Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:05 am GMT

PDB ID	:	2WXD
Title	:	A MICROMOLAR O-SULFATED THIOHYDROXIMATE INHIBITOR BOUND TO PLANT MYROSINASE
Authors	:	Besle, A.; Burmeister, W.P.
Deposited on	:	2009-11-09
Resolution	:	1.60 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 ⓘ) were used in the production of this report:

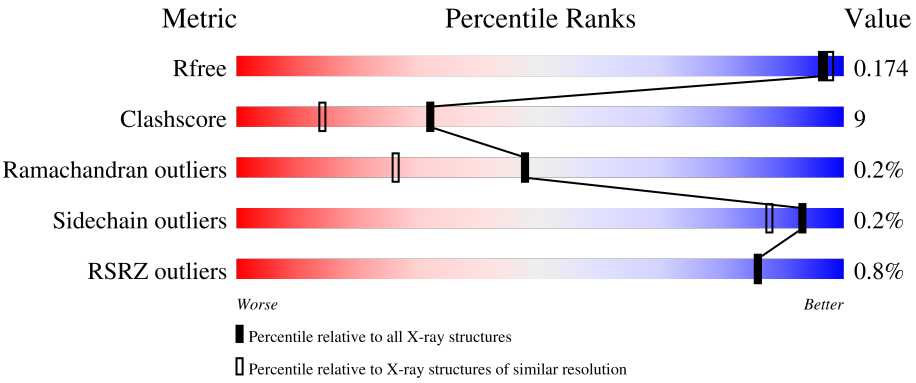
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	M	501	% 81% 17%
2	A	2	100%
2	B	2	100%
2	E	2	100%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
3	C	5	40% 60%
4	D	7	57% 43%

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
5	NAG	M	931	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5238 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.

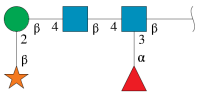
- Molecule 1 is a protein called MYROSINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4082	2617	663	786	16			

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

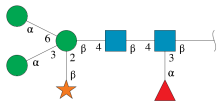
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



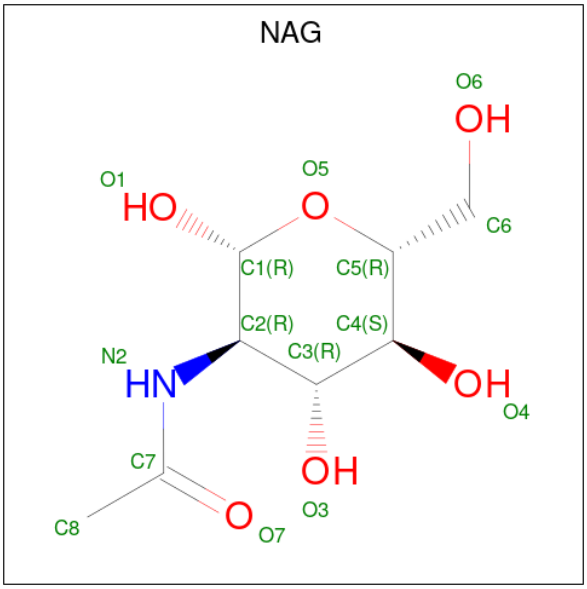
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			58	33	2	23			

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



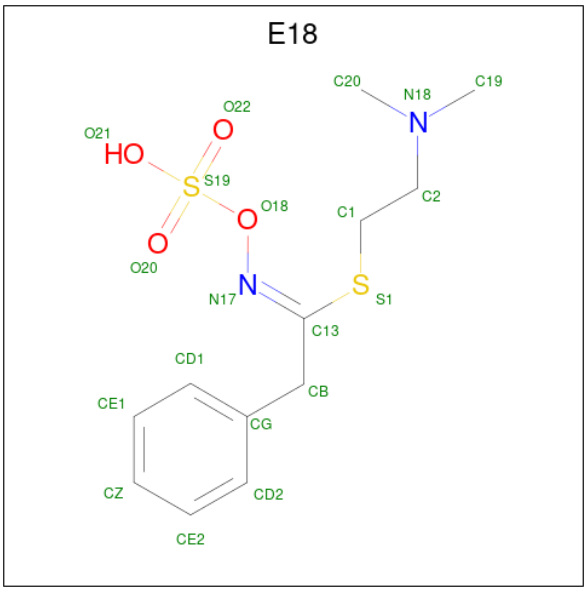
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is 2-(DIMETHYLAMINO)ETHYL (1Z)-2-PHENYL-N-(SULFOOXY)ETHANIMIDOTHIOATE (three-letter code: E18) (formula: $C_{12}H_{18}N_2O_4S_2$).

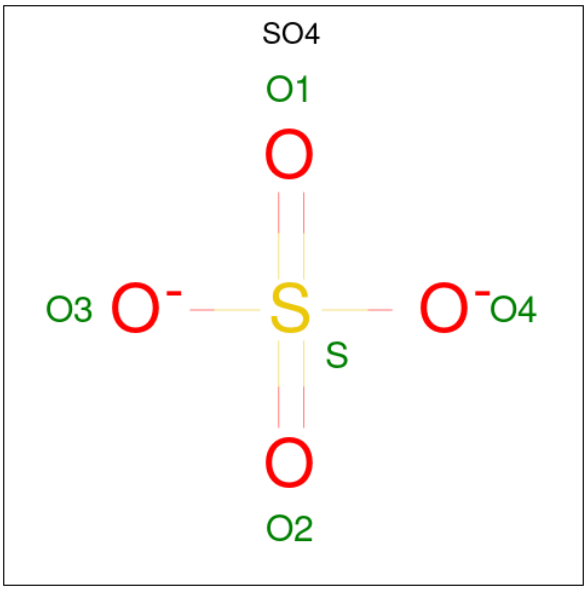


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	M	1	20	12	2	4	2	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

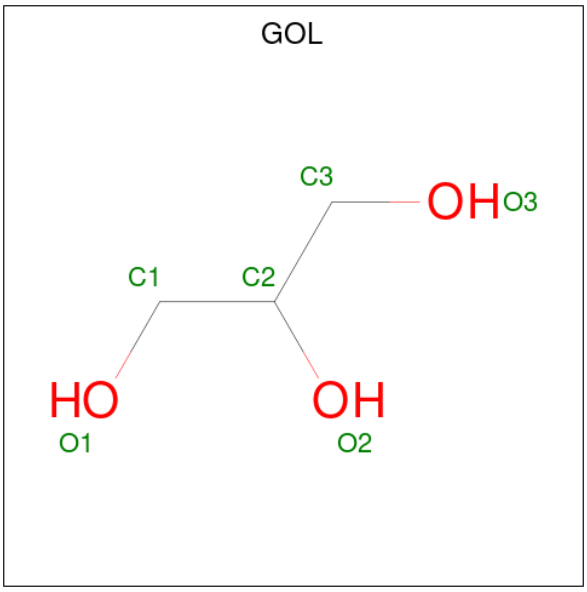
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	M	1	1	1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total O S 10 8 2	0	1
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 7 3 4	0	1
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

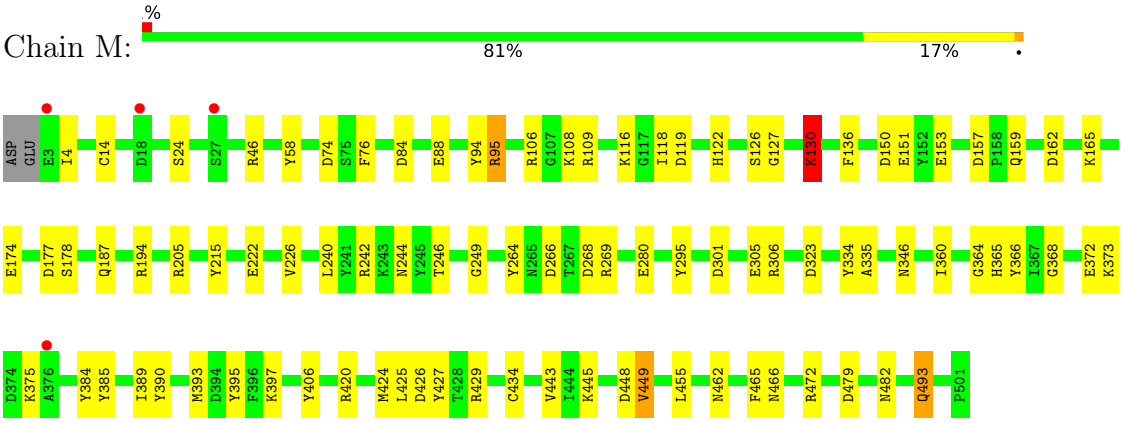
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	764	Total	O	0	0
			764	764		

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.

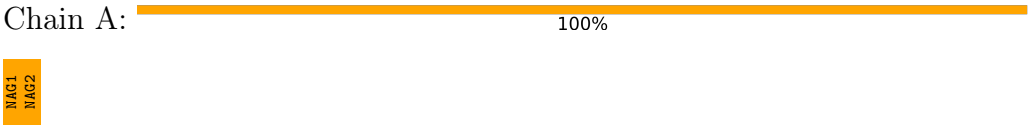
• Molecule 1: MYROSINASE

Chain M:



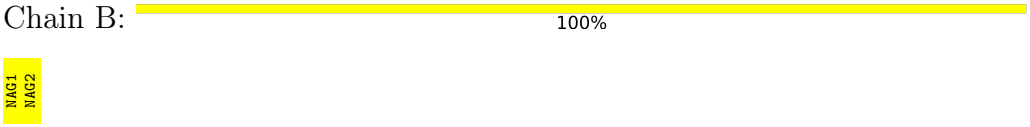
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



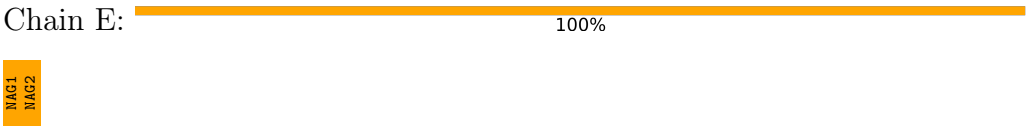
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



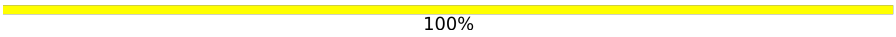
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:

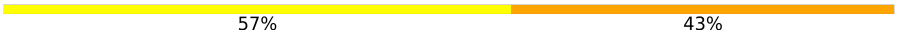


• Molecule 3: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	136.25Å 137.57Å 80.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.78 – 1.60 68.78 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.78-1.60) 99.8 (68.78-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.143 , 0.164 0.153 , 0.174	Depositor DCC
R_{free} test set	5075 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5238	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: GOL, BMA, NAG, FUC, SO4, ZN, MAN, E18, XYP

