



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 AM UTC

PDB ID : 2Q0U / pdb_00002q0u
Title : Structure of Pectenotoxin-2 and Latrunculin B Bound to Actin
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Deposited on : 2007-05-22
Resolution : 1.45 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

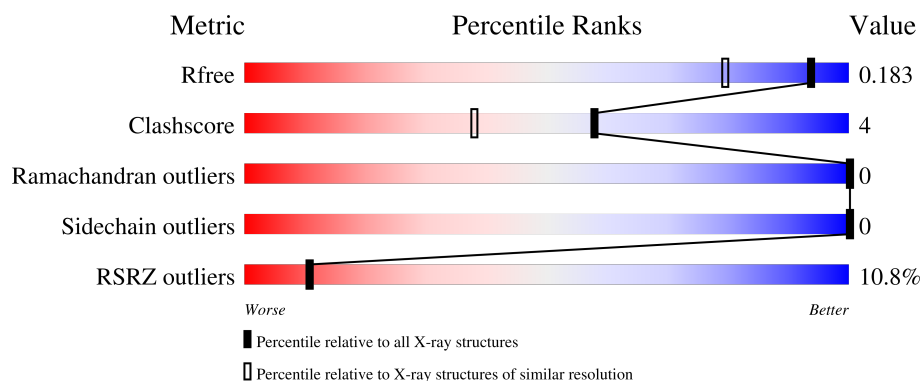
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	375	

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
5	PXT	A	500	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3194 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 Actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	4	0
			2716	1728	447	520	21			

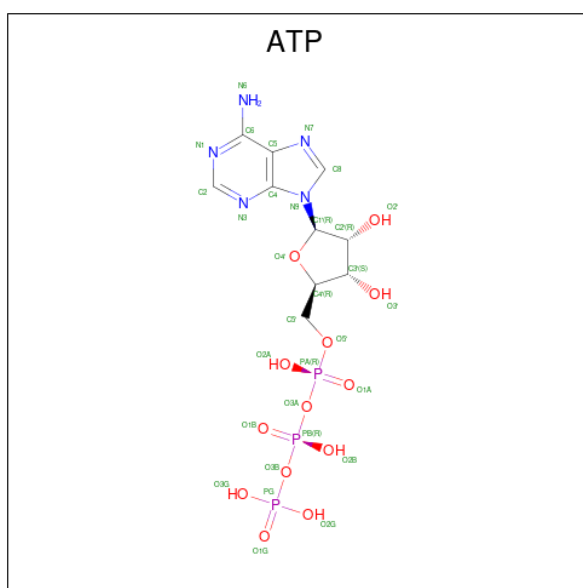
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	modified residue	UNP P68135

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

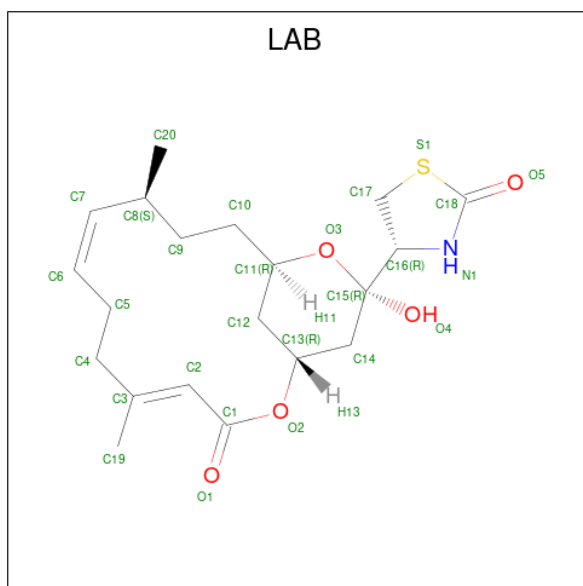
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



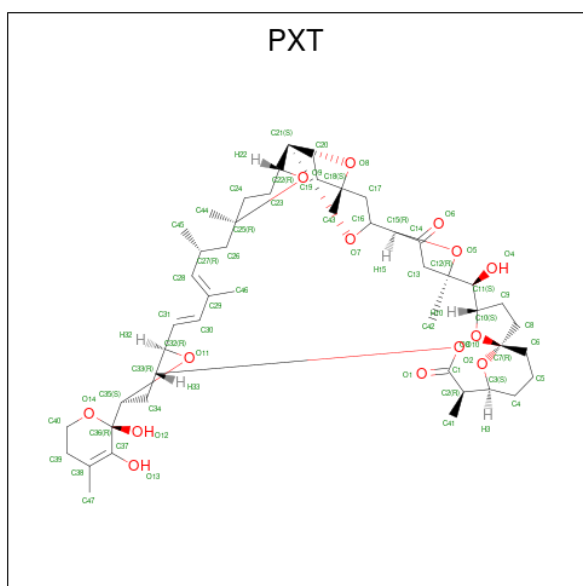
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is LATRUNCULIN B (CCD ID: LAB) (formula: $C_{20}H_{29}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 5 is PECTENOTOXIN-2 (CCD ID: PXT) (formula: $C_{47}H_{68}O_{14}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			61	47	14		

