WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 11:42 pm GMT

PDB ID	:	1E6Z
Title	:	CHITINASE B FROM SERRATIA MARCESCENS WILDTYPE IN COMPLEX WITH CATALYTIC INTERMEDIATE
Authors	:	Komander, D.; Synstad, B.; Eijsink, V.G.H.; Van Aalten, D.M.F.
Deposited on	:	2000-08-23
Resolution	:	1.99 Å(reported)

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
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 ⓘ

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

The reported resolution of this entry is 1.99 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		2.9%
RSRZ outliers		3.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
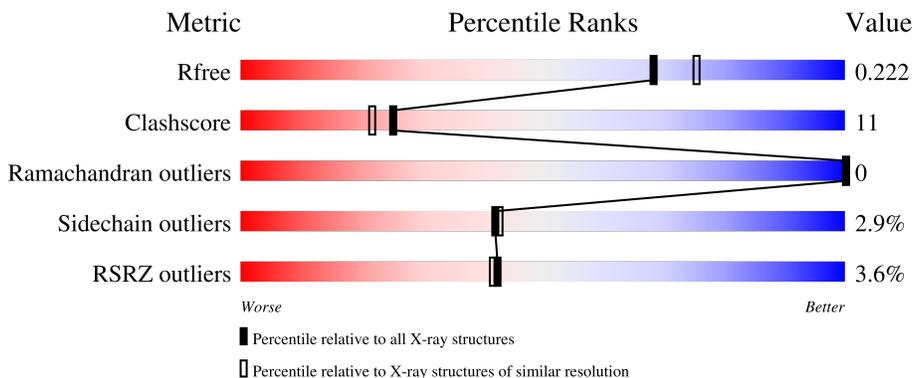
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	498	6% 87% 12% •
1	B	498	% 88% 11% •
2	C	2	50% 50%

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
4	NGO	A	502	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8889 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	6	4	1
			3924	2508	663	739	14			
1	B	498	Total	C	N	O	S	0	8	0
			3940	2517	666	743	14			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is 2-METHYL-4,5-DIHYDRO-(1,2-DIDEOXY-ALPHA-D-GLUCOPYRANOSO)[2,1-D]-1,3-OXAZOLE (three-letter code: NGO) (formula: $C_8H_{14}NO_5$).
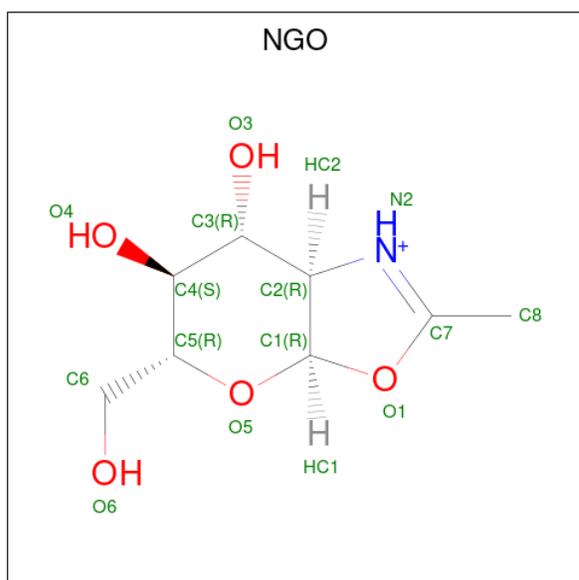
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
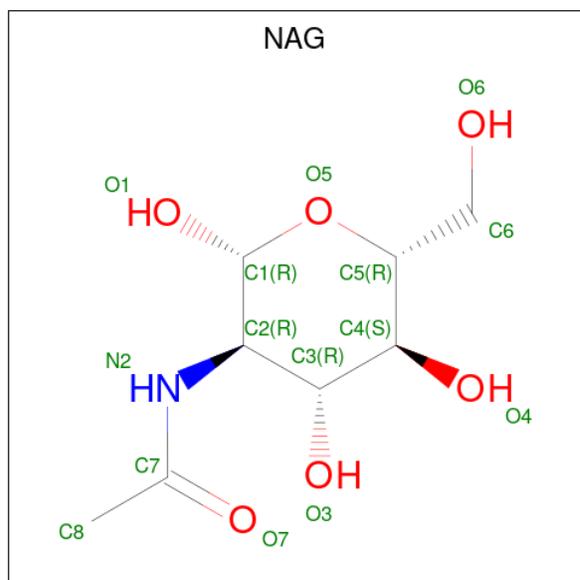
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	474	Total 474	O 474	0	0
6	B	459	Total 459	O 459	0	0

