Full wwPDB X-ray Structure Validation Report

Jun 17, 2024 – 07:06 AM EDT

PDB ID	:	3SJX
Title	:	X-ray structure of human glutamate carboxypeptidase II (the E424A inactive mutant) in complex with N-acetyl-aspartyl-methionine
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Deposited on	:	2011-06-22
Resolution	:	1.66 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

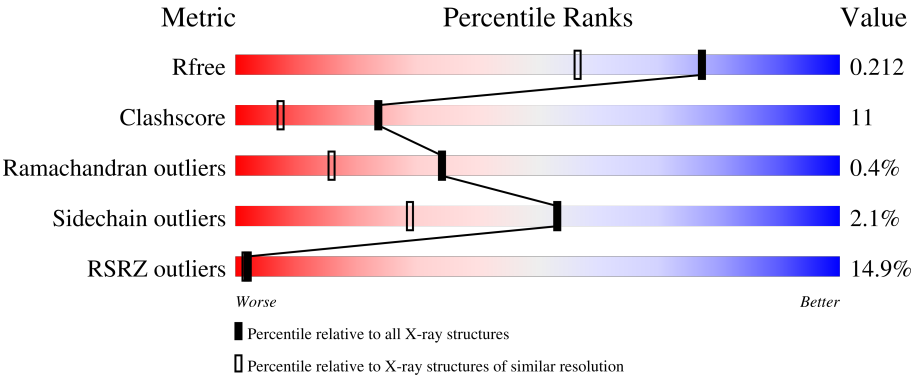
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	709	15%, 80%, 16%, . .
2	B	2	50%, 50%
2	C	2	100%
3	D	4	25%, 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	A	1757	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6633 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	690	Total	C	N	O	S	0	77	0
			6004	3853	1006	1126	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609
A	424	ALA	GLU	engineered mutation	UNP Q04609

- 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			

- 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	D	4	Total C N O 50 28 2 20	0	0	0

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

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

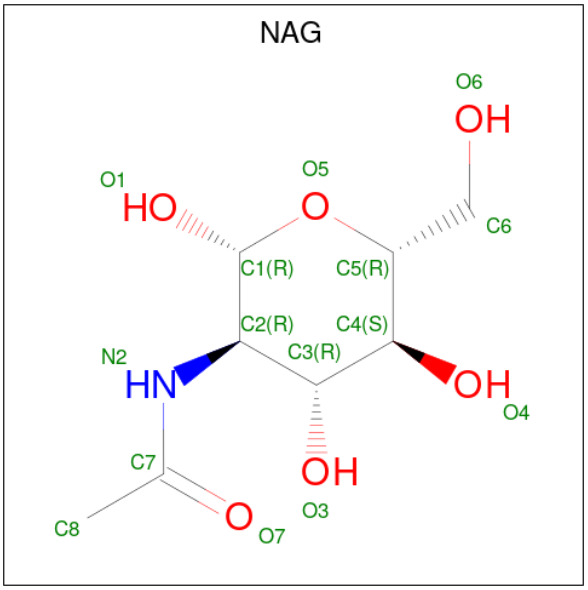
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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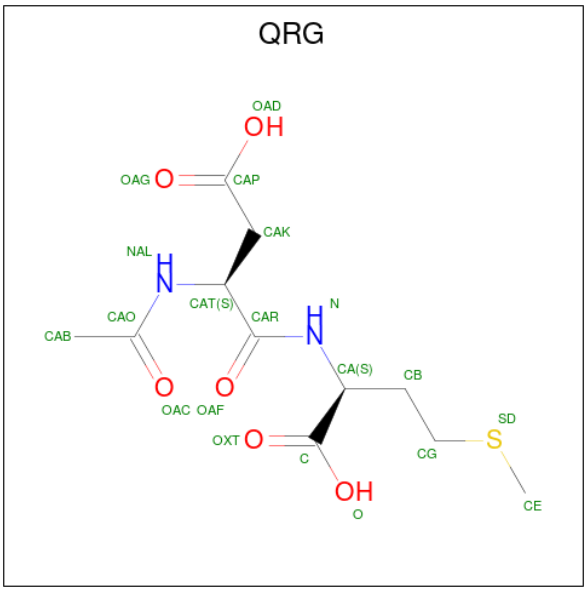
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is N-acetyl-L-alpha-aspartyl-L-methionine (three-letter code: QRG) (formula: $C_{11}H_{18}N_2O_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 20 11 2 6 1	0	0

- Molecule 9 is water.

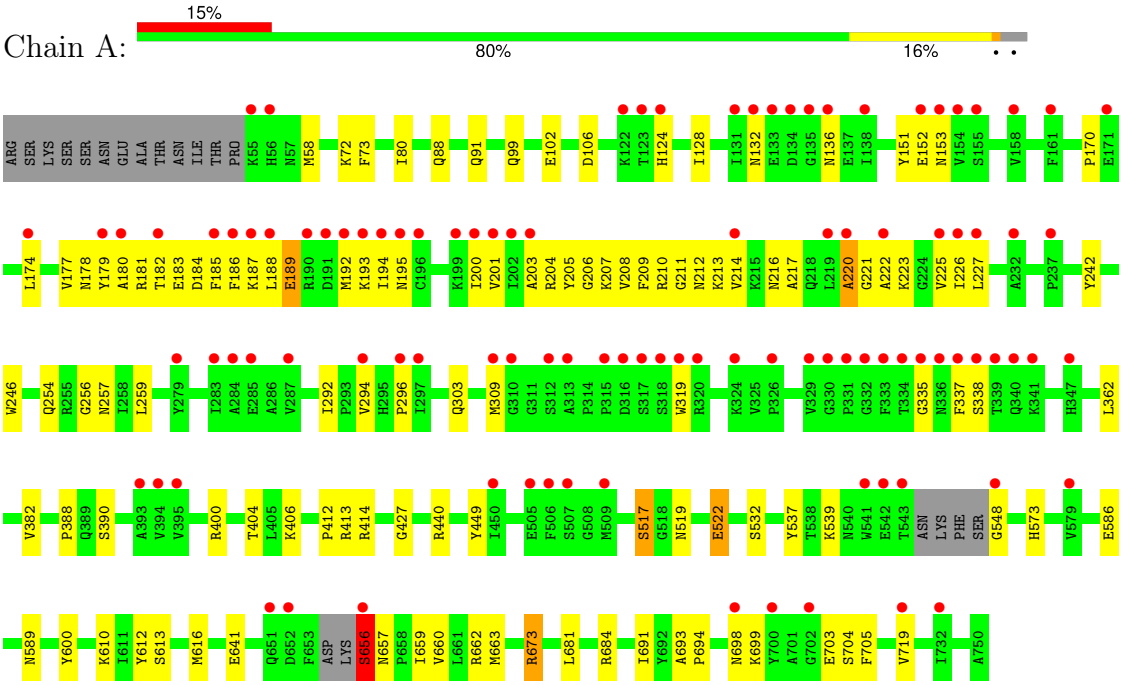
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	457	Total O 457 457	0	0

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

Chain A:

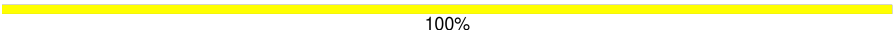


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

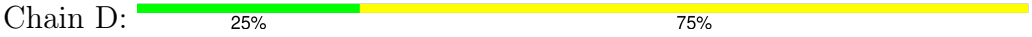
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• 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 D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.54Å 129.94Å 159.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.21 – 1.66 28.21 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.21-1.66) 98.3 (28.21-1.66)	Depositor EDS
R_{merge}	0.62	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 1.66Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.204 0.191 , 0.212	Depositor DCC
R_{free} test set	1815 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6633	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, CA, CL, MAN, QRG, NAG

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	0.90	3/6212 (0.0%)	0.83	6/8405 (0.1%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	GLU	CD-OE2	-7.51	1.17	1.25
1	A	656	SER	CA-CB	6.02	1.61	1.52
1	A	517	SER	CB-OG	5.27	1.49	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	440	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	662	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	413	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	673	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	414	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	662	ARG	CG-CD-NE	-5.33	100.60	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	656	SER	Mainchain

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	6004	0	5806	134	0
2	B	28	0	25	2	0
2	C	28	0	25	0	0
3	D	50	0	43	0	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	20	0	16	1	0
9	A	457	0	0	33	1
All	All	6633	0	5954	136	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 11.

