Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:01 AM EDT

PDB ID	:	3SJE
Title	:	X-ray structure of human glutamate carboxypeptidase II (the E424A inactive mutant) in complex with N-acetyl-aspartyl-aminononanoic acid
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Deposited on	:	2011-06-21
Resolution	:	1.70 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 (i) 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:

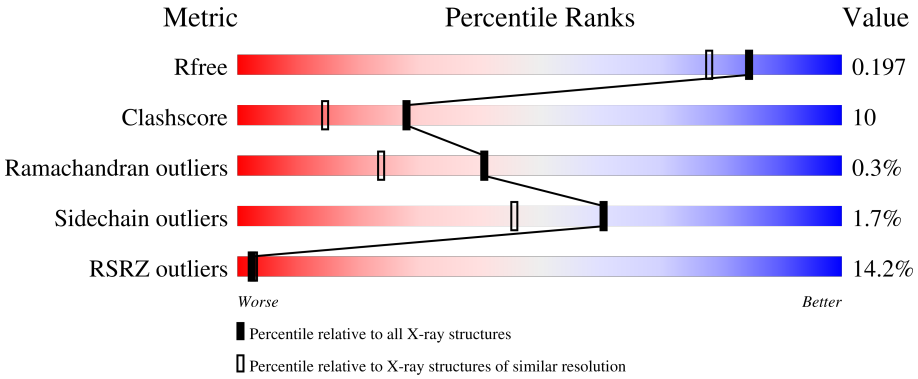
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	14% 84% 12%
2	B	2	50% 50%
2	C	2	100%
2	D	2	100%
3	E	4	100%

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
2	NAG	C	2	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6457 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	57	0
			5853	3756	989	1089	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			
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 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

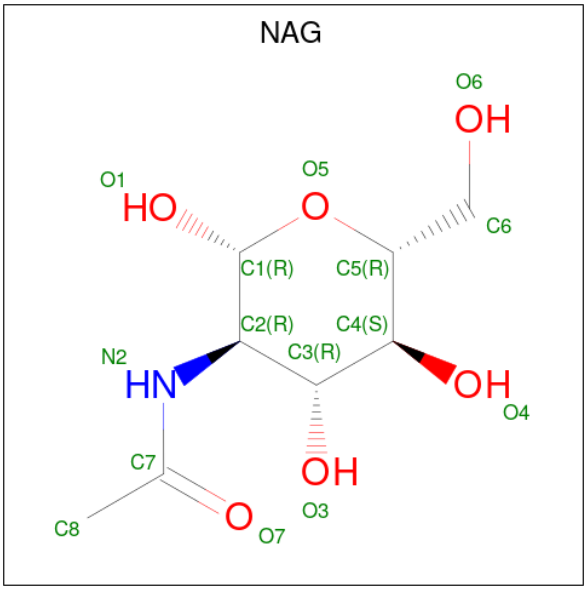
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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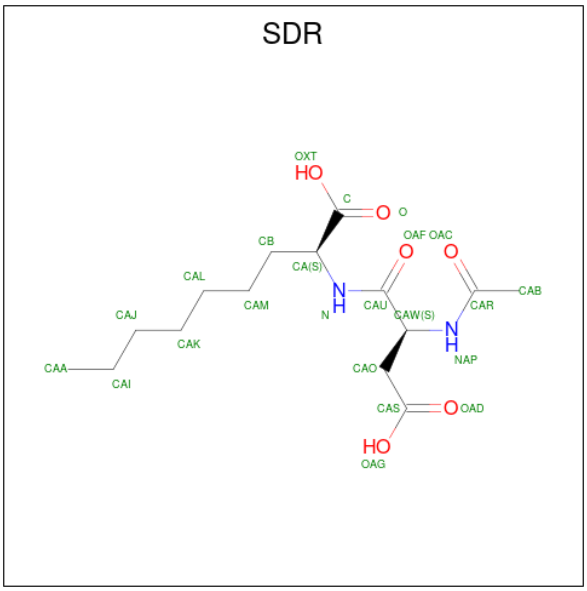
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is (2S)-2-[(N-acetyl-L-alpha-aspartyl)amino]nonanoic acid (three-letter code: SDR) (formula: $C_{15}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 23 15 2 6	0	0

- Molecule 9 is water.

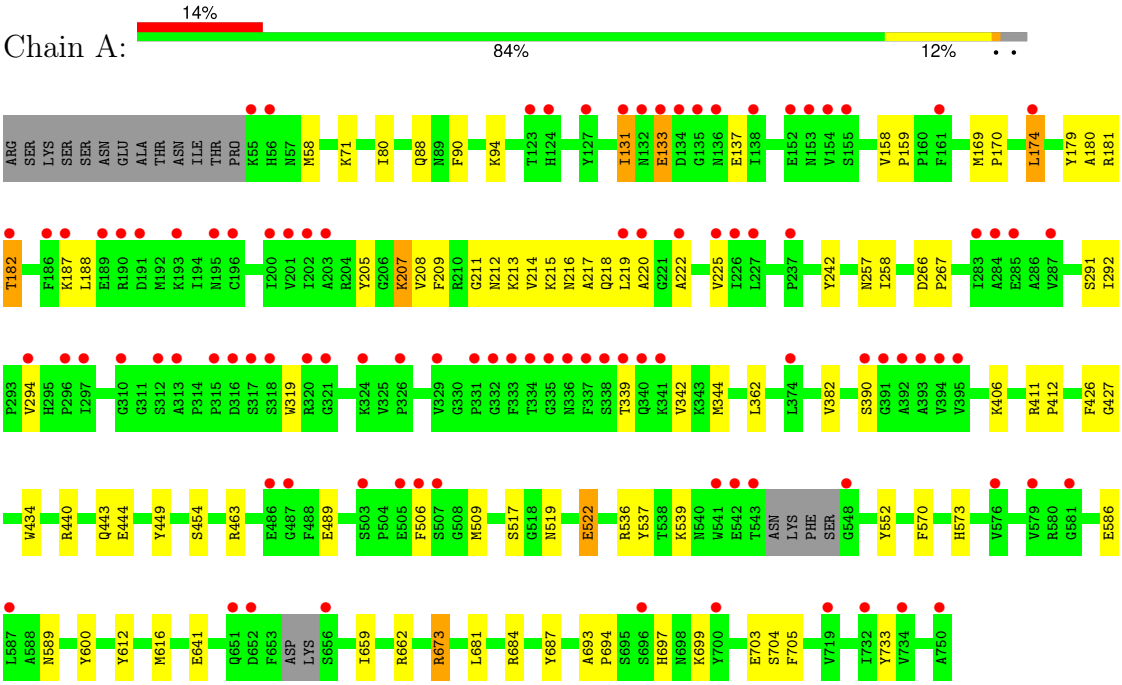
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	401	Total O 401 401	0	0

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:

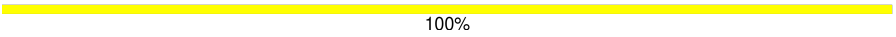


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain C:

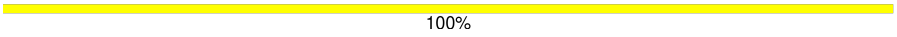


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.82Å 130.23Å 159.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 1.70 29.57 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.57-1.70) 96.6 (29.57-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.188 0.185 , 0.197	Depositor DCC
R_{free} test set	1669 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: CL, MAN, ZN, BMA, SDR, NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.97	5/6068 (0.1%)	0.86	6/8222 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	GLU	CG-CD	5.98	1.60	1.51
1	A	426	PHE	CE2-CZ	5.23	1.47	1.37
1	A	434	TRP	CE3-CZ3	5.22	1.47	1.38
1	A	552	TYR	CE2-CZ	-5.20	1.31	1.38
1	A	449	TYR	CD2-CE2	5.02	1.46	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	673	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	673	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	440	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	662[A]	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	411	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5853	0	5681	114	0
2	B	28	0	25	2	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	E	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	0	0
8	A	23	0	24	7	0
9	A	401	0	0	26	0
All	All	6457	0	5862	118	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 10.

