



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:15 PM UTC

PDB ID : 9WIR / pdb_00009wir
Title : Crystal structure of ADC-227 in the avibactam complex (50 mM for 24 hour)
Authors : Kawai, A.; Doi, Y.
Deposited on : 2025-08-29
Resolution : 2.10 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

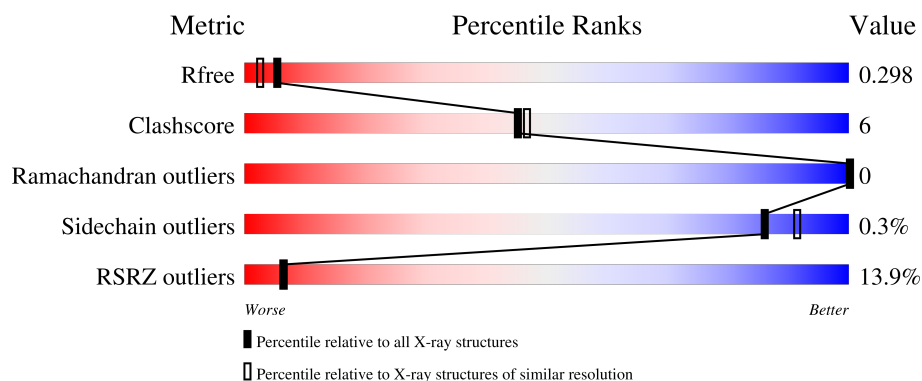
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	363	<div> <div>5%</div> <div>85%</div> <div>13%</div> </div>
1	B	363	<div> <div>23%</div> <div>85%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NXL	B	401	-	-	X	-

2 Entry composition [i](#)

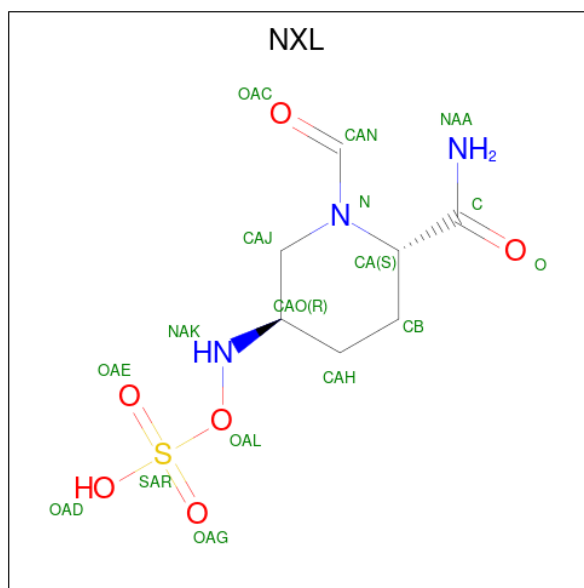
There are 3 unique types of molecules in this entry. The entry contains 5625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2803	1804	464	527	8			
1	B	359	Total	C	N	O	S	0	0	0
			2737	1756	452	521	8			

- Molecule 2 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (CCD ID: NXL) (formula: C₇H₁₃N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	7	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			17	7	3	6	1		

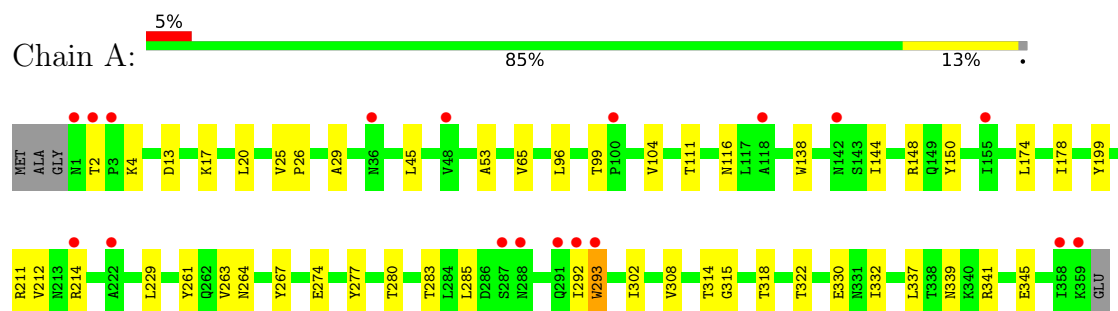
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	4	Total 4	O 4	0	0

