



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:33 PM UTC

PDB ID : 2WZE / pdb_00002wze
Title : High resolution crystallographic structure of the Clostridium thermocellum N-terminal endo-1,4-beta-D-xylanase 10B (Xyn10B) CBM22-1- GH10 modules complexed with xylohexaose
Authors : Najmudin, S.; Pinheiro, B.A.; Romao, M.J.; Prates, J.A.M.; Fontes, C.M.G.A.
Deposited on : 2009-11-27
Resolution : 2.50 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
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

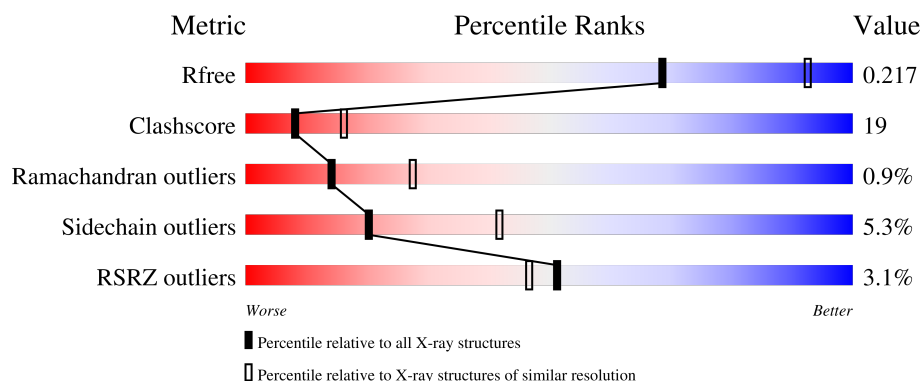
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

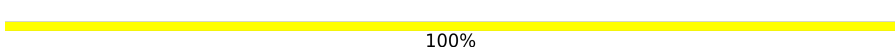
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	A	540	
1	B	540	
2	C	3	
2	D	3	

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	GOL	A	1556	-	-	X	-
4	GOL	A	1557	-	X	-	-
4	GOL	B	1557	-	X	X	-
4	GOL	B	1558	-	-	X	-
4	GOL	B	1559	-	-	X	-
4	GOL	B	1561	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9212 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 ENDO-1,4-BETA-XYLANASE Y.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	Se	0	4	0
			4055	2546	689	802	8	10			
1	B	516	Total	C	N	O	S	Se	0	6	0
			4083	2562	694	809	8	10			

There are 44 discrepancies between the modelled and reference sequences:

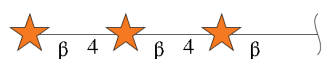
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	expression tag	UNP P51584
A	13	GLY	-	expression tag	UNP P51584
A	14	SER	-	expression tag	UNP P51584
A	15	SER	-	expression tag	UNP P51584
A	16	HIS	-	expression tag	UNP P51584
A	17	HIS	-	expression tag	UNP P51584
A	18	HIS	-	expression tag	UNP P51584
A	19	HIS	-	expression tag	UNP P51584
A	20	HIS	-	expression tag	UNP P51584
A	21	HIS	-	expression tag	UNP P51584
A	22	SER	-	expression tag	UNP P51584
A	23	SER	-	expression tag	UNP P51584
A	24	GLY	-	expression tag	UNP P51584
A	25	LEU	-	expression tag	UNP P51584
A	26	VAL	-	expression tag	UNP P51584
A	27	PRO	-	expression tag	UNP P51584
A	28	ARG	-	expression tag	UNP P51584
A	29	GLY	-	expression tag	UNP P51584
A	30	SER	-	expression tag	UNP P51584
A	31	HIS	-	expression tag	UNP P51584
A	32	MSE	-	expression tag	UNP P51584
B	12	MSE	-	expression tag	UNP P51584
B	13	GLY	-	expression tag	UNP P51584
B	14	SER	-	expression tag	UNP P51584
B	15	SER	-	expression tag	UNP P51584

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP P51584
B	17	HIS	-	expression tag	UNP P51584
B	18	HIS	-	expression tag	UNP P51584
B	19	HIS	-	expression tag	UNP P51584
B	20	HIS	-	expression tag	UNP P51584
B	21	HIS	-	expression tag	UNP P51584
B	22	SER	-	expression tag	UNP P51584
B	23	SER	-	expression tag	UNP P51584
B	24	GLY	-	expression tag	UNP P51584
B	25	LEU	-	expression tag	UNP P51584
B	26	VAL	-	expression tag	UNP P51584
B	27	PRO	-	expression tag	UNP P51584
B	28	ARG	-	expression tag	UNP P51584
B	29	GLY	-	expression tag	UNP P51584
B	30	SER	-	expression tag	UNP P51584
B	31	HIS	-	expression tag	UNP P51584
B	32	MSE	-	expression tag	UNP P51584
A	337	ALA	GLU	engineered mutation	UNP P51584
B	337	ALA	GLU	engineered mutation	UNP P51584

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			28	15	13			
2	D	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

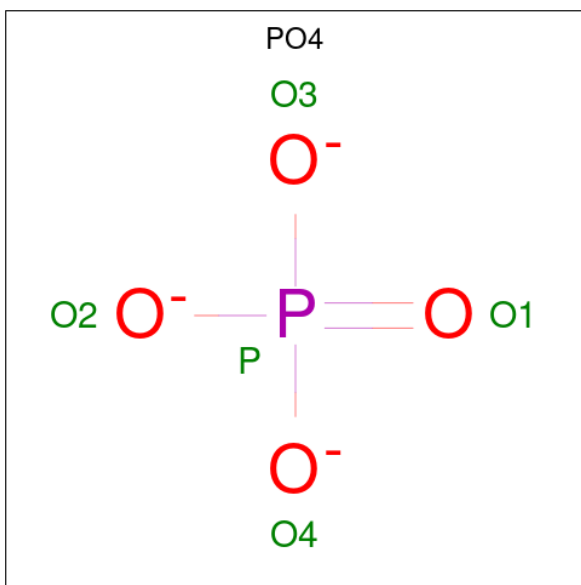
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	422	Total	O	0	0
			422	422		
6	B	512	Total	O	0	0
			512	512		

Chain C:  100%

XYP1
XYP2
XYP3

- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D:  33%  67%

XYP1
XYP2
XYP3

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.04Å 173.04Å 136.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.02 – 2.50 101.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.02-2.50) 100.0 (101.02-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.147 , 0.189 0.177 , 0.217	Depositor DCC
R_{free} test set	4129 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9212	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: CA, PO4, XYP, GOL

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	1.23	7/4146 (0.2%)	1.22	14/5615 (0.2%)
1	B	1.37	8/4180 (0.2%)	1.24	13/5663 (0.2%)
All	All	1.30	15/8326 (0.2%)	1.23	27/11278 (0.2%)

