



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 01:28 pm BST

PDB ID : 2BJJ  
Title : membrane-bound glutamate carboxypeptidase II (GCPII) in complex with 2-PMPA (2-phosphonoMethyl-pentanedioic acid)  
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.  
Deposited on : 2006-12-07  
Resolution : 2.19 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

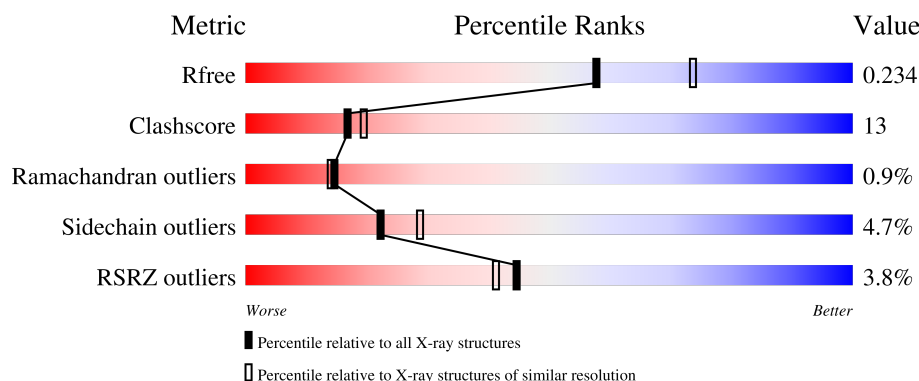
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>...</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	4	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5914 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5318	3430	881	990	17			

- 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

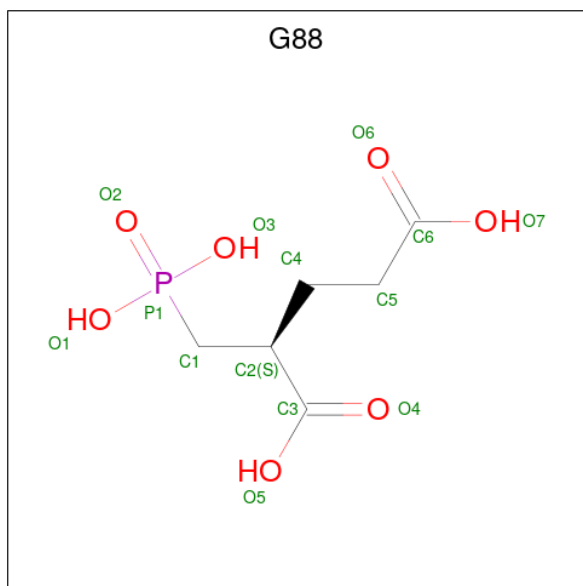
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is (2S)-2-(PHOSPHONOMETHYL)PENTANEDIOIC ACID (three-letter code:

G88) (formula: C<sub>6</sub>H<sub>11</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			14	6	7	1		

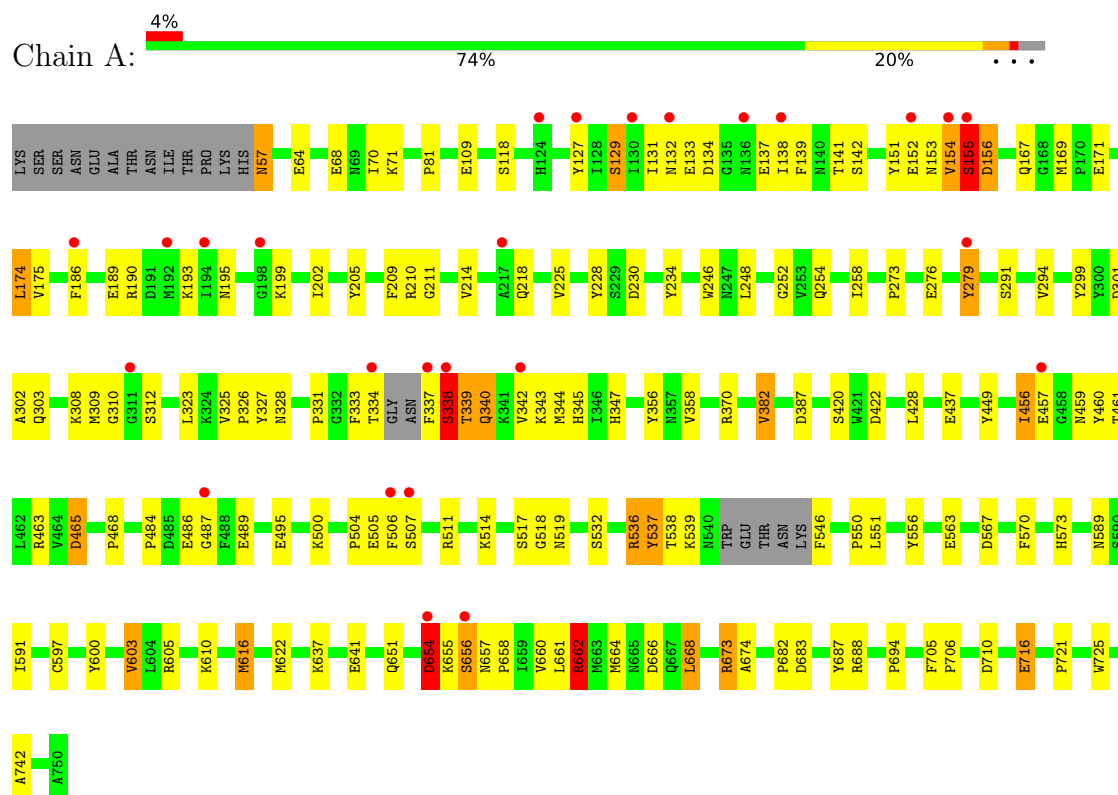
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	402	Total	O	0	0
			402	402		

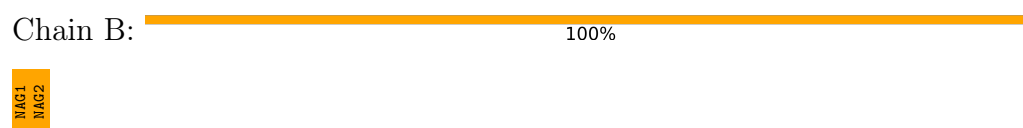
### 3 Residue-property plots

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 2



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



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





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

Chain D:



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

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.75Å 130.98Å 159.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.02 – 2.19 101.02 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.1 (101.02-2.19) 96.1 (101.02-2.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.238 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	1344 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage'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: G88, NAG, CA, MAN, BMA, CL, 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	A	1.12	3/5468 (0.1%)	1.00	15/7431 (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
1	A	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	CYS	CB-SG	5.60	1.91	1.82
1	A	603	VAL	CB-CG2	-5.10	1.42	1.52
1	A	279	TYR	CE2-CZ	5.07	1.45	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	A	662	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	A	654	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	370	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	387	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	339	THR	N-CA-C	-6.21	94.23	111.00
1	A	156	ASP	N-CA-C	5.73	126.47	111.00
1	A	514	LYS	CD-CE-NZ	-5.69	98.61	111.70
1	A	654	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	668	LEU	CB-CG-CD1	5.65	120.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	210	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	688	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	428	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	710	ASP	CB-CG-OD1	5.10	122.89	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	156	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	Peptide
1	A	155	SER	Peptide
1	A	338	SER	Peptide

## 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	5318	0	5004	127	0
2	B	28	0	25	3	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	E	50	0	43	3	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	42	0	39	2	0
8	A	14	0	8	0	0
9	A	402	0	0	39	0
All	All	5914	0	5169	134	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 13.