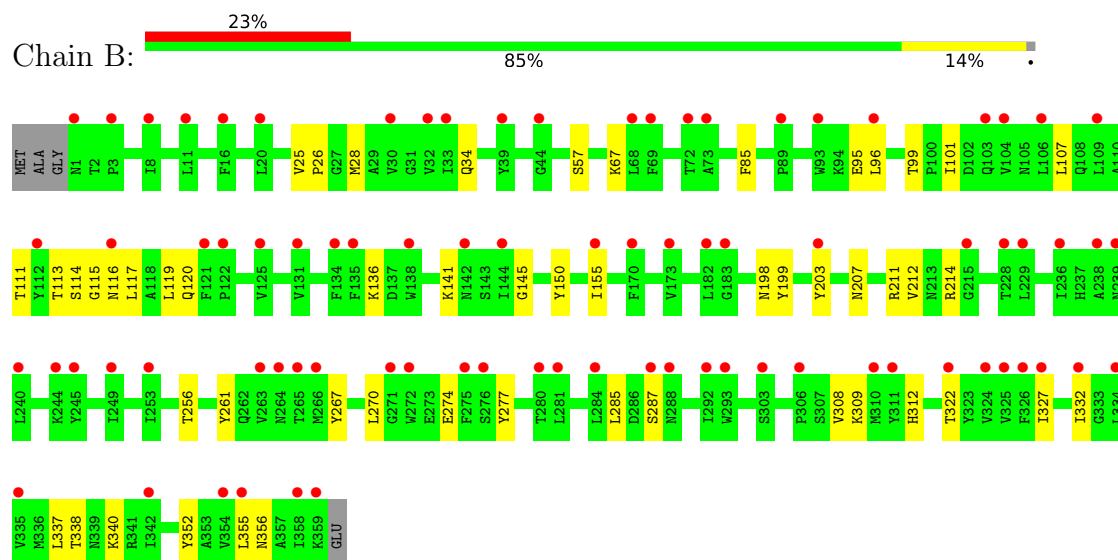
3 Residue-property plots [i](#)

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: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.68Å 75.68Å 206.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.58 – 2.10 40.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.58-2.10) 99.8 (40.58-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.296 0.258 , 0.298	Depositor DCC
R_{free} test set	2046 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5625	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3096e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.09	0/2871	0.26	0/3905
1	B	0.08	0/2805	0.24	0/3830
All	All	0.09	0/5676	0.25	0/7735

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

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	2803	0	2749	30	0
1	B	2737	0	2588	35	0
2	A	17	0	12	2	0
2	B	17	0	12	8	0
3	A	47	0	0	0	0
3	B	4	0	0	0	0
All	All	5625	0	5361	65	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 6.