All (118) 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:703[A]:GLU:C	9:A:2168:HOH:O	1.72	1.23
1:A:703[B]:GLU:HB2	9:A:1912:HOH:O	1.37	1.21
1:A:693[B]:ALA:HB2	9:A:1806:HOH:O	1.48	1.13
1:A:181:ARG:HD3	1:A:207[B]:LYS:HB3	1.23	1.08
1:A:181:ARG:HD3	1:A:207[B]:LYS:CB	1.85	1.06
1:A:215[B]:LYS:O	1:A:218[B]:GLN:HG2	1.61	0.99
1:A:181:ARG:HG2	1:A:208[B]:VAL:HG13	1.43	0.98
1:A:697[B]:HIS:ND1	9:A:2171:HOH:O	1.94	0.98
1:A:208[B]:VAL:HG11	9:A:1909:HOH:O	1.66	0.94
1:A:215[B]:LYS:HA	1:A:218[B]:GLN:HG2	1.56	0.88
1:A:703[A]:GLU:N	9:A:2168:HOH:O	2.05	0.87
1:A:174:LEU:HD11	1:A:342:VAL:CG2	2.04	0.86
1:A:215[B]:LYS:O	1:A:218[B]:GLN:CG	2.24	0.86
1:A:703[A]:GLU:O	9:A:2168:HOH:O	1.83	0.83
1:A:208[B]:VAL:CG1	9:A:1909:HOH:O	2.26	0.82
1:A:641:GLU:HG3	9:A:2183:HOH:O	1.79	0.82
1:A:703[A]:GLU:O	9:A:2169:HOH:O	1.95	0.82
1:A:684:ARG:NH2	1:A:694[B]:PRO:O	2.14	0.81
1:A:215[B]:LYS:O	1:A:219:LEU:N	2.17	0.78
1:A:215[B]:LYS:CA	1:A:218[B]:GLN:HG2	2.14	0.76
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1:SDR:HAA	9:A:2007:HOH:O	1.87	0.75
1:A:131:ILE:HD11	1:A:137:GLU:HG2	1.67	0.74
1:A:215[B]:LYS:C	1:A:218[B]:GLN:HG2	2.08	0.74
1:A:427:GLY:HA2	8:A:1:SDR:HAL	1.69	0.73
1:A:217[B]:ALA:O	1:A:222:ALA:N	2.21	0.73
1:A:174:LEU:HD11	1:A:342:VAL:HG21	1.69	0.72
1:A:182:THR:HG21	1:A:697[A]:HIS:ND1	2.04	0.72
1:A:179:TYR:CD2	1:A:207[B]:LYS:HG3	2.26	0.71
1:A:733:TYR:HE2	9:A:2180:HOH:O	1.74	0.71
1:A:697[B]:HIS:HB2	9:A:2171:HOH:O	1.91	0.71
1:A:58:MET:CE	1:A:586:GLU:HG2	2.21	0.70
1:A:90:PHE:CE2	1:A:94:LYS:HE2	2.26	0.70
1:A:216[B]:ASN:C	1:A:218[B]:GLN:N	2.40	0.70
1:A:209[B]:PHE:CE2	1:A:211:GLY:HA3	2.28	0.69
1:A:536[B]:ARG:N	1:A:536[B]:ARG:HD2	2.06	0.69
1:A:216[B]:ASN:O	1:A:217[B]:ALA:C	2.33	0.67
1:A:684:ARG:NH1	1:A:694[B]:PRO:O	2.29	0.65
1:A:174:LEU:HD12	1:A:174:LEU:N	2.12	0.65
1:A:214[B]:VAL:HG21	1:A:294:VAL:HG21	1.79	0.64
1:A:463:ARG:CZ	1:A:536[B]:ARG:NH2	2.62	0.63
1:A:463:ARG:NH2	1:A:536[B]:ARG:NH2	2.46	0.63
1:A:704[A]:SER:OG	9:A:2167:HOH:O	2.15	0.63
1:A:133:GLU:CD	1:A:133:GLU:H	2.02	0.63
1:A:217[B]:ALA:CB	1:A:225:VAL:HG22	2.29	0.62
1:A:180:ALA:HB3	1:A:213[B]:LYS:HG2	1.82	0.62
1:A:80:ILE:HD12	1:A:88[B]:GLN:HG2	1.81	0.61
1:A:681:LEU:HD11	1:A:693[B]:ALA:HB3	1.83	0.60
9:A:2018:HOH:O	2:B:2:NAG:H81	2.01	0.60
1:A:217[B]:ALA:HB1	1:A:222:ALA:HB3	1.83	0.60
1:A:181:ARG:HD3	1:A:207[B]:LYS:HB2	1.77	0.59
1:A:697[B]:HIS:CG	9:A:2171:HOH:O	2.49	0.59
1:A:217[B]:ALA:O	1:A:222:ALA:HB3	2.03	0.59
1:A:703[B]:GLU:CB	9:A:1912:HOH:O	2.15	0.58
1:A:214[B]:VAL:CG2	1:A:294:VAL:HG21	2.34	0.58
1:A:217[B]:ALA:CA	1:A:222:ALA:HB3	2.34	0.57
1:A:214[B]:VAL:HA	1:A:225:VAL:HG21	1.87	0.57
1:A:217[B]:ALA:HB3	1:A:292:ILE:HD11	1.86	0.56
1:A:684:ARG:CZ	1:A:694[B]:PRO:O	2.53	0.56
1:A:90:PHE:CZ	1:A:94:LYS:HE2	2.42	0.54
1:A:179:TYR:O	1:A:213[B]:LYS:HE3	2.08	0.54
1:A:390:SER:HB2	1:A:573:HIS:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:CD1	1:A:137:GLU:HG2	2.38	0.54
1:A:215[B]:LYS:O	1:A:218[B]:GLN:CA	2.55	0.54
1:A:216[B]:ASN:O	1:A:218[B]:GLN:N	2.41	0.54
1:A:454:SER:OG	8:A:1:SDR:HABA	2.09	0.53
1:A:703[A]:GLU:CA	9:A:2168:HOH:O	2.24	0.53
1:A:174:LEU:N	1:A:174:LEU:CD1	2.73	0.52
1:A:179:TYR:CG	1:A:207[B]:LYS:HG3	2.45	0.52
1:A:217[B]:ALA:CB	1:A:225:VAL:CG2	2.89	0.51
1:A:687:TYR:OH	1:A:699[A]:LYS:HE2	2.10	0.51
1:A:215[B]:LYS:HA	1:A:218[B]:GLN:CG	2.36	0.51
8:A:1:SDR:CAU	9:A:2157:HOH:O	2.59	0.51
1:A:218[B]:GLN:HA	9:A:2017:HOH:O	2.12	0.49
1:A:209[B]:PHE:O	1:A:212[B]:ASN:N	2.44	0.49
1:A:218[A]:GLN:NE2	1:A:291:SER:OG	2.46	0.48
1:A:217[B]:ALA:HB2	1:A:225:VAL:HG22	1.93	0.48
1:A:158[B]:VAL:HG13	1:A:159:PRO:HD2	1.95	0.48
1:A:242:TYR:OH	9:A:2185:HOH:O	1.87	0.48
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.96	0.47
1:A:218[B]:GLN:NE2	9:A:2116:HOH:O	2.47	0.47
1:A:174:LEU:HD13	9:A:2175:HOH:O	2.15	0.47
1:A:517:SER:OG	1:A:522:GLU:OE1	2.32	0.47
1:A:257:ASN:HD21	8:A:1:SDR:CAL	2.28	0.46
1:A:217[B]:ALA:CB	1:A:222:ALA:HB3	2.45	0.46
1:A:427:GLY:CA	8:A:1:SDR:HAL	2.41	0.46
1:A:209[B]:PHE:HB3	1:A:212[B]:ASN:OD1	2.16	0.46
1:A:536[B]:ARG:N	1:A:536[B]:ARG:CD	2.76	0.46
1:A:681:LEU:CD1	1:A:693[B]:ALA:HB3	2.46	0.46
1:A:704[B]:SER:O	1:A:705[B]:PHE:HB2	2.15	0.46
1:A:133:GLU:CD	1:A:133:GLU:N	2.69	0.45
1:A:169:MET:HA	1:A:344:MET:O	2.16	0.45
1:A:174:LEU:HD11	1:A:342:VAL:HG23	1.91	0.45
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.52	0.45
1:A:208[B]:VAL:O	1:A:213[B]:LYS:NZ	2.50	0.45
1:A:58:MET:HE1	1:A:586:GLU:CG	2.43	0.44
1:A:443[B]:GLN:HG3	1:A:444:GLU:CD	2.38	0.44
1:A:216[B]:ASN:O	1:A:220:ALA:N	2.48	0.44
1:A:362:LEU:HD11	1:A:406:LYS:HG3	2.00	0.44
1:A:697[B]:HIS:CB	9:A:2171:HOH:O	2.55	0.43
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.00	0.43
1:A:489:GLU:H	1:A:489:GLU:CD	2.22	0.43
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2193:HOH:O	2:B:2:NAG:H83	2.18	0.43
1:A:212[B]:ASN:ND2	9:A:2160:HOH:O	2.52	0.42
1:A:215[B]:LYS:O	1:A:218[B]:GLN:N	2.53	0.42
1:A:506:PHE:CB	1:A:509:MET:HG3	2.50	0.42
1:A:179:TYR:CG	1:A:207[B]:LYS:CG	3.02	0.42
1:A:659[B]:ILE:HD13	1:A:659[B]:ILE:HA	1.67	0.42
1:A:205[A]:TYR:HA	1:A:213[A]:LYS:HE3	2.00	0.42
1:A:257:ASN:ND2	8:A:1:SDR:HAMA	2.35	0.42
1:A:412:PRO:HA	1:A:589[A]:ASN:OD1	2.20	0.42
1:A:217[B]:ALA:O	1:A:222:ALA:CB	2.67	0.42
1:A:188:LEU:HG	1:A:319:TRP:HH2	1.84	0.41
1:A:133:GLU:HG3	1:A:339:THR:HB	2.01	0.41
1:A:131:ILE:HD13	1:A:131:ILE:HA	2.00	0.40
1:A:170:PRO:HD2	1:A:344:MET:HB2	2.04	0.40
1:A:266:ASP:HA	1:A:267:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	734/709 (104%)	710 (97%)	21 (3%)	3 (0%)	34 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	A	207[A]	LYS
1	A	207[B]	LYS

