



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:40 PM UTC

PDB ID : 9SSI / pdb_00009ssi
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) in complex with Cefditoren
- Streptococcus pneumoniae R6
Authors : Flanders, P.L.; Gillingham, J.R.; Contreras-Martel, C.; Dessen, A.; Carlson,
E.E.; Ambrose, E.A.
Deposited on : 2025-09-25
Resolution : 1.64 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

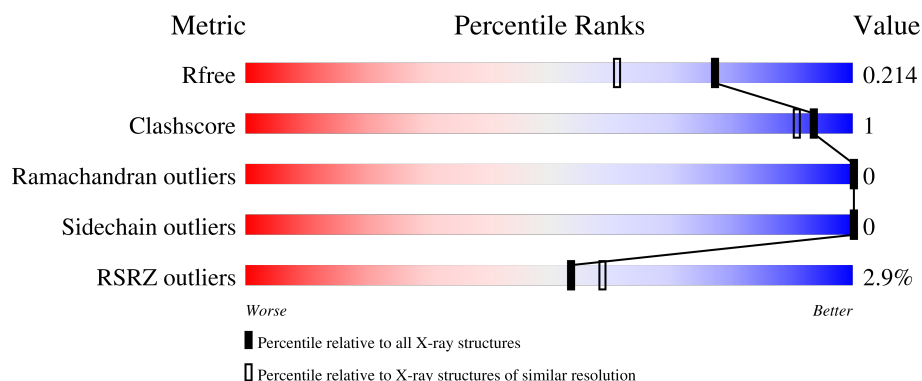
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	494	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4162 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 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	4	0
			3532	2213	600	704	15			

There are 29 discrepancies between the modelled and reference sequences:

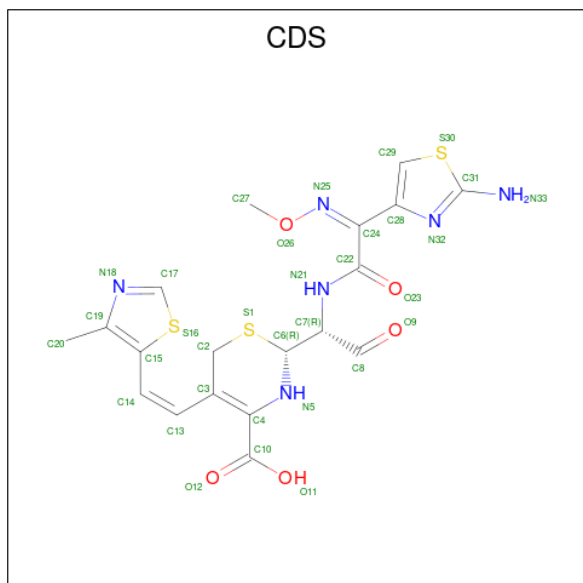
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ASP	-	expression tag	UNP O70038
A	299	ILE	-	expression tag	UNP O70038
A	300	SER	-	expression tag	UNP O70038
A	301	SER	-	expression tag	UNP O70038
A	302	ILE	-	expression tag	UNP O70038
A	303	SER	-	expression tag	UNP O70038
A	304	GLU	-	expression tag	UNP O70038
A	305	ILE	-	expression tag	UNP O70038
A	306	THR	-	expression tag	UNP O70038
A	307	TYR	-	expression tag	UNP O70038
A	308	SER	-	expression tag	UNP O70038
A	309	ASP	-	expression tag	UNP O70038
A	310	GLY	-	expression tag	UNP O70038
A	311	THR	-	expression tag	UNP O70038
A	312	VAL	-	expression tag	UNP O70038
A	313	ILE	-	expression tag	UNP O70038
A	314	ALA	-	expression tag	UNP O70038
A	315	SER	-	expression tag	UNP O70038
A	316	ILE	-	expression tag	UNP O70038
A	317	GLU	-	expression tag	UNP O70038
A	318	SER	-	expression tag	UNP O70038
A	319	ASP	-	expression tag	UNP O70038
A	320	MET	-	expression tag	UNP O70038
A	321	LEU	-	expression tag	UNP O70038
A	322	ARG	-	expression tag	UNP O70038
A	336	GLN	ARG	engineered mutation	UNP O70038
A	656	GLY	ASN	engineered mutation	UNP O70038

