



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 PM UTC

PDB ID : 9QA2 / pdb\_00009qa2  
Title : Drosophila melanogaster angiotensin converting enzyme homologue, AnCE in complex with RW dipeptide  
Authors : Zukowska, J.; Gregory, K.S.; Acharya, K.R.  
Deposited on : 2025-02-27  
Resolution : 1.90 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)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
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

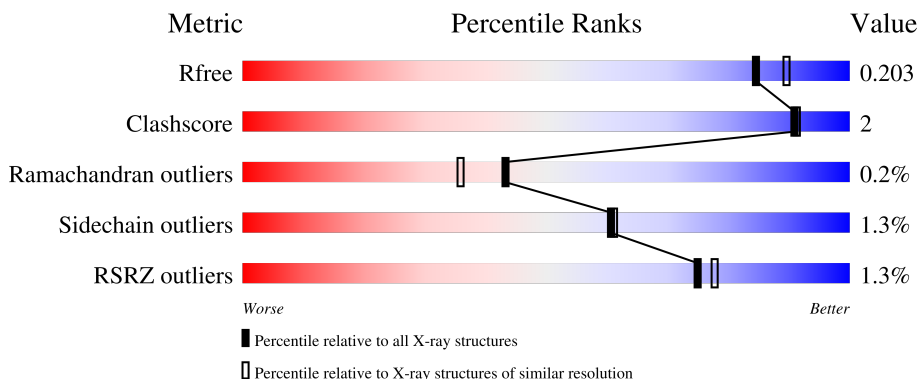
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	B	2	100%
1	C	2	100%
2	A	598	92% (8% outliers)
3	D	6	100%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5549 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 ARG-TRP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	B	2	26	17	6	3	0	0	0
1	C	2	26	17	6	3	0	0	0

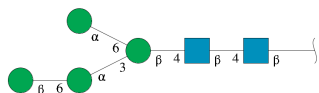
- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	598	4878	3123	805	930	20	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ILE	THR	conflict	UNP Q10714

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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			
3	D	6	72	40	2	30	0	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

- Molecule 5 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
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	4	Total O 4 4	0	0
6	C	6	Total O 6 6	0	0
6	A	508	Total O 508 508	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: ARG-TRP

Chain B:  100%

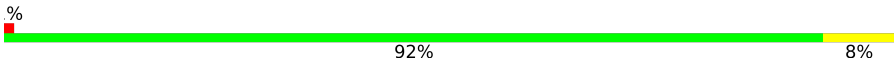
There are no outlier residues recorded for this chain.

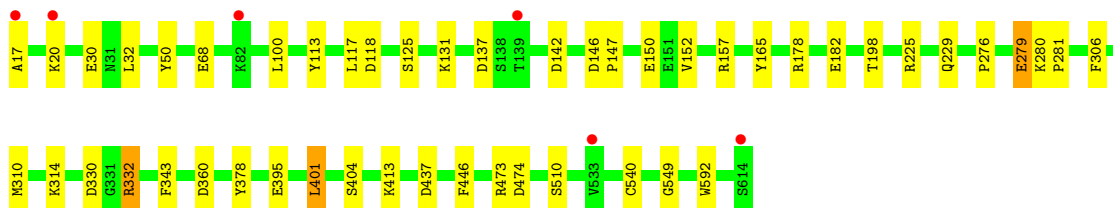
- Molecule 1: ARG-TRP

Chain C:  100%

  
R33  
R34

- Molecule 2: Angiotensin-converting enzyme

Chain A:  %  
92% 8%



- Molecule 3: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

  
MAN1  
MAN2  
MAN3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.89Å 172.89Å 103.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.45 – 1.90 86.45 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.45-1.90) 100.0 (86.45-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.164 , 0.200 0.171 , 0.203	Depositor DCC
$R_{free}$ test set	4427 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.697	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.000 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$ 0.000 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.000 for $-h,2/3^*h+1/3^*k+4/3^*l,1/3^*h+2/3^*k-1/3^*l$ 0.008 for $-1/3^*h-2/3^*k+4/3^*l,-2/3^*h-1/3^*k-4/3^*l,1/3^*h-1/3^*k-1/3^*l$ 0.000 for $1/3^*h+2/3^*k-4/3^*l,-k,-2/3^*h-1/3^*k-1/3^*l$ 0.012 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, BMA, MAN, ZN