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	634/604 (105%)	624 (98%)	10 (2%)	62 48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ILE
1	A	133	GLU
1	A	174	LEU
1	A	182	THR
1	A	187	LYS
1	A	519	ASN
1	A	537	TYR
1	A	539	LYS
1	A	600	TYR
1	A	673	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.57	0	17,19,21	1.26	1 (5%)
2	NAG	B	2	2	14,14,15	0.77	0	17,19,21	1.33	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	1.13	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.50	0	17,19,21	1.18	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.74	0	17,19,21	1.29	1 (5%)
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	1.49	4 (23%)
3	BMA	E	3	3	11,11,12	0.84	0	15,15,17	1.15	1 (6%)
3	MAN	E	4	3	11,11,12	0.62	0	15,15,17	1.18	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	-	0/6/23/26	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	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O7-C7	2.05	1.27	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	O5-C1-C2	-3.45	105.95	111.29
2	B	1	NAG	O5-C1-C2	-3.44	105.97	111.29
2	C	1	NAG	C1-O5-C5	3.38	116.72	112.19
2	B	2	NAG	C2-N2-C7	3.35	127.38	122.90
3	E	2	NAG	C1-O5-C5	3.31	116.63	112.19
3	E	4	MAN	O5-C5-C6	3.18	113.86	107.66
2	C	2	NAG	O7-C7-C8	-2.58	117.45	122.05
3	E	2	NAG	C8-C7-N2	2.53	120.31	116.12
2	D	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	C	2	NAG	C8-C7-N2	2.38	120.06	116.12
3	E	2	NAG	C2-N2-C7	-2.33	119.78	122.90
3	E	3	BMA	O3-C3-C2	-2.31	105.34	110.05
3	E	2	NAG	O7-C7-C8	-2.28	117.99	122.05
2	C	1	NAG	C2-N2-C7	-2.14	120.03	122.90
2	D	2	NAG	O7-C7-C8	-2.04	118.42	122.05
3	E	4	MAN	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (15) 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	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

