:PHE:CE1	2.55	0.41
1:A:74:ALA:HB1	1:A:257:ASP:HA	2.02	0.41
1:A:94:TYR:O	1:A:158:ILE:HG22	2.21	0.41
1:A:716:ILE:CD1	1:A:741:ILE:HD11	2.49	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	673/702 (96%)	606 (90%)	52 (8%)	15 (2%)	6	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	LEU
1	A	369	ALA
1	A	505	LYS
1	A	739	LYS
1	A	106	SER
1	A	175	VAL
1	A	362	SER
1	A	397	ASN
1	A	615	LYS
1	A	632	GLN
1	A	174	GLU
1	A	363	GLU
1	A	246	PRO
1	A	356	GLY
1	A	523	VAL

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	570/590 (97%)	525 (92%)	45 (8%)	12	31

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	101	ASP
1	A	106	SER
1	A	110	LYS
1	A	128	LYS
1	A	135	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	169	GLU
1	A	175	VAL
1	A	187	SER
1	A	208	ASP
1	A	235	THR
1	A	236	TYR
1	A	244	ILE
1	A	283	LYS
1	A	331	SER
1	A	338	THR
1	A	341	VAL
1	A	342	MET
1	A	364	LEU
1	A	409	ASP
1	A	455	SER
1	A	456	VAL
1	A	462	ILE
1	A	489	GLN
1	A	490	THR
1	A	504	SER
1	A	515	MET
1	A	520	THR
1	A	546[A]	LEU
1	A	546[B]	LEU
1	A	556	GLU
1	A	567	ASP
1	A	591	GLN
1	A	596	SER
1	A	614	MET
1	A	622	THR
1	A	632	GLN
1	A	653	LEU
1	A	658	VAL
1	A	667	THR
1	A	698	ASP
1	A	699	MET
1	A	733	ARG
1	A	739	LYS
1	A	745	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	591	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	2.17	4 (20%)	23,44,44	0.98	2 (8%)

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	-	4/8/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1S6	CAY-CAX	7.85	1.50	1.41
2	A	801	1S6	CBC-SAR	-2.90	1.79	1.85
2	A	801	1S6	CAX-NAN	2.36	1.37	1.33
2	A	801	1S6	CB-SAR	-2.16	1.79	1.84

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1S6	OAF-CAU-CAY	-2.57	117.07	120.95
2	A	801	1S6	CA-N-CAU	2.32	125.88	122.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

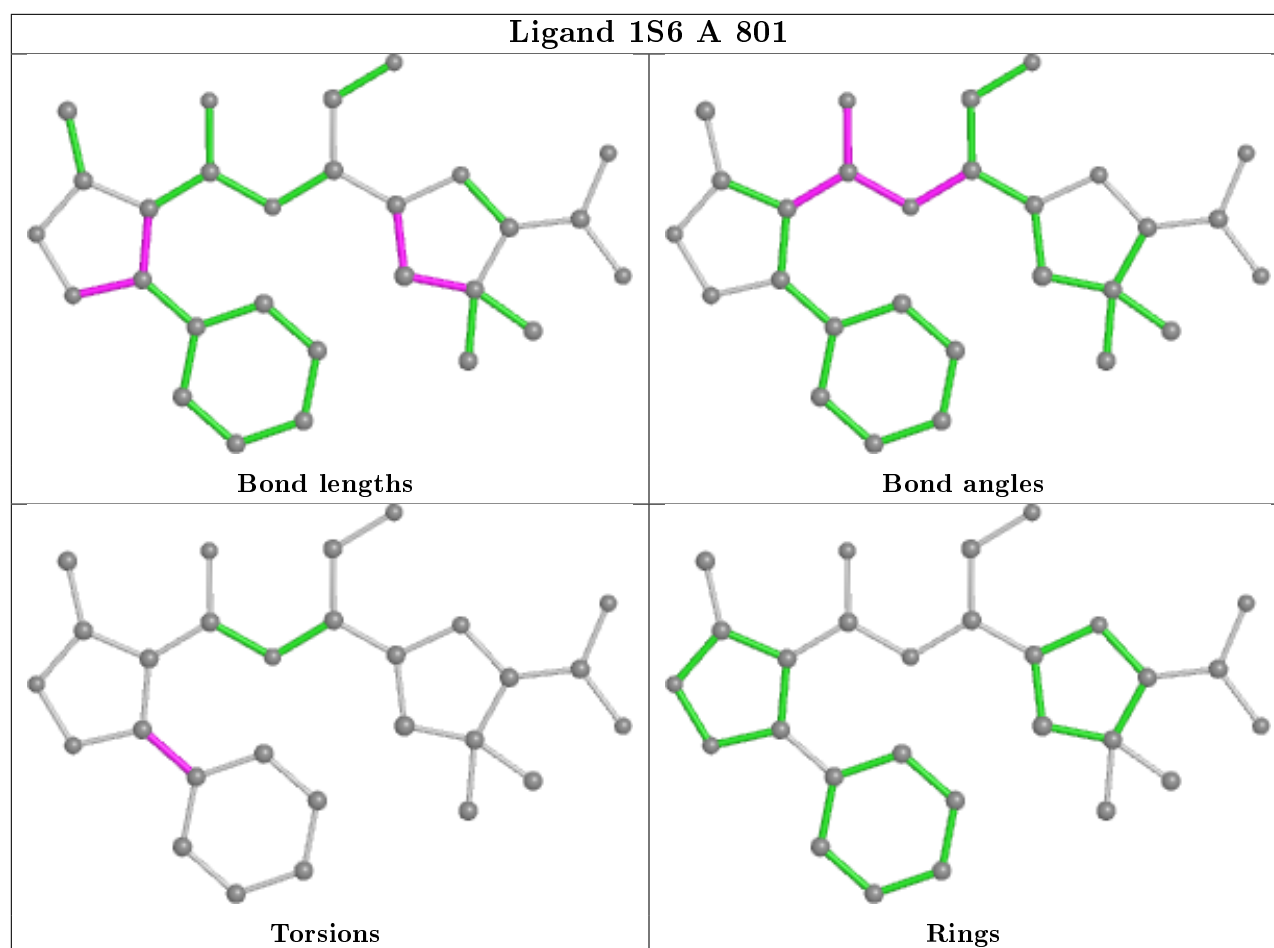
Mol	Chain	Res	Type	Atoms
2	A	801	1S6	CAL-CAW-CAX-NAN
2	A	801	1S6	CAM-CAW-CAX-NAN
2	A	801	1S6	CAL-CAW-CAX-CAY
2	A	801	1S6	CAM-CAW-CAX-CAY