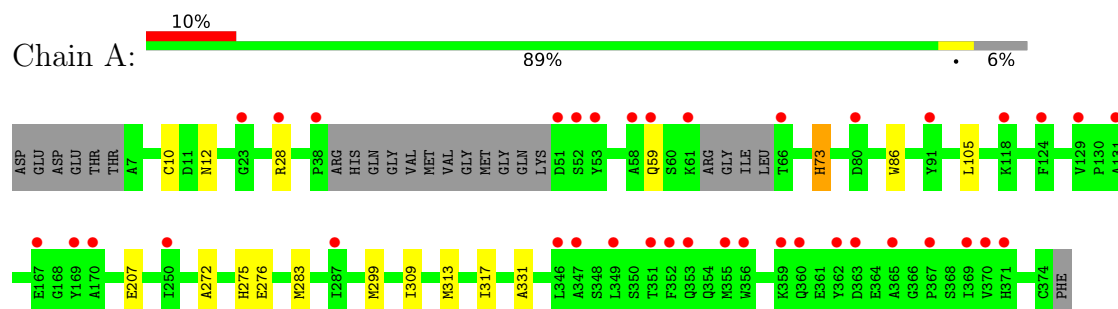
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	357	Total	O	0	0
			357	357		

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: Actin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.68Å 54.34Å 105.89Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	45.00 – 1.45 45.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.00-1.45) 97.8 (45.00-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 1.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.181 0.167 , 0.183	Depositor DCC
R_{free} test set	3096 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3194	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% 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: LAB, ATP, HIC, PXT, CA

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	0.50	0/2771	0.67	0/3757

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	2716	0	2625	22	0
2	A	2	0	0	0	0
3	A	31	0	12	0	0
4	A	27	0	28	4	0
5	A	61	0	65	0	0
6	A	357	0	0	9	1
All	All	3194	0	2730	25	1

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 4.

All (25) 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)
4:A:401:LAB:C8	4:A:401:LAB:C20	1.79	1.58
1:A:73:HIC:HZ1	6:A:858:HOH:O	1.02	1.18
1:A:73:HIC:CZ	6:A:858:HOH:O	1.67	0.95
1:A:299[B]:MET:HE2	1:A:331:ALA:HB2	1.57	0.84
1:A:299[B]:MET:HE1	1:A:309:ILE:HG23	1.67	0.77
1:A:73:HIC:NE2	6:A:858:HOH:O	2.05	0.74
4:A:401:LAB:C20	4:A:401:LAB:C7	2.66	0.73
1:A:283:MET:CE	6:A:771:HOH:O	2.37	0.72
4:A:401:LAB:C20	4:A:401:LAB:C9	2.68	0.71
1:A:275:HIS:HA	1:A:313:MET:HE1	1.76	0.68
1:A:299[B]:MET:HE1	1:A:309:ILE:CG2	2.27	0.64
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.49	0.61
1:A:283:MET:HE1	6:A:771:HOH:O	2.00	0.57
1:A:283:MET:HE3	6:A:771:HOH:O	2.02	0.55
1:A:299[B]:MET:HE2	1:A:331:ALA:CB	2.33	0.54
1:A:10[B]:CYS:HB2	1:A:105:LEU:HD23	1.91	0.52
1:A:12:ASN:ND2	1:A:86:TRP:HE1	2.07	0.51
1:A:10[A]:CYS:HB3	1:A:105:LEU:HD23	1.93	0.48
1:A:73:HIC:CE1	6:A:858:HOH:O	2.57	0.46
1:A:59:GLN:NE2	6:A:856:HOH:O	1.97	0.44
1:A:272:ALA:HB1	1:A:276:GLU:HB3	1.99	0.44
1:A:207:GLU:OE2	4:A:401:LAB:H172	2.20	0.41
1:A:28:ARG:HG2	6:A:623:HOH:O	2.20	0.41
1:A:313:MET:HE2	1:A:317:ILE:HD11	2.02	0.41
1:A:313:MET:HE3	1:A:313:MET:HA	2.02	0.40

All (1) 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)
6:A:837:HOH:O	6:A:846:HOH:O[3_545]	1.52	0.68

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	348/375 (93%)	343 (99%)	5 (1%)	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	284/317 (90%)	284 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	101	HIS
1	A	162	ASN
1	A	225	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	HIC	A	73	1	10,11,12	1.66	2 (20%)	9,14,16	5.80	6 (66%)

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
1	HIC	A	73	1	-	1/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CZ-NE2	4.36	1.58	1.46
1	A	73	HIC	CD2-CG	-2.31	1.32	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	CZ-NE2-CD2	-11.93	110.38	126.03
1	A	73	HIC	CZ-NE2-CE1	7.94	145.45	126.71
1	A	73	HIC	CD2-NE2-CE1	-7.23	103.86	106.71
1	A	73	HIC	CB-CG-CD2	-3.91	120.52	129.96
1	A	73	HIC	NE2-CE1-ND1	-3.91	111.17	112.66
1	A	73	HIC	CB-CG-ND1	3.50	132.20	121.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	LAB	A	401	-	28,29,29	2.35	8 (28%)	29,41,41	2.92	14 (48%)
5	PXT	A	500	-	65,69,69	2.16	13 (20%)	70,111,111	4.10	43 (61%)
3	ATP	A	425	2	32,33,33	1.41	4 (12%)	48,52,52	1.57	10 (20%)