3 Residue-property plots ⓘ

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: CHITINASE B

Chain A:
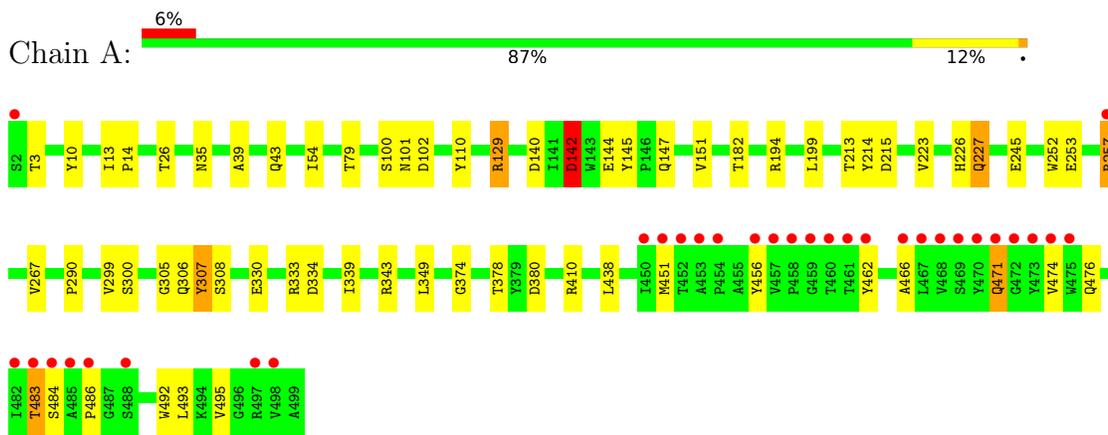
- Molecule 1: CHITINASE B

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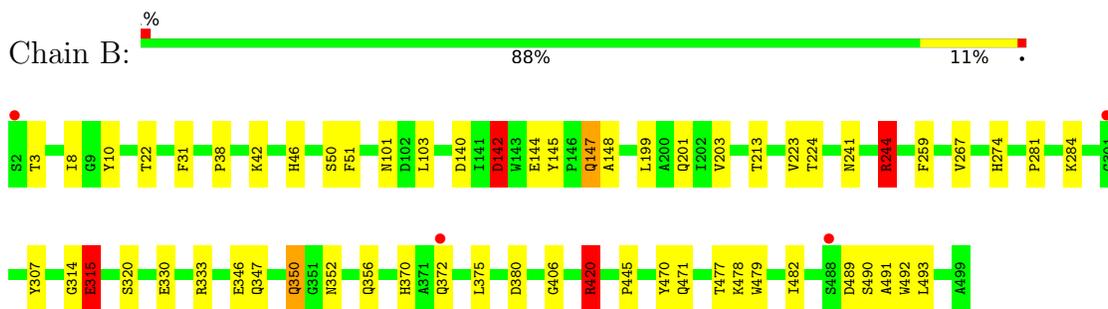
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.80Å 103.81Å 186.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 1.99 47.87 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.87-1.99) 92.9 (47.87-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.225 0.182 , 0.222	Depositor DCC
R_{free} test set	1444 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8889	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NGO, 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	A	2.25	6/4053 (0.1%)	2.56	13/5525 (0.2%)
1	B	10.71	18/4090 (0.4%)	6.23	26/5572 (0.5%)
All	All	7.75	24/8143 (0.3%)	4.77	39/11097 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	2
1	B	0	8
All	All	2	10

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244[A]	ARG	CZ-NH2	267.21	4.80	1.33
1	B	244[B]	ARG	CZ-NH2	267.21	4.80	1.33
1	B	420[A]	ARG	CZ-NH1	246.62	4.53	1.33
1	B	420[B]	ARG	CZ-NH1	246.62	4.53	1.33
1	B	315[A]	GLU	CD-OE1	199.86	3.45	1.25
1	B	315[B]	GLU	CD-OE1	199.86	3.45	1.25
1	B	244[A]	ARG	NE-CZ	165.16	3.47	1.33
1	B	244[B]	ARG	NE-CZ	165.16	3.47	1.33
1	B	315[A]	GLU	CD-OE2	135.94	2.75	1.25
1	B	315[B]	GLU	CD-OE2	135.94	2.75	1.25
1	B	244[A]	ARG	CZ-NH1	109.42	2.75	1.33
1	B	244[B]	ARG	CZ-NH1	109.42	2.75	1.33
1	A	142[A]	ASP	CG-OD1	69.86	2.86	1.25
1	A	142[B]	ASP	CG-OD1	69.86	2.86	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142[A]	ASP	CG-OD2	61.62	2.67	1.25
1	B	142[B]	ASP	CG-OD2	61.62	2.67	1.25
1	A	142[A]	ASP	CG-OD2	54.77	2.51	1.25
1	A	142[B]	ASP	CG-OD2	54.77	2.51	1.25
1	A	129[A]	ARG	CZ-NH2	42.88	1.88	1.33
1	A	129[B]	ARG	CZ-NH2	42.88	1.88	1.33
1	B	420[A]	ARG	CG-CD	8.11	1.72	1.51
1	B	420[B]	ARG	CG-CD	8.11	1.72	1.51
1	B	42[A]	LYS	CE-NZ	6.84	1.66	1.49
1	B	42[B]	LYS	CE-NZ	6.84	1.66	1.49

