



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:13 AM BST

PDB ID : 5O5R
Title : X-ray structure of human glutamate carboxypeptidase II (GCPII) in complex with a urea based inhibitor PSMA 1023
Authors : Motlova, L.; Novakova, Z.; Barinka, C.
Deposited on : 2017-06-02
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

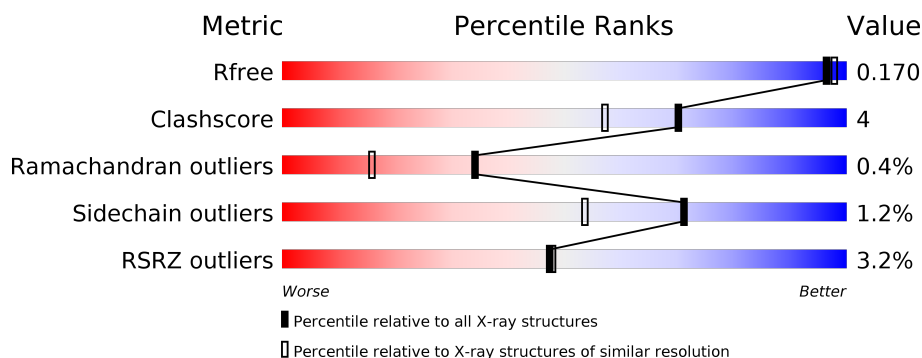
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 on 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	707	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
3	C	3	<div> <div>33%</div> <div>67%</div> </div>
4	D	3	<div> <div>33%</div> <div>67%</div> </div>
5	E	5	<div> <div>80%</div> <div>20%</div> </div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 7009 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.

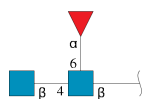
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	75	0
			6081	3895	1021	1140	25			

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



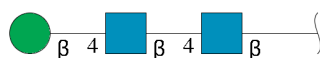
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



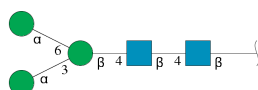
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



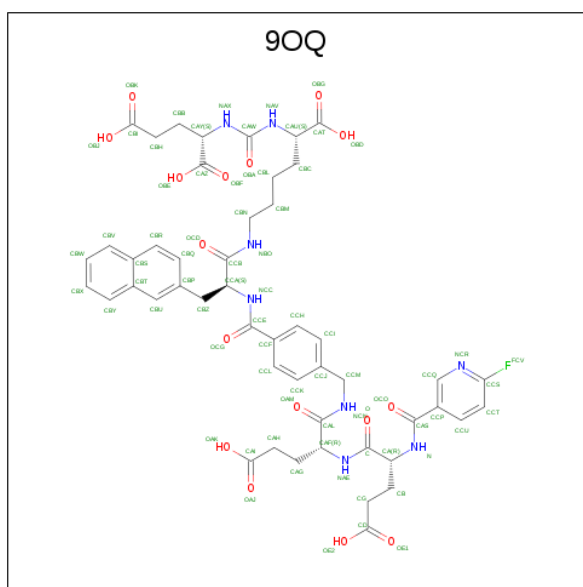
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 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
5	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is (2 {S})-2-[[[(2 {S})-6-[[[(2 {S})-2-[[4-[[[(2 {R})-2-[[[(2 {R})-2-[(6-fluoranylpyridin-3-yl)carbonylamino]-5-oxidanyl-5-oxidanylidene-pentanoyl]amino]-5-oxidanyl-5-oxidanylidene-pentanoyl]amino]methyl]phenyl]carbonylamino]-3-naphthalen-2-yl-propanoyl]amino]-1-oxidanyl-1-oxidanylidene-hexan-2-yl]carbamoylamino]pentanedioic acid (three-letter code: 9OQ) (formula: C₄₉H₅₅FN₈O₁₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			74	49	1	8	16		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		
11	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		

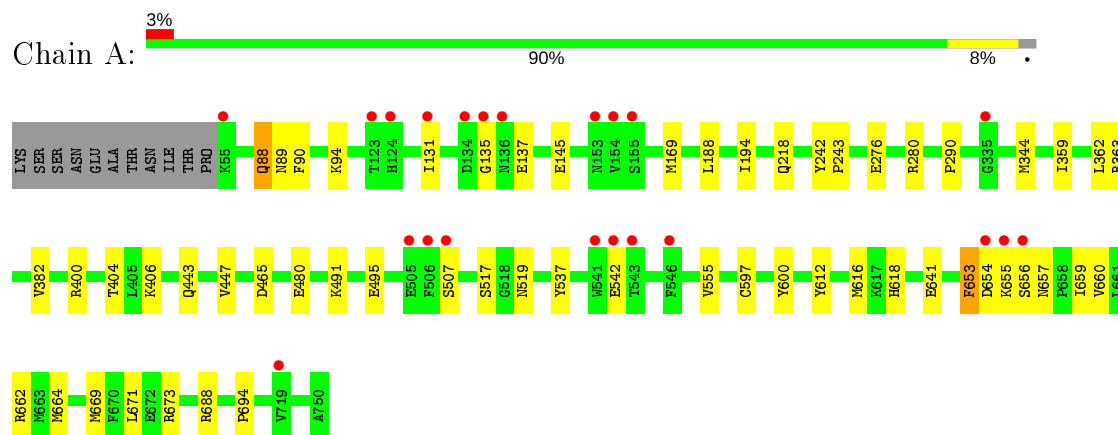
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	624	Total 624	O 624	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: Glutamate carboxypeptidase 2



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



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



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



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain E:



MAG1
MAG2
BOA3
MAT4
MAT5

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.51Å 130.20Å 159.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 1.65 49.13 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.13-1.65) 99.0 (49.13-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.124 , 0.160 0.139 , 0.170	Depositor DCC
R_{free} test set	6313 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7009	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, EDO, FUC, PEG, 9OQ, MAN