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
4	LAB	A	401	-	-	3/21/49/49	0/2/3/3
5	PXT	A	500	-	1/1/22/25	8/47/152/152	0/1/9/9
3	ATP	A	425	2	-	2/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	PXT	C38-C37	10.65	1.47	1.33
4	A	401	LAB	C20-C8	7.32	1.79	1.53
4	A	401	LAB	C4-C3	-6.47	1.37	1.51
5	A	500	PXT	C34-C33	-6.45	1.39	1.52
5	A	500	PXT	O8-C18	-4.47	1.40	1.46
5	A	500	PXT	O10-C1	4.46	1.44	1.34
3	A	425	ATP	C5-C4	4.35	1.46	1.39
5	A	500	PXT	O10-C33	3.48	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	PXT	C33-C32	-3.24	1.48	1.53
5	A	500	PXT	C30-C29	2.97	1.52	1.46
3	A	425	ATP	PB-O3B	2.93	1.62	1.59
5	A	500	PXT	O12-C36	2.82	1.44	1.39
4	A	401	LAB	C16-N1	2.76	1.50	1.46
5	A	500	PXT	O13-C37	2.70	1.41	1.32
3	A	425	ATP	C4-N9	-2.68	1.32	1.37
5	A	500	PXT	C16-C15	-2.59	1.48	1.52
4	A	401	LAB	O3-C15	-2.57	1.39	1.43
3	A	425	ATP	PA-O3A	2.45	1.62	1.59
5	A	500	PXT	O7-C16	-2.32	1.39	1.44
4	A	401	LAB	C19-C3	2.21	1.56	1.50
5	A	500	PXT	C15-C14	-2.15	1.49	1.52
4	A	401	LAB	O4-C15	2.13	1.44	1.40
4	A	401	LAB	C8-C7	2.08	1.57	1.51
4	A	401	LAB	C10-C11	2.07	1.58	1.51
5	A	500	PXT	O5-C12	-2.00	1.43	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	PXT	O8-C21-C20	-16.16	85.08	105.09
5	A	500	PXT	O8-C18-C19	-11.51	85.18	103.65
5	A	500	PXT	O8-C18-C17	8.62	120.69	106.54
5	A	500	PXT	C39-C38-C37	-7.78	111.41	121.66
5	A	500	PXT	C40-O14-C36	7.44	122.45	113.99
5	A	500	PXT	O7-C16-C17	6.66	121.59	110.17
5	A	500	PXT	C25-C26-C27	6.30	127.11	116.25
4	A	401	LAB	O2-C13-C12	-5.97	93.75	107.77
4	A	401	LAB	O3-C11-C12	5.84	119.28	109.02
5	A	500	PXT	C34-C33-C32	5.75	116.77	103.07
4	A	401	LAB	C9-C8-C7	5.35	125.30	110.64
5	A	500	PXT	O8-C18-C43	5.31	114.65	107.88
5	A	500	PXT	C7-O2-C3	5.30	124.00	114.06
4	A	401	LAB	C12-C13-C14	5.28	121.43	111.02
4	A	401	LAB	C12-C11-C10	5.24	123.01	113.28
5	A	500	PXT	O12-C36-O14	-5.08	105.67	111.39
4	A	401	LAB	O4-C15-O3	-4.85	100.58	110.00
5	A	500	PXT	C5-C6-C7	4.64	117.58	111.55
5	A	500	PXT	C6-C5-C4	4.56	118.70	111.33
5	A	500	PXT	O5-C12-C11	4.51	110.32	106.20
3	A	425	ATP	C5-C4-N3	-4.39	120.67	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	PXT	O11-C32-C31	4.35	120.04	110.17
5	A	500	PXT	C42-C12-C11	-4.18	107.80	112.23
5	A	500	PXT	C45-C27-C28	3.94	120.60	110.04
5	A	500	PXT	C5-C4-C3	3.87	118.53	110.90
3	A	425	ATP	N3-C4-N9	3.80	133.63	127.17
5	A	500	PXT	O14-C40-C39	3.78	116.94	111.28
5	A	500	PXT	C26-C27-C28	3.64	121.47	110.27
5	A	500	PXT	C44-C25-C24	-3.60	107.51	113.64
3	A	425	ATP	C4-N9-C8	3.60	109.51	105.74
5	A	500	PXT	C33-O10-C1	3.54	123.21	117.85
5	A	500	PXT	O11-C32-C33	-3.51	99.11	104.26
5	A	500	PXT	C27-C28-C29	3.44	134.01	128.13
5	A	500	PXT	C24-C25-C26	3.35	120.78	112.77
5	A	500	PXT	C4-C3-C2	3.25	119.11	114.50
5	A	500	PXT	O2-C3-C4	3.18	116.11	110.17
3	A	425	ATP	C4-C5-N7	-3.12	107.02	110.58
5	A	500	PXT	C32-C31-C30	-3.09	118.89	125.10
5	A	500	PXT	C30-C29-C28	-3.09	110.53	118.82
5	A	500	PXT	C23-C22-C21	3.00	121.26	116.06
5	A	500	PXT	C20-C21-C22	3.00	117.13	111.10
5	A	500	PXT	C16-C15-C14	-2.98	105.53	112.58
4	A	401	LAB	C17-S1-C18	2.92	93.73	92.04
3	A	425	ATP	N3-C2-N1	-2.90	124.19	128.58
4	A	401	LAB	C20-C8-C7	-2.90	104.79	110.82
4	A	401	LAB	O4-C15-C14	-2.78	100.86	109.80
5	A	500	PXT	C47-C38-C37	-2.77	115.58	121.52
3	A	425	ATP	C2-N3-C4	2.71	118.44	111.83
5	A	500	PXT	O11-C35-C34	2.69	108.05	104.16
4	A	401	LAB	C14-C15-C16	2.64	118.89	113.75
5	A	500	PXT	C46-C29-C28	2.62	130.61	123.21
5	A	500	PXT	C7-O3-C10	2.61	113.41	107.70
4	A	401	LAB	C19-C3-C4	-2.58	110.75	115.23
5	A	500	PXT	O10-C1-O1	2.53	128.53	123.95
5	A	500	PXT	C45-C27-C26	2.49	117.86	110.75
5	A	500	PXT	O10-C33-C34	-2.46	103.28	109.21
4	A	401	LAB	C5-C4-C3	2.42	121.21	113.19
4	A	401	LAB	C4-C3-C2	2.42	128.87	121.90
5	A	500	PXT	O13-C37-C38	-2.31	111.00	121.00
3	A	425	ATP	C5-N7-C8	2.31	107.08	103.45
3	A	425	ATP	N9-C8-N7	-2.30	110.67	113.94
5	A	500	PXT	O1-C1-C2	-2.16	118.48	124.11
3	A	425	ATP	C2-N1-C6	2.16	122.28	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	425	ATP	N6-C6-N1	2.13	123.13	118.38
5	A	500	PXT	C3-C2-C1	2.12	113.62	109.91
5	A	500	PXT	O5-C12-C42	-2.07	104.22	108.05
4	A	401	LAB	C20-C8-C9	-2.04	105.06	110.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	500	PXT	C27