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244[A]	ARG	NE-CZ-NH2	-187.15	26.73	120.30
1	B	244[B]	ARG	NE-CZ-NH2	-187.15	26.73	120.30
1	B	244[A]	ARG	NE-CZ-NH1	-157.37	41.62	120.30
1	B	244[B]	ARG	NE-CZ-NH1	-157.37	41.62	120.30
1	B	420[A]	ARG	NE-CZ-NH1	-138.44	51.08	120.30
1	B	420[B]	ARG	NE-CZ-NH1	-138.44	51.08	120.30
1	B	244[A]	ARG	NH1-CZ-NH2	-94.40	15.56	119.40
1	B	244[B]	ARG	NH1-CZ-NH2	-94.40	15.56	119.40
1	B	315[A]	GLU	OE1-CD-OE2	-70.08	39.20	123.30
1	B	315[B]	GLU	OE1-CD-OE2	-70.08	39.20	123.30
1	A	142[A]	ASP	CB-CG-OD1	-68.12	56.99	118.30
1	A	142[B]	ASP	CB-CG-OD1	-68.12	56.99	118.30
1	A	129[A]	ARG	NE-CZ-NH2	-67.27	86.67	120.30
1	A	129[B]	ARG	NE-CZ-NH2	-67.27	86.67	120.30
1	B	142[A]	ASP	CB-CG-OD2	-65.65	59.22	118.30
1	B	142[B]	ASP	CB-CG-OD2	-65.65	59.22	118.30
1	B	244[A]	ARG	CD-NE-CZ	-57.39	43.25	123.60
1	B	244[B]	ARG	CD-NE-CZ	-57.39	43.25	123.60
1	A	142[A]	ASP	CB-CG-OD2	-55.56	68.29	118.30
1	A	142[B]	ASP	CB-CG-OD2	-55.56	68.29	118.30
1	B	203[A]	VAL	CG1-CB-CG2	-55.44	22.20	110.90
1	B	203[B]	VAL	CG1-CB-CG2	-55.44	22.20	110.90
1	A	79[A]	THR	OG1-CB-CG2	-44.06	8.65	110.00
1	A	79[B]	THR	OG1-CB-CG2	-44.06	8.65	110.00
1	B	315[A]	GLU	CG-CD-OE1	-42.61	33.09	118.30
1	B	315[B]	GLU	CG-CD-OE1	-42.61	33.09	118.30
1	A	142[A]	ASP	OD1-CG-OD2	-39.84	47.60	123.30
1	A	142[B]	ASP	OD1-CG-OD2	-39.84	47.60	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129[A]	ARG	NH1-CZ-NH2	30.20	152.62	119.40
1	A	129[B]	ARG	NH1-CZ-NH2	30.20	152.62	119.40
1	B	315[A]	GLU	CG-CD-OE2	-28.92	60.47	118.30
1	B	315[B]	GLU	CG-CD-OE2	-28.92	60.47	118.30
1	B	420[A]	ARG	NH1-CZ-NH2	18.70	139.97	119.40
1	B	420[B]	ARG	NH1-CZ-NH2	18.70	139.97	119.40
1	B	142[A]	ASP	OD1-CG-OD2	17.35	156.26	123.30
1	B	142[B]	ASP	OD1-CG-OD2	17.35	156.26	123.30
1	A	100	SER	N-CA-C	5.36	125.46	111.00
1	B	420[A]	ARG	CG-CD-NE	-5.10	101.10	111.80
1	B	420[B]	ARG	CG-CD-NE	-5.10	101.10	111.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	79[A]	THR	CB
1	A	79[B]	THR	CB

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142[A]	ASP	Sidechain
1	A	142[B]	ASP	Sidechain
1	B	142[A]	ASP	Sidechain
1	B	142[B]	ASP	Sidechain
1	B	244[A]	ARG	Sidechain
1	B	244[B]	ARG	Sidechain
1	B	315[A]	GLU	Sidechain
1	B	315[B]	GLU	Sidechain
1	B	420[A]	ARG	Sidechain
1	B	420[B]	ARG	Sidechain

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	3924	0	3754	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3940	0	3763	87	0
2	C	29	0	27	4	0
3	A	5	0	0	0	0
3	B	15	0	0	0	0
4	A	14	0	14	12	0
4	B	14	0	14	5	0
5	B	15	0	15	0	0
6	A	474	0	0	8	0
6	B	459	0	0	6	0
All	All	8889	0	7587	166	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 11.