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	0.61	0/6290	0.74	4/8513 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	363	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	662[A]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	465	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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	6081	0	5908	44	1
2	B	28	0	25	1	0
3	C	38	0	34	0	0
4	D	39	0	34	0	0
5	E	61	0	52	0	1
6	A	74	0	0	0	0
7	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
11	A	14	0	20	0	0
12	A	4	0	6	0	0
13	A	624	0	0	7	0
All	All	7009	0	6118	45	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (45) 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:653[B]:PHE:CD2	1:A:654[B]:ASP:N	2.10	1.17
1:A:443[B]:GLN:NE2	13:A:905:HOH:O	1.77	1.14
1:A:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.60	1.01
1:A:653[B]:PHE:CG	1:A:654[B]:ASP:N	2.13	0.98
1:A:654[A]:ASP:O	1:A:654[A]:ASP:OD1	1.92	0.87
1:A:88[A]:GLN:H	1:A:88[A]:GLN:HE21	1.26	0.83
1:A:491[B]:LYS:HD2	1:A:495[B]:GLU:OE1	1.84	0.77
1:A:653[B]:PHE:O	1:A:654[B]:ASP:HB2	1.84	0.76
1:A:654[A]:ASP:OD1	1:A:657[A]:ASN:HB3	1.88	0.73
1:A:242:TYR:OH	13:A:906:HOH:O	2.11	0.68
1:A:653[B]:PHE:CG	1:A:654[B]:ASP:H	1.50	0.68
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.35	0.67
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.95	0.67
1:A:447:VAL:HG22	1:A:669[B]:MET:CE	2.26	0.66
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.87	0.62
1:A:188[B]:LEU:HG	1:A:194[B]:ILE:HB	1.82	0.60
1:A:447:VAL:HG22	1:A:669[B]:MET:HE1	1.83	0.59
1:A:218[B]:GLN:HE22	1:A:290:PRO:HA	1.69	0.58
1:A:653[B]:PHE:CD2	1:A:654[B]:ASP:CA	2.88	0.56
1:A:90:PHE:CE2	1:A:94[A]:LYS:HE2	2.42	0.54
1:A:145:GLU:OE1	1:A:555[B]:VAL:HG23	2.08	0.54
1:A:362:LEU:CD1	1:A:406:LYS:HD2	2.37	0.54
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.43	0.53
1:A:89[B]:ASN:C	1:A:89[B]:ASN:OD1	2.48	0.53
1:A:280[B]:ARG:NH1	1:A:280[B]:ARG:HG3	2.25	0.52
1:A:641:GLU:HG3	13:A:1234:HOH:O	2.10	0.52
1:A:555[B]:VAL:O	1:A:555[B]:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688[B]:ARG:NH2	13:A:909:HOH:O	2.31	0.49
1:A:359[B]:ILE:N	1:A:359[B]:ILE:HD12	2.27	0.49
1:A:654[A]:ASP:OD1	1:A:657[A]:ASN:CB	2.60	0.47
1:A:618:HIS:HD2	13:A:1100:HOH:O	1.99	0.46
1:A:131[A]:ILE:HG22	1:A:137:GLU:HG2	1.98	0.46
1:A:218[B]:GLN:HE22	1:A:290:PRO:CA	2.28	0.44
1:A:169:MET:HA	1:A:344:MET:O	2.18	0.44
1:A:131[B]:ILE:HD11	1:A:135:GLY:HA2	1.99	0.44
1:A:280[B]:ARG:CG	1:A:280[B]:ARG:HH11	2.30	0.44
1:A:242:TYR:CG	1:A:243:PRO:HA	2.53	0.44
1:A:659[B]:ILE:HA	1:A:659[B]:ILE:HD13	1.81	0.43
1:A:656[B]:SER:O	1:A:656[B]:SER:OG	2.36	0.43
1:A:669[B]:MET:HE2	1:A:669[B]:MET:HB2	1.29	0.43
1:A:653[B]:PHE:CE2	1:A:654[B]:ASP:HA	2.54	0.42
1:A:280[B]:ARG:HG3	1:A:280[B]:ARG:HH11	1.85	0.41
1:A:480:GLU:HG3	13:A:1467:HOH:O	2.21	0.41
1:A:517:SER:HB2	1:A:694:PRO:HG3	2.02	0.41
13:A:1429:HOH:O	2:B:2:NAG:H81	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276[B]:GLU:OE1	5:E:3:BMA:O2[2_565]	2.19	0.01

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	767/707 (108%)	745 (97%)	17 (2%)	5 (1%)	22 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	655[A]	LYS
1	A	655[B]	LYS
1	A	653[A]	PHE
1	A	653[B]	PHE
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	666/603 (110%)	657 (99%)	9 (1%)	67 46

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88[A]	GLN
1	A	88[B]	GLN
1	A	507[A]	SER
1	A	507[B]	SER
1	A	519	ASN
1	A	537	TYR
1	A	542	GLU
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	618	HIS

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 ⓘ

13 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	0.24	0	17,19,21	0.84	0
2	NAG	B	2	2	14,14,15	0.68	0	17,19,21	1.36	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.45	0	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	0.40	0	17,19,21	1.02	1 (5%)
3	FUC	C	3	3	10,10,11	0.73	0	14,14,16	1.00	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.55	0	17,19,21	1.39	1 (5%)
4	NAG	D	2	4	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
4	BMA	D	3	4	11,11,12	0.63	0	15,15,17	0.80	0
5	NAG	E	1	1,5	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
5	NAG	E	2	5	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
5	BMA	E	3	5	11,11,12	0.54	0	15,15,17	1.23	2 (13%)
5	MAN	E	4	5	11,11,12	0.59	0	15,15,17	1.11	2 (13%)
5	MAN	E	5	5	11,11,12	0.75	0	15,15,17	1.29	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	C	3	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	4.62	129.48	122.90
2	B	2	NAG	C2-N2-C7	3.44	127.80	122.90
5	E	1	NAG	O5-C1-C2	-3.14	106.33	111.29
4	D	2	NAG	C8-C7-N2	2.94	121.08	116.10
5	E	1	NAG	C1-O5-C5	2.74	115.90	112.19
5	E	5	MAN	O5-C5-C6	2.61	111.29	107.20
5	E	5	MAN	O5-C1-C2	2.34	114.39	110.77
3	C	3	FUC	O5-C1-C2	2.33	114.37	110.77
5	E	3	BMA	O3-C3-C2	-2.25	105.68	109.99
5	E	2	NAG	C4-C3-C2	-2.23	107.75	111.02
3	C	2	NAG	O4-C4-C5	2.18	114.71	109.30
5	E	4	MAN	C1-O5-C5	2.15	115.10	112.19
4	D	2	NAG	C2-N2-C7	2.11	125.90	122.90
5	E	3	BMA	C1-O5-C5	-2.10	109.35	112.19
5	E	2	NAG	C8-C7-N2	2.08	119.62	116.10
5	E	4	MAN	O5-C5-C6	2.04	110.41	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2