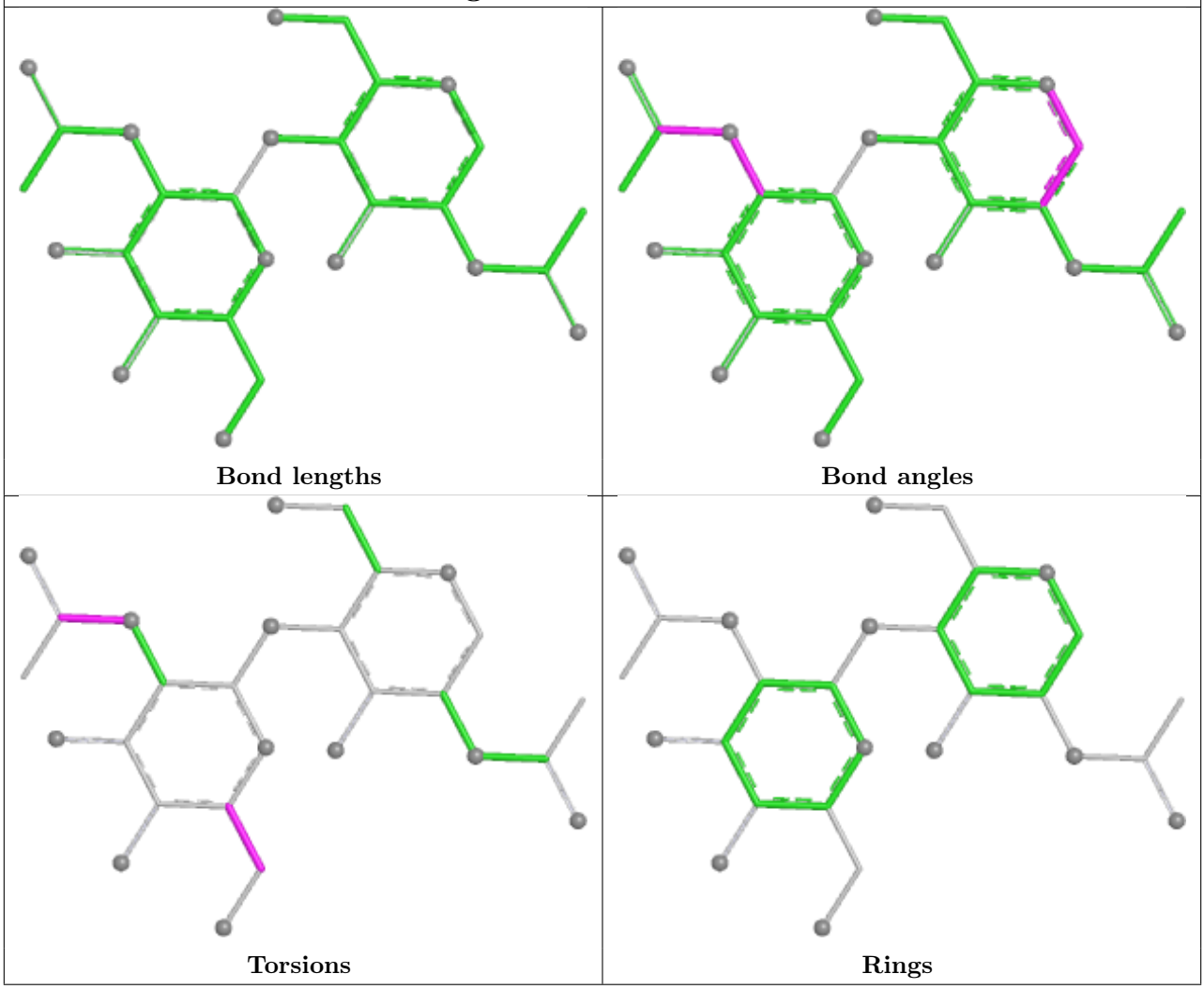
There are no ring outliers.

1 monomer is involved in 2 short contacts:

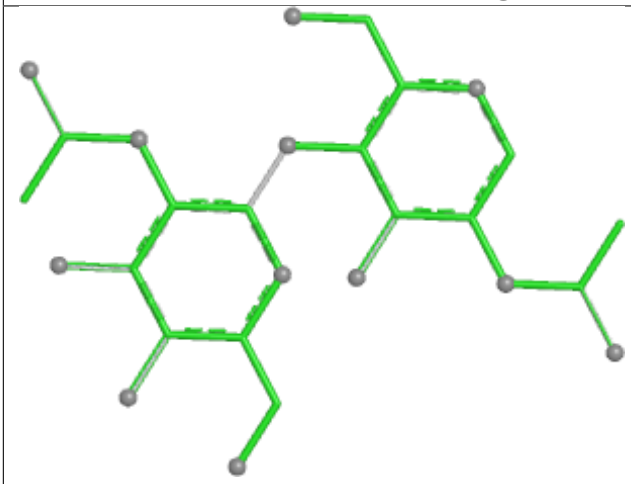
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0