All (166) 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:B:315[B]:GLU:CD	1:B:315[B]:GLU:CG	1.90	1.39
1:A:129[B]:ARG:CZ	1:A:129[B]:ARG:NH2	1.83	1.38
1:A:129[A]:ARG:NH2	1:A:129[A]:ARG:CZ	1.88	1.35
1:B:315[B]:GLU:OE2	1:B:315[B]:GLU:HG3	1.44	1.14
4:A:502:NGO:HC4	6:A:650:HOH:O	1.46	1.13
1:A:142[B]:ASP:HB3	1:A:142[B]:ASP:OD1	1.51	1.10
1:B:315[A]:GLU:OE2	1:B:315[A]:GLU:HG2	1.54	1.06
1:A:10:TYR:CZ	4:A:502:NGO:HC81	1.91	1.05
1:A:142[B]:ASP:OD2	1:A:142[B]:ASP:CG	1.98	1.02
1:B:244[A]:ARG:NH2	1:B:244[A]:ARG:HH11	1.56	1.01
1:B:244[B]:ARG:HH11	1:B:244[B]:ARG:NE	1.57	1.00
1:B:142[A]:ASP:OD2	1:B:142[A]:ASP:HB3	1.64	0.98
1:B:142[B]:ASP:OD2	1:B:142[B]:ASP:HB2	1.64	0.97
1:B:315[A]:GLU:HG2	1:B:315[A]:GLU:OE1	1.65	0.96
1:B:244[B]:ARG:HH11	1:B:244[B]:ARG:NH2	1.65	0.93
1:A:483:THR:HG21	1:B:103:LEU:HD11	1.50	0.93
1:A:142[A]:ASP:OD2	1:A:142[A]:ASP:HB2	1.69	0.92
1:B:244[A]:ARG:HH11	1:B:244[A]:ARG:NE	1.67	0.92
1:A:142[B]:ASP:OD2	4:A:502:NGO:HC83	1.70	0.91
1:A:129[B]:ARG:NH2	1:A:129[B]:ARG:NE	2.19	0.90
1:A:142[A]:ASP:HB2	1:A:142[A]:ASP:OD1	1.73	0.89
1:A:10:TYR:CZ	4:A:502:NGO:C8	2.55	0.88
4:A:502:NGO:HC2	6:A:697:HOH:O	1.72	0.87
1:A:253:GLU:O	1:A:257:ARG:HG2	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:504:NGO:HC2	6:B:872:HOH:O	1.75	0.86
1:A:129[A]:ARG:NH2	1:A:129[A]:ARG:NE	2.24	0.85
6:A:997:HOH:O	2:C:2:NAG:H81	1.76	0.84
1:B:244[A]:ARG:CZ	1:B:244[A]:ARG:HD2	2.08	0.82
1:B:244[A]:ARG:NH2	1:B:244[A]:ARG:NH1	2.27	0.82
1:B:244[B]:ARG:NH2	1:B:244[B]:ARG:NH1	2.29	0.81
1:B:244[B]:ARG:NE	1:B:244[B]:ARG:NH2	2.30	0.79
1:B:244[B]:ARG:NE	1:B:244[B]:ARG:NH1	2.30	0.79
1:B:350:GLN:NE2	6:B:601:HOH:O	2.16	0.79
1:B:244[A]:ARG:NH2	1:B:244[A]:ARG:NE	2.31	0.79
1:B:142[A]:ASP:OD2	1:B:142[A]:ASP:CB	2.29	0.79
1:B:142[B]:ASP:OD2	1:B:142[B]:ASP:CB	2.30	0.79
1:B:244[A]:ARG:CZ	1:B:244[A]:ARG:CD	2.61	0.78
1:B:244[A]:ARG:NE	1:B:244[A]:ARG:NH1	2.31	0.77
1:B:241:ASN:O	1:B:244[A]:ARG:HG2	1.85	0.77
1:A:142[B]:ASP:OD2	1:A:142[B]:ASP:CB	2.33	0.76
1:B:244[A]:ARG:NH2	1:B:244[A]:ARG:HE	1.84	0.75
1:A:483:THR:CG2	1:B:103:LEU:HD11	2.18	0.74
1:B:315[A]:GLU:OE1	1:B:315[A]:GLU:CG	2.37	0.72
1:B:244[B]:ARG:NH2	1:B:244[B]:ARG:HE	1.86	0.72
1:A:483:THR:HG21	1:B:103:LEU:CD1	2.21	0.71
1:A:451:MET:HB2	1:A:474:VAL:HG21	1.72	0.71
1:A:142[B]:ASP:HB3	1:A:142[B]:ASP:OD2	1.91	0.71
1:B:315[B]:GLU:CG	1:B:315[B]:GLU:OE1	2.38	0.71
1:A:142[A]:ASP:OD2	1:A:142[A]:ASP:CB	2.38	0.69
1:A:142[A]:ASP:OD1	1:A:142[A]:ASP:CB	2.40	0.69
1:A:299[B]:VAL:HG23	1:A:308:SER:HB3	1.74	0.68
1:B:315[B]:GLU:HG3	1:B:315[B]:GLU:OE1	1.94	0.67
1:B:10:TYR:CZ	4:B:504:NGO:HC82	2.30	0.67
1:B:244[B]:ARG:CZ	1:B:244[B]:ARG:HD2	2.24	0.67
1:B:315[B]:GLU:CD	1:B:315[B]:GLU:OE1	2.34	0.66
1:A:330:GLU:HG2	6:A:796:HOH:O	1.96	0.65
1:B:315[A]:GLU:OE2	1:B:315[A]:GLU:CG	2.39	0.64
1:B:199:LEU:HD21	1:B:274:HIS:CD2	2.33	0.64
