



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:27 AM UTC

PDB ID : 3FED / pdb\_00003fed  
Title : The high resolution structure of human glutamate carboxypeptidase III (GCPIII/NAALADase II) in complex with a transition state analog of Glu-Glu  
Authors : Lubkowski, J.; Barinka, C.; Hlouchova, K.  
Deposited on : 2008-11-28  
Resolution : 1.29 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](mailto: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>.

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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)  
Xtrriage (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

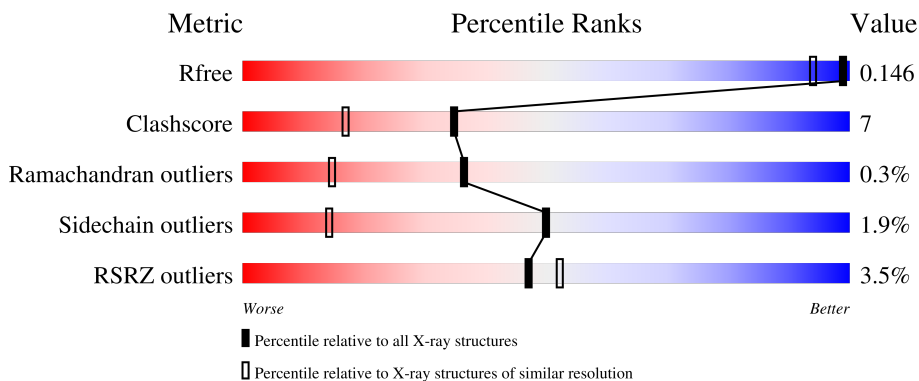
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


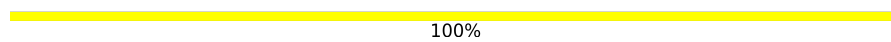
The reported resolution of this entry is 1.29 Å.

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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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  $\geq 3$ , 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	707	 3% 86% 10% ..
2	B	2	 100%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6774 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 Glutamate carboxypeptidase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	690	5819	3765	966	1074	14	0	67	0

There are 2 discrepancies between the modelled and reference sequences:

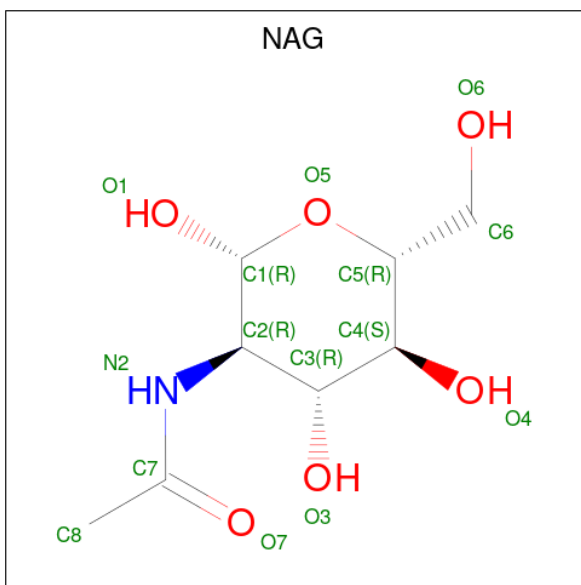
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ARG	-	expression tag	UNP Q9Y3Q0
A	35	SER	-	expression tag	UNP Q9Y3Q0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

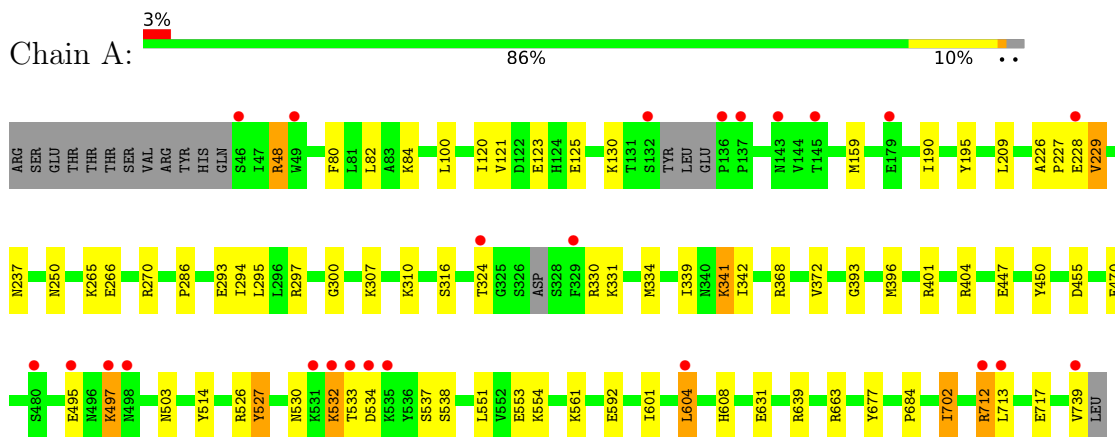
- Molecule 7 is (2S)-2-[(S)-[(3S)-3-amino-3-carboxypropyl](hydroxy)phosphoryl]methyl}pentanedioic acid (CCD ID: BIX) (formula: C<sub>10</sub>H<sub>18</sub>NO<sub>8</sub>P).