All (136) 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:217[B]:ALA:C	1:A:222[B]:ALA:HB3	1.32	1.43
1:A:217[B]:ALA:O	1:A:222[B]:ALA:N	1.56	1.38
1:A:703[A]:GLU:C	9:A:2238:HOH:O	1.66	1.33
1:A:703[A]:GLU:CB	9:A:2243:HOH:O	1.67	1.29
1:A:216[B]:ASN:O	1:A:220[B]:ALA:HB3	1.33	1.25
1:A:703[A]:GLU:CA	9:A:2243:HOH:O	1.65	1.25
1:A:703[A]:GLU:HB3	9:A:2243:HOH:O	1.24	1.24
1:A:217[B]:ALA:O	1:A:222[B]:ALA:CA	1.86	1.23
1:A:217[B]:ALA:O	1:A:222[B]:ALA:CB	1.85	1.23
1:A:217[B]:ALA:CA	1:A:222[B]:ALA:HB3	1.72	1.18
1:A:693[B]:ALA:HB2	9:A:2228:HOH:O	1.48	1.12
1:A:217[B]:ALA:C	1:A:222[B]:ALA:CB	2.19	1.11
1:A:703[A]:GLU:C	9:A:2243:HOH:O	1.75	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151[B]:TYR:O	1:A:153:ASN:N	1.89	1.05
1:A:217[B]:ALA:O	1:A:222[B]:ALA:HB3	1.47	1.05
1:A:703[A]:GLU:O	9:A:2243:HOH:O	1.71	1.04
1:A:703[B]:GLU:CB	9:A:1912:HOH:O	2.06	1.03
1:A:703[B]:GLU:HB2	9:A:1912:HOH:O	1.60	1.01
1:A:217[B]:ALA:CA	1:A:222[B]:ALA:CB	2.39	0.98
1:A:181[B]:ARG:HB2	1:A:184[B]:ASP:OD2	1.64	0.97
1:A:185[A]:PHE:O	1:A:189:GLU:HG2	1.67	0.95
1:A:221[A]:GLY:O	1:A:222[A]:ALA:O	1.86	0.94
1:A:208[B]:VAL:HG11	9:A:1909:HOH:O	1.73	0.89
1:A:217[B]:ALA:HB1	1:A:222[B]:ALA:CB	2.07	0.84
1:A:703[A]:GLU:N	9:A:2238:HOH:O	2.08	0.83
1:A:208[B]:VAL:CG1	9:A:1909:HOH:O	2.26	0.82
1:A:217[B]:ALA:CB	1:A:222[B]:ALA:HB3	2.10	0.81
1:A:72[A]:LYS:C	1:A:73:PHE:CA	2.49	0.81
1:A:209[B]:PHE:CE2	1:A:211:GLY:HA3	2.17	0.80
1:A:641:GLU:HG3	9:A:2251:HOH:O	1.81	0.79
1:A:610[B]:LYS:HD2	9:A:2244:HOH:O	1.83	0.78
1:A:217[B]:ALA:CB	1:A:222[B]:ALA:CB	2.63	0.77
1:A:703[A]:GLU:O	9:A:2238:HOH:O	1.80	0.76
1:A:72[B]:LYS:C	1:A:73:PHE:CA	2.52	0.76
1:A:216[B]:ASN:O	1:A:220[B]:ALA:CB	2.26	0.76
1:A:362:LEU:CD1	1:A:406:LYS:HD2	2.16	0.75
1:A:704[A]:SER:OG	9:A:2085:HOH:O	2.00	0.75
1:A:703[B]:GLU:HB3	9:A:1912:HOH:O	1.76	0.75
1:A:699[A]:LYS:NZ	9:A:2210:HOH:O	2.21	0.74
1:A:613[B]:SER:OG	9:A:2244:HOH:O	2.05	0.73
1:A:58:MET:CE	1:A:586:GLU:HG2	2.18	0.73
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.70	0.72
1:A:217[B]:ALA:HA	1:A:222[B]:ALA:CB	2.19	0.72
1:A:684:ARG:NH2	1:A:694[B]:PRO:O	2.23	0.71
1:A:214[B]:VAL:HA	1:A:225[B]:VAL:HG21	1.72	0.70
1:A:217[B]:ALA:HA	1:A:222[B]:ALA:HB2	1.73	0.69
1:A:610[B]:LYS:CE	9:A:2244:HOH:O	2.41	0.69
1:A:174:LEU:HB2	1:A:309:MET:HE3	1.74	0.68
9:A:2018:HOH:O	2:B:2:NAG:H81	1.92	0.68
1:A:91[A]:GLN:OE1	9:A:2216:HOH:O	2.12	0.67
1:A:217[B]:ALA:HB1	1:A:222[B]:ALA:HB1	1.78	0.66
1:A:179[B]:TYR:O	1:A:213[B]:LYS:HE3	1.96	0.66
1:A:182[B]:THR:O	1:A:186[B]:PHE:N	2.26	0.65
1:A:242:TYR:OH	9:A:2252:HOH:O	1.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:HB2	7:A:1759:NAG:N2	2.14	0.63
1:A:182[B]:THR:O	1:A:185[B]:PHE:HB2	1.99	0.62
1:A:703[A]:GLU:N	9:A:2243:HOH:O	2.07	0.62
1:A:217[B]:ALA:CB	1:A:225[B]:VAL:HG22	2.29	0.61
1:A:183[B]:GLU:HA	1:A:186[B]:PHE:HB2	1.81	0.61
1:A:185[A]:PHE:O	1:A:189:GLU:CG	2.48	0.60
1:A:189:GLU:HG3	9:A:2250:HOH:O	2.02	0.60
1:A:703[A]:GLU:CA	9:A:2238:HOH:O	2.23	0.59
1:A:362:LEU:HD11	1:A:406:LYS:HD2	1.85	0.58
1:A:209[B]:PHE:O	1:A:212[B]:ASN:N	2.35	0.58
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.39	0.58
1:A:179[B]:TYR:CD2	1:A:207[B]:LYS:HG3	2.39	0.57
1:A:400:ARG:O	1:A:404:THR:HG23	2.05	0.57
1:A:517:SER:HB3	1:A:699[A]:LYS:HG2	1.87	0.56
1:A:188:LEU:HG	1:A:319:TRP:HH2	1.70	0.56
1:A:684:ARG:NH1	1:A:694[B]:PRO:O	2.39	0.55
1:A:80:ILE:HD12	1:A:88[B]:GLN:HG2	1.88	0.55
1:A:180[B]:ALA:HB3	1:A:213[B]:LYS:HG2	1.88	0.55
1:A:180[B]:ALA:HB2	1:A:203:ALA:HB2	1.89	0.54
1:A:698[B]:ASN:HB2	9:A:1996:HOH:O	2.07	0.54
1:A:181[B]:ARG:HG2	1:A:208[B]:VAL:CG1	2.37	0.54
1:A:517:SER:OG	1:A:522:GLU:OE2	2.21	0.54
1:A:412:PRO:HA	1:A:589[B]:ASN:OD1	2.07	0.53
1:A:656:SER:O	1:A:656:SER:OG	2.26	0.53
1:A:610[B]:LYS:CD	9:A:2244:HOH:O	2.45	0.53
1:A:179[B]:TYR:HB3	1:A:206[B]:GLY:O	2.09	0.52
1:A:208[B]:VAL:HG12	9:A:1909:HOH:O	2.03	0.52
1:A:610[A]:LYS:HD3	9:A:2085:HOH:O	2.10	0.52
1:A:205[A]:TYR:HA	1:A:213[A]:LYS:HE3	1.92	0.51
1:A:704[B]:SER:O	1:A:705[B]:PHE:HB2	2.10	0.51
1:A:390[A]:SER:HB2	1:A:573:HIS:NE2	2.26	0.51
1:A:179[B]:TYR:CD1	1:A:207[B]:LYS:HG2	2.46	0.51
1:A:217[B]:ALA:HB1	1:A:222[B]:ALA:HB3	1.80	0.51
1:A:610[B]:LYS:HE3	9:A:2244:HOH:O	2.10	0.50
1:A:179[B]:TYR:CD2	1:A:179[B]:TYR:N	2.80	0.49
1:A:681:LEU:HD11	1:A:693[B]:ALA:HB3	1.95	0.49
1:A:181[B]:ARG:HG2	1:A:208[B]:VAL:HG13	1.94	0.48
1:A:181[B]:ARG:CB	1:A:184[B]:ASP:OD2	2.33	0.48
1:A:208[B]:VAL:O	1:A:213[B]:LYS:NZ	2.47	0.48
1:A:217[B]:ALA:CB	1:A:225[B]:VAL:CG2	2.92	0.47
1:A:257[B]:ASN:OD1	1:A:259:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[B]:VAL:CG2	1:A:294:VAL:HG21	2.45	0.46
1:A:217[B]:ALA:HB3	1:A:225[B]:VAL:CG2	2.45	0.46
1:A:691:ILE:O	1:A:704[A]:SER:HA	2.15	0.46
1:A:205[A]:TYR:CE1	1:A:254:GLN:HB3	2.51	0.46
1:A:179[A]:TYR:O	1:A:180[A]:ALA:HB3	2.16	0.46
1:A:684:ARG:CZ	1:A:694[B]:PRO:O	2.63	0.46
1:A:214[B]:VAL:HG21	1:A:294:VAL:HG21	1.98	0.45
1:A:177:VAL:CG2	1:A:180[B]:ALA:HA	2.47	0.45
1:A:217[B]:ALA:HB2	1:A:225[B]:VAL:HG22	1.97	0.45
1:A:180[B]:ALA:HB3	1:A:213[B]:LYS:CG	2.47	0.45
1:A:179[B]:TYR:CG	1:A:207[B]:LYS:CG	3.00	0.45
1:A:180[B]:ALA:HB2	1:A:203:ALA:CB	2.47	0.44
1:A:335:GLY:HA2	1:A:338:SER:HB3	2.00	0.44
1:A:174:LEU:HA	1:A:200:ILE:O	2.18	0.44
1:A:106:ASP:OD1	1:A:406:LYS:HE3	2.18	0.43
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.18	0.43
1:A:170:PRO:HB3	1:A:223[A]:LYS:HE2	2.00	0.43
1:A:179[B]:TYR:OH	1:A:204:ARG:CZ	2.66	0.43
1:A:657[B]:ASN:HB3	1:A:660[B]:VAL:HB	2.00	0.43
1:A:539:LYS:NZ	1:A:548:GLY:O	2.47	0.42
9:A:2172:HOH:O	2:B:2:NAG:H83	2.19	0.42
1:A:58:MET:HE1	1:A:586:GLU:CG	2.46	0.42
1:A:246:TRP:CD1	7:A:1760:NAG:H83	2.54	0.42
1:A:192:MET:HB3	1:A:194:ILE:HD12	2.02	0.42
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.42
1:A:181[B]:ARG:HG2	1:A:208[B]:VAL:HG11	2.01	0.42
1:A:58:MET:HE2	1:A:586:GLU:HG2	2.00	0.41
1:A:427:GLY:HA2	8:A:1:QRG:SD	2.60	0.41
1:A:449:TYR:O	1:A:532:SER:HA	2.19	0.41
1:A:132:ASN:ND2	1:A:136:ASN:HB2	2.36	0.41
1:A:183[B]:GLU:O	1:A:186[B]:PHE:HB2	2.21	0.41
1:A:185[A]:PHE:O	1:A:189:GLU:OE2	2.39	0.41
1:A:693[B]:ALA:CB	9:A:2228:HOH:O	2.27	0.41
1:A:178:ASN:HD22	1:A:181[B]:ARG:NH2	2.19	0.41
1:A:128:ILE:HD13	1:A:226:ILE:HG12	2.03	0.41
1:A:189:GLU:O	1:A:193:LYS:HA	2.21	0.41
1:A:217[B]:ALA:HB3	1:A:292:ILE:HD11	2.03	0.41
1:A:209[B]:PHE:CD2	1:A:211:GLY:HA3	2.53	0.40
1:A:210[A]:ARG:CZ	1:A:256:GLY:HA3	2.51	0.40