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	425	ATP	PB-O3B-PG-O1G
5	A	500	PXT	O5-C15-C16-C17
5	A	500	PXT	C1-C2-C3-O2
5	A	500	PXT	O9-C25-C26-C27
4	A	401	LAB	C9-C10-C11-C12
4	A	401	LAB	O1-C1-C2-C3
5	A	500	PXT	O10-C1-C2-C3
4	A	401	LAB	O2-C1-C2-C3
5	A	500	PXT	O1-C1-C2-C3
5	A	500	PXT	C1-C2-C3-C4
5	A	500	PXT	C10-C11-C12-O5
5	A	500	PXT	C25-C26-C27-C45
3	A	425	ATP	PG-O3B-PB-O2B

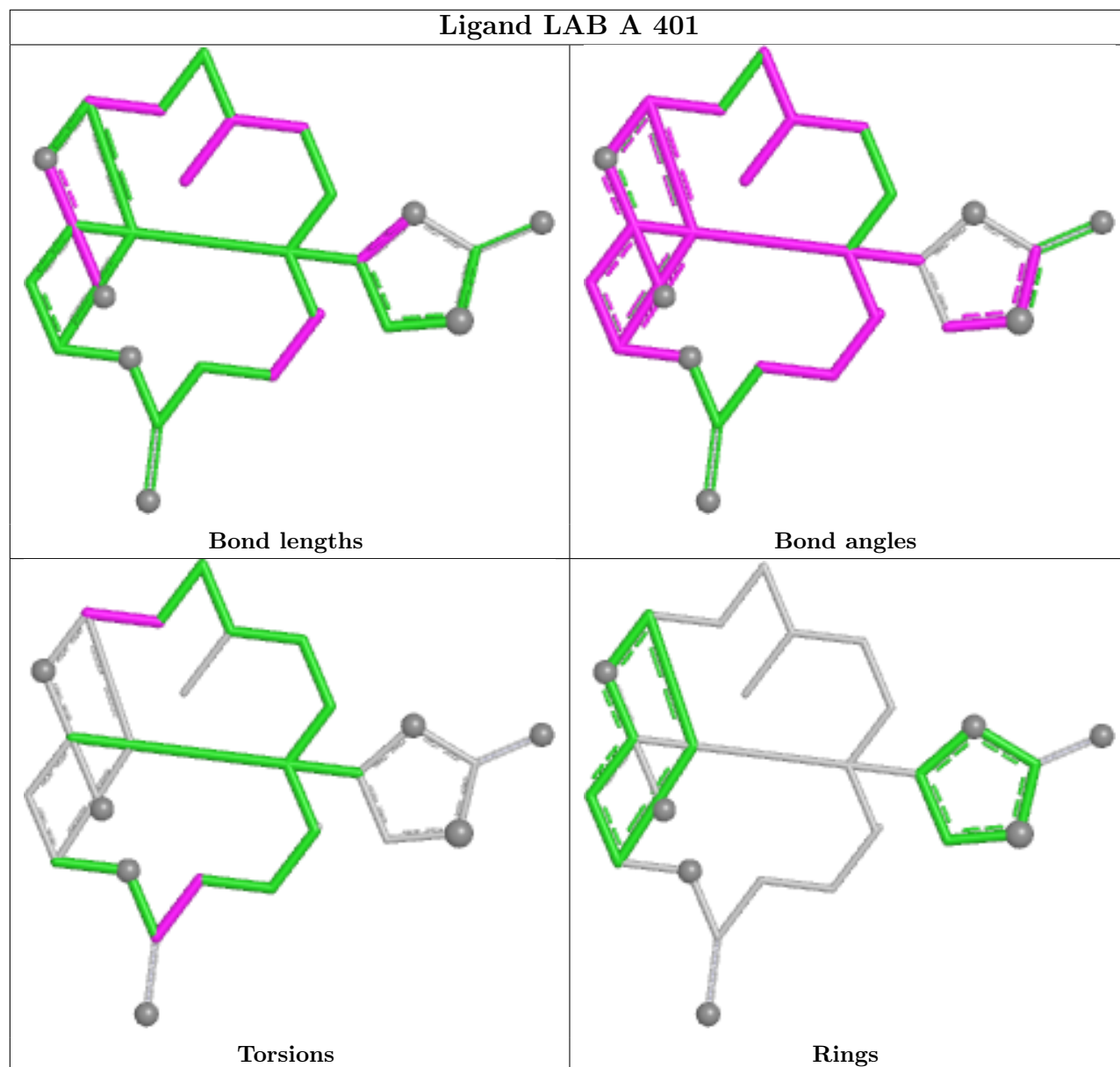
There are no ring outliers.

