Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:18 PM JST

PDB ID	:	5XQO
Title	:	Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from Penicillium chrysogenum complexed with tetrameric substrate
Authors	:	Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on	:	2017-06-07
Resolution	:	3.20 Å(reported)

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

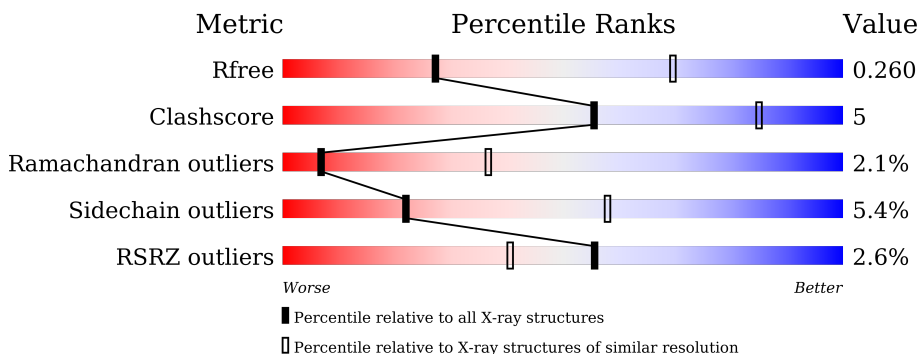|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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		0.260
Clashscore		5
Ramachandran outliers		2.1%
Sidechain outliers		5.4%
RSRZ outliers		2.6%

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	906	2% 83% 15% ••
1	B	906	3% 80% 16% • •
2	C	4	25% 75%
3	D	4	75% 25%

2 Entity composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14092 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 Pcrglx protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	Se	0	0	0
			7017	4476	1178	1357	3	3			
1	B	881	Total	C	N	O	S	Se	0	0	0
			6870	4392	1153	1319	3	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	PHE	TYR	engineered mutation	UNP A0A0C6EFY4
B	458	PHE	TYR	engineered mutation	UNP A0A0C6EFY4

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose.
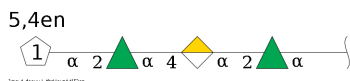
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 3 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-3)-alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose.
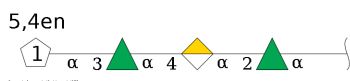
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total 44	C 24	O 20	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	54	Total 54	O 54	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: Pcrglx protein

- Molecule 1: Pcrglx protein

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose

Chain C:

• Molecule 3: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-3)-alpha-L-rhamnopyranose-(1-4)-alpha-D-galactopyranuronic acid-(1-2)-alpha-L-rhamnopyranose
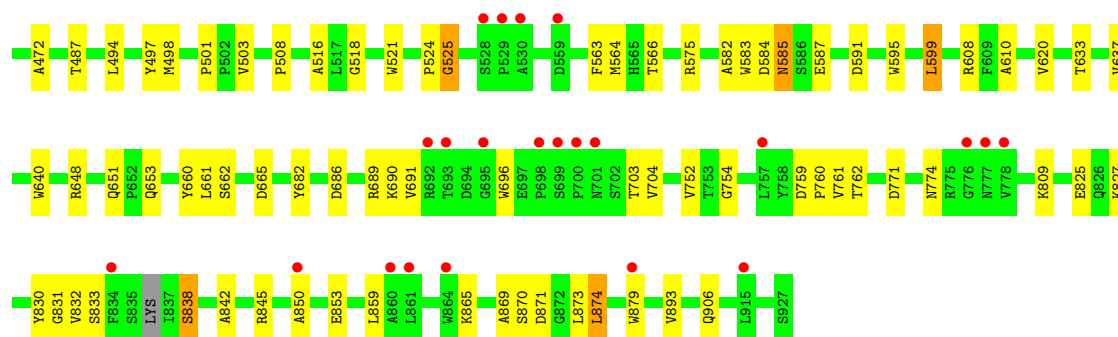
Chain D:
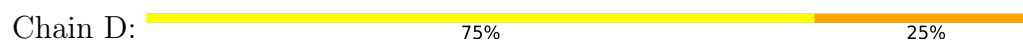
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.44Å 166.44Å 171.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.58 – 3.20 48.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (119.58-3.20) 99.5 (48.56-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.40 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.191 , 0.264 0.195 , 0.260	Depositor DCC
R_{free} test set	2100 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	87.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14092	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: CA, ADA, RAM, GAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.54	0/7218	0.76	0/9854
1	B	0.57	0/7069	0.77	1/9655 (0.0%)
All	All	0.56	0/14287	0.77	1/19509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	665	ASP	CB-CG-OD1	5.36	123.13	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7017	0	6566	68	0
1	B	6870	0	6391	70	0
2	C	44	0	32	5	0
3	D	44	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	61	0	0	3	0
5	B	54	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14092	0	13015	137	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 5.