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Chain	Residue	Modelled	Actual	Comment	Reference
A	686	GLN	ARG	engineered mutation	UNP O70038
A	687	GLN	ARG	engineered mutation	UNP O70038

- Molecule 2 is (2R)-2-[(1R)-1-{[(2Z)-2-(2-AMINO-1,3-THIAZOL-4-YL)-2-(METHOXYIMINO)ACETYL]AMINO}-2-OXOETHYL]-5-[(Z)-2-(4-METHYL-1,3-THIAZOL-5-YL)VINY]-3,6-DIHYDRO-2H-1,3-THIAZINE-4-CARBOXYLIC ACID (CCD ID: CDS) (formula: C₁₉H₂₀N₆O₅S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	19	6	5	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	Cl	0	0
			27	27		

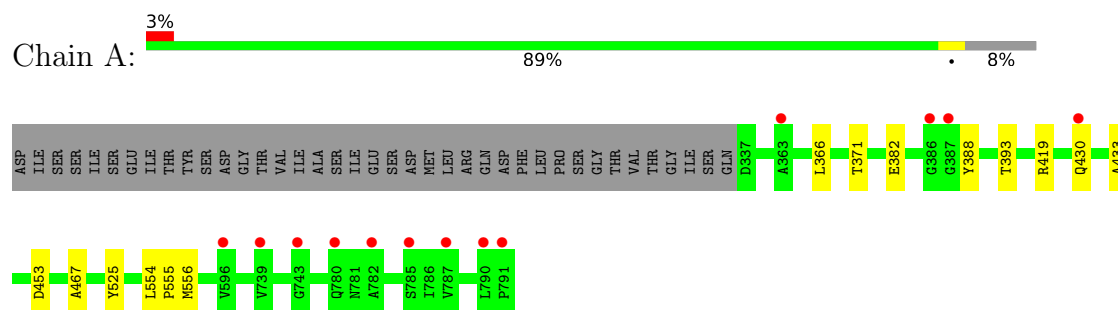
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	570	Total	O	0	0
			570	570		

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: Penicillin-binding protein 1B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.94Å 149.05Å 98.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 1.64 48.47 – 1.64	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.47-1.64) 97.8 (48.47-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.174 , 0.203 0.187 , 0.214	Depositor DCC
R_{free} test set	2145 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4162	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: CL, CDS

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	0.59	0/3618	0.84	2/4909 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	371	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	453	ASP	CB-CA-C	5.27	118.36	110.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	ARG	Sidechain

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	3532	0	3418	8	0
2	A	33	0	18	3	0
3	A	27	0	0	0	0
4	A	570	0	0	1	0
All	All	4162	0	3436	10	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 1.

All (10) 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:556:MET:O	2:A:801:CDS:H29	2.00	0.60
2:A:801:CDS:O11	2:A:801:CDS:H13	2.07	0.54
1:A:430:GLN:HG3	4:A:1142:HOH:O	2.09	0.52
1:A:393:THR:HB	1:A:433:ALA:HB1	1.92	0.50
1:A:554:LEU:N	1:A:555:PRO:HD2	2.29	0.48
1:A:382:GLU:HG3	1:A:388:TYR:CE2	2.50	0.47
1:A:525:TYR:HB2	1:A:555:PRO:HG3	1.98	0.45
2:A:801:CDS:O11	2:A:801:CDS:C13	2.67	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.94	0.42
1:A:467:ALA:HB2	1:A:555:PRO:HB3	2.03	0.41

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	457/494 (92%)	447 (98%)	10 (2%)	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	377/408 (92%)	377 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	396	GLN
1	A	444	GLN
1	A	448	ASN
1	A	635	ASN
1	A	781	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 27 are 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	CDS	A	801	1	32,35,35	1.95	10 (31%)	35,48,48	3.74	8 (22%)

