



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:03 AM BST

PDB ID : 5FO8  
Title : Crystal Structure of Human Complement C3b in Complex with MCP (CCP1-4)  
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.  
Deposited on : 2015-11-18  
Resolution : 2.40 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

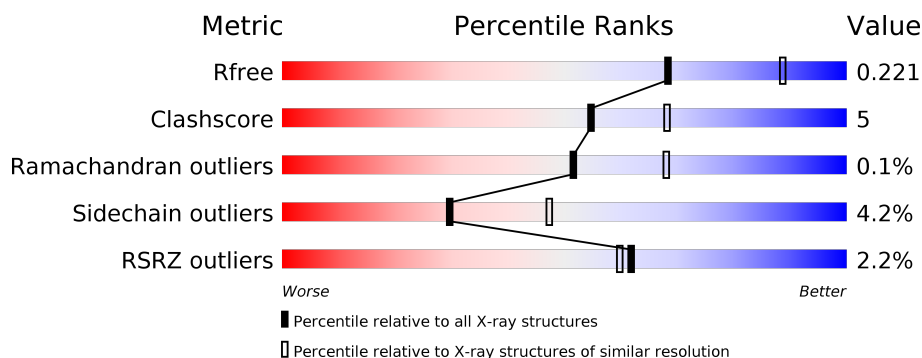
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	645	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 84%, yellow 14%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>
2	B	915	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 83%, yellow 14%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>83%</span> <span>14%</span> <span>..</span> </div> </div>
3	C	252	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 46%, yellow 0%, grey 49%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>46%</span> <span>..</span> <span>49%</span> </div> </div>
4	D	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>50%</span> <span>50%</span> </div> </div>
5	E	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>33%</span> <span>67%</span> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13810 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 COMPLEMENT C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			

- Molecule 2 is a protein called COMPLEMENT C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	894	Total	C	N	O	S	0	1	0
			7145	4530	1201	1376	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called MEMBRANE COFACTOR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			999	644	157	189	9			

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



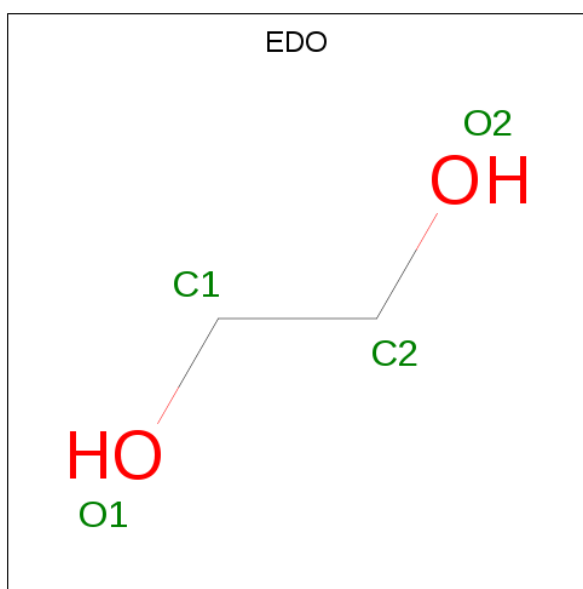
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

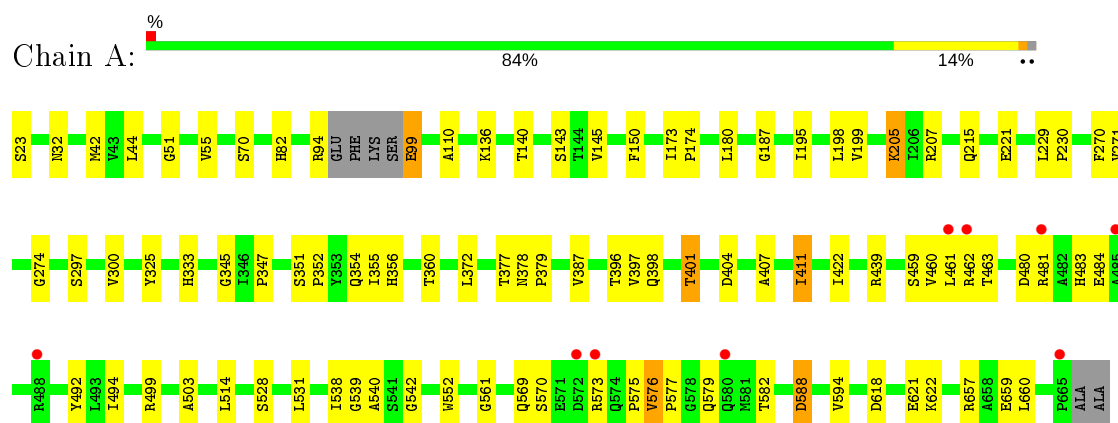
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total 172	O 172	0	0
7	B	293	Total 293	O 293	0	0
7	C	27	Total 27	O 27	0	0