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	B	0.62	0/27	0.55	0/34
1	C	0.73	0/27	1.34	0/34
2	A	0.69	0/5004	1.12	13/6779 (0.2%)
All	All	0.69	0/5058	1.12	13/6847 (0.2%)

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
2	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	343	PHE	CA-CB-CG	-6.55	107.25	113.80
2	A	332	ARG	CB-CG-CD	-6.25	96.92	111.30
2	A	279	GLU	CB-CA-C	-6.08	97.86	109.95
2	A	198	THR	CA-CB-OG1	-5.53	101.30	109.60
2	A	401	LEU	N-CA-CB	5.50	118.29	110.16
2	A	474	ASP	CA-CB-CG	5.49	118.09	112.60
2	A	314	LYS	N-CA-CB	-5.42	102.37	110.17
2	A	437	ASP	CA-CB-CG	5.40	118.00	112.60
2	A	68	GLU	CB-CA-C	-5.39	101.68	110.85
2	A	118	ASP	CA-CB-CG	5.37	117.97	112.60
2	A	157	ARG	NE-CZ-NH2	-5.30	114.42	119.20
2	A	150	GLU	CB-CG-CD	5.21	121.45	112.60
2	A	413	LYS	CD-CE-NZ	-5.09	95.60	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	473	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	B	26	0	22	0	0
1	C	26	0	22	0	0
2	A	4878	0	4680	17	0
3	D	72	0	61	0	0
4	A	1	0	0	0	0
5	A	28	0	26	0	0
6	A	508	0	0	3	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
All	All	5549	0	4811	17	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 2.

All (17) 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)
2:A:17:ALA:HB3	6:A:1212:HOH:O	1.93	0.69
2:A:306:PHE:CD1	2:A:401:LEU:HD13	2.40	0.56
2:A:279:GLU:HG2	6:A:1102:HOH:O	2.06	0.55
2:A:113:TYR:CE2	2:A:117:LEU:HD11	2.45	0.51
2:A:276:PRO:HB3	2:A:592:TRP:CH2	2.48	0.48
2:A:152:VAL:HG11	2:A:165:TYR:CD2	2.49	0.48
2:A:32:LEU:HD23	2:A:100:LEU:HD13	1.98	0.45
2:A:178:ARG:NE	2:A:182:GLU:OE2	2.46	0.45
2:A:310:MET:O	2:A:549:GLY:HA3	2.18	0.44
2:A:330:ASP:OD1	2:A:332:ARG:HD3	2.18	0.44
2:A:395:GLU:HB2	2:A:510:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:146:ASP:HA	2:A:147:PRO:HA	1.84	0.42
2:A:280:LYS:HB3	2:A:281:PRO:HD2	2.03	0.41
2:A:131:LYS:HD2	2:A:142:ASP:HA	2.02	0.41
2:A:17:ALA:CB	6:A:1212:HOH:O	2.62	0.41
2:A:50:TYR:OH	2:A:125:SER:HB3	2.22	0.40
2:A:225:ARG:O	2:A:229:GLN:HG2	2.22	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
2	A	596/598 (100%)	589 (99%)	6 (1%)	1 (0%)	43 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	137	ASP