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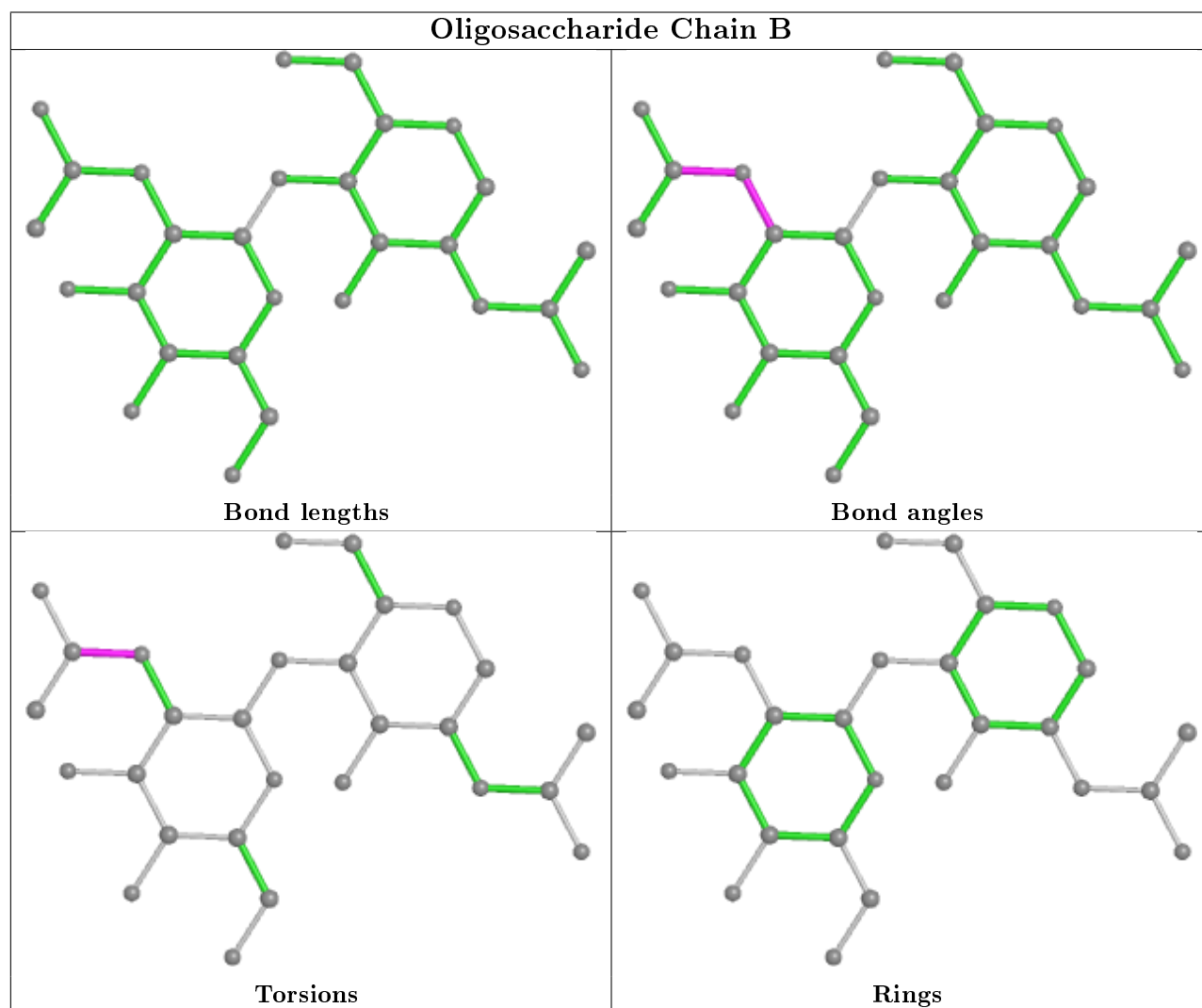
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6

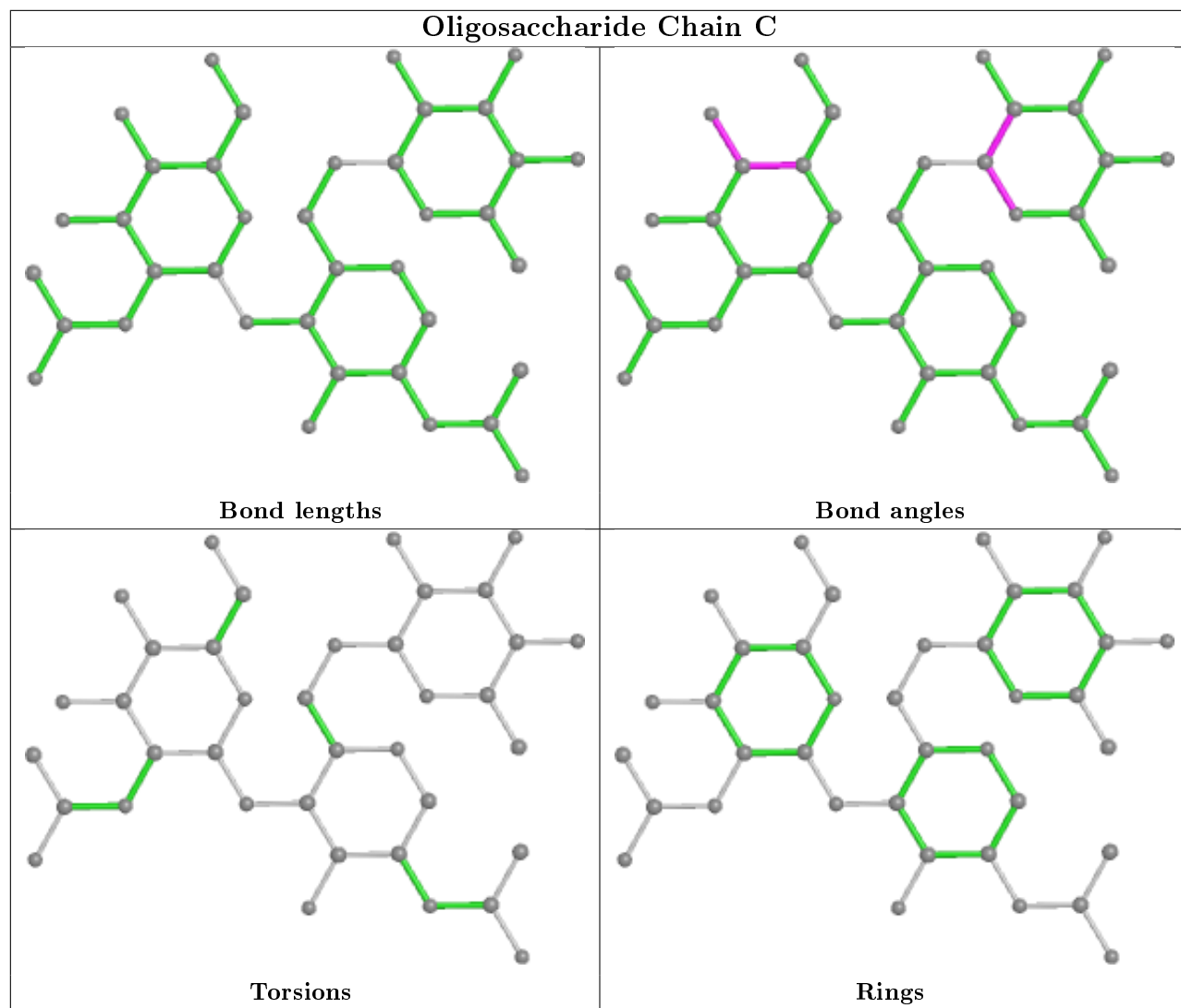
There are no ring outliers.