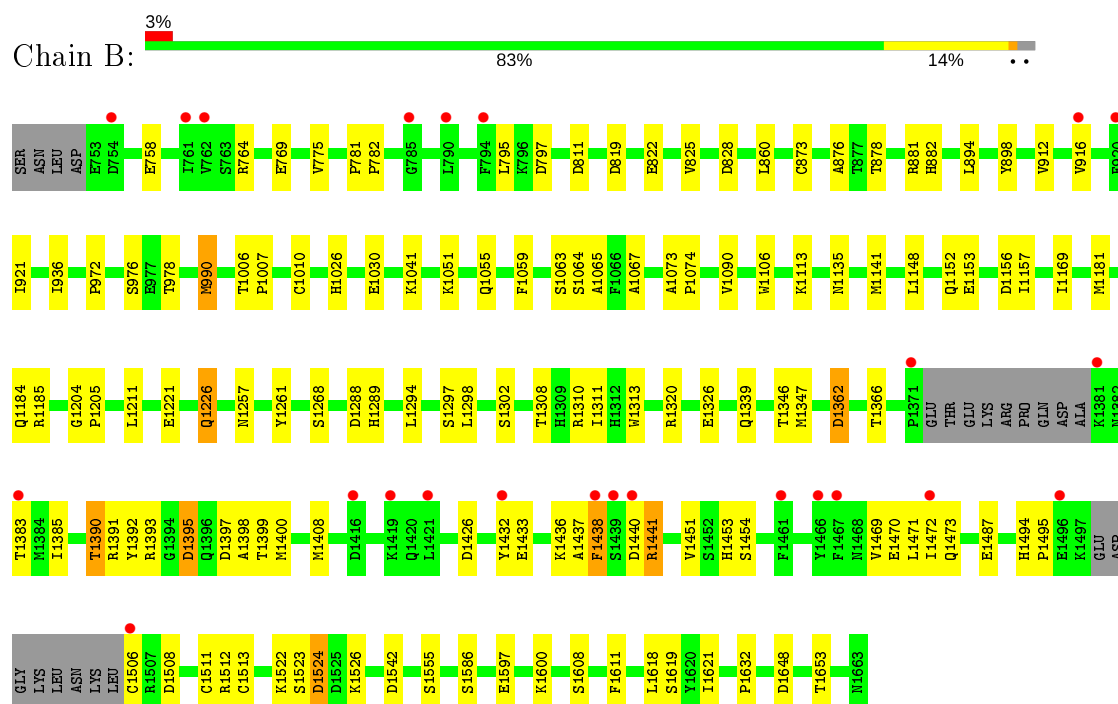
### 3 Residue-property plots

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: COMPLEMENT C3



#### • Molecule 2: COMPLEMENT C3



#### • Molecule 3: MEMBRANE COFACTOR PROTEIN



GLY	GLY	GLY	PRO	PRO	THR	PHE	GLU	ALA	MET	GLU	LEU	ILE	GLY	LYS	LYS	PRO	TYR	TYR	ILE	GLY	GLU	ARG	VAL	ASP	TYR	GLN	TYR	LYS	CYS	LYS	LYS	GLY	TYR	TYR	ILE	PRO	PRO	ILE	GLY	ALA	THR	HIS	THR	ILE	CYS	ASP	GLU	ARG	ASN	HIS	THR	TRP	VAL	PRO	ILE	SER	ASP	ALA	LYS	ALA	CYS							
TYR	ARG	GLU	THR	CYS	PRO	TYR	ILE	ARG	ASP	PRO	LEU	ASN	GLY	GLN	ALA	VAL	PRO	ALA	ASN	GLY	THR	TYR	PHE	GLY	VAL	TYR	GLN	MET	HIS	CYS	PHE	ILE	CYS	ASN	GLU	PHE	TYR	TYR	PRO	PRO	ILE	GLY	ALA	GLU	THR	HIS	THR	ILE	LEU	CYS	ASP	GLU	LEU	LYS	GLY	SER	TRP	VAL	ILE	ALA	PRO	THR	SER	GLY	LYS	ALA	PRO	CYS



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



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.83Å 130.63Å 233.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 2.40 65.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.02-2.40) 95.2 (65.31-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.188 , 0.219 0.191 , 0.221	Depositor DCC
$R_{free}$ test set	4928 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, EDO