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	0	2
1	B	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	THR	CA-CB	7.25	1.65	1.53
1	B	188	VAL	CA-CB	6.28	1.62	1.54
1	A	318	ALA	CA-CB	-6.17	1.43	1.53
1	A	476	ALA	CA-CB	6.14	1.62	1.53
1	A	427	SER	C-O	5.91	1.31	1.23
1	B	456	VAL	C-O	5.57	1.29	1.24
1	B	492	THR	CA-C	-5.41	1.45	1.52
1	B	51	LEU	CA-C	5.36	1.59	1.52
1	A	401	ASP	N-CA	5.17	1.52	1.46
1	B	219	ILE	N-CA	-5.17	1.40	1.46
1	A	394	ASN	N-CA	5.12	1.52	1.46
1	A	275	GLY	C-O	5.09	1.29	1.23
1	B	166	SER	C-O	-5.09	1.19	1.24
1	B	495	LYS	N-CA	-5.05	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYS	CA-C	5.04	1.59	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	N-CA-C	-8.91	95.69	108.96
1	B	493	SER	N-CA-C	8.57	121.91	108.79
1	A	518	ALA	CA-C-N	-7.98	111.39	121.04
1	A	518	ALA	C-N-CA	-7.98	111.39	121.04
1	A	514	GLY	N-CA-C	-7.01	104.00	112.48
1	A	60	VAL	N-CA-C	6.86	117.71	108.11
1	B	217	SER	N-CA-C	6.80	119.56	111.33
1	A	359	ASN	CB-CA-C	-6.62	101.06	111.51
1	A	141	GLU	N-CA-C	6.45	118.92	108.41
1	B	281	HIS	N-CA-C	-6.27	105.46	113.23
1	B	123	GLU	N-CA-C	6.26	118.10	111.28
1	B	86	GLU	CB-CA-C	5.96	119.57	109.80
1	A	271	ILE	N-CA-C	-5.86	99.97	108.17
1	B	466	GLU	CA-CB-CG	-5.85	102.41	114.10
1	B	473	GLN	N-CA-C	-5.85	104.99	111.36
1	B	367	ILE	CB-CA-C	-5.39	105.02	112.24
1	B	515	SER	CA-CB-OG	-5.39	100.32	111.10
1	B	509	ALA	N-CA-C	-5.38	106.49	113.16
1	A	539	ILE	N-CA-C	5.37	113.18	107.76
1	B	132	ILE	N-CA-C	-5.36	108.06	113.47
1	A	370	ASP	N-CA-CB	-5.32	102.64	111.57
1	A	41	PHE	N-CA-C	5.30	122.09	110.80
1	A	249	ASN	N-CA-C	5.26	118.48	111.75
1	A	475	GLN	N-CA-C	-5.18	105.71	111.36
1	B	174	ASP	N-CA-C	5.16	118.37	111.24
1	A	425	MSE	CG-SE-CE	-5.15	87.60	98.92
1	B	492	THR	N-CA-C	-5.05	100.03	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	GLY	Peptide
1	A	494	SER	Peptide
1	B	494	SER	Peptide

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	4055	0	3865	185	0
1	B	4083	0	3893	107	0
2	C	28	0	0	0	0
2	D	28	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	48	13	0
4	B	36	0	47	21	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	422	0	0	77	1
6	B	512	0	0	59	1
All	All	9212	0	7853	312	1

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 19.