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	CDS	A	801	1	-	10/24/43/43	0/2/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CDS	C31-S30	-4.46	1.68	1.74
2	A	801	CDS	C29-S30	-3.78	1.62	1.71
2	A	801	CDS	C31-N32	3.62	1.36	1.31
2	A	801	CDS	C15-C19	3.53	1.42	1.37
2	A	801	CDS	O11-C10	-3.34	1.21	1.30
2	A	801	CDS	C4-C10	3.31	1.53	1.48
2	A	801	CDS	C17-N18	2.71	1.37	1.30
2	A	801	CDS	C4-C3	2.37	1.42	1.37
2	A	801	CDS	C19-N18	2.29	1.41	1.38
2	A	801	CDS	C14-C15	-2.07	1.39	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CDS	C29-S30-C31	17.54	96.40	88.84
2	A	801	CDS	C13-C3-C4	-7.88	115.72	122.02
2	A	801	CDS	S30-C31-N32	-6.44	109.47	114.54
2	A	801	CDS	S16-C17-N18	-4.74	112.01	116.08
2	A	801	CDS	S30-C31-N33	3.44	124.99	120.99
2	A	801	CDS	C15-C19-N18	-3.02	112.22	114.97
2	A	801	CDS	O12-C10-C4	-2.34	116.13	120.20