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)
9:A:1904:HOH:O	9:A:2168:HOH:O[2_565]	1.85	0.35

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	749/709 (106%)	716 (96%)	28 (4%)	5 (1%)	22 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152[A]	GLU
1	A	152[B]	GLU
1	A	220[A]	ALA
1	A	220[B]	ALA
1	A	382	VAL

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	646/604 (107%)	633 (98%)	13 (2%)	55 32

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	HIS

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Mol	Chain	Res	Type
1	A	187[A]	LYS
1	A	187[B]	LYS
1	A	189	GLU
1	A	201	VAL
1	A	303	GLN
1	A	337	PHE
1	A	388	PRO
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG
1	A	719	VAL

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

Mol	Chain	Res	Type
1	A	136	ASN

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)

8 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	0.46	0	17,19,21	1.31	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	1.44	2 (11%)
2	NAG	C	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	0.66	0
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.08	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.34	3 (17%)
3	NAG	D	2	3	14,14,15	0.65	0	17,19,21	1.30	2 (11%)
3	BMA	D	3	3	11,11,12	0.70	0	15,15,17	0.82	0
3	MAN	D	4	3	11,11,12	0.66	0	15,15,17	1.17	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	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	-	0/2/19/22	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	O7-C7	2.83	1.29	1.23
3	D	1	NAG	C1-C2	2.16	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C2-N2-C7	4.43	128.84	122.90
3	D	1	NAG	O5-C1-C2	-3.72	105.54	111.29
2	B	1	NAG	O5-C1-C2	-3.24	106.27	111.29
3	D	4	MAN	O5-C5-C6	2.89	113.29	107.66
3	D	2	NAG	C3-C4-C5	-2.54	105.62	110.23
3	D	2	NAG	C8-C7-N2	2.50	120.26	116.12
2	B	2	NAG	C1-O5-C5	2.43	115.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C8-C7-N2	2.26	119.86	116.12
3	D	1	NAG	C1-O5-C5	2.21	115.14	112.19
3	D	1	NAG	O4-C4-C5	-2.20	103.91	109.32
3	D	4	MAN	C1-O5-C5	2.20	115.13	112.19

There are no chirality outliers.