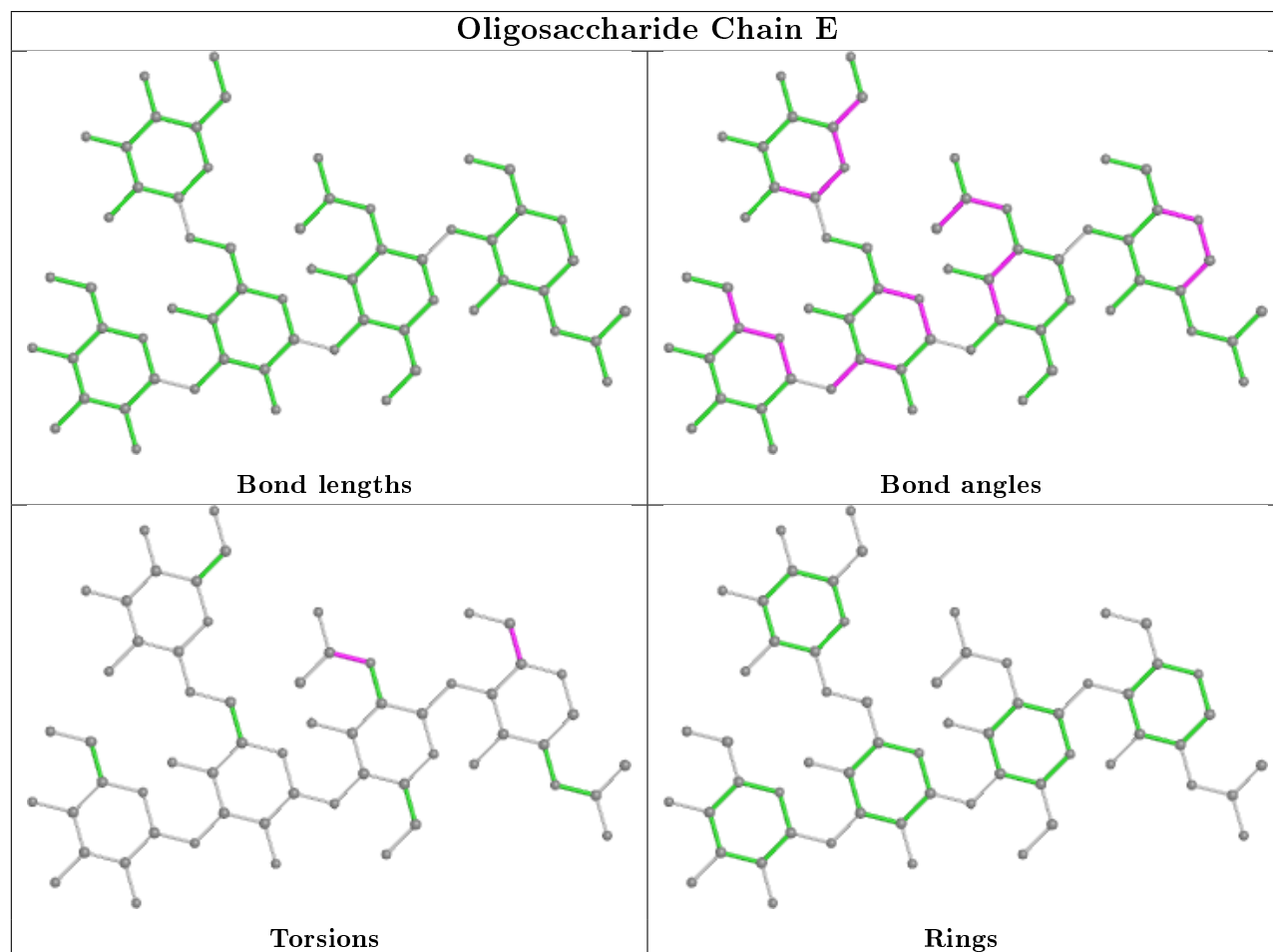
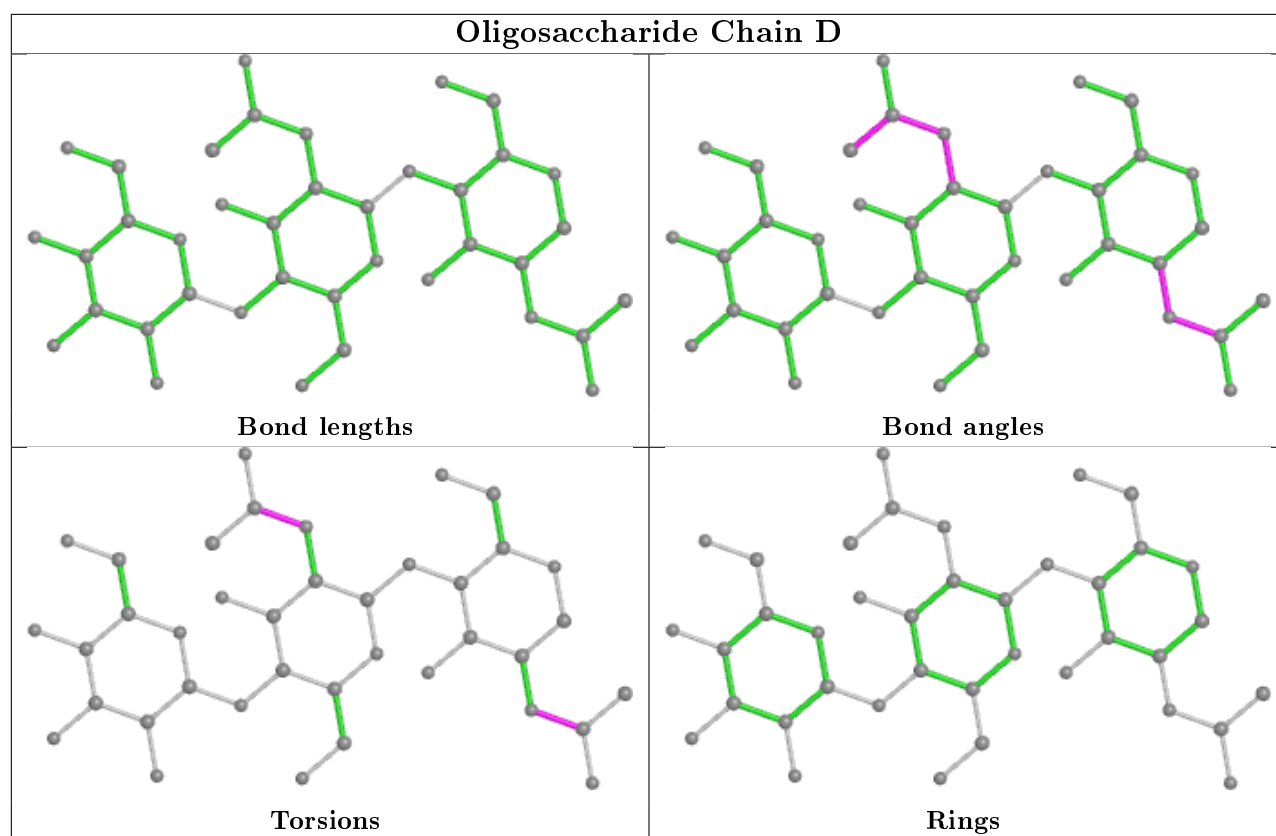
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	3	BMA	0	1
2	B	2	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 oligosaccharide.