All (134) 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:657:ASN:ND2	1:A:660:VAL:HG23	1.71	1.05
1:A:651:GLN:CG	9:A:2143:HOH:O	2.05	1.03
1:A:616:MET:HE3	1:A:616:MET:HA	1.44	0.98
9:A:2399:HOH:O	3:E:4:MAN:H61	1.66	0.95
1:A:589:ASN:HB2	9:A:2264:HOH:O	1.65	0.95
1:A:563:GLU:HG2	9:A:2255:HOH:O	1.70	0.91
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.36	0.88
9:A:2396:HOH:O	3:E:3:BMA:H5	1.75	0.86
1:A:134:ASP:CA	9:A:2036:HOH:O	2.31	0.77
1:A:133:GLU:CA	9:A:2035:HOH:O	2.33	0.74
1:A:57:ASN:N	9:A:2001:HOH:O	2.21	0.73
1:A:133:GLU:N	9:A:2035:HOH:O	2.21	0.73
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.69	0.73
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.00	0.72
1:A:109:GLU:HG2	9:A:2020:HOH:O	1.89	0.72
1:A:338:SER:HB2	1:A:339:THR:HB	1.72	0.71
1:A:660:VAL:O	1:A:664:MET:HG2	1.90	0.71
1:A:154:VAL:CA	9:A:2055:HOH:O	2.39	0.70
1:A:654:ASP:OD1	1:A:656:SER:HB3	1.92	0.69
2:B:1:NAG:H61	2:B:2:NAG:C1	2.22	0.69
1:A:616:MET:HA	1:A:616:MET:CE	2.22	0.69
1:A:337:PHE:N	9:A:2154:HOH:O	2.27	0.68
1:A:167:GLN:HG2	1:A:347:HIS:HA	1.77	0.67
9:A:2398:HOH:O	3:E:4:MAN:H2	1.96	0.66
1:A:193:LYS:CB	9:A:2034:HOH:O	2.44	0.65
1:A:716:GLU:H	1:A:716:GLU:CD	2.00	0.65
1:A:138:ILE:N	1:A:138:ILE:HD13	2.11	0.64
1:A:151:TYR:C	1:A:153:ASN:H	1.99	0.64
1:A:486:GLU:CG	9:A:2220:HOH:O	2.45	0.64
1:A:174:LEU:HD22	1:A:342:VAL:HG21	1.79	0.64
1:A:132:ASN:HD22	1:A:138:ILE:HD11	1.63	0.63
9:A:2217:HOH:O	2:D:1:NAG:H83	1.98	0.63
1:A:337:PHE:O	1:A:339:THR:N	2.32	0.62
1:A:131:ILE:HD11	1:A:171:GLU:OE2	1.99	0.62
1:A:657:ASN:HD22	1:A:660:VAL:HG21	1.62	0.62
1:A:68:GLU:CG	9:A:2010:HOH:O	2.47	0.62
1:A:151:TYR:C	1:A:153:ASN:N	2.49	0.61
1:A:657:ASN:HD21	1:A:660:VAL:HG23	1.62	0.61
1:A:637:LYS:NZ	1:A:641:GLU:OE1	2.32	0.61
1:A:616:MET:HE3	1:A:622:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:CB	9:A:2081:HOH:O	2.49	0.60
1:A:456:ILE:HD12	1:A:573:HIS:CE1	2.36	0.60
1:A:456:ILE:HG12	1:A:456:ILE:O	1.99	0.60
1:A:591:ILE:HG23	1:A:661:LEU:HD21	1.82	0.60
1:A:682:PRO:O	1:A:683:ASP:HB2	2.00	0.60
1:A:654:ASP:OD1	1:A:656:SER:CB	2.50	0.59
9:A:2012:HOH:O	2:B:1:NAG:H82	2.01	0.59
1:A:589:ASN:CB	9:A:2264:HOH:O	2.36	0.58
1:A:563:GLU:CG	9:A:2255:HOH:O	2.39	0.57
1:A:171:GLU:HA	1:A:342:VAL:O	2.05	0.57
1:A:246:TRP:CD1	7:A:1761:NAG:H83	2.41	0.56
1:A:131:ILE:HG22	1:A:137:GLU:HG3	1.88	0.56
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.40	0.56
1:A:308:LYS:O	1:A:333:PHE:HB3	2.05	0.56
1:A:539:LYS:CD	9:A:2248:HOH:O	2.53	0.56
1:A:460:TYR:CE1	1:A:500:LYS:HD3	2.41	0.56
1:A:505:GLU:CA	9:A:2223:HOH:O	2.53	0.56
9:A:2383:HOH:O	2:B:2:NAG:H81	2.06	0.55
1:A:225:VAL:O	1:A:294:VAL:HA	2.06	0.55
1:A:234:TYR:O	1:A:550:PRO:HB3	2.06	0.55
1:A:309:MET:HE2	1:A:328:ASN:O	2.06	0.55
1:A:616:MET:CE	1:A:622:MET:SD	2.96	0.54
1:A:459:ASN:OD1	7:A:1761:NAG:H2	2.07	0.54
1:A:337:PHE:O	1:A:338:SER:C	2.46	0.54
1:A:171:GLU:HB3	1:A:343:LYS:HG3	1.90	0.54
1:A:666:ASP:OD2	9:A:2322:HOH:O	2.18	0.53
1:A:129:SER:HA	1:A:139:PHE:O	2.09	0.53
1:A:468:PRO:HG2	1:A:603:VAL:HG21	1.90	0.53
1:A:138:ILE:O	2:C:1:NAG:H82	2.08	0.53