All (10) 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
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

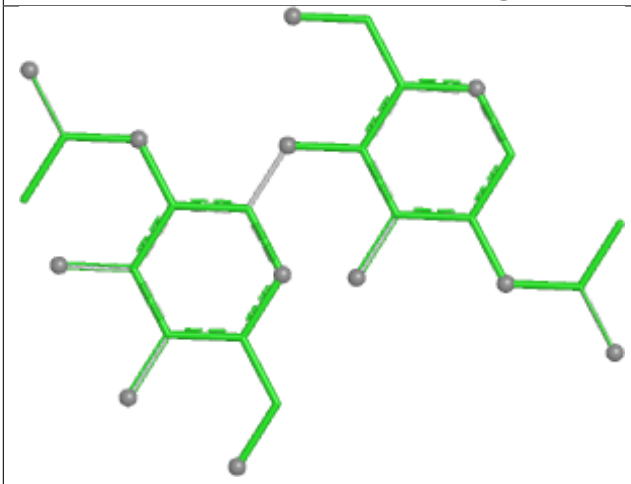
There are no ring outliers.

1 monomer is involved in 2 short contacts:

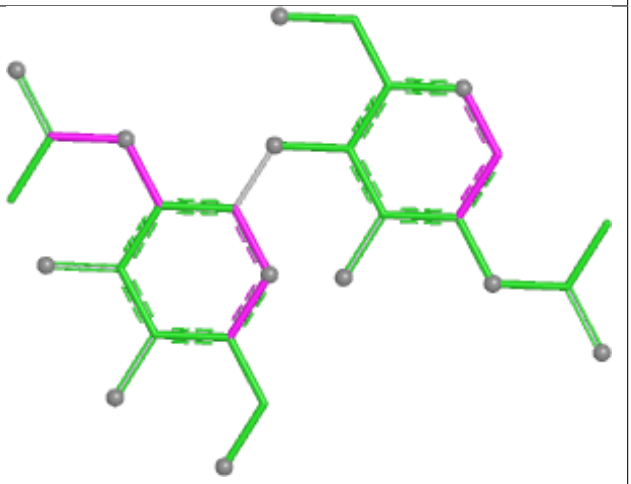
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