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	0.27	0/5079	0.47	0/6902
2	B	0.29	1/7291 (0.0%)	0.46	1/9872 (0.0%)
3	C	0.25	0/1029	0.42	0/1399
All	All	0.28	1/13399 (0.0%)	0.46	1/18173 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1511	CYS	CB-SG	5.39	1.91	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1362	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4979	0	5037	55	0
2	B	7145	0	7070	80	0
3	C	999	0	962	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	25	2	0
5	E	39	0	34	0	0
6	A	16	0	24	1	0
6	B	112	0	168	12	0
7	A	172	0	0	4	0
7	B	293	0	0	17	1
7	C	27	0	0	0	0
All	All	13810	0	13320	137	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 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)
2:B:1586:SER:OG	7:B:2246:HOH:O	1.83	0.91
2:B:873:CYS:HG	2:B:1513:CYS:HG	1.09	0.85
1:A:351:SER:O	7:A:2090:HOH:O	2.00	0.79
2:B:1010:CYS:SG	7:B:2078:HOH:O	2.42	0.77
2:B:819:ASP:O	7:B:2035:HOH:O	2.03	0.76
2:B:1297:SER:HG	2:B:1308:THR:HG1	1.31	0.73
2:B:1313:TRP:O	7:B:2231:HOH:O	2.07	0.71
2:B:822:GLU:OE1	7:B:2037:HOH:O	2.08	0.70
1:A:503:ALA:H	4:D:1:NAG:H81	1.55	0.70
1:A:94:ARG:NH1	1:A:99:GLU:OE1	2.23	0.70
1:A:387:VAL:H	1:A:401:THR:HG22	1.56	0.70
1:A:576:VAL:HG12	1:A:579:GLN:HB2	1.74	0.69
1:A:462:ARG:NH2	1:A:552:TRP:O	2.27	0.68
2:B:1288:ASP:OD1	2:B:1289:HIS:ND1	2.29	0.67
2:B:1310:ARG:O	2:B:1320:ARG:NH2	2.29	0.66
2:B:1611:PHE:HD1	2:B:1618:LEU:HD21	1.59	0.65
1:A:569:GLN:HA	1:A:570:SER:HB3	1.77	0.65
2:B:1508:ASP:OD1	2:B:1512:ARG:NH2	2.29	0.65
2:B:1524:ASP:N	2:B:1524:ASP:OD1	2.26	0.64
1:A:32:ASN:OD1	7:A:2004:HOH:O	2.16	0.63
1:A:594:VAL:HG12	2:B:775:VAL:HG22	1.81	0.63
2:B:916:VAL:HG12	2:B:921:ILE:HB	1.82	0.62
1:A:136:LYS:NZ	2:B:769:GLU:OE1	2.33	0.61
2:B:1339:GLN:HG2	6:B:2682:EDO:H11	1.83	0.60
2:B:972:PRO:HB3	2:B:1621:ILE:HD12	1.83	0.60
1:A:481:ARG:HD3	1:A:484:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ILE:HD13	1:A:531:LEU:HD23	1.84	0.59
1:A:480:ASP:OD1	1:A:483:HIS:ND1	2.34	0.58
2:B:758:GLU:OE1	2:B:881:ARG:NH2	2.36	0.58
1:A:51:GLY:O	1:A:82:HIS:HE1	1.86	0.57
1:A:588:ASP:OD1	1:A:588:ASP:N	2.33	0.56
1:A:576:VAL:HG22	1:A:577:PRO:HD2	1.87	0.56
1:A:205:LYS:HG3	1:A:221:GLU:HG2	1.88	0.56
1:A:198:LEU:HD13	2:B:1347:MET:HG3	1.87	0.55
3:C:213:ASN:HB2	3:C:215:VAL:HG22	1.87	0.55
1:A:140:THR:O	1:A:143:SER:OG	2.24	0.55
1:A:378:ASN:OD1	7:A:2091:HOH:O	2.18	0.55
1:A:360:THR:HG21	1:A:372:LEU:HD23	1.88	0.55
1:A:271:VAL:HG11	1:A:300:VAL:HG11	1.88	0.55
2:B:1141:MET:HG3	6:B:2678:EDO:H11	1.87	0.54
1:A:503:ALA:N	4:D:1:NAG:H81	2.22	0.54
1:A:461:LEU:HD11	1:A:463:THR:HG23	1.88	0.54
2:B:1226:GLN:NE2	7:B:2200:HOH:O	2.40	0.53
1:A:99:GLU:OE1	1:A:99:GLU:HA	2.08	0.53
2:B:1261:TYR:OH	2:B:1268:SER:HB2	2.08	0.53
3:C:251:THR:HG22	3:C:269:VAL:HG22	1.90	0.53
2:B:1073:ALA:HA	6:B:2673:EDO:H22	1.90	0.53
2:B:1597:GLU:HB2	2:B:1600:LYS:HG3	1.91	0.52
2:B:1395:ASP:N	2:B:1395:ASP:OD1	2.42	0.52
1:A:539:GLY:HA2	1:A:540:ALA:HB3	1.91	0.52
3:C:166:PRO:HG2	3:C:220:ALA:HB2	1.92	0.52
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.92	0.51
2:B:1007:PRO:HG3	7:B:2095:HOH:O	2.09	0.51
2:B:1221:GLU:OE1	7:B:2194:HOH:O	2.20	0.51
2:B:882:HIS:NE2	2:B:898:TYR:HE1	2.10	0.50
2:B:1611:PHE:CD1	2:B:1618:LEU:HD21	2.44	0.50
6:B:2666:EDO:O2	7:B:2190:HOH:O	2.19	0.50
1:A:483:HIS:CE1	1:A:540:ALA:HB2	2.47	0.50
2:B:876:ALA:HB2	2:B:882:HIS:HB3	1.94	0.50
1:A:32:ASN:HD22	1:A:657:ARG:HH11	1.59	0.49
1:A:573:ARG:HG2	1:A:575:PRO:HD3	1.94	0.49
2:B:1041:LYS:O	6:B:2675:EDO:O2	2.30	0.49
2:B:1362:ASP:O	2:B:1390:THR:HA	2.12	0.49
