



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 02:51 PM UTC

PDB ID : 8TX9 / pdb_00008tx9
Title : Nan Regulatory Protein (core isomerase domain) from Streptococcus pneumoniae
Authors : Wood, D.M.; Horne, C.R.; Panjikar, S.; Dobson, R.C.J.
Deposited on : 2023-08-23
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

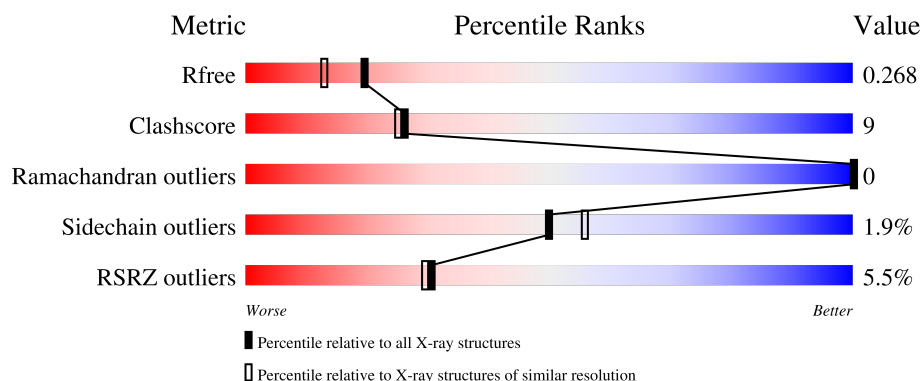
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	286	6% 53% 14% 33%
1	B	286	5% 50% 14% 36%
1	C	286	% 56% 10% 34%
1	D	286	% 52% 12% 34%

2 Entry composition [i](#)

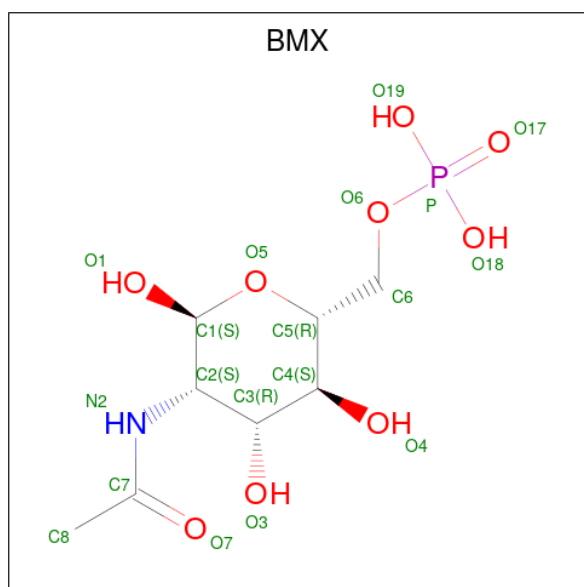
There are 4 unique types of molecules in this entry. The entry contains 12246 atoms, of which 5994 are hydrogens and 0 are deuteriums.

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 MurR/RpiR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	H	N	O	S	0	0	0
			3054	972	1526	255	293	8			
1	C	187	Total	C	H	N	O	S	Se	11	4
			3047	969	1523	250	293	9	3		0
1	D	185	Total	C	H	N	O	S		0	0
			2969	946	1484	244	287	8			0
1	B	181	Total	C	H	N	O	S		0	0
			2892	924	1441	237	282	8			0

- Molecule 2 is 2-acetamido-2-deoxy-6-O-phosphono-alpha-D-mannopyranose (CCD ID: BMX) (formula: C₈H₁₆NO₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			24	8	5	1	9	1		
2	C	1	Total	C	H	N	O	P	0	0
			24	8	5	1	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	P	
			24	8	5	1	9	1	
2	B	1	Total	C	H	N	O	P	
			24	8	5	1	9	1	

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

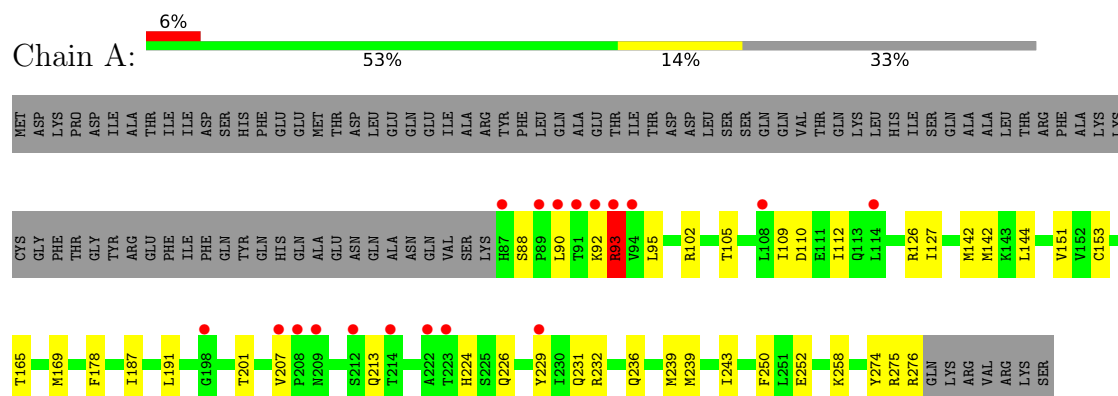
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O		
			21	21	0	0
4	C	75	Total	O		
			75	75	0	0
4	D	60	Total	O		
			60	60	0	0
4	B	28	Total	O		
			28	28	0	0