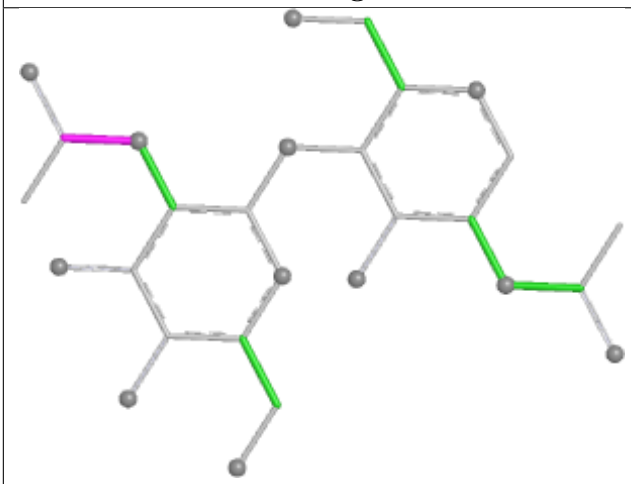
Oligosaccharide Chain B



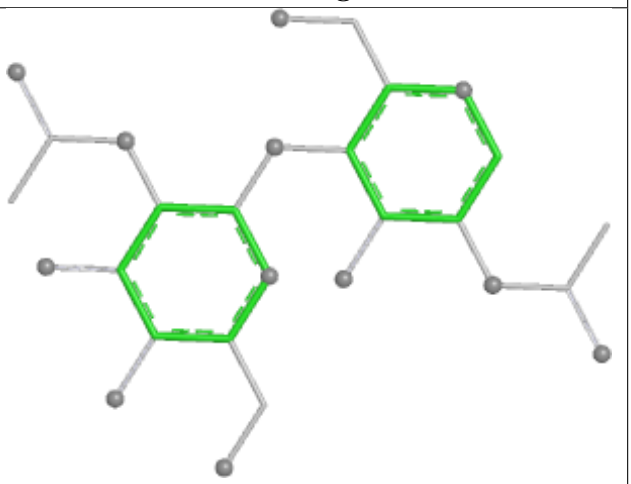
Bond lengths



Bond angles

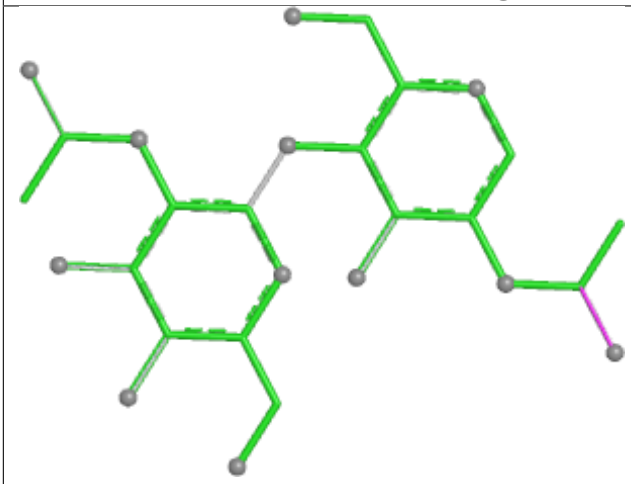


Torsions

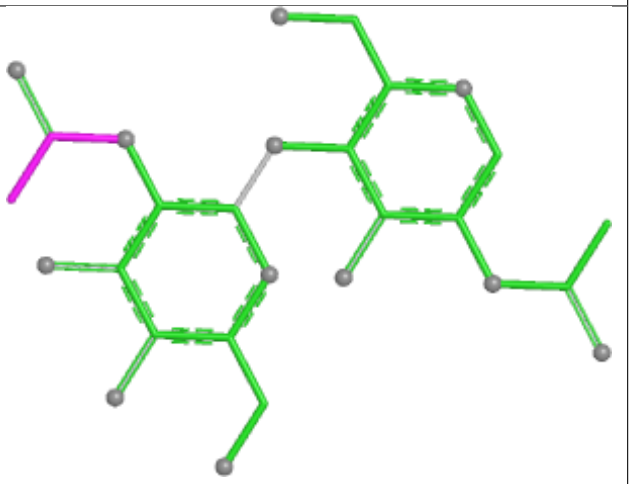


Rings

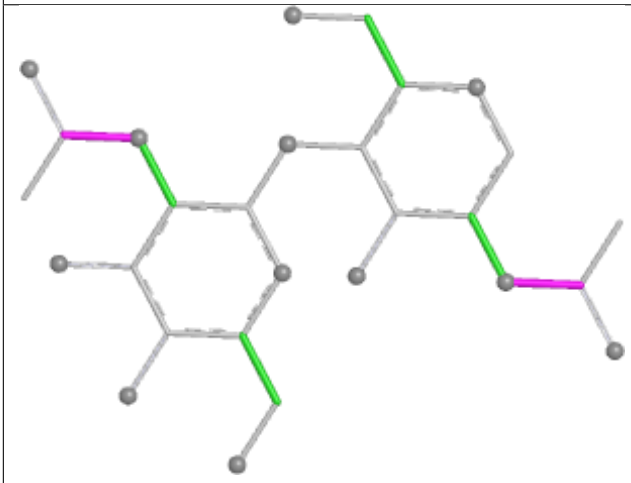
Oligosaccharide Chain C



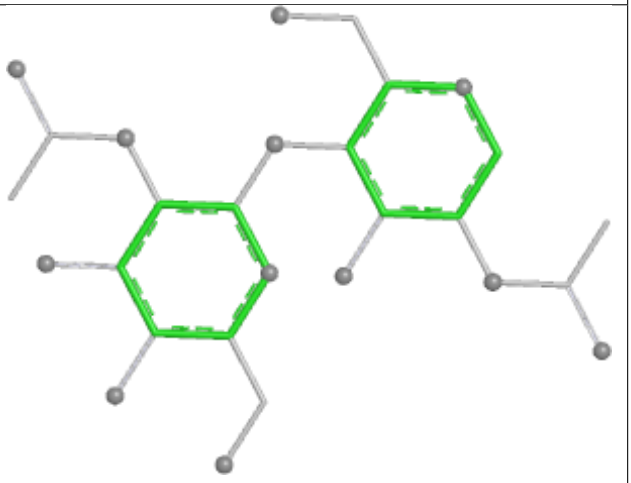
Bond lengths



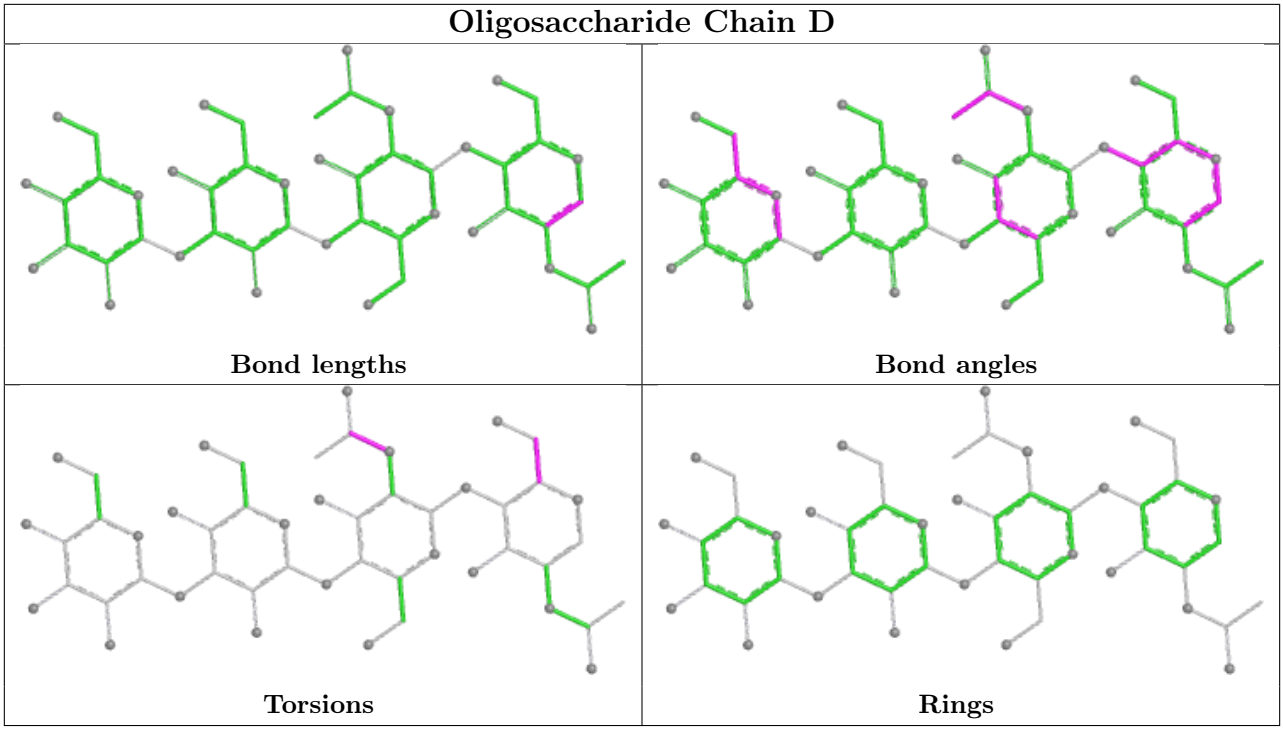
Bond angles



Torsions



Rings



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	NAG	A	1757	1	14,14,15	0.54	0	17,19,21	1.84	4 (23%)
7	NAG	A	1759	1	14,14,15	0.91	1 (7%)	17,19,21	1.60	3 (17%)
8	QRG	A	1	4	19,19,19	1.18	2 (10%)	24,24,24	1.23	2 (8%)
7	NAG	A	1760	1	14,14,15	0.85	0	17,19,21	1.58	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
7	NAG	A	1757	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1759	1	-	2/6/23/26	0/1/1/1
8	QRG	A	1	4	-	3/24/24/24	-
7	NAG	A	1760	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1759	NAG	C1-C2	2.80	1.56	1.52
8	A	1	QRG	CA-N	2.15	1.50	1.45
8	A	1	QRG	OAG-CAP	2.08	1.28	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1757	NAG	C1-O5-C5	5.11	119.03	112.19
7	A	1759	NAG	C1-O5-C5	3.96	117.49	112.19
7	A	1759	NAG	C2-N2-C7	3.17	127.15	122.90
8	A	1	QRG	CB-CA-N	-2.85	105.27	110.91
7	A	1757	NAG	C3-C4-C5	2.85	115.39	110.23
7	A	1760	NAG	O5-C1-C2	-2.80	106.97	111.29
7	A	1760	NAG	C1-O5-C5	2.63	115.71	112.19
7	A	1760	NAG	C8-C7-N2	2.60	120.42	116.12
7	A	1760	NAG	O7-C7-C8	-2.55	117.51	122.05
7	A	1757	NAG	O5-C5-C4	2.41	116.69	110.83
7	A	1759	NAG	O5-C1-C2	-2.38	107.61	111.29
8	A	1	QRG	CAK-CAT-CAR	-2.20	105.37	110.57
7	A	1757	NAG	O3-C3-C2	-2.04	105.15	109.40

There are no chirality outliers.