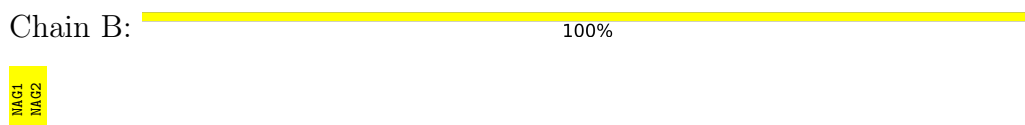
### 3 Residue-property plots [i](#)

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: Glutamate carboxypeptidase III



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.73Å 104.09Å 77.63Å 90.00° 108.19° 90.00°	Depositor
Resolution (Å)	25.00 – 1.29 25.00 – 1.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-1.29) 98.7 (25.00-1.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.29Å)	Xtrriage
Refinement program	REFMAC 5.4.0057	Depositor
R, $R_{free}$	0.131 , 0.147 0.140 , 0.146	Depositor DCC
$R_{free}$ test set	11403 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BIX, ZN, CL, 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	0.88	1/6185 (0.0%)	0.90	0/8361

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	ARG	CG-CD	-5.49	1.35	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	TYR	Sidechain
1	A	404	ARG	Sidechain
1	A	514	TYR	Sidechain
1	A	663	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

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	5819	0	5852	88	0
2	B	28	0	25	0	0
3	A	42	0	39	1	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	20	0	14	0	0
8	A	861	0	0	29	2
All	All	6774	0	5930	89	2

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 7.