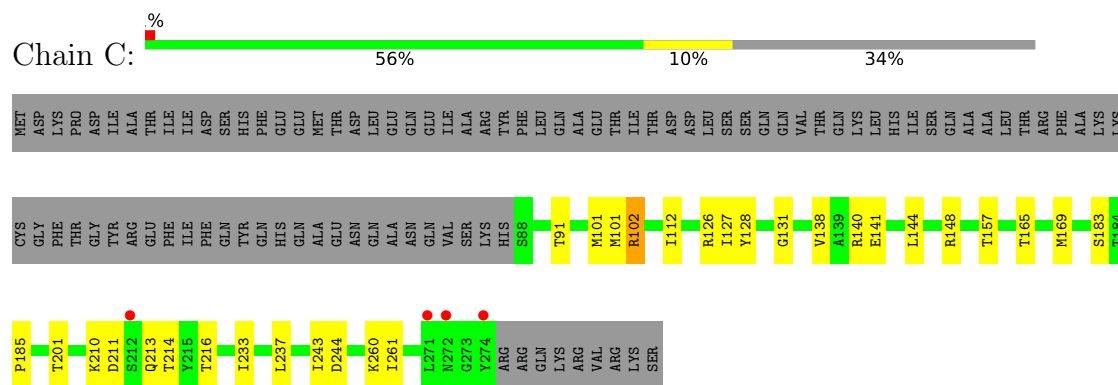
3 Residue-property plots [i](#)

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.

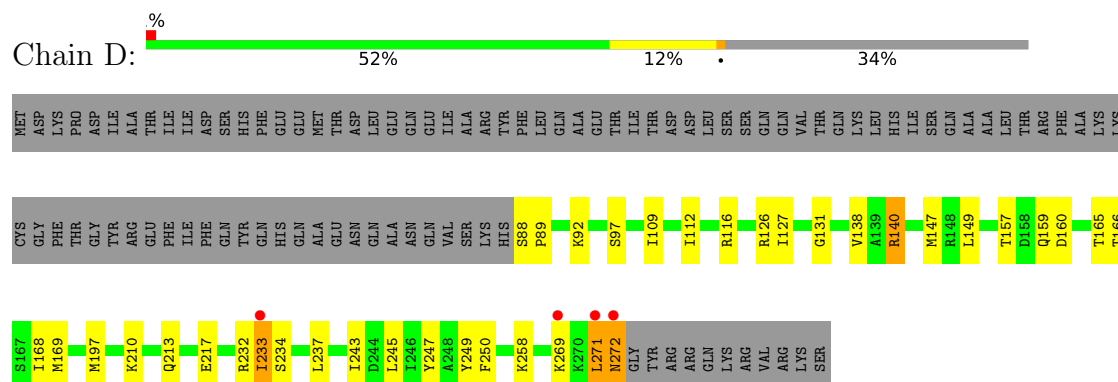
- Molecule 1: MurR/RpiR family transcriptional regulator



- Molecule 1: MurR/RpiR family transcriptional regulator



- Molecule 1: MurR/RpiR family transcriptional regulator



Chain B:

5% 50% 14% 36%

Label	Color
NET	Grey
ASP	Grey
LYS	Grey
PRO	Grey
ASP	Grey
ILE	Grey
ALA	Grey
THR	Grey
ILE	Grey
ILE	Grey
ASP	Grey
SER	Grey
HIS	Grey
PHE	Grey
GLU	Grey
GLU	Grey
MET	Grey
THR	Grey
ASP	Grey
GLN	Grey
LEU	Grey
GLN	Grey
GLU	Grey
ILE	Grey
ALA	Grey
ALA	Grey
THR	Grey
ILE	Grey
THR	Grey
ASP	Grey
ASP	Grey
LEU	Grey
SER	Grey
SER	Grey
GLN	Grey
GLN	Grey
VAL	Grey
THR	Grey
GLN	Grey
LYS	Grey
LEU	Grey
THR	Grey
PHE	Grey
ARG	Grey
ALA	Grey
LYS	Grey
LYS	Grey
CYS	Grey
GLY	Grey
PHE	Grey
THR	Grey
GLY	Yellow
TYR	Grey
ARG	Grey
GLU	Grey
PHE	Grey
ILE	Grey
PHE	Grey
GLN	Grey
TYR	Grey
HIS	Grey
GLN	Grey
ALA	Grey
GLU	Grey
ASN	Grey
ALA	Grey
ASN	Grey
GLN	Grey
VAL	Grey
SER	Grey
LYS	Grey
HIS	Grey
S88	Red
P89	Red
L90	Red
L95	Yellow
M101	Yellow
M101	Yellow
R102	Yellow
E103	Yellow
Q104	Yellow
L108	Yellow
A118	Red
E122	Yellow
D123	Yellow
A124	Yellow
F125	Yellow
R126	Yellow
I127	Yellow
Y128	Yellow
F129	Yellow
E141	Yellow
M142	Yellow
M142	Yellow
K143	Yellow
L144	Yellow
R145	Yellow
F146	Yellow
L149	Red
G150	Yellow
V151	Yellow
V152	Yellow
C153	Yellow
M169	Yellow
V175	Yellow
G182	Yellow
L189	Yellow
V207	Red
P208	Yellow
N209	Yellow
K210	Yellow
D211	Red
S212	Red
Q213	Red
T214	Yellow
L220	Red
V221	Yellow
A222	Yellow
T223	Yellow
H224	Yellow
T230	Red
Q231	Yellow
K232	Yellow
L240	Yellow
T243	Red
Y247	Red
A248	Yellow
Y249	Red
E252	Yellow
I253	Yellow
N254	Yellow
E255	Yellow
E256	Yellow
S257	Yellow
K260	Yellow
W266	Red
E267	Yellow
N268	Yellow
LYS	Grey
LYS	Grey
LEU	Grey
ASN	Grey
GLY	Grey
TYR	Grey
ARG	Grey

