



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:01 PM EDT

PDB ID : 5OJ1 / pdb_00005oj1
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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

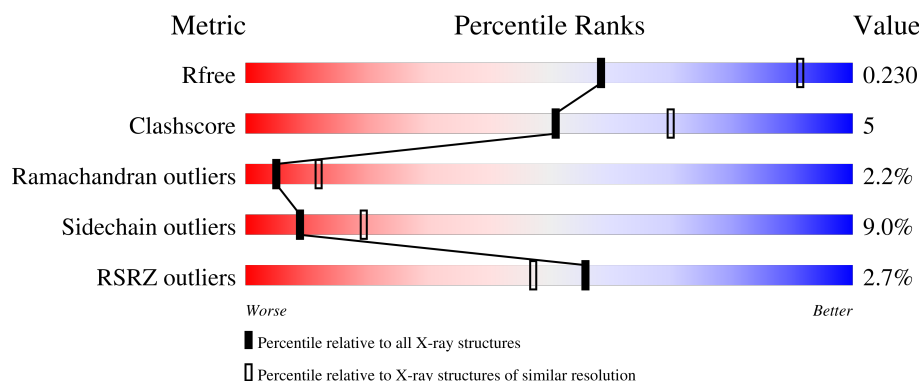
1 Overall quality at a glance

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 ≥ 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	

2 Entry composition [i](#)

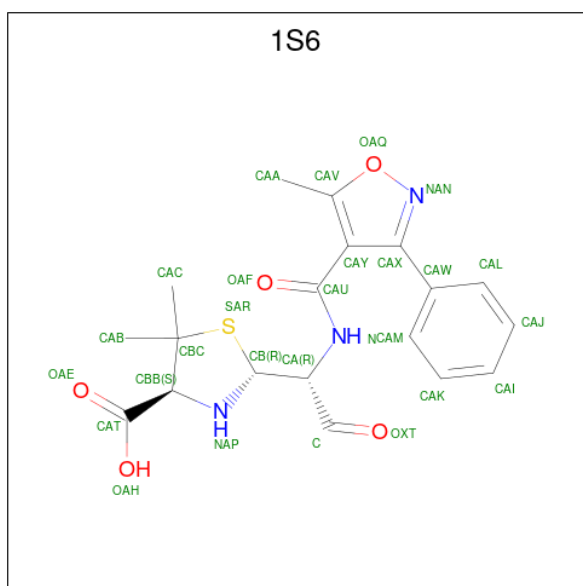
There are 4 unique types of molecules in this entry. The entry contains 5267 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	675	5197	3265	862	1047	23	0	2	0

- Molecule 2 is (2R,4S)-5,5-dimethyl-2-[(1R)-1-[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbonyl]amino]-2-oxoethyl]-1,3-thiazolidine-4-carboxylic acid (CCD ID: 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 SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is water.

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

i

- 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 87.33 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.33-2.85) 99.9 (87.33-2.85)	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)	0.33 , 48.9	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	0.98	4/5289 (0.1%)	1.08	3/7167 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	THR	CA-C	6.50	1.60	1.53
1	A	158	ILE	CA-CB	5.18	1.60	1.54
1	A	573	VAL	C-O	-5.16	1.18	1.24
1	A	183	SER	CA-C	5.12	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	N-CA-C	7.03	123.95	109.34
1	A	604	ALA	N-CA-C	5.32	118.24	111.69
1	A	526	THR	N-CA-C	5.30	117.82	109.39

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	54	0
2	A	28	0	19	0	0
3	A	1	0	0	0	0
4	A	41	0	0	0	0
All	All	5267	0	5137	54	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 (54) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:632:GLN:CD	1:A:632:GLN:N	2.74	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:488:ASP:CG	1:A:490:THR:HG23	2.43	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:360:ASN:O	1:A:361:SER:C	2.59	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:277:MET:HE1	1:A:289:MET:HG2	2.01	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:700:TYR:CD1	1:A:700:TYR:C	2.99	0.41
1:A:290:THR:HG22	1:A:291:ALA:N	2.36	0.41
1:A:361:SER:C	1:A:363:GLU:N	2.76	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

5.3.1 Protein backbone

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%)	5 12

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%)	518 (91%)	52 (9%)	9 19

All (52) 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	135	SER
1	A	163	MET
1	A	168	LYS
1	A	169	GLU
1	A	175	VAL
1	A	181	THR
1	A	198	ILE
1	A	208	ASP
1	A	226	ILE
1	A	235	THR
1	A	244	ILE
1	A	338	THR
1	A	341	VAL
1	A	342	MET
1	A	364	LEU
1	A	365	LYS
1	A	381	THR
1	A	387	THR
1	A	455	SER
1	A	456	VAL
1	A	462	ILE
1	A	489	GLN
1	A	490	THR
1	A	503	VAL
1	A	504	SER
1	A	515	MET
1	A	520	THR
1	A	523	VAL
1	A	537	VAL
1	A	546[A]	LEU
1	A	546[B]	LEU
1	A	556	GLU
1	A	591	GLN
1	A	596	SER
1	A	614	MET
1	A	622	THR
1	A	625	LYS
1	A	630	VAL