All (137) 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:24:CYS:SG	5:B:1114:HOH:O	2.34	0.84
1:A:157:ILE:HA	1:A:204:ILE:HD11	1.70	0.73
1:B:288:ILE:HD13	1:B:349:TYR:CE1	2.29	0.67
1:A:708:LEU:HG	1:A:755:SER:HA	1.78	0.66
1:B:825:GLU:CB	5:B:1149:HOH:O	2.46	0.63
1:B:277:PRO:O	1:B:417:ASP:O	2.18	0.61
1:A:672:LEU:HD13	1:A:721:ILE:HG21	1.82	0.60
1:B:363:LYS:HD3	1:B:374:ILE:HD11	1.84	0.60
1:B:246:ALA:O	1:B:247:ASN:HB2	2.02	0.58
1:A:310:ARG:HD2	1:A:335:ARG:HD2	1.86	0.58
1:B:157:ILE:HA	1:B:204:ILE:HD11	1.86	0.58
1:B:280:GLY:N	5:B:1101:HOH:O	2.36	0.58
1:A:902:ASN:HD22	2:C:3:RAM:H62	1.68	0.57
1:A:773:GLY:O	1:A:775:ARG:N	2.37	0.57
1:A:324:GLN:HG2	5:A:1161:HOH:O	2.02	0.57
1:A:190:ARG:HD2	1:B:178:GLN:HE22	1.70	0.57
1:A:564:MSE:HE1	1:A:576:TYR:HB3	1.86	0.57
1:B:346:TRP:CD2	1:B:363:LYS:HE3	2.41	0.56
1:B:873:LEU:O	1:B:874:LEU:HB2	2.06	0.56
1:A:902:ASN:ND2	2:C:3:RAM:H62	2.22	0.55
1:B:236:LEU:HD21	1:B:257:ILE:HD11	1.89	0.55
1:B:595:TRP:CE2	1:B:610:ALA:HB1	2.42	0.55
1:B:268:THR:HG22	1:B:432:PRO:HB3	1.89	0.54
1:A:754:GLY:HA2	1:A:779:SER:HB3	1.90	0.54
1:A:839:LEU:HB3	1:A:842:ALA:HB3	1.90	0.54
1:A:817:TYR:O	1:A:862:ARG:NH2	2.40	0.54
1:A:754:GLY:O	1:A:755:SER:OG	2.25	0.54
1:B:236:LEU:CD2	1:B:257:ILE:HD11	2.38	0.54
2:C:1:RAM:O3	2:C:2:ADA:H5	2.07	0.54
1:B:236:LEU:HG	1:B:257:ILE:HD11	1.90	0.53
1:A:114:VAL:O	1:A:117:SER:OG	2.27	0.53
1:B:236:LEU:CG	1:B:257:ILE:HD11	2.40	0.52
1:A:575:ARG:HD3	1:B:307:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:THR:HG21	1:B:640:TRP:HA	1.90	0.52
1:A:580:GLY:O	1:A:635:HIS:HD2	1.94	0.51
1:B:566:THR:O	1:B:575:ARG:HG3	2.10	0.51
1:A:550:GLU:HG2	1:A:555:TYR:OH	2.11	0.51
1:A:692:ARG:HD3	1:A:696:TRP:HB3	1.92	0.51
1:B:258:VAL:HG22	1:B:472:ALA:HB2	1.92	0.51
1:B:383:LEU:HD23	1:B:384:ALA:N	2.26	0.50
1:B:89:TRP:CD1	1:B:660:TYR:CD2	2.99	0.50
1:A:31:VAL:HG12	1:A:104:TYR:HB2	1.93	0.50
1:A:741:ILE:HG23	1:A:808:PHE:CD1	2.47	0.50
1:A:333:GLU:CG	5:A:1108:HOH:O	2.60	0.50
1:B:661:LEU:O	1:B:662:SER:CB	2.60	0.49
1:B:64:LEU:HD11	1:B:104:TYR:HB3	1.95	0.49
1:B:246:ALA:O	1:B:247:ASN:CB	2.59	0.49
1:B:438:PHE:CE1	1:B:637:VAL:HB	2.47	0.49
1:A:26:SER:HA	1:A:108:ALA:O	2.12	0.49
1:B:447:TYR:CD2	1:B:690:LYS:HA	2.48	0.49
1:A:586:SER:OG	1:A:617:THR:HG21	2.12	0.49
1:B:761:VAL:HG23	1:B:762:THR:HG23	1.95	0.49
1:A:694:ASP:O	1:A:696:TRP:N	2.45	0.49
1:B:135:ASN:CB	5:B:1152:HOH:O	2.61	0.48
1:B:759:ASP:OD1	1:B:761:VAL:HG22	2.13	0.48
1:B:845:ARG:NH1	1:B:906:GLN:OE1	2.47	0.48
1:A:237:PRO:HG2	1:A:258:VAL:HB	1.95	0.48
1:A:361:LEU:HG	1:A:374:ILE:HD12	1.96	0.48
1:A:217:LEU:HD13	1:A:243:TYR:CE1	2.48	0.48
1:B:361:LEU:HB3	1:B:374:ILE:HB	1.96	0.47
1:A:260:ASP:N	1:A:260:ASP:OD1	2.46	0.47
1:A:74:LEU:HD11	1:A:92:HIS:HB3	1.96	0.47
1:A:685:LEU:HD11	1:A:689:ARG:NH1	2.29	0.47
1:B:686:ASP:HB3	1:B:689:ARG:HB3	1.95	0.47
1:A:40:TYR:OH	1:A:42:ALA:HB2	2.15	0.47
1:A:589:SER:HB3	1:A:592:LEU:HD12	1.96	0.47
1:A:201:ASP:OD2	1:A:227:THR:HG21	2.15	0.47
1:A:52:GLN:HA	1:A:82:TRP:CD1	2.50	0.46
1:A:554:TRP:HE1	1:A:564:MSE:HE2	1.80	0.46
1:B:382:GLY:O	1:B:498:MSE:HE1	2.15	0.46