1:A:175:VAL:HG23	1:A:199:LYS:HG3	1.91	0.53
1:A:109:GLU:HB2	9:A:2089:HOH:O	2.08	0.53
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.44	0.53
1:A:457:GLU:OE2	1:A:538:THR:OG1	2.23	0.53
1:A:456:ILE:HD12	1:A:573:HIS:HE1	1.74	0.52
1:A:279:TYR:HD2	9:A:2129:HOH:O	1.93	0.52
1:A:662:ARG:HD2	9:A:2322:HOH:O	2.10	0.51
1:A:495:GLU:CB	9:A:2098:HOH:O	2.58	0.51
1:A:248:LEU:HD11	1:A:252:GLY:HA3	1.92	0.51
1:A:57:ASN:N	1:A:57:ASN:HD22	2.10	0.50
1:A:457:GLU:HG3	1:A:538:THR:HA	1.92	0.49
1:A:310:GLY:O	1:A:328:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:O	1:A:327:TYR:HB2	2.13	0.49
1:A:465:ASP:N	1:A:465:ASP:OD1	2.46	0.48
1:A:273:PRO:HB3	1:A:437:GLU:HB2	1.96	0.48
1:A:334:THR:C	9:A:2152:HOH:O	2.52	0.48
1:A:463:ARG:HD3	1:A:536:ARG:CZ	2.44	0.48
1:A:507:SER:C	9:A:2225:HOH:O	2.52	0.48
1:A:70:ILE:HG21	1:A:573:HIS:HB3	1.96	0.47
1:A:141:THR:HG22	1:A:301:ASP:HB3	1.96	0.47
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.49	0.47
1:A:656:SER:O	1:A:658:PRO:HD3	2.14	0.47
1:A:489:GLU:H	1:A:489:GLU:CD	2.18	0.47
1:A:721:PRO:O	1:A:725:TRP:HD1	1.98	0.47
1:A:129:SER:HB3	1:A:137:GLU:HG2	1.96	0.46
1:A:589:ASN:CG	9:A:2264:HOH:O	2.50	0.46
1:A:186:PHE:O	1:A:190:ARG:HB2	2.15	0.46
1:A:64:GLU:O	1:A:64:GLU:HG3	2.15	0.46
1:A:546:PHE:N	9:A:2243:HOH:O	2.48	0.46
1:A:132:ASN:ND2	1:A:138:ILE:HD11	2.29	0.46
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.98	0.46
1:A:487:GLY:HA2	1:A:489:GLU:OE2	2.17	0.45
1:A:299:TYR:HA	1:A:302:ALA:HB3	1.98	0.45
1:A:674:ALA:HB1	1:A:742:ALA:HA	1.99	0.45
1:A:449:TYR:O	1:A:532:SER:HA	2.17	0.45
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.52	0.45
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.99	0.44
1:A:127:TYR:O	1:A:345:HIS:HD2	2.00	0.44
1:A:276:GLU:H	1:A:276:GLU:HG2	1.66	0.44
1:A:517:SER:OG	1:A:518:GLY:N	2.50	0.44
1:A:155:SER:O	1:A:156:ASP:CB	2.66	0.44
1:A:214:VAL:O	1:A:218:GLN:HB2	2.18	0.43
1:A:461:THR:HA	1:A:537:TYR:CE2	2.53	0.43
1:A:655:LYS:HB2	9:A:2317:HOH:O	2.18	0.43
1:A:308:LYS:O	1:A:333:PHE:CB	2.66	0.43
1:A:504:PRO:HG3	1:A:511:ARG:NH2	2.33	0.43
1:A:81:PRO:HA	1:A:382:VAL:O	2.18	0.43
1:A:155:SER:O	1:A:156:ASP:CG	2.57	0.43
1:A:169:MET:HA	1:A:344:MET:O	2.19	0.42
1:A:507:SER:CA	9:A:2225:HOH:O	2.66	0.42
1:A:610:LYS:CG	9:A:2151:HOH:O	2.67	0.42
1:A:218:GLN:OE1	1:A:291:SER:N	2.34	0.42
1:A:487:GLY:CA	1:A:489:GLU:OE2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HB	1:A:420:SER:HB3	2.02	0.42
1:A:195:ASN:HB3	9:A:2083:HOH:O	2.19	0.41
1:A:567:ASP:OD2	1:A:570:PHE:HA	2.19	0.41
1:A:705:PHE:N	1:A:706:PRO:CD	2.83	0.41
1:A:334:THR:HG22	9:A:2152:HOH:O	2.19	0.41
1:A:325:VAL:HB	1:A:326:PRO:HD2	2.03	0.41
1:A:174:LEU:O	1:A:331:PRO:HA	2.21	0.41
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.56	0.41
1:A:486:GLU:CB	9:A:2220:HOH:O	2.69	0.40
1:A:131:ILE:O	1:A:340:GLN:HB3	2.22	0.40
1:A:308:LYS:O	1:A:333:PHE:HA	2.21	0.40
1:A:356:TYR:O	1:A:422:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	681/707 (96%)	640 (94%)	35 (5%)	6 (1%)	14	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	338	SER
1	A	506	PHE
1	A	152	GLU
1	A	155	SER
1	A	382	VAL