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	1S6	1	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 ⓘ

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, 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	675/702 (96%)	0.01	27 (4%) 38 32	35, 65, 128, 171	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	5.6
1	A	250	GLN	4.8
1	A	137	VAL	3.9
1	A	241	LEU	3.6
1	A	242	GLY	3.5
1	A	169	GLU	3.3
1	A	318	ILE	3.2
1	A	321	ASP	3.1
1	A	750	ASP	3.1
1	A	102	GLU	3.0
1	A	108	THR	2.8
1	A	210	SER	2.8
1	A	136	TYR	2.8
1	A	557	LYS	2.8
1	A	319	THR	2.8
1	A	141	LEU	2.7
1	A	320	GLU	2.6
1	A	722	GLY	2.6
1	A	744	ILE	2.6
1	A	103	ASN	2.4
1	A	151	PHE	2.4
1	A	96	VAL	2.3
1	A	723	SER	2.2
1	A	146	LEU	2.2
1	A	104	TYR	2.2
1	A	531	SER	2.1
1	A	211	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

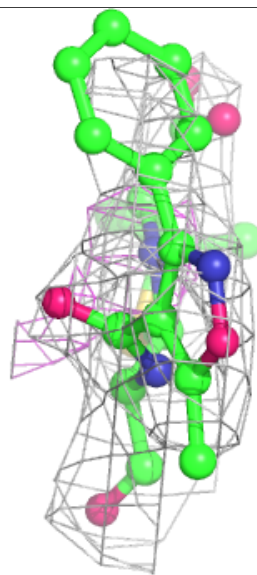
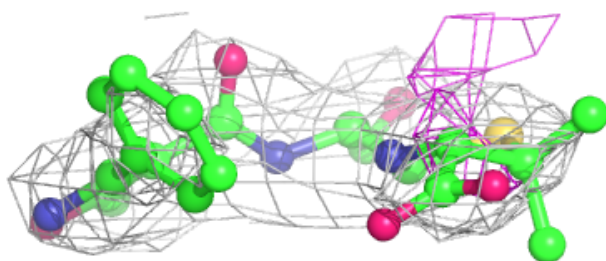
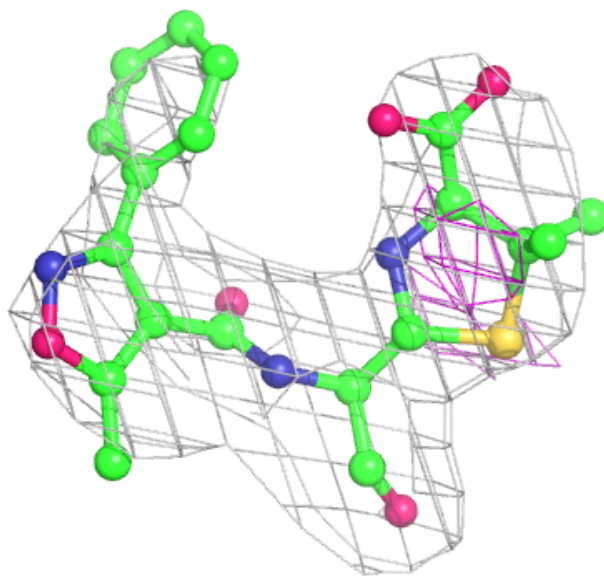
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1S6	A	801	28/28	0.91	0.33	62,113,126,133	0
3	NA	A	802	1/1	0.98	0.49	57,57,57,57	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 1S6 A 801:

$2mF_o-DF_c$ (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.