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Mol	Chain	Res	Type
1	A	632	GLN
1	A	634	SER
1	A	641	VAL
1	A	653	LEU
1	A	658	VAL
1	A	667	THR
1	A	698	ASP
1	A	699	MET
1	A	739	LYS
1	A	745	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	143	GLN
1	A	276	GLN
1	A	351	ASN
1	A	390	GLN
1	A	397	ASN
1	A	436	GLN
1	A	452	GLN
1	A	470	ASN
1	A	495	GLN
1	A	591	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	25,30,30	1.99	7 (28%)	34,44,44	2.42	9 (26%)

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	-	6/16/37/37	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1S6	CAY-CAV	5.71	1.47	1.36
2	A	801	1S6	CAX-NAN	3.40	1.37	1.31
2	A	801	1S6	CAY-CAX	3.36	1.50	1.43
2	A	801	1S6	OAQ-NAN	-3.24	1.36	1.42
2	A	801	1S6	CBC-SAR	-3.01	1.79	1.85
2	A	801	1S6	CB-SAR	-2.29	1.79	1.84
2	A	801	1S6	CAW-CAX	2.05	1.51	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1S6	OAQ-CAV-CAY	-6.78	104.09	109.38
2	A	801	1S6	CAY-CAX-NAN	-5.85	105.26	111.43
2	A	801	1S6	CAW-CAX-NAN	5.38	127.43	118.75
2	A	801	1S6	CAV-OAQ-NAN	4.86	113.91	108.51
2	A	801	1S6	OAQ-NAN-CAX	3.78	109.94	105.91
2	A	801	1S6	CAX-CAY-CAV	3.32	106.79	104.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1S6	OAF-CAU-CAY	-2.98	117.07	121.53
2	A	801	1S6	OAQ-CAV-CAA	2.61	120.62	116.59
2	A	801	1S6	C-CA-N	-2.09	106.50	109.80

There are no chirality outliers.

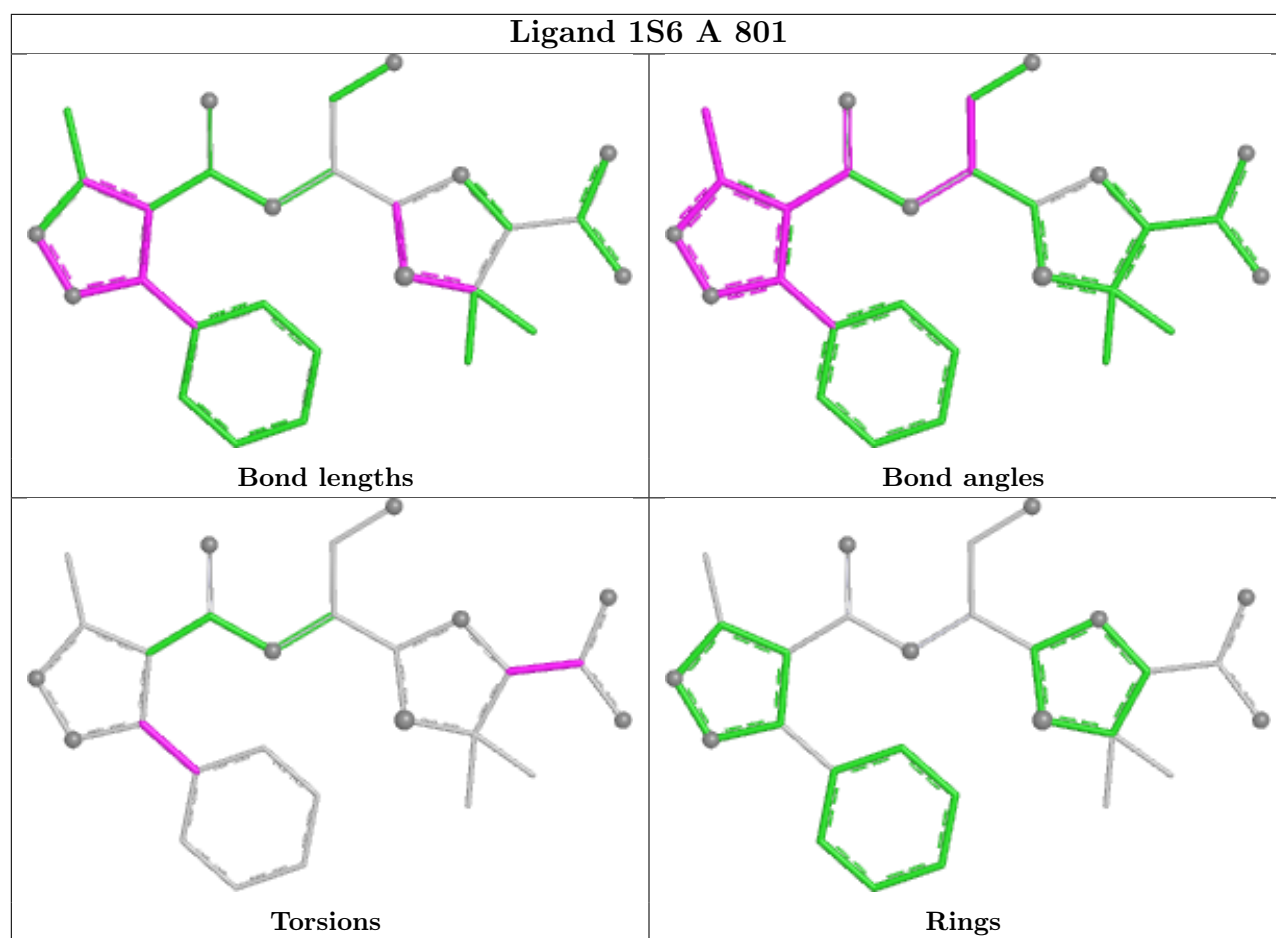
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	1S6	OAE-CAT-CBB-CBC
2	A	801	1S6	OAQ-CAT-CBB-CBC
2	A	801	1S6	CAL-CAW-CAX-CAY
2	A	801	1S6	CAM-CAW-CAX-CAY
2	A	801	1S6	CAM-CAW-CAX-NAN
2	A	801	1S6	CAL-CAW-CAX-NAN