1:A:401:THR:HA	1:A:407:ALA:HB2	1.94	0.49
1:A:657:ARG:NH2	7:A:2159:HOH:O	2.42	0.49
2:B:1156:ASP:OD2	3:C:245:LYS:NZ	2.39	0.49
2:B:873:CYS:HG	2:B:1513:CYS:CB	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1257:ASN:HB3	6:B:2691:EDO:H22	1.95	0.48
2:B:1051:LYS:HE3	2:B:1055:GLN:OE1	2.13	0.48
1:A:145:VAL:HG23	1:A:195:ILE:HD11	1.94	0.48
2:B:1398:ALA:HB3	2:B:1451:VAL:HB	1.95	0.48
2:B:1487:GLU:HG2	6:B:2671:EDO:H22	1.94	0.47
2:B:860:LEU:HD22	2:B:916:VAL:HG21	1.96	0.47
2:B:1454:SER:O	7:B:2241:HOH:O	2.20	0.47
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.96	0.47
1:A:539:GLY:HA3	1:A:542:GLY:N	2.29	0.47
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.49	0.47
1:A:561:GLY:HA3	1:A:588:ASP:OD2	2.14	0.47
1:A:492:TYR:HB2	1:A:531:LEU:HD21	1.97	0.47
2:B:1408:MET:SD	2:B:1495:PRO:HD3	2.55	0.46
2:B:1362:ASP:OD1	2:B:1393:ARG:NH2	2.48	0.46
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.51	0.46
1:A:42:MET:HE1	1:A:110:ALA:HB2	1.98	0.45
2:B:1181:MET:HB3	6:B:2677:EDO:H21	1.98	0.45
2:B:1438:PHE:C	2:B:1440:ASP:H	2.20	0.45
2:B:978:THR:HG23	2:B:1346:THR:HG22	1.98	0.45
1:A:354:GLN:HG3	1:A:377:THR:OG1	2.17	0.45
2:B:1648:ASP:OD1	6:B:2687:EDO:O1	2.25	0.44
2:B:1437:ALA:HA	2:B:1441:ARG:NE	2.33	0.44
2:B:1135:ASN:O	7:B:2149:HOH:O	2.21	0.44
1:A:356:HIS:ND1	6:A:1666:EDO:H21	2.33	0.44
2:B:1113:LYS:HD3	2:B:1113:LYS:HA	1.83	0.44
2:B:1436:LYS:HA	2:B:1436:LYS:HD2	1.83	0.44
1:A:205:LYS:HD2	1:A:207:ARG:NH2	2.33	0.43
1:A:372:LEU:HD11	1:A:422:ILE:HG21	1.99	0.43
1:A:618:ASP:O	1:A:622:LYS:HG2	2.18	0.43
2:B:1397:ASP:OD1	2:B:1453:HIS:ND1	2.45	0.43
2:B:1026:HIS:ND1	7:B:2082:HOH:O	2.04	0.43
2:B:1152:GLN:NE2	7:B:2157:HOH:O	2.40	0.43
1:A:352:PRO:O	1:A:379:PRO:HD3	2.18	0.43
2:B:1067:ALA:HB2	2:B:1074:PRO:HA	2.00	0.43
2:B:1090:VAL:HG21	2:B:1157:ILE:HD13	2.00	0.43
2:B:1632:PRO:O	6:B:2681:EDO:O1	2.28	0.43
3:C:263:ASP:HB2	3:C:284:LEU:HD22	2.01	0.43
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.90	0.42
1:A:150:PHE:HA	1:A:187:GLY:O	2.19	0.42
2:B:1184:GLN:NE2	7:B:2173:HOH:O	2.50	0.42
2:B:1399:THR:OG1	2:B:1400:MET:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG11	1:A:411:ILE:HG22	2.01	0.42
1:A:528:SER:OG	1:A:621:GLU:OE2	2.28	0.42
2:B:873:CYS:SG	2:B:1513:CYS:C	2.98	0.42
2:B:1010:CYS:HA	2:B:1059:PHE:CZ	2.54	0.42
2:B:1362:ASP:OD2	2:B:1391:ARG:NH2	2.53	0.42
2:B:1608:SER:HA	2:B:1611:PHE:CE2	2.55	0.42
1:A:229:LEU:HA	1:A:230:PRO:HD3	1.91	0.42
1:A:404:ASP:N	1:A:404:ASP:OD1	2.53	0.42
2:B:1063:SER:O	2:B:1064:SER:HB2	2.20	0.42
1:A:355:ILE:O	1:A:439:ARG:NH1	2.52	0.42
2:B:1204:GLY:HA3	2:B:1205:PRO:HD3	1.91	0.41
2:B:1211:LEU:HB3	6:B:2666:EDO:H12	2.01	0.41
1:A:345:GLY:O	1:A:347:PRO:HD3	2.20	0.41
1:A:270:PHE:HD2	2:B:1400:MET:HE3	1.85	0.41
2:B:781:PRO:HA	2:B:782:PRO:HD3	1.82	0.41
2:B:976:SER:N	7:B:2056:HOH:O	2.13	0.41
2:B:1006:THR:HA	2:B:1007:PRO:HD3	1.86	0.41
2:B:1522:LYS:HA	2:B:1522:LYS:HD3	1.86	0.41
2:B:1185:ARG:NH1	7:B:2144:HOH:O	2.20	0.41
2:B:1065:ALA:HB2	2:B:1106:TRP:CD2	2.56	0.41
1:A:136:LYS:HB2	1:A:136:LYS:HE3	1.89	0.41
2:B:1294:LEU:HB2	2:B:1311:ILE:HB	2.01	0.41
2:B:795:LEU:HD13	2:B:825:VAL:HG22	2.03	0.41
2:B:1148:LEU:HD11	2:B:1169:ILE:HG23	2.02	0.41
2:B:1030:GLU:HG2	7:B:2081:HOH:O	2.20	0.40
3:C:194:ALA:HA	3:C:195:PRO:HD3	1.93	0.40
2:B:1653:THR:HG21	6:B:2680:EDO:H22	2.03	0.40
2:B:990:MET:HE2	2:B:990:MET:HB3	1.91	0.40
1:A:539:GLY:HA3	1:A:542:GLY:H	1.85	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)
7:B:2137:HOH:O	7:B:2291:HOH:O[1_545]	2.02	0.18