All (65) 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:293:TRP:CD1	1:A:293:TRP:H	2.00	0.77
1:B:96:LEU:HD22	1:B:101:ILE:HD11	1.72	0.72
1:B:267:TYR:HB2	1:B:274:GLU:HB2	1.78	0.64
1:B:111:THR:HB	1:B:261:TYR:HE2	1.61	0.64
1:B:352:TYR:O	1:B:356:ASN:ND2	2.29	0.63
1:A:293:TRP:H	1:A:293:TRP:HD1	1.49	0.60
1:B:150:TYR:HE1	2:B:401:NXL:H3	1.64	0.60
1:B:277:TYR:HB3	1:B:308:VAL:HG12	1.84	0.60
1:B:120:GLN:NE2	2:B:401:NXL:NAA	2.50	0.59
1:B:150:TYR:CE1	2:B:401:NXL:H3	2.39	0.57
1:A:277:TYR:HB3	1:A:308:VAL:HG12	1.87	0.57
1:A:267:TYR:HB2	1:A:274:GLU:HB2	1.87	0.57
1:B:256:THR:HA	1:B:270:LEU:HB2	1.87	0.56
1:B:119:LEU:HD11	2:B:401:NXL:H11	1.86	0.56
1:A:45:LEU:HA	1:A:53:ALA:HA	1.89	0.55
1:B:150:TYR:CE1	2:B:401:NXL:NAK	2.75	0.55
1:A:26:PRO:HB2	1:A:339:ASN:HD21	1.71	0.55
1:A:111:THR:HB	1:A:261:TYR:HE2	1.72	0.54
1:A:199:TYR:O	1:A:211:ARG:NH2	2.41	0.53
1:B:327:ILE:HD12	1:B:332:ILE:HD11	1.89	0.53
1:B:120:GLN:NE2	2:B:401:NXL:H6	2.08	0.51
1:B:285:LEU:O	1:B:287:SER:N	2.40	0.51
1:A:280:THR:HG23	1:A:283:THR:H	1.76	0.50
1:A:148:ARG:HH12	1:A:292:ILE:HA	1.77	0.50
1:A:285:LEU:HD22	1:A:345:GLU:HG2	1.92	0.50
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.93	0.50
1:A:212:VAL:HG22	1:A:214:ARG:H	1.75	0.50
1:A:318:THR:HA	1:A:341:ARG:HH21	1.80	0.47
1:A:330:GLU:HB2	1:A:332:ILE:HG12	1.97	0.47
1:B:95:GLU:O	1:B:136:LYS:NZ	2.46	0.47
1:B:322:THR:HG23	1:B:337:LEU:HD23	1.97	0.46
1:A:111:THR:HB	1:A:261:TYR:CE2	2.51	0.45
1:A:148:ARG:HH12	1:A:292:ILE:HG12	1.82	0.45
1:B:28:MET:HG3	1:B:338:THR:HG22	1.98	0.45
1:B:203:TYR:HB3	1:B:207:ASN:HA	1.99	0.45
1:B:116:ASN:HB2	1:B:141:LYS:HG3	1.99	0.45
1:B:113:THR:HB	1:B:145:GLY:HA2	1.97	0.45
1:B:96:LEU:O	1:B:99:THR:OG1	2.28	0.44
1:B:26:PRO:HG2	1:B:203:TYR:CD1	2.53	0.44
1:A:96:LEU:O	1:A:99:THR:OG1	2.27	0.44
1:A:104:VAL:HG22	1:A:144:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:HG3	1:B:332:ILE:HG22	2.00	0.44
1:A:20:LEU:HD23	1:A:25:VAL:HB	1.99	0.43
1:B:277:TYR:H	1:B:309:LYS:HA	1.84	0.43
1:B:332:ILE:HD12	1:B:355:LEU:HB3	1.99	0.43
1:A:2:THR:HG22	1:A:4:LYS:H	1.84	0.43
1:A:116:ASN:O	1:A:138:TRP:NE1	2.43	0.43
1:B:120:GLN:NE2	2:B:401:NXL:C	2.82	0.42
1:B:114:SER:OG	1:B:115:GLY:N	2.51	0.42
1:A:322:THR:HG23	1:A:337:LEU:HD23	2.01	0.42
1:B:25:VAL:HG13	1:B:340:LYS:HB3	2.01	0.42
1:A:29:ALA:HB1	1:A:229:LEU:HD22	2.00	0.42
1:A:314:THR:OG1	2:A:401:NXL:OAG	2.30	0.41
1:B:67:LYS:HE3	1:B:155:ILE:HG21	2.03	0.41
1:A:65:VAL:HG23	1:A:315:GLY:HA3	2.03	0.41
1:B:57:SER:O	1:B:198:ASN:HB3	2.20	0.41
1:A:13:ASP:O	1:A:17:LYS:HB3	2.20	0.41
1:A:261:TYR:HA	1:A:302:ILE:HG13	2.03	0.41
1:B:150:TYR:CE1	2:B:401:NXL:CAJ	3.04	0.41
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.95	0.41
1:A:150:TYR:HE2	2:A:401:NXL:H3	1.86	0.40
1:A:263:VAL:HG12	1:A:264:ASN:ND2	2.36	0.40
1:B:199:TYR:CZ	1:B:211:ARG:HD3	2.57	0.40
1:A:174:LEU:HA	1:A:178:ILE:HB	2.02	0.40
1:B:212:VAL:HG22	1:B:214:ARG:H	1.87	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	357/363 (98%)	342 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	357/363 (98%)	339 (95%)	18 (5%)	0	100	100
All	All	714/726 (98%)	681 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	298/317 (94%)	297 (100%)	1 (0%)	86	91
1	B	280/317 (88%)	279 (100%)	1 (0%)	84	89
All	All	578/634 (91%)	576 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	TRP
1	B	312	HIS