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, 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%)	-0.21	18 (2%) 56 47	20, 65, 128, 171	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	5.1
1	A	233	ILE	4.0
1	A	250	GLN	3.6
1	A	241	LEU	3.4
1	A	245	VAL	3.2
1	A	108	THR	3.1
1	A	251	VAL	3.0
1	A	244	ILE	2.7
1	A	234	ILE	2.6
1	A	72	VAL	2.6
1	A	107	ALA	2.3
1	A	106	SER	2.3
1	A	236	TYR	2.3
1	A	628	GLU	2.2
1	A	105	LYS	2.1
1	A	740	ASP	2.1
1	A	146	LEU	2.0
1	A	625	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

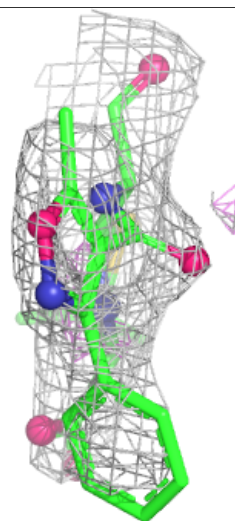
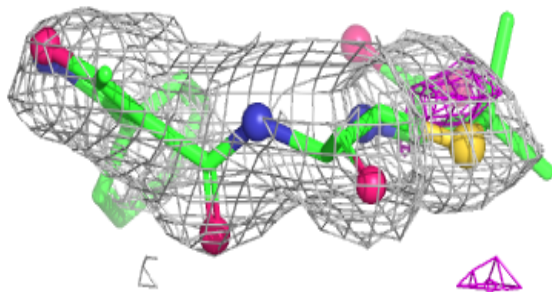
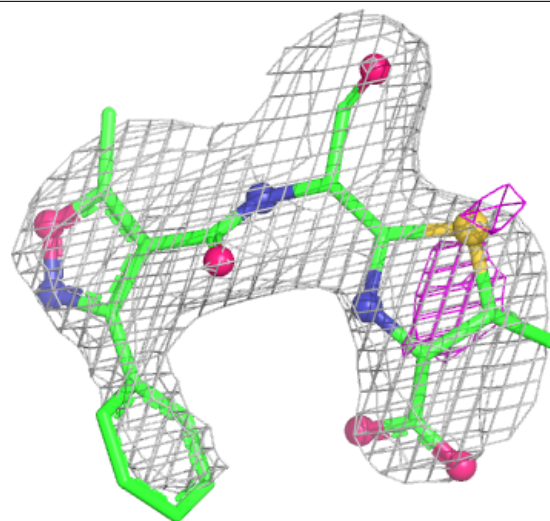
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1S6	A	801	28/28	0.90	0.15	62,113,126,133	0
3	NA	A	802	1/1	0.94	0.24	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.