



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID : 3I5O / pdb_00003i5o
Title : The X-ray crystal structure of a thermophilic cellobiose binding protein bound with cellopentaose
Authors : Cuneo, M.J.; Hellinga, H.W.
Deposited on : 2009-07-06
Resolution : 1.50 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

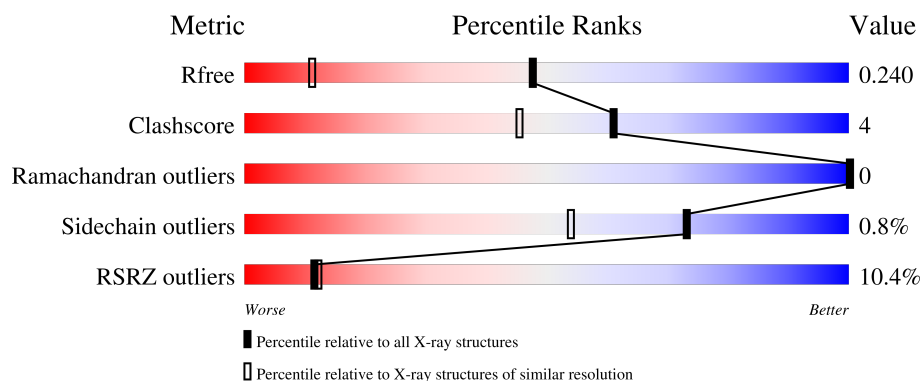
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	592	9% 92% 6%
1	B	592	11% 91% 7%
2	C	5	100%
2	D	5	100%

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
2	BGC	D	3	-	-	X	-
2	BGC	D	4	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10662 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 Oligopeptide ABC transporter, periplasmic oligopeptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	14	0
			4853	3189	771	877	16			
1	B	582	Total	C	N	O	S	0	5	0
			4810	3153	766	878	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q9WXN8
A	585	HIS	-	expression tag	UNP Q9WXN8
A	586	HIS	-	expression tag	UNP Q9WXN8
A	587	HIS	-	expression tag	UNP Q9WXN8
A	588	HIS	-	expression tag	UNP Q9WXN8
A	589	HIS	-	expression tag	UNP Q9WXN8
A	590	HIS	-	expression tag	UNP Q9WXN8
B	-1	MET	-	expression tag	UNP Q9WXN8
B	585	HIS	-	expression tag	UNP Q9WXN8
B	586	HIS	-	expression tag	UNP Q9WXN8
B	587	HIS	-	expression tag	UNP Q9WXN8
B	588	HIS	-	expression tag	UNP Q9WXN8
B	589	HIS	-	expression tag	UNP Q9WXN8
B	590	HIS	-	expression tag	UNP Q9WXN8

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total 56	C 30	O 26	0	0	0
2	D	5	Total 56	C 30	O 26	0	0	0

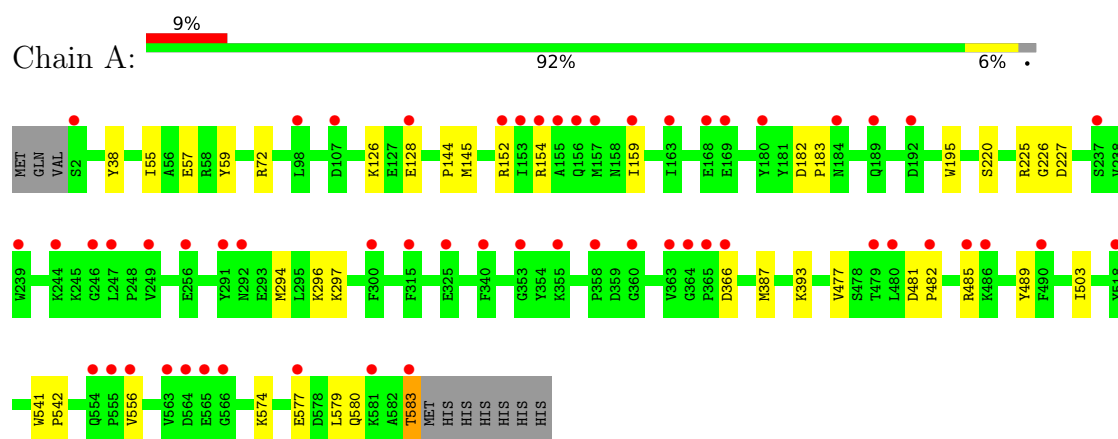
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total 454	O 454	0	0
3	B	433	Total 433	O 433	0	0