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	M	1.42	20/4284 (0.5%)	1.35	45/5824 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	390	TYR	CE2-CZ	-9.47	1.26	1.38
1	M	178	SER	CB-OG	9.17	1.54	1.42
1	M	24	SER	CB-OG	6.99	1.51	1.42
1	M	222	GLU	CD-OE2	6.96	1.33	1.25
1	M	372	GLU	CD-OE1	6.93	1.33	1.25
1	M	151	GLU	CD-OE2	-6.89	1.18	1.25
1	M	264	TYR	CE1-CZ	-6.32	1.30	1.38
1	M	434	CYS	CB-SG	-6.04	1.72	1.82
1	M	14	CYS	CB-SG	5.98	1.92	1.82
1	M	493	GLN	CD-OE1	-5.59	1.11	1.24
1	M	24	SER	CA-CB	5.41	1.61	1.52
1	M	390	TYR	CD2-CE2	5.35	1.47	1.39
1	M	127	GLY	N-CA	-5.21	1.38	1.46
1	M	226	VAL	CB-CG2	5.20	1.63	1.52
1	M	395	TYR	CD1-CE1	-5.19	1.31	1.39
1	M	449[A]	VAL	CB-CG1	5.18	1.63	1.52
1	M	449[B]	VAL	CB-CG1	5.18	1.63	1.52
1	M	335	ALA	CA-CB	5.13	1.63	1.52
1	M	427	TYR	CZ-OH	5.07	1.46	1.37
1	M	406	TYR	CE1-CZ	-5.00	1.32	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	242	ARG	NE-CZ-NH2	-11.80	114.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	205	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	M	268	ASP	CB-CG-OD1	8.62	126.06	118.30
1	M	426	ASP	CB-CG-OD1	8.33	125.80	118.30
1	M	242	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	M	269	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	M	106	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	M	425	LEU	CB-CG-CD1	-7.33	98.53	111.00
1	M	94	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	M	301	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	M	215	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	M	153	GLU	OE1-CD-OE2	-6.61	115.37	123.30
1	M	334	TYR	CZ-CE2-CD2	6.60	125.74	119.80
1	M	420	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	M	390	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	M	266	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	M	323	ASP	CB-CG-OD2	6.45	124.10	118.30
1	M	46	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	M	306	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	M	429	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	M	448	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	M	280	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	M	162	ASP	CB-CG-OD2	-5.98	112.91	118.30
1	M	385	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	M	472	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	M	84	ASP	CB-CG-OD1	5.78	123.50	118.30
1	M	76	PHE	CB-CG-CD2	-5.78	116.76	120.80
1	M	74	ASP	CB-CG-OD1	5.71	123.44	118.30
1	M	157	ASP	CB-CG-OD1	5.68	123.41	118.30
1	M	424	MET	CG-SD-CE	5.66	109.26	100.20
1	M	109	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	M	448	ASP	CB-CG-OD1	5.42	123.18	118.30
1	M	479	ASP	CB-CG-OD1	5.36	123.12	118.30
1	M	150	ASP	CB-CG-OD2	5.34	123.11	118.30
1	M	130	LYS	CB-CG-CD	5.32	125.44	111.60
1	M	58	TYR	CB-CG-CD2	5.26	124.16	121.00
1	M	94	TYR	CB-CG-CD2	5.25	124.15	121.00
1	M	84	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	M	295	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	M	109	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	M	119	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	M	194[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	M	194[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	95	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	M	434	CYS	CA-CB-SG	5.00	123.00	114.00

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	M	4082	0	3830	51	0
2	A	28	0	26	2	0
2	B	28	0	25	0	0
2	E	28	0	26	2	0
2	F	28	0	25	0	0
3	C	58	0	43	4	0
4	D	80	0	60	3	0
5	M	56	0	52	18	0
6	M	20	0	18	2	0
7	M	1	0	0	0	0
8	M	40	0	0	0	0
9	M	25	0	30	4	0
10	M	764	0	0	25	5
All	All	5238	0	4135	68	5

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 9.

All (68) 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:M:346:ASN:HD21	5:M:971:NAG:C1	0.99	1.61
1:M:244:ASN:HD21	5:M:931:NAG:C1	0.92	1.57
1:M:373:LYS:NZ	10:M:3539:HOH:O	1.81	1.14
1:M:130:LYS:HB3	10:M:3254:HOH:O	1.49	1.12
1:M:493:GLN:NE2	10:M:3675:HOH:O	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1501:E18:H11C	10:M:3641:HOH:O	1.60	1.00
9:M:2511:GOL:H11	10:M:3756:HOH:O	1.61	0.99
1:M:346:ASN:HD21	5:M:971:NAG:C2	1.80	0.95
1:M:246:THR:HG22	10:M:3377:HOH:O	1.67	0.93
1:M:165:LYS:NZ	5:M:931:NAG:H82	1.82	0.92
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.39	0.88
3:C:2:NAG:C4	3:C:3:BMA:C1	2.52	0.86
10:M:3708:HOH:O	4:D:1:NAG:H83	1.74	0.85
1:M:126[B]:SER:OG	10:M:3244:HOH:O	1.93	0.85
2:E:1:NAG:C4	2:E:2:NAG:C1	2.55	0.84
1:M:482:ASN:CG	5:M:991:NAG:C1	2.48	0.81
2:A:1:NAG:C4	2:A:2:NAG:C1	2.58	0.80
4:D:3:BMA:C6	4:D:6:MAN:C1	2.60	0.80
3:C:3:BMA:C2	3:C:4:XYP:C1	2.59	0.79
1:M:346:ASN:CG	5:M:971:NAG:C1	2.57	0.72
1:M:88[A]:GLU:OE2	10:M:3168:HOH:O	2.07	0.71
1:M:240:LEU:HD13	5:M:931:NAG:H83	1.71	0.71
1:M:177:ASP:OD1	10:M:3324:HOH:O	2.08	0.70
1:M:482:ASN:ND2	5:M:991:NAG:C2	2.54	0.68
9:M:2511:GOL:H32	10:M:3700:HOH:O	1.93	0.67
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD1	2.22	0.66
1:M:244:ASN:CG	5:M:931:NAG:C1	2.61	0.66
1:M:462:ASN:ND2	10:M:3639:HOH:O	2.29	0.66
1:M:165:LYS:NZ	5:M:931:NAG:C8	2.57	0.65
1:M:244:ASN:ND2	5:M:931:NAG:O5	2.28	0.65
1:M:116:LYS:HG2	10:M:3224:HOH:O	1.95	0.65
2:E:1:NAG:O4	2:E:2:NAG:O5	2.16	0.63
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.81	0.62
1:M:165:LYS:HZ2	5:M:931:NAG:H82	1.65	0.61
1:M:88[B]:GLU:CD	10:M:3167:HOH:O	2.38	0.60
1:M:108:LYS:HD2	10:M:3304:HOH:O	2.01	0.60
1:M:165:LYS:HZ2	5:M:931:NAG:C8	2.15	0.59
4:D:3:BMA:O6	4:D:6:MAN:C2	2.49	0.58
1:M:159:GLN:NE2	10:M:3296:HOH:O	2.37	0.57
2:A:1:NAG:O4	2:A:2:NAG:C2	2.49	0.55
6:M:1501:E18:C1	10:M:3641:HOH:O	2.32	0.55
1:M:365:HIS:HD2	10:M:3247:HOH:O	1.89	0.54
1:M:240:LEU:CD1	5:M:931:NAG:H83	2.35	0.54
1:M:118[B]:ILE:HD12	1:M:174:GLU:HG3	1.90	0.53
1:M:130:LYS:CB	10:M:3254:HOH:O	2.27	0.53
1:M:365:HIS:HE1	10:M:3532:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:249:GLY:HA3	9:M:2513:GOL:H12	1.92	0.51
1:M:360[A]:ILE:HD11	1:M:364:GLY:HA2	1.92	0.51
3:C:2:NAG:O4	3:C:3:BMA:C2	2.50	0.51
1:M:443:VAL:HG13	1:M:449[B]:VAL:HG21	1.92	0.50
1:M:465:PHE:O	1:M:466[A]:ASN:HB2	2.12	0.49
1:M:122:HIS:HE1	1:M:174:GLU:O	1.97	0.48
1:M:482:ASN:ND2	5:M:991:NAG:O5	2.38	0.47
1:M:397:LYS:HB2	1:M:449[B]:VAL:HG12	1.97	0.47
1:M:368:GLY:HA3	1:M:384:TYR:O	2.16	0.46
9:M:2511:GOL:H2	10:M:3409:HOH:O	2.16	0.46
5:M:931:NAG:H81	10:M:3366:HOH:O	2.15	0.46
1:M:375:LYS:N	10:M:3543:HOH:O	2.37	0.45
1:M:465:PHE:O	1:M:466[A]:ASN:CB	2.66	0.43
1:M:130:LYS:HB3	10:M:3094:HOH:O	2.17	0.43
1:M:482:ASN:OD1	5:M:991:NAG:C1	2.67	0.43
1:M:95:ARG:HB2	1:M:455:LEU:HD13	2.01	0.43
1:M:389:ILE:O	1:M:393:MET:HG2	2.19	0.42
1:M:88[A]:GLU:CG	10:M:3168:HOH:O	2.68	0.41
1:M:95:ARG:HA	1:M:136:PHE:O	2.21	0.40
3:C:3:BMA:H2	3:C:4:XYP:C1	2.49	0.40

All (5) 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)
10:M:3250:HOH:O	10:M:3250:HOH:O[4_576]	1.49	0.71
10:M:3285:HOH:O	10:M:3285:HOH:O[3_656]	1.66	0.54
10:M:3198:HOH:O	10:M:3741:HOH:O[3_656]	2.12	0.08
10:M:3255:HOH:O	10:M:3715:HOH:O[6_565]	2.18	0.02
10:M:3285:HOH:O	10:M:3743:HOH:O[3_656]	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	M	518/501 (103%)	504 (97%)	13 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

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	M	454/437 (104%)	453 (100%)	1 (0%)	93 88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	122	HIS
1	M	244	ASN
1	M	346	ASN
1	M	365	HIS

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)

20 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	A	1	2,1	14,14,15	1.44	2 (14%)	17,19,21	1.71	3 (17%)
2	NAG	A	2	2	14,14,15	0.89	0	17,19,21	1.51	4 (23%)
2	NAG	B	1	2,1	14,14,15	1.93	5 (35%)	17,19,21	1.87	4 (23%)
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	2.73	9 (52%)
3	NAG	C	1	3,1	14,14,15	1.45	2 (14%)	17,19,21	1.99	6 (35%)
3	NAG	C	2	3	14,14,15	1.08	2 (14%)	17,19,21	1.77	7 (41%)
3	BMA	C	3	3	11,11,12	1.00	1 (9%)	15,15,17	2.56	4 (26%)
3	XYP	C	4	3	9,9,10	1.18	1 (11%)	10,12,14	2.35	5 (50%)
3	FUC	C	5	3	10,10,11	0.70	0	14,14,16	1.53	4 (28%)
4	NAG	D	1	1,4	14,14,15	2.04	6 (42%)	17,19,21	2.13	4 (23%)
4	NAG	D	2	4	14,14,15	2.05	5 (35%)	17,19,21	2.69	8 (47%)
4	BMA	D	3	4	11,11,12	1.49	1 (9%)	15,15,17	2.29	6 (40%)
4	XYP	D	4	4	9,9,10	0.47	0	10,12,14	2.40	3 (30%)
4	MAN	D	5	4	11,11,12	0.83	0	15,15,17	1.80	3 (20%)
4	MAN	D	6	4	11,11,12	1.14	0	15,15,17	1.35	3 (20%)
4	FUC	D	7	4	10,10,11	1.25	1 (10%)	14,14,16	2.19	6 (42%)
2	NAG	E	1	2,1	14,14,15	0.84	0	17,19,21	1.75	4 (23%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	1.41	2 (11%)
2	NAG	F	1	2,1	14,14,15	1.86	5 (35%)	17,19,21	1.70	5 (29%)
2	NAG	F	2	2	14,14,15	1.25	2 (14%)	17,19,21	2.11	7 (41%)