All (89) 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:604[A]:LEU:HD23	1:A:604[A]:LEU:O	1.21	1.27
1:A:604[A]:LEU:HD23	1:A:604[A]:LEU:C	1.65	1.17
1:A:80:PHE:CE2	1:A:84[A]:LYS:HE2	1.82	1.14
1:A:250[B]:ASN:ND2	8:A:1090:HOH:O	1.88	1.06
1:A:80:PHE:HE2	1:A:84[A]:LYS:HZ3	1.02	0.96
1:A:604[A]:LEU:C	1:A:604[A]:LEU:CD2	2.37	0.96
1:A:80:PHE:CE2	1:A:84[A]:LYS:CE	2.49	0.94
1:A:341[A]:LYS:HE2	8:A:987:HOH:O	1.68	0.91
1:A:712:ARG:HH21	1:A:712:ARG:HG2	1.38	0.89
1:A:266[A]:GLU:OE1	8:A:1100:HOH:O	1.92	0.86
1:A:396[B]:MET:HE3	1:A:401:ARG:NH1	1.90	0.85
1:A:341[A]:LYS:CE	8:A:987:HOH:O	2.25	0.83
1:A:608:HIS:CD2	1:A:702[A]:ILE:HD11	2.14	0.82
1:A:604[A]:LEU:O	1:A:604[A]:LEU:CD2	2.17	0.82
1:A:293[B]:GLU:OE2	8:A:1164:HOH:O	1.96	0.81
1:A:631[B]:GLU:HG3	8:A:1406:HOH:O	1.80	0.80
1:A:80:PHE:HE2	1:A:84[A]:LYS:NZ	1.80	0.80
1:A:80:PHE:CE2	1:A:84[A]:LYS:NZ	2.49	0.79
1:A:713:LEU:HD12	8:A:911:HOH:O	1.86	0.75
1:A:229[A]:VAL:HG13	1:A:237:ASN:ND2	2.02	0.73
1:A:84[B]:LYS:HE3	8:A:959:HOH:O	1.89	0.72
1:A:226:ALA:HB3	1:A:229[A]:VAL:HG11	1.71	0.72
1:A:561[B]:LYS:HD3	8:A:1153:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:CD1	8:A:911:HOH:O	2.39	0.70
1:A:48:ARG:HH22	1:A:470:GLU:CD	1.99	0.69
1:A:534:ASP:OD2	8:A:884:HOH:O	2.12	0.67
3:A:1756:NAG:O4	8:A:853:HOH:O	2.13	0.67
1:A:530:ASN:OD1	1:A:532:LYS:HG3	1.96	0.66
1:A:80:PHE:CD2	1:A:84[A]:LYS:HE2	2.32	0.64
1:A:120:ILE:HD11	1:A:295:LEU:HD23	1.78	0.64
1:A:396[B]:MET:CE	1:A:401:ARG:NH1	2.59	0.63
1:A:554[A]:LYS:HG2	8:A:1335:HOH:O	1.99	0.62
1:A:532:LYS:HD2	1:A:533:THR:HG23	1.83	0.61
1:A:80:PHE:CZ	1:A:84[A]:LYS:HE2	2.35	0.57
1:A:639[B]:ARG:NE	8:A:1417:HOH:O	2.14	0.57
1:A:310[B]:LYS:NZ	1:A:316:SER:O	2.37	0.57
1:A:48:ARG:NH2	1:A:470:GLU:OE2	2.38	0.56
1:A:592[B]:GLU:CD	8:A:1251:HOH:O	2.48	0.56
1:A:341[A]:LYS:HE2	1:A:342:ILE:H	1.69	0.56
1:A:229[A]:VAL:HG13	1:A:237:ASN:HD21	1.70	0.56
1:A:396[B]:MET:HE3	1:A:401:ARG:HH11	1.70	0.55
1:A:226:ALA:HB3	1:A:229[A]:VAL:CG1	2.35	0.54
1:A:121[B]:VAL:CG1	1:A:125:GLU:HA	2.37	0.54
1:A:739:VAL:CG1	8:A:1532:HOH:O	2.56	0.53