1:B:435:LEU:HB3	1:B:468:PRO:HG3	1.96	0.46
1:B:45:THR:HA	1:B:92:HIS:O	2.16	0.46
1:B:521:TRP:CE2	1:B:599:LEU:HD23	2.50	0.46
1:B:31:VAL:HG12	1:B:104:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	1:A:341:LYS:CB	2.64	0.46
1:A:549:ILE:HD11	1:A:609:PHE:CE2	2.50	0.46
1:A:155:ASN:ND2	1:A:201:ASP:HB3	2.31	0.46
1:B:696:TRP:HB2	5:B:1109:HOH:O	2.15	0.45
1:A:124:SER:O	1:A:125:ALA:HB3	2.16	0.45
1:A:889:VAL:HG23	5:A:1141:HOH:O	2.16	0.45
1:B:689:ARG:O	1:B:691:VAL:N	2.48	0.44
1:A:595:TRP:CE2	1:A:610:ALA:HB1	2.53	0.44
1:B:524:PRO:O	1:B:525:GLY:C	2.56	0.44
1:B:703:THR:HA	1:B:760:PRO:HD2	1.98	0.44
1:A:589:SER:OG	1:A:786:VAL:O	2.29	0.44
1:A:633:THR:HG21	1:A:640:TRP:HA	1.98	0.44
1:B:584:ASP:O	1:B:585:ASN:C	2.55	0.44
1:A:456:ILE:HD11	1:B:308:LEU:HD13	1.99	0.44
1:A:791:GLU:OE1	1:A:791:GLU:N	2.46	0.43
1:B:873:LEU:O	1:B:874:LEU:CB	2.67	0.43
1:A:257:ILE:CD1	1:A:270:LEU:HD21	2.48	0.43
1:A:648:ARG:NH2	2:C:1:RAM:O3	2.52	0.43
1:B:682:TYR:HB3	1:B:704:VAL:HG11	1.99	0.43
1:B:293:VAL:HG12	1:B:294:ASP:HB2	1.99	0.43
1:B:653:GLN:NE2	5:B:1102:HOH:O	2.50	0.43
1:A:310:ARG:NH2	3:D:4:GAD:O6B	2.52	0.43
1:B:494:LEU:O	1:B:497:TYR:HB3	2.18	0.43
1:B:564:MSE:HE2	1:B:583:TRP:CE2	2.54	0.42
1:B:865:LYS:O	1:B:869:ALA:HB3	2.18	0.42
1:A:473:ARG:HD3	1:A:557:PHE:O	2.19	0.42
1:B:752:VAL:HG21	1:B:830:TYR:CZ	2.55	0.42
1:B:842:ALA:O	1:B:845:ARG:HD3	2.18	0.42
1:A:580:GLY:O	1:A:635:HIS:CD2	2.72	0.42
1:B:456:ILE:HG23	1:B:457:THR:HG23	2.01	0.42
1:B:89:TRP:NE1	1:B:516:ALA:HB1	2.34	0.42
1:B:352:THR:HB	1:B:354:LEU:HD21	2.00	0.42
1:A:599:LEU:HD21	1:A:661:LEU:HD11	2.01	0.42
1:A:241:ARG:NH2	1:A:670:GLU:OE2	2.53	0.42
1:A:253:VAL:HB	1:A:477:VAL:HB	2.02	0.42
1:B:827:LYS:HA	1:B:831:GLY:HA2	2.01	0.42
1:B:382:GLY:HA3	1:B:401:PHE:CG	2.55	0.41
1:A:405:TYR:CD1	1:A:405:TYR:C	2.94	0.41
1:B:870:SER:OG	1:B:871:ASP:N	2.53	0.41
1:B:43:GLY:HA3	1:B:245:TYR:CD2	2.55	0.41
1:A:583:TRP:CG	1:A:639:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ILE:HG23	1:A:808:PHE:CG	2.56	0.41
1:A:781:SER:HB3	1:A:784:ASN:ND2	2.35	0.41
1:B:145:GLU:HB3	1:B:249:ALA:HB2	2.01	0.41
1:B:305:ILE:HD12	1:B:305:ILE:HA	1.86	0.41
1:A:89:TRP:CD2	1:A:660:TYR:HB3	2.56	0.41
1:B:850:ALA:HB3	1:B:859:LEU:HD21	2.02	0.41
1:B:873:LEU:HD13	1:B:879:TRP:CH2	2.56	0.41
1:A:746:ASN:HD22	1:A:746:ASN:N	2.19	0.41
1:A:345:THR:HG23	1:A:345:THR:O	2.21	0.41
1:B:340:LEU:HD23	1:B:343:ILE:HD12	2.02	0.41
1:B:346:TRP:CE3	1:B:363:LYS:HE3	2.56	0.41
1:A:45:THR:HA	1:A:92:HIS:O	2.21	0.40
1:A:456:ILE:HG23	1:A:457:THR:HG23	2.03	0.40
2:C:1:RAM:O3	2:C:2:ADA:C5	2.69	0.40
1:A:210:ASN:O	1:A:216:THR:HA	2.20	0.40
1:A:478:TYR:CD1	1:A:498:MSE:HG3	2.56	0.40
1:B:385:TYR:CD1	1:B:385:TYR:C	2.94	0.40
1:A:759:ASP:OD1	1:A:761:VAL:HG22	2.22	0.40
1:A:277:PRO:O	1:A:417:ASP:O	2.39	0.40
1:A:750:GLY:O	1:A:753:THR:HB	2.20	0.40
1:B:34:LEU:HD22	1:B:503:VAL:HG11	2.04	0.40
1:B:501:PRO:O	1:B:608:ARG:NH2	2.52	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	893/906 (99%)	805 (90%)	74 (8%)	14 (2%)	9	43
1	B	873/906 (96%)	773 (88%)	77 (9%)	23 (3%)	5	31
All	All	1766/1812 (98%)	1578 (89%)	151 (9%)	37 (2%)	7	37