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	147.58Å 147.58Å 82.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.23 – 2.01 42.23 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.23-2.01) 94.2 (42.23-2.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.01Å)	Xtriage
Refinement program	REFMAC 8.0.013, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.271 0.217 , 0.268	Depositor DCC
R_{free} test set	2836 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12246	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, BMX

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	0.65	0/1555	0.85	0/2099
1	B	0.64	0/1477	0.80	1/1997 (0.1%)
1	C	0.93	1/1547 (0.1%)	0.87	1/2082 (0.0%)
1	D	0.71	0/1511	0.84	1/2041 (0.0%)
All	All	0.74	1/6090 (0.0%)	0.84	3/8219 (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
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101[B]	MSE	C-N	-19.38	1.08	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	GLU	CA-CB-CG	-5.73	102.63	114.10
1	B	210	LYS	N-CA-C	-5.41	106.73	113.38
1	D	233	ILE	CA-CB-CG1	5.09	119.05	110.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	ARG	Sidechain
1	B	145	ARG	Sidechain
1	C	102	ARG	Sidechain
1	D	140	ARG	Sidechain
1	D	232	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	1528	1526	1524	41	0
1	B	1451	1441	1441	37	0
1	C	1524	1523	1514	19	0
1	D	1485	1484	1484	31	0
2	A	19	5	13	3	0
2	B	19	5	13	0	0
2	C	19	5	13	0	0
2	D	19	5	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	0	0	0
4	B	28	0	0	0	0
4	C	75	0	0	0	0
4	D	60	0	0	0	0
All	All	6252	5994	6016	113	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 9.

The worst 5 of 113 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:102:ARG:NH1	1:B:95:LEU:HD12	1.78	0.97
1:B:149:LEU:HD11	1:B:247:TYR:CE1	2.13	0.84
1:A:95:LEU:HD22	1:B:102:ARG:NH1	2.01	0.76
2:A:301:BMX:H82C	2:A:301:BMX:H4	1.70	0.73
1:B:182:GLY:O	1:B:188:LEU:HD11	1.88	0.72

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	188/286 (66%)	187 (100%)	1 (0%)	0	100	100
1	B	179/286 (63%)	173 (97%)	6 (3%)	0	100	100
1	C	183/286 (64%)	180 (98%)	3 (2%)	0	100	100
1	D	183/286 (64%)	180 (98%)	3 (2%)	0	100	100
All	All	733/1144 (64%)	720 (98%)	13 (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	170/254 (67%)	165 (97%)	5 (3%)	37	40
1	B	163/254 (64%)	159 (98%)	4 (2%)	42	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	171/254 (67%)	170 (99%)	1 (1%)	78	85
1	D	167/254 (66%)	164 (98%)	3 (2%)	51	58
All	All	671/1016 (66%)	658 (98%)	13 (2%)	50	56

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	271	LEU
1	D	272	ASN
1	B	254	ASN
1	B	213	GLN
1	B	214	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	236	GLN
1	B	106	GLN
1	B	263	ASN
1	C	236	GLN
1	C	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	BMX	B	301	-	19,19,19	1.64	5 (26%)	27,28,28	1.95	8 (29%)
2	BMX	C	301	-	19,19,19	1.78	4 (21%)	27,28,28	1.83	7 (25%)
2	BMX	A	301	-	19,19,19	1.75	5 (26%)	27,28,28	2.16	6 (22%)
2	BMX	D	301	-	19,19,19	1.62	4 (21%)	27,28,28	1.61	7 (25%)

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	BMX	B	301	-	-	1/10/30/30	0/1/1/1
2	BMX	C	301	-	-	3/10/30/30	0/1/1/1
2	BMX	A	301	-	-	9/10/30/30	0/1/1/1
2	BMX	D	301	-	-	0/10/30/30	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BMX	C7-N2	3.71	1.46	1.34
2	C	301	BMX	C2-N2	3.68	1.51	1.45
2	C	301	BMX	C7-N2	3.66	1.46	1.34
2	A	301	BMX	C2-N2	3.53	1.51	1.45
2	D	301	BMX	C7-N2	3.44	1.45	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	BMX	C8-C7-N2	6.88	127.52	116.12
2	A	301	BMX	O7-C7-N2	-4.59	113.86	121.98
2	B	301	BMX	C1-C2-N2	-4.42	105.60	110.73
2	B	301	BMX	O5-C1-C2	4.27	113.81	109.52
2	C	301	BMX	O5-C5-C4	3.70	116.37	109.70