## 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	635/645 (98%)	617 (97%)	17 (3%)	1 (0%)	47	62
2	B	889/915 (97%)	860 (97%)	29 (3%)	0	100	100
3	C	127/252 (50%)	123 (97%)	4 (3%)	0	100	100
All	All	1651/1812 (91%)	1600 (97%)	50 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	GLU

### 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	563/567 (99%)	541 (96%)	22 (4%)	32	50
2	B	792/810 (98%)	757 (96%)	35 (4%)	28	45
3	C	114/222 (51%)	110 (96%)	4 (4%)	36	55
All	All	1469/1599 (92%)	1408 (96%)	61 (4%)	30	47

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	70	SER

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Mol	Chain	Res	Type
1	A	99	GLU
1	A	180	LEU
1	A	199	VAL
1	A	205	LYS
1	A	215	GLN
1	A	297	SER
1	A	333	HIS
1	A	396	THR
1	A	398	GLN
1	A	401	THR
1	A	411	ILE
1	A	459	SER
1	A	460	VAL
1	A	499	ARG
1	A	514	LEU
1	A	538	ILE
1	A	576	VAL
1	A	582	THR
1	A	588	ASP
1	A	660	LEU
2	B	811	ASP
2	B	828	ASP
2	B	878	THR
2	B	894	LEU
2	B	912	VAL
2	B	936	ILE
2	B	990	MET
2	B	1153	GLU
2	B	1226	GLN
2	B	1298	LEU
2	B	1302	SER
2	B	1326	GLU
2	B	1366	THR
2	B	1383	THR
2	B	1385	ILE
2	B	1390	THR
2	B	1395	ASP
2	B	1426	ASP
2	B	1432	TYR
2	B	1433	GLU
2	B	1438	PHE
2	B	1441	ARG

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Mol	Chain	Res	Type
2	B	1469	VAL
2	B	1470	GLU
2	B	1471	LEU
2	B	1472	ILE
2	B	1473	GLN
2	B	1494	HIS
2	B	1506	CYS
2	B	1523	SER
2	B	1524	ASP
2	B	1526	LYS
2	B	1542	ASP
2	B	1555	SER
2	B	1619	SER
3	C	179	GLU
3	C	215	VAL
3	C	284	LEU
3	C	286	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	82	HIS
2	B	919	HIS

### 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 ⓘ

5 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
4	NAG	D	1	1,4	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	0.81	0
5	NAG	E	1	2,5	14,14,15	0.52	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	14,14,15	0.58	0	17,19,21	1.15	2 (11%)
5	BMA	E	3	5	11,11,12	0.83	0	15,15,17	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	2.74	115.91	112.19
5	E	2	NAG	C3-C4-C5	2.68	115.03	110.24
5	E	2	NAG	C4-C3-C2	2.49	114.67	111.02
4	D	1	NAG	O5-C1-C2	-2.17	107.86	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2

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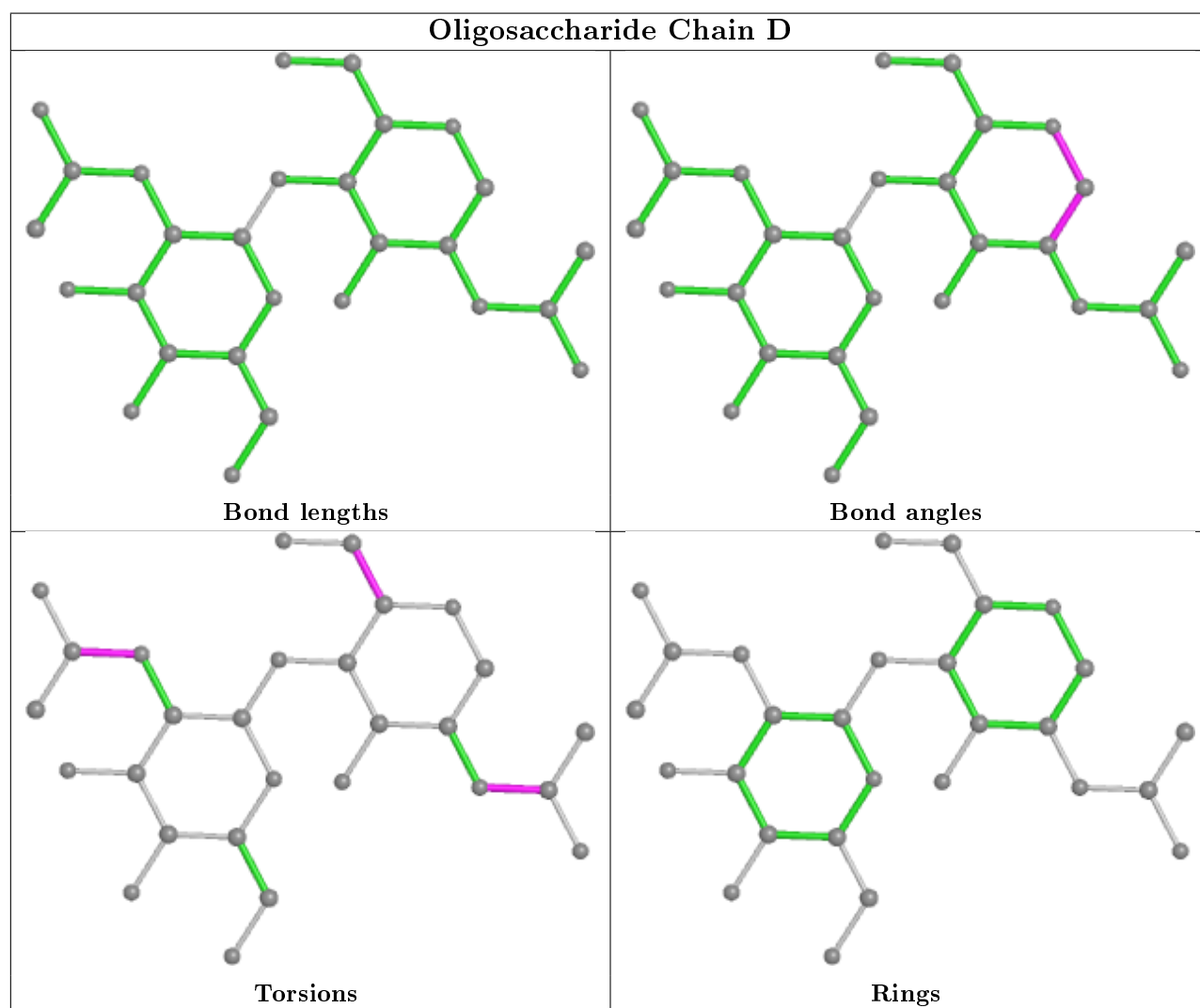
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6