2	A	801	CDS	C14-C15-S16	-2.26	119.60	122.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

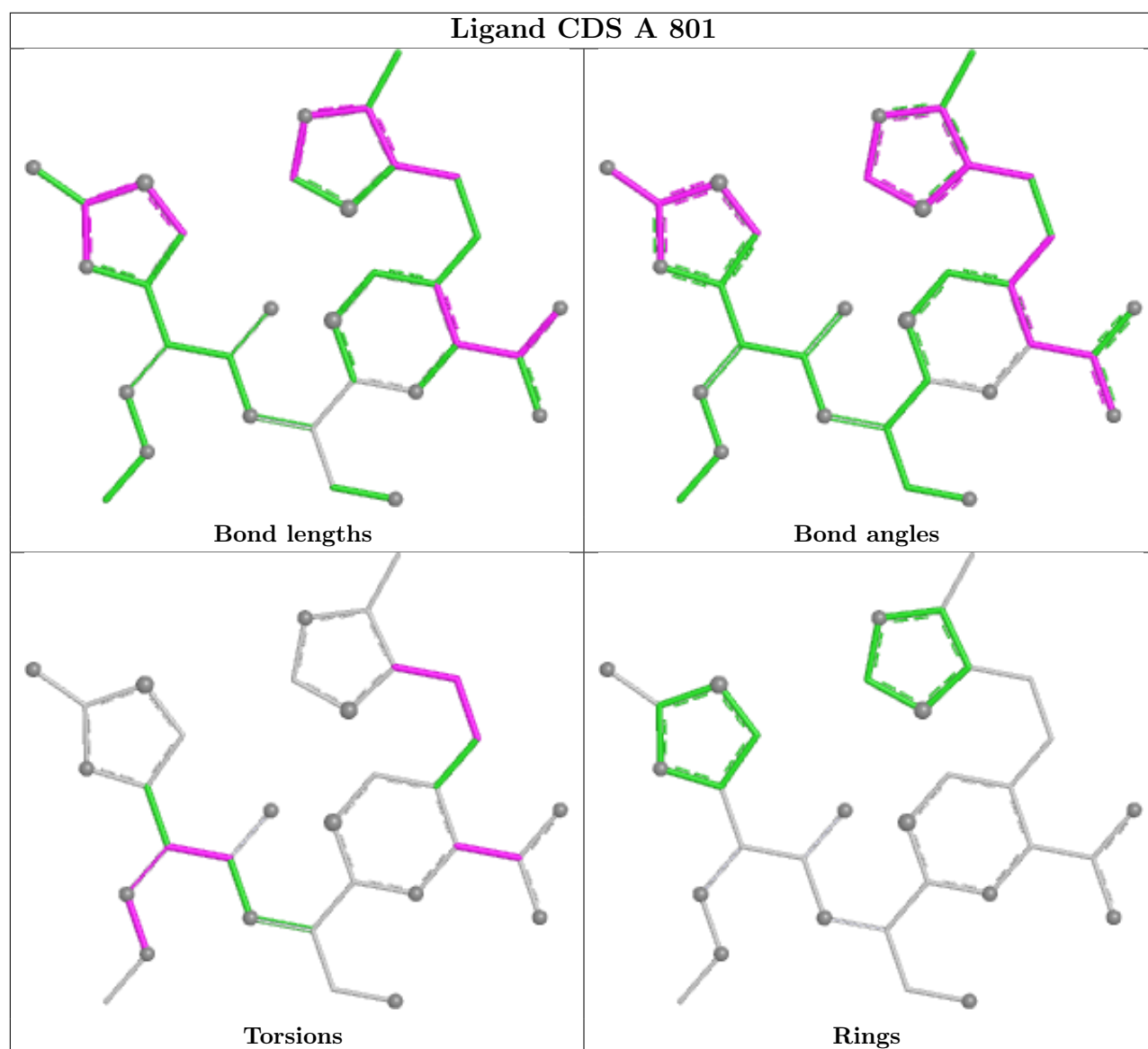
Mol	Chain	Res	Type	Atoms
2	A	801	CDS	C28-C24-N25-O26
2	A	801	CDS	C24-N25-O26-C27
2	A	801	CDS	O11-C10-C4-N5
2	A	801	CDS	C3-C13-C14-C15
2	A	801	CDS	C22-C24-N25-O26
2	A	801	CDS	O23-C22-C24-C28
2	A	801	CDS	O23-C22-C24-N25
2	A	801	CDS	C13-C14-C15-S16
2	A	801	CDS	C13-C14-C15-C19
2	A	801	CDS	O12-C10-C4-N5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CDS	3	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	455/494 (92%)	0.03	13 (2%) 53 59	17, 31, 65, 121	4 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	PRO	3.7
1	A	386	GLY	3.5
1	A	743	GLY	2.8
1	A	387	GLY	2.6
1	A	780	GLN	2.6
1	A	739	VAL	2.4
1	A	785	SER	2.4
1	A	787	VAL	2.3
1	A	596	VAL	2.2
1	A	430	GLN	2.1
1	A	790	LEU	2.1
1	A	363	ALA	2.1
1	A	782	ALA	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](#)