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	695	GLY
1	A	748	THR
1	A	774	ASN
1	B	231	ASP
1	B	525	GLY
1	B	832	VAL
1	B	833	SER
1	A	341	LYS
1	A	579	GLY
1	A	755	SER
1	B	137	ASP
1	B	202	GLY
1	B	230	THR
1	B	247	ASN
1	B	278	LEU
1	B	433	LEU
1	B	518	GLY
1	B	838	SER
1	B	874	LEU
1	A	277	PRO
1	A	697	GLU
1	A	124	SER
1	A	651	GLN
1	B	585	ASN
1	B	651	GLN
1	B	771	ASP
1	A	125	ALA
1	A	870	SER
1	B	164	LYS
1	B	339	ARG
1	B	774	ASN
1	A	776	GLY
1	A	874	LEU
1	B	582	ALA
1	B	754	GLY
1	B	112	GLY
1	B	193	SER

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	719/742 (97%)	677 (94%)	42 (6%)	20	55
1	B	694/742 (94%)	660 (95%)	34 (5%)	25	61
All	All	1413/1484 (95%)	1337 (95%)	76 (5%)	22	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	58	GLN
1	A	113	CYS
1	A	148	VAL
1	A	165	SER
1	A	167	LYS
1	A	172	ASN
1	A	186	ASN
1	A	201	ASP
1	A	206	GLU
1	A	209	VAL
1	A	215	ARG
1	A	257	ILE
1	A	277	PRO
1	A	315	GLU
1	A	329	THR
1	A	332	TRP
1	A	335	ARG
1	A	366	LYS
1	A	381	GLU
1	A	394	LEU
1	A	416	SER
1	A	418	THR
1	A	420	GLU
1	A	448	GLU
1	A	475	SER
1	A	493	SER

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Mol	Chain	Res	Type
1	A	505	VAL
1	A	563	PHE
1	A	588	LEU
1	A	591	ASP
1	A	622	VAL
1	A	655	ARG
1	A	699	SER
1	A	803	ASP
1	A	804	ILE
1	A	853	GLU
1	A	855	LYS
1	A	862	ARG
1	A	865	LYS
1	A	889	VAL
1	A	921	SER
1	B	26	SER
1	B	28	SER
1	B	65	THR
1	B	79	THR
1	B	111	LEU
1	B	137	ASP
1	B	140	THR
1	B	145	GLU
1	B	213	SER
1	B	247	ASN
1	B	250	THR
1	B	252	LYS
1	B	270	LEU
1	B	282	GLU
1	B	305	ILE
1	B	310	ARG
1	B	329	THR
1	B	341	LYS
1	B	361	LEU
1	B	391	GLN
1	B	451	LEU
1	B	454	LEU
1	B	487	THR
1	B	508	PRO
1	B	563	PHE
1	B	587	GLU
1	B	591	ASP

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Mol	Chain	Res	Type
1	B	599	LEU
1	B	620	VAL
1	B	648	ARG
1	B	809	LYS
1	B	838	SER
1	B	853	GLU
1	B	893	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	515	GLN
1	A	635	HIS
1	A	746	ASN
1	A	810	GLN
1	A	902	ASN
1	B	178	GLN
1	B	203	ASN
1	B	391	GLN
1	B	515	GLN
1	B	653	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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	RAM	C	1	2	11,11,11	0.62	0	15,16,16	1.55	4 (26%)
2	ADA	C	2	2	12,12,13	0.75	0	14,17,19	2.57	4 (28%)
2	RAM	C	3	2	10,10,11	0.76	0	14,14,16	1.71	5 (35%)
2	GAD	C	4	2	10,11,11	2.28	2 (20%)	13,15,15	2.71	5 (38%)
3	RAM	D	1	3	11,11,11	0.89	0	15,16,16	1.66	5 (33%)
3	ADA	D	2	1,3	12,12,13	0.79	0	14,17,19	1.88	3 (21%)
3	RAM	D	3	3	10,10,11	3.17	3 (30%)	14,14,16	5.87	9 (64%)
3	GAD	D	4	3	10,11,11	2.61	2 (20%)	13,15,15	4.52	5 (38%)