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	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	XYP	C	4	3	-	-	0/1/1/1
3	FUC	C	5	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	XYP	D	4	4	-	-	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	FUC	D	7	4	-	-	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-5.07	1.35	1.43
4	D	2	NAG	C1-C2	4.76	1.59	1.52
2	F	1	NAG	O5-C1	-4.43	1.36	1.43
2	B	1	NAG	C2-N2	-4.30	1.39	1.46
3	C	1	NAG	O4-C4	4.04	1.52	1.43
2	A	1	NAG	O5-C1	-3.65	1.37	1.43
4	D	3	BMA	O4-C4	3.54	1.51	1.43
2	B	1	NAG	O5-C1	-3.32	1.38	1.43
4	D	1	NAG	O5-C5	3.18	1.49	1.43
2	F	1	NAG	C2-N2	-3.05	1.41	1.46
4	D	2	NAG	C4-C5	2.99	1.59	1.53
4	D	2	NAG	O7-C7	2.75	1.29	1.23
2	B	1	NAG	C3-C2	2.72	1.58	1.52
3	C	1	NAG	C1-C2	2.66	1.56	1.52
4	D	2	NAG	O4-C4	-2.64	1.36	1.43
3	C	4	XYP	C4-C3	2.60	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C8-C7	2.53	1.55	1.50
2	B	1	NAG	O4-C4	2.38	1.48	1.43
4	D	1	NAG	O7-C7	2.33	1.28	1.23
3	C	2	NAG	O5-C1	-2.27	1.40	1.43
4	D	7	FUC	C2-C3	-2.18	1.49	1.52
2	F	1	NAG	O4-C4	2.09	1.47	1.43
3	C	2	NAG	C1-C2	2.09	1.55	1.52
4	D	1	NAG	C1-C2	2.08	1.55	1.52
2	F	1	NAG	C4-C5	2.07	1.57	1.53
2	B	1	NAG	C4-C3	-2.05	1.47	1.52
2	F	1	NAG	C1-C2	2.04	1.55	1.52
2	F	2	NAG	C1-C2	2.04	1.55	1.52
2	A	1	NAG	O5-C5	2.03	1.47	1.43
4	D	2	NAG	O5-C5	-2.03	1.39	1.43
4	D	1	NAG	C4-C3	-2.02	1.47	1.52
4	D	1	NAG	C3-C2	2.01	1.56	1.52
3	C	3	BMA	O5-C5	2.01	1.47	1.43

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	-6.44	103.47	112.19
3	C	3	BMA	C1-O5-C5	-6.40	103.52	112.19
4	D	2	NAG	O3-C3-C2	-6.40	96.23	109.47
4	D	4	XYP	C1-C2-C3	-5.37	103.07	109.67
4	D	3	BMA	O3-C3-C4	-5.07	98.62	110.35
3	C	4	XYP	O3-C3-C2	-4.94	100.53	109.99
4	D	1	NAG	C1-O5-C5	-4.77	105.73	112.19
4	D	1	NAG	O5-C5-C6	-4.62	99.97	107.20
4	D	2	NAG	C8-C7-N2	-4.54	108.42	116.10
4	D	7	FUC	O3-C3-C2	-4.34	101.69	109.99
2	E	2	NAG	C1-O5-C5	-4.30	106.37	112.19
2	F	2	NAG	C1-O5-C5	-4.17	106.54	112.19
3	C	3	BMA	C2-C3-C4	-4.12	103.77	110.89
4	D	3	BMA	C1-O5-C5	-4.10	106.63	112.19
4	D	1	NAG	O3-C3-C2	4.03	117.80	109.47
2	F	2	NAG	O5-C1-C2	-4.01	104.96	111.29
4	D	5	MAN	O3-C3-C4	3.99	119.58	110.35
3	C	3	BMA	O3-C3-C4	3.98	119.55	110.35
2	B	1	NAG	O5-C1-C2	-3.89	105.14	111.29
2	B	2	NAG	O7-C7-C8	-3.88	114.84	122.06
2	E	1	NAG	C3-C4-C5	3.74	116.91	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C8-C7-N2	-3.69	109.84	116.10
4	D	7	FUC	O5-C5-C6	3.69	115.27	107.33
2	A	2	NAG	C2-N2-C7	3.56	127.97	122.90
3	C	5	FUC	O2-C2-C3	-3.52	103.08	110.14
4	D	5	MAN	O3-C3-C2	-3.47	103.34	109.99
2	A	1	NAG	O5-C5-C6	3.46	112.64	107.20
4	D	4	XYP	C5-C4-C3	3.32	113.74	109.67
4	D	2	NAG	C4-C3-C2	-3.26	106.24	111.02
2	B	1	NAG	C1-O5-C5	-3.26	107.78	112.19
4	D	2	NAG	O5-C1-C2	-3.24	106.18	111.29
4	D	7	FUC	C1-O5-C5	3.21	120.06	112.78
3	C	2	NAG	O7-C7-C8	-3.19	116.12	122.06
2	E	1	NAG	O4-C4-C5	-3.15	101.47	109.30
2	B	2	NAG	C3-C4-C5	3.15	115.86	110.24
4	D	2	NAG	O5-C5-C6	3.14	112.13	107.20
2	B	2	NAG	O4-C4-C3	-3.14	103.10	110.35
2	B	2	NAG	C4-C3-C2	3.09	115.54	111.02
2	F	2	NAG	O4-C4-C3	-3.02	103.36	110.35
4	D	3	BMA	O2-C2-C1	-3.01	102.99	109.15
4	D	7	FUC	C6-C5-C4	-2.97	107.59	113.07
2	F	1	NAG	C2-N2-C7	2.97	127.13	122.90
3	C	1	NAG	O4-C4-C5	-2.96	101.95	109.30
3	C	1	NAG	O5-C1-C2	-2.96	106.62	111.29
2	B	2	NAG	C8-C7-N2	2.95	121.10	116.10
4	D	3	BMA	C3-C4-C5	-2.95	104.98	110.24
2	B	2	NAG	C1-C2-N2	2.95	115.52	110.49
3	C	2	NAG	O4-C4-C3	-2.92	103.59	110.35
2	F	1	NAG	C4-C3-C2	2.90	115.28	111.02
4	D	7	FUC	O2-C2-C3	2.87	115.88	110.14
2	A	2	NAG	C1-O5-C5	-2.87	108.31	112.19
3	C	1	NAG	O5-C5-C4	-2.86	103.87	110.83
3	C	4	XYP	O3-C3-C4	2.84	115.44	109.99
2	E	1	NAG	O5-C1-C2	-2.79	106.88	111.29
4	D	4	XYP	C5-O5-C1	-2.78	107.25	111.52
2	F	2	NAG	C4-C3-C2	-2.77	106.96	111.02
2	A	1	NAG	O6-C6-C5	2.76	120.75	111.29
3	C	2	NAG	O3-C3-C2	-2.73	103.81	109.47
2	A	1	NAG	C4-C3-C2	-2.71	107.05	111.02
2	F	1	NAG	C3-C4-C5	-2.71	105.41	110.24
2	B	1	NAG	O7-C7-C8	2.70	127.06	122.06
3	C	3	BMA	O2-C2-C1	-2.66	103.70	109.15
4	D	6	MAN	O2-C2-C1	-2.64	103.76	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O7-C7-N2	-2.62	117.13	121.95
2	E	1	NAG	C1-C2-N2	-2.62	106.02	110.49
3	C	2	NAG	O5-C5-C4	-2.57	104.56	110.83
4	D	3	BMA	C2-C3-C4	2.57	115.35	110.89
2	F	2	NAG	O7-C7-N2	2.52	126.58	121.95
3	C	4	XYP	C4-C3-C2	-2.49	107.96	110.92
2	F	2	NAG	C1-C2-N2	-2.45	106.31	110.49
3	C	4	XYP	C5-C4-C3	2.44	112.67	109.67
2	B	2	NAG	O5-C1-C2	2.41	115.09	111.29
3	C	1	NAG	O4-C4-C3	-2.39	104.82	110.35
4	D	5	MAN	O5-C1-C2	2.38	114.45	110.77
2	A	2	NAG	O4-C4-C3	-2.38	104.84	110.35
3	C	2	NAG	C1-O5-C5	2.33	115.34	112.19
4	D	2	NAG	C3-C4-C5	2.31	114.36	110.24
2	F	1	NAG	O4-C4-C5	-2.28	103.63	109.30
3	C	1	NAG	C1-C2-N2	-2.27	106.61	110.49
3	C	5	FUC	O5-C5-C4	2.23	113.53	109.52
2	A	2	NAG	C4-C3-C2	2.23	114.28	111.02
4	D	6	MAN	O5-C5-C6	2.19	110.64	107.20
2	B	2	NAG	O3-C3-C4	-2.17	105.32	110.35
3	C	4	XYP	O4-C4-C3	2.16	114.47	110.14
2	F	1	NAG	C1-C2-N2	2.14	114.15	110.49
3	C	2	NAG	O7-C7-N2	2.13	125.86	121.95
4	D	2	NAG	C1-O5-C5	-2.12	109.32	112.19
4	D	2	NAG	O7-C7-C8	2.09	125.94	122.06
2	E	2	NAG	O4-C4-C3	2.08	115.16	110.35
3	C	2	NAG	O6-C6-C5	-2.07	104.18	111.29
3	C	5	FUC	O4-C4-C5	-2.06	105.10	109.67
4	D	7	FUC	C1-C2-C3	2.05	112.18	109.67
3	C	5	FUC	O5-C5-C6	-2.04	102.94	107.33
2	F	2	NAG	O6-C6-C5	-2.04	104.30	111.29
4	D	3	BMA	C1-C2-C3	-2.03	107.17	109.67
4	D	1	NAG	C4-C3-C2	-2.02	108.06	111.02
4	D	6	MAN	C2-C3-C4	2.00	114.36	110.89

There are no chirality outliers.