### 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	B	2/2 (100%)	2 (100%)	0	100 100
1	C	2/2 (100%)	2 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	520/520 (100%)	513 (99%)	7 (1%)	61	61
All	All	524/524 (100%)	517 (99%)	7 (1%)	61	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	LYS
2	A	30	GLU
2	A	360	ASP
2	A	378	TYR
2	A	404	SER
2	A	446	PHE
2	A	540	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 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	$\# Z  > 2$
3	NAG	D	1	2,3	14,14,15	0.48	0	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	2	3	14,14,15	0.51	0	17,19,21	1.37	2 (11%)
3	BMA	D	3	3	11,11,12	0.72	0	15,15,17	1.13	1 (6%)
3	MAN	D	4	3	11,11,12	0.93	1 (9%)	15,15,17	1.96	3 (20%)
3	BMA	D	5	3	11,11,12	1.14	1 (9%)	15,15,17	2.26	6 (40%)
3	MAN	D	6	3	11,11,12	1.04	1 (9%)	15,15,17	1.65	3 (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
3	NAG	D	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	BMA	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	BMA	C2-C3	-3.25	1.47	1.52
3	D	6	MAN	C2-C3	2.61	1.56	1.52
3	D	4	MAN	C4-C5	2.56	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	4.70	118.49	112.19
3	D	1	NAG	C2-N2-C7	4.13	128.44	122.90
3	D	5	BMA	C1-C2-C3	4.04	115.53	109.64
3	D	5	BMA	O3-C3-C4	4.03	119.87	110.38
3	D	6	MAN	C1-C2-C3	4.02	115.49	109.64
3	D	5	BMA	C3-C4-C5	-3.51	103.87	110.23
3	D	5	BMA	C2-C3-C4	-3.32	105.01	110.86
3	D	6	MAN	C1-O5-C5	3.23	116.51	112.19
3	D	2	NAG	C2-N2-C7	3.17	127.14	122.90
3	D	4	MAN	O5-C5-C6	-3.13	101.58	107.66
3	D	3	BMA	C1-O5-C5	3.10	116.34	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	O2-C2-C3	3.09	116.54	110.15
3	D	5	BMA	C1-O5-C5	2.81	115.95	112.19
3	D	6	MAN	O3-C3-C2	2.63	115.42	110.05
3	D	2	NAG	O7-C7-N2	-2.44	117.67	121.98
3	D	5	BMA	O2-C2-C3	-2.30	105.39	110.15

There are no chirality outliers.

