



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 PM UTC

PDB ID : 1W9D / pdb_00001w9d
Title : S. alba myrosinase in complex with S-ethyl phenylacetothiohydroximate-O-sulfate
Authors : Bourderioux, A.; Lefoix, M.; Gueyrard, D.; Tatibouet, A.; Cottaz, S.; Arzt, S.; Burmeister, W.P.; Rollin, P.
Deposited on : 2004-10-08
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

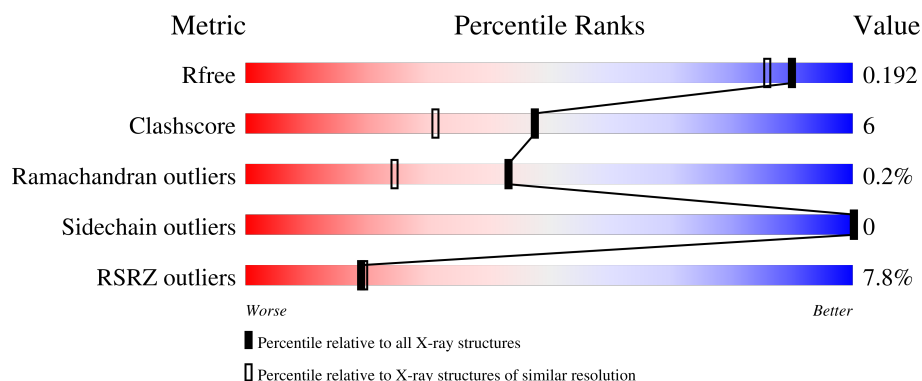
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	501	 8% 89% 11%
2	A	2	 50% 50%
2	D	2	 100%
3	B	5	 100%

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Mol	Chain	Length	Quality of chain
4	C	7	 86%14%

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
6	SEH	M	999	-	-	X	-
9	GOL	M	1513	-	X	-	-
9	GOL	M	1514	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5112 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 GLYCOSIDASE.

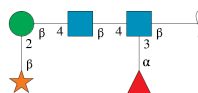
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	0	0
			4016	2571	659	770	16			

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



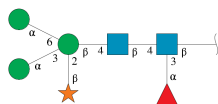
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



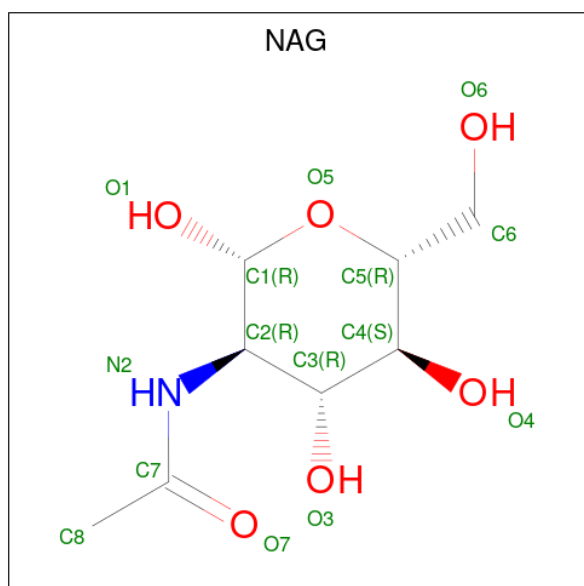
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

- 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.



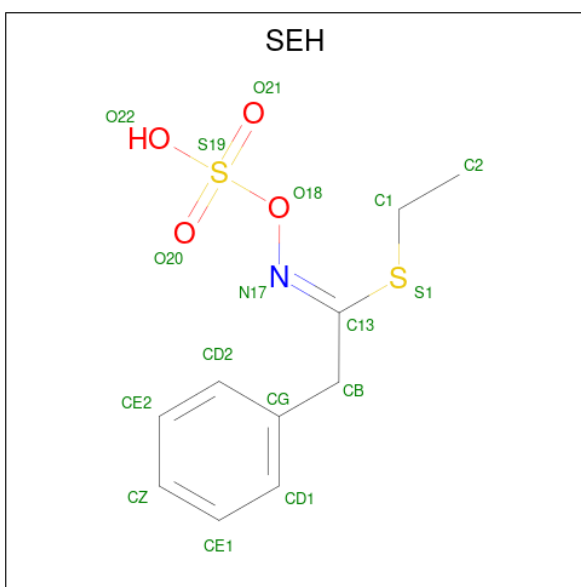
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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
			15	8	1	6		
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 S-BENZYL PHENYLACETOTHIOHYDROXIMATE-O-SULFATE (CCD ID: SEH) (formula: $C_{10}H_{13}NO_4S_2$).

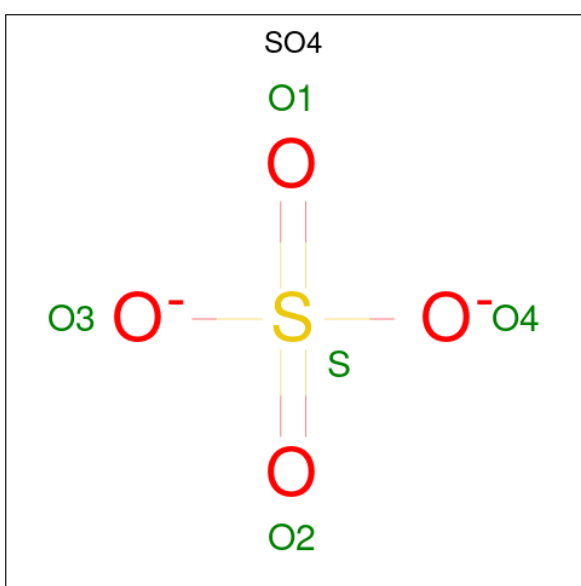


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	M	1	Total	C	N	O	S	0	0
			17	10	1	4	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

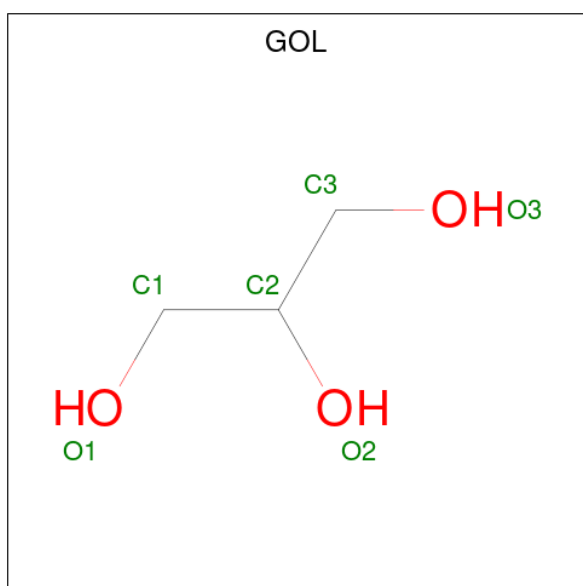
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 (CCD ID: 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 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0