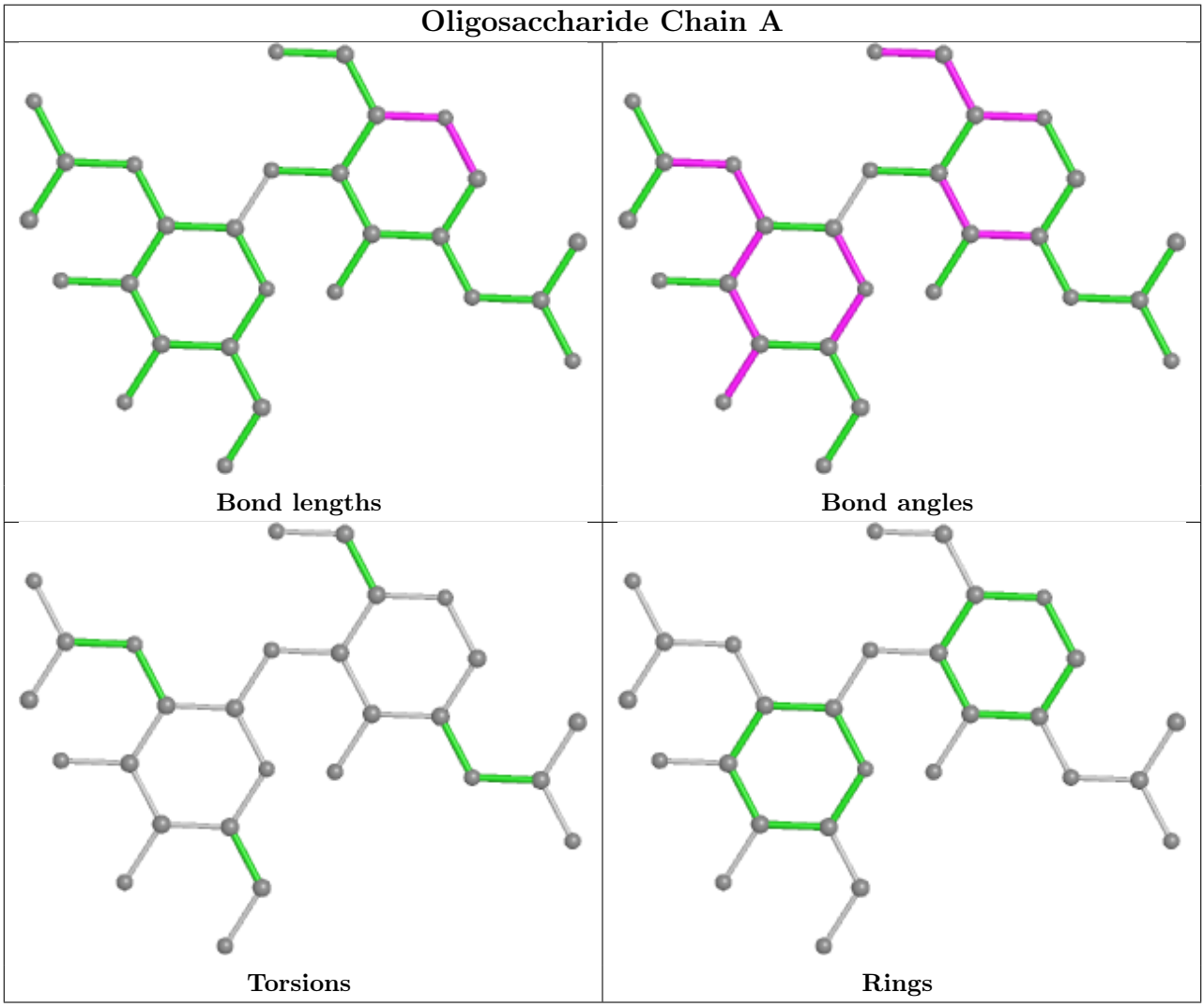
There are no torsion outliers.

There are no ring outliers.

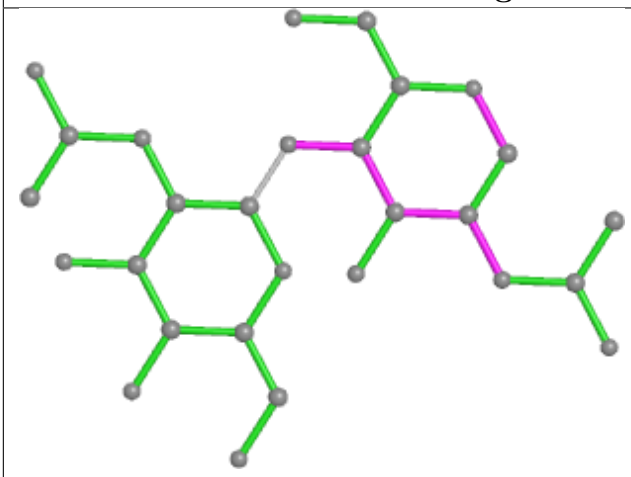
10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	XYP	2	0
4	D	3	BMA	2	0
4	D	1	NAG	1	0
2	E	2	NAG	2	0
2	A	1	NAG	2	0
3	C	3	BMA	4	0
4	D	6	MAN	2	0
3	C	2	NAG	2	0
2	A	2	NAG	2	0
2	E	1	NAG	2	0

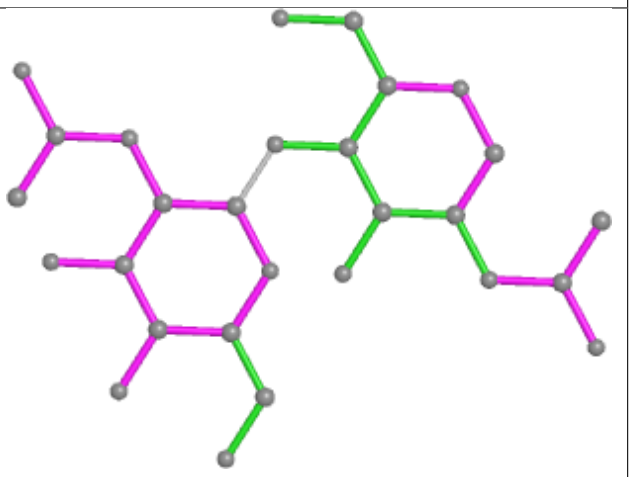
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