1:A:447[B]:GLU:CD	1:A:526:ARG:NE	2.67	0.53
1:A:631[A]:GLU:HG3	8:A:1142:HOH:O	2.07	0.53
1:A:712:ARG:HG2	1:A:712:ARG:NH2	2.16	0.53
1:A:608:HIS:HD2	1:A:702[A]:ILE:HD11	1.67	0.52
1:A:300:GLY:HA3	1:A:324[B]:THR:HG23	1.92	0.52
1:A:639[B]:ARG:NH1	8:A:1417:HOH:O	2.38	0.52
1:A:330[B]:ARG:HD3	1:A:331:LYS:HG2	1.92	0.52
1:A:209:LEU:HG	8:A:1217:HOH:O	2.10	0.51
1:A:130[B]:LYS:NZ	8:A:1461:HOH:O	2.44	0.51
1:A:339[B]:ILE:HD11	8:A:1292:HOH:O	2.09	0.51
1:A:497:LYS:H	1:A:497:LYS:CD	2.24	0.51
1:A:497:LYS:H	1:A:497:LYS:CE	2.24	0.50
1:A:159:MET:HA	1:A:334:MET:O	2.12	0.49
1:A:227:PRO:O	1:A:228:GLU:HG2	2.11	0.49
1:A:712:ARG:HH21	1:A:712:ARG:CG	2.15	0.49
1:A:82[A]:LEU:HD23	1:A:368:ARG:HG2	1.93	0.49
1:A:294[B]:ILE:HD13	1:A:297:ARG:HH22	1.78	0.48
1:A:307:LYS:NZ	8:A:1017:HOH:O	2.45	0.48
1:A:341[A]:LYS:HE2	1:A:342:ILE:N	2.29	0.47
1:A:554[A]:LYS:HE2	8:A:1335:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLY:HA2	1:A:396[A]:MET:HE3	1.96	0.47
1:A:265[B]:LYS:HD2	8:A:963:HOH:O	2.16	0.46
1:A:455[B]:ASP:OD1	8:A:1467:HOH:O	2.20	0.46
1:A:447[B]:GLU:HG2	1:A:527:TYR:O	2.15	0.46
1:A:553:GLU:OE1	1:A:554[A]:LYS:HE2	2.15	0.46
1:A:717[A]:GLU:HG2	8:A:1510:HOH:O	2.16	0.45
1:A:601:ILE:HD12	1:A:604[A]:LEU:HD13	1.99	0.45
1:A:447[B]:GLU:CD	1:A:526:ARG:HE	2.25	0.45
1:A:190[B]:ILE:HD13	1:A:334:MET:HG3	1.98	0.44
1:A:712:ARG:NH2	1:A:712:ARG:CG	2.79	0.44
1:A:123:GLU:HA	1:A:330[B]:ARG:HD2	2.00	0.43
1:A:537:SER:O	1:A:538:SER:C	2.61	0.43
1:A:447[B]:GLU:OE1	1:A:526:ARG:CZ	2.65	0.43
1:A:310[B]:LYS:HE3	1:A:310[B]:LYS:HB3	1.83	0.43
1:A:341[A]:LYS:HE3	8:A:987:HOH:O	2.06	0.43
1:A:677:TYR:CZ	1:A:684:PRO:HG2	2.54	0.43
1:A:84[B]:LYS:HD3	1:A:100[B]:LEU:HD11	2.01	0.43
1:A:447[B]:GLU:OE1	1:A:526:ARG:NE	2.53	0.42
1:A:604[A]:LEU:CD2	1:A:702[A]:ILE:HD12	2.49	0.42
1:A:450:TYR:CG	1:A:530:ASN:HB2	2.55	0.41
1:A:455[A]:ASP:OD2	1:A:503:ASN:HB2	2.20	0.41
1:A:739:VAL:HG12	8:A:1531:HOH:O	2.20	0.41
1:A:121[B]:VAL:HG11	1:A:125:GLU:HA	2.03	0.41
1:A:84[B]:LYS:HE2	8:A:1015:HOH:O	2.21	0.41
1:A:604[A]:LEU:HD21	1:A:702[A]:ILE:HD12	2.02	0.41