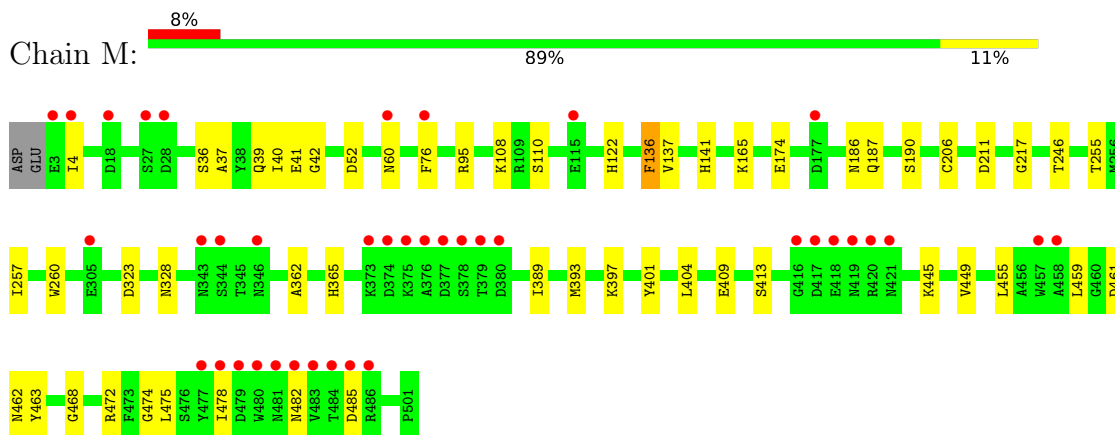
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	761	Total O 761 761	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.

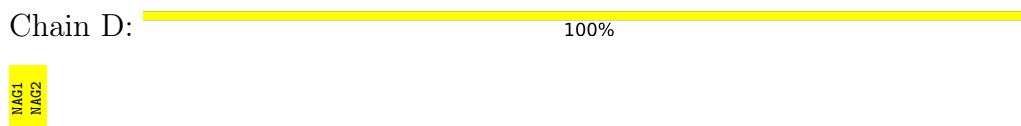
- Molecule 1: GLYCOSIDASE



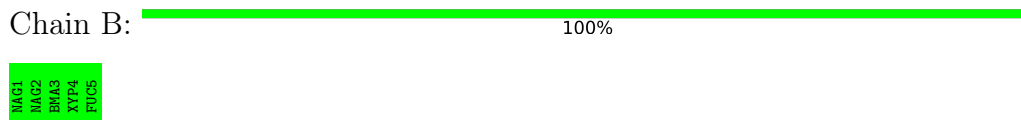
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 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



- 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 C:  86% 14%

NAG1	NAG2	EMA3	XYP4	MAN5	MAN6	FUC7
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.60 35.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.00-1.60) 99.2 (35.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.195 0.195 , 0.192	Depositor DCC
R_{free} test set	7352 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5112	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, FUC, SEH, GOL, BMA, XYP, SO4, 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	M	0.34	0/4137	0.89	20/5624 (0.4%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	190	SER	N-CA-C	9.21	121.01	110.97
1	M	41	GLU	N-CA-C	7.62	120.69	111.40
1	M	475	LEU	N-CA-C	-6.92	104.84	113.28
1	M	40	ILE	N-CA-C	6.76	120.15	113.53
1	M	401	TYR	N-CA-C	6.75	120.97	111.52
1	M	474	GLY	N-CA-C	6.67	120.74	112.14
1	M	42	GLY	N-CA-C	-6.48	105.03	112.29
1	M	137	VAL	N-CA-C	6.36	117.02	107.80
1	M	257	ILE	N-CA-C	-6.02	99.91	108.58
1	M	37	ALA	N-CA-C	5.98	117.47	111.07
1	M	52	ASP	N-CA-C	-5.93	104.74	111.14
1	M	459	LEU	N-CA-C	-5.89	104.93	111.71
1	M	323	ASP	N-CA-C	-5.82	106.31	113.41
1	M	217	GLY	N-CA-C	5.62	118.10	111.63
1	M	136	PHE	N-CA-C	-5.22	98.88	108.02
1	M	485	ASP	N-CA-C	5.22	117.86	110.50
1	M	404	LEU	N-CA-C	-5.21	101.47	109.76
1	M	40	ILE	CB-CA-C	-5.20	105.56	110.65
1	M	76	PHE	N-CA-C	-5.07	105.67	111.14
1	M	260	TRP	N-CA-C	-5.02	102.63	110.42

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	M	4016	0	3772	26	0
2	A	28	0	25	0	0
2	D	28	0	25	1	0
3	B	58	0	42	0	0
4	C	80	0	60	1	0
5	M	85	0	80	7	0
6	M	17	0	13	18	0
7	M	1	0	0	0	0
8	M	20	0	0	0	0
9	M	18	0	24	15	0
10	M	761	0	0	8	0
All	All	5112	0	4041	46	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 6.

All (46) 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)
6:M:999:SEH:H2C1	9:M:1514:GOL:C1	1.44	1.48
6:M:999:SEH:C2	9:M:1514:GOL:H32	1.58	1.31
6:M:999:SEH:C2	9:M:1514:GOL:H12	1.63	1.28
6:M:999:SEH:C2	9:M:1514:GOL:C1	2.15	1.25
6:M:999:SEH:H2C3	9:M:1514:GOL:C3	1.71	1.16
6:M:999:SEH:H2C2	9:M:1514:GOL:H31	1.39	1.00
6:M:999:SEH:H2C3	9:M:1514:GOL:H32	0.94	0.94
6:M:999:SEH:C2	9:M:1514:GOL:H31	1.90	0.88
6:M:999:SEH:H2C2	9:M:1514:GOL:C3	1.94	0.86
6:M:999:SEH:H2C2	9:M:1514:GOL:C1	2.14	0.76
6:M:999:SEH:C2	9:M:1514:GOL:C2	2.63	0.76
6:M:999:SEH:C2	9:M:1514:GOL:H11	2.15	0.76
1:M:246:THR:HG22	10:M:2380:HOH:O	1.84	0.76
6:M:999:SEH:H2C1	9:M:1514:GOL:C2	2.16	0.76
10:M:2714:HOH:O	4:C:3:BMA:H61	1.85	0.75
1:M:165:LYS:NZ	5:M:931:NAG:H81	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:999:SEH:H2C1	9:M:1514:GOL:H12	0.72	0.70
1:M:60:ASN:ND2	5:M:961:NAG:H1	2.08	0.68
1:M:165:LYS:HZ1	5:M:931:NAG:H81	1.56	0.68
1:M:462:ASN:HB3	10:M:2635:HOH:O	1.95	0.67
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.77	0.64
6:M:999:SEH:H2C2	9:M:1514:GOL:H11	1.75	0.64
5:M:971:NAG:H82	10:M:2504:HOH:O	2.06	0.55
1:M:108:LYS:HE3	1:M:110:SER:OG	2.06	0.55
1:M:461:ASP:O	1:M:478:ILE:HD12	2.07	0.55
6:M:999:SEH:C1	10:M:2148:HOH:O	2.58	0.52
1:M:95:ARG:HB2	1:M:455:LEU:HD13	1.92	0.51
1:M:165:LYS:NZ	5:M:931:NAG:C8	2.72	0.50
1:M:365:HIS:HE1	10:M:2531:HOH:O	1.94	0.50
6:M:999:SEH:H2C2	10:M:2148:HOH:O	2.11	0.50
1:M:95:ARG:HA	1:M:136:PHE:O	2.15	0.46
1:M:39:GLN:O	1:M:462:ASN:HB2	2.17	0.45
1:M:328:ASN:CG	1:M:409:GLU:HB2	2.40	0.45
1:M:362:ALA:HB3	2:D:1:NAG:H82	2.00	0.44
1:M:482:ASN:HD22	5:M:991:NAG:H82	1.83	0.43
1:M:463:TYR:CE1	1:M:468:GLY:HA2	2.54	0.43
1:M:186:ASN:HA	1:M:255:THR:HB	2.02	0.42
1:M:389:ILE:O	1:M:393:MET:HG2	2.20	0.42
1:M:397:LYS:HD2	1:M:449:VAL:HA	2.00	0.41
1:M:36:SER:HB2	1:M:141:HIS:CG	2.55	0.41
1:M:95:ARG:NH1	1:M:409:GLU:HG3	2.35	0.41
1:M:165:LYS:HZ3	5:M:931:NAG:C8	2.34	0.41
1:M:122:HIS:HE1	1:M:174:GLU:O	2.03	0.41
6:M:999:SEH:H1C2	10:M:2148:HOH:O	2.20	0.40
1:M:413:SER:HA	1:M:472:ARG:O	2.22	0.40
1:M:206:CYS:SG	1:M:211:ASP:HB3	2.61	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	M	497/501 (99%)	480 (97%)	16 (3%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	435/437 (100%)	435 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	122	HIS
1	M	230	GLN
1	M	297	GLN
1	M	365	HIS
1	M	402	ASN
1	M	410	ASN
1	M	462	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	1,2	14,14,15	0.41	0	17,19,21	0.66	0
2	NAG	A	2	2	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
3	NAG	B	1	1,3	14,14,15	0.43	0	17,19,21	0.65	0
3	NAG	B	2	3	14,14,15	0.40	0	17,19,21	0.67	0
3	BMA	B	3	3	11,11,12	0.32	0	15,15,17	0.25	0
3	XYP	B	4	3	9,9,10	0.44	0	10,12,14	0.35	0
3	FUC	B	5	3	10,10,11	0.38	0	14,14,16	0.31	0
4	NAG	C	1	1,4	14,14,15	0.40	0	17,19,21	0.64	0
4	NAG	C	2	4	14,14,15	0.39	0	17,19,21	0.74	0
4	BMA	C	3	4	11,11,12	0.36	0	15,15,17	0.44	0
4	XYP	C	4	4	9,9,10	0.42	0	10,12,14	0.42	0
4	MAN	C	5	4	11,11,12	0.34	0	15,15,17	0.55	0
4	MAN	C	6	4	11,11,12	0.35	0	15,15,17	0.50	0
4	FUC	C	7	4	10,10,11	0.37	0	14,14,16	0.31	0
2	NAG	D	1	1,2	14,14,15	0.51	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.40	0	17,19,21	0.71	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	MAN	C	6	4	-	2/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	C2-N2-C7	-2.21	119.94	122.90
2	D	2	NAG	C2-N2-C7	-2.17	119.99	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