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	RAM	C	1	2	-	-	0/1/1/1
2	ADA	C	2	2	-	0/4/21/24	0/1/1/1
2	RAM	C	3	2	-	-	0/1/1/1
2	GAD	C	4	2	-	0/4/17/17	0/1/1/1
3	RAM	D	1	3	-	-	0/1/1/1
3	ADA	D	2	1,3	-	2/4/21/24	0/1/1/1
3	RAM	D	3	3	-	-	0/1/1/1
3	GAD	D	4	3	-	2/4/17/17	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	RAM	C2-C3	8.71	1.65	1.52
3	D	4	GAD	O5-C5	7.17	1.47	1.37
2	C	4	GAD	O5-C5	6.19	1.46	1.37
3	D	3	RAM	O3-C3	3.57	1.51	1.43
3	D	3	RAM	C4-C3	2.65	1.59	1.52
3	D	4	GAD	O5-C1	-2.56	1.41	1.45
2	C	4	GAD	C3-C4	2.23	1.53	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	RAM	O3-C3-C2	13.43	135.71	109.99
3	D	3	RAM	C1-C2-C3	11.75	124.11	109.67
3	D	4	GAD	O5-C5-C4	-10.12	116.26	124.81
3	D	3	RAM	O5-C1-C2	-8.83	97.14	110.77
3	D	4	GAD	C1-C2-C3	7.93	119.42	109.67
3	D	4	GAD	O5-C5-C6	7.63	122.97	111.52
2	C	2	ADA	O4-C4-C5	7.54	126.65	109.74
2	C	4	GAD	O5-C5-C4	-7.30	118.65	124.81
3	D	4	GAD	C3-C4-C5	-5.20	112.81	121.60
3	D	3	RAM	C3-C4-C5	4.43	116.68	109.77
3	D	3	RAM	O3-C3-C4	-4.24	100.54	110.35
3	D	2	ADA	O5-C1-C2	-4.21	104.27	110.77
3	D	3	RAM	O2-C2-C3	4.09	118.33	110.14
3	D	2	ADA	C3-C4-C5	-4.07	102.27	109.25
2	C	4	GAD	O5-C5-C6	4.05	117.60	111.52
3	D	3	RAM	O2-C2-C1	-4.01	100.94	109.15
2	C	3	RAM	C1-C2-C3	3.63	114.13	109.67
2	C	1	RAM	O5-C5-C6	3.27	113.77	106.70
3	D	1	RAM	O5-C5-C4	3.27	115.39	109.52
2	C	2	ADA	O4-C4-C3	3.25	117.87	110.35
2	C	4	GAD	O6B-C6-C5	3.15	122.06	114.20
3	D	1	RAM	O2-C2-C3	3.00	117.29	110.35
3	D	1	RAM	O5-C1-C2	2.88	115.42	110.28
2	C	3	RAM	C2-C3-C4	2.62	115.43	110.89
2	C	2	ADA	O2-C2-C3	2.51	115.16	110.14
3	D	4	GAD	O2-C2-C1	2.48	114.24	109.15
2	C	3	RAM	C3-C4-C5	2.37	113.46	109.77
3	D	3	RAM	O4-C4-C5	-2.28	104.61	109.67
2	C	4	GAD	C1-O5-C5	2.28	120.37	115.58
2	C	2	ADA	O6B-C6-C5	2.25	121.89	113.65
2	C	4	GAD	C1-C2-C3	2.24	112.42	109.67
2	C	1	RAM	O5-C1-C2	2.22	114.25	110.28
2	C	1	RAM	O1-C1-C2	-2.19	102.86	109.03
2	C	3	RAM	C1-O5-C5	2.16	117.66	112.78
3	D	3	RAM	C2-C3-C4	-2.14	107.19	110.89
3	D	1	RAM	C6-C5-C4	-2.13	109.14	113.07
2	C	1	RAM	O2-C2-C3	-2.04	105.64	110.35
3	D	1	RAM	C4-C3-C2	-2.02	107.30	110.82
3	D	2	ADA	O4-C4-C5	2.02	114.27	109.74
2	C	3	RAM	O5-C5-C4	2.01	113.12	109.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	GAD	O5-C5-C6-O6A
3	D	4	GAD	O5-C5-C6-O6B
3	D	2	ADA	O5-C5-C6-O6B
3	D	2	ADA	O5-C5-C6-O6A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	GAD	1	0
2	C	3	RAM	2	0
2	C	2	ADA	2	0
2	C	1	RAM	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 oligosaccharide.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths   Bond angles