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	297	ASN
1	B	120	GLN
1	B	149	GLN
1	B	241	ASN
1	B	288	ASN
1	B	291	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 oligosaccharides 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	NXL	A	401	1	14,17,17	2.68	4 (28%)	16,24,24	1.52	3 (18%)
2	NXL	B	401	1	14,17,17	2.71	4 (28%)	16,24,24	1.50	3 (18%)

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	NXL	A	401	1	-	2/5/25/25	0/1/1/1
2	NXL	B	401	1	-	2/5/25/25	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NXL	C-NAA	6.20	1.47	1.32
2	A	401	NXL	C-NAA	6.19	1.47	1.32
2	B	401	NXL	CAN-N	6.11	1.45	1.34
2	A	401	NXL	CAN-N	6.03	1.45	1.34
2	B	401	NXL	CAJ-N	2.71	1.51	1.47
2	A	401	NXL	O-C	-2.69	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NXL	O-C	-2.64	1.19	1.23
2	A	401	NXL	CAJ-N	2.49	1.50	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NXL	OAG-SAR-OAE	-2.90	101.04	112.24
2	A	401	NXL	OAG-SAR-OAE	-2.89	101.07	112.24
2	B	401	NXL	CAH-CAO-CAJ	2.38	112.80	109.71
2	A	401	NXL	CAH-CAO-CAJ	2.32	112.72	109.71
2	A	401	NXL	OAC-CAN-N	-2.15	120.09	125.34
2	B	401	NXL	OAC-CAN-N	-2.09	120.23	125.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NXL	NAA-C-CA-CB
2	A	401	NXL	O-C-CA-CB
2	B	401	NXL	O-C-CA-CB
2	B	401	NXL	NAA-C-CA-CB