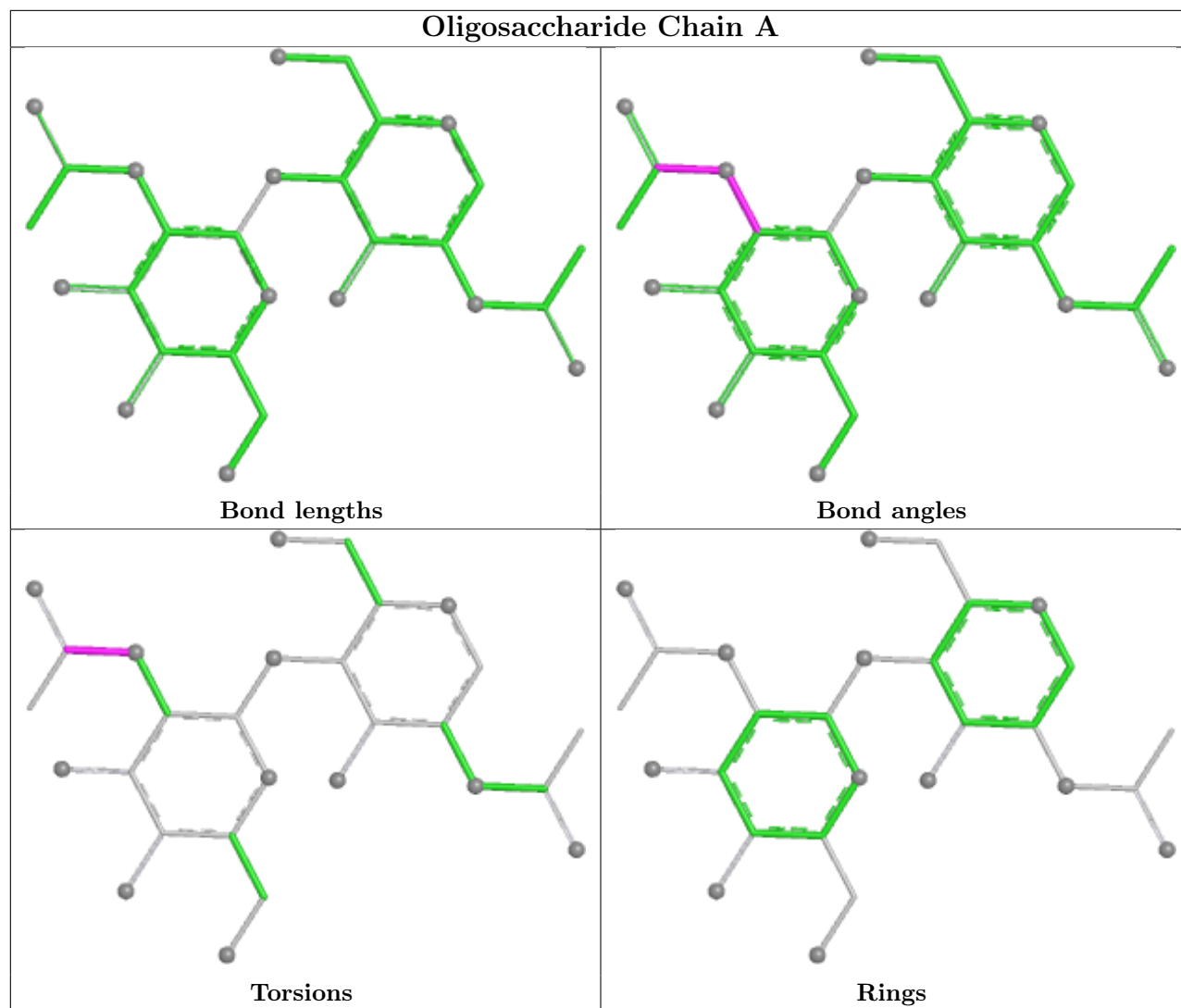
Mol	Chain	Res	Type	Atoms
2	A	2	NAG	C8-C7-N2-C2
2	A	2	NAG	O7-C7-N2-C2
4	C	6	MAN	O5-C5-C6-O6
4	C	6	MAN	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6