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

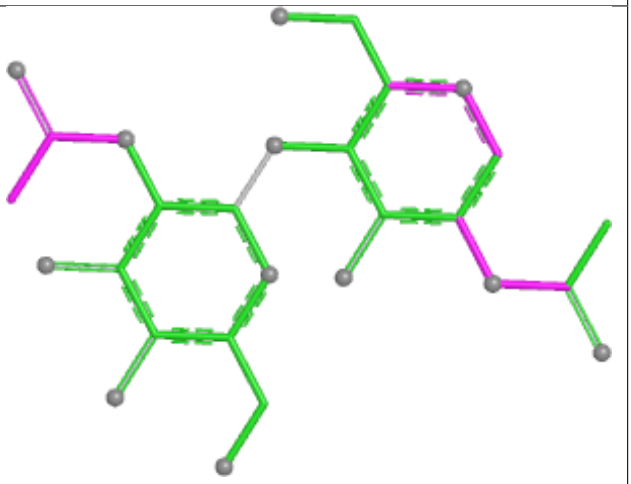
Oligosaccharide Chain B



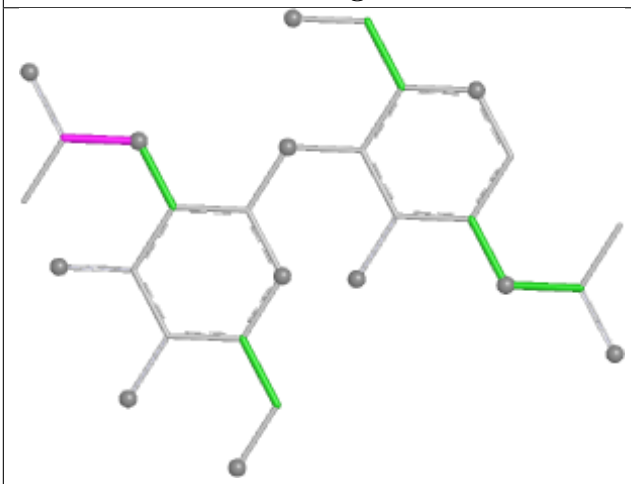
Oligosaccharide Chain C



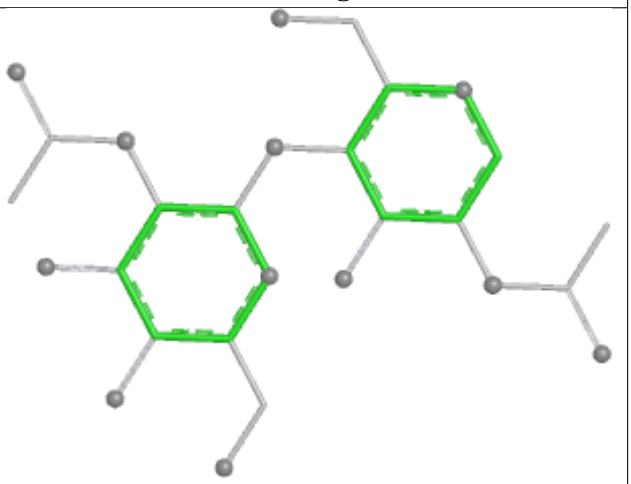
Bond lengths



Bond angles

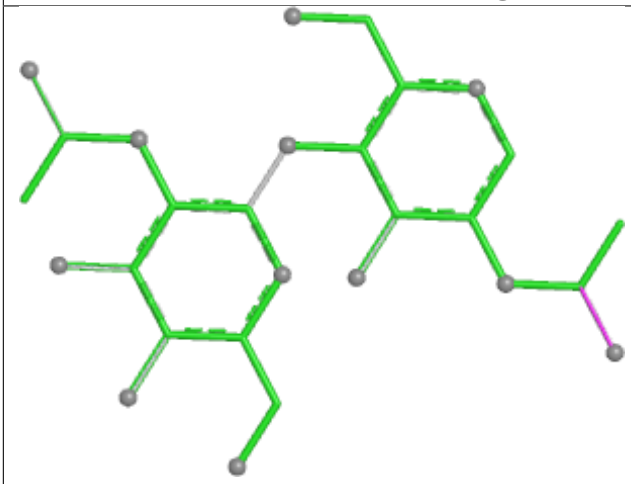


Torsions

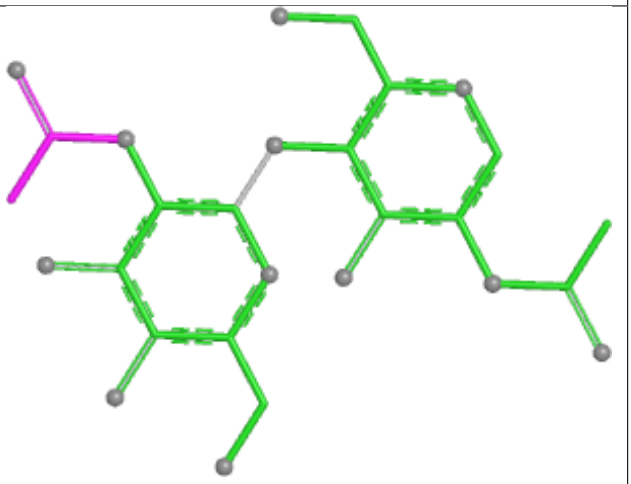


Rings

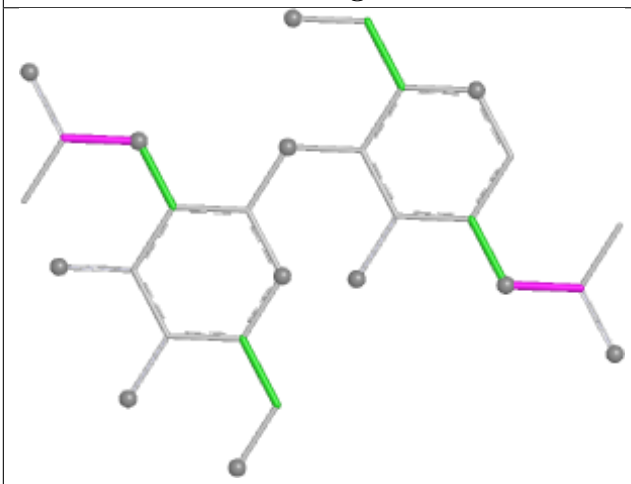
Oligosaccharide Chain D



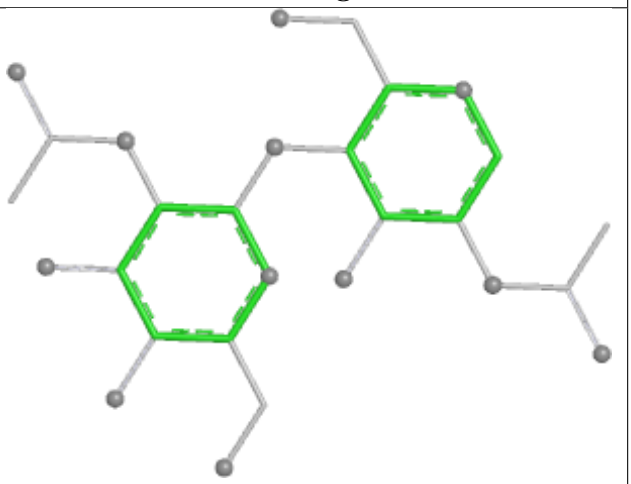
Bond lengths



Bond angles

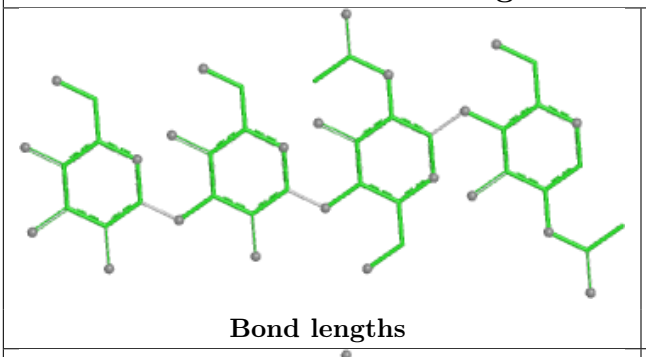


Torsions

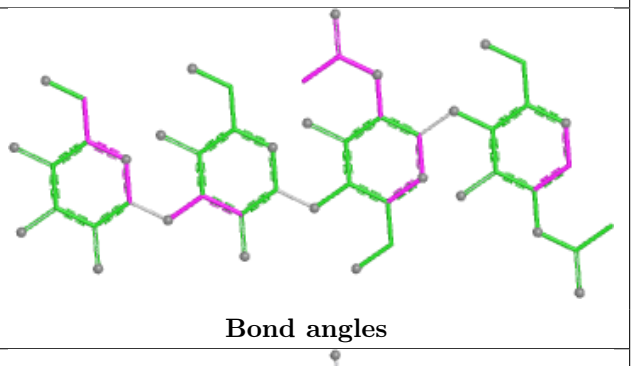


Rings

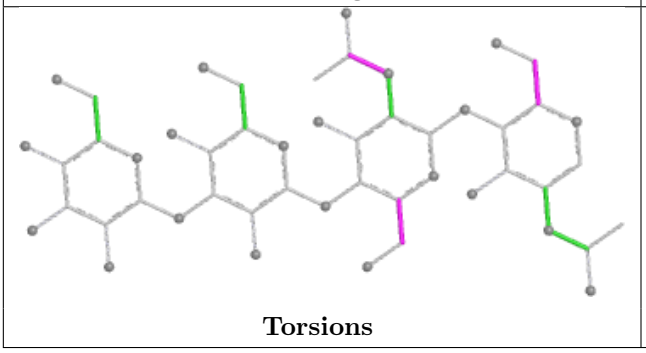
Oligosaccharide Chain E



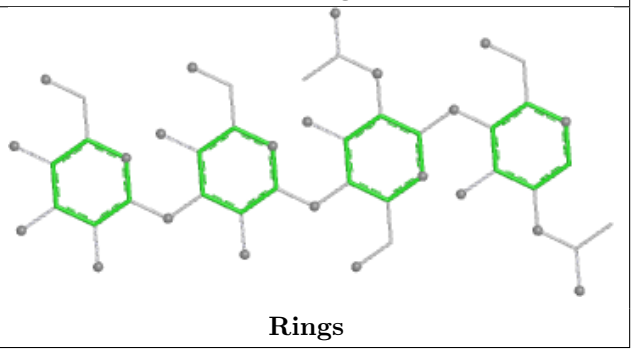
Bond lengths



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	$\#\|Z\| > 2$
8	SDR	A	1	4	22,22,22	1.13	0	27,27,27	1.12	1 (3%)
7	NAG	A	1760	1	14,14,15	0.73	0	17,19,21	1.68	3 (17%)
7	NAG	A	1759	1	14,14,15	0.51	0	17,19,21	1.57	2 (11%)
7	NAG	A	1757	1	14,14,15	0.65	0	17,19,21	1.18	1 (5%)