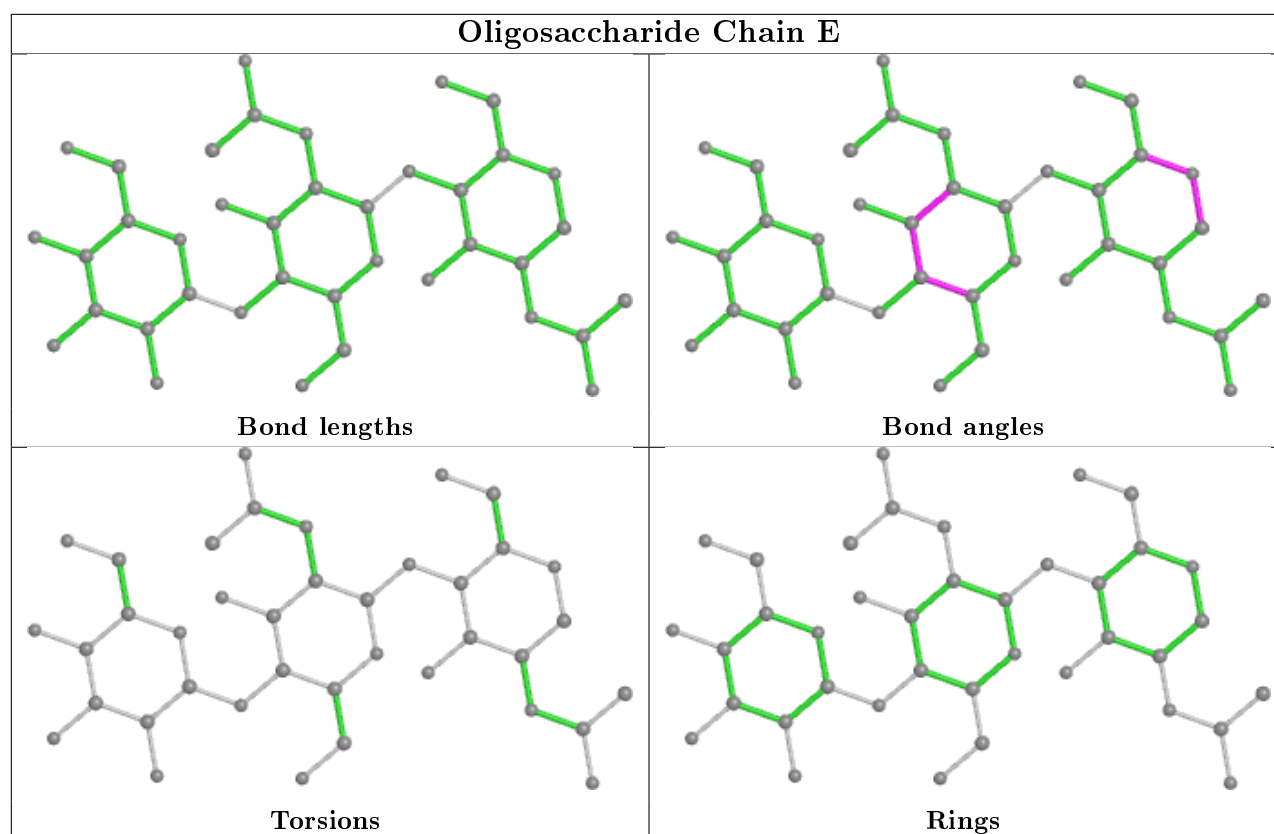
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	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](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	EDO	B	2684	-	3,3,3	0.47	0	2,2,2	0.12	0
6	EDO	B	2665	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	B	2685	-	3,3,3	0.43	0	2,2,2	0.41	0
6	EDO	B	2682	-	3,3,3	0.47	0	2,2,2	0.30	0
6	EDO	B	2683	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	B	2669	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	B	2664	-	3,3,3	0.45	0	2,2,2	0.42	0
6	EDO	B	2687	-	3,3,3	0.46	0	2,2,2	0.37	0
6	EDO	B	2676	-	3,3,3	0.47	0	2,2,2	0.27	0
6	EDO	B	2681	-	3,3,3	0.46	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	1667	-	3,3,3	0.45	0	2,2,2	0.32	0
6	EDO	B	2688	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	B	2689	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	B	2666	-	3,3,3	0.45	0	2,2,2	0.30	0
6	EDO	B	2668	-	3,3,3	0.47	0	2,2,2	0.22	0
6	EDO	B	2667	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	A	1666	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	B	2680	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	A	1669	-	3,3,3	0.47	0	2,2,2	0.29	0
6	EDO	B	2679	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	B	2672	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	B	2678	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	B	2686	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	B	2677	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	B	2690	-	3,3,3	0.48	0	2,2,2	0.40	0
6	EDO	B	2673	-	3,3,3	0.47	0	2,2,2	0.39	0
6	EDO	A	1668	-	3,3,3	0.47	0	2,2,2	0.33	0
6	EDO	B	2675	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	B	2674	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	B	2671	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	B	2691	-	3,3,3	0.43	0	2,2,2	0.44	0
6	EDO	B	2670	-	3,3,3	0.45	0	2,2,2	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	2684	-	-	0/1/1/1	-
6	EDO	B	2665	-	-	0/1/1/1	-
6	EDO	B	2685	-	-	0/1/1/1	-
6	EDO	B	2682	-	-	0/1/1/1	-
6	EDO	B	2683	-	-	0/1/1/1	-
6	EDO	B	2669	-	-	0/1/1/1	-
6	EDO	B	2664	-	-	0/1/1/1	-
6	EDO	B	2687	-	-	1/1/1/1	-
6	EDO	B	2676	-	-	0/1/1/1	-
6	EDO	B	2681	-	-	0/1/1/1	-
6	EDO	A	1667	-	-	0/1/1/1	-
6	EDO	B	2688	-	-	0/1/1/1	-
6	EDO	B	2689	-	-	0/1/1/1	-
6	EDO	B	2666	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	2668	-	-	0/1/1/1	-
6	EDO	B	2667	-	-	1/1/1/1	-
6	EDO	A	1666	-	-	0/1/1/1	-
6	EDO	B	2680	-	-	0/1/1/1	-
6	EDO	A	1669	-	-	1/1/1/1	-
6	EDO	B	2679	-	-	1/1/1/1	-
6	EDO	B	2672	-	-	0/1/1/1	-
6	EDO	B	2678	-	-	0/1/1/1	-
6	EDO	B	2686	-	-	0/1/1/1	-
6	EDO	B	2677	-	-	0/1/1/1	-
6	EDO	B	2690	-	-	0/1/1/1	-
6	EDO	B	2673	-	-	0/1/1/1	-
6	EDO	A	1668	-	-	0/1/1/1	-
6	EDO	B	2675	-	-	0/1/1/1	-
6	EDO	B	2674	-	-	0/1/1/1	-
6	EDO	B	2671	-	-	0/1/1/1	-
6	EDO	B	2691	-	-	0/1/1/1	-
6	EDO	B	2670	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2687	EDO	O1-C1-C2-O2
6	A	1669	EDO	O1-C1-C2-O2
6	B	2667	EDO	O1-C1-C2-O2
6	B	2679	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2682	EDO	1	0
6	B	2687	EDO	1	0
6	B	2681	EDO	1	0
6	B	2666	EDO	2	0
6	A	1666	EDO	1	0
6	B	2680	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2678	EDO	1	0
6	B	2677	EDO	1	0
6	B	2673	EDO	1	0
6	B	2675	EDO	1	0
6	B	2671	EDO	1	0
6	B	2691	EDO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	639/645 (99%)	-0.13	9 (1%) 75 73	38, 64, 99, 164	0
2	B	894/915 (97%)	-0.04	24 (2%) 54 52	26, 64, 118, 157	0
3	C	129/252 (51%)	-0.04	4 (3%) 49 47	43, 71, 101, 122	0
All	All	1662/1812 (91%)	-0.07	37 (2%) 62 60	26, 65, 110, 164	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	PRO	6.7
2	B	1466	TYR	5.9
2	B	1438	PHE	4.3
2	B	790	LEU	4.2
1	A	481	ARG	3.8
3	C	160	VAL	3.8
1	A	461	LEU	3.4
3	C	213	ASN	3.4
2	B	916	VAL	3.3
2	B	1432	TYR	3.2
3	C	177	GLU	3.2
1	A	572	ASP	3.1
2	B	762	VAL	3.1
2	B	1416	ASP	3.1
2	B	1381	LYS	2.8
2	B	785	GLY	2.8
2	B	761	ILE	2.7
1	A	573	ARG	2.6
2	B	1467	PHE	2.6
3	C	159	LYS	2.6
2	B	1419	LYS	2.5
2	B	1383	THR	2.4
2	B	1439	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	485	ALA	2.4
2	B	754	ASP	2.3
1	A	580	GLN	2.3
2	B	1472	ILE	2.3
2	B	1421	LEU	2.3
2	B	1496	GLU	2.2
2	B	920	PHE	2.2
1	A	462	ARG	2.2
1	A	488	ARG	2.2
2	B	1461	PHE	2.1
2	B	1506	CYS	2.1
2	B	1440	ASP	2.1
2	B	794	PHE	2.1
2	B	1371	PRO	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](#)