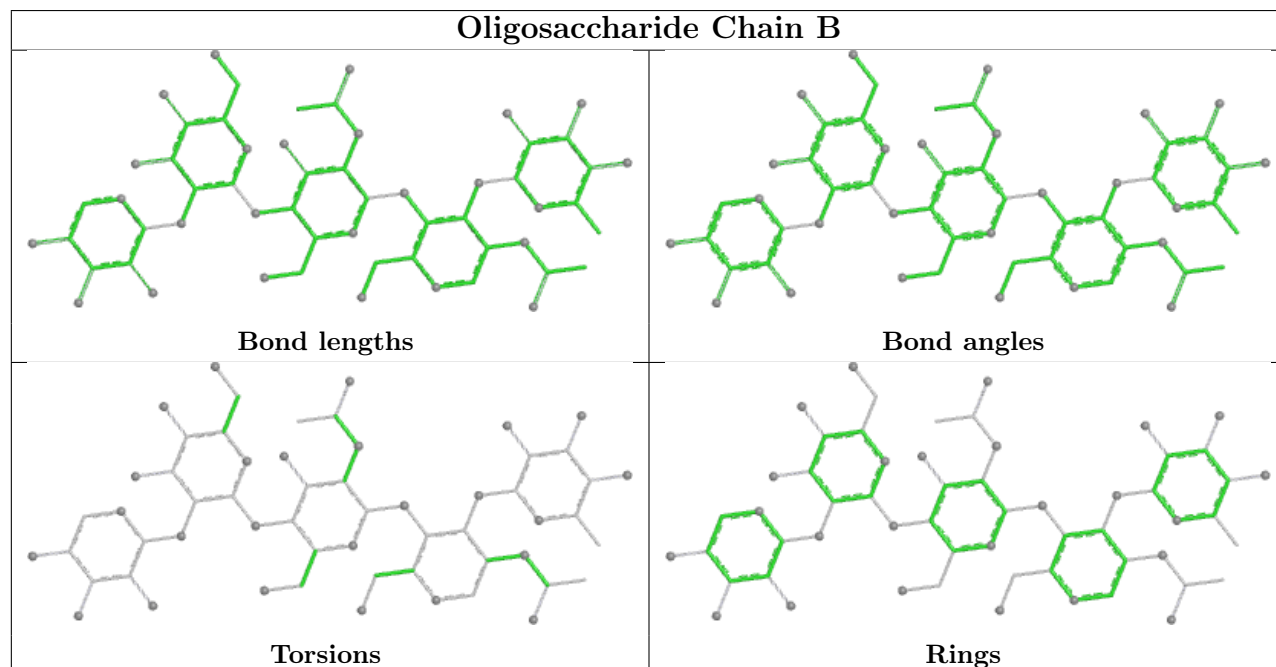
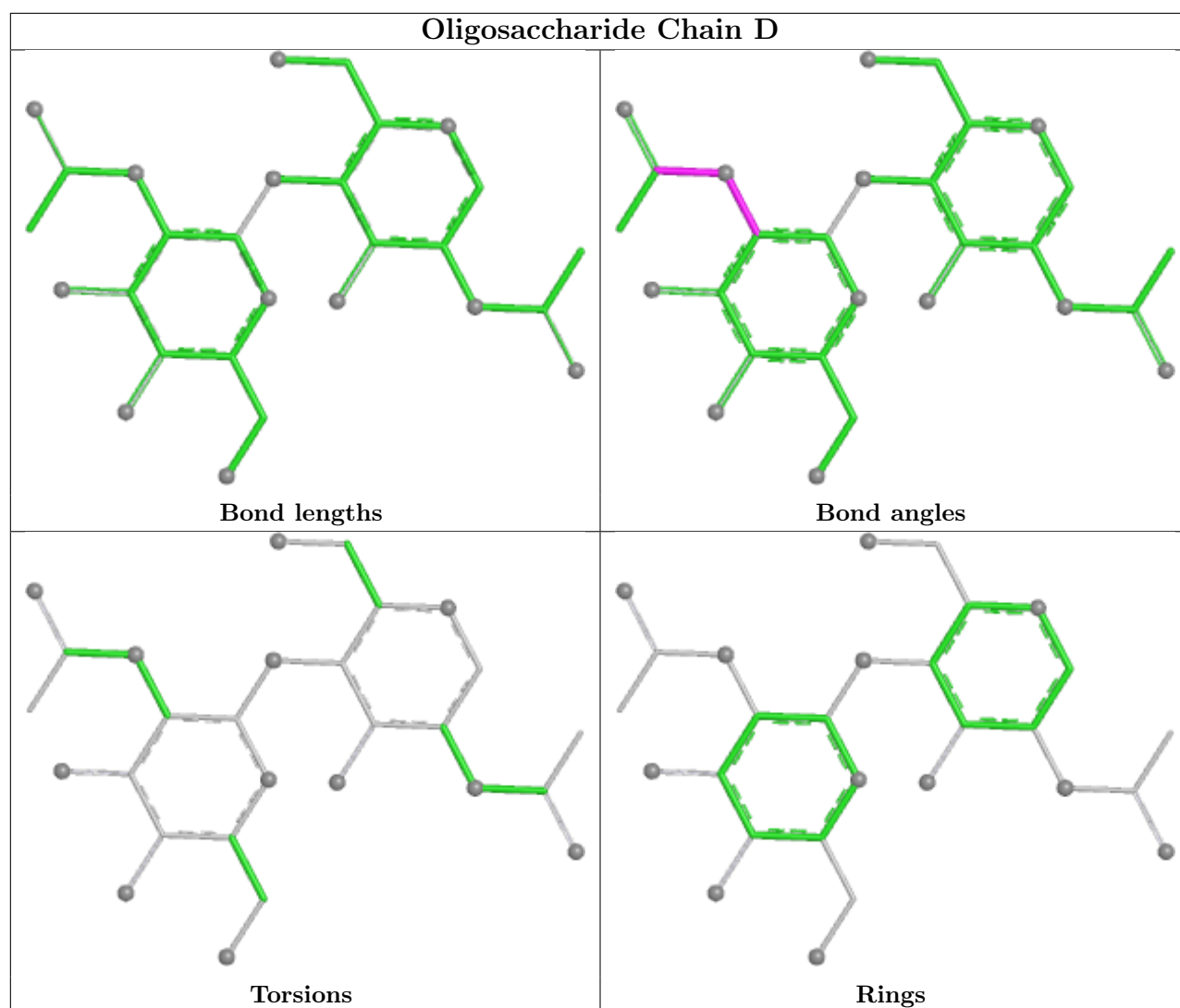
There are no ring outliers.