All (2) 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)
8:A:885:HOH:O	8:A:1243:HOH:O[2_555]	1.93	0.27
8:A:993:HOH:O	8:A:1190:HOH:O[2_555]	2.08	0.12

## 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	749/707 (106%)	728 (97%)	19 (2%)	2 (0%)	36 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	VAL
1	A	286	PRO

### 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	656/606 (108%)	641 (98%)	15 (2%)	44 9

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	229[A]	VAL
1	A	229[B]	VAL
1	A	341[A]	LYS
1	A	341[B]	LYS
1	A	495	GLU
1	A	497	LYS
1	A	527	TYR
1	A	532	LYS
1	A	551	LEU
1	A	604[A]	LEU
1	A	604[B]	LEU
1	A	702[A]	ILE
1	A	702[B]	ILE
1	A	712	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	340	ASN
1	A	441	ASN
1	A	563	GLN
1	A	611	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](#)

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.77	0	17,19,21	1.04	1 (5%)
2	NAG	B	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.27	2 (11%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-3.08	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-3.53	105.83	111.29
2	B	2	NAG	O5-C1-C2	-3.19	106.36	111.29
2	B	2	NAG	C1-C2-N2	2.23	113.95	110.43

There are no chirality outliers.

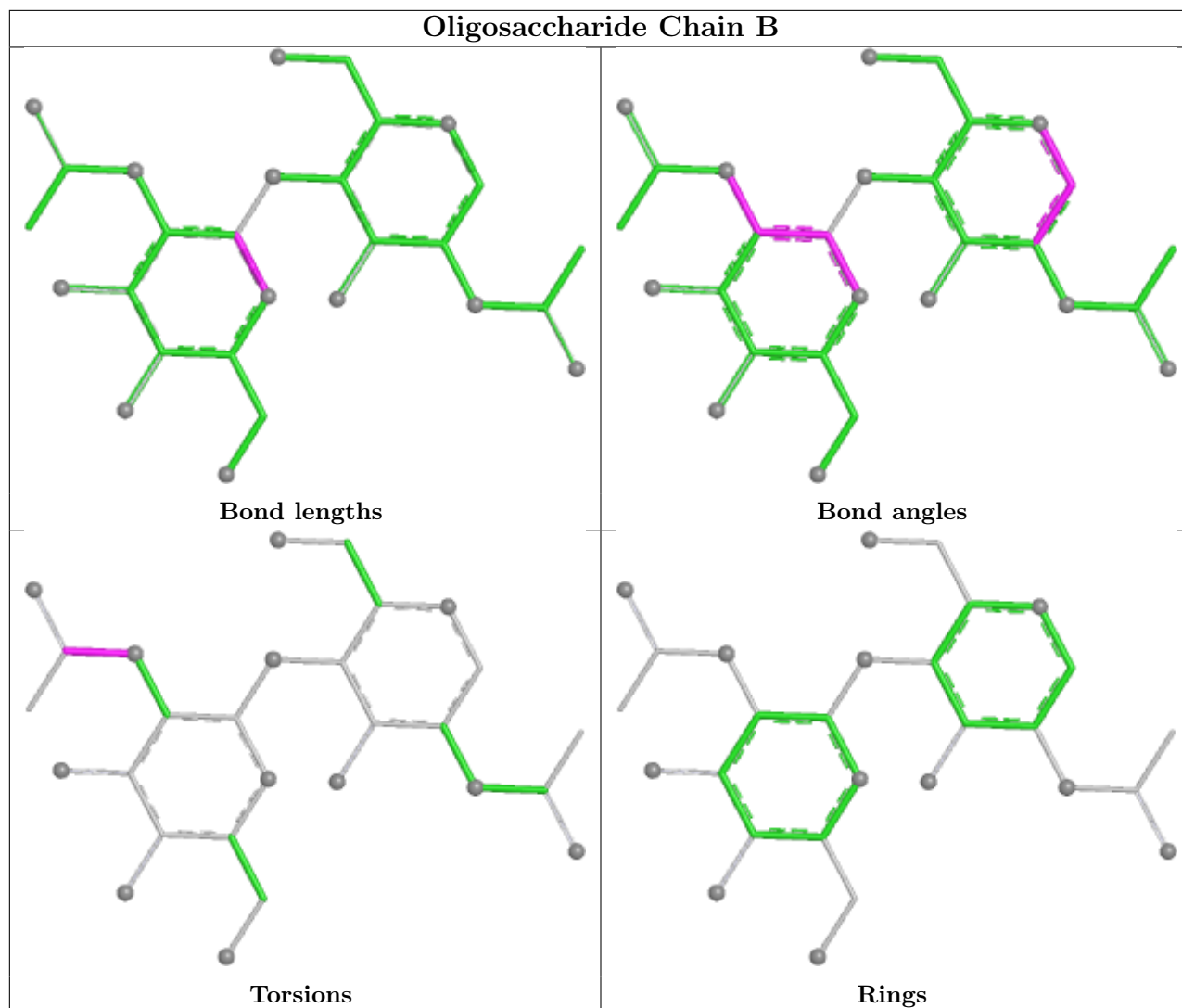
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

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 oligosaccharide.



## 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$
7	BIX	A	1	4	14,19,19	2.26	3 (21%)	13,26,26	1.29	2 (15%)
3	NAG	A	1758	1	14,14,15	0.68	0	17,19,21	1.31	3 (17%)
3	NAG	A	1757	1	14,14,15	1.45	1 (7%)	17,19,21	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1756	1	14,14,15	0.62	0	17,19,21	1.25	2 (11%)

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
7	BIX	A	1	4	-	3/24/24/24	-
3	NAG	A	1758	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1757	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1756	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	BIX	P6-C1	6.59	1.86	1.79
3	A	1757	NAG	O5-C1	-5.09	1.35	1.43
7	A	1	BIX	OE2-CD	-2.65	1.22	1.30
7	A	1	BIX	O-C	2.19	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1757	NAG	C1-C2-N2	-3.06	105.61	110.43
3	A	1758	NAG	O3-C3-C2	-2.72	103.75	109.40
3	A	1758	NAG	O5-C1-C2	-2.41	107.57	111.29
3	A	1756	NAG	C1-C2-N2	2.39	114.19	110.43
3	A	1757	NAG	C3-C4-C5	2.34	114.48	110.23
7	A	1	BIX	OC-C-CA	2.33	120.21	114.16
3	A	1758	NAG	C1-C2-N2	-2.33	106.76	110.43
3	A	1756	NAG	O5-C1-C2	-2.20	107.89	111.29
7	A	1	BIX	OC-C-O	-2.00	119.54	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	BIX	CA-C1-P6-O6
7	A	1	BIX	CA-C1-P6-C5
3	A	1757	NAG	O5-C5-C6-O6