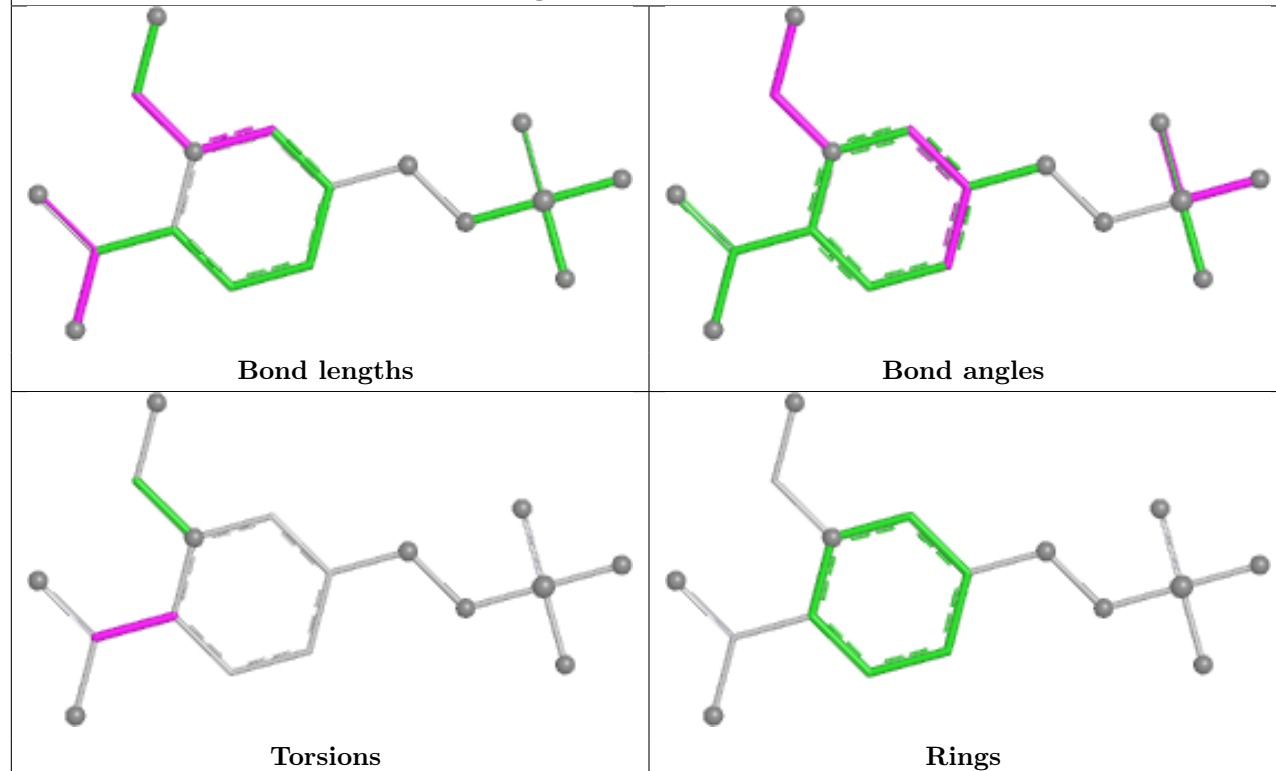
There are no ring outliers.

2 monomers are involved in 10 short contacts:

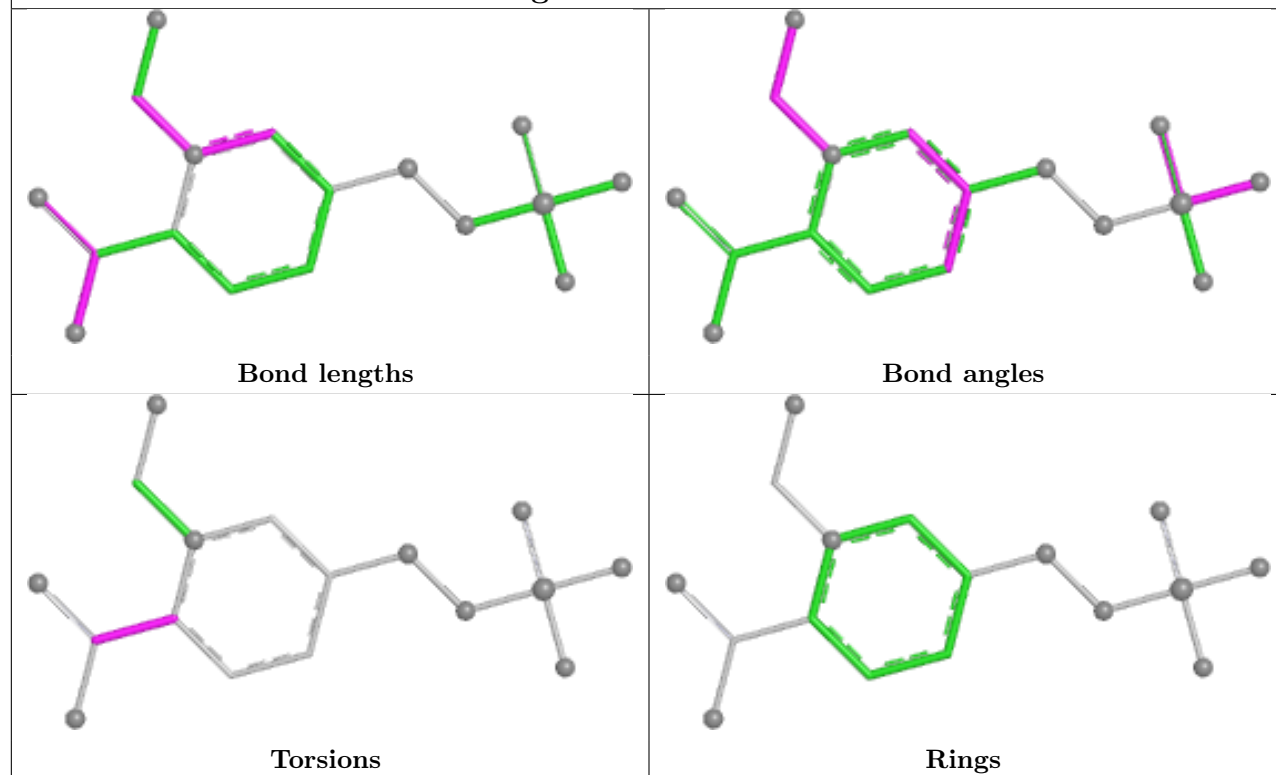
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NXL	2	0
2	B	401	NXL	8	0