Torsions   Rings
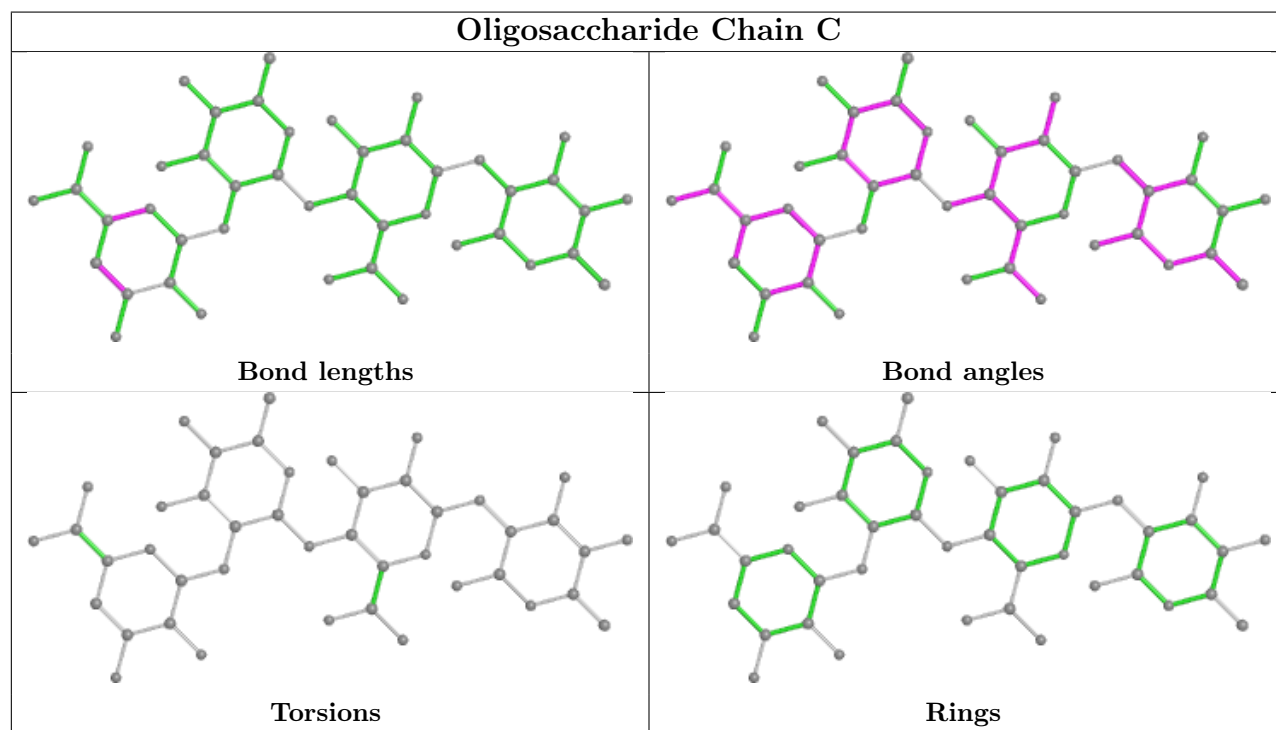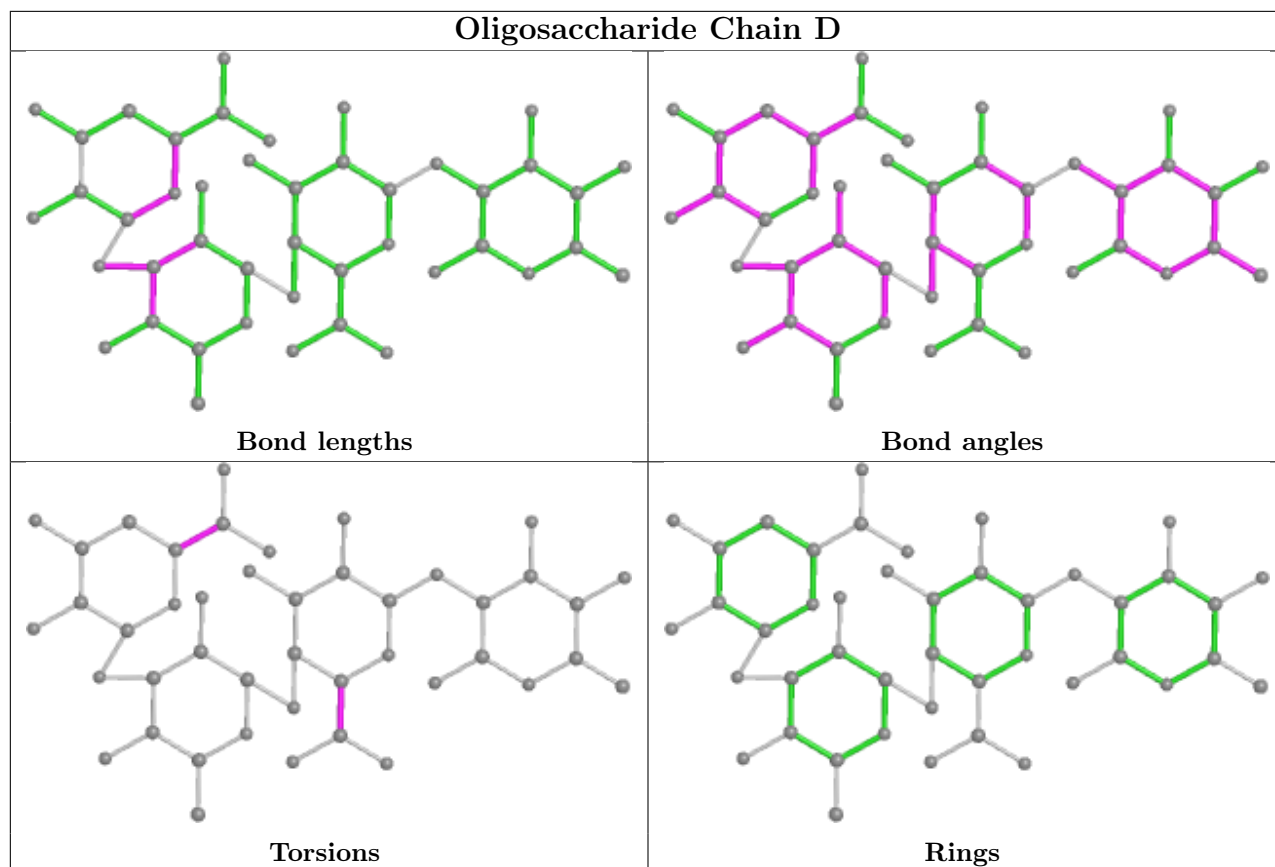
5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	896/906 (98%)	0.02	15 (1%)	70	57	62, 84, 111, 156	0
1	B	878/906 (96%)	0.16	31 (3%)	44	28	60, 90, 119, 159	0
All	All	1774/1812 (97%)	0.09	46 (2%)	56	40	60, 87, 117, 159	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	4.4
1	B	777	ASN	4.1
1	B	701	ASN	4.0
1	A	66	GLY	3.7
1	B	860	ALA	3.7
1	B	700	PRO	3.7
1	A	228	ASP	3.6
1	A	373	ASN	3.4
1	A	332	TRP	3.4
1	A	342	TRP	3.1
1	B	698	PRO	3.0
1	B	695	GLY	2.9
1	B	778	VAL	2.9
1	B	528	SER	2.8
1	A	67	ASP	2.8
1	B	463	PRO	2.7
1	B	861	LEU	2.7
1	A	101	TYR	2.7
1	A	139	LEU	2.7
1	B	864	TRP	2.6
1	B	776	GLY	2.6