All (312) 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:493:SER:HA	1:B:494:SER:OG	1.30	1.21
1:A:169:ASP:HB3	6:A:2107:HOH:O	1.36	1.19
1:A:425:MSE:HE3	1:A:449:TYR:CD2	1.76	1.18
1:A:77:SER:HB3	6:A:2034:HOH:O	1.45	1.16
4:B:1556:GOL:H31	6:B:2497:HOH:O	1.46	1.11
1:A:527[B]:GLN:OE1	6:A:2389:HOH:O	1.66	1.11
1:A:136:ASP:HB2	6:A:2077:HOH:O	1.49	1.10
1:A:448:LYS:HE2	6:A:2332:HOH:O	1.51	1.10
1:A:539:ILE:HD13	6:A:2398:HOH:O	1.51	1.10
1:A:493:SER:HA	1:A:494:SER:HB2	1.19	1.09
1:A:425:MSE:HE3	1:A:449:TYR:HD2	1.10	1.09
1:A:493:SER:HA	1:A:494:SER:CB	1.83	1.08
1:A:300:VAL:HG21	1:A:305:MSE:HE2	1.17	1.08
1:A:198[B]:MSE:HE3	1:A:539:ILE:H	1.14	1.07
1:A:300:VAL:HG21	1:A:305:MSE:CE	1.84	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:HD2	6:A:2111:HOH:O	1.57	1.04
1:B:493:SER:OG	1:B:494:SER:HB2	1.59	1.03
1:A:108:THR:HG22	6:A:2061:HOH:O	1.59	1.02
4:B:1561:GOL:H11	6:B:2510:HOH:O	1.60	1.01
1:A:436:PHE:H	4:A:1556:GOL:H11	1.22	1.01
1:A:527[B]:GLN:NE2	6:A:2390:HOH:O	1.93	1.01
1:A:179:ARG:HB2	1:A:180:LYS:HB3	1.39	1.00
1:B:413:ASN:HB2	6:B:2362:HOH:O	1.59	1.00
1:A:466:GLU:HG2	6:A:2340:HOH:O	1.62	1.00
4:B:1561:GOL:H12	6:B:2509:HOH:O	1.60	1.00
1:B:244:GLN:HG2	6:B:2206:HOH:O	1.60	0.99
1:A:493:SER:OG	1:A:494:SER:HB3	1.62	0.99
1:A:300:VAL:CG2	1:A:305:MSE:CE	2.43	0.95
1:A:89:PHE:CE1	6:A:2138:HOH:O	2.19	0.94
1:A:179:ARG:CB	1:A:180:LYS:HB3	1.99	0.91
1:B:493:SER:HA	1:B:494:SER:CB	2.01	0.91
1:A:493:SER:HB2	6:A:2369:HOH:O	1.70	0.89
1:A:198[B]:MSE:HE3	1:A:539:ILE:N	1.86	0.89
4:B:1558:GOL:H12	6:B:2502:HOH:O	1.72	0.89
1:A:300:VAL:CG2	1:A:305:MSE:HE2	2.02	0.88
1:A:436:PHE:N	4:A:1556:GOL:H11	1.89	0.88
1:A:448:LYS:CE	6:A:2332:HOH:O	2.12	0.88
1:A:198[B]:MSE:CE	1:A:539:ILE:H	1.87	0.86
1:A:270:ASN:HB2	6:A:2199:HOH:O	1.75	0.86
1:A:76:ARG:NH2	1:A:166:SER:O	2.09	0.86
1:B:493:SER:CB	1:B:494:SER:HB2	2.04	0.85
1:A:425:MSE:SE	6:A:2291:HOH:O	2.44	0.85
1:A:527[B]:GLN:HG2	6:A:2391:HOH:O	1.76	0.85
1:B:32:MSE:HE2	6:B:2006:HOH:O	1.76	0.84
1:A:89:PHE:CE2	1:A:214:VAL:HG22	2.12	0.84
1:B:404:ARG:HH12	4:B:1561:GOL:H2	1.41	0.84
1:A:211:SER:HB2	6:A:2136:HOH:O	1.78	0.83
1:A:493:SER:CA	1:A:494:SER:CB	2.55	0.83
1:B:204:ARG:HH21	4:B:1559:GOL:H32	1.42	0.83
1:B:234:ASN:HA	1:B:237:LYS:HD2	1.58	0.83
1:B:237:LYS:HE2	1:B:280:TRP:CZ3	2.13	0.82
1:A:539:ILE:HA	6:A:2398:HOH:O	1.79	0.82
4:A:1558:GOL:H31	6:A:2416:HOH:O	1.80	0.82
1:B:493:SER:CA	1:B:494:SER:OG	2.23	0.81
1:B:495:LYS:HE2	6:B:2364:HOH:O	1.80	0.81
1:A:300:VAL:HG22	1:A:305:MSE:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:THR:HB	6:B:2084:HOH:O	1.80	0.81
1:A:300:VAL:CG2	1:A:305:MSE:HE3	2.09	0.80
1:B:75:ASN:HB2	6:B:2034:HOH:O	1.80	0.79
4:B:1559:GOL:H31	6:B:2506:HOH:O	1.82	0.78
1:A:110:THR:HG21	1:A:136:ASP:HB3	1.64	0.78
1:B:237:LYS:HE2	1:B:280:TRP:HZ3	1.48	0.78
1:B:493:SER:CA	1:B:494:SER:CB	2.61	0.78
1:A:113:PHE:HA	6:A:2066:HOH:O	1.84	0.77
2:D:2:XYP:O4	2:D:3:XYP:C2	2.32	0.77
1:A:527[A]:GLN:HG2	6:A:2391:HOH:O	1.85	0.77
1:A:116:SER:HB2	6:A:2067:HOH:O	1.83	0.77
1:A:237:LYS:HE2	1:A:280:TRP:CZ3	2.19	0.77
1:A:425:MSE:CE	1:A:449:TYR:CD2	2.65	0.76
1:A:198[B]:MSE:HE1	1:A:538:ILE:H	1.48	0.76
1:A:180:LYS:HA	1:A:180:LYS:HE2	1.66	0.75
1:A:153:LYS:HG3	6:A:2094:HOH:O	1.86	0.75
4:B:1557:GOL:C3	6:B:2500:HOH:O	2.35	0.75
1:A:425:MSE:HE3	1:A:449:TYR:CE2	2.21	0.74
1:A:535:VAL:HG13	6:A:2122:HOH:O	1.88	0.73
1:B:67:GLY:HA2	6:B:2022:HOH:O	1.87	0.73
4:A:1558:GOL:O1	6:A:2417:HOH:O	2.07	0.73
1:A:488:ASP:HB3	6:A:2357:HOH:O	1.88	0.73
2:D:2:XYP:C4	2:D:3:XYP:C1	2.66	0.73
1:A:34:TYR:CE1	6:A:2113:HOH:O	2.40	0.73
1:B:494:SER:CB	6:B:2445:HOH:O	2.36	0.73
1:A:493:SER:CA	1:A:494:SER:HB2	2.10	0.73
1:B:466:GLU:HG2	6:B:2409:HOH:O	1.89	0.73
1:A:469:LYS:HZ1	4:B:1558:GOL:H31	1.55	0.72
1:B:493:SER:HA	1:B:494:SER:HG	1.54	0.72
1:A:274:ARG:HE	1:A:457:GLN:NE2	1.87	0.72
4:B:1561:GOL:H31	6:B:2356:HOH:O	1.90	0.72
4:A:1560:GOL:C1	6:A:2400:HOH:O	2.37	0.72
1:A:473[A]:GLN:HG2	6:A:2348:HOH:O	1.90	0.71
1:B:80:SER:HA	6:B:2041:HOH:O	1.89	0.71
1:A:469:LYS:NZ	4:B:1558:GOL:H31	2.06	0.71
1:A:179:ARG:CA	1:A:180:LYS:HB3	2.21	0.71
4:B:1557:GOL:C2	6:B:2500:HOH:O	2.37	0.70
1:B:144:GLU:HG3	6:B:2064:HOH:O	1.91	0.70
1:B:494:SER:HB2	6:B:2445:HOH:O	1.91	0.70
1:A:179:ARG:CA	1:A:180:LYS:CB	2.71	0.69
1:A:76:ARG:HH12	1:A:164:THR:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:SER:OG	1:B:494:SER:CB	2.39	0.69
1:A:471:SER:HB2	1:A:473[A]:GLN:OE1	1.93	0.68
1:A:34:TYR:CD2	6:A:2005:HOH:O	2.46	0.68
1:A:153:LYS:HE2	1:A:154:THR:HG23	1.75	0.68
1:A:180:LYS:CG	6:A:2052:HOH:O	2.41	0.68