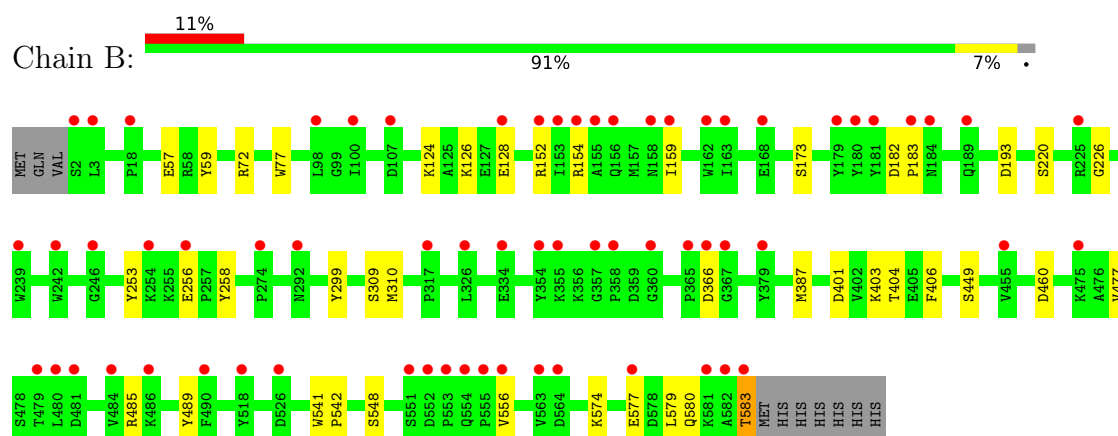
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

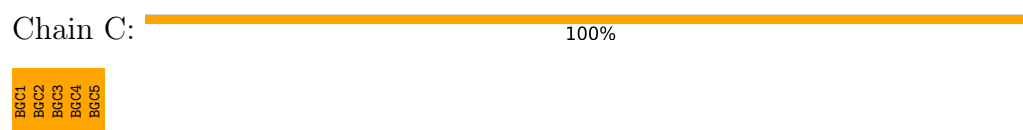
- Molecule 1: Oligopeptide ABC transporter, periplasmic oligopeptide-binding protein



- Molecule 1: Oligopeptide ABC transporter, periplasmic oligopeptide-binding protein



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



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

Chain D:  100%

BCC1
BCC2
BCC3
BCC4
BCC5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.11Å 101.46Å 108.29Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	48.67 – 1.50 48.67 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.67-1.50) 96.3 (48.67-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.50Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.225 (Not available) , 0.240	Depositor DCC
R_{free} test set	10325 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	1.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10662	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: BGC

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	0.37	0/5038	0.68	1/6879 (0.0%)
1	B	0.36	0/4980	0.67	0/6798
All	All	0.36	0/10018	0.68	1/13677 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ILE	N-CA-C	5.31	113.28	107.60

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	4853	0	4671	27	0
1	B	4810	0	4617	30	0
2	C	56	0	52	8	0
2	D	56	0	52	11	0
3	A	454	0	0	2	0
3	B	433	0	0	5	0
All	All	10662	0	9392	73	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 4.