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	SDR	A	1	4	-	4/27/27/27	-
7	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1759	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1757	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1759	NAG	C1-O5-C5	4.90	118.76	112.19
7	A	1760	NAG	O5-C1-C2	-3.84	105.35	111.29
7	A	1757	NAG	C1-C2-N2	-3.18	105.42	110.43
7	A	1760	NAG	O5-C5-C6	2.79	113.09	107.66
7	A	1760	NAG	C1-O5-C5	2.67	115.76	112.19
8	A	1	SDR	CB-CA-N	-2.63	105.71	110.91
7	A	1759	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1759	NAG	O5-C5-C6-O6
7	A	1759	NAG	C4-C5-C6-O6
7	A	1757	NAG	C8-C7-N2-C2
7	A	1757	NAG	O7-C7-N2-C2
7	A	1759	NAG	C8-C7-N2-C2
7	A	1759	NAG	O7-C7-N2-C2
8	A	1	SDR	CAI-CAJ-CAK-CAL
8	A	1	SDR	CAJ-CAK-CAL-CAM
8	A	1	SDR	CAW-CAO-CAS-OAD
8	A	1	SDR	CAW-CAO-CAS-OAG
7	A	1757	NAG	O5-C5-C6-O6

There are no ring outliers.

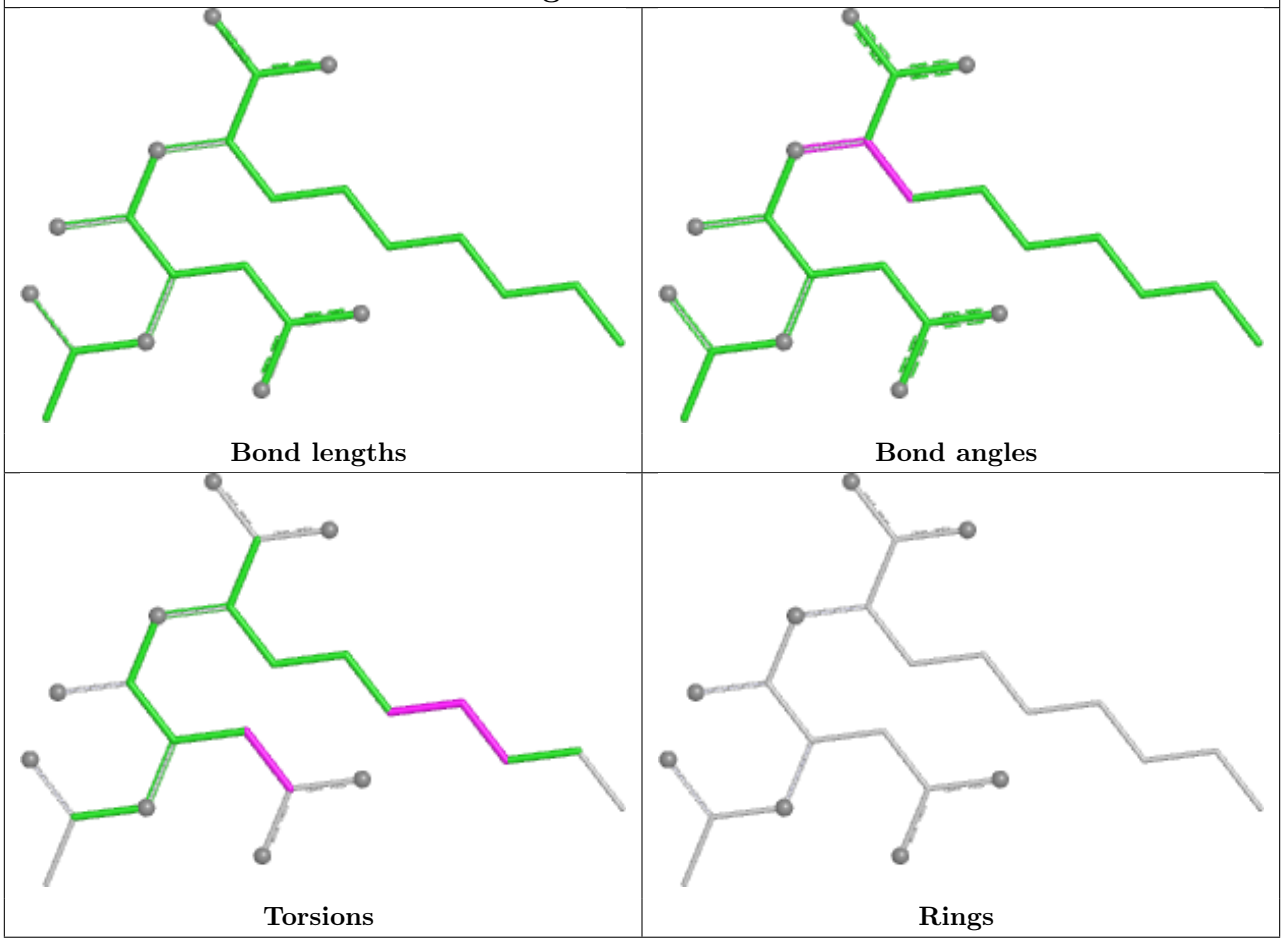
1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1	SDR	7	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 SDR 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%)	0.69	98 (14%)	2	3	17, 30, 62, 82	5 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541[A]	TRP	10.6
1	A	543	THR	8.2
1	A	135	GLY	6.7
1	A	153	ASN	6.1
1	A	337	PHE	6.0
1	A	719	VAL	5.8
1	A	542	GLU	5.7
1	A	507	SER	5.6
1	A	505	GLU	5.5
1	A	219	LEU	5.3
1	A	506	PHE	5.0
1	A	133	GLU	4.9
1	A	124	HIS	4.7
1	A	334	THR	4.7
1	A	155	SER	4.7
1	A	226	ILE	4.5
1	A	202	ILE	4.4
1	A	700[A]	TYR	4.3
1	A	55	LYS	4.2
1	A	656[A]	SER	4.1
1	A	196	CYS	4.0
1	A	335	GLY	4.0
1	A	338	SER	3.9
1	A	329	VAL	3.9
1	A	227	LEU	3.9
1	A	152	GLU	3.9
1	A	189	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	312	SER	3.8
1	A	200	ILE	3.8
1	A	225	VAL	3.8
1	A	134	ASP	3.7
1	A	394	VAL	3.6
1	A	317	SER	3.6
1	A	652	ASP	3.6
1	A	324	LYS	3.5
1	A	341	LYS	3.4
1	A	136	ASN	3.4
1	A	237	PRO	3.4
1	A	732	ILE	3.4
1	A	186	PHE	3.3
1	A	191	ASP	3.3
1	A	287	VAL	3.3
1	A	138	ILE	3.3
1	A	395	VAL	3.3
1	A	123	THR	3.2
1	A	318	SER	3.2
1	A	336	ASN	3.2
1	A	284	ALA	3.1
1	A	201	VAL	3.1
1	A	193	LYS	3.1
1	A	579	VAL	3.1
1	A	174	LEU	3.0
1	A	154	VAL	2.8
1	A	296	PRO	2.8
1	A	132	ASN	2.8
1	A	487	GLY	2.7
1	A	486	GLU	2.7
1	A	190	ARG	2.7
1	A	333	PHE	2.6
1	A	182	THR	2.6
1	A	340	GLN	2.6
1	A	222	ALA	2.6
1	A	313	ALA	2.6
1	A	195	ASN	2.5
1	A	56	HIS	2.5
1	A	320	ARG	2.5
1	A	392	ALA	2.5
1	A	187	LYS	2.5
1	A	331	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	548	GLY	2.5
1	A	651	GLN	2.5
1	A	316	ASP	2.4
1	A	339	THR	2.4
1	A	503	SER	2.4
1	A	310	GLY	2.4
1	A	131	ILE	2.4
1	A	283	ILE	2.4
1	A	297	ILE	2.4
1	A	391	GLY	2.4
1	A	220	ALA	2.3
1	A	393	ALA	2.3
1	A	587	LEU	2.3
1	A	734	VAL	2.3
1	A	315	PRO	2.3
1	A	294	VAL	2.2
1	A	750	ALA	2.2
1	A	285	GLU	2.2
1	A	374	LEU	2.2
1	A	696[A]	SER	2.2
1	A	321	GLY	2.2
1	A	332	GLY	2.2
1	A	576	VAL	2.1
1	A	127	TYR	2.1
1	A	326	PRO	2.1
1	A	161	PHE	2.0
1	A	581	GLY	2.0
1	A	203	ALA	2.0
1	A	390	SER	2.0