1:B:244[B]:ARG:NH1	1:B:244[B]:ARG:CZ	2.61	0.63
1:A:129[B]:ARG:NH2	1:A:129[B]:ARG:HE	1.94	0.62
1:B:10:TYR:OH	4:B:504:NGO:C8	2.45	0.62
1:A:142[B]:ASP:OD1	1:A:142[B]:ASP:CB	2.37	0.62
1:B:420[A]:ARG:HD3	1:B:420[A]:ARG:NH1	2.15	0.62
2:C:2:NAG:H3	2:C:2:NAG:H83	1.82	0.62
1:A:129[A]:ARG:NH2	1:A:129[A]:ARG:HE	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142[A]:ASP:OD2	1:A:142[A]:ASP:OD1	2.19	0.61
1:B:315[A]:GLU:OE2	1:B:315[A]:GLU:OE1	2.18	0.61
1:A:10:TYR:CE1	4:A:502:NGO:HC81	2.34	0.61
1:B:315[B]:GLU:OE2	1:B:315[B]:GLU:OE1	2.19	0.61
1:B:489:ASP:OD2	1:B:491:ALA:HB3	2.01	0.60
1:B:147:GLN:HE21	1:B:148:ALA:H	1.48	0.60
1:A:299[B]:VAL:HG12	1:A:374:GLY:O	2.02	0.60
1:B:244[A]:ARG:CZ	1:B:244[A]:ARG:HD3	2.29	0.60
1:A:142[B]:ASP:OD1	1:A:142[B]:ASP:OD2	2.19	0.59
1:A:299[B]:VAL:HG23	1:A:308:SER:CB	2.31	0.59
1:A:10:TYR:OH	4:A:502:NGO:C8	2.50	0.58
1:B:10:TYR:CZ	4:B:504:NGO:C8	2.86	0.58
1:A:299[B]:VAL:HG12	1:A:374:GLY:C	2.25	0.57
1:B:489:ASP:HB3	6:B:621:HOH:O	2.04	0.57
1:B:244[B]:ARG:HE	1:B:244[B]:ARG:HH21	1.51	0.57
1:A:10:TYR:CE2	4:A:502:NGO:C8	2.87	0.56
1:A:471:GLN:O	1:A:471:GLN:HG3	2.05	0.56
1:A:226:HIS:HD2	6:A:666:HOH:O	1.89	0.56
1:B:244[B]:ARG:CZ	1:B:244[B]:ARG:CD	2.85	0.55
1:A:486:PRO:HA	1:A:492:TRP:CD1	2.42	0.55
1:A:142[B]:ASP:OD1	1:A:144:GLU:OE2	2.26	0.54
1:B:244[A]:ARG:HE	1:B:244[A]:ARG:HH21	1.56	0.54
1:A:343:ARG:HH11	1:A:410:ARG:NH1	2.07	0.53
1:B:201:GLN:HG3	6:B:933:HOH:O	2.08	0.53
1:A:101:ASN:HA	1:A:144:GLU:O	2.09	0.53
1:A:226:HIS:HE1	1:A:306:GLN:OE1	1.93	0.52
1:A:471:GLN:O	1:A:471:GLN:CG	2.59	0.51
1:A:215:ASP:H	1:A:227:GLN:NE2	2.09	0.51
1:B:10:TYR:OH	4:B:504:NGO:HC82	2.08	0.51
1:B:346:GLU:O	1:B:350:GLN:HG2	2.10	0.51
1:A:10:TYR:CE2	4:A:502:NGO:HC82	2.45	0.51
1:B:244[A]:ARG:CZ	1:B:244[A]:ARG:NH1	2.75	0.50
1:A:456:TYR:CE1	1:A:462:TYR:HE2	2.30	0.49
1:B:482:ILE:HD12	1:B:491:ALA:HB1	1.94	0.49
1:B:8:ILE:HG12	1:B:46:HIS:HB2	1.94	0.49
1:A:307:TYR:CD1	1:A:307:TYR:N	2.81	0.49
1:A:486:PRO:HG3	1:A:492:TRP:CZ2	2.48	0.49
1:A:142[A]:ASP:OD2	1:A:142[A]:ASP:CG	2.51	0.49
1:B:101:ASN:HA	1:B:144:GLU:O	2.12	0.48
1:B:478:LYS:HE3	1:B:490:SER:O	2.13	0.48
1:A:483:THR:HG23	1:A:483:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:O	1:B:307:TYR:HA	2.13	0.48
1:B:330:GLU:HG3	1:B:333:ARG:NH2	2.29	0.48
1:A:252:TRP:HB2	1:B:244[A]:ARG:HB2	1.95	0.47
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.50	0.47
1:A:257:ARG:CZ	1:A:493:LEU:HD21	2.44	0.47
1:B:223:VAL:HG12	1:B:307:TYR:HA	1.98	0.46
1:B:356:GLN:HG3	6:B:881:HOH:O	2.15	0.46
1:B:370:HIS:CE1	1:B:372:GLN:HB2	2.51	0.46
1:A:471:GLN:O	1:A:471:GLN:NE2	2.48	0.45
1:A:245:GLU:HG3	1:B:478:LYS:HD2	1.98	0.45
1:A:299[B]:VAL:HG21	1:A:305:GLY:HA2	1.98	0.45
1:A:299[B]:VAL:HG22	1:A:300:SER:N	2.32	0.45
1:A:466:ALA:O	1:A:476:GLN:HA	2.16	0.45
1:A:483:THR:CG2	1:A:483:THR:O	2.64	0.45