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

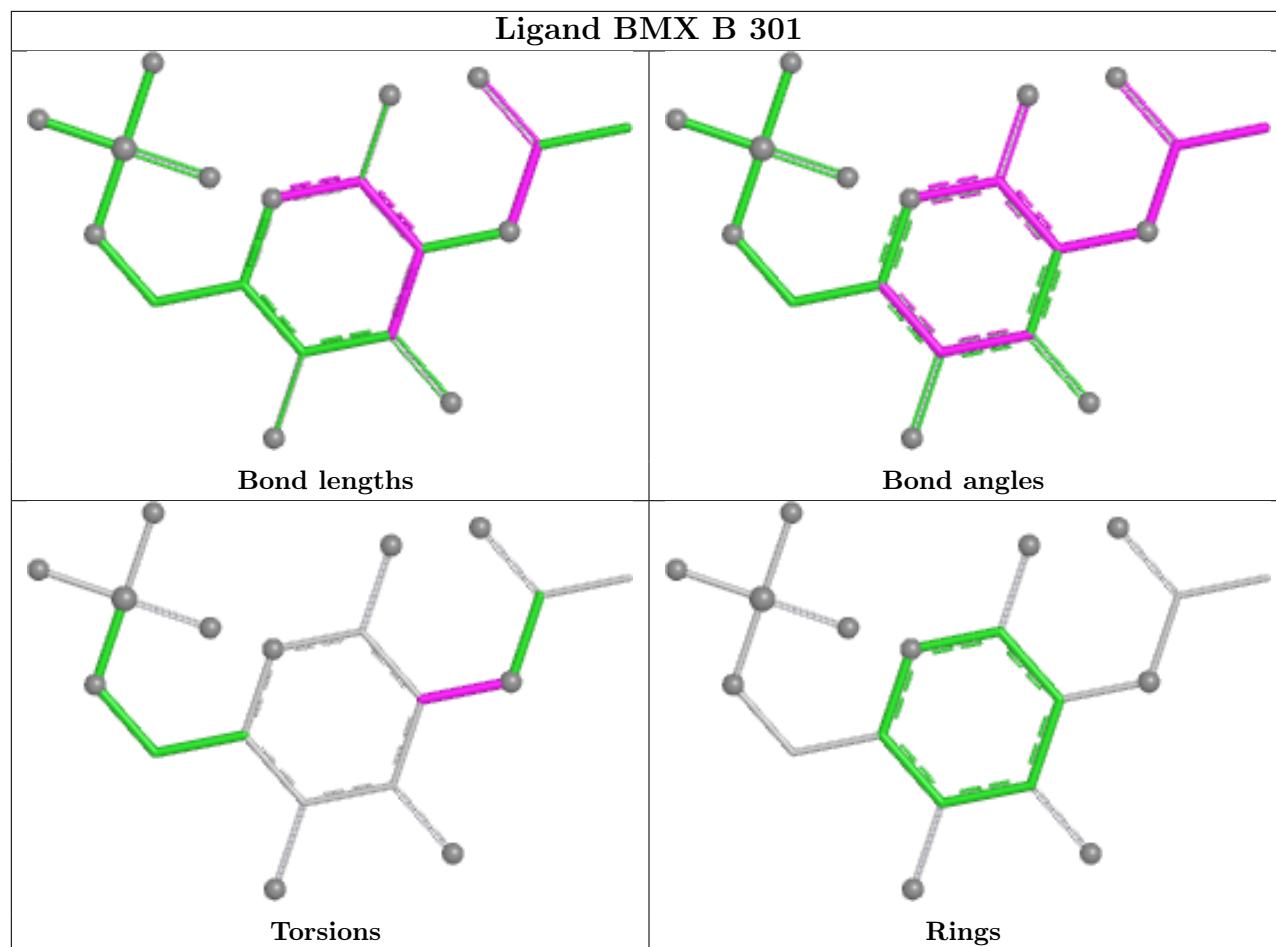
Mol	Chain	Res	Type	Atoms
2	A	301	BMX	C4-C5-C6-O6
2	A	301	BMX	O5-C5-C6-O6
2	A	301	BMX	C6-O6-P-O19
2	A	301	BMX	C6-O6-P-O17
2	A	301	BMX	C6-O6-P-O18

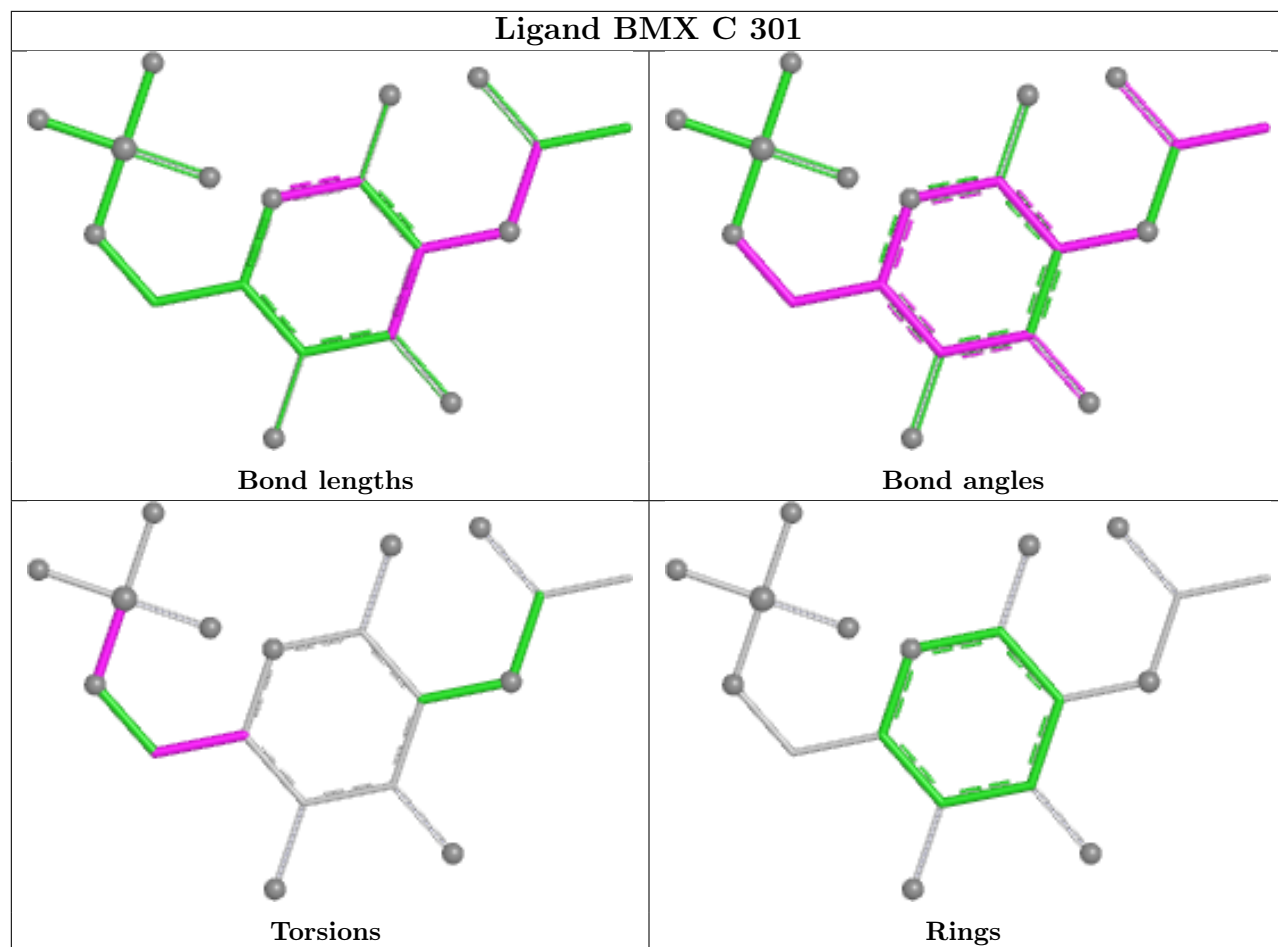
There are no ring outliers.