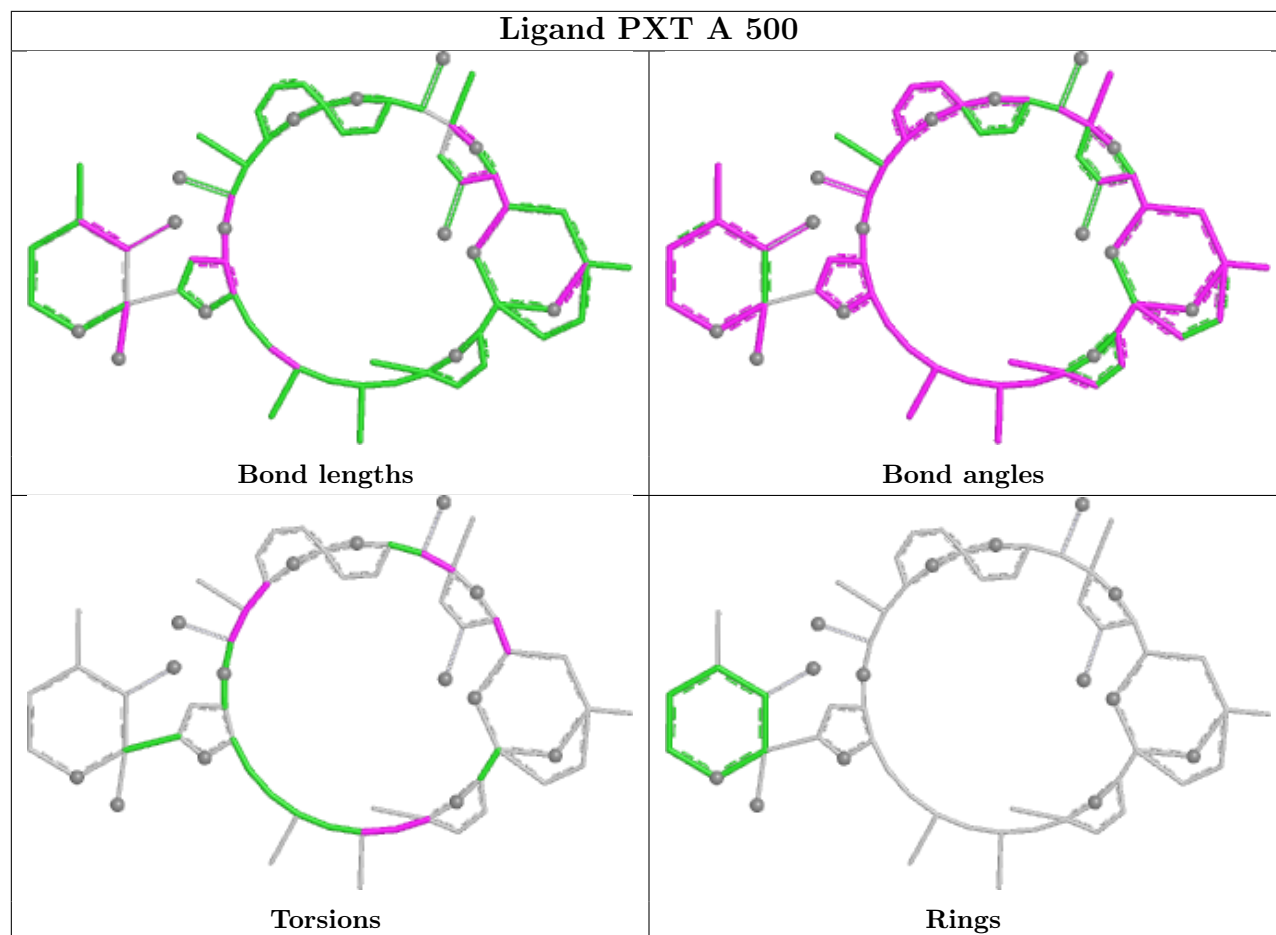
1 monomer is involved in 4 short contacts:

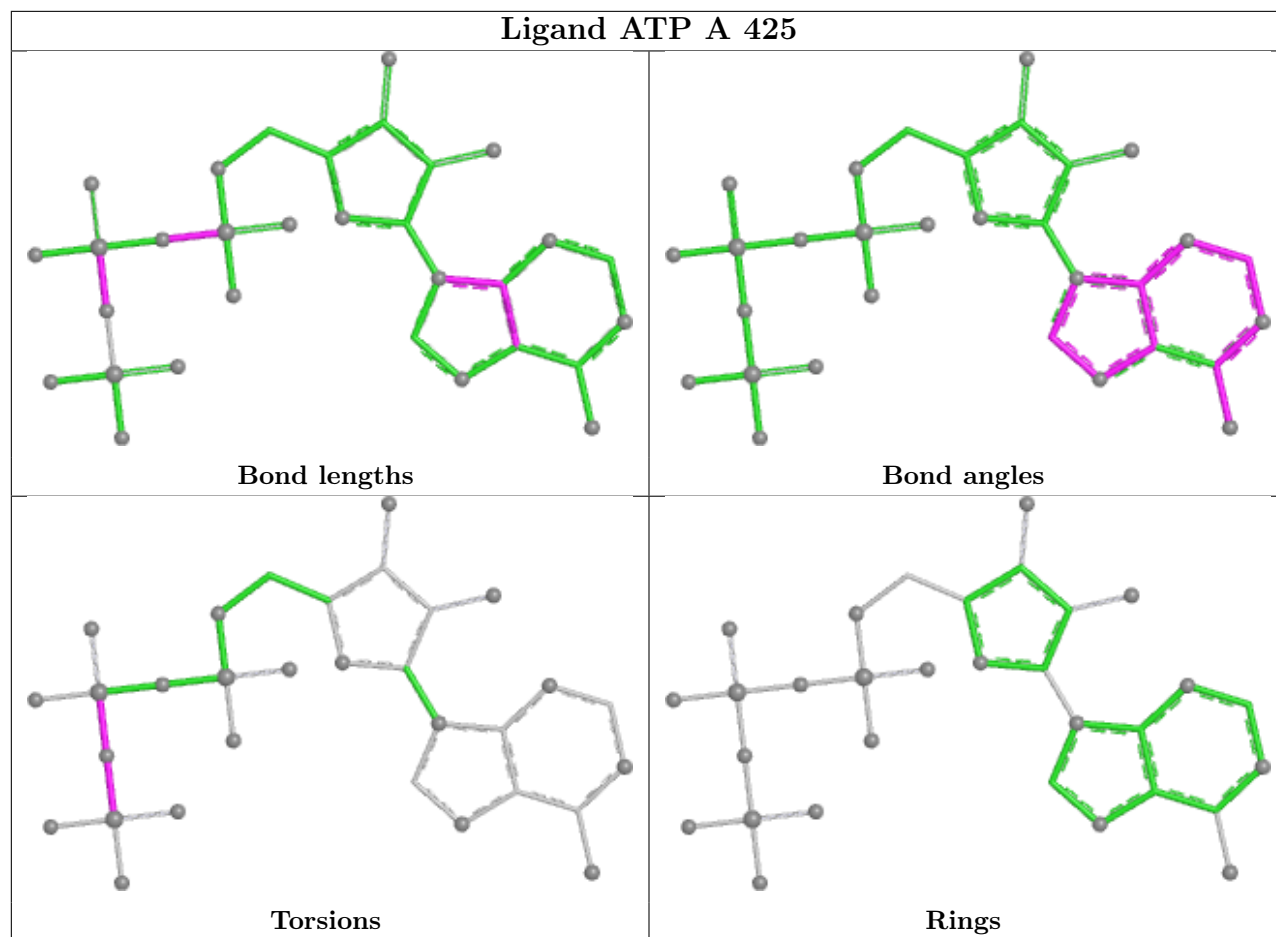
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	LAB	4	0

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	351/375 (93%)	0.39	38 (10%)	11 11	5, 13, 27, 31	14 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LYS	9.8
1	A	51	ASP	8.5
1	A	66	THR	7.4
1	A	53	TYR	5.7
1	A	371[A]	HIS	5.0
1	A	169	TYR	4.9
1	A	352	PHE	3.9
1	A	365	ALA	3.6
1	A	362	TYR	3.3
1	A	91	TYR	3.2
1	A	80	ASP	2.9
1	A	287	ILE	2.8
1	A	349	LEU	2.8
1	A	363	ASP	2.8
1	A	38	PRO	2.8
1	A	360	GLN	2.7
1	A	129	VAL	2.6
1	A	250	ILE	2.5
1	A	367	PRO	2.5
1	A	351	THR	2.5
1	A	118	LYS	2.3
1	A	369	ILE	2.3
1	A	355	MET	2.3
1	A	353	GLN	2.2
1	A	59	GLN	2.2
1	A	356	TRP	2.2
1	A	23	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	131	ALA	2.1
1	A	28	ARG	2.1
1	A	124	PHE	2.1
1	A	170	ALA	2.1
1	A	370[A]	VAL	2.1
1	A	347	ALA	2.1
1	A	167	GLU	2.0
1	A	359	LYS	2.0
1	A	58	ALA	2.0
1	A	346	LEU	2.0
1	A	52	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	A	73	11/12	0.88	0.14	11,13,21,22	0