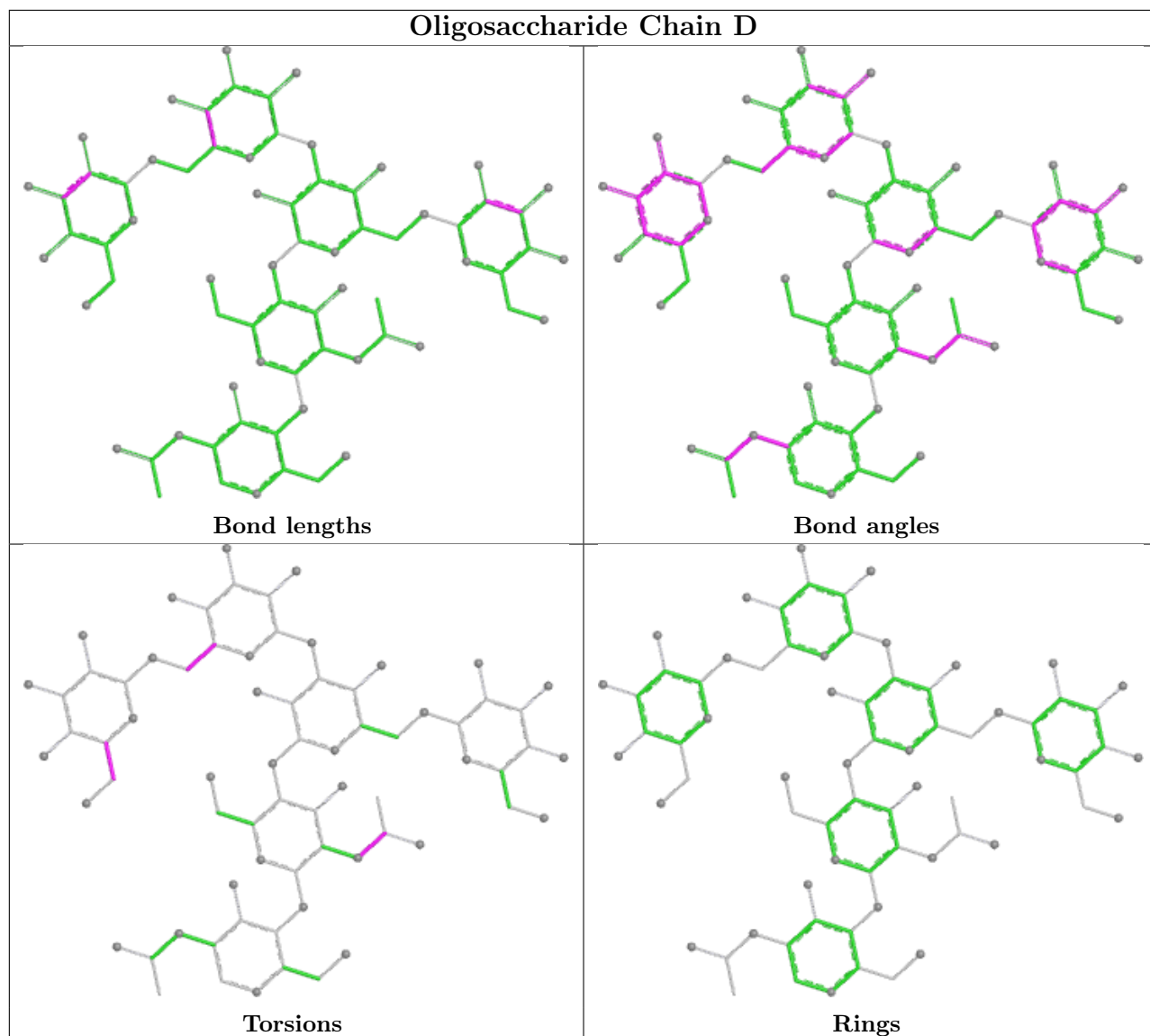
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	5	BMA	O5-C5-C6-O6
3	D	5	BMA	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
5	NAG	A	703	2	14,14,15	0.37	0	17,19,21	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	702	2	14,14,15	0.48	0	17,19,21	1.53	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
5	NAG	A	703	2	-	2/6/23/26	0/1/1/1
5	NAG	A	702	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	NAG	C1-C2-N2	-4.62	103.15	110.43
5	A	703	NAG	C3-C4-C5	-2.36	105.95	110.23
5	A	703	NAG	C1-O5-C5	2.31	115.28	112.19
5	A	702	NAG	C4-C3-C2	2.03	113.99	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	NAG	C8-C7-N2-C2
5	A	702	NAG	O7-C7-N2-C2
5	A	703	NAG	C4-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	B	2/2 (100%)	0.36	0 <b>100</b> <b>100</b>	39, 39, 39, 41	0
1	C	2/2 (100%)	2.29	2 (100%) <b>0</b> <b>0</b>	46, 46, 46, 64	0
2	A	598/598 (100%)	-0.02	6 (1%) <b>79</b> <b>82</b>	22, 31, 50, 71	0
All	All	602/602 (100%)	-0.01	8 (1%) <b>75</b> <b>78</b>	22, 31, 50, 71	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	17	ALA	4.6
2	A	82	LYS	4.4
2	A	614	SER	3.1
2	A	139	THR	2.7
2	A	20	LYS	2.5
1	C	33	ARG	2.3
1	C	34	TRP	2.3
2	A	533	VAL	2.0