All (73) 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)
2:D:2:BGC:HD	2:D:3:BGC:C1	1.86	0.85
1:A:296:LYS:O	1:B:152:ARG:HD3	1.77	0.84
2:D:3:BGC:HD	2:D:4:BGC:C1	1.90	0.82
2:D:4:BGC:HD	2:D:5:BGC:C1	2.01	0.73
1:A:57:GLU:HB3	1:A:72:ARG:HG2	1.70	0.72
1:B:57:GLU:HB3	1:B:72:ARG:HG2	1.70	0.72
2:D:2:BGC:C4	2:D:3:BGC:C1	2.69	0.70
2:D:3:BGC:C4	2:D:4:BGC:C1	2.70	0.70
2:C:2:BGC:C4	2:C:3:BGC:C1	2.70	0.69
2:C:4:BGC:C4	2:C:5:BGC:C1	2.73	0.66
2:C:3:BGC:C4	2:C:4:BGC:C1	2.73	0.66
1:A:485:ARG:HG2	1:A:489:TYR:CE2	2.33	0.64
1:B:485:ARG:HG2	1:B:489:TYR:CE2	2.33	0.64
1:A:126:LYS:HG2	1:A:128:GLU:OE2	2.01	0.60
2:D:4:BGC:C4	2:D:5:BGC:C1	2.79	0.60
1:B:126:LYS:HG2	1:B:128:GLU:OE2	2.02	0.59
1:A:55[B]:ILE:HD13	1:A:195:TRP:CZ2	2.37	0.58
1:A:393:LYS:HE2	1:B:193:ASP:OD2	2.04	0.56
2:C:3:BGC:O4	2:C:4:BGC:C2	2.53	0.56
1:A:297:LYS:HA	1:B:152:ARG:HG3	1.88	0.55
1:A:366:ASP:OD2	1:A:366:ASP:C	2.50	0.54
2:D:1:BGC:C4	2:D:2:BGC:C1	2.86	0.53
1:A:182:ASP:HB2	1:A:183:PRO:CD	2.38	0.53
1:B:366:ASP:C	1:B:366:ASP:OD2	2.51	0.53
1:A:182:ASP:HB2	1:A:183:PRO:HD2	1.91	0.52
1:B:182:ASP:HB2	1:B:183:PRO:CD	2.39	0.52
1:B:154:ARG:HB2	1:B:159:ILE:HD11	1.92	0.51
1:B:182:ASP:HB2	1:B:183:PRO:HD2	1.92	0.51
2:C:2:BGC:O4	2:C:3:BGC:C2	2.58	0.51
1:A:154:ARG:HB2	1:A:159:ILE:HD11	1.92	0.51
1:A:128:GLU:H	1:A:128:GLU:CD	2.20	0.50
2:D:2:BGC:O4	2:D:3:BGC:C2	2.60	0.50
1:A:485:ARG:HG2	1:A:489:TYR:CZ	2.47	0.50
2:C:1:BGC:C4	2:C:2:BGC:C1	2.90	0.50
1:B:128:GLU:H	1:B:128:GLU:CD	2.20	0.49
2:D:3:BGC:O4	2:D:4:BGC:C2	2.59	0.49
2:C:1:BGC:O4	2:C:2:BGC:C2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HG2	1:B:489:TYR:CZ	2.47	0.49
2:D:4:BGC:O4	2:D:5:BGC:C2	2.61	0.48
2:C:4:BGC:O4	2:C:5:BGC:C2	2.61	0.47
1:B:256:GLU:CG	3:B:2655:HOH:O	2.62	0.47
1:B:579:LEU:C	1:B:579:LEU:HD23	2.41	0.46
1:A:579:LEU:C	1:A:579:LEU:HD23	2.40	0.46
1:B:299:TYR:CD2	1:B:387:MET:CE	2.99	0.46
1:B:574:LYS:HA	1:B:577:GLU:OE1	2.16	0.45
1:A:574:LYS:HA	1:A:577:GLU:OE1	2.16	0.45
1:A:152:ARG:HE	1:A:152:ARG:HB3	1.50	0.45
1:B:152:ARG:HE	1:B:152:ARG:HB3	1.57	0.45
1:B:124:LYS:NZ	3:B:2667:HOH:O	2.50	0.44
1:B:256:GLU:HG3	3:B:2655:HOH:O	2.17	0.44
1:B:541:TRP:CG	1:B:542:PRO:HD3	2.53	0.44
1:B:548:SER:HB2	3:B:2375:HOH:O	2.19	0.43
1:B:226:GLY:HA2	3:B:2360:HOH:O	2.19	0.43
1:A:38:TYR:CG	1:A:145[A]:MET:HE1	2.54	0.42
1:A:226:GLY:HA2	3:A:2355:HOH:O	2.19	0.42
1:A:225[A]:ARG:NH1	1:A:227:ASP:OD2	2.53	0.42
1:A:294[B]:MET:HE2	1:A:387[B]:MET:HG2	2.00	0.42
2:D:1:BGC:O4	2:D:2:BGC:C2	2.66	0.42
1:A:144:PRO:O	1:A:145[A]:MET:HE2	2.19	0.42
1:B:59:TYR:CD1	1:B:59:TYR:C	2.98	0.42
1:B:309:SER:O	1:B:310:MET:HB2	2.20	0.42
1:A:580:GLN:O	1:A:583:THR:OG1	2.34	0.41
1:B:401:ASP:OD1	1:B:403[B]:LYS:NZ	2.53	0.41
1:A:541:TRP:CG	1:A:542:PRO:HD3	2.55	0.41
1:B:580:GLN:O	1:B:583:THR:OG1	2.33	0.41
1:A:38:TYR:CD1	1:A:145[A]:MET:HE1	2.56	0.41
1:B:404:THR:HB	1:B:406:PHE:CZ	2.56	0.41
1:B:253:TYR:HB2	1:B:258:TYR:HA	2.03	0.41
1:B:449:SER:HB2	1:B:460:ASP:HB3	2.02	0.41
1:A:59:TYR:CD1	1:A:59:TYR:C	2.99	0.41
1:A:225[A]:ARG:HG3	3:A:2416:HOH:O	2.20	0.40
1:A:481:ASP:HA	1:A:482:PRO:HD3	1.93	0.40
1:B:77:TRP:CZ3	1:B:173:SER:HB3	2.57	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	594/592 (100%)	578 (97%)	16 (3%)	0	100	100
1	B	585/592 (99%)	570 (97%)	15 (3%)	0	100	100
All	All	1179/1184 (100%)	1148 (97%)	31 (3%)	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	509/514 (99%)	505 (99%)	4 (1%)	73	54
1	B	506/514 (98%)	502 (99%)	4 (1%)	73	54
All	All	1015/1028 (99%)	1007 (99%)	8 (1%)	73	54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	SER
1	A	477	VAL
1	A	556	VAL
1	A	583	THR
1	B	220	SER
1	B	477	VAL
1	B	556	VAL
1	B	583	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	GLN
1	B	487	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 ⓘ