All (7) 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	1759	NAG	O5-C5-C6-O6
8	A	1	QRG	CAT-CAK-CAP-OAD
8	A	1	QRG	CAT-CAK-CAP-OAG
8	A	1	QRG	OAF-CAR-CAT-NAL
7	A	1759	NAG	C4-C5-C6-O6

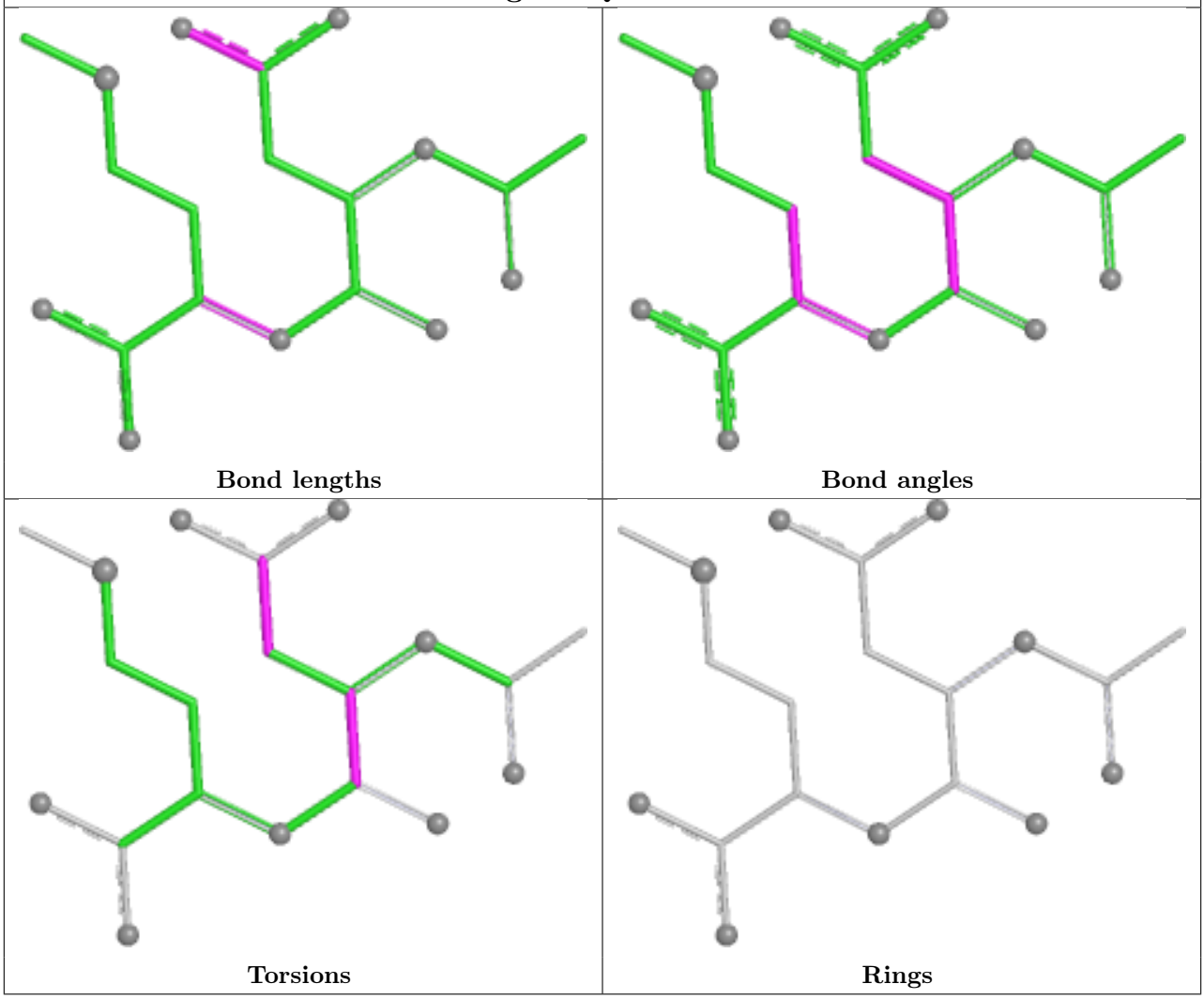
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1759	NAG	1	0
8	A	1	QRG	1	0
7	A	1760	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 then 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.

Ligand QRG A 1



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^{th} 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	690/709 (97%)	0.68	103 (14%) 2 2	15, 27, 60, 78	5 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	8.5
1	A	135	GLY	7.5
1	A	543	THR	7.5
1	A	337	PHE	6.4
1	A	155	SER	6.2
1	A	186[A]	PHE	5.7
1	A	317	SER	5.5
1	A	138	ILE	5.4
1	A	318	SER	5.3
1	A	153	ASN	5.2
1	A	136	ASN	5.2
1	A	506	PHE	5.2
1	A	542	GLU	4.9
1	A	133	GLU	4.5
1	A	154	VAL	4.5
1	A	507	SER	4.5
1	A	55	LYS	4.5
1	A	202	ILE	4.4
1	A	284	ALA	4.3
1	A	226	ILE	4.3
1	A	134	ASP	4.2
1	A	200	ILE	4.2
1	A	310	GLY	4.1
1	A	656	SER	4.1
1	A	329	VAL	4.0
1	A	222[A]	ALA	4.0
1	A	124	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	719	VAL	4.0
1	A	315	PRO	3.9
1	A	341	LYS	3.9
1	A	287	VAL	3.9
1	A	225[A]	VAL	3.9
1	A	227	LEU	3.8
1	A	333	PHE	3.8
1	A	131	ILE	3.8
1	A	194	ILE	3.8
1	A	336	ASN	3.8
1	A	331	PRO	3.7
1	A	338	SER	3.7
1	A	340	GLN	3.7
1	A	195	ASN	3.7
1	A	123	THR	3.5
1	A	339	THR	3.5
1	A	182[A]	THR	3.5
1	A	652	ASP	3.4
1	A	187[A]	LYS	3.3
1	A	505[A]	GLU	3.2
1	A	732	ILE	3.2
1	A	185[A]	PHE	3.2
1	A	132	ASN	3.1
1	A	316	ASP	3.1
1	A	700[A]	TYR	3.1
1	A	201	VAL	3.0
1	A	152[A]	GLU	3.0
1	A	174	LEU	3.0
1	A	312	SER	2.9
1	A	319	TRP	2.9
1	A	199	LYS	2.9
1	A	294	VAL	2.8
1	A	334	THR	2.7
1	A	219[A]	LEU	2.7
1	A	158[A]	VAL	2.7
1	A	191	ASP	2.6
1	A	335	GLY	2.6
1	A	651	GLN	2.6
1	A	220[A]	ALA	2.6
1	A	330	GLY	2.5
1	A	332	GLY	2.5
1	A	203	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	2.5
1	A	179[A]	TYR	2.5
1	A	196	CYS	2.5
1	A	450	ILE	2.5
1	A	698[A]	ASN	2.5
1	A	188	LEU	2.5
1	A	122	LYS	2.4
1	A	285	GLU	2.4
1	A	190	ARG	2.3
1	A	313	ALA	2.3
1	A	56	HIS	2.3
1	A	297	ILE	2.3
1	A	283	ILE	2.3
1	A	161	PHE	2.3
1	A	320	ARG	2.3
1	A	193	LYS	2.3
1	A	309	MET	2.3
1	A	324	LYS	2.3
1	A	579	VAL	2.2
1	A	192	MET	2.2
1	A	326	PRO	2.2
1	A	214[A]	VAL	2.2
1	A	395	VAL	2.1
1	A	171	GLU	2.1
1	A	509	MET	2.1
1	A	347	HIS	2.1
1	A	393	ALA	2.1
1	A	296	PRO	2.1
1	A	180[A]	ALA	2.1
1	A	232	ALA	2.1
1	A	279[A]	TYR	2.0
1	A	548	GLY	2.0
1	A	237	PRO	2.0
1	A	702[A]	GLY	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)