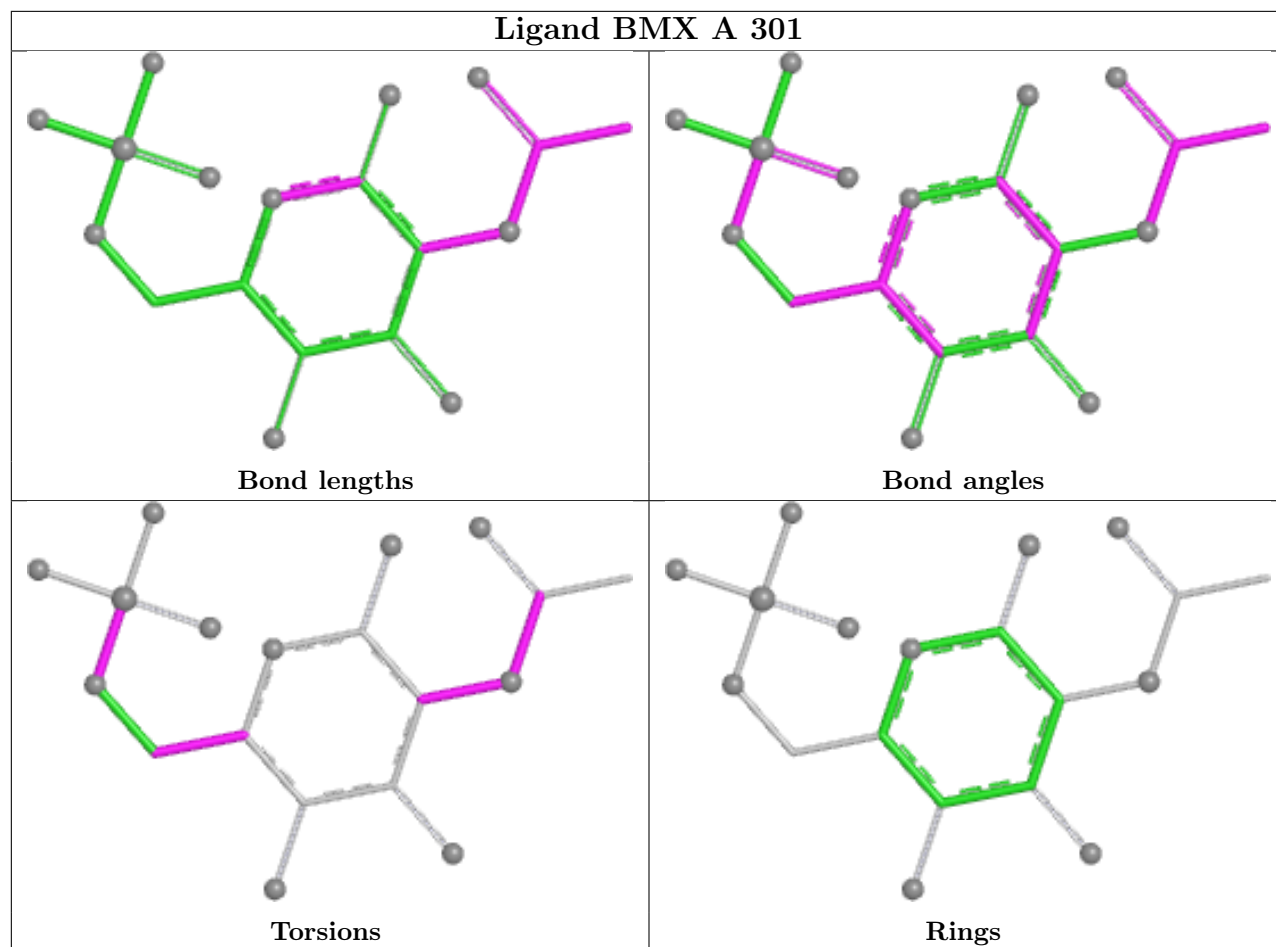
1 monomer is involved in 3 short contacts:

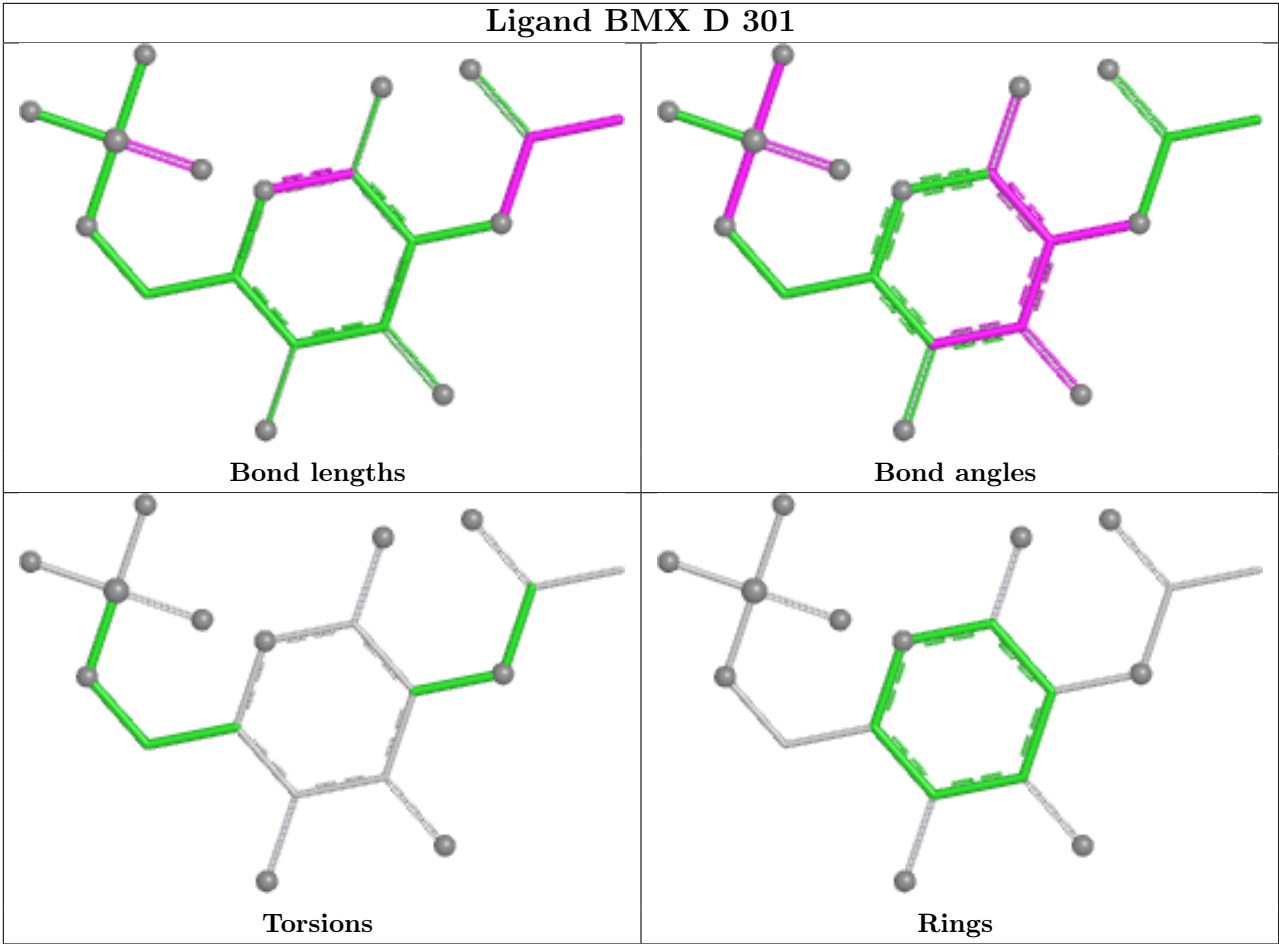
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BMX	3	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	101[A]:MET	C	102:ARG	N	1.08
1	C	101[B]:MSE	C	102:ARG	N	1.08

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	193/286 (67%)	0.90	18 (9%) 14 13	44, 74, 110, 138	0
1	B	184/286 (64%)	0.81	15 (8%) 17 16	46, 71, 104, 149	0
1	C	184/286 (64%)	-0.02	4 (2%) 62 61	18, 49, 92, 126	1 (0%)
1	D	188/286 (65%)	0.27	4 (2%) 63 63	34, 60, 93, 123	0
All	All	749/1144 (65%)	0.49	41 (5%) 30 29	18, 64, 104, 149	1 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	6.8
1	C	274	TYR	6.4
1	D	233	ILE	4.7
1	A	87	HIS	4.7
1	A	222	ALA	3.8

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](#)