1:A:144:GLU:HA	1:A:145:TYR:CG	2.53	0.44
1:B:31:PHE:CG	1:B:406:GLY:HA2	2.52	0.44
1:A:227:GLN:HE21	1:A:227:GLN:HB2	1.67	0.44
1:A:215:ASP:H	1:A:227:GLN:HE21	1.64	0.44
1:B:477:THR:HG23	1:B:492:TRP:CZ3	2.53	0.44
1:A:451:MET:CB	1:A:474:VAL:HG21	2.44	0.44
1:A:102:ASP:OD2	1:A:194:ARG:NH2	2.42	0.44
1:A:147:GLN:O	1:A:151:VAL:HG23	2.18	0.43
1:B:142[B]:ASP:OD2	1:B:142[B]:ASP:CG	2.56	0.43
1:A:142[B]:ASP:OD2	4:A:502:NGO:C8	2.54	0.43
2:C:2:NAG:C1	2:C:2:NAG:H82	2.49	0.43
1:B:370:HIS:HE1	1:B:372:GLN:HB2	1.83	0.43
4:A:502:NGO:C2	6:A:697:HOH:O	2.47	0.43
2:C:2:NAG:H3	2:C:2:NAG:C8	2.47	0.43
1:B:479:TRP:CD1	1:B:482:ILE:HD11	2.54	0.42
1:B:314:GLY:N	1:B:315[A]:GLU:OE1	2.52	0.42
1:B:445:PRO:HB3	6:B:781:HOH:O	2.19	0.42
1:A:39:ALA:O	1:A:43:GLN:HG3	2.19	0.42
1:B:50:SER:HA	1:B:51:PHE:HA	1.75	0.42
1:B:478:LYS:HE2	1:B:493:LEU:HB2	2.00	0.42
1:A:330:GLU:O	1:A:333:ARG:HG2	2.20	0.42
1:B:244[B]:ARG:NH1	1:B:244[B]:ARG:CD	2.82	0.42
1:A:54:ILE:HD12	1:A:110:TYR:CD2	2.55	0.42
1:B:244[A]:ARG:NH1	1:B:244[A]:ARG:CD	2.83	0.42
1:B:281:PRO:HG2	1:B:284:LYS:HG3	2.02	0.42
1:A:10:TYR:OH	4:A:502:NGO:HC83	2.18	0.41
1:A:484:SER:HA	6:A:966:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:HB2	1:B:51:PHE:CG	2.55	0.41
1:B:140:ASP:OD2	1:B:142[A]:ASP:OD1	2.38	0.41
1:B:142[B]:ASP:OD1	1:B:144:GLU:OE2	2.39	0.41
1:B:347:GLN:HE21	1:B:347:GLN:HB3	1.64	0.41
1:B:144:GLU:HA	1:B:145:TYR:CG	2.56	0.41
1:A:333:ARG:HG3	1:A:334:ASP:N	2.34	0.41
1:A:13:ILE:HA	1:A:14:PRO:HD3	1.88	0.41
1:A:213:THR:HB	1:A:267:VAL:HG22	2.02	0.41
1:A:493:LEU:O	1:A:495:VAL:HG13	2.21	0.41
1:A:140:ASP:HA	1:A:182:THR:O	2.21	0.41
1:B:244[A]:ARG:NH2	1:B:259:PHE:O	2.54	0.41
1:B:213:THR:HB	1:B:267:VAL:HG22	2.04	0.40
1:A:129[B]:ARG:HE	1:A:129[B]:ARG:HH21	1.68	0.40
1:A:223:VAL:HG13	6:A:962:HOH:O	2.21	0.40
1:B:470:TYR:CE2	1:B:471:GLN:HG3	2.55	0.40
1:A:214:TYR:O	1:A:215:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	500/498 (100%)	486 (97%)	14 (3%)	0	100	100
1	B	504/498 (101%)	494 (98%)	10 (2%)	0	100	100
All	All	1004/996 (101%)	980 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2　Protein sidechains　ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/404 (101%)	393 (96%)	15 (4%)	34	32
1	B	411/404 (102%)	403 (98%)	8 (2%)	57	61
All	All	819/808 (101%)	796 (97%)	23 (3%)	42	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	26	THR
1	A	35	ASN
1	A	199	LEU
1	A	227	GLN
1	A	257	ARG
1	A	290	PRO
1	A	307	TYR
1	A	339	ILE
1	A	349	LEU
1	A	378	THR
1	A	380	ASP
1	A	438	LEU
1	A	471	GLN
1	A	483	THR
1	B	3	THR
1	B	22	THR
1	B	147	GLN
1	B	320	SER
1	B	350	GLN
1	B	352	ASN
1	B	375	LEU
1	B	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	112	ASN
1	A	147	GLN
1	A	226	HIS
1	A	227	GLN
1	B	57	ASN
1	B	147	GLN
1	B	167	GLN
1	B	273	GLN
1	B	347	GLN
1	B	350	GLN
1	B	352	ASN
1	B	394	GLN
1	B	431	GLN