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

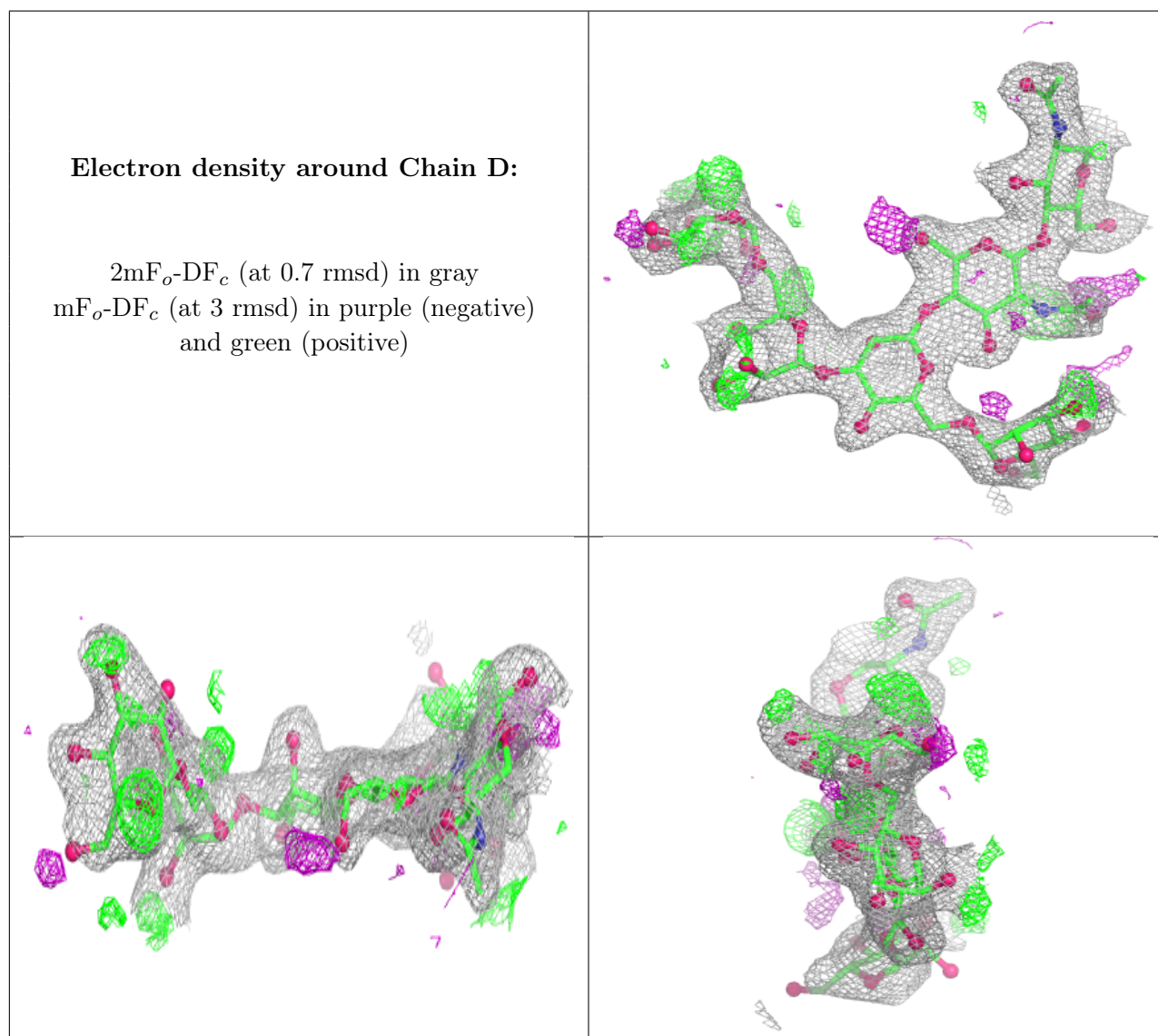
There are no non-standard protein/DNA/RNA residues in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
3	MAN	D	6	11/12	0.76	0.17	71,84,94,99	0
3	BMA	D	5	11/12	0.84	0.19	49,66,77,106	0
3	MAN	D	4	11/12	0.88	0.13	46,56,61,62	0
3	BMA	D	3	11/12	0.91	0.11	46,58,68,75	0
3	NAG	D	2	14/15	0.91	0.11	34,41,53,63	0
3	NAG	D	1	14/15	0.97	0.07	27,32,37,39	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.