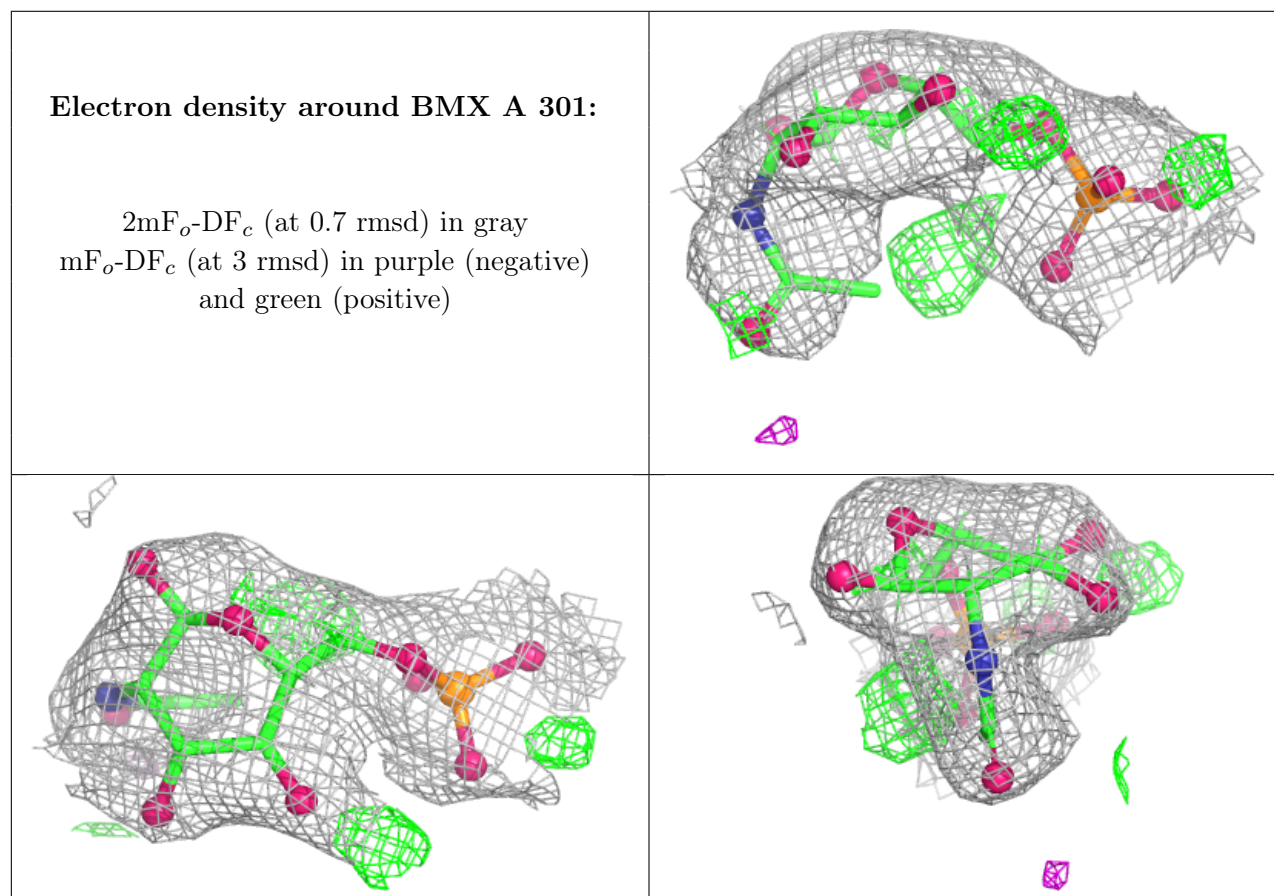
There are no oligosaccharides in this entry.

6.4 Ligands [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.

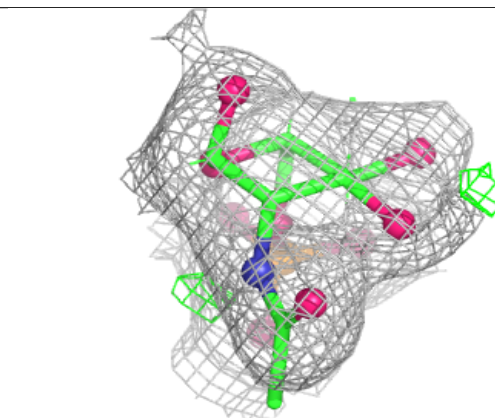
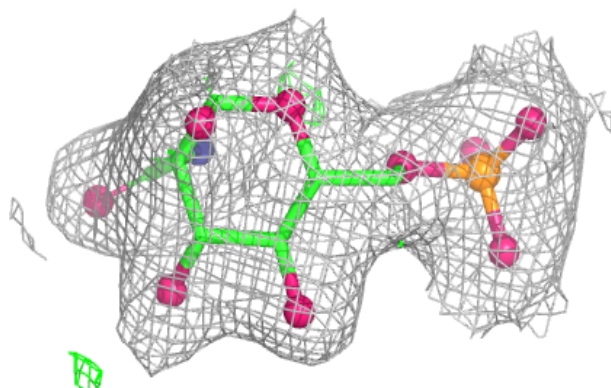
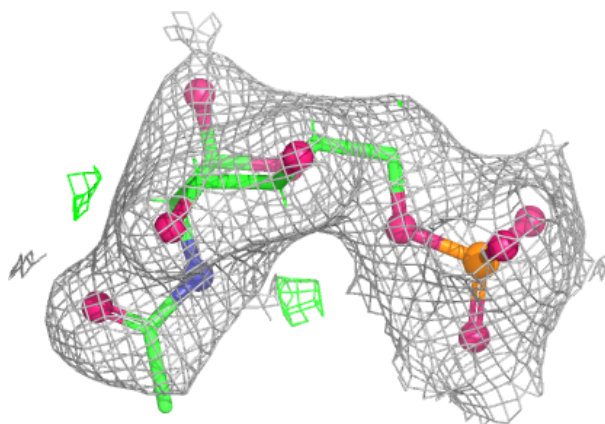
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	302	1/1	0.74	0.22	66,66,66,66	0
2	BMX	A	301	19/19	0.89	0.13	63,77,99,103	0
3	NA	B	302	1/1	0.94	0.15	57,57,57,57	0
2	BMX	B	301	19/19	0.96	0.07	40,46,56,87	0
2	BMX	D	301	19/19	0.97	0.08	41,50,63,74	0
3	NA	D	302	1/1	0.98	0.11	27,27,27,27	0
2	BMX	C	301	19/19	0.98	0.07	32,44,60,61	0
3	NA	C	302	1/1	0.99	0.13	31,31,31,31	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.