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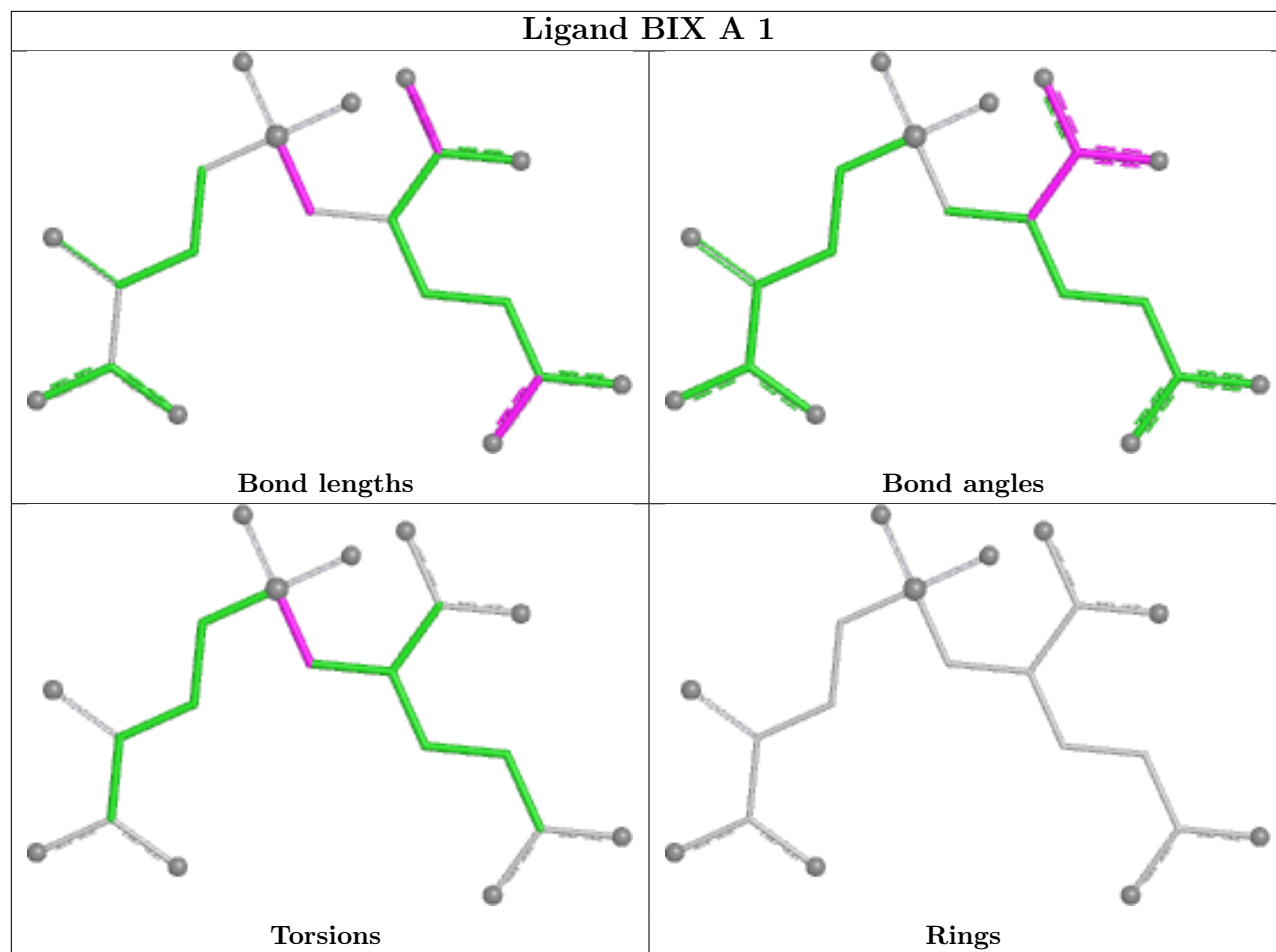
Mol	Chain	Res	Type	Atoms
7	A	1	BIX	CA-C1-P6-O61

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1756	NAG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	690/707 (97%)	0.05	24 (3%) 47 52	7, 14, 28, 45	67 (9%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	PRO	4.7
1	A	739	VAL	4.3
1	A	532	LYS	3.8
1	A	145[A]	THR	3.5
1	A	49	TRP	3.4
1	A	535	LYS	3.3
1	A	480	SER	3.1
1	A	712	ARG	3.1
1	A	531	LYS	3.0
1	A	533	THR	3.0
1	A	228	GLU	3.0
1	A	604[A]	LEU	2.6
1	A	143	ASN	2.6
1	A	534	ASP	2.5
1	A	132[A]	SER	2.4
1	A	329	PHE	2.2
1	A	498	ASN	2.2
1	A	324[A]	THR	2.2
1	A	497	LYS	2.1
1	A	179	GLU	2.1
1	A	713	LEU	2.1
1	A	137	PRO	2.0
1	A	495	GLU	2.0
1	A	46	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