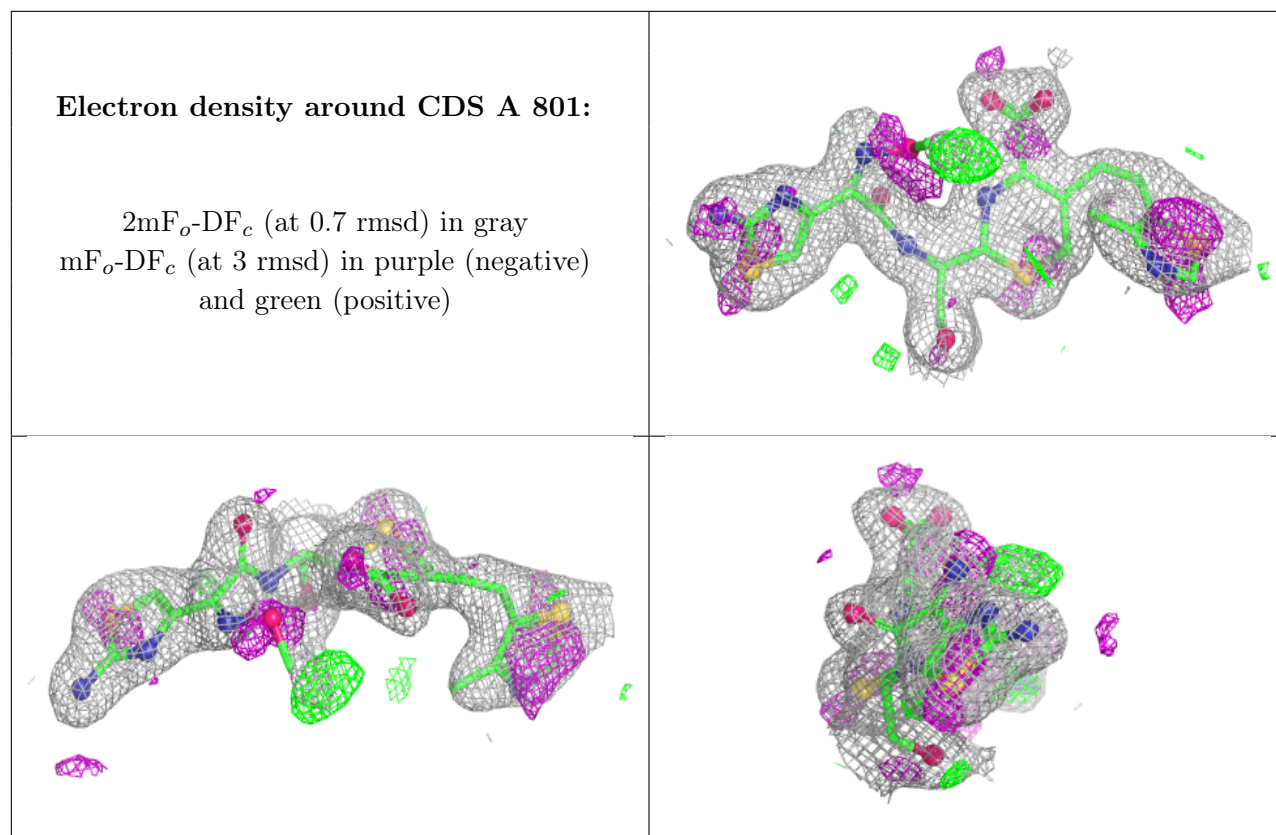
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	CL	A	824	1/1	0.89	0.17	52,52,52,52	0
3	CL	A	818	1/1	0.91	0.14	65,65,65,65	0
3	CL	A	807	1/1	0.91	0.13	55,55,55,55	0
3	CL	A	825	1/1	0.91	0.18	57,57,57,57	0
3	CL	A	809	1/1	0.92	0.18	57,57,57,57	0
3	CL	A	822	1/1	0.93	0.12	38,38,38,38	0
3	CL	A	819	1/1	0.94	0.15	53,53,53,53	0
3	CL	A	810	1/1	0.94	0.13	43,43,43,43	0
3	CL	A	817	1/1	0.94	0.15	43,43,43,43	0
3	CL	A	806	1/1	0.94	0.22	58,58,58,58	0
3	CL	A	805	1/1	0.95	0.08	42,42,42,42	0
3	CL	A	815	1/1	0.95	0.16	41,41,41,41	0
3	CL	A	823	1/1	0.95	0.19	63,63,63,63	0
3	CL	A	808	1/1	0.95	0.18	49,49,49,49	0
2	CDS	A	801	33/33	0.95	0.11	24,39,66,80	0
3	CL	A	828	1/1	0.95	0.12	55,55,55,55	0
3	CL	A	821	1/1	0.96	0.15	44,44,44,44	0
3	CL	A	827	1/1	0.96	0.15	47,47,47,47	0
3	CL	A	803	1/1	0.96	0.20	49,49,49,49	0
3	CL	A	826	1/1	0.97	0.13	57,57,57,57	0
3	CL	A	812	1/1	0.97	0.15	36,36,36,36	0
3	CL	A	804	1/1	0.97	0.09	43,43,43,43	0
3	CL	A	820	1/1	0.98	0.13	41,41,41,41	0
3	CL	A	813	1/1	0.98	0.08	37,37,37,37	0
3	CL	A	814	1/1	0.98	0.16	40,40,40,40	0
3	CL	A	802	1/1	0.99	0.07	32,32,32,32	0
3	CL	A	811	1/1	0.99	0.06	34,34,34,34	0
3	CL	A	816	1/1	0.99	0.04	27,27,27,27	1

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.