6.3 Carbohydrates [i](#)

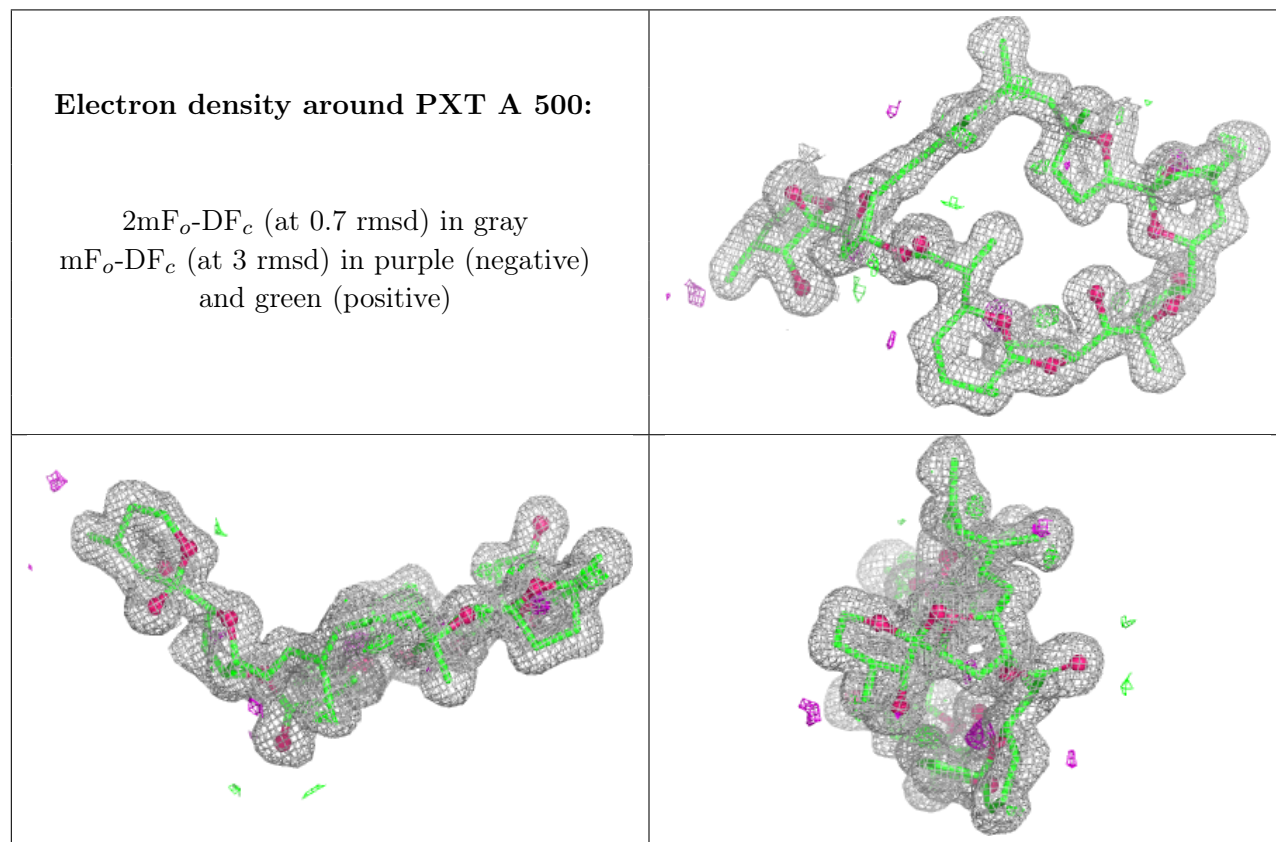
There are no oligosaccharides in this entry.

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.