10 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	BGC	C	1	2	12,12,12	0.44	0	17,17,17	1.40	2 (11%)
2	BGC	C	2	2	11,11,12	0.59	0	15,15,17	3.19	4 (26%)
2	BGC	C	3	2	11,11,12	0.63	0	15,15,17	3.09	6 (40%)
2	BGC	C	4	2	11,11,12	0.64	0	15,15,17	3.17	5 (33%)
2	BGC	C	5	2	11,11,12	0.56	0	15,15,17	2.19	3 (20%)
2	BGC	D	1	2	12,12,12	0.43	0	17,17,17	1.47	2 (11%)
2	BGC	D	2	2	11,11,12	0.59	0	15,15,17	2.87	4 (26%)
2	BGC	D	3	2	11,11,12	0.64	0	15,15,17	3.06	7 (46%)
2	BGC	D	4	2	11,11,12	0.44	0	15,15,17	3.14	4 (26%)
2	BGC	D	5	2	11,11,12	0.58	0	15,15,17	2.07	3 (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
2	BGC	C	1	2	-	1/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1	2	-	1/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	BGC	D	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BGC	C1-O5-C5	-8.28	101.08	112.19
2	D	4	BGC	C1-O5-C5	-8.11	101.32	112.19
2	C	3	BGC	C1-O5-C5	-7.71	101.85	112.19
2	C	4	BGC	C1-O5-C5	-7.69	101.88	112.19
2	D	3	BGC	C1-O5-C5	-7.68	101.89	112.19
2	C	4	BGC	C1-C2-C3	-7.00	99.45	109.64
2	D	2	BGC	C1-O5-C5	-6.97	102.84	112.19
2	D	4	BGC	C1-C2-C3	-6.85	99.68	109.64
2	C	3	BGC	C1-C2-C3	-6.23	100.57	109.64
2	D	3	BGC	C1-C2-C3	-6.20	100.62	109.64
2	C	5	BGC	C1-C2-C3	-5.70	101.34	109.64
2	C	2	BGC	C1-C2-C3	-5.46	101.70	109.64
2	D	5	BGC	C1-C2-C3	-5.20	102.07	109.64
2	D	5	BGC	C1-O5-C5	-5.11	105.34	112.19
2	D	2	BGC	O4-C4-C3	-4.89	98.85	110.38
2	D	2	BGC	C1-C2-C3	-4.87	102.55	109.64
2	C	5	BGC	C1-O5-C5	-4.79	105.76	112.19
2	C	2	BGC	C3-C4-C5	4.73	118.81	110.23
2	C	2	BGC	O4-C4-C3	-4.53	99.71	110.38
2	D	1	BGC	C3-C4-C5	4.35	118.12	110.23
2	C	4	BGC	C3-C4-C5	4.26	117.95	110.23
2	D	2	BGC	C3-C4-C5	4.04	117.56	110.23
2	C	1	BGC	C3-C4-C5	3.71	116.96	110.23
2	C	3	BGC	O4-C4-C3	-3.64	100.36	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BGC	C3-C4-C5	3.57	116.70	110.23
2	D	4	BGC	C3-C4-C5	3.50	116.58	110.23
2	C	4	BGC	O4-C4-C3	-3.24	102.74	110.38
2	D	3	BGC	O4-C4-C5	-3.22	101.40	109.32
2	D	3	BGC	C3-C4-C5	3.09	115.83	110.23
2	D	4	BGC	O4-C4-C3	-2.95	103.43	110.38
2	D	3	BGC	O4-C4-C3	-2.88	103.58	110.38
2	C	1	BGC	O5-C1-C2	-2.57	105.78	110.30
2	D	3	BGC	O5-C5-C6	2.55	112.62	107.66
2	C	3	BGC	O5-C5-C4	-2.25	105.36	110.83
2	C	3	BGC	O5-C5-C6	2.21	111.96	107.66
2	D	1	BGC	O5-C1-C2	-2.20	106.42	110.30
2	D	5	BGC	O5-C1-C2	-2.08	105.83	110.79
2	C	4	BGC	C2-C3-C4	-2.07	107.21	110.86
2	C	5	BGC	O5-C1-C2	-2.05	105.89	110.79
2	D	3	BGC	O5-C5-C4	-2.03	105.89	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