### 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	536/603 (89%)	511 (95%)	25 (5%)	22	29

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	118	SER
1	A	142	SER
1	A	155	SER
1	A	174	LEU
1	A	202	ILE
1	A	303	GLN
1	A	312	SER
1	A	323	LEU
1	A	340	GLN
1	A	456	ILE
1	A	465	ASP
1	A	484	PRO
1	A	519	ASN
1	A	536	ARG
1	A	537	TYR
1	A	600	TYR
1	A	605	ARG
1	A	616	MET
1	A	654	ASP
1	A	656	SER
1	A	662	ARG
1	A	668	LEU
1	A	673	ARG
1	A	716	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	618	HIS
1	A	657	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 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	2,1	14,14,15	0.67	0	17,19,21	2.00	6 (35%)
2	NAG	B	2	2	14,14,15	0.77	0	17,19,21	2.00	6 (35%)
2	NAG	C	1	2,1	14,14,15	0.94	2 (14%)	17,19,21	1.48	3 (17%)
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	1.79	3 (17%)
2	NAG	D	1	2,1	14,14,15	1.10	0	17,19,21	1.87	2 (11%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	1.75	5 (29%)
3	NAG	E	1	3,1	14,14,15	0.80	0	17,19,21	1.70	6 (35%)
3	NAG	E	2	3	14,14,15	0.79	0	17,19,21	1.57	2 (11%)
3	BMA	E	3	3	11,11,12	0.85	0	15,15,17	1.83	5 (33%)
3	MAN	E	4	3	11,11,12	0.60	0	15,15,17	1.84	2 (13%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	1/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.21	1.55	1.52
2	C	1	NAG	C4-C5	2.13	1.57	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	O5-C5-C6	5.37	115.62	107.20
2	D	2	NAG	C2-N2-C7	-4.95	115.85	122.90
2	B	1	NAG	C2-N2-C7	-4.82	116.04	122.90
2	D	1	NAG	C1-O5-C5	4.61	118.43	112.19
3	E	3	BMA	C1-O5-C5	4.28	117.99	112.19
2	C	2	NAG	C1-O5-C5	4.28	117.99	112.19
2	B	2	NAG	C1-O5-C5	4.09	117.74	112.19
2	B	2	NAG	C2-N2-C7	4.04	128.66	122.90
2	D	1	NAG	O5-C1-C2	-4.02	104.95	111.29
3	E	2	NAG	C1-O5-C5	3.95	117.55	112.19
2	C	2	NAG	C4-C3-C2	3.84	116.64	111.02
2	C	1	NAG	C1-O5-C5	3.61	117.08	112.19
3	E	1	NAG	O5-C1-C2	-3.23	106.19	111.29
2	B	1	NAG	O5-C1-C2	-3.10	106.40	111.29
2	B	1	NAG	O5-C5-C6	3.05	111.98	107.20
2	B	2	NAG	C8-C7-N2	2.95	121.10	116.10
3	E	4	MAN	O2-C2-C1	2.91	115.10	109.15
3	E	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	B	1	NAG	C3-C4-C5	-2.84	105.18	110.24
2	B	1	NAG	O4-C4-C3	-2.74	104.02	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	O3-C3-C4	-2.74	104.03	110.35
3	E	1	NAG	C6-C5-C4	-2.69	106.70	113.00
3	E	2	NAG	C8-C7-N2	2.69	120.65	116.10
3	E	1	NAG	C4-C3-C2	2.53	114.72	111.02
3	E	3	BMA	O5-C1-C2	2.52	114.66	110.77
2	B	2	NAG	O7-C7-N2	-2.45	117.44	121.95
3	E	3	BMA	O5-C5-C6	2.43	111.02	107.20
3	E	1	NAG	O5-C5-C6	-2.41	103.43	107.20
2	B	1	NAG	O3-C3-C2	2.39	114.42	109.47
2	D	2	NAG	C1-O5-C5	2.29	115.29	112.19
2	B	2	NAG	C4-C3-C2	2.28	114.36	111.02
2	B	2	NAG	C1-C2-N2	-2.27	106.61	110.49
3	E	3	BMA	C3-C4-C5	2.26	114.27	110.24
2	D	2	NAG	C1-C2-N2	-2.16	106.80	110.49
2	C	1	NAG	O4-C4-C5	2.15	114.64	109.30
2	D	2	NAG	C8-C7-N2	2.11	119.67	116.10
2	C	2	NAG	O4-C4-C5	2.10	114.52	109.30
3	E	1	NAG	C2-N2-C7	-2.10	119.91	122.90
2	D	2	NAG	O4-C4-C5	2.02	114.31	109.30
2	C	1	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	4	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6

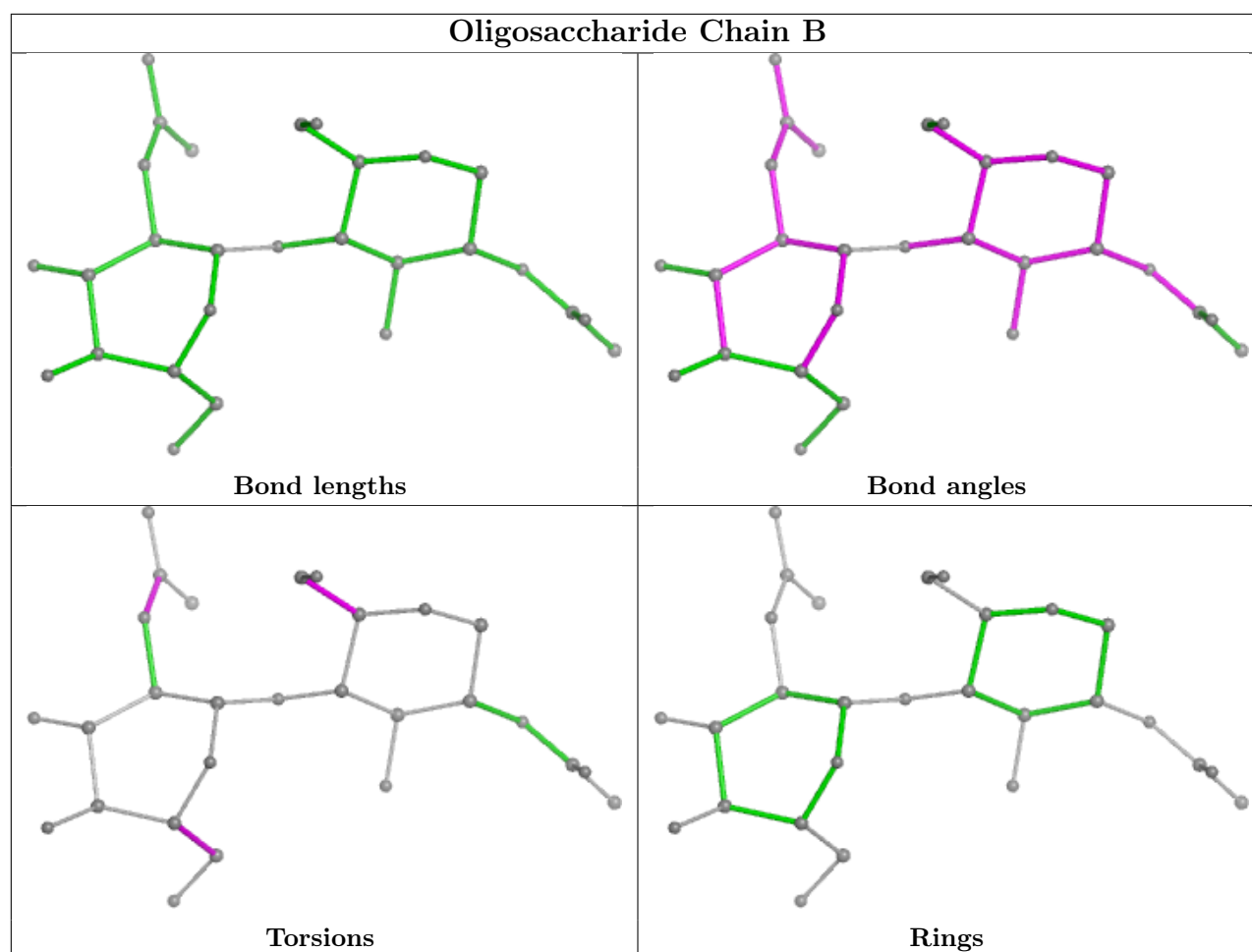
All (1) ring outliers are listed below:

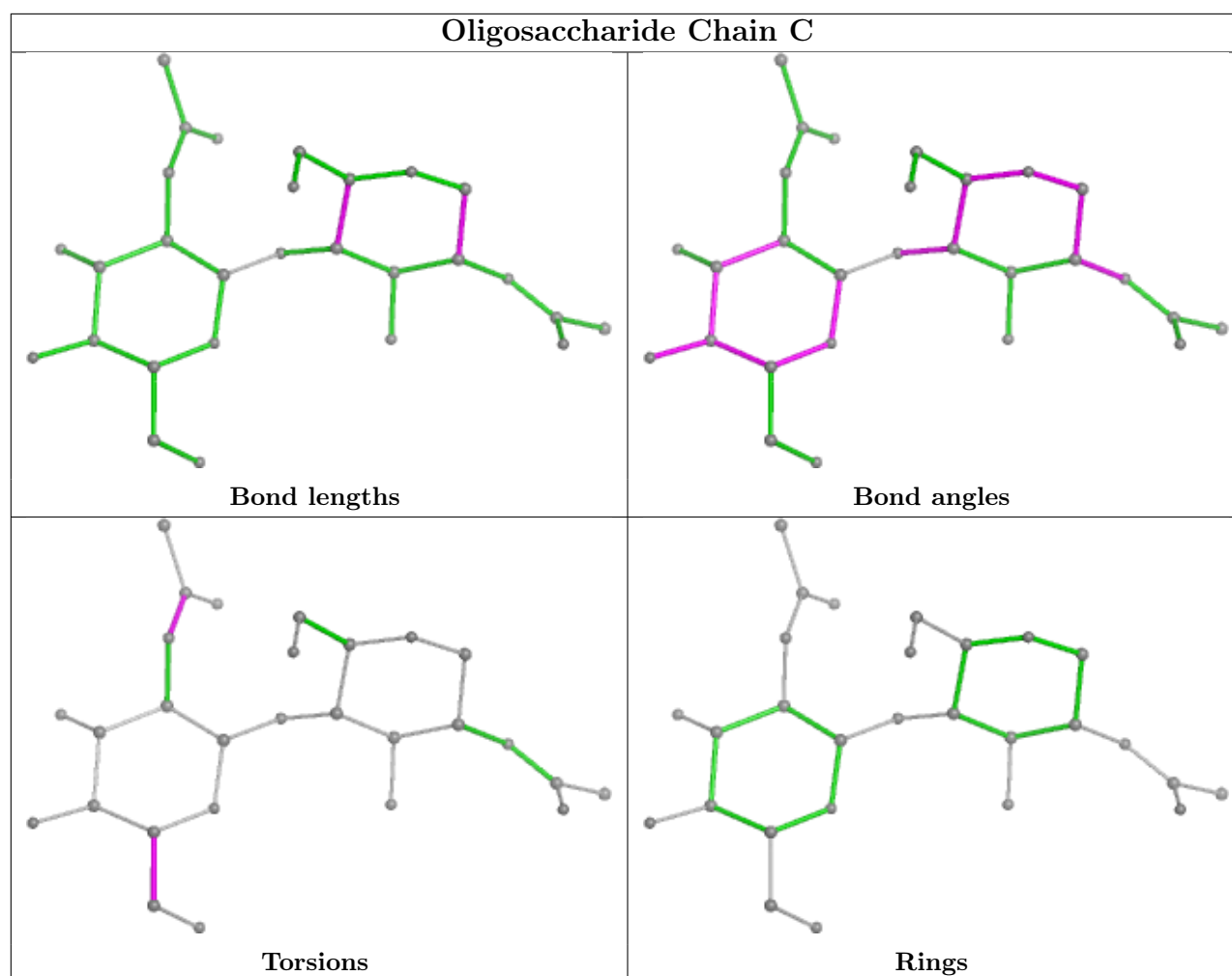
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	C1-C2-C3-C4-C5-O5

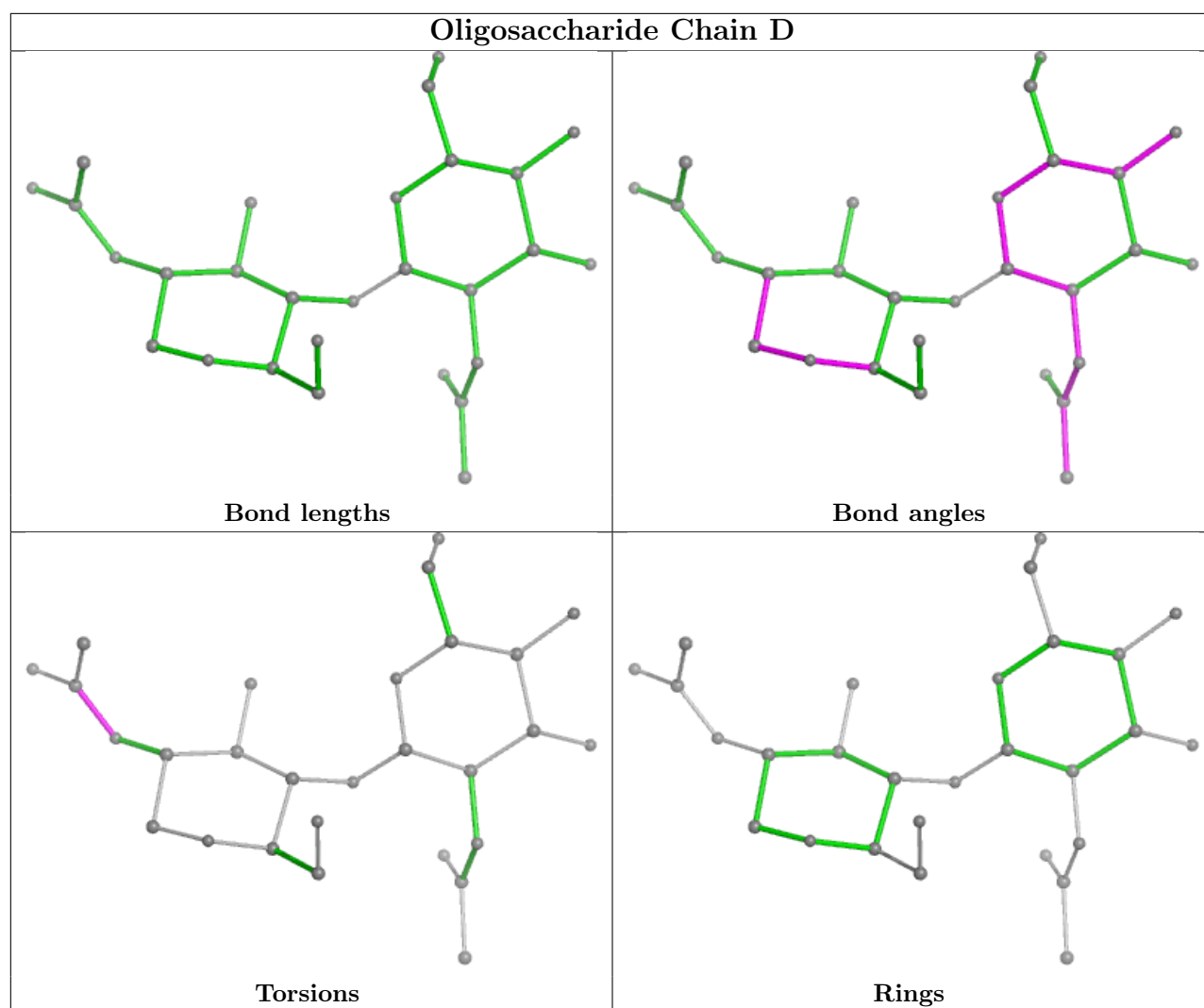
6 monomers are involved in 8 short contacts:

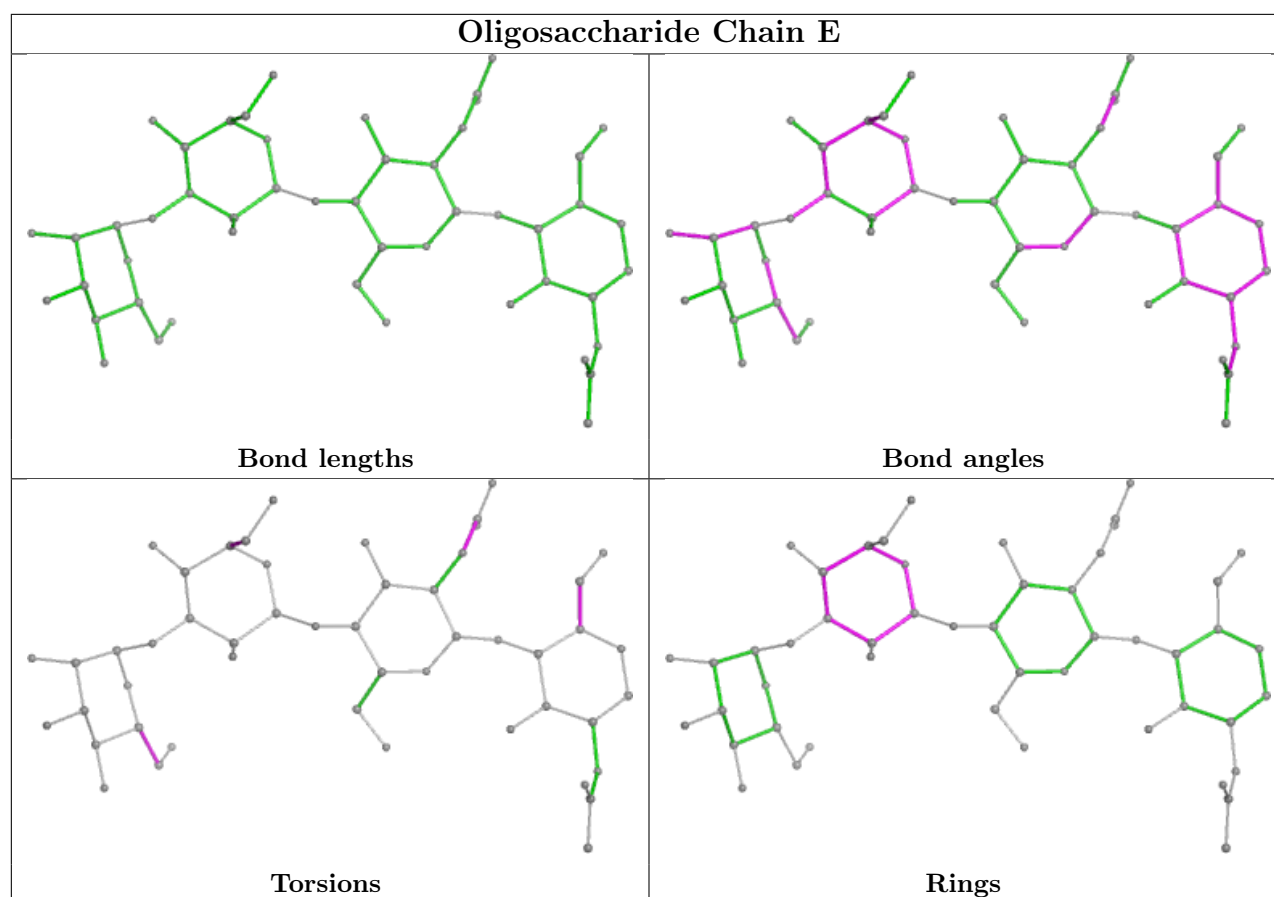
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
3	E	3	BMA	1	0
2	B	2	NAG	2	0
2	B	1	NAG	2	0
2	C	1	NAG	1	0
3	E	4	MAN	2	0

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	$\# Z  > 2$
8	G88	A	1768	4	12,13,13	4.47	4 (33%)	17,18,18	2.35	8 (47%)
7	NAG	A	1757	1	14,14,15	0.80	0	17,19,21	2.16	6 (35%)
7	NAG	A	1761	1	14,14,15	0.67	1 (7%)	17,19,21	2.80	7 (41%)
7	NAG	A	1760	1	14,14,15	1.23	1 (7%)	17,19,21	2.24	4 (23%)

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
8	G88	A	1768	4	-	5/14/14/14	-
7	NAG	A	1757	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1761	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1760	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1768	G88	P1-O2	12.59	1.76	1.50
8	A	1768	G88	P1-O3	7.41	1.71	1.54
8	A	1768	G88	O4-C3	3.88	1.34	1.22
7	A	1760	NAG	C1-C2	2.46	1.56	1.52
8	A	1768	G88	O5-C3	-2.10	1.23	1.30
7	A	1761	NAG	C1-C2	2.07	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1761	NAG	C4-C3-C2	-8.30	98.85	111.02
7	A	1760	NAG	C1-O5-C5	7.46	122.30	112.19
7	A	1757	NAG	O5-C5-C6	4.94	114.95	107.20
8	A	1768	G88	O3-P1-C1	4.07	116.69	106.74
7	A	1761	NAG	C1-O5-C5	3.94	117.53	112.19
8	A	1768	G88	O2-P1-C1	-3.93	104.27	111.54
7	A	1761	NAG	C3-C4-C5	-3.87	103.34	110.24
7	A	1757	NAG	C2-N2-C7	-3.83	117.45	122.90
8	A	1768	G88	O5-C3-C2	3.73	123.96	114.21
8	A	1768	G88	O5-C3-O4	-3.68	115.74	124.09
8	A	1768	G88	O7-C6-C5	3.09	123.96	114.03
7	A	1761	NAG	O4-C4-C5	3.02	116.79	109.30
7	A	1760	NAG	C4-C3-C2	-3.00	106.62	111.02
7	A	1757	NAG	O5-C1-C2	-2.75	106.94	111.29
7	A	1761	NAG	O3-C3-C2	2.54	114.72	109.47
7	A	1757	NAG	C4-C3-C2	2.53	114.73	111.02
7	A	1757	NAG	O5-C5-C4	-2.42	104.93	110.83
7	A	1761	NAG	O5-C5-C6	2.30	110.82	107.20
7	A	1760	NAG	O5-C5-C6	2.28	110.78	107.20
8	A	1768	G88	O7-C6-O6	-2.27	117.64	123.30
8	A	1768	G88	C4-C2-C3	-2.27	105.84	111.01
7	A	1757	NAG	C1-O5-C5	-2.26	109.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1761	NAG	C2-N2-C7	-2.11	119.89	122.90
7	A	1760	NAG	O3-C3-C2	2.11	113.83	109.47
8	A	1768	G88	O3-P1-O2	-2.09	106.85	112.39