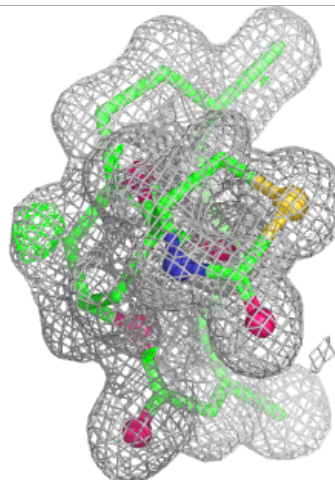
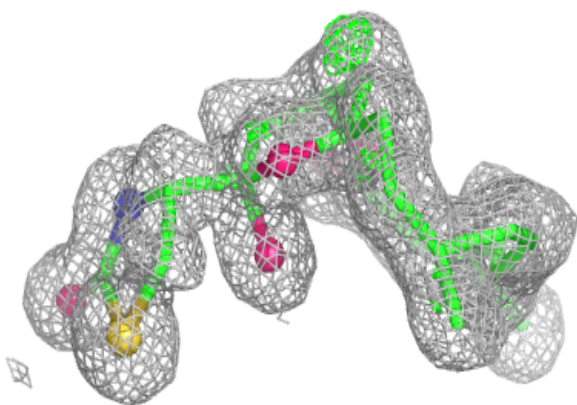
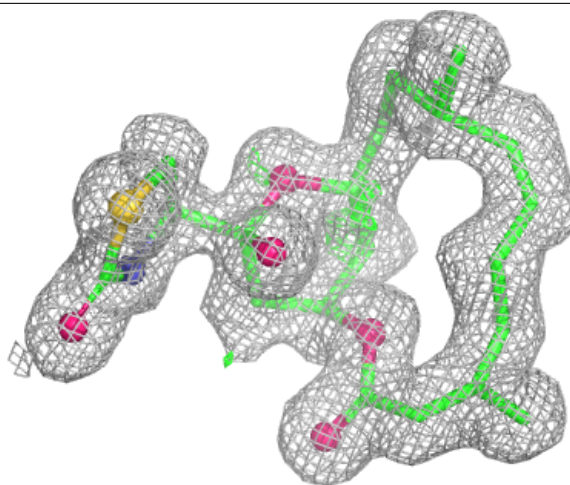
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PXT	A	500	61/61	0.91	0.09	12,15,16,18	0
4	LAB	A	401	27/27	0.97	0.06	10,11,13,14	0
3	ATP	A	425	31/31	0.99	0.04	7,8,9,9	0
2	CA	A	501	1/1	1.00	0.02	7,7,7,7	0
2	CA	A	400	1/1	1.00	0.01	9,9,9,9	0

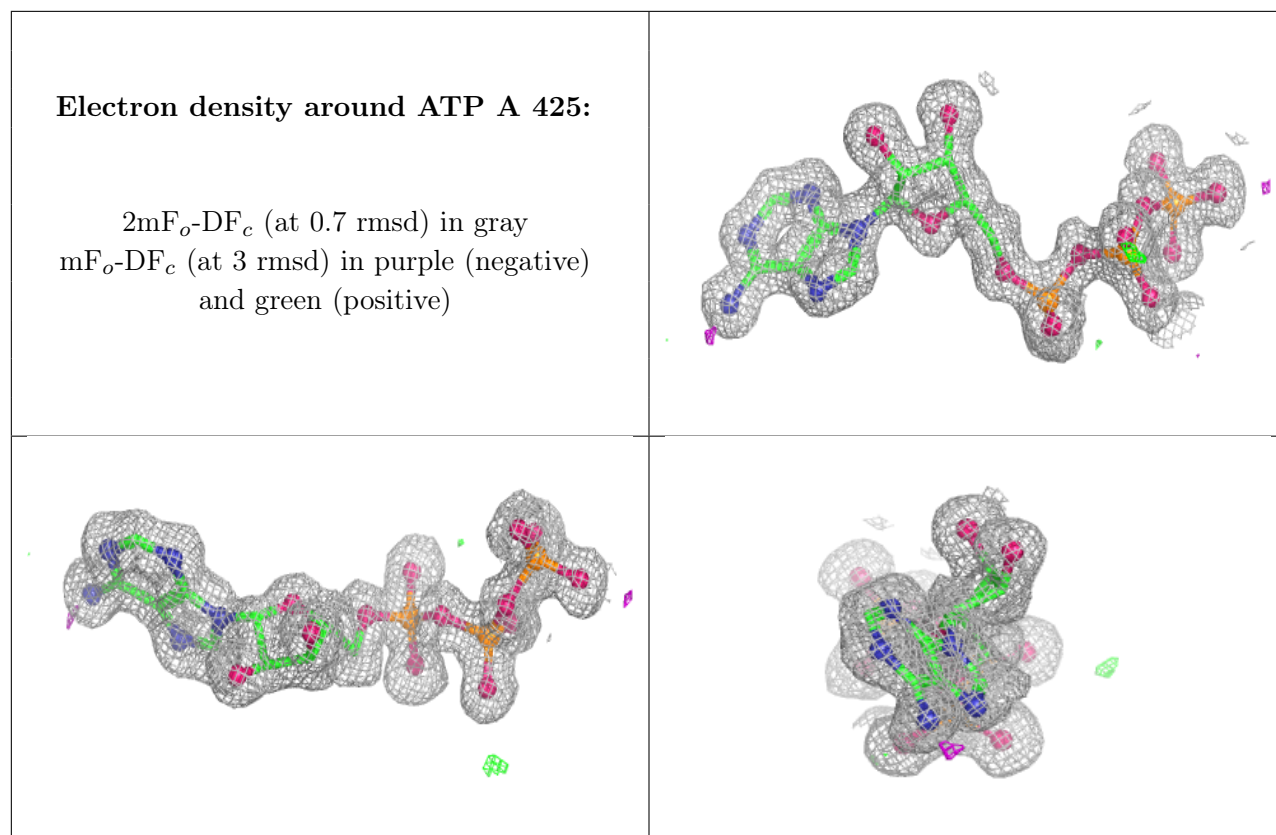
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around LAB A 401:

$2mF_o-DF_c$ (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.