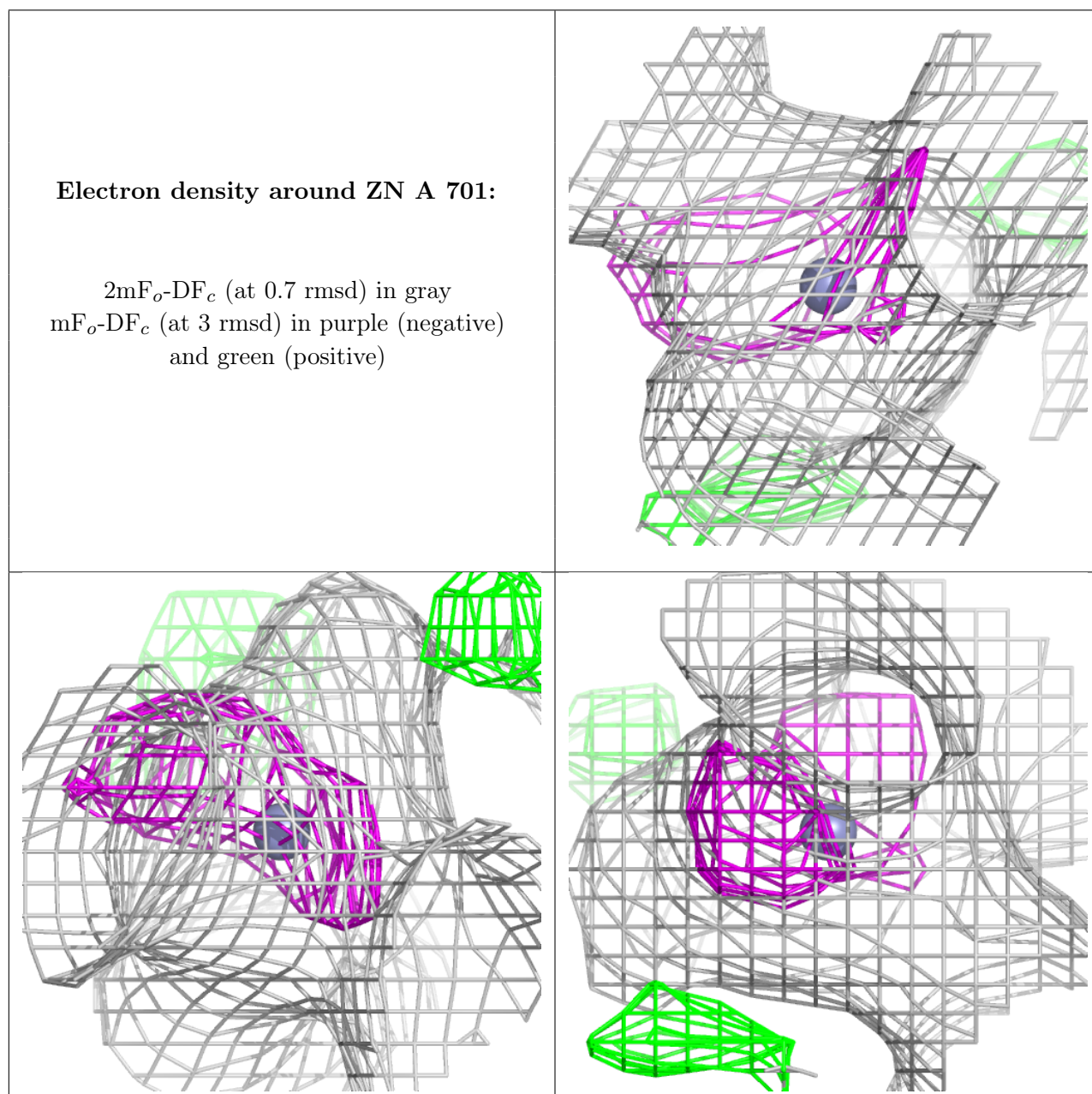
## 6.4 Ligands [i](#)

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
5	NAG	A	702	14/15	0.76	0.17	58,68,85,88	0
5	NAG	A	703	14/15	0.78	0.17	52,76,93,96	0
4	ZN	A	701	1/1	1.00	0.04	28,28,28,28	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.