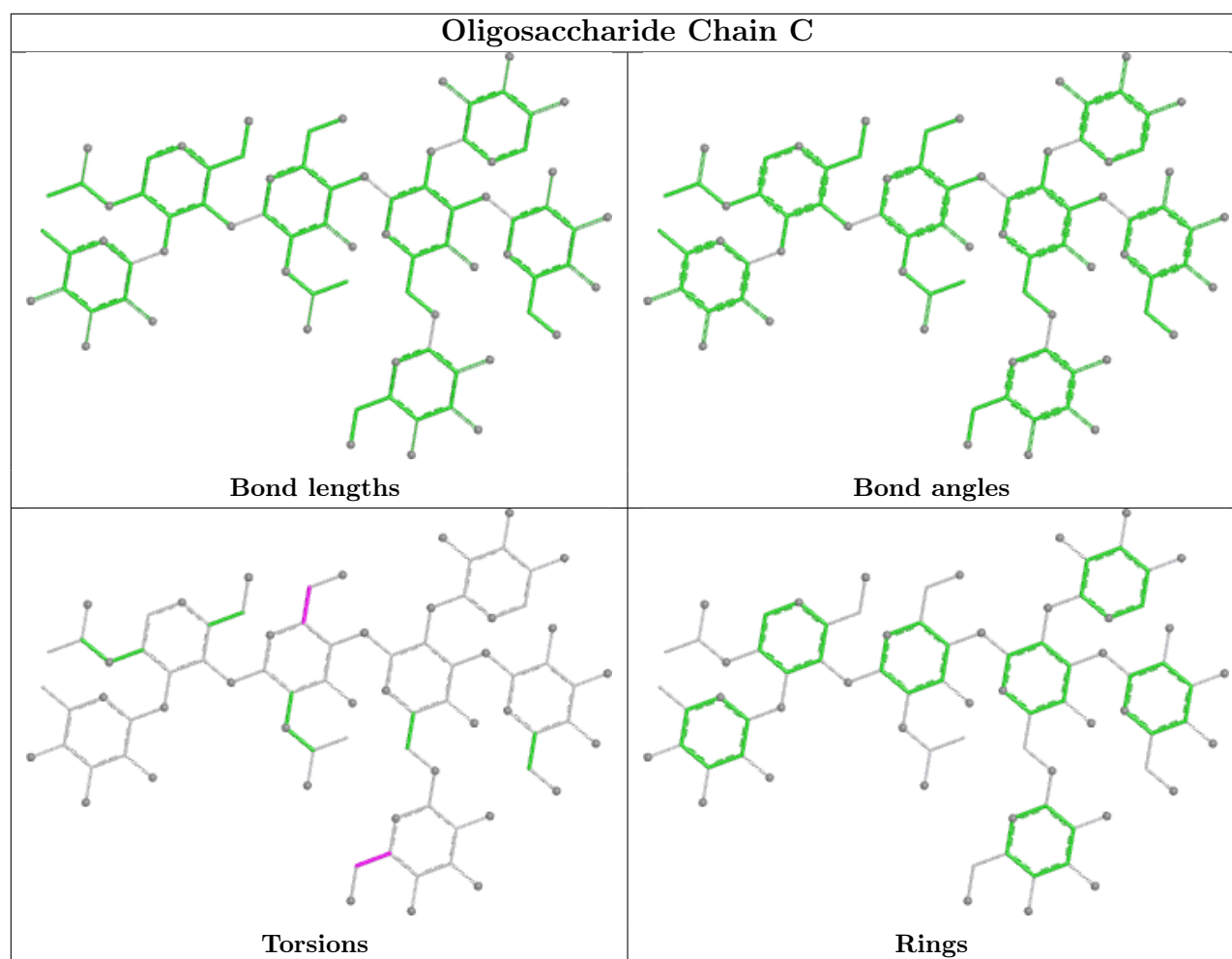
2 monomers are involved in 2 short contacts:

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

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







5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	SO4	M	1505	-	4,4,4	0.36	0	6,6,6	0.08	0
8	SO4	M	1504	-	4,4,4	0.38	0	6,6,6	0.08	0
8	SO4	M	1506	-	4,4,4	0.37	0	6,6,6	0.07	0
5	NAG	M	971	1	14,14,15	0.41	0	17,19,21	0.69	1 (5%)
5	NAG	M	991	1	14,14,15	0.42	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	961	-	15,15,15	0.30	0	21,21,21	0.58	0
5	NAG	M	911	1	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
8	SO4	M	1503	-	4,4,4	0.36	0	6,6,6	0.07	0
9	GOL	M	1512	-	5,5,5	1.07	0	5,5,5	1.05	0
5	NAG	M	931	1	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
5	NAG	M	901	1	14,14,15	0.42	0	17,19,21	0.68	0
9	GOL	M	1514	6	5,5,5	0.64	0	5,5,5	1.20	1 (20%)
9	GOL	M	1513	-	5,5,5	2.68	2 (40%)	5,5,5	1.84	2 (40%)
6	SEH	M	999	9	14,17,17	0.54	0	16,22,22	0.73	0

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
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1
5	NAG	M	991	1	-	2/6/23/26	0/1/1/1
5	NAG	M	961	-	-	2/6/26/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
9	GOL	M	1512	-	-	0/4/4/4	-
5	NAG	M	931	1	-	2/6/23/26	0/1/1/1
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
9	GOL	M	1514	6	-	0/4/4/4	-
9	GOL	M	1513	-	-	3/4/4/4	-
6	SEH	M	999	9	-	2/6/13/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1513	GOL	O1-C1	4.03	1.59	1.42
9	M	1513	GOL	C1-C2	3.78	1.66	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1513	GOL	O2-C2-C1	3.10	122.00	109.18
9	M	1513	GOL	O3-C3-C2	2.48	121.54	110.38
9	M	1514	GOL	C3-C2-C1	-2.45	102.80	111.80
5	M	931	NAG	C2-N2-C7	-2.18	119.98	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	971	NAG	C2-N2-C7	-2.08	120.11	122.90
5	M	911	NAG	C2-N2-C7	-2.07	120.13	122.90
5	M	991	NAG	C2-N2-C7	-2.05	120.15	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
5	M	961	NAG	C8-C7-N2-C2
5	M	961	NAG	O7-C7-N2-C2
5	M	971	NAG	C8-C7-N2-C2
5	M	971	NAG	O7-C7-N2-C2
5	M	991	NAG	C8-C7-N2-C2
5	M	991	NAG	O7-C7-N2-C2
9	M	1513	GOL	O1-C1-C2-C3
9	M	1513	GOL	C1-C2-C3-O3
9	M	1513	GOL	O1-C1-C2-O2
6	M	999	SEH	CB-C13-S1-C1
6	M	999	SEH	C2-C1-S1-C13

