



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

PDB ID : 5FO8 / pdb_00005fo8
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

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

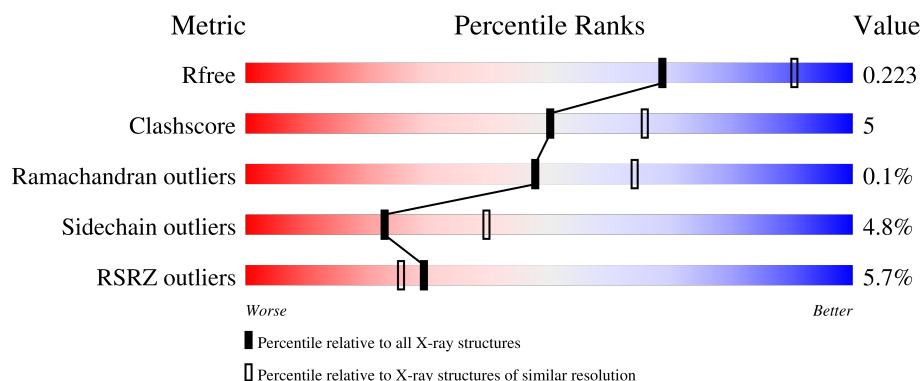
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	645	4% 84% 15% ..
2	B	915	7% 82% 15% ..
3	C	252	4% 46% 5% 49%
4	D	2	50% 50%
5	E	3	33% 67%

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.

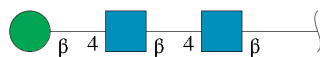
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			999	644	157	189	9			

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



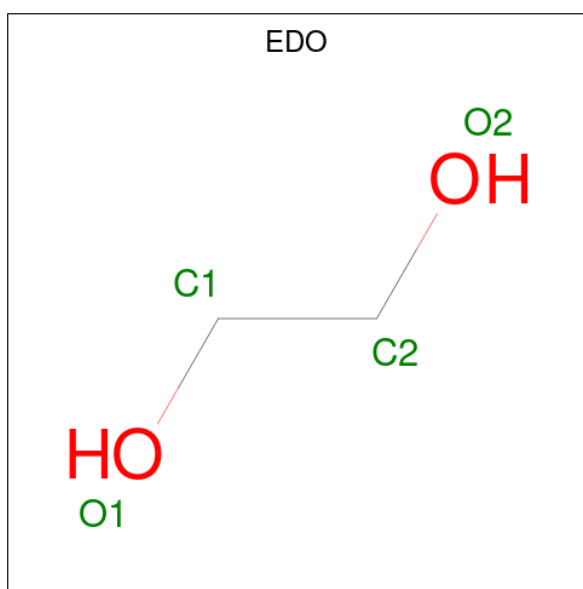
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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	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		

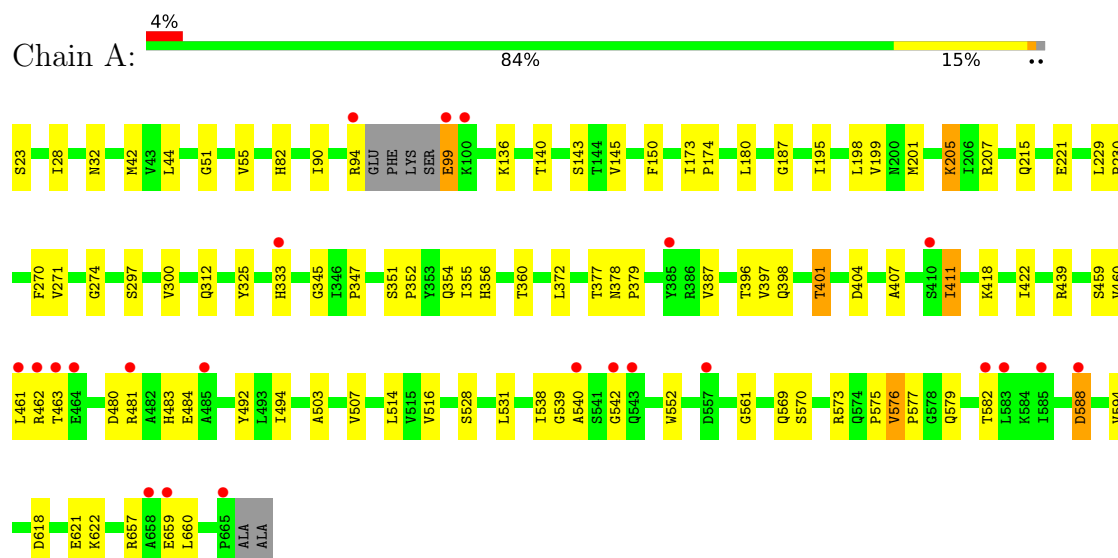
- Molecule 7 is water.