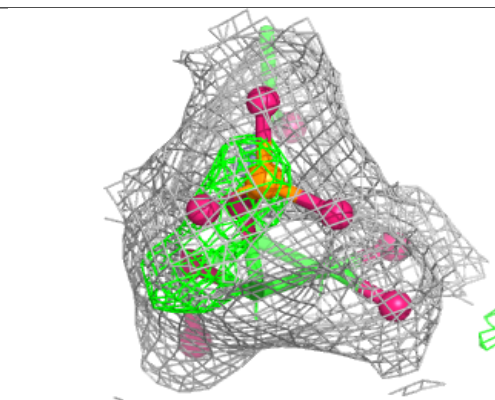
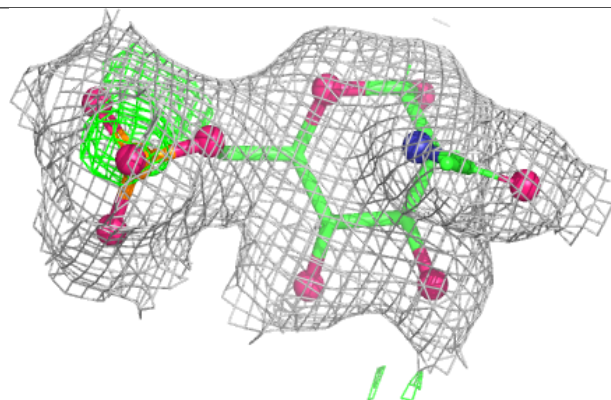
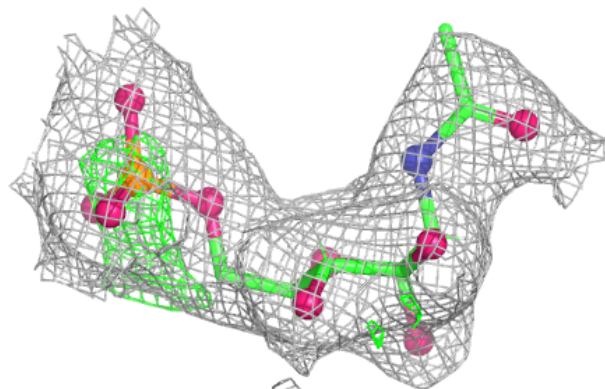


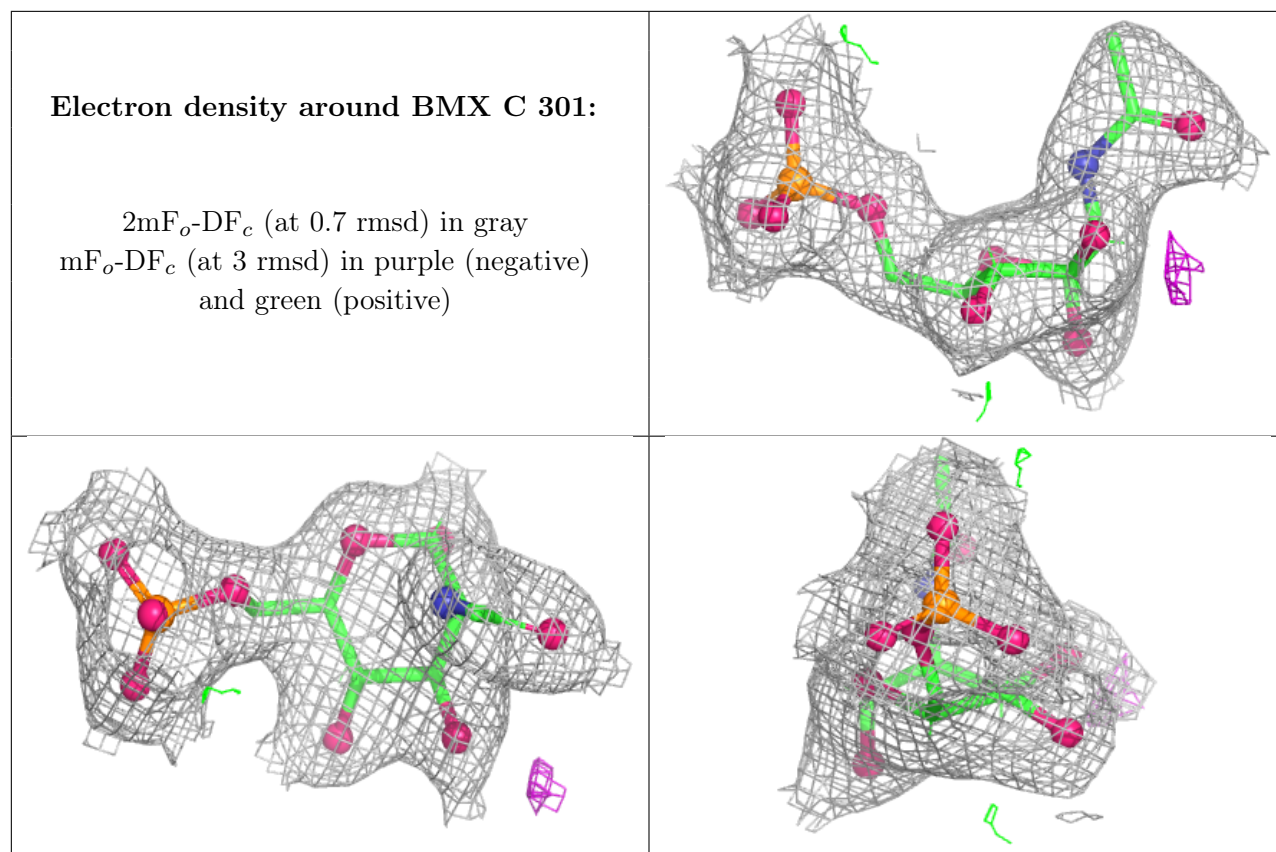
Electron density around BMX B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BMX D 301:**

$2mF_o-DF_c$ (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.