1:B:86:GLU:OE1	1:B:157[B]:ASN:OD1	2.12	0.68
1:A:110:THR:CG2	1:A:136:ASP:HB3	2.23	0.67
1:A:415:TYR:OH	1:A:495:LYS:HE2	1.94	0.67
1:A:433:MSE:HE1	1:A:477:ASP:O	1.93	0.67
1:B:204:ARG:HH21	4:B:1559:GOL:C3	2.07	0.67
1:A:440:GLN:HG3	6:A:2322:HOH:O	1.95	0.67
1:A:198[C]:MSE:HE3	1:A:544:TRP:CZ2	2.29	0.67
1:A:234:ASN:HA	1:A:237:LYS:HD2	1.76	0.66
1:A:473[A]:GLN:CD	1:A:473[A]:GLN:H	2.04	0.66
1:A:176:THR:HG22	6:A:2110:HOH:O	1.95	0.65
1:A:237:LYS:HE2	1:A:280:TRP:HZ3	1.61	0.65
1:A:425:MSE:CE	1:A:449:TYR:HD2	1.97	0.65
1:A:180:LYS:HG2	6:A:2052:HOH:O	1.96	0.65
1:B:89:PHE:HA	6:B:2051:HOH:O	1.96	0.65
1:A:268:GLN:HG2	6:A:2192:HOH:O	1.96	0.65
1:A:179:ARG:HA	1:A:180:LYS:CB	2.28	0.64
1:B:141:GLU:HA	6:B:2109:HOH:O	1.97	0.64
4:B:1561:GOL:C1	6:B:2509:HOH:O	2.30	0.64
4:A:1558:GOL:C3	6:A:2416:HOH:O	2.42	0.64
1:B:88:GLY:HA3	1:B:215:ASN:OD1	1.98	0.64
1:A:35:GLU:HA	1:A:178:THR:HG22	1.79	0.64
1:B:225:ARG:HD3	6:B:2193:HOH:O	1.96	0.64
1:B:58:THR:HG22	6:B:2018:HOH:O	1.97	0.64
4:B:1557:GOL:C1	6:B:2500:HOH:O	2.47	0.64
1:A:433:MSE:HE3	1:A:477:ASP:HB3	1.79	0.63
1:B:120:LEU:HG	6:B:2089:HOH:O	1.98	0.63
1:B:493:SER:CB	1:B:494:SER:CB	2.76	0.62
1:A:118:SER:OG	1:A:129:LYS:HB3	2.00	0.61
4:A:1556:GOL:H2	6:A:2412:HOH:O	1.99	0.61
1:B:58:THR:HG23	1:B:322:ARG:NH1	2.15	0.61
1:A:463:ILE:HD12	1:A:479:TYR:CD1	2.36	0.61
1:A:549:ASN:HB3	6:A:2406:HOH:O	2.00	0.61
1:B:198[B]:MSE:HG2	1:B:544:TRP:CE2	2.35	0.61
1:A:167:THR:HG23	6:A:2106:HOH:O	1.99	0.60
1:A:87:LYS:HB2	1:A:91:LEU:HD22	1.82	0.60
1:A:130:GLU:HB2	6:A:2091:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB3	6:A:2074:HOH:O	2.02	0.60
4:B:1557:GOL:H31	6:B:2500:HOH:O	1.96	0.60
1:A:198[B]:MSE:HE1	1:A:538:ILE:N	2.17	0.59
1:A:493:SER:CB	1:A:494:SER:HB3	2.31	0.59
1:A:440:GLN:CG	6:A:2322:HOH:O	2.48	0.59
1:A:289:PHE:HA	1:A:305:MSE:HE1	1.84	0.59
1:B:495:LYS:CE	6:B:2364:HOH:O	2.42	0.59
1:A:180:LYS:HA	1:A:180:LYS:CE	2.32	0.59
1:A:473[A]:GLN:CG	6:A:2348:HOH:O	2.51	0.58
1:A:198[B]:MSE:HG3	1:A:539:ILE:HB	1.84	0.58
1:A:198[B]:MSE:HE2	1:A:199:TYR:OH	2.03	0.58
1:A:179:ARG:HA	1:A:180:LYS:HB2	1.85	0.58
1:A:211:SER:CB	6:A:2136:HOH:O	2.45	0.58
1:A:469:LYS:NZ	4:B:1558:GOL:C3	2.67	0.58
1:B:186:ASN:O	1:B:187:THR:HB	2.02	0.58
1:A:457:GLN:HG2	1:A:500:ALA:HB3	1.86	0.58
1:B:33:ASP:HB3	6:B:2005:HOH:O	2.04	0.58
1:A:198[B]:MSE:HE3	1:A:539:ILE:HG12	1.85	0.57
1:A:220:LYS:HE3	6:A:2148:HOH:O	2.04	0.57
4:A:1556:GOL:H12	1:B:469:LYS:HZ2	1.69	0.57
1:A:433:MSE:CE	1:A:477:ASP:C	2.77	0.57
1:B:239:ASP:HB3	6:B:2203:HOH:O	2.03	0.57
1:A:40:THR:O	1:A:42:GLU:HG2	2.05	0.57
1:A:34:TYR:HE1	6:A:2113:HOH:O	1.84	0.57
1:B:135:LYS:HB2	6:B:2097:HOH:O	2.04	0.57
1:B:493:SER:HB2	6:B:2442:HOH:O	2.04	0.57
1:A:463:ILE:HD12	1:A:479:TYR:CG	2.40	0.57
1:B:198[A]:MSE:HG2	1:B:544:TRP:CE2	2.39	0.57
4:A:1556:GOL:H12	1:B:469:LYS:NZ	2.19	0.57
1:A:464:SER:HB2	4:A:1559:GOL:H31	1.87	0.56
4:A:1556:GOL:C2	6:A:2412:HOH:O	2.50	0.56
1:A:541:GLN:HA	1:A:544:TRP:CE2	2.40	0.56
1:B:204:ARG:NH2	4:B:1559:GOL:H32	2.15	0.56
1:A:86[B]:GLU:HG3	1:A:157:ASN:OD1	2.05	0.55
1:A:388:ASN:HB3	6:A:2283:HOH:O	2.05	0.55
1:B:113:PHE:HA	6:B:2077:HOH:O	2.05	0.55
1:B:463:ILE:HD12	1:B:479:TYR:CD1	2.42	0.55
1:A:128:ASN:CB	6:A:2073:HOH:O	2.55	0.55
1:A:164:THR:HG22	6:A:2066:HOH:O	2.06	0.55
1:B:125:GLU:OE2	1:B:125:GLU:HA	2.07	0.54
1:A:494:SER:HB2	6:A:2371:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:HB2	1:B:161[B]:SER:OG	2.07	0.54
1:B:214:VAL:HG13	1:B:214:VAL:O	2.07	0.54
1:A:425:MSE:CE	1:A:449:TYR:CE2	2.87	0.54
1:A:214:VAL:HG12	1:A:215:ASN:ND2	2.23	0.54
1:B:53:VAL:HB	6:B:2014:HOH:O	2.08	0.53
1:B:135:LYS:HB3	1:B:145:ILE:HD12	1.89	0.53
1:A:60:VAL:HG23	1:A:63:GLU:HB2	1.91	0.53
1:A:198[B]:MSE:HE2	1:A:199:TYR:CZ	2.44	0.53
1:B:116:SER:HB2	1:B:161[B]:SER:HG	1.74	0.53
1:A:90:TYR:HA	6:A:2149:HOH:O	2.08	0.53
1:B:436:PHE:HB2	4:B:1558:GOL:H32	1.91	0.52
1:B:497:LYS:HE3	6:B:2436:HOH:O	2.09	0.52
1:B:32:MSE:HG3	1:B:33:ASP:N	2.25	0.52
1:A:180:LYS:HG3	6:A:2052:HOH:O	2.06	0.52
1:B:375:GLU:HG2	6:B:2329:HOH:O	2.10	0.52
1:A:33:ASP:HA	6:A:2002:HOH:O	2.08	0.51
1:A:198[B]:MSE:SE	1:A:536:ALA:HA	2.61	0.51
1:B:86:GLU:HG2	6:B:2021:HOH:O	2.09	0.51
1:A:535:VAL:HG22	6:A:2122:HOH:O	2.09	0.51
1:A:34:TYR:O	1:A:179:ARG:O	2.27	0.51
1:A:95:VAL:HG11	6:A:2111:HOH:O	2.10	0.51
1:A:108:THR:HA	6:A:2059:HOH:O	2.10	0.51
1:A:128:ASN:HB2	6:A:2073:HOH:O	2.10	0.51
1:A:34:TYR:HD2	6:A:2005:HOH:O	1.87	0.50
1:B:208:VAL:HG21	1:B:504:TRP:CE3	2.47	0.50
1:B:401[A]:ASP:OD1	1:B:402:HIS:N	2.44	0.50
1:A:76:ARG:HH12	1:A:164:THR:N	2.09	0.50
1:A:189:TYR:CE2	1:A:191:ALA:HA	2.47	0.50