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 ⓘ

2 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	C	1	2	15,15,15	0.60	0	21,21,21	0.76	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	1.15	2 (11%)

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	C	1	2	-	0/6/26/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	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(^{o})	Ideal(^{o})
2	C	2	NAG	C8-C7-N2	2.25	119.90	116.10
2	C	2	NAG	C4-C3-C2	-2.13	107.90	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	4	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 C

Bond lengths

Bond angles

Torsions

Rings
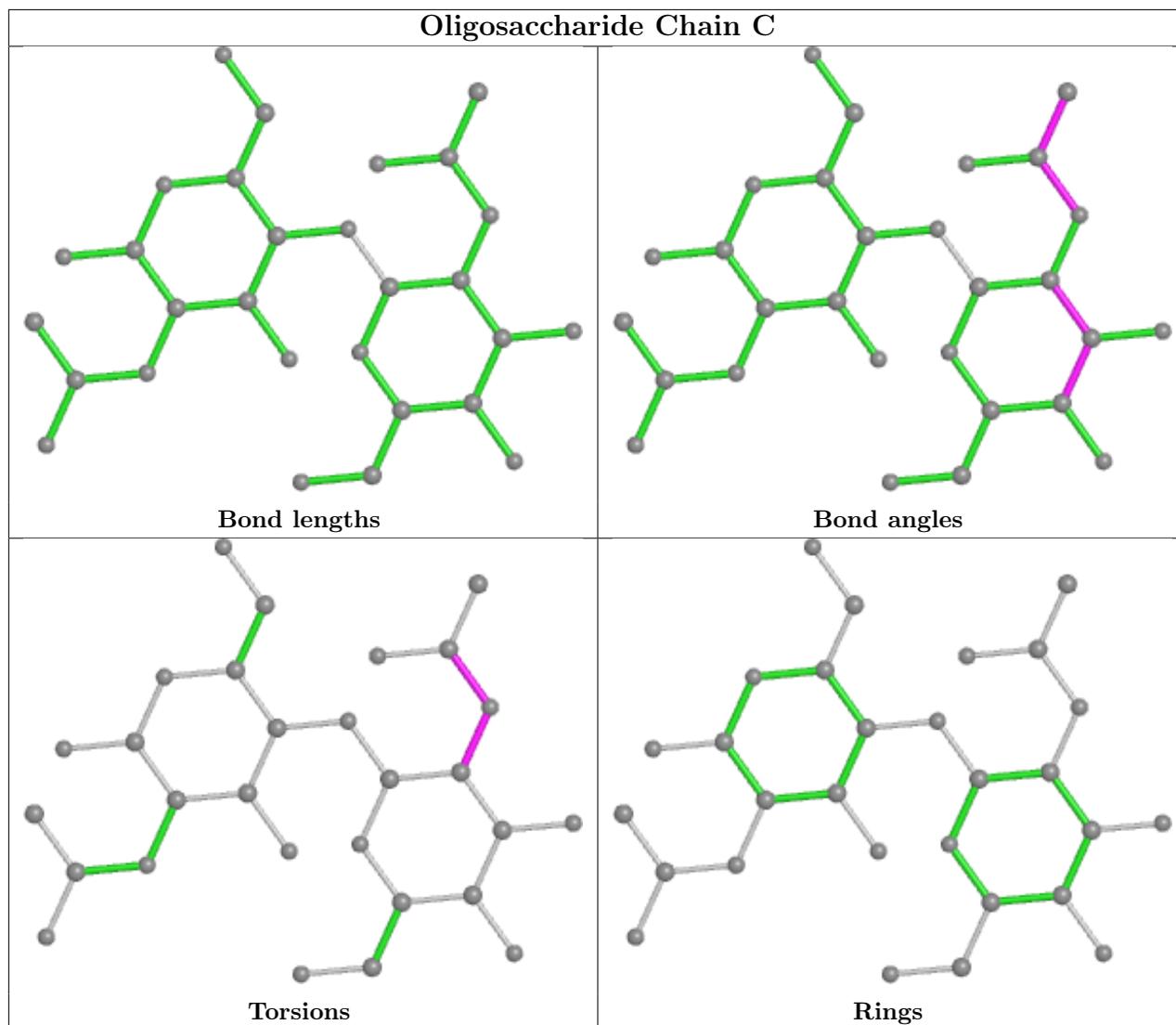
5.6 Ligand geometry ⓘ

7 ligands 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	#$|Z| > 2$
3	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	B	501	-	4,4,4	0.30	0	6,6,6	0.09	0
5	NAG	B	505	-	15,15,15	0.57	0	21,21,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NGO	A	502	-	15,15,15	3.03	3 (20%)	15,22,22	3.11	4 (26%)
4	NGO	B	504	-	15,15,15	2.24	4 (26%)	15,22,22	2.16	2 (13%)
3	SO4	A	501	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	B	503	-	4,4,4	0.28	0	6,6,6	0.08	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	B	505	-	-	3/6/26/26	0/1/1/1
4	NGO	A	502	-	-	0/2/30/30	0/2/2/2
4	NGO	B	504	-	-	2/2/30/30	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	NGO	C2-N2	-10.28	1.36	1.47
4	B	504	NGO	C2-N2	-7.06	1.39	1.47
4	A	502	NGO	C1-C2	4.07	1.60	1.52
4	B	504	NGO	C1-C2	2.72	1.58	1.52
4	B	504	NGO	O1-C1	-2.68	1.40	1.45
4	A	502	NGO	O1-C1	-2.38	1.41	1.45
4	B	504	NGO	C7-N2	2.07	1.35	1.27

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	NGO	O1-C7-C8	8.61	122.80	114.90
4	B	504	NGO	O1-C7-C8	7.39	121.68	114.90
4	A	502	NGO	C8-C7-N2	-5.74	118.43	127.04
4	A	502	NGO	O5-C1-O1	5.10	118.32	109.24
4	B	504	NGO	C8-C7-N2	-3.28	122.12	127.04
4	A	502	NGO	C1-O1-C7	-2.13	103.93	106.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	505	NAG	C1-C2-N2-C7
5	B	505	NAG	C8-C7-N2-C2
5	B	505	NAG	O7-C7-N2-C2
4	B	504	NGO	O5-C5-C6-O6
4	B	504	NGO	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	NGO	12	0
4	B	504	NGO	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	498/498 (100%)	0.04	32 (6%)	19	18	10, 19, 44, 52	2 (0%)
1	B	498/498 (100%)	-0.10	4 (0%)	86	85	11, 20, 36, 48	0
All	All	996/996 (100%)	-0.03	36 (3%)	42	42	10, 19, 40, 52	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	TYR	6.4
1	A	457	VAL	5.8
1	A	459	GLY	5.2
1	A	498	VAL	5.0
1	A	458	PRO	4.6
1	A	461	THR	4.5
1	A	460	THR	4.2
1	A	454	PRO	4.0
1	A	453	ALA	3.8
1	A	470	TYR	3.7
1	A	484	SER	3.7
1	A	452	THR	3.6
1	A	485	ALA	3.5
1	A	473	TYR	3.5
1	A	471	GLN	3.4
1	A	466	ALA	3.3
1	A	474	VAL	3.2
1	A	483	THR	2.8
1	A	469	SER	2.6
1	A	486	PRO	2.6
1	B	2	SER	2.6
1	A	462	TYR	2.5
1	A	2	SER	2.5
1	A	472	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	301	GLY	2.4
1	A	468	VAL	2.4
1	A	488	SER	2.4
1	B	488	SER	2.3
1	B	372	GLN	2.2
1	A	467	LEU	2.2
1	A	482	ILE	2.2
1	A	451	MET	2.2
1	A	475	TRP	2.1
1	A	497	ARG	2.1
1	A	257	ARG	2.0
1	A	450	ILE	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	C	2	14/15	0.94	0.11	19,23,26,31	0
2	NAG	C	1	15/15	0.95	0.10	19,22,25,29	0