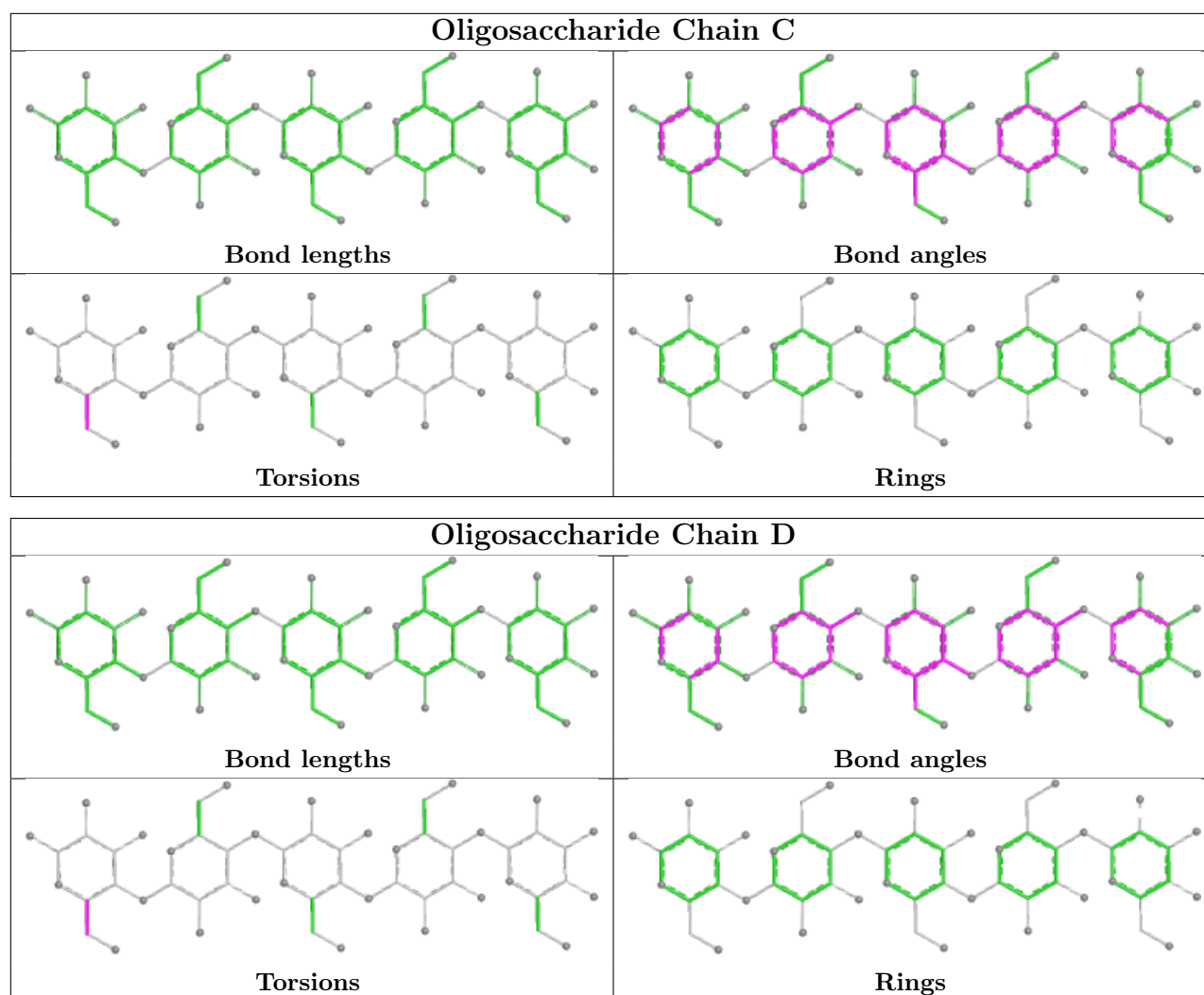
Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	BGC	6	0
2	D	5	BGC	3	0
2	C	1	BGC	2	0
2	D	1	BGC	2	0
2	C	5	BGC	2	0
2	D	3	BGC	6	0
2	C	3	BGC	4	0
2	C	2	BGC	4	0
2	D	2	BGC	5	0
2	C	4	BGC	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.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	582/592 (98%)	0.74	56 (9%)	13 14	7, 20, 37, 55	14 (2%)
1	B	582/592 (98%)	0.87	65 (11%)	10 10	8, 21, 38, 55	5 (0%)
All	All	1164/1184 (98%)	0.80	121 (10%)	11 12	7, 21, 37, 55	19 (1%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	5.5
1	B	2	SER	5.1
1	A	152	ARG	5.0
1	B	556	VAL	4.7
1	A	556	VAL	4.7
1	B	552	ASP	4.4
1	B	152	ARG	4.3
1	B	155	ALA	4.3
1	B	256	GLU	4.2
1	A	563	VAL	4.2
1	A	365	PRO	4.1
1	B	563	VAL	4.1
1	A	155	ALA	4.1
1	B	555	PRO	4.0
1	A	256	GLU	3.8
1	B	154	ARG	3.8
1	B	553	PRO	3.7
1	B	583	THR	3.7
1	A	239	TRP	3.7
1	B	163	ILE	3.5
1	A	583	THR	3.5
1	B	554	GLN	3.5
1	B	358	PRO	3.4
1	B	100	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	239	TRP	3.4
1	B	168	GLU	3.4
1	B	334	GLU	3.3
1	B	128	GLU	3.3
1	A	168	GLU	3.1
1	B	480	LEU	3.1
1	A	581	LYS	3.1
1	A	363	VAL	3.1
1	B	484	VAL	3.1
1	A	246	GLY	3.0
1	A	169	GLU	2.9
1	A	189	GLN	2.9
1	B	360	GLY	2.9
1	A	163	ILE	2.9
1	A	98	LEU	2.9
1	B	98	LEU	2.9
1	B	367	GLY	2.9
1	A	358	PRO	2.8
1	A	247	LEU	2.8
1	B	479	THR	2.8
1	A	128	GLU	2.8
1	A	355	LYS	2.8