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1757	NAG	C8-C7-N2-C2
7	A	1757	NAG	O7-C7-N2-C2
7	A	1761	NAG	C4-C5-C6-O6
7	A	1761	NAG	O5-C5-C6-O6
8	A	1768	G88	C1-C2-C3-O5
8	A	1768	G88	C1-C2-C3-O4
8	A	1768	G88	C2-C1-P1-O3
8	A	1768	G88	C2-C1-P1-O1
8	A	1768	G88	C4-C5-C6-O7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1761	NAG	2	0

## 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, 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	687/707 (97%)	0.03	26 (3%) 44 41	25, 41, 68, 75	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	656	SER	3.2
1	A	130	ILE	3.2
1	A	194	ILE	3.0
1	A	654	ASP	3.0
1	A	138	ILE	2.8
1	A	311	GLY	2.7
1	A	334	THR	2.7
1	A	152	GLU	2.7
1	A	127	TYR	2.6
1	A	338	SER	2.4
1	A	124	HIS	2.4
1	A	487	GLY	2.3
1	A	507	SER	2.3
1	A	186	PHE	2.3
1	A	198	GLY	2.3
1	A	337	PHE	2.3
1	A	217	ALA	2.2
1	A	506	PHE	2.2
1	A	457	GLU	2.2
1	A	136	ASN	2.2
1	A	132	ASN	2.1
1	A	154	VAL	2.1
1	A	155	SER	2.1
1	A	342	VAL	2.1
1	A	192	MET	2.1
1	A	279	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

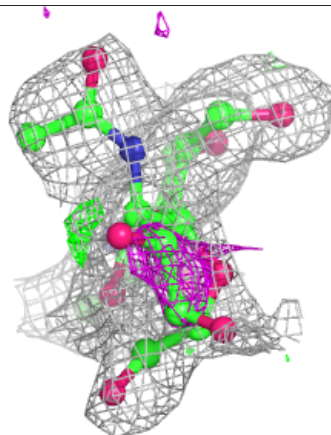
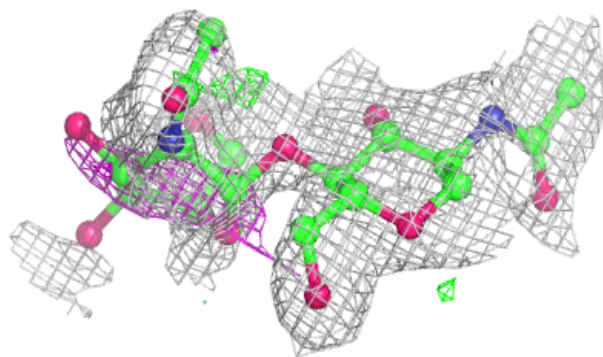
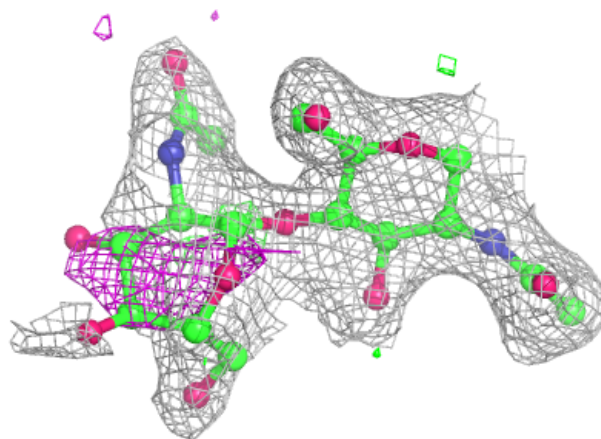
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.72	0.17	72,75,75,75	0
2	NAG	C	2	14/15	0.84	0.13	75,75,75,75	0
2	NAG	C	1	14/15	0.86	0.11	68,72,75,75	0
3	NAG	E	2	14/15	0.86	0.13	67,72,75,75	0
3	MAN	E	4	11/12	0.86	0.13	75,75,75,75	0
3	BMA	E	3	11/12	0.90	0.12	74,75,75,75	0
2	NAG	B	1	14/15	0.91	0.09	53,60,66,72	0
2	NAG	D	2	14/15	0.93	0.09	57,61,67,70	0
3	NAG	E	1	14/15	0.95	0.07	29,43,58,62	0
2	NAG	D	1	14/15	0.95	0.06	46,50,53,55	0

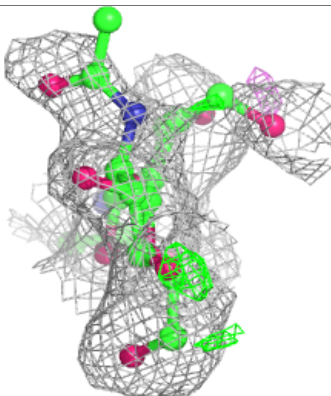
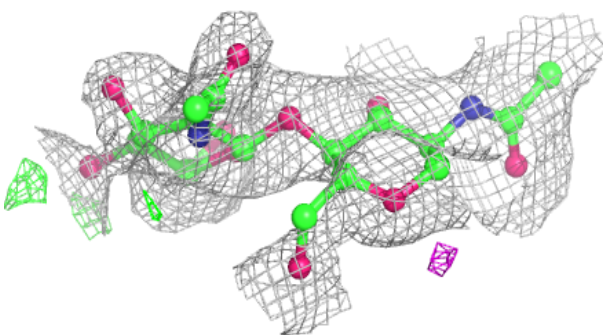
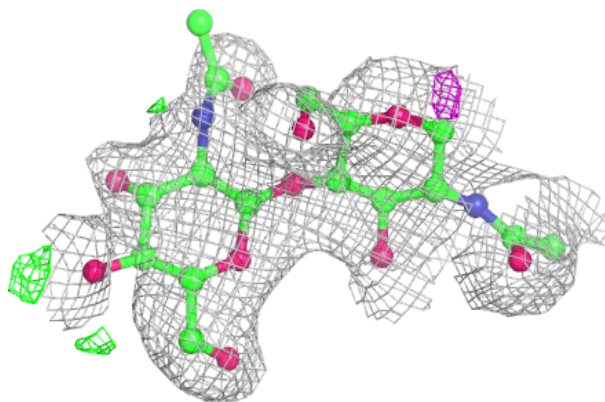
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain B:**