5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	NAG	A	807	1	14,14,15	0.61	0	17,19,21	2.24	3 (17%)
11	PEG	A	822	-	6,6,6	0.60	0	5,5,5	0.47	0
11	PEG	A	821	-	6,6,6	0.54	0	5,5,5	0.40	0
7	NAG	A	824	1	14,14,15	0.75	0	17,19,21	1.58	2 (11%)
7	NAG	A	816	1	14,14,15	0.77	0	17,19,21	1.73	3 (17%)
12	EDO	A	823	-	3,3,3	0.57	0	2,2,2	0.44	0
6	9OQ	A	801	8	62,77,77	1.82	4 (6%)	82,103,103	3.02	20 (24%)

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	NAG	A	807	1	-	0/6/23/26	0/1/1/1
11	PEG	A	822	-	-	3/4/4/4	-
11	PEG	A	821	-	-	0/4/4/4	-
7	NAG	A	824	1	-	2/6/23/26	0/1/1/1
7	NAG	A	816	1	-	2/6/23/26	0/1/1/1
12	EDO	A	823	-	-	1/1/1/1	-
6	9OQ	A	801	8	-	7/66/80/80	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	9OQ	CCM-NCN	-11.50	1.23	1.46
6	A	801	9OQ	CCS-NCR	4.26	1.35	1.30
6	A	801	9OQ	CCT-CCS	3.51	1.41	1.37
6	A	801	9OQ	CBZ-CCA	2.03	1.59	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	9OQ	CCQ-NCR-CCS	18.26	121.70	115.75
6	A	801	9OQ	CCT-CCS-NCR	-12.97	119.72	126.83
7	A	807	NAG	C1-O5-C5	7.90	122.90	112.19
6	A	801	9OQ	FCV-CCS-CCT	6.47	123.36	118.71
6	A	801	9OQ	CCM-NCN-CAL	-4.98	115.18	122.34
7	A	816	NAG	C1-O5-C5	4.75	118.63	112.19
7	A	824	NAG	O5-C5-C6	4.57	114.37	107.20
6	A	801	9OQ	CCU-CCT-CCS	4.41	119.64	116.35
6	A	801	9OQ	CA-N-CAS	3.47	130.09	121.60
6	A	801	9OQ	OCO-CAS-CCP	-3.38	114.91	120.94
6	A	801	9OQ	CAG-CAF-NAE	-3.05	104.71	110.88
6	A	801	9OQ	FCV-CCS-NCR	3.02	116.92	114.95
7	A	816	NAG	O5-C1-C2	-2.94	106.64	111.29
6	A	801	9OQ	CCP-CAS-N	2.89	122.59	117.06
6	A	801	9OQ	CCA-CCB-NBO	-2.78	110.93	116.54
6	A	801	9OQ	CCK-CCL-CCF	-2.73	117.60	120.78
6	A	801	9OQ	CB-CA-N	2.73	116.39	110.88
7	A	807	NAG	O5-C5-C6	2.56	111.21	107.20
7	A	807	NAG	C6-C5-C4	-2.37	107.45	113.00
6	A	801	9OQ	CBB-CAY-NAX	2.37	113.64	110.19
7	A	824	NAG	C1-C2-N2	-2.34	106.48	110.49
6	A	801	9OQ	CCJ-CCM-NCN	-2.20	108.33	113.05
6	A	801	9OQ	CAF-NAE-C	2.20	126.39	121.67
6	A	801	9OQ	CAF-CAL-NCN	2.07	120.72	116.54
7	A	816	NAG	O5-C5-C6	2.06	110.43	107.20
6	A	801	9OQ	CCM-CCJ-CCI	-2.04	116.69	120.91
6	A	801	9OQ	CAL-CAF-NAE	2.04	116.70	111.16
6	A	801	9OQ	CG-CB-CA	2.03	117.21	113.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	9OQ	CB-CA-N-CAS
6	A	801	9OQ	CA-CB-CG-CD
6	A	801	9OQ	CAL-CAF-NAE-C
7	A	824	NAG	O5-C5-C6-O6
7	A	824	NAG	C4-C5-C6-O6
7	A	816	NAG	C4-C5-C6-O6
7	A	816	NAG	O5-C5-C6-O6
11	A	822	PEG	O1-C1-C2-O2