1	B	180	TYR	2.8
1	B	518	TYR	2.8
1	A	292	ASN	2.7
1	B	242	TRP	2.7
1	A	482	PRO	2.7
1	A	244	LYS	2.6
1	B	3	LEU	2.6
1	A	325	GLU	2.6
1	A	564	ASP	2.6
1	B	181	TYR	2.6
1	B	577	GLU	2.6
1	B	183	PRO	2.6
1	B	274	PRO	2.6
1	A	485	ARG	2.5
1	B	107	ASP	2.5
1	B	551	SER	2.5
1	B	292	ASN	2.5
1	A	154	ARG	2.5
1	B	225	ARG	2.5
1	A	364	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	581	LYS	2.5
1	B	564	ASP	2.5
1	B	246	GLY	2.4
1	A	159	ILE	2.4
1	B	153	ILE	2.4
1	A	184	ASN	2.4
1	B	490	PHE	2.4
1	A	565	GLU	2.4
1	B	156	GLN	2.4
1	A	353	GLY	2.4
1	B	365	PRO	2.4
1	A	291	TYR	2.4
1	A	555	PRO	2.4
1	A	480	LEU	2.4
1	B	184	ASN	2.4
1	A	577	GLU	2.4
1	A	107	ASP	2.3
1	B	355	LYS	2.3
1	A	249	VAL	2.3
1	A	366	ASP	2.3
1	B	159	ILE	2.3
1	B	326	LEU	2.3
1	A	566	GLY	2.2
1	B	158	ASN	2.2
1	B	379	TYR	2.2
1	B	189	GLN	2.2
1	A	479	THR	2.2
1	B	486	LYS	2.2
1	A	360	GLY	2.2
1	B	354	TYR	2.2
1	B	18	PRO	2.2
1	B	366	ASP	2.2
1	B	455	VAL	2.2
1	A	486	LYS	2.2
1	B	317	PRO	2.1
1	B	179	TYR	2.1
1	B	162	TRP	2.1
1	A	192	ASP	2.1
1	B	475	LYS	2.1
1	A	300	PHE	2.1
1	A	315	PHE	2.1
1	A	237	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	481	ASP	2.1
1	A	157	MET	2.1
1	A	156	GLN	2.1
1	A	340	PHE	2.1
1	B	582	ALA	2.1
1	B	254	LYS	2.1
1	A	153	ILE	2.1
1	A	180	TYR	2.1
1	A	554	GLN	2.1
1	A	490	PHE	2.0
1	A	518	TYR	2.0
1	B	357	GLY	2.0
1	B	526	ASP	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](#)