1	B	693	THR	2.6
1	B	757	LEU	2.5
1	B	444	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	559	ASP	2.4
1	B	529	PRO	2.4
1	B	915	LEU	2.4
1	B	699	SER	2.3
1	B	834	PHE	2.3
1	A	360	GLY	2.2
1	A	231	ASP	2.2
1	B	879	TRP	2.2
1	A	337	SER	2.2
1	B	230	THR	2.2
1	B	323	GLY	2.2
1	B	850	ALA	2.1
1	B	692	ARG	2.1
1	B	389	ALA	2.1
1	A	229	GLY	2.1
1	B	192	ASN	2.1
1	B	530	ALA	2.1
1	A	834	PHE	2.1
1	B	139	LEU	2.1
1	A	805	PRO	2.1
1	B	278	LEU	2.1
1	B	332	TRP	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.
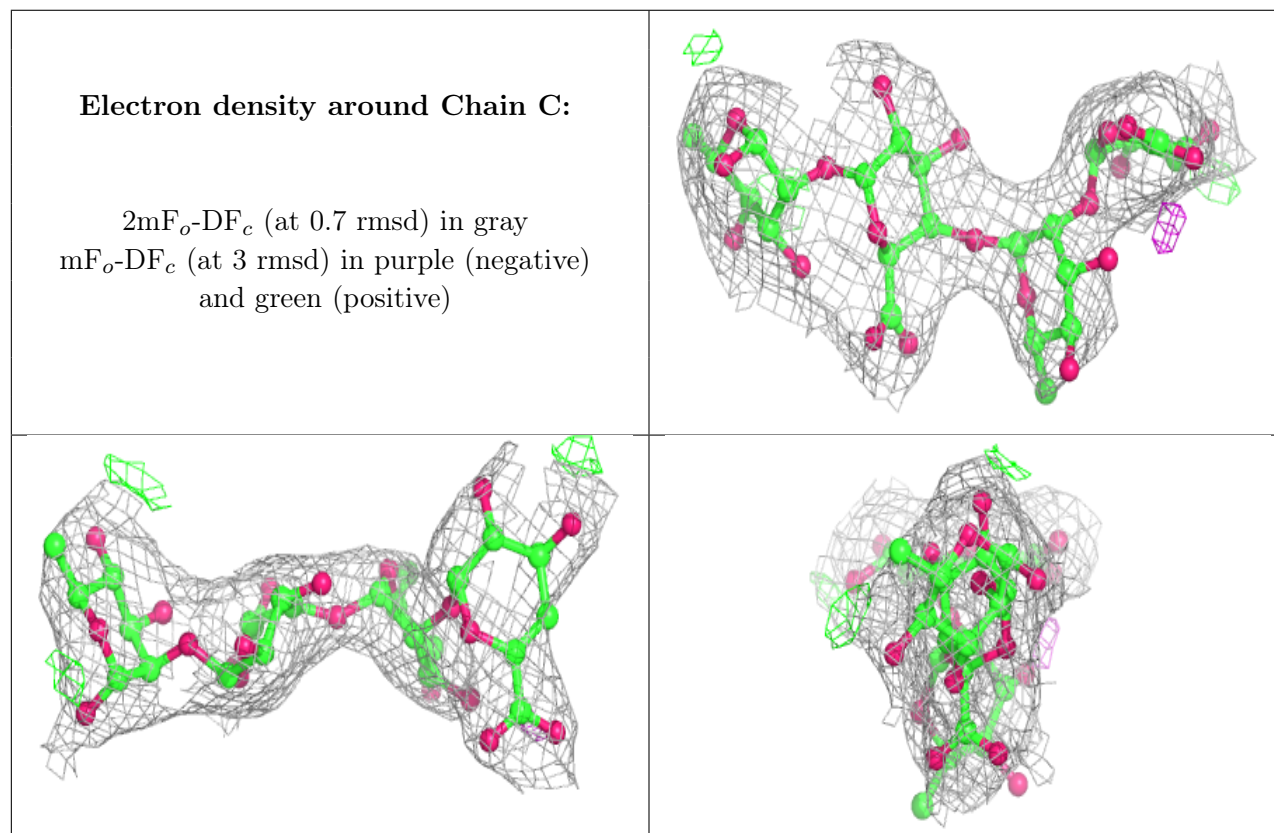
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	RAM	D	3	10/11	0.85	0.21	100,139,152,168	0
2	GAD	C	4	11/11	0.86	0.22	89,104,110,113	0