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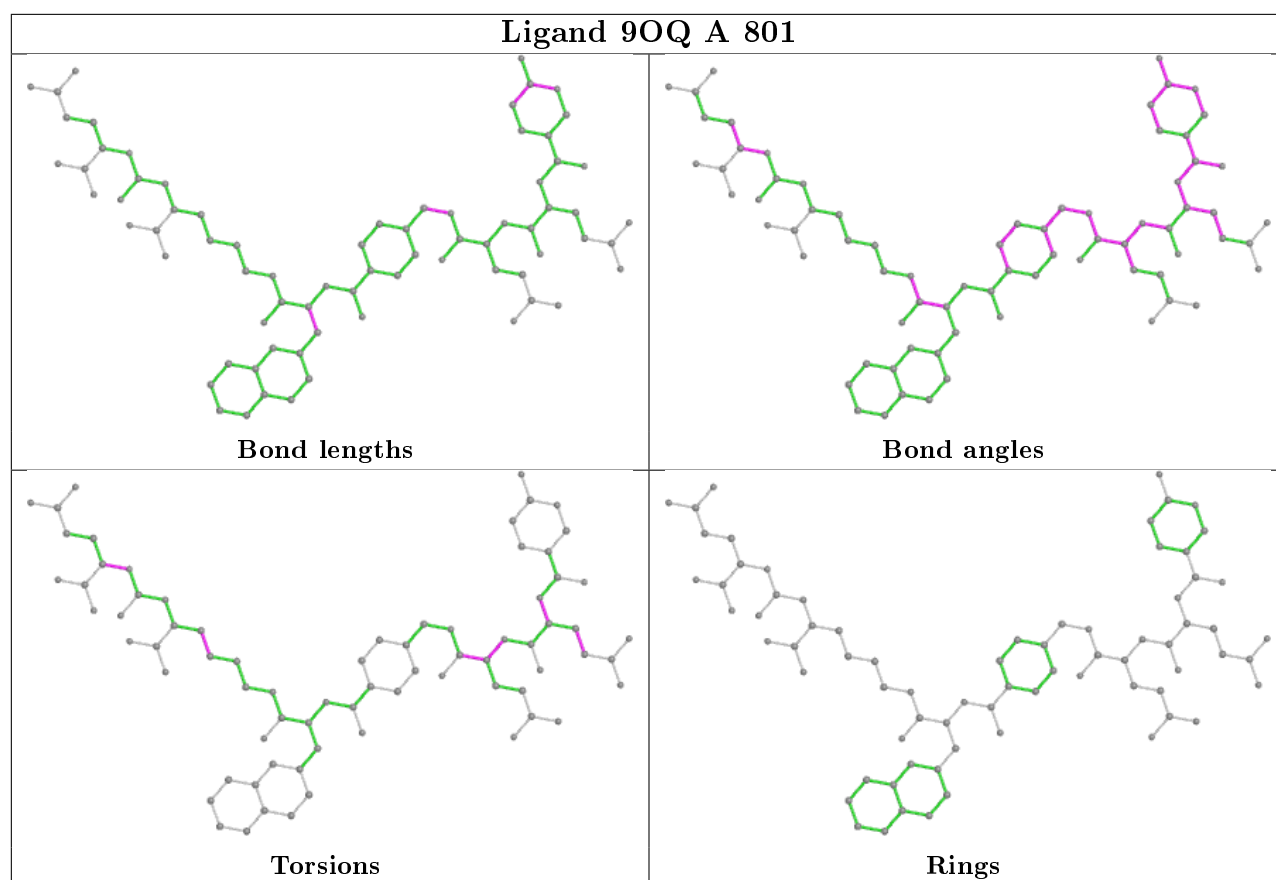
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Mol	Chain	Res	Type	Atoms
12	A	823	EDO	O1-C1-C2-O2
6	A	801	9OQ	CAZ-CAY-NAX-CAW
6	A	801	9OQ	CAG-CAF-CAL-OAM
11	A	822	PEG	C4-C3-O2-C2
6	A	801	9OQ	NAE-CAF-CAL-OAM
6	A	801	9OQ	CAU-CBC-CBL-CBM
11	A	822	PEG	C1-C2-O2-C3

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 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, 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	696/707 (98%)	-0.10	22 (3%)	47 48	22, 33, 56, 97	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654[A]	ASP	4.2
1	A	155[A]	SER	4.2
1	A	542	GLU	4.1
1	A	656[A]	SER	3.6
1	A	506	PHE	3.6
1	A	153	ASN	3.4
1	A	541	TRP	3.4
1	A	507[A]	SER	3.4
1	A	655[A]	LYS	3.4
1	A	131[A]	ILE	3.0
1	A	546	PHE	3.0
1	A	55	LYS	2.8
1	A	135	GLY	2.7
1	A	123	THR	2.7
1	A	719	VAL	2.6
1	A	505[A]	GLU	2.6
1	A	134	ASP	2.5
1	A	154	VAL	2.4
1	A	335	GLY	2.3
1	A	543	THR	2.1
1	A	136	ASN	2.1
1	A	124	HIS	2.1

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

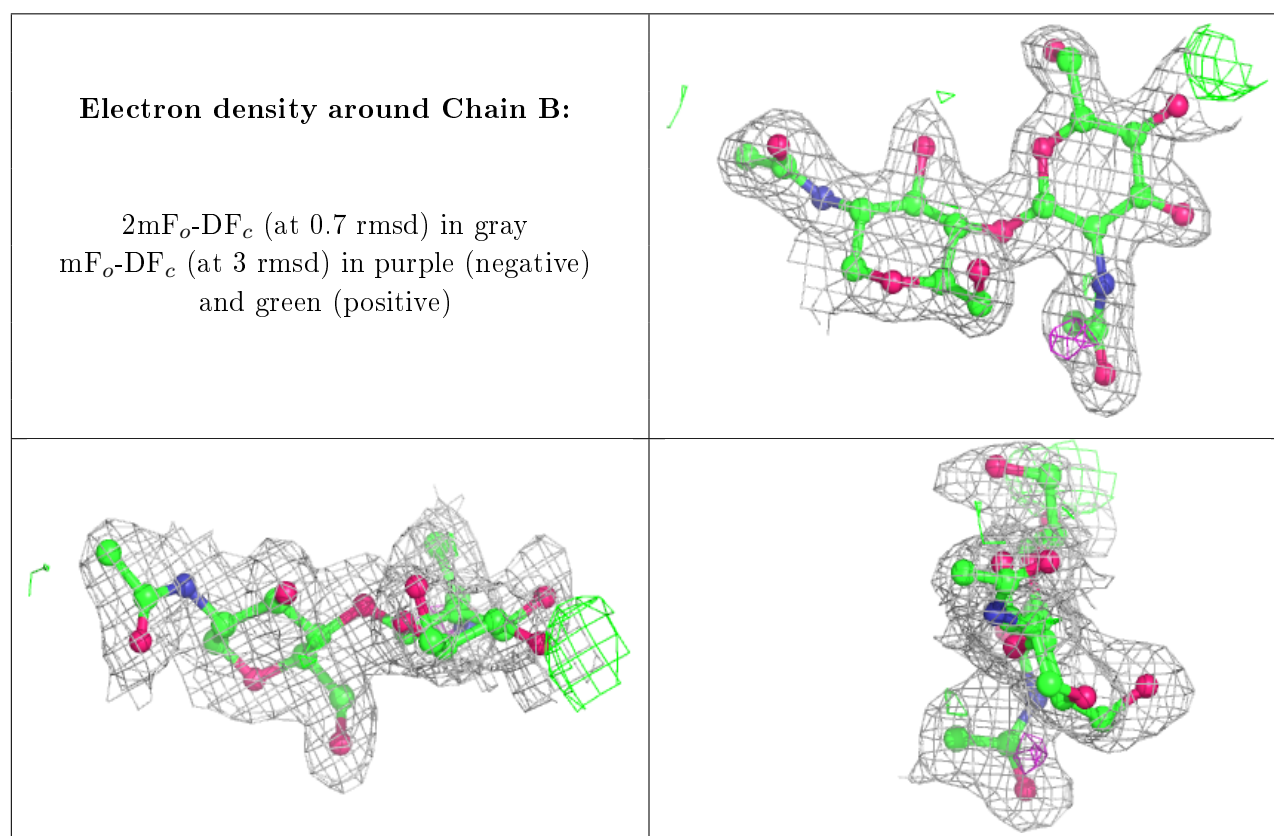
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