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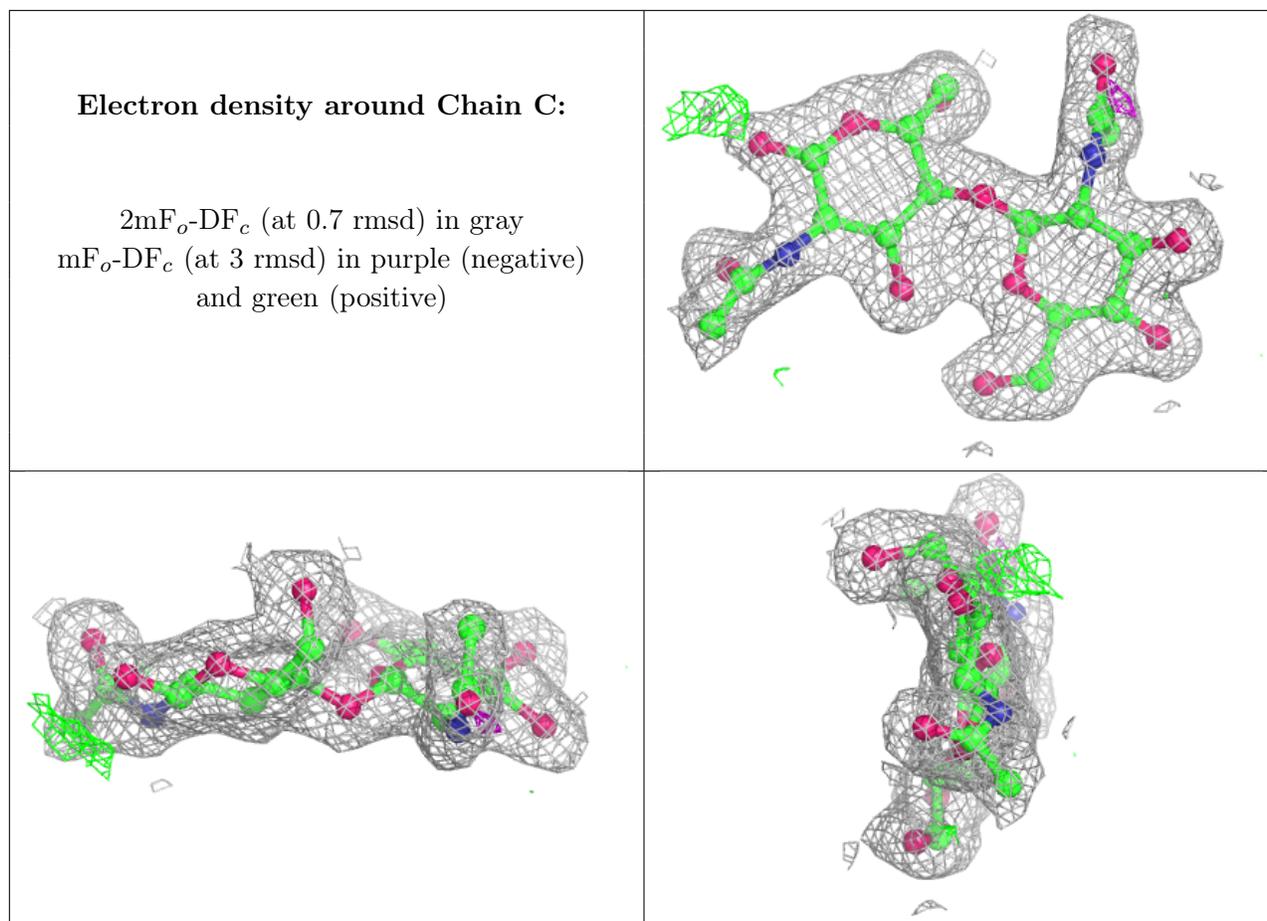
Electron density around Chain C:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NGO	A	502	14/14	0.67	0.39	21,27,30,32	14
4	NGO	B	504	14/14	0.73	0.33	23,28,32,34	14
5	NAG	B	505	15/15	0.80	0.19	47,49,54,56	0
3	SO4	B	502	5/5	0.93	0.17	57,58,59,60	0
3	SO4	B	503	5/5	0.96	0.17	51,52,53,54	0
3	SO4	B	501	5/5	0.97	0.17	50,51,52,53	0
3	SO4	A	501	5/5	0.98	0.11	37,38,41,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.