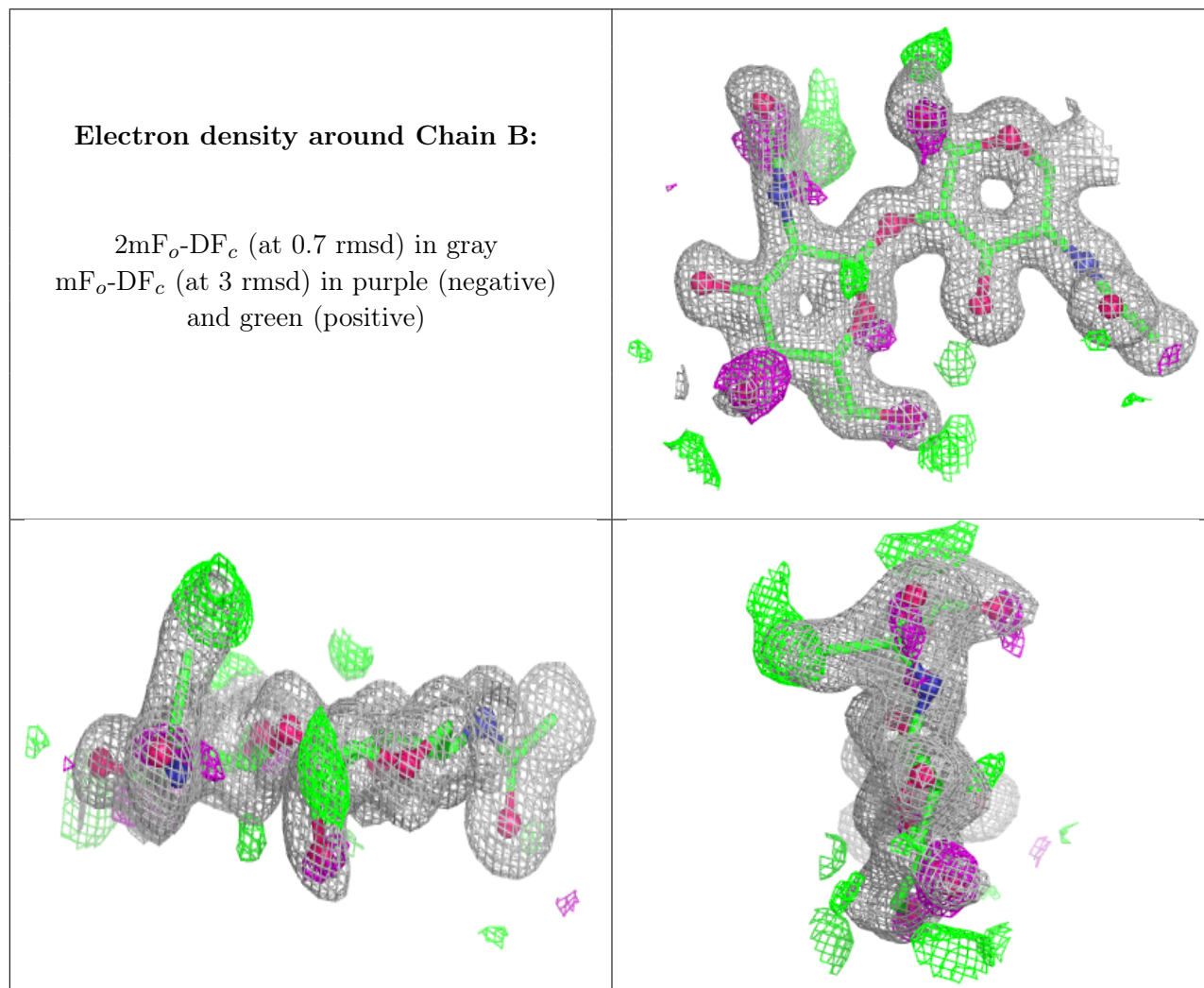
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.82	0.14	23,29,33,39	0
2	NAG	B	1	14/15	0.97	0.07	13,16,24,32	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