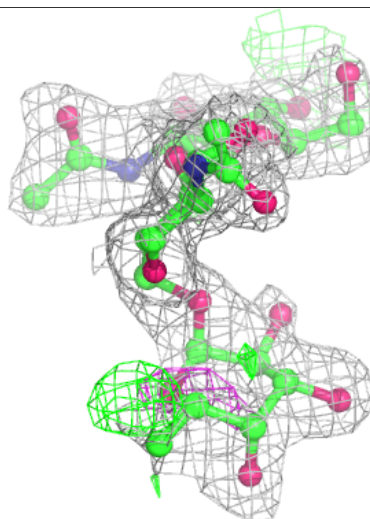
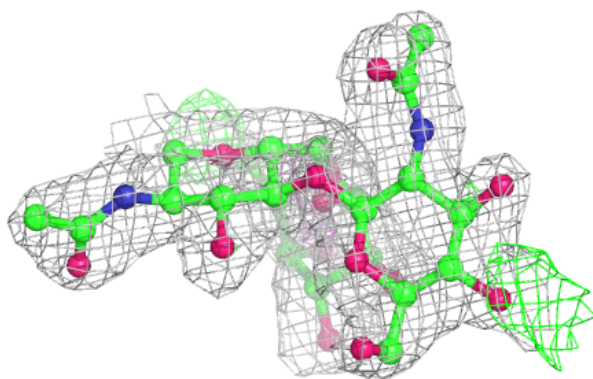
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	D	3	11/12	0.69	0.21	64,75,88,88	0
2	NAG	B	2	14/15	0.75	0.27	43,59,67,69	0
3	FUC	C	3	10/11	0.75	0.31	65,72,76,78	0
5	MAN	E	5	11/12	0.76	0.21	62,68,77,89	0
3	NAG	C	2	14/15	0.91	0.24	60,64,75,78	0
3	NAG	C	1	14/15	0.93	0.19	47,50,56,58	0
5	NAG	E	2	14/15	0.93	0.12	41,46,65,67	0
5	NAG	E	1	14/15	0.94	0.08	29,36,45,54	0
5	BMA	E	3	11/12	0.94	0.10	43,50,55,61	0
2	NAG	B	1	14/15	0.95	0.13	38,47,54,59	0
4	NAG	D	2	14/15	0.95	0.10	41,49,61,65	0
5	MAN	E	4	11/12	0.95	0.08	48,54,62,62	0
4	NAG	D	1	14/15	0.97	0.07	33,38,47,56	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.



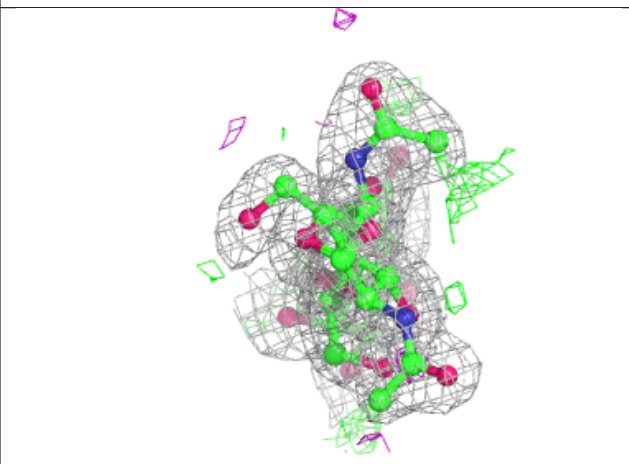
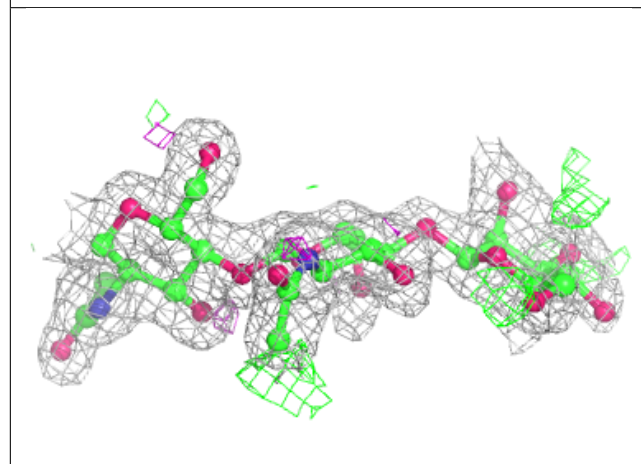
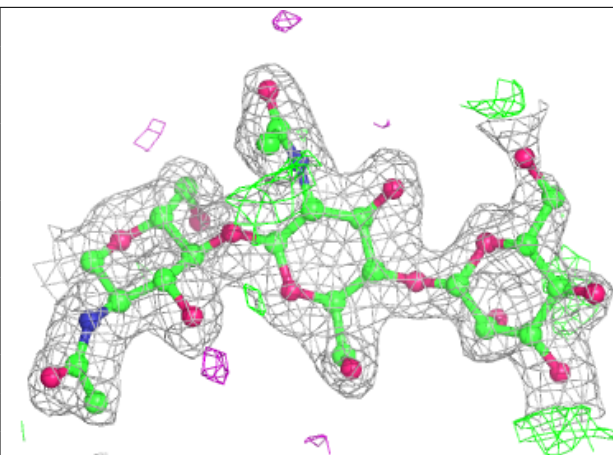
Electron density around Chain C:

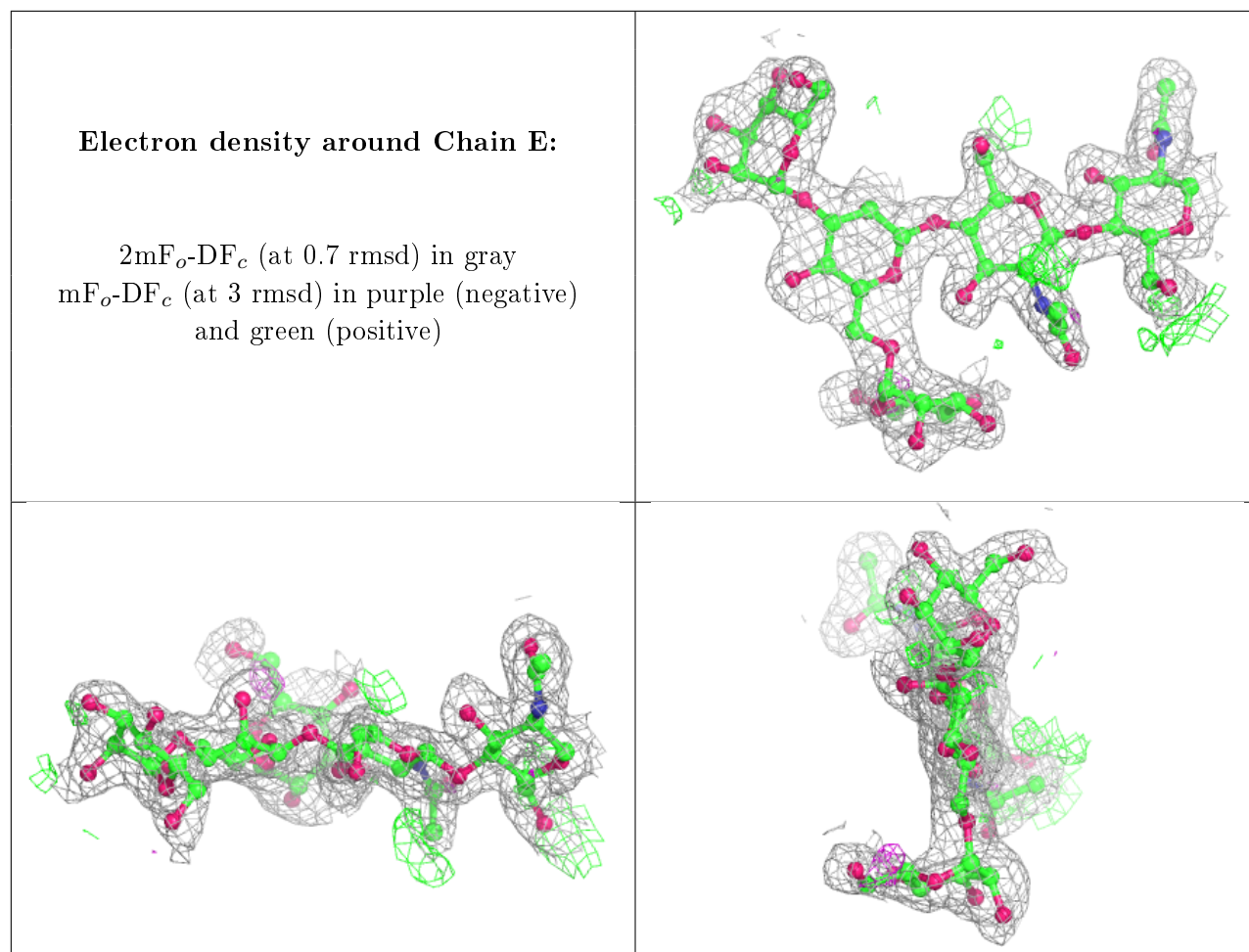
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)



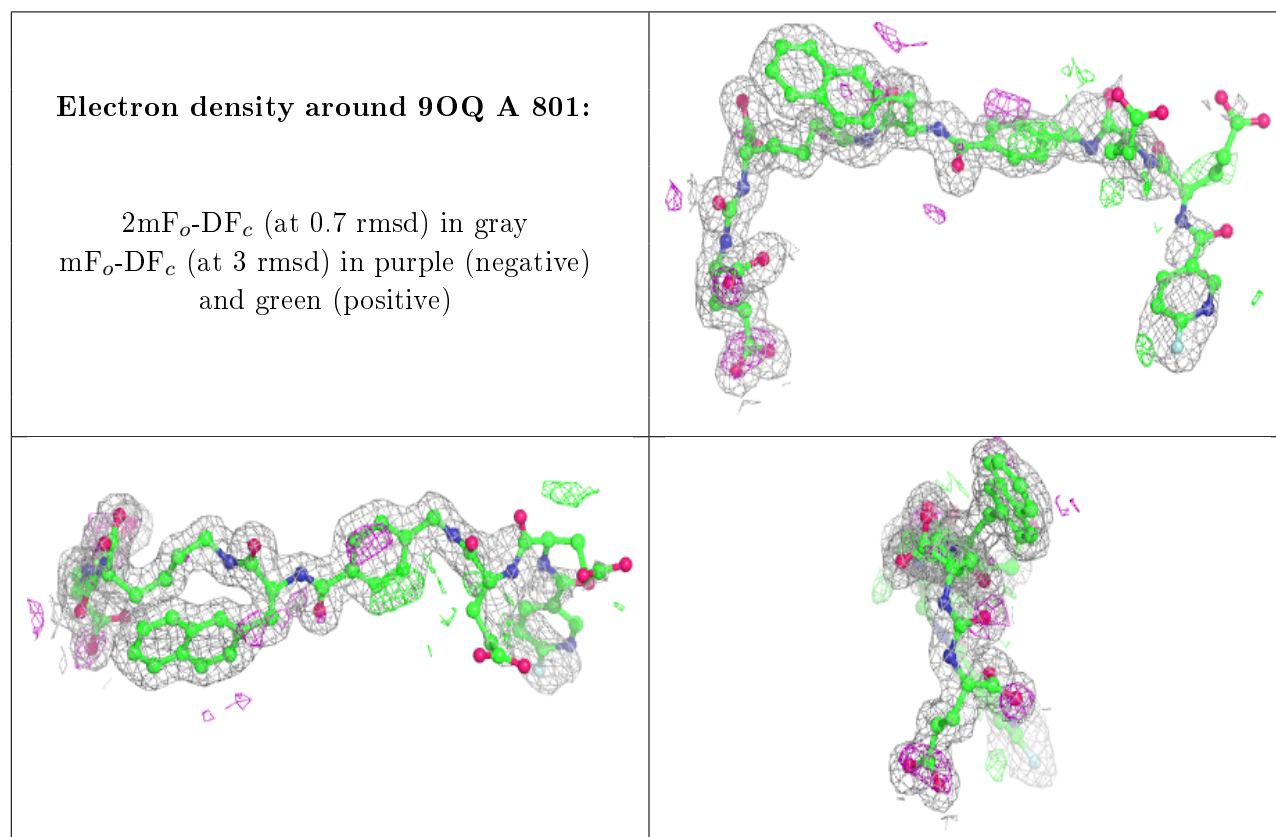


6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	PEG	A	822	7/7	0.77	0.12	59,82,88,92	0
7	NAG	A	807	14/15	0.82	0.24	73,81,92,94	0
11	PEG	A	821	7/7	0.87	0.13	62,65,68,69	0
7	NAG	A	816	14/15	0.89	0.13	37,61,75,81	0
7	NAG	A	824	14/15	0.90	0.26	48,63,80,85	0
12	EDO	A	823	4/4	0.92	0.15	48,57,58,78	0
6	9OQ	A	801	74/74	0.94	0.14	23,29,133,147	0
10	CL	A	820	1/1	0.99	0.10	31,31,31,31	0
8	ZN	A	817	1/1	1.00	0.06	25,25,25,25	0
9	CA	A	819	1/1	1.00	0.09	23,23,23,23	0
8	ZN	A	818	1/1	1.00	0.05	26,26,26,26	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.