1:A:40:THR:O	1:A:42:GLU:N	2.44	0.50
1:A:198[B]:MSE:CE	1:A:535:VAL:O	2.60	0.49
1:B:118:SER:HB2	6:B:2082:HOH:O	2.11	0.49
1:B:121:ASP:C	6:B:2084:HOH:O	2.56	0.49
1:A:63:GLU:O	1:A:142:TRP:HZ2	1.96	0.49
1:A:215:ASN:HB3	6:A:2099:HOH:O	2.12	0.48
1:A:45:PHE:CD1	1:A:71:MSE:HE1	2.49	0.48
1:B:372:LYS:HE2	6:B:2260:HOH:O	2.14	0.48
1:A:34:TYR:CD1	6:A:2113:HOH:O	2.63	0.48
1:A:309:LEU:HD13	1:A:364:TRP:CH2	2.49	0.48
1:A:84:TYR:HE1	6:A:2042:HOH:O	1.97	0.48
1:A:212:GLY:N	6:A:2136:HOH:O	2.47	0.48
1:A:198[B]:MSE:CG	1:A:539:ILE:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:CYS:HB3	1:B:257:ASN:CG	2.39	0.47
1:A:268:GLN:OE1	4:A:1561:GOL:H11	2.14	0.47
1:A:289:PHE:HA	1:A:305:MSE:CE	2.44	0.47
1:B:92:ASP:HB2	1:B:95:VAL:CG2	2.44	0.47
1:A:433:MSE:HE1	1:A:477:ASP:C	2.40	0.47
4:A:1560:GOL:H12	6:A:2400:HOH:O	2.08	0.47
1:B:37:VAL:HB	1:B:177:ILE:HG13	1.97	0.47
1:B:270:ASN:HB2	6:B:2234:HOH:O	2.14	0.47
1:A:111:GLU:HA	1:A:111:GLU:OE1	2.15	0.47
2:D:2:XYP:O4	2:D:3:XYP:O5	2.30	0.47
1:A:164:THR:HG21	1:A:168:VAL:CG1	2.45	0.47
1:B:81:ASP:O	1:B:163:THR:HG22	2.15	0.47
1:B:137:VAL:HG22	1:B:143:THR:HG21	1.97	0.46
1:A:433:MSE:CE	1:A:477:ASP:HB3	2.43	0.46
1:A:425:MSE:CE	6:A:2291:HOH:O	2.62	0.46
1:A:128:ASN:HB3	6:A:2073:HOH:O	2.15	0.46
1:B:58:THR:HG23	1:B:322:ARG:HH12	1.80	0.46
1:B:494:SER:HA	1:B:497:LYS:NZ	2.30	0.46
1:A:129:LYS:HB2	1:A:129:LYS:NZ	2.31	0.46
1:A:215:ASN:HB2	6:A:2137:HOH:O	2.15	0.46
1:A:198[B]:MSE:SE	1:A:536:ALA:C	3.10	0.45
1:A:388:ASN:HD22	1:A:388:ASN:H	1.63	0.45
1:A:189:TYR:N	6:A:2114:HOH:O	2.49	0.45
1:B:75:ASN:N	6:B:2034:HOH:O	2.50	0.45
1:B:108:THR:HA	6:B:2070:HOH:O	2.16	0.45
1:B:95:VAL:HG11	6:B:2140:HOH:O	2.16	0.45
1:A:86[A]:GLU:CD	6:A:2042:HOH:O	2.58	0.44
1:B:32:MSE:N	6:B:2001:HOH:O	2.50	0.44
1:A:527[A]:GLN:CG	6:A:2391:HOH:O	2.56	0.44
1:B:126:GLU:HG3	6:B:2088:HOH:O	2.17	0.44
1:B:494:SER:HB3	6:B:2445:HOH:O	2.10	0.44
1:A:549:ASN:HA	6:A:2405:HOH:O	2.17	0.44
1:B:32:MSE:HG3	1:B:33:ASP:H	1.82	0.44
1:A:129:LYS:NZ	6:A:2071:HOH:O	2.50	0.44
1:A:392:TYR:CE2	1:A:422:GLY:HA3	2.53	0.44
1:B:92:ASP:HB2	1:B:95:VAL:HG21	2.00	0.44
1:B:283:GLN:H	4:B:1557:GOL:C2	2.30	0.44
1:A:189:TYR:HE2	1:A:191:ALA:HA	1.82	0.44
1:A:198[C]:MSE:HG2	1:A:544:TRP:CE2	2.53	0.44
1:B:129:LYS:HE3	6:B:2093:HOH:O	2.17	0.43
1:A:274:ARG:HE	1:A:457:GLN:HE22	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:SER:CB	1:A:473[A]:GLN:OE1	2.65	0.43
1:B:59:ALA:HB2	1:B:71:MSE:HE1	1.99	0.43
1:A:127:GLU:HB2	1:B:126:GLU:OE1	2.18	0.43
1:A:153:LYS:CG	6:A:2094:HOH:O	2.56	0.43
1:B:193:ALA:HB1	1:B:198[A]:MSE:HE3	2.00	0.43
1:A:388:ASN:H	1:A:388:ASN:ND2	2.16	0.43
1:A:532:TYR:C	1:A:532:TYR:CD2	2.97	0.43
1:B:96:GLU:O	6:B:2056:HOH:O	2.21	0.43
1:A:507:ASN:C	1:A:507:ASN:OD1	2.62	0.43
1:B:161[A]:SER:HB2	6:B:2129:HOH:O	2.18	0.43
1:A:279:VAL:HG13	1:A:364:TRP:CE2	2.53	0.43
1:A:85:SER:OG	1:A:87:LYS:HE2	2.19	0.43
1:A:37:VAL:HB	1:A:177:ILE:HG13	2.01	0.43
1:B:270:ASN:CB	6:B:2234:HOH:O	2.66	0.43
1:A:493:SER:CA	1:A:494:SER:HB3	2.38	0.43
1:A:97:TYR:O	1:A:148:LYS:HA	2.19	0.43
1:A:469:LYS:HZ2	4:B:1558:GOL:C3	2.31	0.43
1:A:466:GLU:CG	6:A:2340:HOH:O	2.41	0.42
1:A:471:SER:OG	1:A:474:GLN:HG3	2.18	0.42
1:B:119:TYR:N	6:B:2082:HOH:O	2.47	0.42
1:B:186:ASN:O	1:B:187:THR:CB	2.65	0.42
1:B:433:MSE:HE2	6:B:2373:HOH:O	2.20	0.42
1:B:433:MSE:HE2	1:B:433:MSE:HB2	1.92	0.42
1:A:153:LYS:HE2	1:A:154:THR:CG2	2.45	0.42
1:A:396:TYR:HB3	1:A:426:GLN:OE1	2.20	0.42
1:A:460:GLU:HG2	1:A:504:TRP:CE3	2.55	0.42
1:B:122:SER:N	6:B:2084:HOH:O	2.52	0.42
1:B:215:ASN:HB3	6:B:2179:HOH:O	2.20	0.42
1:A:72:MSE:HG3	1:A:171:ILE:HG12	2.01	0.42
1:A:433:MSE:HE2	1:A:477:ASP:C	2.43	0.42
1:B:164:THR:HG21	1:B:168:VAL:HG12	2.01	0.42
1:B:123:GLU:HB3	6:B:2123:HOH:O	2.19	0.42
1:A:169:ASP:CB	6:A:2107:HOH:O	2.20	0.41
1:A:415:TYR:HH	1:A:495:LYS:HE2	1.85	0.41
1:A:68:THR:HA	6:A:2007:HOH:O	2.20	0.41
1:B:460:GLU:O	1:B:461:LEU:C	2.62	0.41
1:A:179:ARG:HA	1:A:180:LYS:HB3	1.94	0.41
1:B:86:GLU:CD	1:B:157[B]:ASN:OD1	2.63	0.41
1:B:310:GLU:HG3	1:B:380:TYR:CD1	2.55	0.41
1:B:241:THR:O	1:B:254:VAL:HA	2.21	0.41
1:B:492:THR:HG22	1:B:493:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:HA	1:A:178:THR:O	2.21	0.41
1:B:129:LYS:NZ	6:B:2095:HOH:O	2.53	0.41
1:B:493:SER:OG	1:B:494:SER:CA	2.69	0.41
1:B:544:TRP:CD1	1:B:544:TRP:N	2.86	0.41
1:A:45:PHE:CG	1:A:71:MSE:HE1	2.56	0.40
1:B:67:GLY:CA	6:B:2022:HOH:O	2.59	0.40
1:B:532:TYR:CD2	1:B:532:TYR:C	2.99	0.40
1:A:401:ASP:HB2	6:A:2296:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2364:HOH:O	6:B:2255:HOH:O[6_765]	2.13	0.07