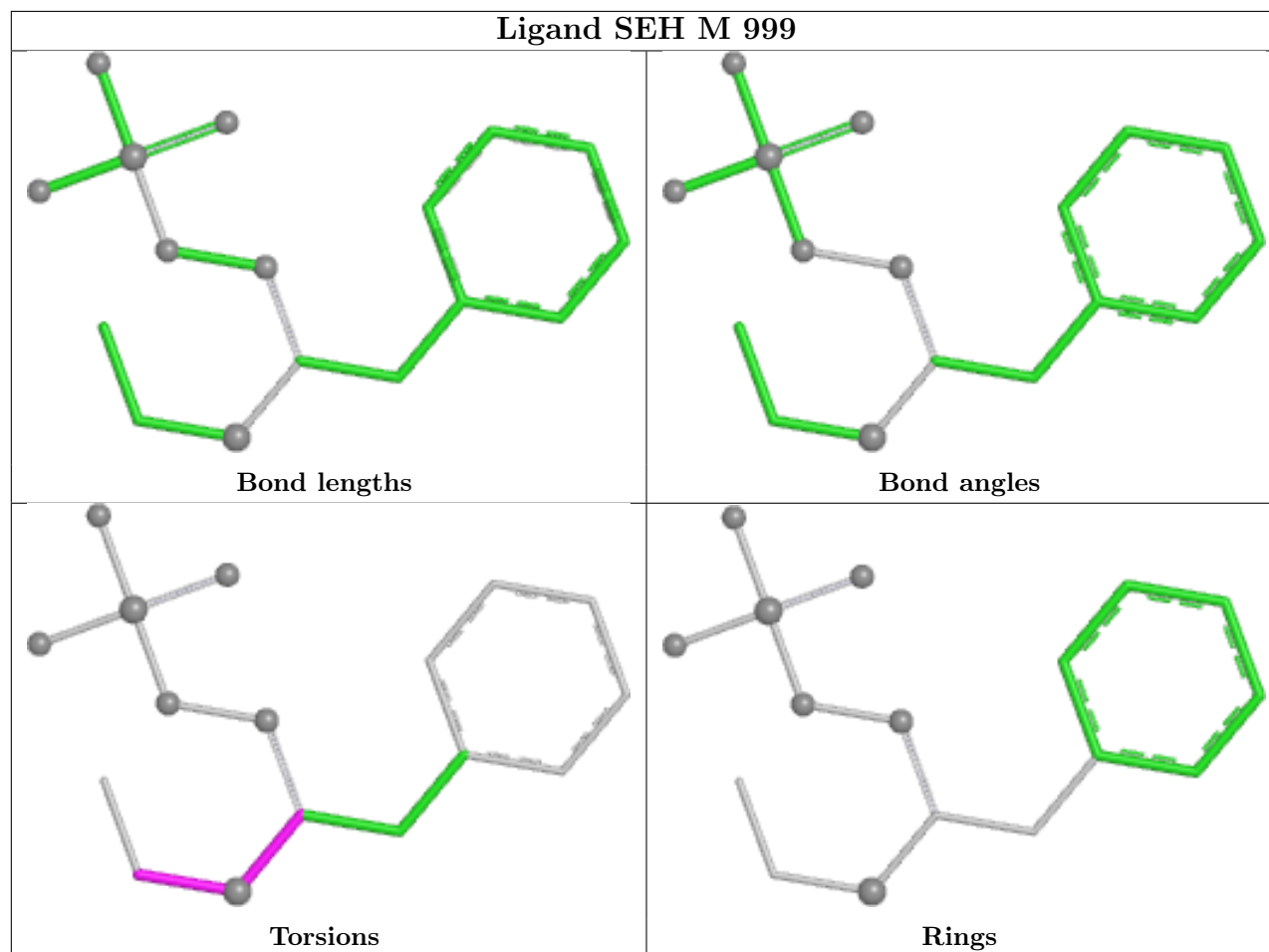
There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	971	NAG	1	0
5	M	991	NAG	1	0
5	M	961	NAG	1	0
5	M	931	NAG	4	0
9	M	1514	GOL	15	0
6	M	999	SEH	18	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	499/501 (99%)	0.01	39 (7%) 19 19	6, 11, 28, 56	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	8.7
1	M	458	ALA	7.4
1	M	417	ASP	5.6
1	M	375	LYS	5.4
1	M	378	SER	5.2
1	M	483	VAL	5.1
1	M	374	ASP	4.5
1	M	486	ARG	4.2
1	M	380	ASP	4.2
1	M	416	GLY	4.0
1	M	3	GLU	3.9
1	M	482	ASN	3.8
1	M	377	ASP	3.8
1	M	27	SER	3.5
1	M	305	GLU	3.4
1	M	379	THR	3.4
1	M	373	LYS	3.4
1	M	485	ASP	3.4
1	M	484	THR	3.4
1	M	478	ILE	3.4
1	M	421	ASN	3.3
1	M	18	ASP	3.2
1	M	4	ILE	3.2
1	M	480	TRP	3.0
1	M	420	ARG	3.0
1	M	343	ASN	2.8
1	M	346	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	481	ASN	2.8
1	M	60	ASN	2.6
1	M	477	TYR	2.6
1	M	115	GLU	2.5
1	M	76	PHE	2.5
1	M	418	GLU	2.4
1	M	419	ASN	2.4
1	M	28	ASP	2.4
1	M	344	SER	2.3
1	M	479	ASP	2.3
1	M	457	TRP	2.1
1	M	177	ASP	2.0

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

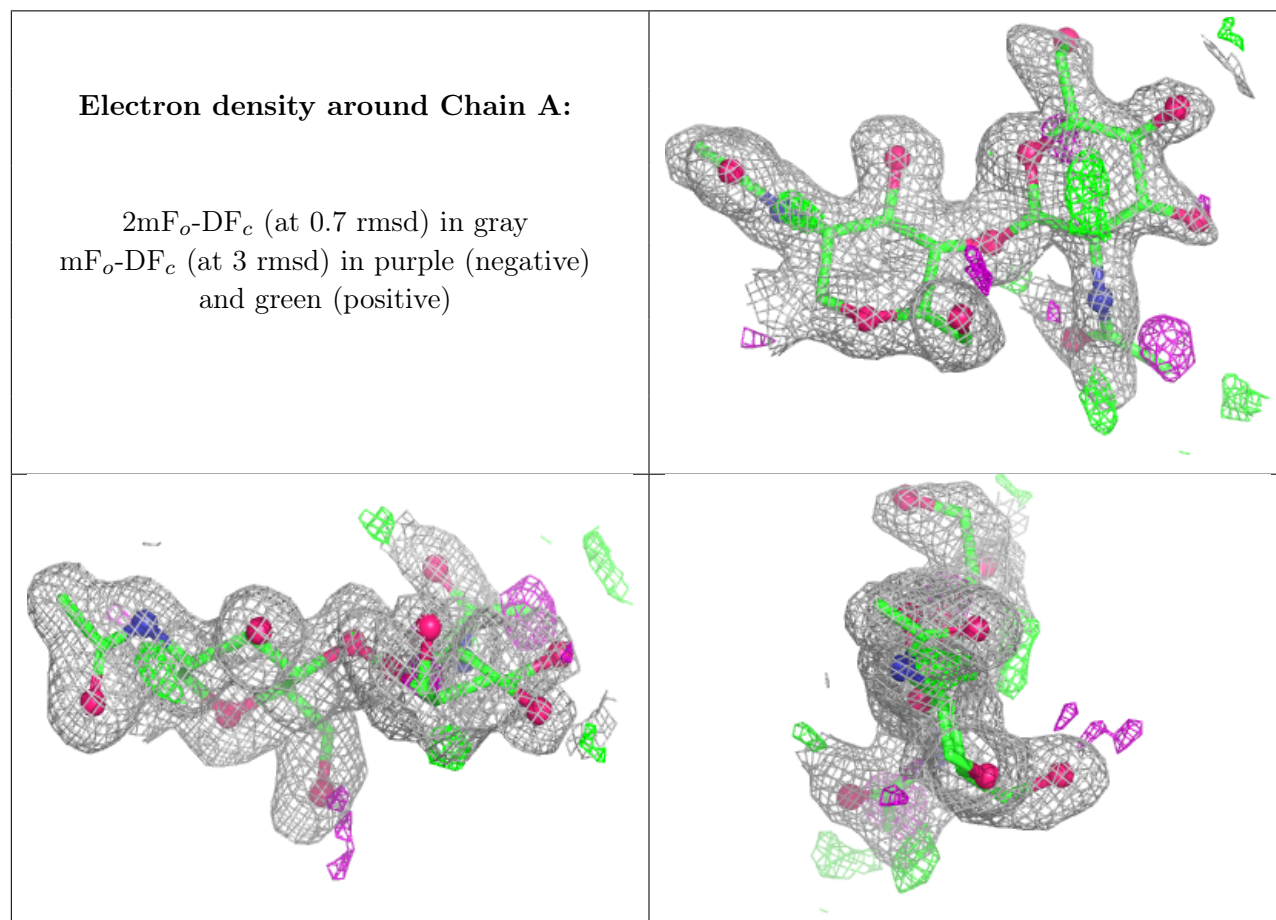
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