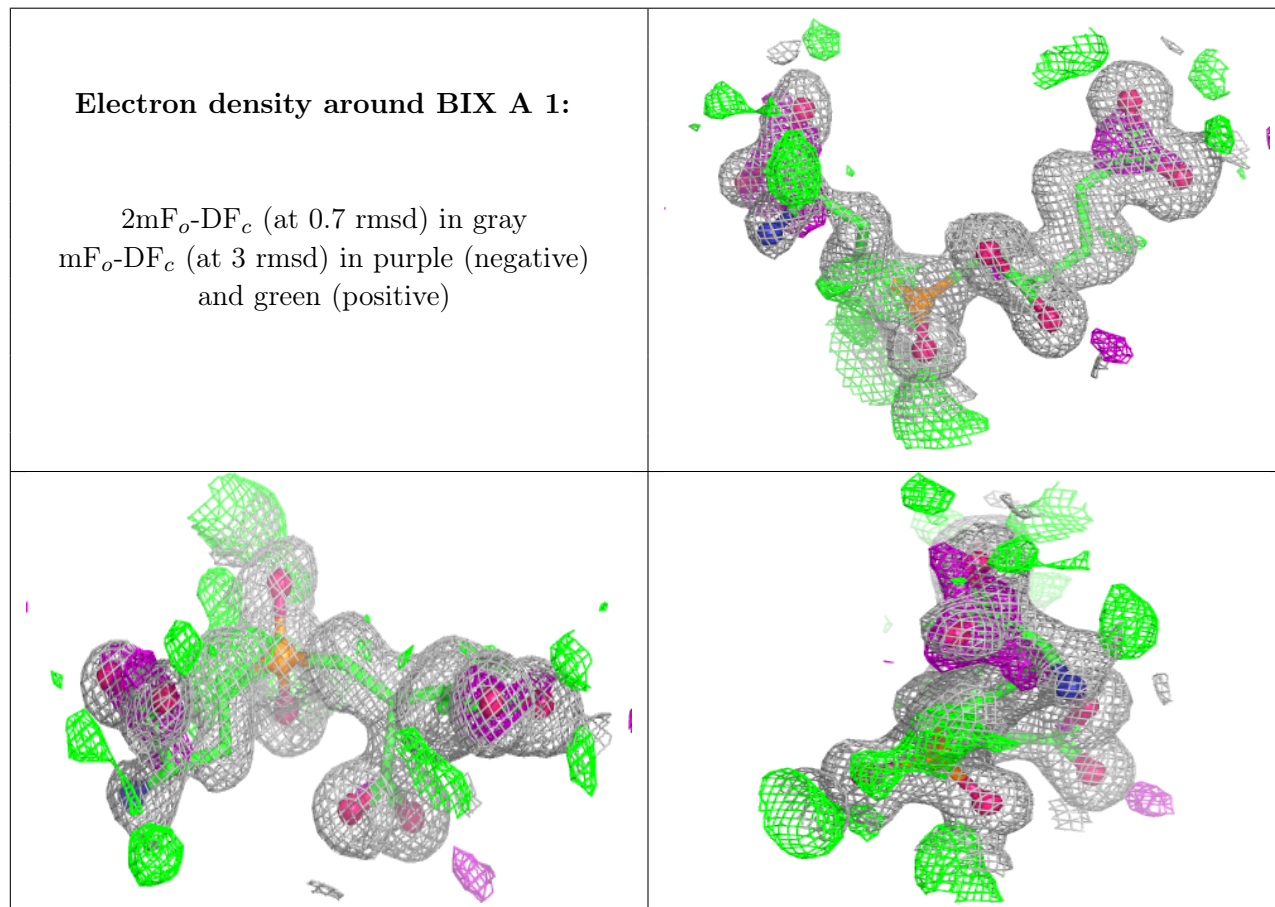


## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	1757	14/15	0.62	0.20	38,45,48,49	0
3	NAG	A	1756	14/15	0.92	0.09	23,27,32,33	0
3	NAG	A	1758	14/15	0.93	0.09	18,23,30,34	0
7	BIX	A	1	20/20	0.95	0.11	9,13,25,25	20
5	CL	A	1754	1/1	0.99	0.03	14,14,14,14	1
4	ZN	A	1751	1/1	1.00	0.04	10,10,10,10	0
6	CA	A	1755	1/1	1.00	0.03	9,9,9,9	0
4	ZN	A	1752	1/1	1.00	0.05	10,10,10,10	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.