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	513/540 (95%)	485 (94%)	23 (4%)	5 (1%)	12	24
1	B	518/540 (96%)	488 (94%)	26 (5%)	4 (1%)	16	31
All	All	1031/1080 (96%)	973 (94%)	49 (5%)	9 (1%)	14	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PHE
1	A	180	LYS
1	B	187	THR
1	B	494	SER
1	A	33	ASP

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Mol	Chain	Res	Type
1	A	494	SER
1	A	62	ASN
1	B	188	VAL
1	B	214	VAL

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	436/443 (98%)	411 (94%)	25 (6%)	18	39
1	B	441/443 (100%)	419 (95%)	22 (5%)	22	44
All	All	877/886 (99%)	830 (95%)	47 (5%)	20	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	91	LEU
1	A	116	SER
1	A	120	LEU
1	A	123	GLU
1	A	128	ASN
1	A	129	LYS
1	A	143	THR
1	A	153	LYS
1	A	164	THR
1	A	167	THR
1	A	176	THR
1	A	177	ILE
1	A	179	ARG
1	A	214	VAL
1	A	245	SER
1	A	261	SER
1	A	268	GLN
1	A	347	ARG

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	382	ARG
1	A	409	SER
1	A	420	LEU
1	A	511	THR
1	A	535	VAL
1	B	53	VAL
1	B	58	THR
1	B	77	SER
1	B	86	GLU
1	B	89	PHE
1	B	95	VAL
1	B	125	GLU
1	B	128	ASN
1	B	134	THR
1	B	157[A]	ASN
1	B	157[B]	ASN
1	B	164	THR
1	B	165	ASP
1	B	177	ILE
1	B	178	THR
1	B	218	SER
1	B	268	GLN
1	B	382	ARG
1	B	473	GLN
1	B	480	LYS
1	B	511	THR
1	B	525	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	298	ASN
1	A	366	GLN
1	A	388	ASN
1	A	416	ASN
1	A	440	GLN
1	A	447	GLN
1	A	457	GLN
1	B	251	ASN
1	B	283	GLN

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Mol	Chain	Res	Type
1	B	302	GLN
1	B	307	GLN
1	B	315	ASN
1	B	328	ASN
1	B	366	GLN
1	B	394	ASN
1	B	413	ASN
1	B	434	ASN
1	B	447	GLN
1	B	484	GLN
1	B	541	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 ⓘ

6 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	XYP	C	1	2	10,10,10	1.01	0	14,14,14	1.88	3 (21%)
2	XYP	C	2	2	9,9,10	1.41	2 (22%)	10,12,14	1.39	1 (10%)
2	XYP	C	3	2	9,9,10	1.18	1 (11%)	10,12,14	2.65	6 (60%)
2	XYP	D	1	2	10,10,10	1.39	0	14,14,14	1.67	3 (21%)
2	XYP	D	2	2	9,9,10	1.41	1 (11%)	10,12,14	2.02	3 (30%)
2	XYP	D	3	2	9,9,10	1.00	0	10,12,14	2.05	3 (30%)

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	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
2	XYP	D	1	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1
2	XYP	D	3	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	XYP	O5-C5	3.91	1.50	1.43
2	C	2	XYP	C4-C3	-3.22	1.47	1.52
2	C	2	XYP	O4-C4	2.45	1.48	1.43
2	C	3	XYP	O4-C4	2.39	1.48	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	XYP	C5-O5-C1	5.19	119.80	111.42
2	C	1	XYP	C5-O5-C1	4.42	121.64	112.46
2	D	2	XYP	O4-C4-C5	3.94	118.25	109.22
2	D	1	XYP	C5-O5-C1	3.87	120.50	112.46
2	D	3	XYP	C5-C4-C3	3.78	115.15	109.64
2	C	3	XYP	C1-C2-C3	-3.67	104.30	109.64
2	D	3	XYP	C5-O5-C1	3.45	116.98	111.42
2	C	3	XYP	O3-C3-C2	-3.19	103.54	110.05
2	C	2	XYP	O4-C4-C5	3.17	116.49	109.22
2	C	1	XYP	O3-C3-C4	-3.10	103.74	110.05
2	D	2	XYP	C5-O5-C1	3.07	116.37	111.42
2	D	3	XYP	C4-C3-C2	-2.78	107.62	110.92
2	C	1	XYP	O1-C1-O5	-2.63	103.17	109.91
2	C	3	XYP	O4-C4-C5	2.61	115.20	109.22
2	C	3	XYP	O4-C4-C3	2.51	115.34	110.15
2	D	2	XYP	C4-C3-C2	2.24	113.58	110.92
2	D	1	XYP	O5-C5-C4	-2.16	105.63	110.79
2	C	3	XYP	O3-C3-C4	-2.04	105.89	110.05
2	D	1	XYP	O2-C2-C3	2.02	115.13	110.38

There are no chirality outliers.