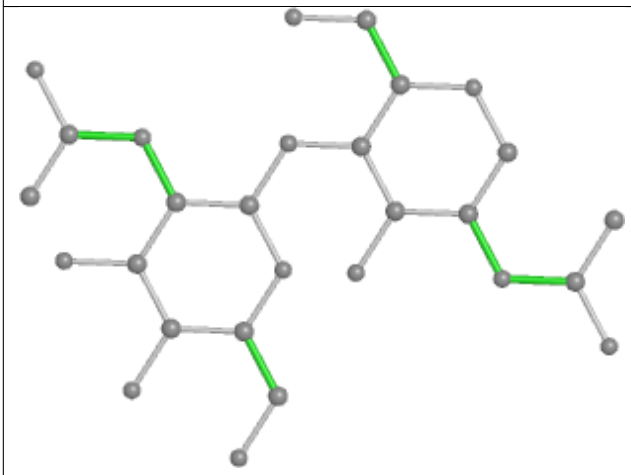
Oligosaccharide Chain B



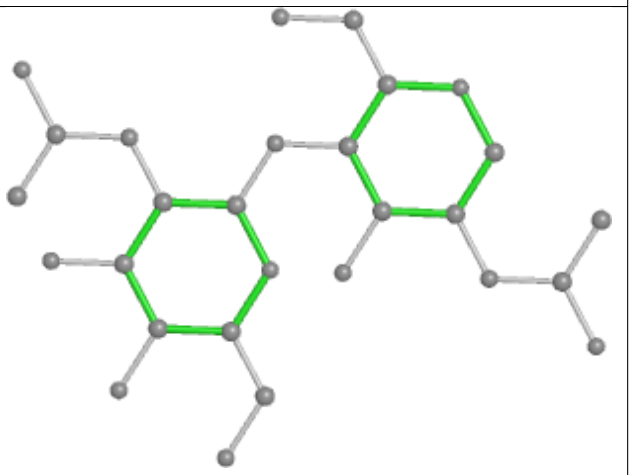
Bond lengths



Bond angles

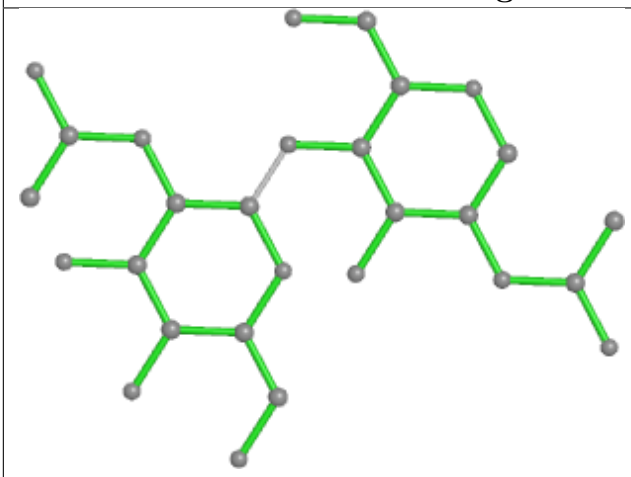


Torsions

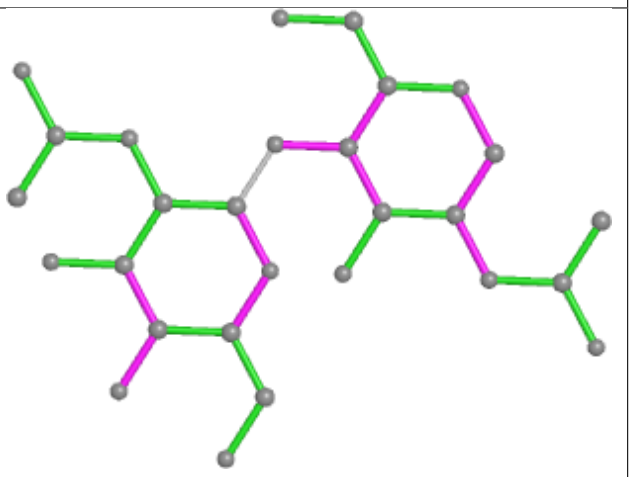


Rings

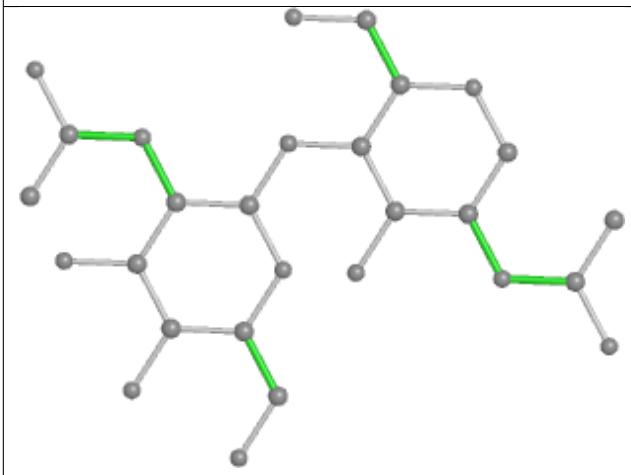
Oligosaccharide Chain E



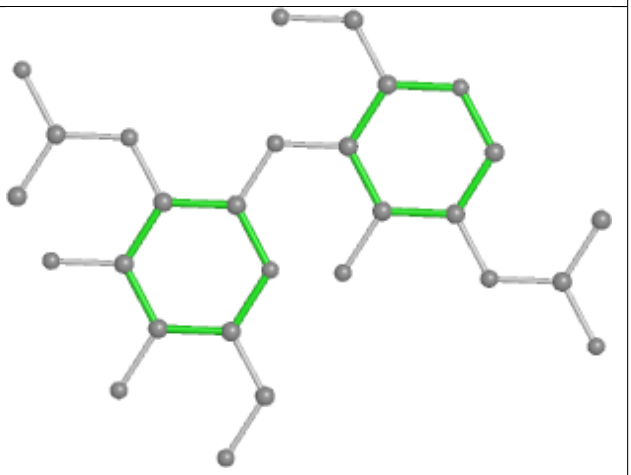
Bond lengths



Bond angles

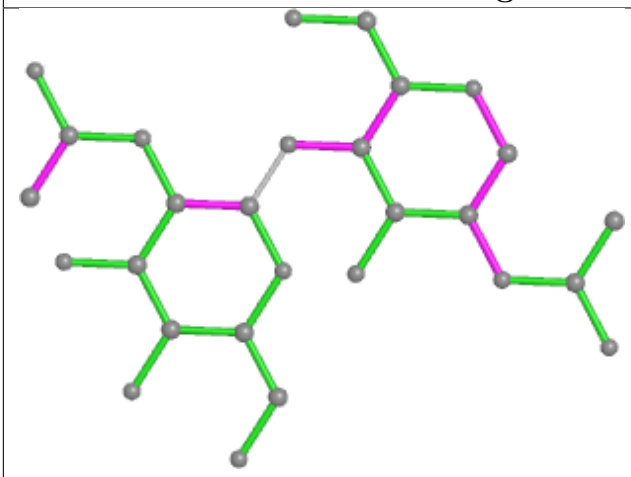


Torsions

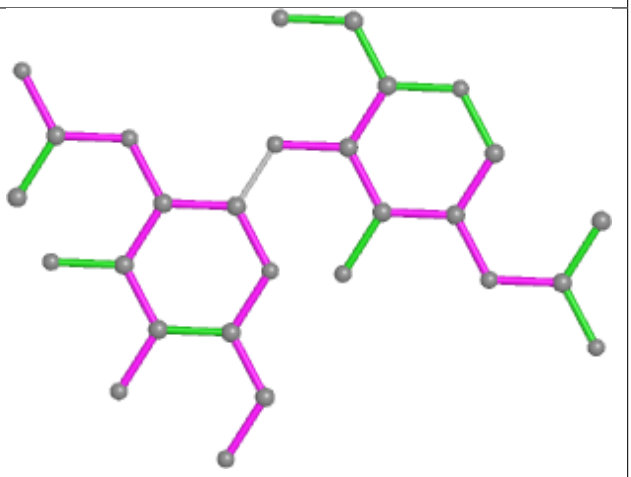


Rings

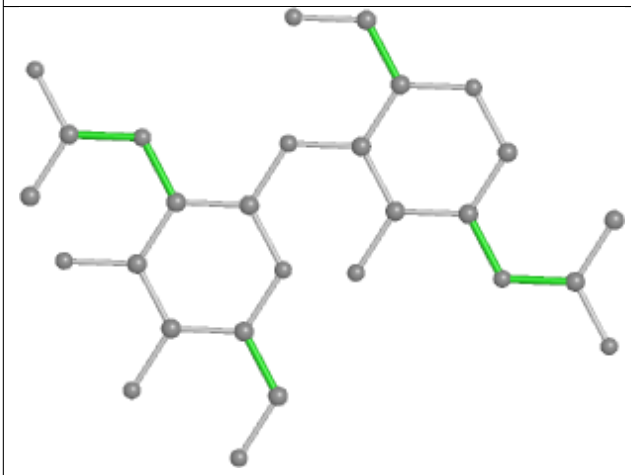
Oligosaccharide Chain F



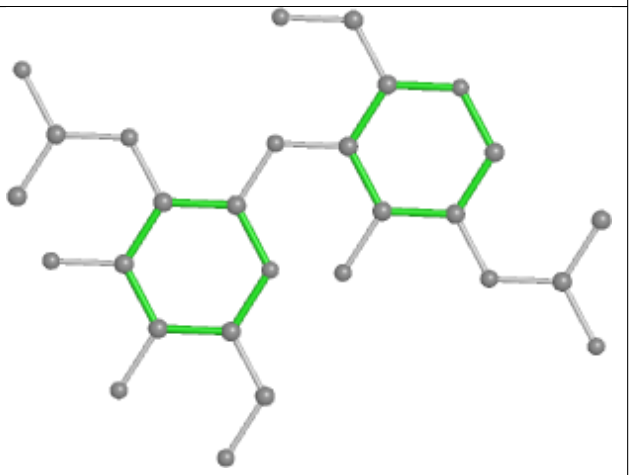
Bond lengths



Bond angles

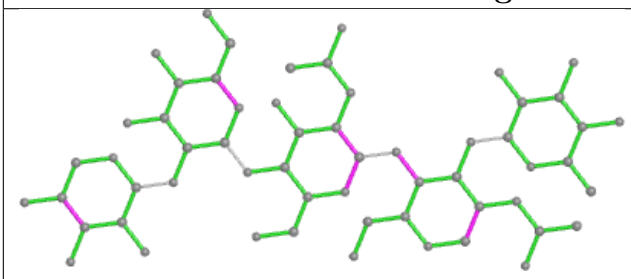


Torsions

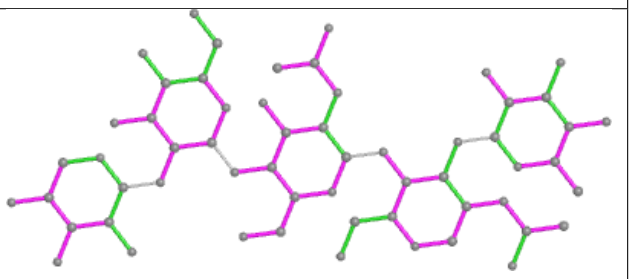


Rings

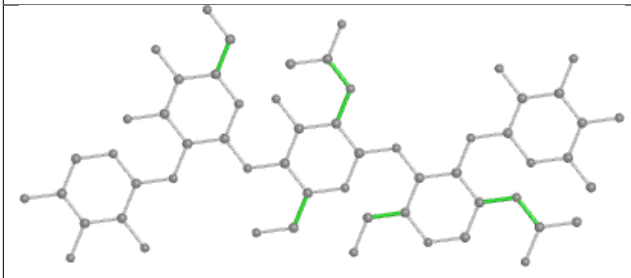
Oligosaccharide Chain C



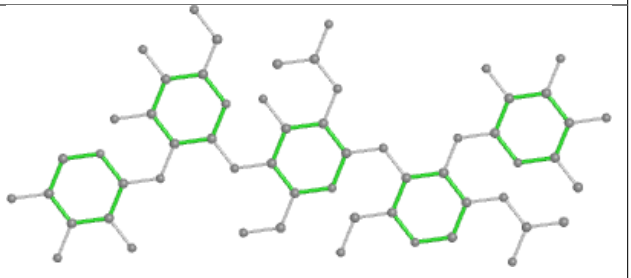
Bond lengths



Bond angles

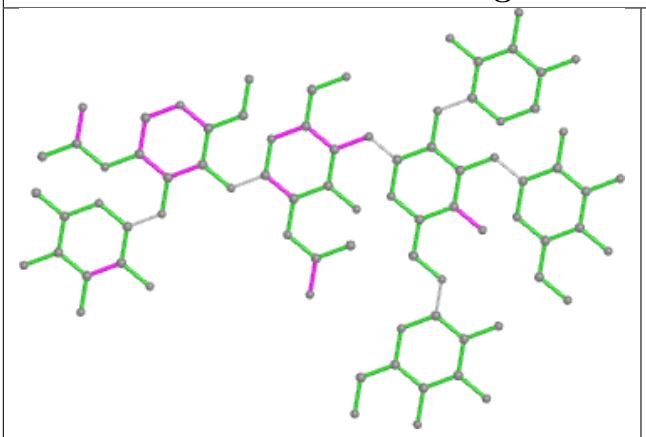


Torsions

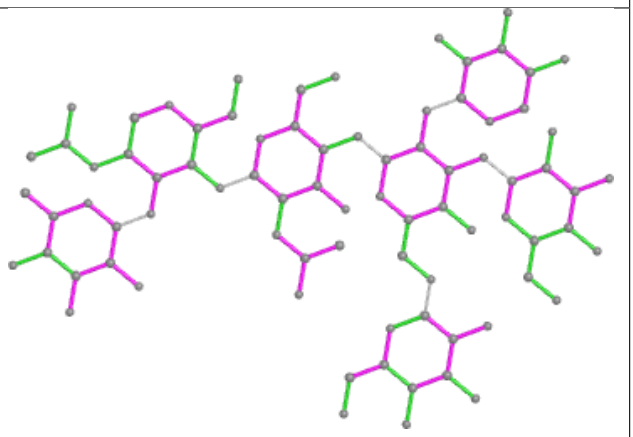


Rings

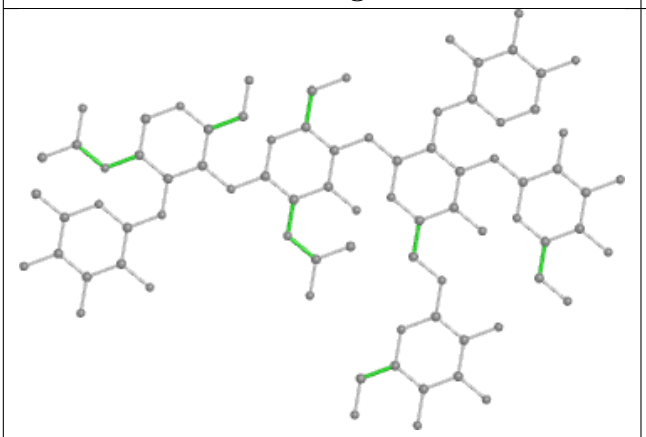
Oligosaccharide Chain D



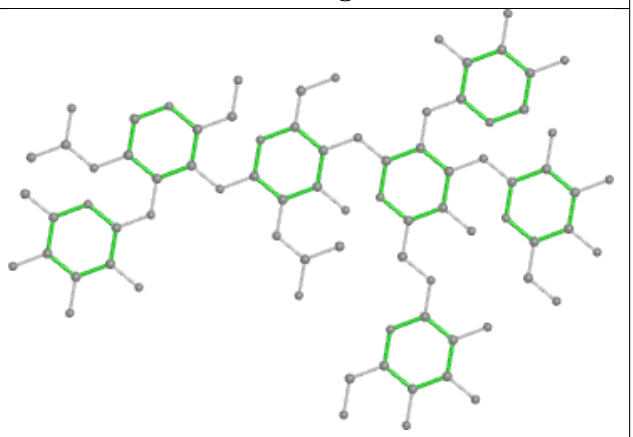
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
9	GOL	M	2513	-	5,5,5	0.54	0	5,5,5	0.84	0
5	NAG	M	901	1	14,14,15	1.15	1 (7%)	17,19,21	2.11	6 (35%)
5	NAG	M	931	1	14,14,15	0.88	0	17,19,21	2.36	6 (35%)
8	SO4	M	1503[A]	-	4,4,4	0.51	0	6,6,6	0.73	0
6	E18	M	1501	-	17,20,20	1.37	1 (5%)	17,26,26	3.05	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	M	971	1	14,14,15	0.60	0	17,19,21	1.39	3 (17%)
5	NAG	M	991	1	14,14,15	1.11	1 (7%)	17,19,21	1.70	3 (17%)
8	SO4	M	1505	-	4,4,4	0.39	0	6,6,6	1.06	0
9	GOL	M	2511	-	5,5,5	0.53	0	5,5,5	1.06	0
9	GOL	M	2512[B]	-	5,5,5	0.93	0	5,5,5	2.50	1 (20%)
8	SO4	M	1506	-	4,4,4	0.43	0	6,6,6	0.76	0
8	SO4	M	1503[B]	-	4,4,4	0.38	0	6,6,6	1.55	2 (33%)
8	SO4	M	1504	-	4,4,4	0.69	0	6,6,6	1.13	0
8	SO4	M	1509	-	4,4,4	0.30	0	6,6,6	0.27	0
8	SO4	M	1507	-	4,4,4	0.55	0	6,6,6	1.04	0
9	GOL	M	2512[A]	-	5,5,5	0.92	0	5,5,5	2.51	1 (20%)
8	SO4	M	1508	-	4,4,4	0.59	0	6,6,6	1.79	2 (33%)
9	GOL	M	2514	-	5,5,5	0.46	0	5,5,5	1.14	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	M	2513	-	-	0/4/4/4	-
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
5	NAG	M	931	1	-	3/6/23/26	0/1/1/1
6	E18	M	1501	-	-	4/8/16/16	0/1/1/1
5	NAG	M	971	1	-	0/6/23/26	0/1/1/1
5	NAG	M	991	1	-	0/6/23/26	0/1/1/1
9	GOL	M	2512[B]	-	-	2/4/4/4	-
9	GOL	M	2511	-	-	2/4/4/4	-
9	GOL	M	2512[A]	-	-	1/4/4/4	-
9	GOL	M	2514	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1501	E18	O18-N17	-4.37	1.36	1.45
5	M	901	NAG	O5-C1	-3.12	1.38	1.43