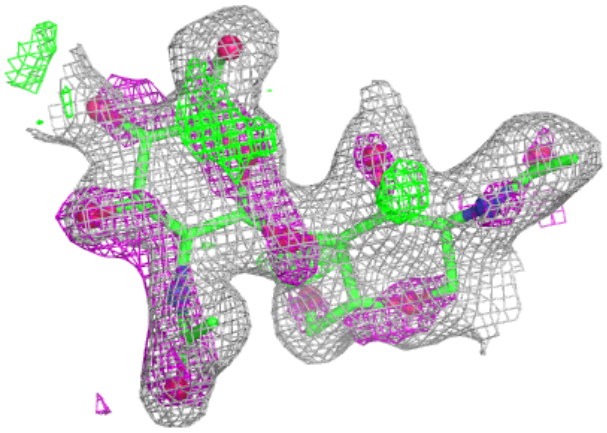
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

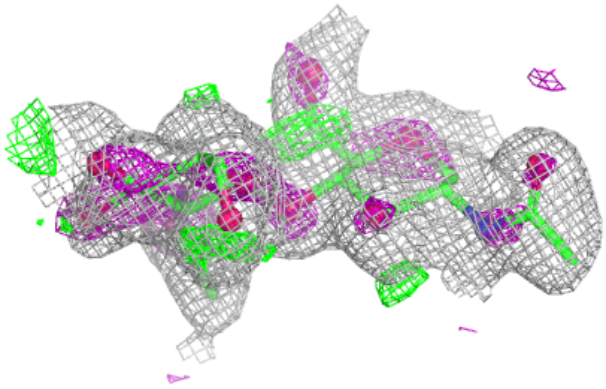
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.70	0.33	27,33,36,38	0
2	NAG	C	2	14/15	0.85	0.27	20,28,33,37	0
3	BMA	D	3	11/12	0.86	0.23	30,33,37,37	0
3	NAG	D	2	14/15	0.88	0.29	26,31,40,41	0
2	NAG	C	1	14/15	0.89	0.15	16,18,27,29	0
3	MAN	D	4	11/12	0.90	0.28	34,36,40,40	0
3	NAG	D	1	14/15	0.93	0.12	12,18,23,33	0
2	NAG	B	1	14/15	0.93	0.19	20,25,33,34	0

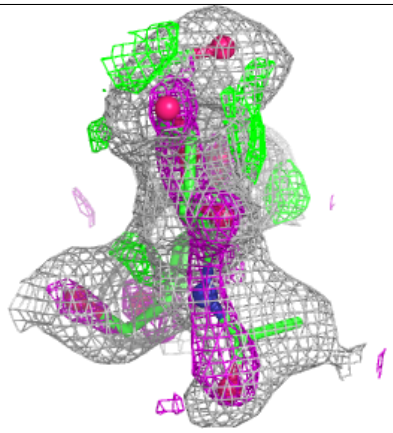
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