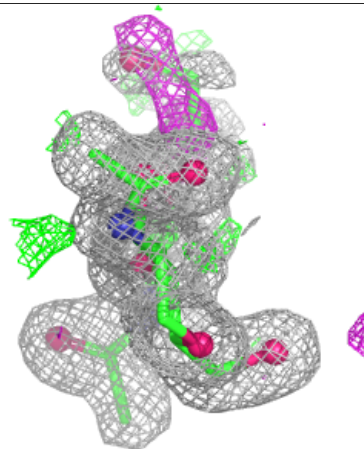
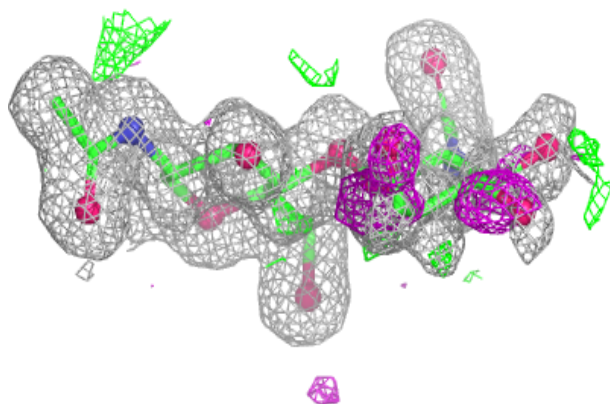
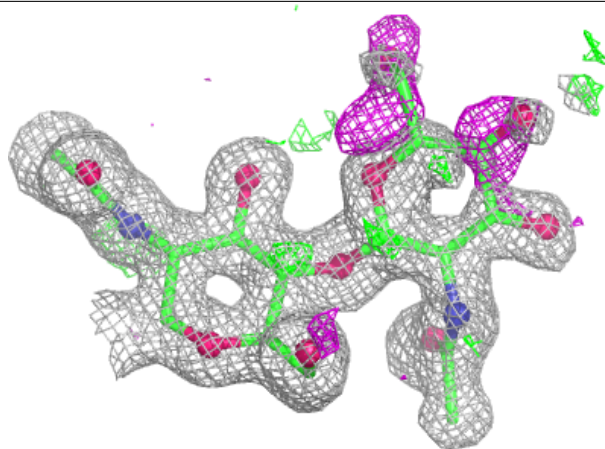
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	17,22,27,30	0
2	NAG	A	2	14/15	-	-	37,40,42,43	0
4	BMA	C	3	11/12	0.59	0.19	43,46,48,51	0
4	XYP	C	4	9/10	0.61	0.19	48,49,52,52	0
3	NAG	B	2	14/15	0.65	0.20	28,32,39,40	0
4	NAG	C	2	14/15	0.86	0.14	23,30,33,36	0
3	BMA	B	3	11/12	-	-	45,48,49,50	0
3	XYP	B	4	9/10	-	-	51,52,53,53	0
3	FUC	B	5	10/11	-	-	29,33,36,38	0
2	NAG	D	2	14/15	0.89	0.14	22,27,34,35	0
4	NAG	C	1	14/15	0.92	0.09	19,22,25,26	0
3	NAG	B	1	14/15	0.93	0.10	16,19,23,26	0
2	NAG	D	1	14/15	0.93	0.10	10,14,15,18	0
4	MAN	C	5	11/12	-	-	43,49,49,49	0
4	MAN	C	6	11/12	-	-	53,55,56,56	0
4	FUC	C	7	10/11	-	-	25,26,30,31	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.



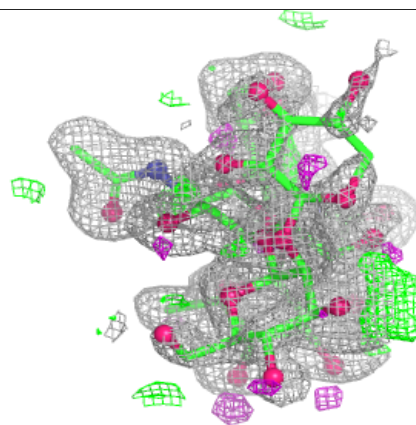
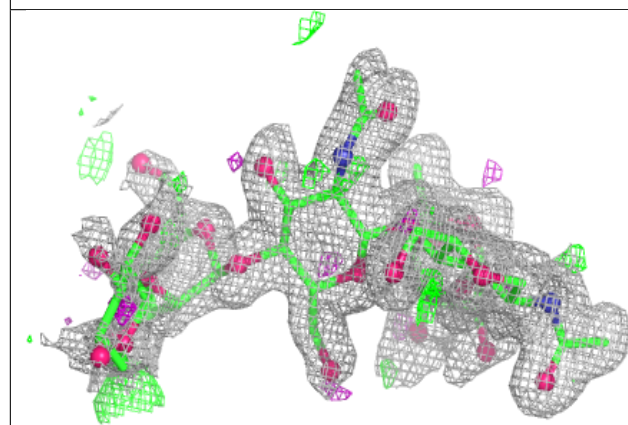
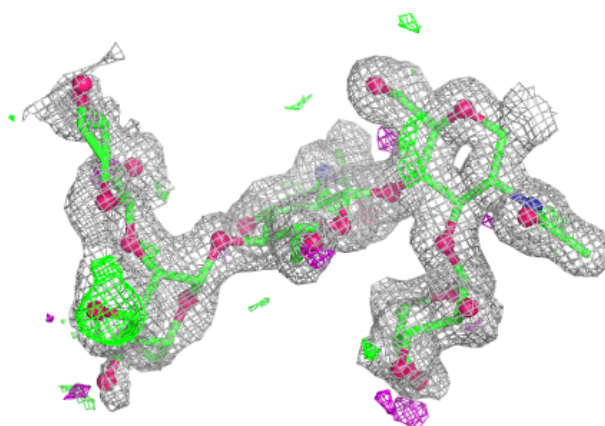
Electron density around Chain D:

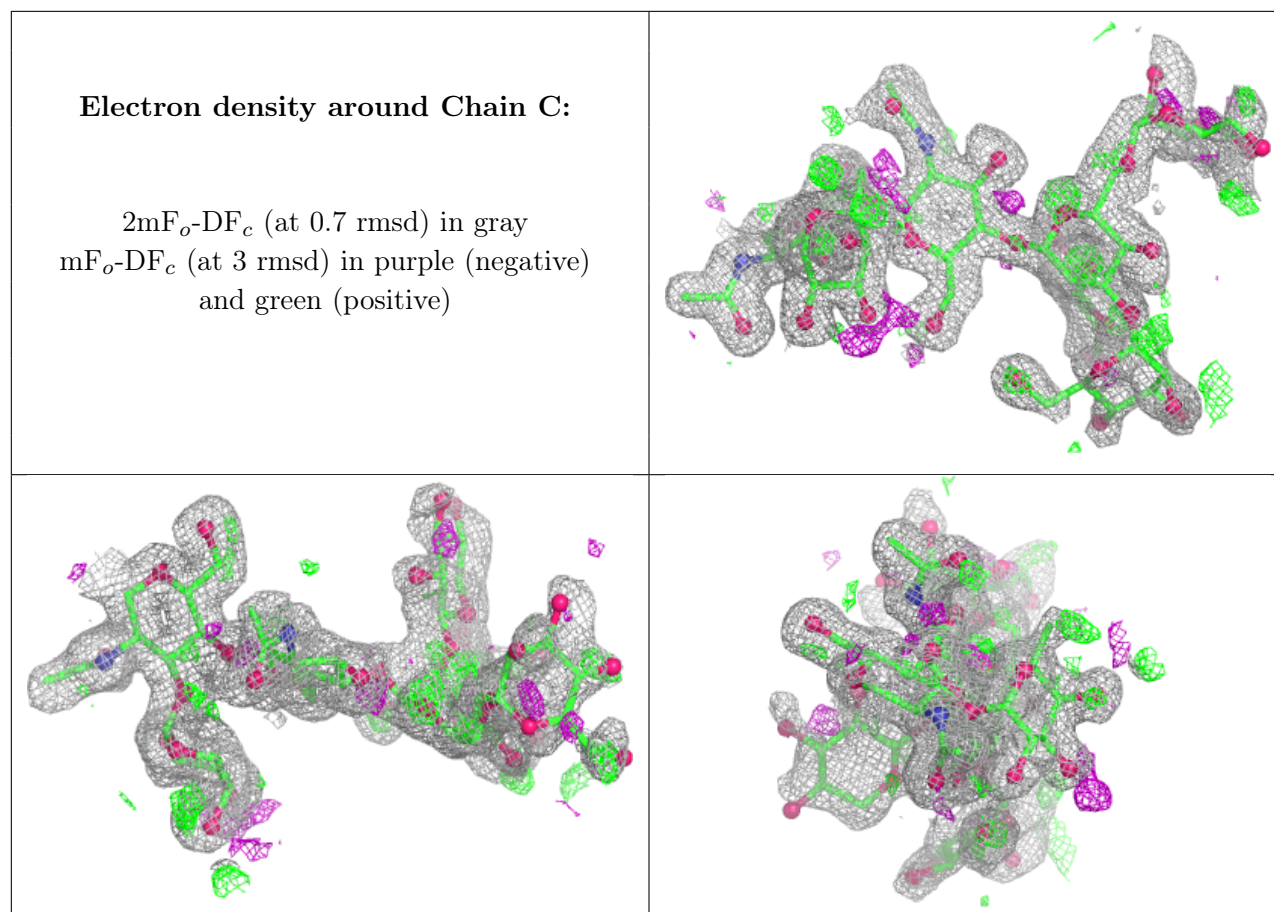
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain B:

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





6.4 Ligands [i](#)

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

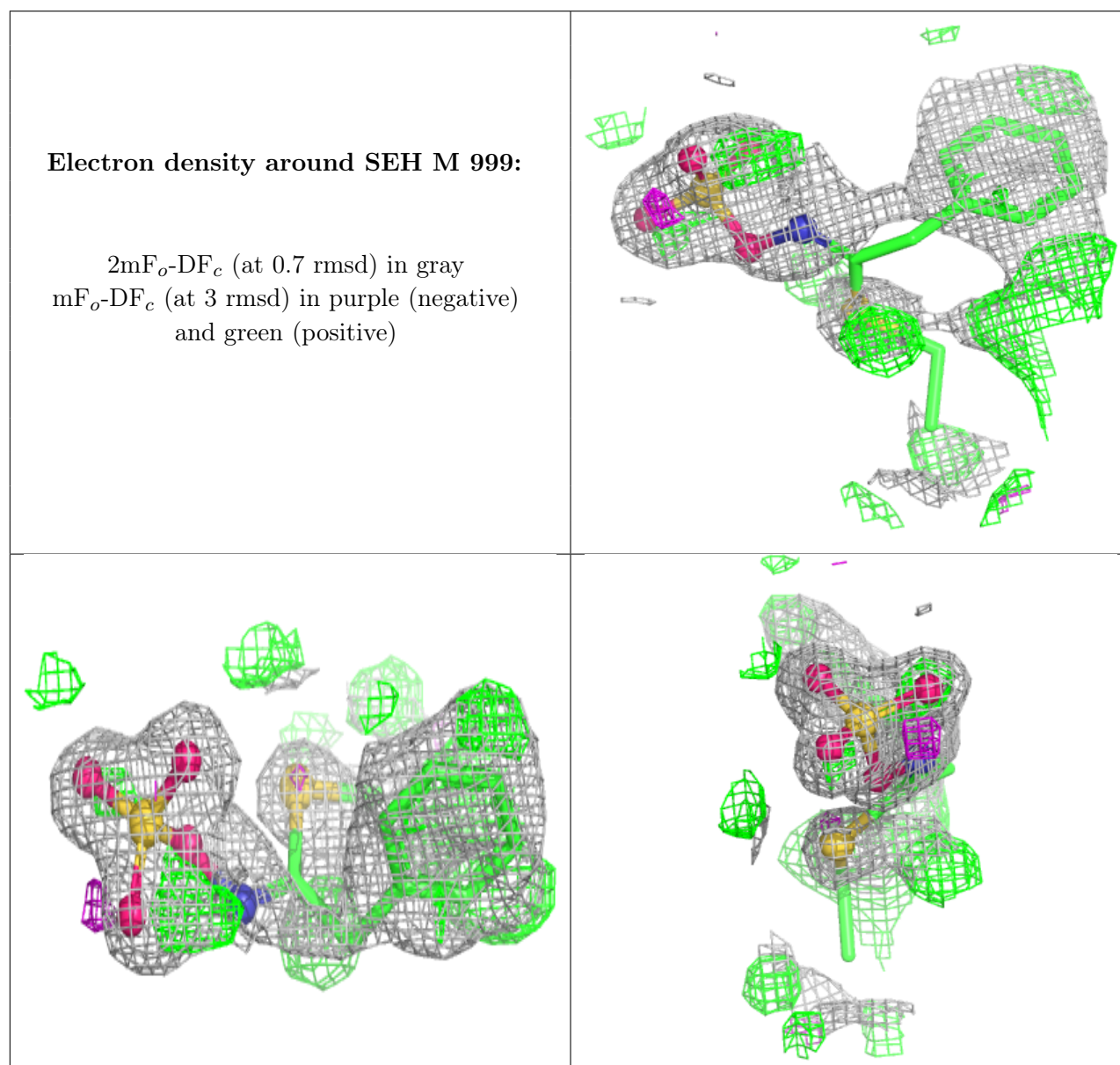
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	M	961	15/15	0.35	0.30	82,82,83,83	0
5	NAG	M	971	14/15	0.46	0.21	50,55,56,57	0
5	NAG	M	991	14/15	0.59	0.22	55,57,59,60	0
8	SO4	M	1505	5/5	0.62	0.20	66,66,67,67	0
5	NAG	M	931	14/15	0.63	0.21	38,42,44,46	0
5	NAG	M	901	14/15	0.76	0.17	29,33,38,39	0
8	SO4	M	1504	5/5	0.78	0.17	40,43,44,44	0
6	SEH	M	999	17/17	0.81	0.24	24,27,35,36	17
9	GOL	M	1514	6/6	0.85	0.14	9,12,14,15	0
9	GOL	M	1513	6/6	0.87	0.20	20,30,33,40	0
5	NAG	M	911	14/15	0.89	0.11	22,27,30,32	0
9	GOL	M	1512	6/6	0.91	0.17	18,25,30,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	M	1503	5/5	0.94	0.10	33,36,37,39	0
8	SO4	M	1506	5/5	0.97	0.06	20,21,23,25	0
7	ZN	M	1502	1/1	0.99	0.02	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.