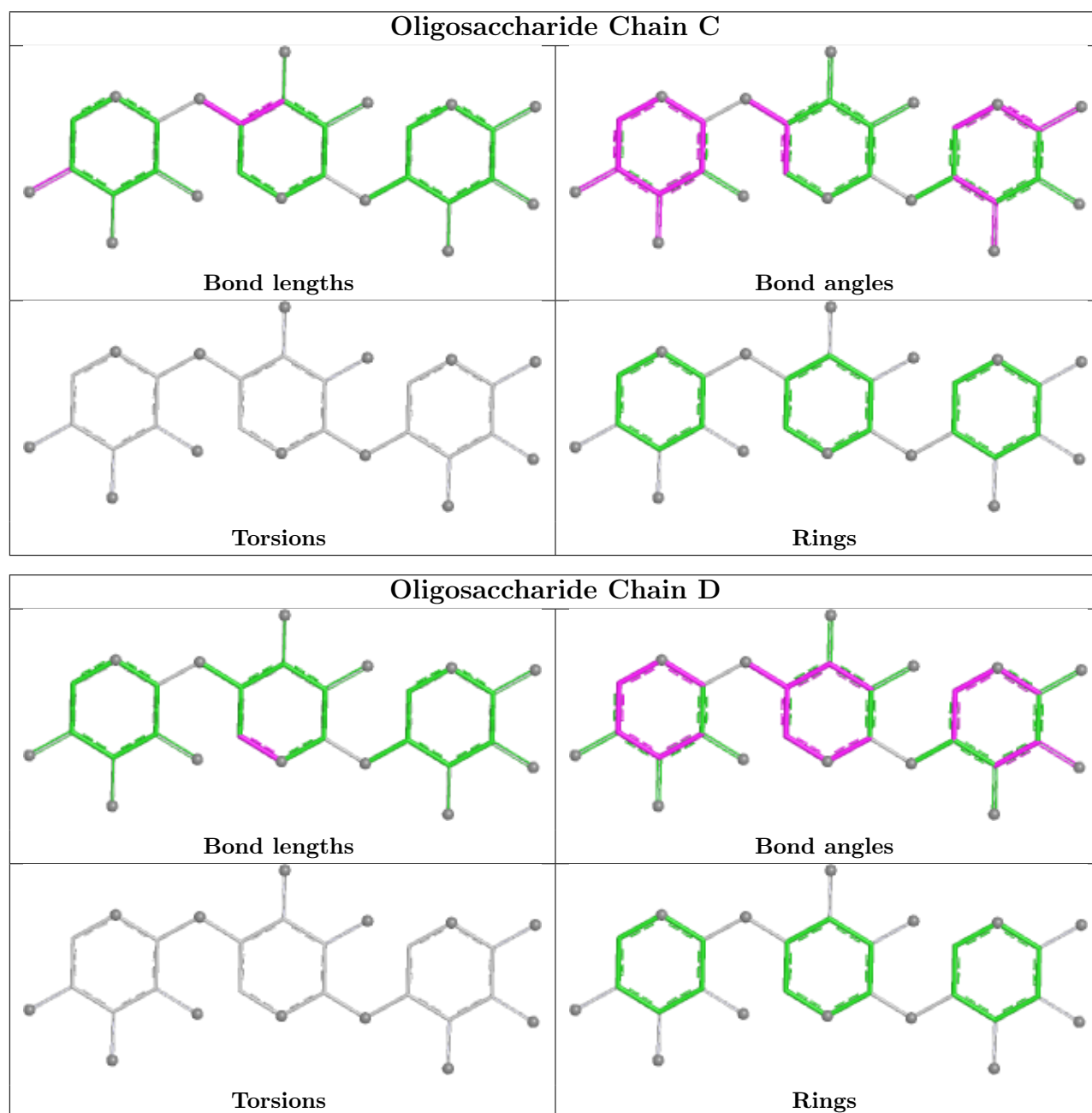
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	XYP	3	0
2	D	3	XYP	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.



5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are 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
4	GOL	B	1558	-	5,5,5	0.61	0	5,5,5	0.80	0
4	GOL	A	1558	-	5,5,5	1.00	0	5,5,5	1.37	1 (20%)
4	GOL	B	1560	-	5,5,5	0.41	0	5,5,5	0.94	0
4	GOL	B	1559	-	5,5,5	0.50	0	5,5,5	1.28	0
4	GOL	B	1556	-	5,5,5	0.73	0	5,5,5	0.63	0
5	PO4	A	1562	-	4,4,4	1.41	1 (25%)	6,6,6	1.63	1 (16%)
4	GOL	B	1561	-	5,5,5	0.69	0	5,5,5	1.28	0
4	GOL	A	1560	-	5,5,5	0.44	0	5,5,5	0.83	0
4	GOL	A	1561	-	5,5,5	0.49	0	5,5,5	1.45	0
5	PO4	B	1562	-	4,4,4	1.06	0	6,6,6	1.23	1 (16%)
4	GOL	B	1557	-	5,5,5	1.81	1 (20%)	5,5,5	2.69	3 (60%)
4	GOL	A	1557	-	5,5,5	1.35	1 (20%)	5,5,5	2.51	3 (60%)
4	GOL	A	1556	-	5,5,5	0.82	0	5,5,5	1.00	1 (20%)
4	GOL	A	1559	-	5,5,5	1.29	0	5,5,5	1.97	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1558	-	-	2/4/4/4	-
4	GOL	A	1558	-	-	4/4/4/4	-
4	GOL	B	1560	-	-	2/4/4/4	-
4	GOL	B	1559	-	-	4/4/4/4	-
4	GOL	B	1556	-	-	4/4/4/4	-
4	GOL	B	1561	-	-	4/4/4/4	-
4	GOL	A	1560	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1561	-	-	0/4/4/4	-
4	GOL	B	1557	-	-	3/4/4/4	-
4	GOL	A	1557	-	-	4/4/4/4	-
4	GOL	A	1556	-	-	1/4/4/4	-
4	GOL	A	1559	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1557	GOL	C1-C2	2.88	1.62	1.51
5	A	1562	PO4	P-O1	2.54	1.56	1.50
4	A	1557	GOL	C3-C2	2.28	1.60	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1559	GOL	O3-C3-C2	4.10	128.82	110.38
4	A	1557	GOL	O3-C3-C2	3.87	127.81	110.38
4	B	1557	GOL	O1-C1-C2	3.71	127.08	110.38
4	B	1557	GOL	O2-C2-C1	3.69	124.46	109.18
4	A	1557	GOL	O2-C2-C1	-3.50	94.69	109.18
5	A	1562	PO4	O4-P-O2	-2.43	100.36	107.91
4	A	1558	GOL	O3-C3-C2	2.29	120.68	110.38
4	B	1557	GOL	C3-C2-C1	2.28	120.14	111.80
5	B	1562	PO4	O4-P-O3	2.15	114.60	107.91
4	A	1557	GOL	C3-C2-C1	2.01	119.17	111.80
4	A	1556	GOL	O2-C2-C1	-2.01	100.86	109.18

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1557	GOL	O1-C1-C2-O2
4	A	1557	GOL	O1-C1-C2-C3
4	A	1558	GOL	C1-C2-C3-O3
4	A	1559	GOL	O1-C1-C2-O2
4	A	1559	GOL	O1-C1-C2-C3
4	A	1559	GOL	C1-C2-C3-O3
4	A	1560	GOL	C1-C2-C3-O3
4	B	1557	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1557	GOL	C1-C2-C3-O3
4	B	1559	GOL	O1-C1-C2-O2
4	B	1559	GOL	O1-C1-C2-C3
4	B	1559	GOL	C1-C2-C3-O3
4	B	1561	GOL	O1-C1-C2-C3
4	A	1556	GOL	C1-C2-C3-O3
4	A	1557	GOL	C1-C2-C3-O3
4	A	1558	GOL	O1-C1-C2-C3
4	B	1556	GOL	O1-C1-C2-C3
4	B	1556	GOL	C1-C2-C3-O3
4	B	1558	GOL	C1-C2-C3-O3
4	B	1560	GOL	O1-C1-C2-C3
4	B	1561	GOL	C1-C2-C3-O3
4	A	1558	GOL	O2-C2-C3-O3
4	B	1556	GOL	O1-C1-C2-O2
4	B	1559	GOL	O2-C2-C3-O3
4	B	1560	GOL	O1-C1-C2-O2
4	A	1557	GOL	O2-C2-C3-O3
4	A	1560	GOL	O2-C2-C3-O3
4	A	1558	GOL	O1-C1-C2-O2
4	A	1559	GOL	O2-C2-C3-O3
4	B	1558	GOL	O2-C2-C3-O3
4	B	1561	GOL	O1-C1-C2-O2
4	B	1557	GOL	O2-C2-C3-O3
4	B	1556	GOL	O2-C2-C3-O3
4	B	1561	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1558	GOL	6	0
4	A	1558	GOL	3	0
4	B	1559	GOL	4	0
4	B	1556	GOL	1	0
4	B	1561	GOL	5	0
4	A	1560	GOL	2	0
4	A	1561	GOL	1	0
4	B	1557	GOL	5	0
4	A	1556	GOL	6	0
4	A	1559	GOL	1	0