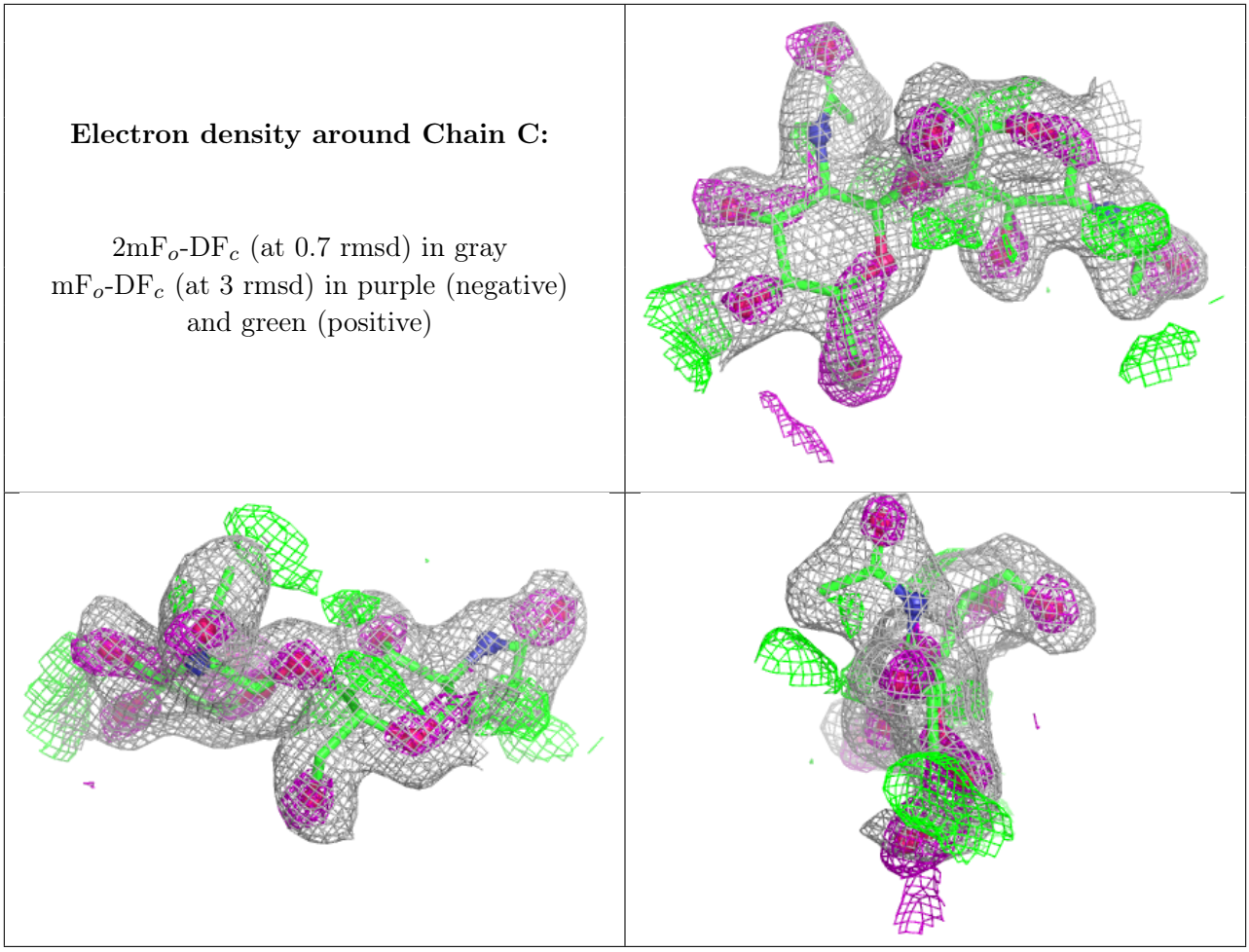






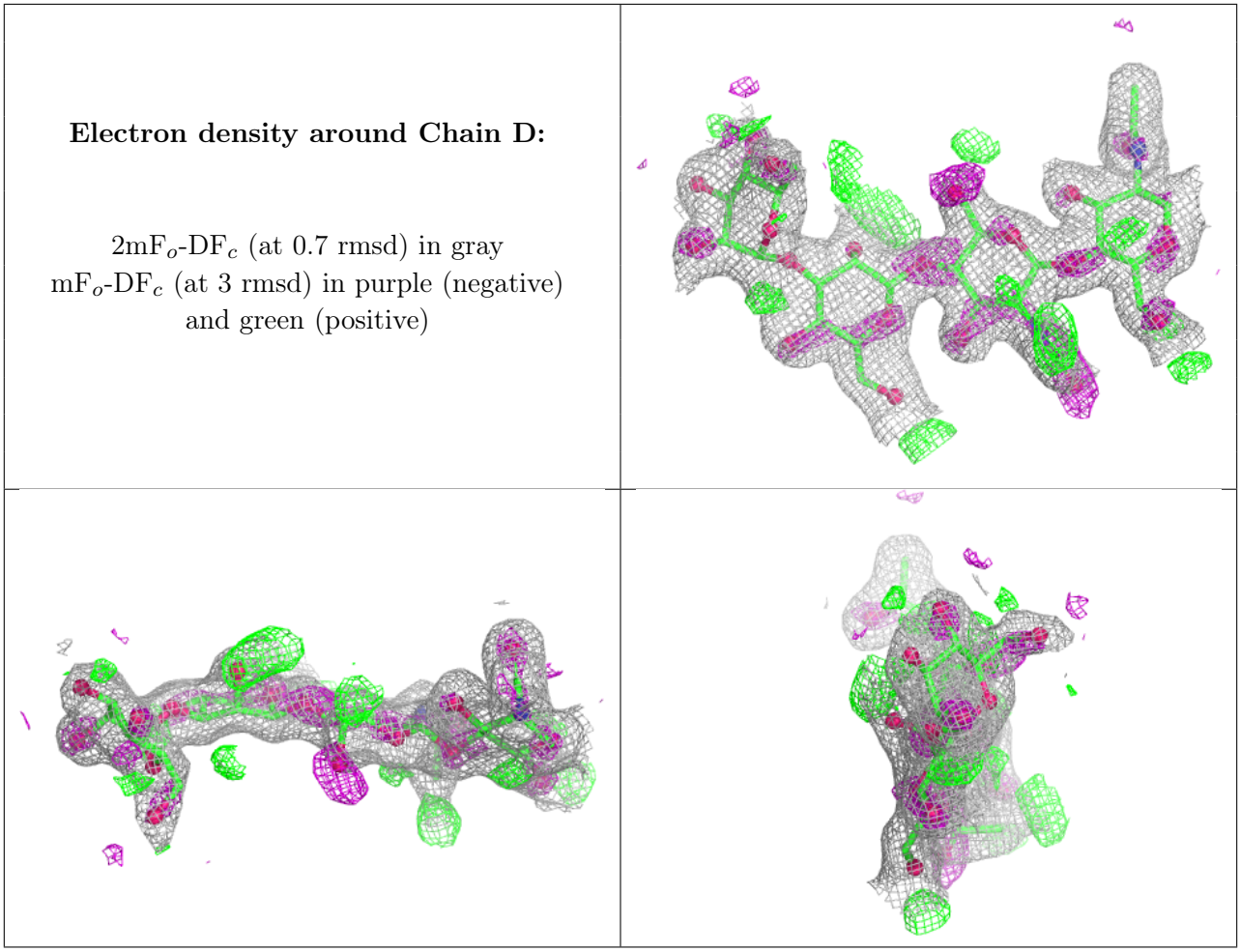
Electron density around Chain C:

$2mF_o$-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

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^{th} 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.

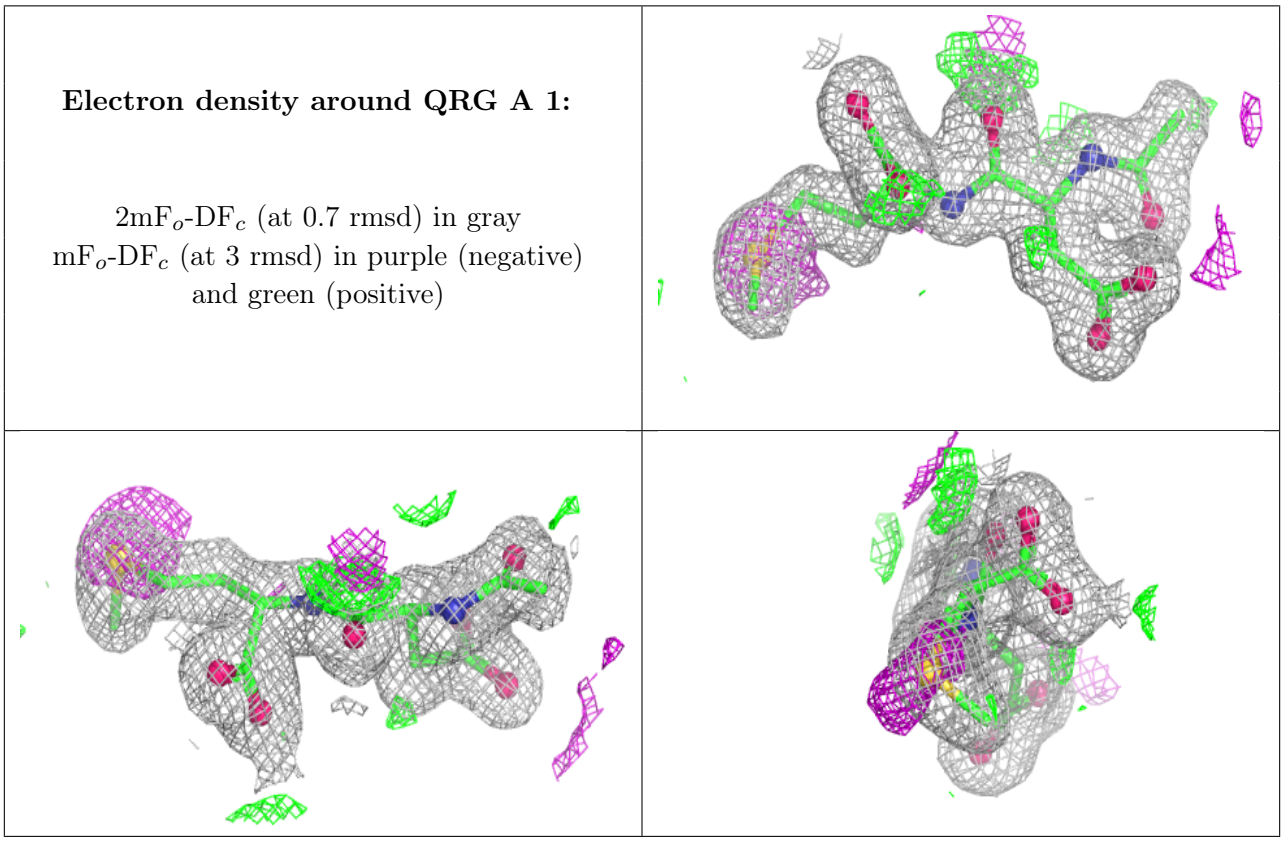
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	1759	14/15	0.56	0.39	58,62,65,65	0
7	NAG	A	1757	14/15	0.68	0.45	38,43,46,47	0
7	NAG	A	1760	14/15	0.82	0.22	18,27,30,31	0
8	QRG	A	1	20/20	0.93	0.09	22,26,36,37	0
4	ZN	A	1752	1/1	0.99	0.03	14,14,14,14	0
6	CL	A	1754	1/1	0.99	0.04	17,17,17,17	0
4	ZN	A	1751	1/1	0.99	0.02	14,14,14,14	0
5	CA	A	1753	1/1	1.00	0.04	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QRG A 1:

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



6.5 Other polymers (i)

There are no such residues in this entry.