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.

Ligand NXL A 401



Ligand NXL B 401



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	359/363 (98%)	0.54	18 (5%) 34 36	42, 62, 94, 119	0
1	B	359/363 (98%)	1.38	82 (22%) 2 2	52, 93, 126, 163	0
All	All	718/726 (98%)	0.96	100 (13%) 6 6	42, 75, 122, 163	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	VAL	4.6
1	B	284	LEU	4.5
1	A	292	ILE	4.4
1	B	265	THR	4.4
1	B	324	VAL	4.4
1	B	325	VAL	4.2
1	B	106	LEU	4.2
1	B	334	LEU	4.1
1	B	355	LEU	4.0
1	A	293	TRP	3.9
1	B	72	THR	3.9
1	B	327	ILE	3.7
1	A	48	VAL	3.6
1	B	73	ALA	3.6
1	B	112	TYR	3.5
1	A	1	ASN	3.4
1	B	263	VAL	3.4
1	A	118	ALA	3.3
1	B	281	LEU	3.3
1	B	354	VAL	3.3
1	B	1	ASN	3.3
1	B	238	ALA	3.3
1	B	342	ILE	3.2
1	B	229	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	266	MET	3.0
1	A	291	GLN	3.0
1	B	264	ASN	3.0
1	B	293	TRP	3.0
1	B	249	ILE	2.9
1	B	135	PHE	2.9
1	B	245	TYR	2.9
1	B	272	TRP	2.9
1	B	16	PHE	2.9
1	B	303	SER	2.8
1	B	173	VAL	2.8
1	B	69	PHE	2.8
1	B	253	ILE	2.8
1	B	358	ILE	2.7
1	B	116	ASN	2.7
1	B	244	LYS	2.7
1	A	288	ASN	2.6
1	B	11	LEU	2.6
1	B	96	LEU	2.6
1	B	155	ILE	2.6
1	B	182	LEU	2.6
1	B	322	THR	2.6
1	A	222	ALA	2.5
1	B	170	PHE	2.5
1	B	32	VAL	2.5
1	B	131	VAL	2.5
1	B	39	TYR	2.5
1	A	36	ASN	2.5
1	B	125	VAL	2.4
1	B	236	ILE	2.5
1	B	275	PHE	2.4
1	B	203	TYR	2.4
1	B	280	THR	2.4
1	B	288	ASN	2.4
1	B	121	PHE	2.3
1	A	358	ILE	2.3
1	A	3	PRO	2.3
1	B	122	PRO	2.3
1	B	68	LEU	2.3
1	B	276	SER	2.3
1	B	326	PHE	2.3
1	B	228	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	215	GLY	2.3
1	B	109	LEU	2.3
1	B	138	TRP	2.3
1	B	93	TRP	2.2
1	A	2	THR	2.2
1	B	332	ILE	2.2
1	B	240	LEU	2.2
1	B	287	SER	2.2
1	B	89	PRO	2.2
1	B	144	ILE	2.2
1	A	359	LYS	2.2
1	B	239	ASN	2.2
1	A	287	SER	2.1
1	A	142	ASN	2.1
1	B	311	TYR	2.1
1	B	8	ILE	2.1
1	B	33	ILE	2.1
1	B	359	LYS	2.1
1	B	44	GLY	2.1
1	B	292	ILE	2.1
1	B	30	VAL	2.1
1	B	20	LEU	2.1
1	B	310	MET	2.1
1	B	103	GLN	2.1
1	A	100	PRO	2.1
1	B	3	PRO	2.1
1	B	306	PRO	2.1
1	B	183	GLY	2.1
1	B	271	GLY	2.1
1	A	214	ARG	2.0
1	A	155	ILE	2.0
1	B	104	VAL	2.0
1	B	134	PHE	2.0
1	B	142	ASN	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](#)