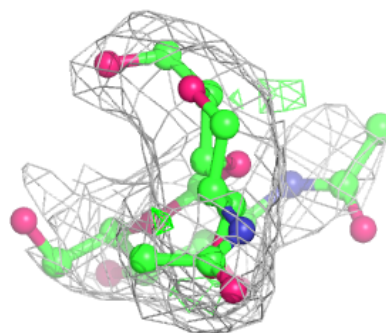
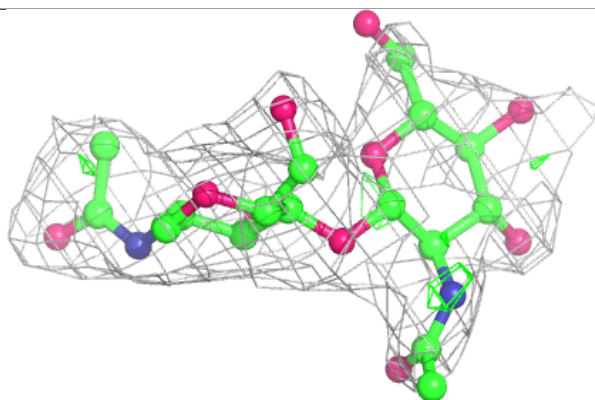
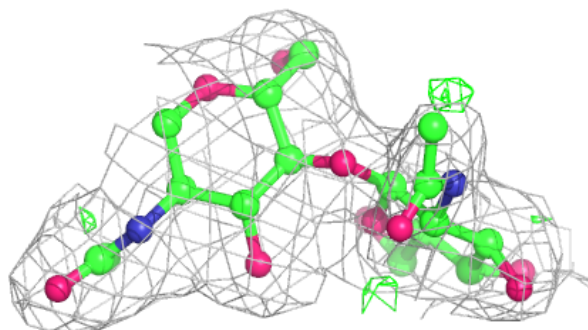
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	E	3	11/12	0.74	0.26	122,143,153,153	0
5	NAG	E	2	14/15	0.76	0.23	102,132,138,142	0
4	NAG	D	2	14/15	0.82	0.17	94,112,117,117	0
5	NAG	E	1	14/15	0.88	0.16	94,100,108,121	0
4	NAG	D	1	14/15	0.93	0.14	67,79,90,101	0