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

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

6.3 Carbohydrates (i)

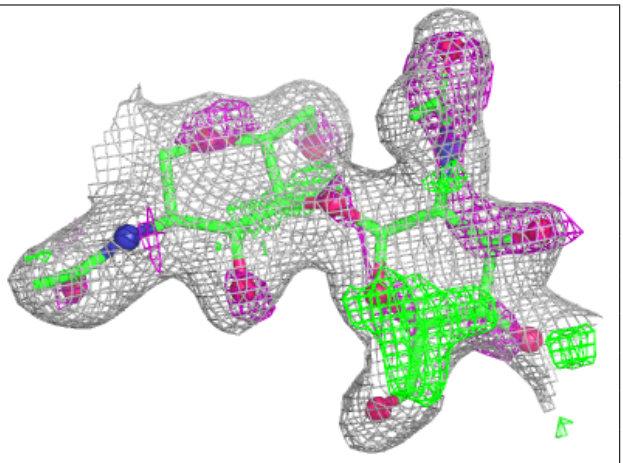
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

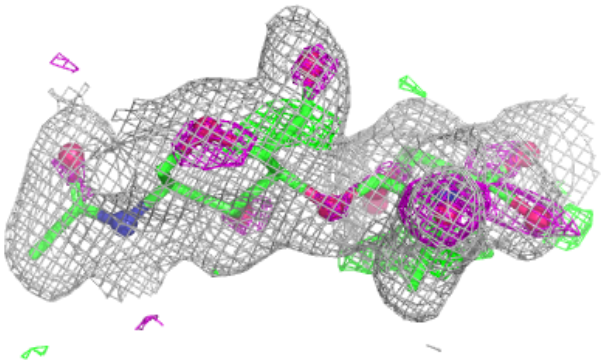
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	1	14/15	0.71	0.38	28,33,35,45	0
2	NAG	C	2	14/15	0.71	0.48	51,54,57,57	0
2	NAG	B	2	14/15	0.79	0.32	30,36,41,42	0
2	NAG	D	2	14/15	0.82	0.27	24,29,33,39	0
3	NAG	E	2	14/15	0.87	0.30	27,31,41,42	0
3	MAN	E	4	11/12	0.90	0.29	36,39,42,43	0
3	BMA	E	3	11/12	0.91	0.24	32,36,39,40	0
2	NAG	B	1	14/15	0.91	0.15	24,29,36,38	0
2	NAG	D	1	14/15	0.92	0.17	17,21,30,34	0
3	NAG	E	1	14/15	0.94	0.10	14,20,24,35	0

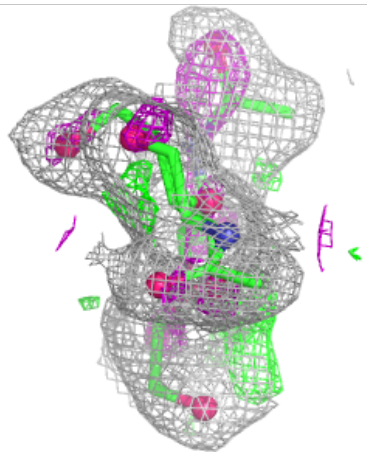
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

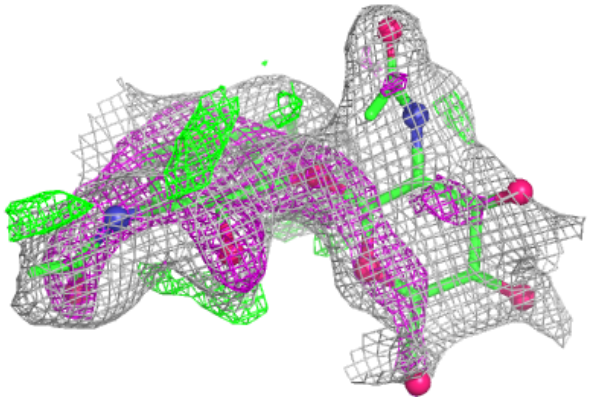


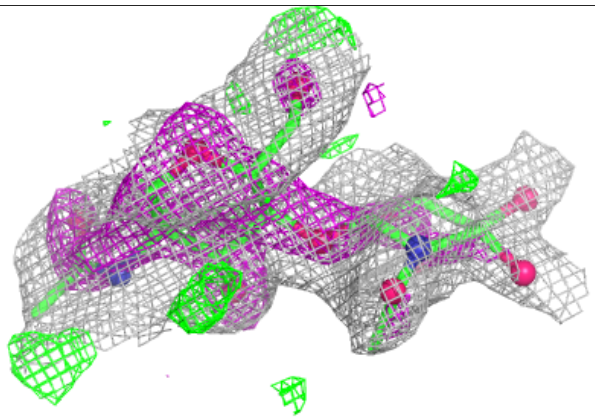


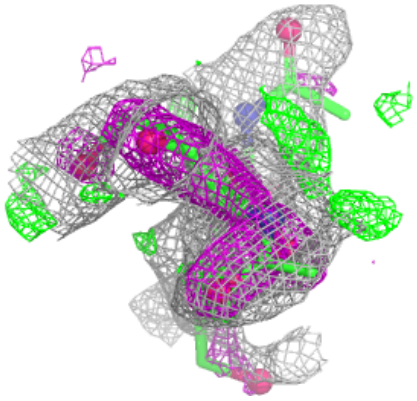


Electron density around Chain C:

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

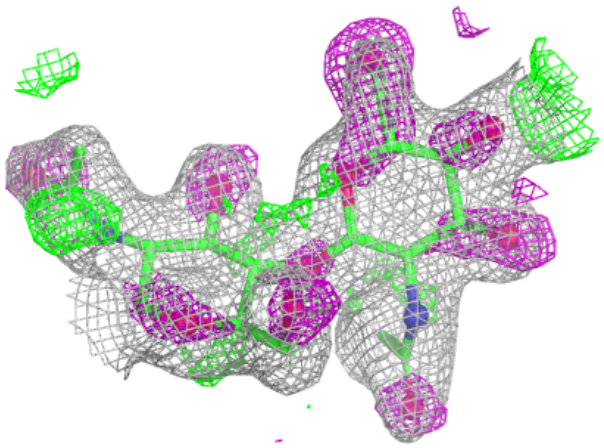


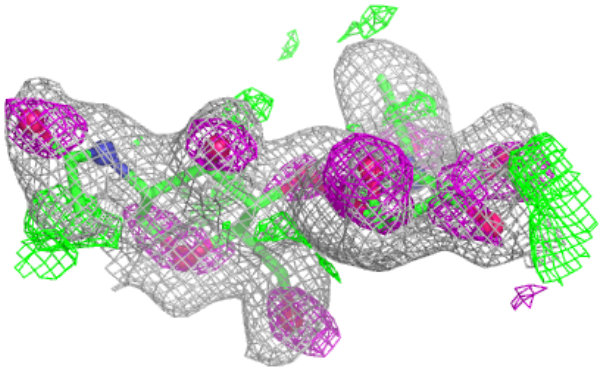


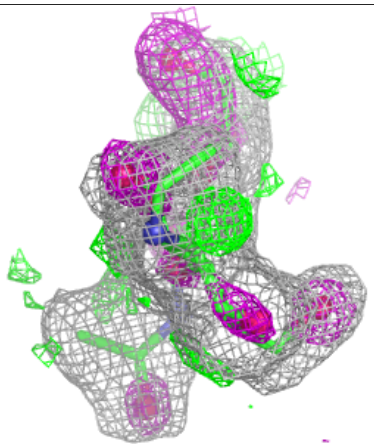


Electron density around Chain D:

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

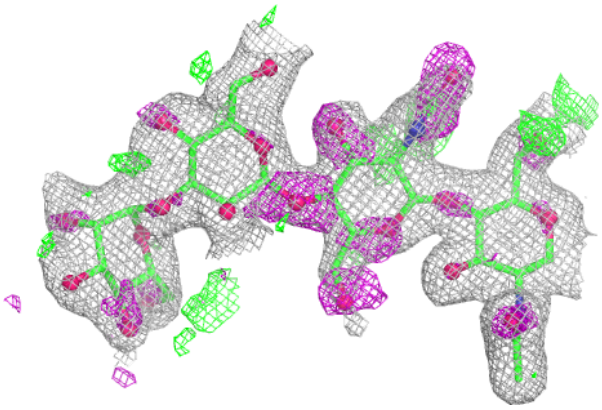


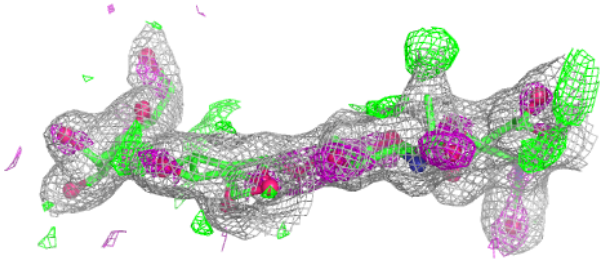


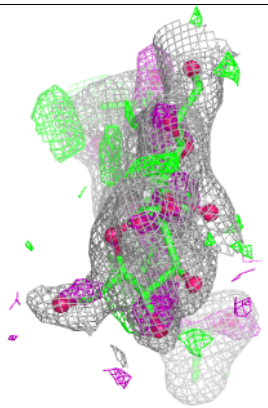


Electron density around Chain E:

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







6.4 Ligands

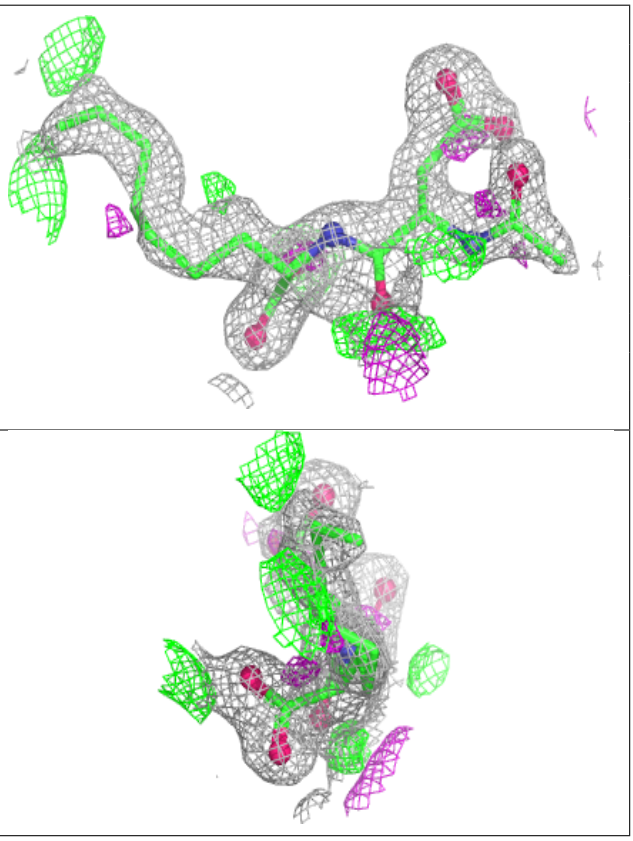
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.65	0.36	59,63,64,64	0
7	NAG	A	1757	14/15	0.67	0.37	38,44,48,50	0
7	NAG	A	1760	14/15	0.82	0.22	20,34,40,40	0
8	SDR	A	1	23/23	0.86	0.18	31,36,43,44	23
6	CL	A	1754	1/1	0.98	0.05	23,23,23,23	0
4	ZN	A	1751	1/1	0.99	0.02	16,16,16,16	0
5	CA	A	1753	1/1	1.00	0.05	15,15,15,15	0
4	ZN	A	1752	1/1	1.00	0.03	15,15,15,15	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 SDR 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.