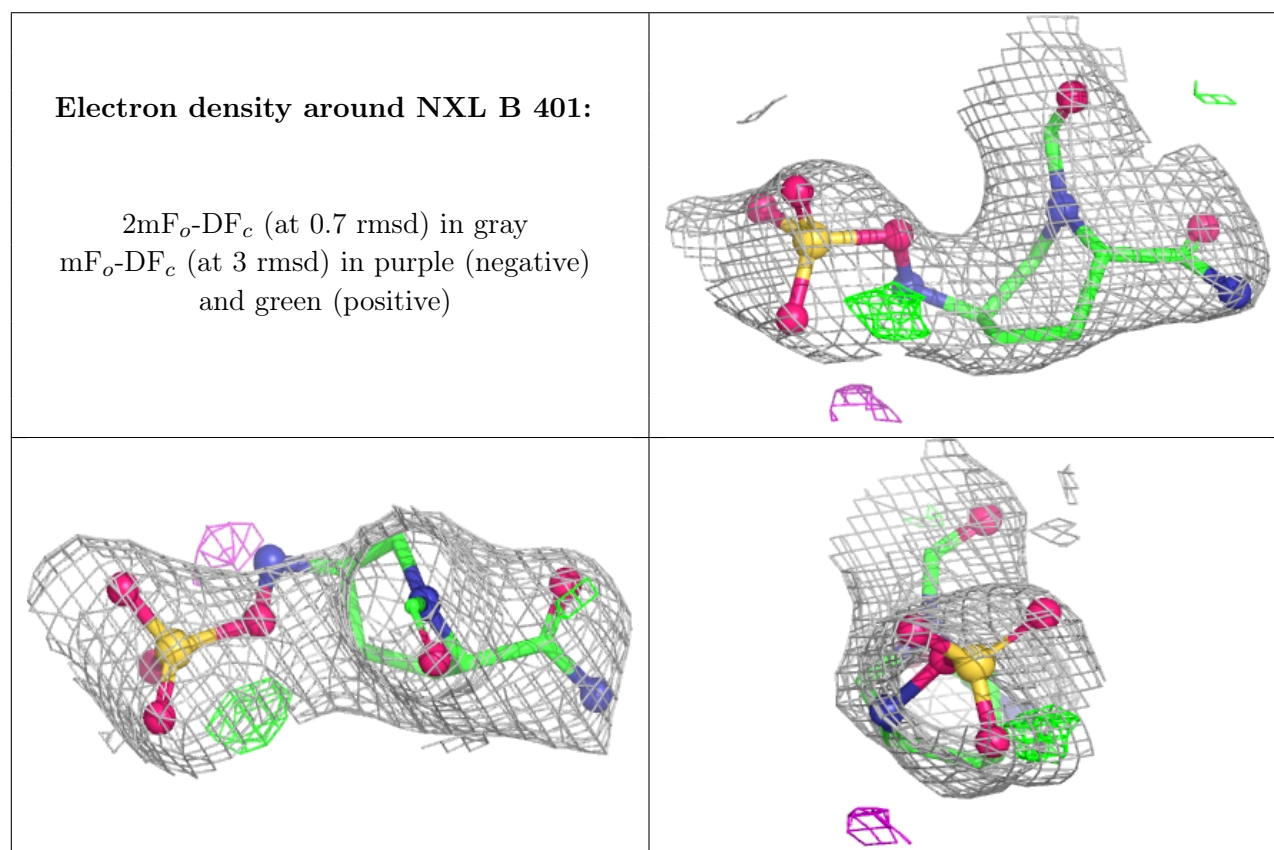
There are no oligosaccharides in this entry.