3	RAM	D	1	11/11	0.92	0.15	99,103,108,120	0
3	GAD	D	4	11/11	0.92	0.16	100,114,134,138	0
2	RAM	C	3	10/11	0.93	0.18	104,106,115,125	0
3	ADA	D	2	12/13	0.93	0.14	81,102,118,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADA	C	2	12/13	0.94	0.18	73,84,88,103	0
2	RAM	C	1	11/11	0.96	0.20	73,76,83,84	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.
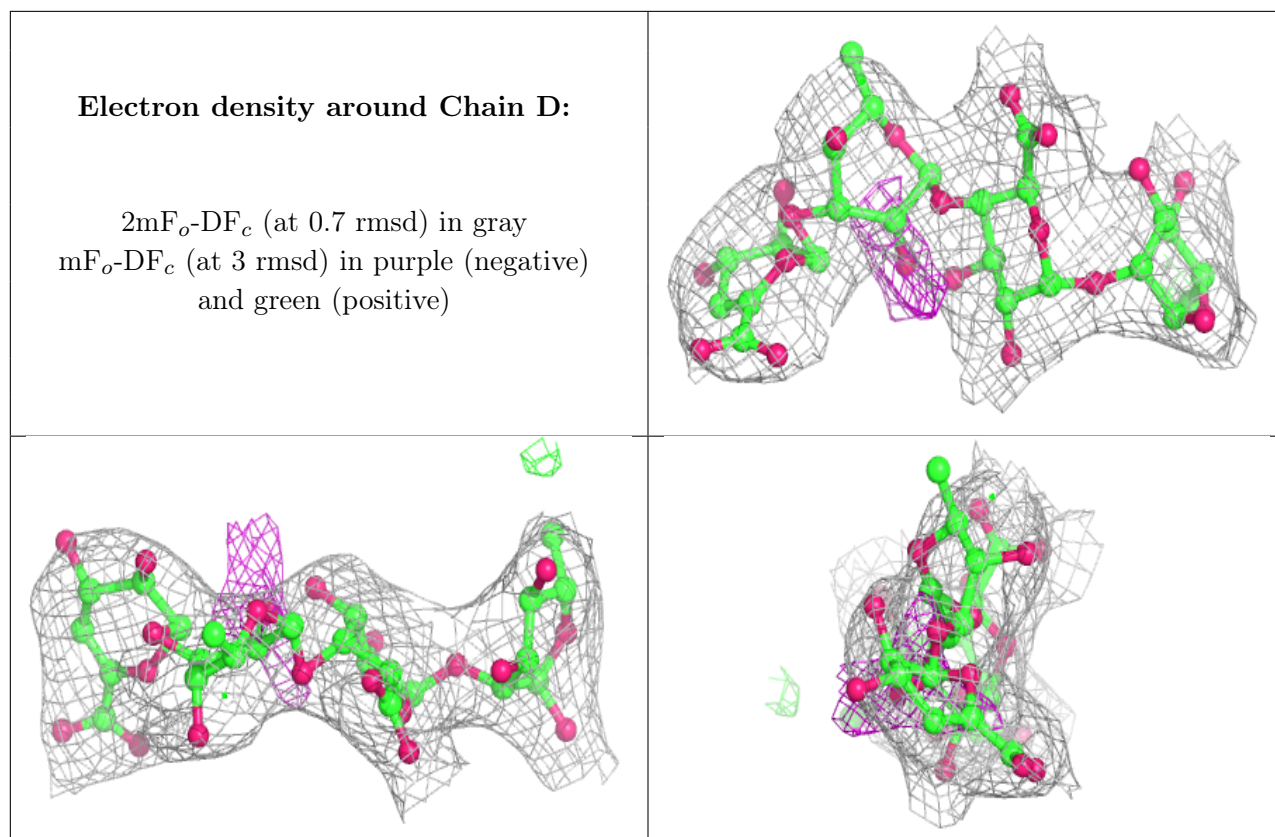
Electron density around Chain C:

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

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (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	CA	B	1001	1/1	0.98	0.27	57,57,57,57	0
4	CA	A	1001	1/1	0.99	0.25	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.