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	A	504/540 (93%)	-0.04	16 (3%)	50	46	27, 57, 113, 139	3 (0%)
1	B	507/540 (93%)	-0.31	15 (2%)	52	48	23, 46, 102, 145	5 (0%)
All	All	1011/1080 (93%)	-0.18	31 (3%)	51	47	23, 52, 109, 145	8 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	GLY	8.8
1	B	188	VAL	6.8
1	B	187	THR	5.8
1	B	181	GLY	4.4
1	A	34	TYR	4.2
1	B	180	LYS	4.0
1	B	124	THR	3.6
1	B	108	THR	3.5
1	A	153	LYS	3.3
1	A	124	THR	3.2
1	A	108	THR	3.2
1	B	95	VAL	3.1
1	B	153	LYS	3.1
1	A	109	GLY	3.0
1	A	134	THR	2.9
1	A	148	LYS	2.8
1	A	189	TYR	2.7
1	A	129	LYS	2.6
1	A	33	ASP	2.5
1	B	186	ASN	2.5
1	B	126	GLU	2.4
1	B	110	THR	2.3
1	A	138	VAL	2.1
1	A	110	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	SER	2.1
1	A	131	VAL	2.1
1	B	33	ASP	2.1
1	A	190	ALA	2.1
1	B	148	LYS	2.1
1	A	128	ASN	2.0
1	B	34	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

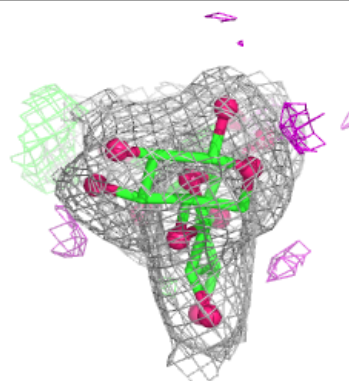
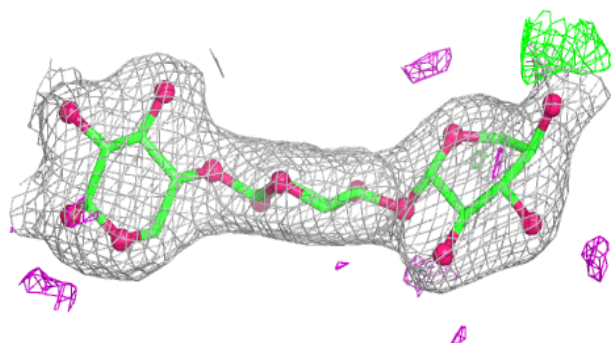
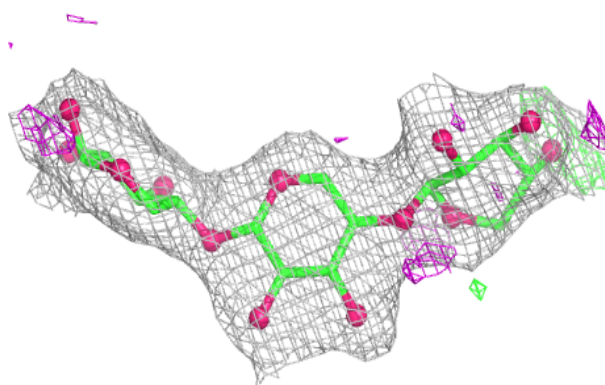
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYP	C	3	9/10	0.90	0.13	56,65,74,78	0
2	XYP	D	3	9/10	0.94	0.10	61,66,70,77	0
2	XYP	C	2	9/10	0.98	0.05	30,33,39,40	0
2	XYP	D	1	10/10	0.99	0.04	29,33,36,38	0
2	XYP	D	2	9/10	0.99	0.04	30,34,41,43	0
2	XYP	C	1	10/10	0.99	0.05	35,36,38,40	0

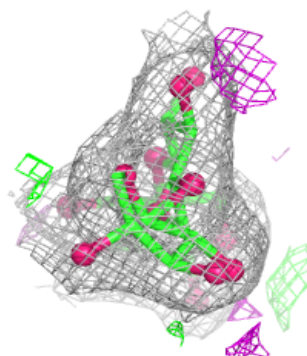
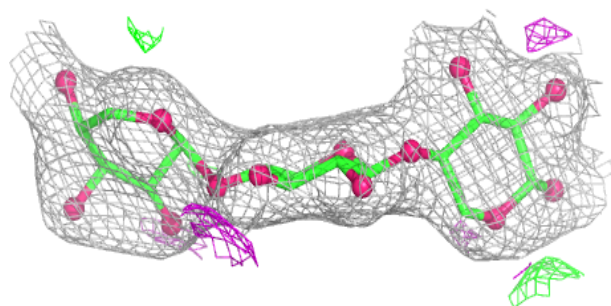
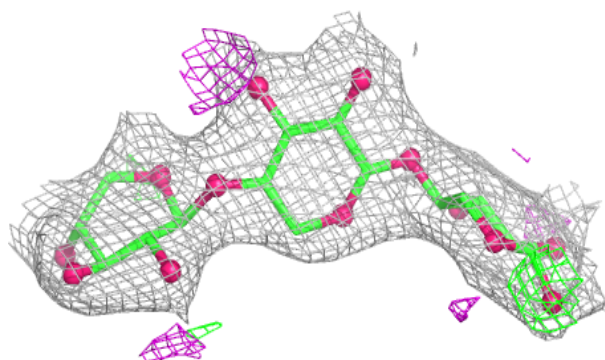
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	B	1558	6/6	0.86	0.18	64,75,78,78	0
4	GOL	A	1561	6/6	0.87	0.23	91,99,100,103	0
4	GOL	A	1559	6/6	0.87	0.22	51,66,67,67	0
4	GOL	B	1561	6/6	0.87	0.16	81,82,84,84	0
4	GOL	B	1557	6/6	0.88	0.18	51,62,67,67	0
4	GOL	A	1558	6/6	0.89	0.23	81,87,89,91	0
4	GOL	A	1556	6/6	0.89	0.16	67,74,75,77	0
4	GOL	A	1557	6/6	0.90	0.20	56,65,69,70	0
4	GOL	B	1559	6/6	0.92	0.15	74,78,81,81	0
5	PO4	B	1562	5/5	0.92	0.10	97,98,102,103	0
4	GOL	A	1560	6/6	0.93	0.13	73,74,77,80	0
4	GOL	B	1560	6/6	0.93	0.14	66,72,75,79	0
5	PO4	A	1562	5/5	0.94	0.13	72,73,77,78	0
4	GOL	B	1556	6/6	0.97	0.11	51,62,69,78	0
3	CA	A	1552	1/1	0.98	0.05	76,76,76,76	0
3	CA	B	1552	1/1	0.99	0.03	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.