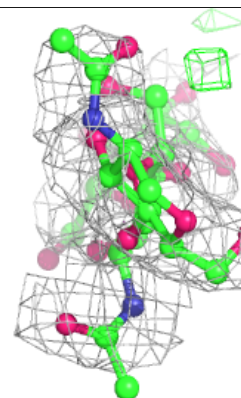
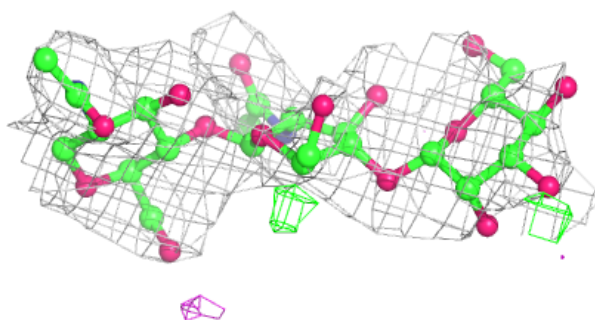
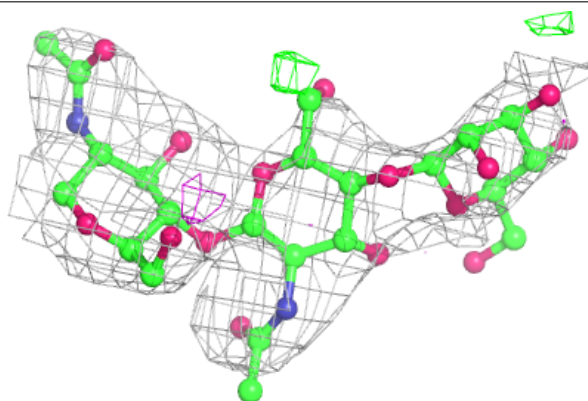
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain D:**

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

**Electron density around Chain E:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	A	1669	4/4	0.63	0.27	99,99,100,101	0
6	EDO	B	2674	4/4	0.68	0.34	82,87,93,96	0
6	EDO	B	2668	4/4	0.75	0.27	82,82,84,84	0
6	EDO	B	2665	4/4	0.77	0.15	88,90,92,93	0
6	EDO	A	1668	4/4	0.79	0.18	92,92,95,96	0
6	EDO	B	2688	4/4	0.82	0.20	76,78,82,85	0
6	EDO	B	2686	4/4	0.83	0.23	70,75,86,92	0
6	EDO	B	2673	4/4	0.83	0.18	70,70,75,77	1
6	EDO	B	2677	4/4	0.84	0.21	85,87,88,88	0
6	EDO	B	2671	4/4	0.84	0.17	76,76,76,85	1
6	EDO	B	2682	4/4	0.85	0.48	77,81,86,91	0
6	EDO	B	2672	4/4	0.85	0.17	74,74,76,78	0
6	EDO	B	2679	4/4	0.86	0.21	68,73,77,82	0
6	EDO	B	2676	4/4	0.86	0.24	65,66,77,82	0
6	EDO	B	2666	4/4	0.87	0.23	59,60,62,63	2
6	EDO	B	2681	4/4	0.89	0.21	91,92,92,98	0
6	EDO	A	1667	4/4	0.89	0.19	90,90,92,93	0
6	EDO	B	2680	4/4	0.90	0.23	78,86,89,91	0
6	EDO	B	2675	4/4	0.90	0.22	48,50,51,55	3
6	EDO	A	1666	4/4	0.91	0.19	79,82,83,85	0
6	EDO	B	2684	4/4	0.92	0.19	36,43,55,66	0
6	EDO	B	2678	4/4	0.92	0.33	62,63,64,65	0
6	EDO	B	2689	4/4	0.92	0.21	62,65,71,73	0
6	EDO	B	2685	4/4	0.93	0.18	48,58,61,64	0
6	EDO	B	2669	4/4	0.93	0.14	87,87,88,88	0
6	EDO	B	2687	4/4	0.94	0.21	51,53,55,59	0
6	EDO	B	2691	4/4	0.94	0.26	47,54,66,77	0
6	EDO	B	2664	4/4	0.95	0.18	42,56,63,72	0
6	EDO	B	2667	4/4	0.95	0.20	64,65,68,76	1
6	EDO	B	2683	4/4	0.96	0.17	55,56,56,57	0
6	EDO	B	2690	4/4	0.97	0.17	33,38,48,54	0
6	EDO	B	2670	4/4	0.97	0.27	45,47,48,49	3

## 6.5 Other polymers ⓘ

There are no such residues in this entry.