5	M	991	NAG	C1-C2	2.58	1.56	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1501	E18	C1-S1-C13	11.51	121.86	102.41
5	M	901	NAG	C8-C7-N2	5.69	125.73	116.10
9	M	2512[A]	GOL	O2-C2-C3	5.30	132.46	109.12
9	M	2512[B]	GOL	O2-C2-C3	5.30	132.46	109.12
5	M	931	NAG	C2-N2-C7	4.88	129.85	122.90
5	M	931	NAG	C1-O5-C5	-4.17	106.54	112.19
5	M	931	NAG	O7-C7-C8	-4.08	114.48	122.06
5	M	991	NAG	C1-O5-C5	-3.99	106.78	112.19
5	M	991	NAG	O5-C5-C6	3.34	112.45	107.20
6	M	1501	E18	CB-CG-CD1	-3.01	116.58	120.89
5	M	931	NAG	C8-C7-N2	2.98	121.15	116.10
5	M	931	NAG	C1-C2-N2	-2.94	105.47	110.49
5	M	901	NAG	O7-C7-C8	-2.86	116.74	122.06
8	M	1503[B]	SO4	O4-S-O3	2.77	120.88	109.06
8	M	1508	SO4	O4-S-O1	2.75	123.68	109.31
5	M	901	NAG	O4-C4-C3	2.69	116.56	110.35
8	M	1508	SO4	O3-S-O1	-2.66	95.44	109.31
8	M	1503[B]	SO4	O4-S-O2	-2.52	96.17	109.31
5	M	931	NAG	O5-C5-C4	-2.42	104.93	110.83
5	M	901	NAG	O7-C7-N2	-2.41	117.52	121.95
5	M	991	NAG	C8-C7-N2	2.38	120.13	116.10
5	M	971	NAG	C1-O5-C5	-2.31	109.06	112.19
5	M	971	NAG	O4-C4-C3	-2.19	105.29	110.35
5	M	901	NAG	O3-C3-C4	2.19	115.41	110.35
9	M	2514	GOL	O3-C3-C2	2.17	120.61	110.20
5	M	901	NAG	C1-C2-N2	2.08	114.04	110.49
5	M	971	NAG	C4-C3-C2	-2.07	107.98	111.02
6	M	1501	E18	CE1-CD1-CG	-2.07	117.46	120.63

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	1501	E18	CB-C13-S1-C1
6	M	1501	E18	C2-C1-S1-C13
9	M	2511	GOL	C1-C2-C3-O3
9	M	2512[B]	GOL	C1-C2-C3-O3
9	M	2514	GOL	O1-C1-C2-C3
6	M	1501	E18	S1-C1-C2-N18
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
9	M	2512[B]	GOL	O2-C2-C3-O3
9	M	2511	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	M	2514	GOL	O1-C1-C2-O2
9	M	2512[A]	GOL	C1-C2-C3-O3
5	M	931	NAG	C4-C5-C6-O6
6	M	1501	E18	C13-CB-CG-CD2

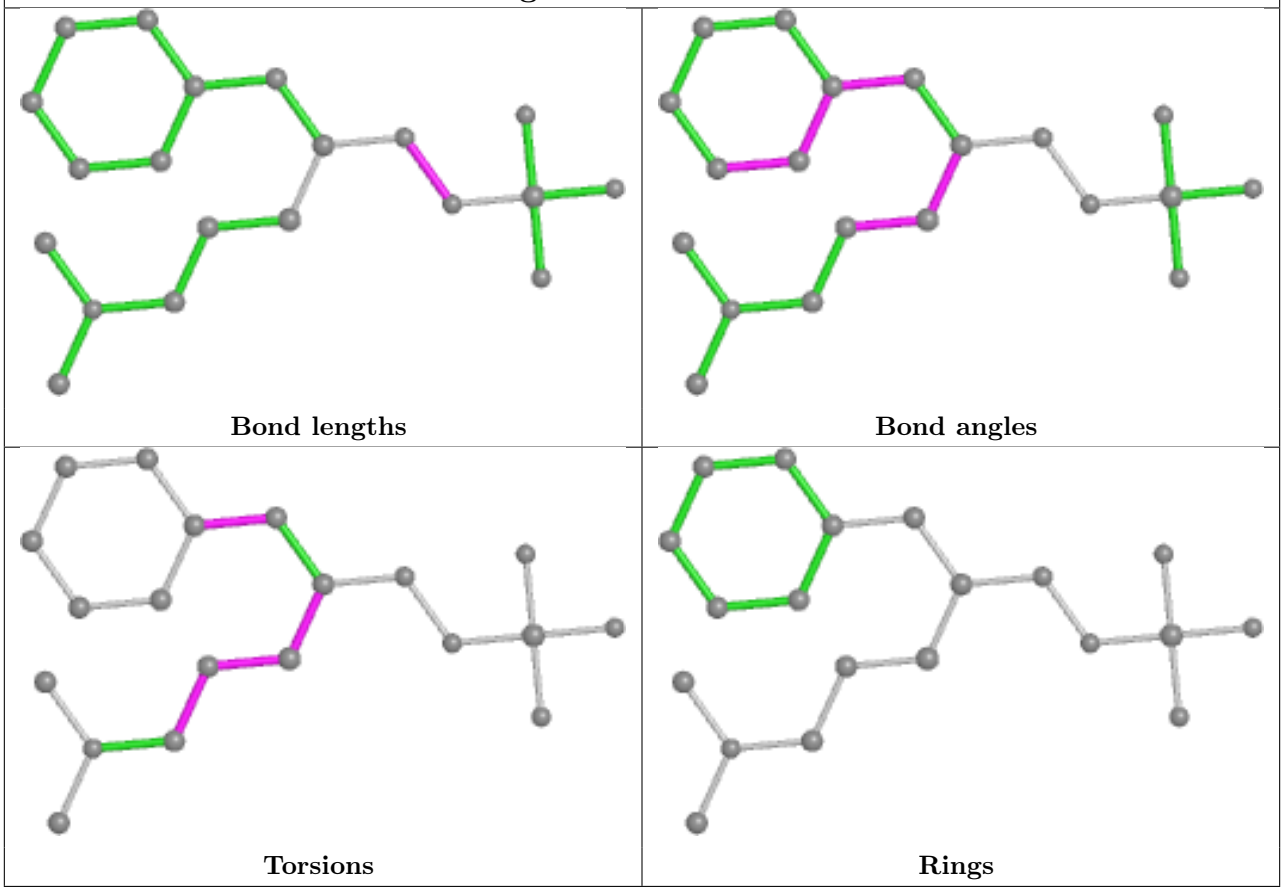
There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	2513	GOL	1	0
5	M	931	NAG	11	0
6	M	1501	E18	2	0
5	M	971	NAG	3	0
5	M	991	NAG	4	0
9	M	2511	GOL	3	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 E18 M 1501



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	M	499/501 (99%)	-0.34	4 (0%)	86	86	7, 11, 24, 51	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	3	GLU	3.2
1	M	18	ASP	2.1
1	M	376	ALA	2.1
1	M	27	SER	2.1

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	MAN	D	6	11/12	0.64	0.28	35,43,44,45	0
2	NAG	B	2	14/15	0.69	0.32	38,45,54,57	0
2	NAG	E	1	14/15	0.71	0.29	39,46,61,63	0
3	BMA	C	3	11/12	0.75	0.20	37,39,46,47	0
2	NAG	A	2	14/15	0.76	0.34	37,42,47,48	0
4	MAN	D	5	11/12	0.78	0.27	36,42,48,52	0
2	NAG	E	2	14/15	0.79	0.19	40,46,52,53	0
3	XYP	C	4	9/10	0.79	0.23	37,41,43,45	0