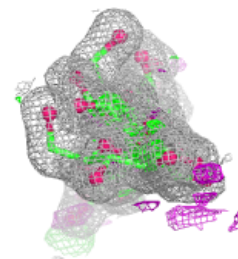
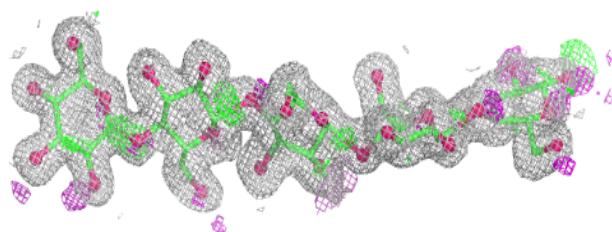
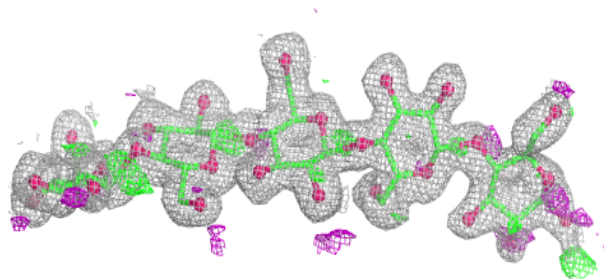
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BGC	C	1	12/12	0.79	0.17	23,29,33,37	1
2	BGC	D	1	12/12	0.80	0.18	23,30,34,38	0
2	BGC	C	2	11/12	0.91	0.10	17,19,25,25	0
2	BGC	D	2	11/12	0.91	0.10	17,19,24,26	0
2	BGC	C	4	11/12	0.92	0.09	12,15,19,23	0
2	BGC	D	3	11/12	0.92	0.09	17,18,20,21	0
2	BGC	D	4	11/12	0.92	0.09	13,15,21,26	0
2	BGC	C	3	11/12	0.93	0.08	15,17,21,22	0
2	BGC	C	5	11/12	0.93	0.07	12,13,15,15	0
2	BGC	D	5	11/12	0.95	0.07	13,14,16,16	0