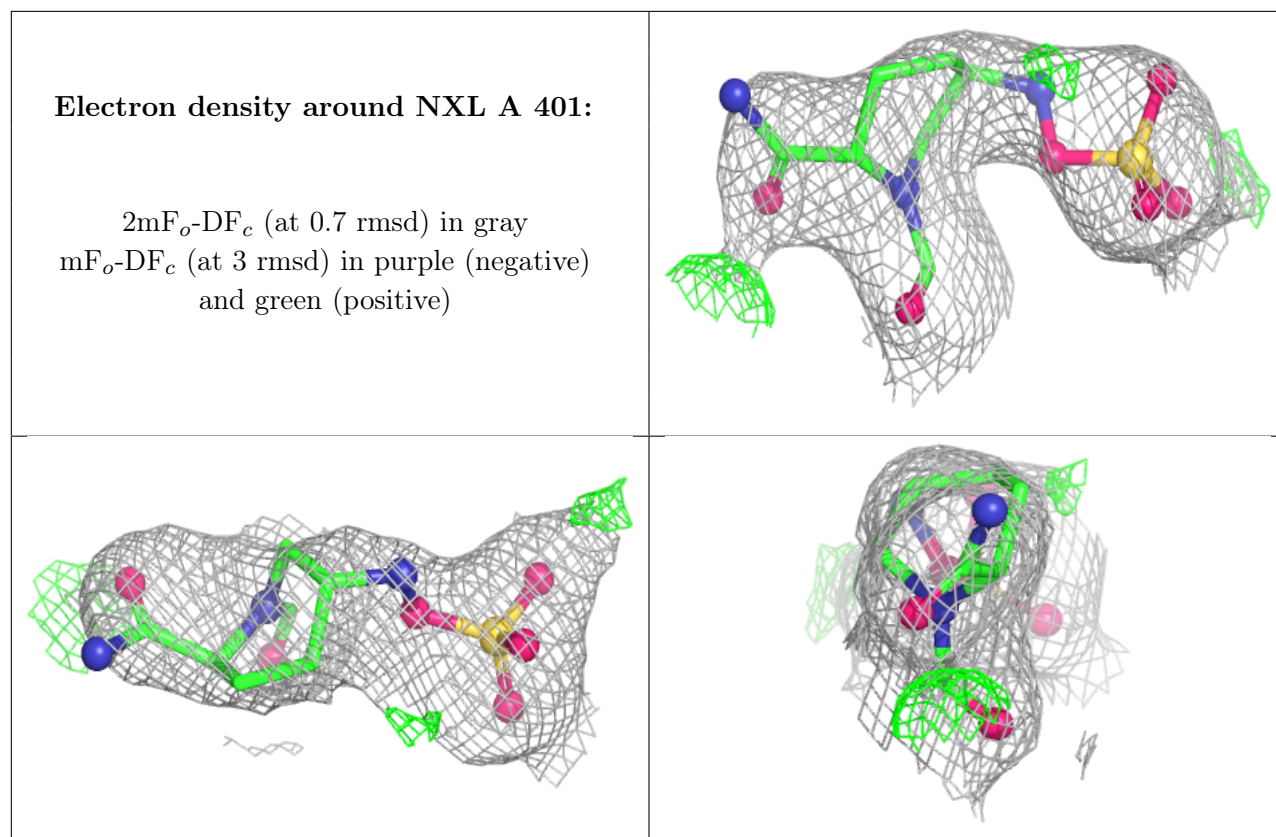
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	NXL	B	401	17/17	0.77	0.14	68,74,97,98	17
2	NXL	A	401	17/17	0.85	0.13	56,70,83,87	17

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.