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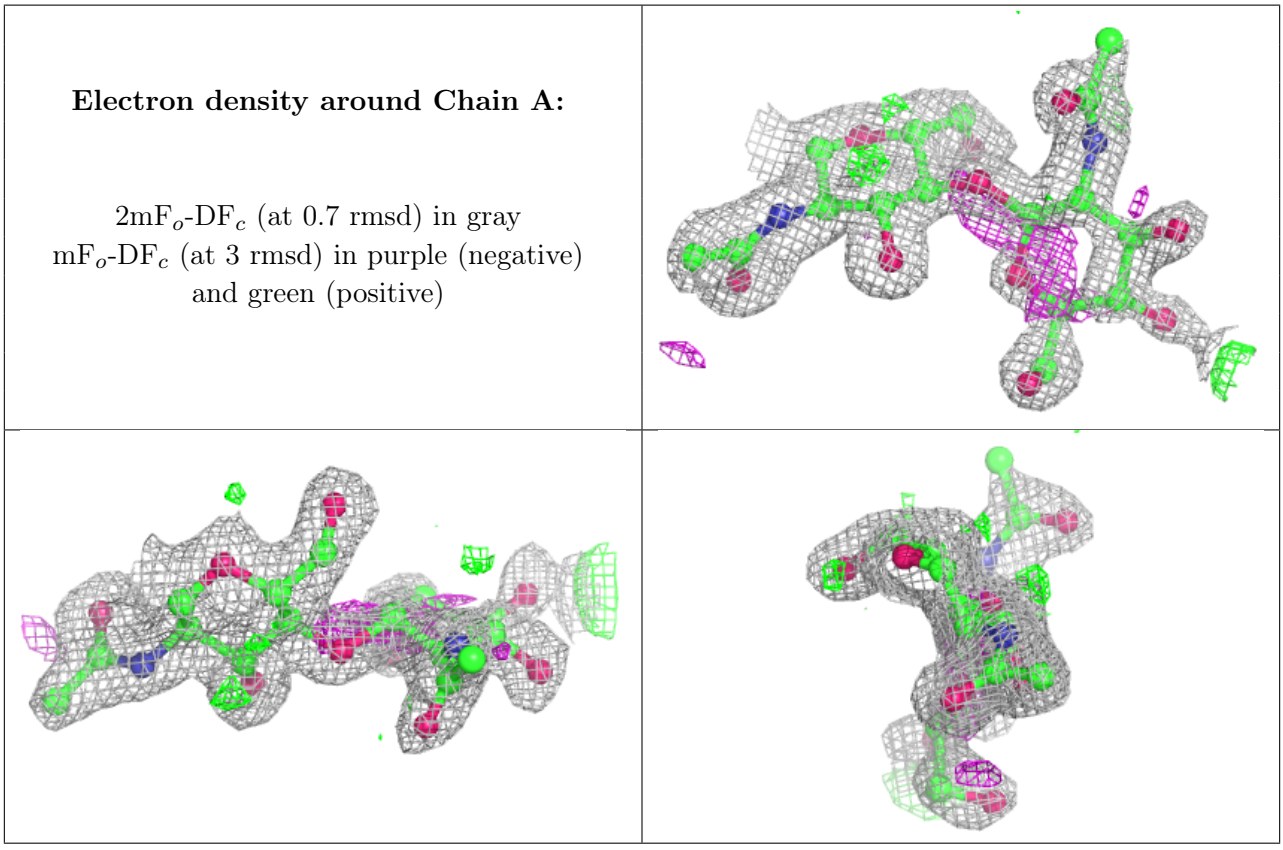
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	14/15	0.82	0.22	22,37,46,48	0
4	NAG	D	2	14/15	0.88	0.15	19,23,30,33	0
3	FUC	C	5	10/11	0.90	0.12	22,31,36,42	0
2	NAG	A	1	14/15	0.90	0.17	19,27,31,33	0
3	NAG	C	2	14/15	0.91	0.12	20,27,32,39	0
4	BMA	D	3	11/12	0.91	0.16	22,26,30,33	0
4	XYP	D	4	9/10	0.93	0.18	30,38,43,47	0
4	NAG	D	1	14/15	0.94	0.09	16,19,25,27	0
3	NAG	C	1	14/15	0.94	0.08	12,15,18,18	0
4	FUC	D	7	10/11	0.94	0.12	22,25,30,31	0
2	NAG	B	1	14/15	0.95	0.08	14,24,28,35	0
2	NAG	F	1	14/15	0.96	0.07	11,14,18,19	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.

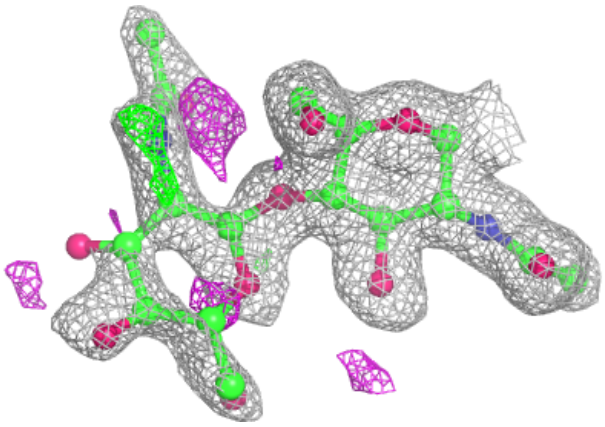
Electron density around Chain A:

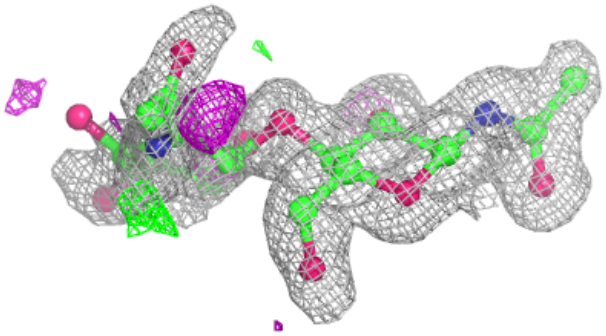
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

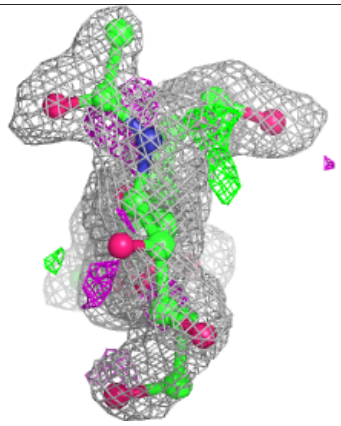


Electron density around Chain B:

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

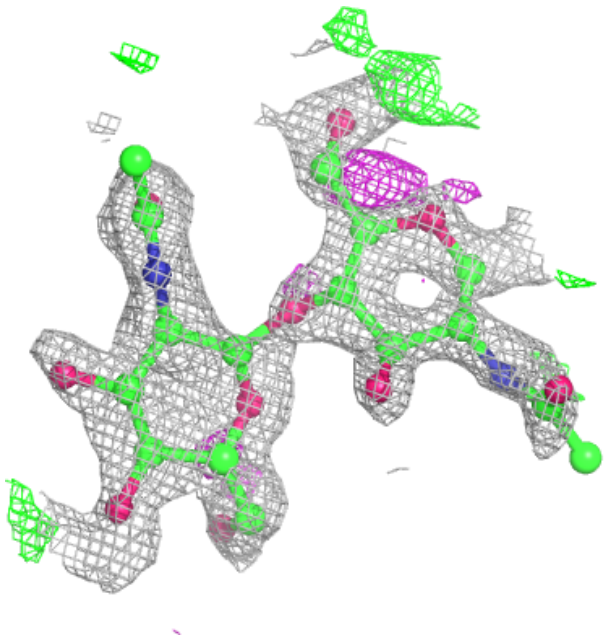


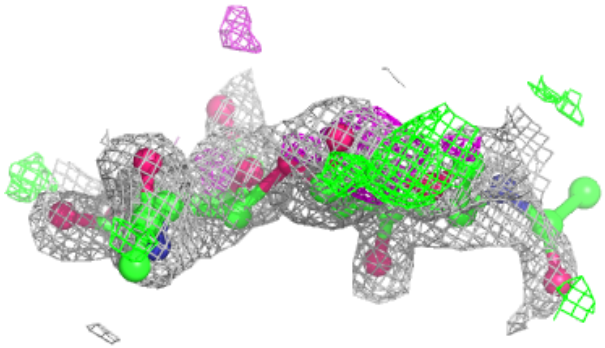


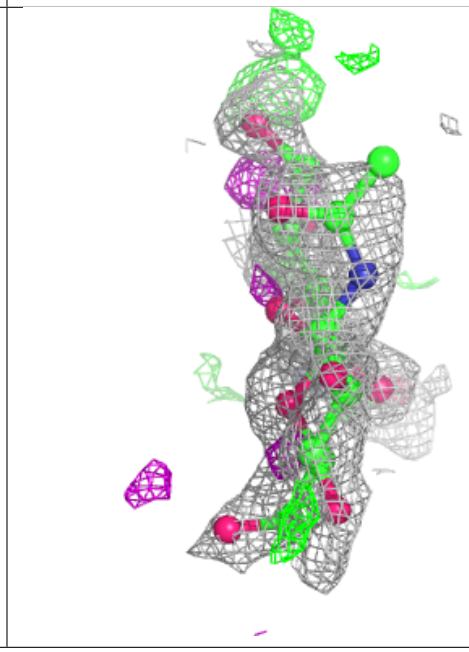


Electron density around Chain E:

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

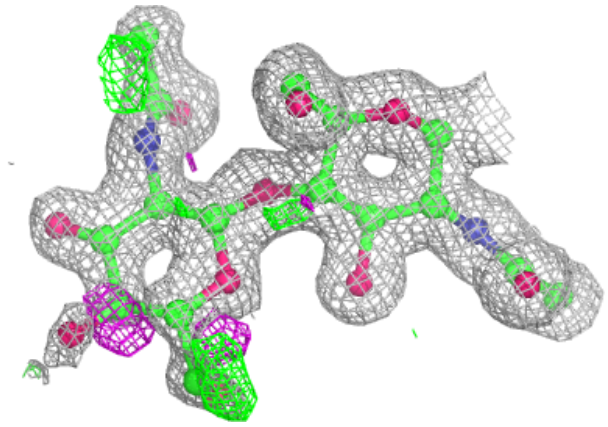


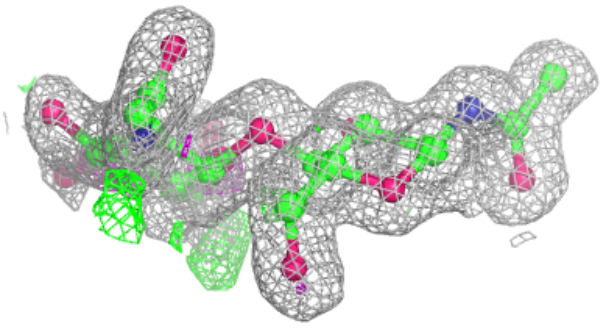


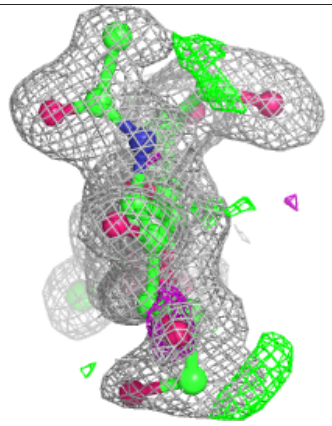


Electron density around Chain F:

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

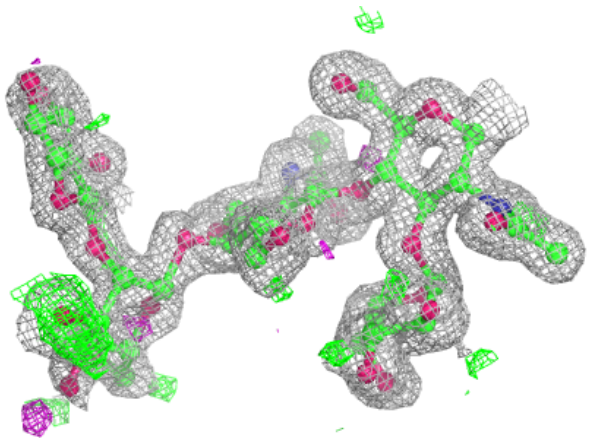


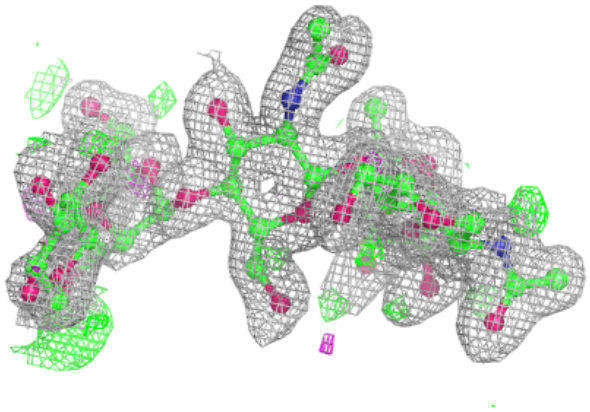


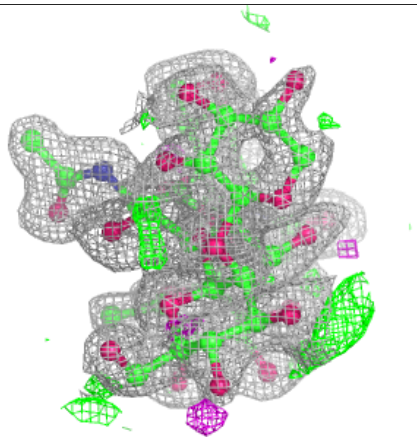


Electron density around Chain C:

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

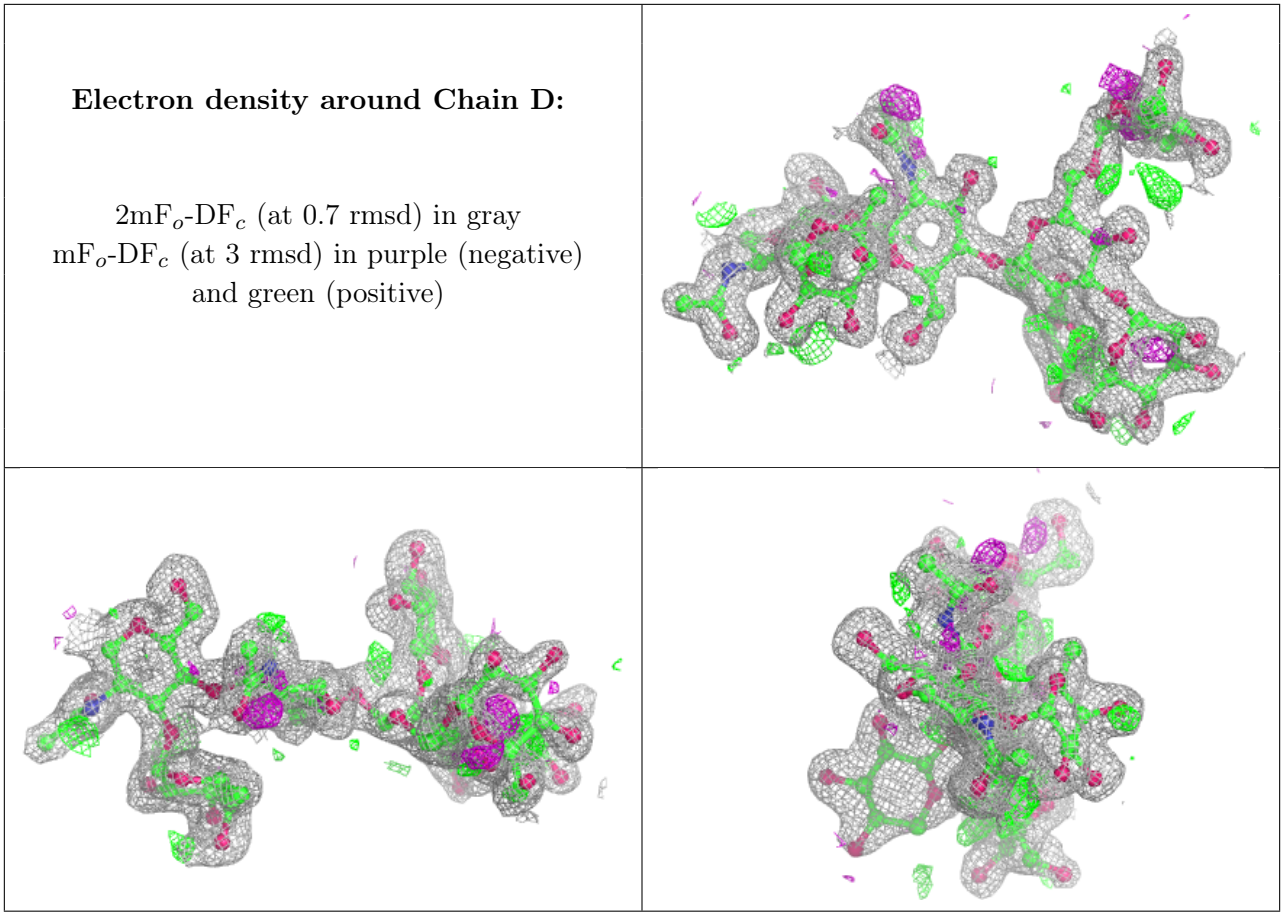






Electron density around Chain D:

$2mF_o$-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
9	GOL	M	2514	6/6	0.68	0.18	37,45,45,46	6
8	SO4	M	1508	5/5	0.74	0.20	18,29,40,41	5
5	NAG	M	971	14/15	0.76	0.23	57,60,62,62	0
9	GOL	M	2511	6/6	0.77	0.22	34,36,36,40	6
5	NAG	M	991	14/15	0.78	0.20	30,39,49,53	0
8	SO4	M	1509	5/5	0.82	0.19	36,39,42,42	5
5	NAG	M	931	14/15	0.84	0.27	37,54,64,90	0
5	NAG	M	901	14/15	0.89	0.15	24,36,41,46	0
8	SO4	M	1503[A]	5/5	0.89	0.17	24,29,44,45	5
8	SO4	M	1503[B]	5/5	0.89	0.17	18,26,32,32	5
8	SO4	M	1507	5/5	0.89	0.17	25,36,41,43	5
9	GOL	M	2512[B]	6/6	0.90	0.15	14,16,22,23	1

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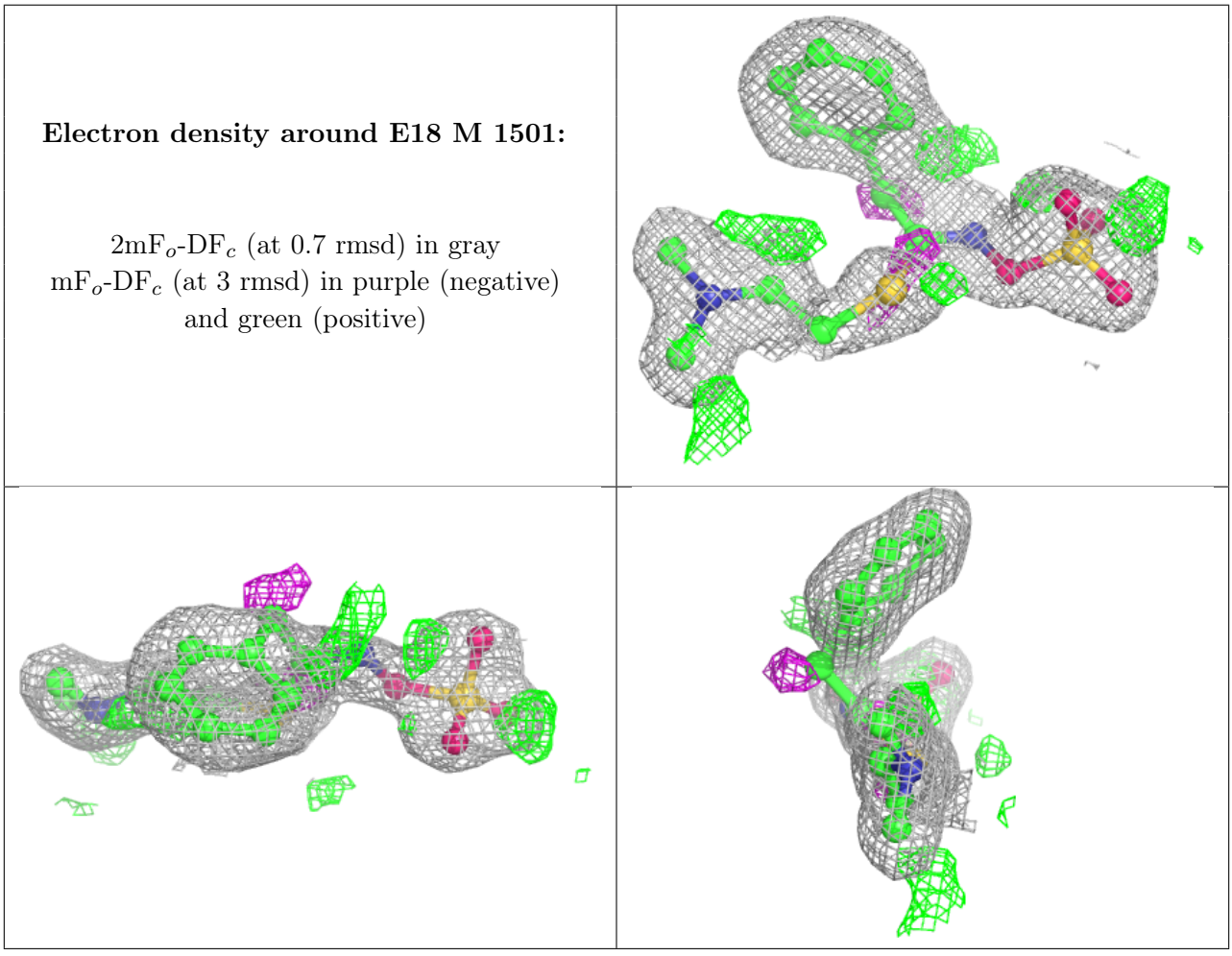
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	M	2512[A]	6/6	0.90	0.15	8,16,22,23	1
6	E18	M	1501	20/20	0.91	0.15	16,23,39,40	20
9	GOL	M	2513	6/6	0.96	0.11	14,27,30,37	6
8	SO4	M	1505	5/5	0.97	0.08	19,25,31,32	5
8	SO4	M	1504	5/5	0.98	0.10	20,22,31,31	5
8	SO4	M	1506	5/5	0.99	0.07	19,19,23,27	0
7	ZN	M	1502	1/1	1.00	0.07	8,8,8,8	1

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 E18 M 1501:

$2mF_o$-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

There are no such residues in this entry.