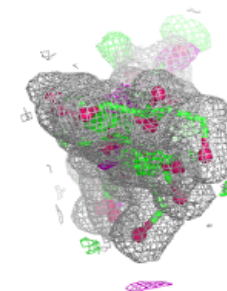
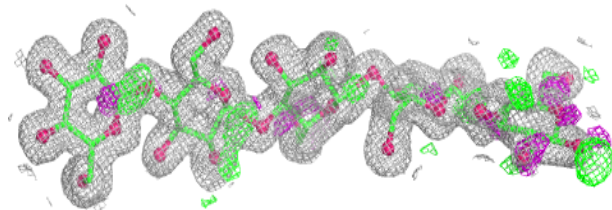
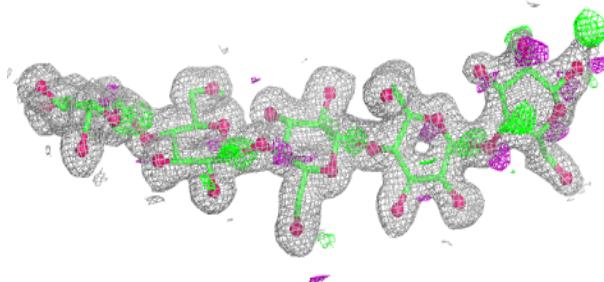
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.