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

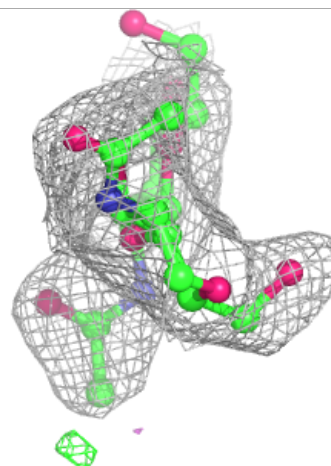
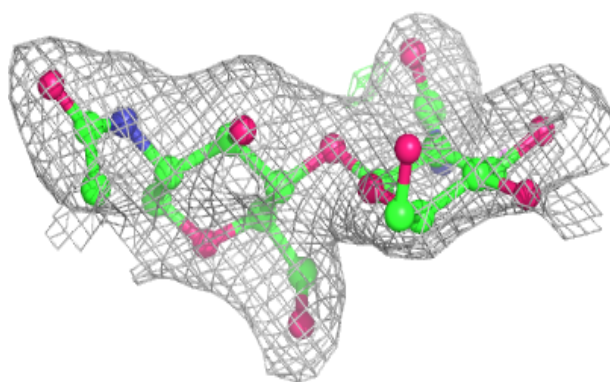
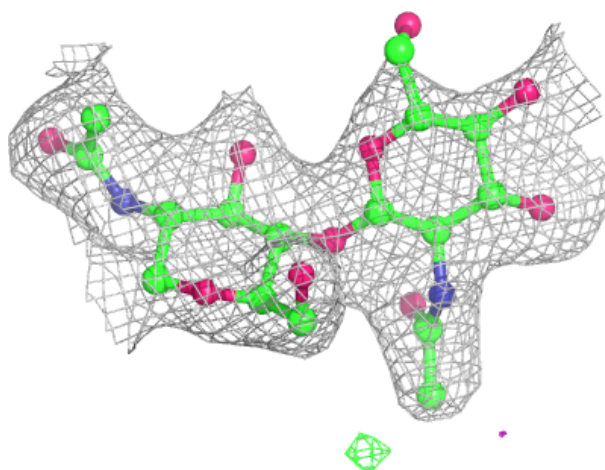
**Electron density around Chain C:**

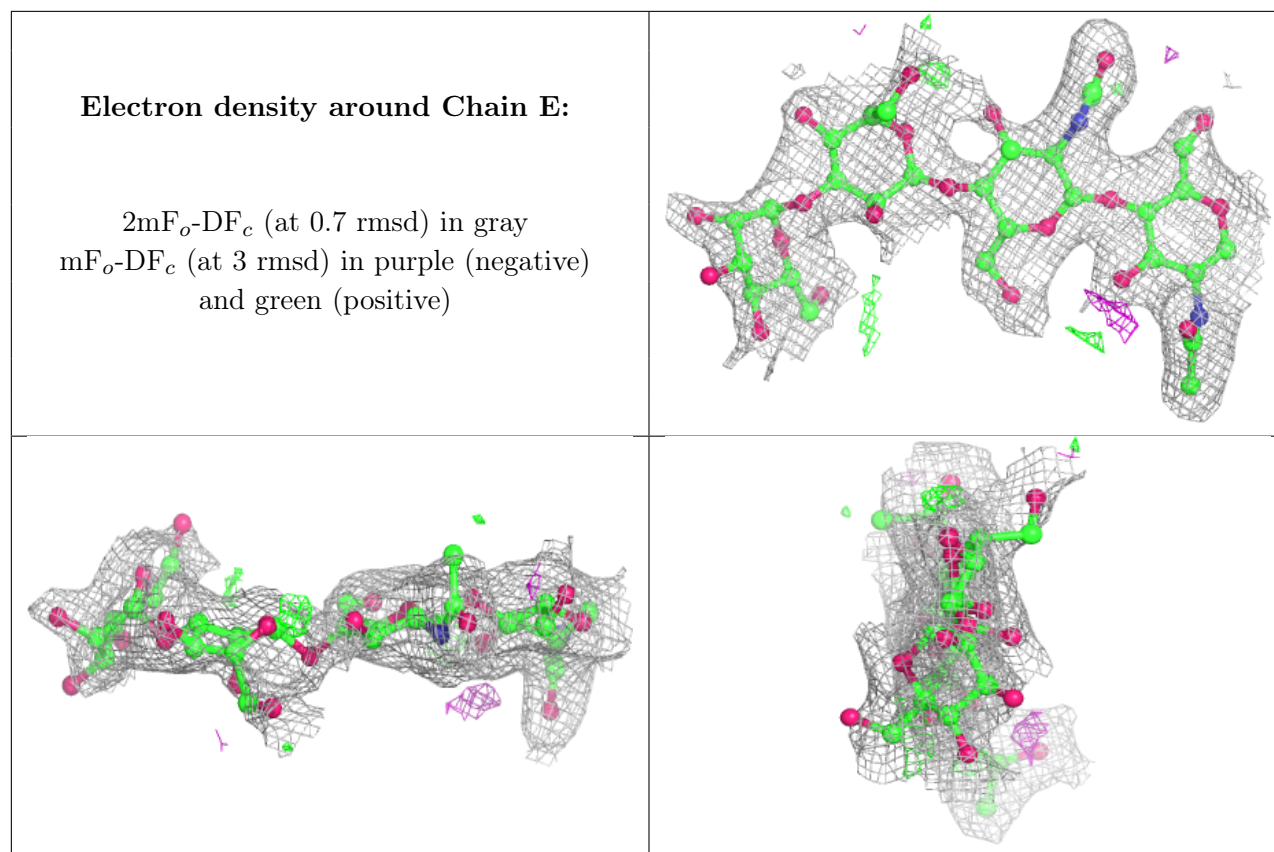
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

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





## 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( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	1760	14/15	0.49	0.19	75,75,75,75	0
7	NAG	A	1757	14/15	0.72	0.13	73,75,75,75	0
7	NAG	A	1761	14/15	0.83	0.13	52,70,75,75	0
8	G88	A	1768	14/14	0.97	0.08	29,34,39,40	0
4	ZN	A	1752	1/1	0.98	0.14	49,49,49,49	0
5	CA	A	1753	1/1	0.99	0.01	30,30,30,30	0
6	CL	A	1754	1/1	0.99	0.04	37,37,37,37	0
4	ZN	A	1751	1/1	0.99	0.12	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.