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

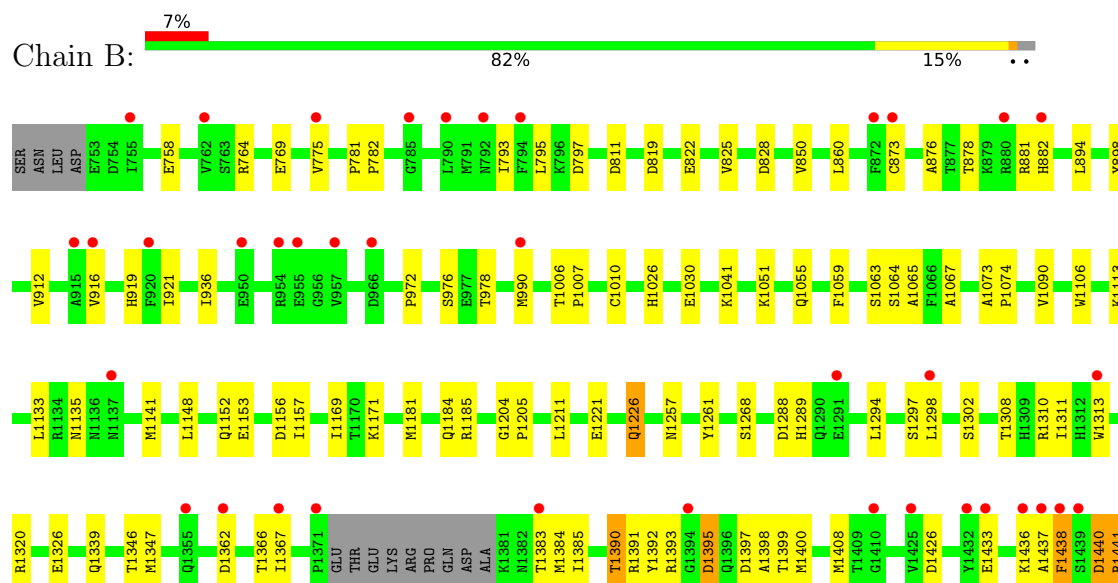
3 Residue-property plots [i](#)

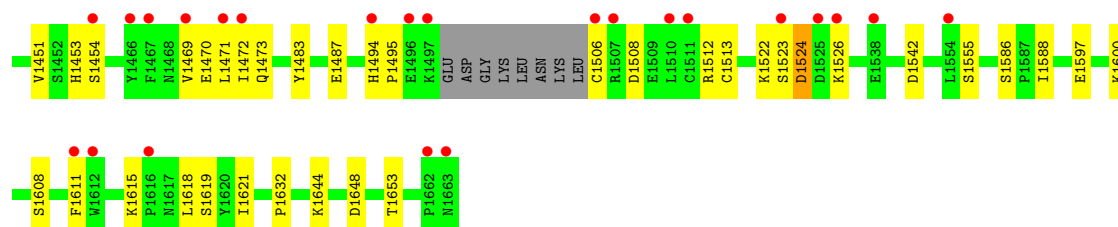
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COMPLEMENT C3

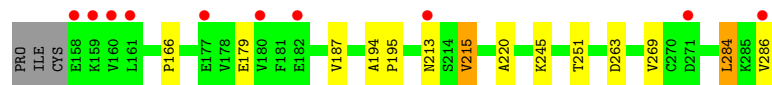
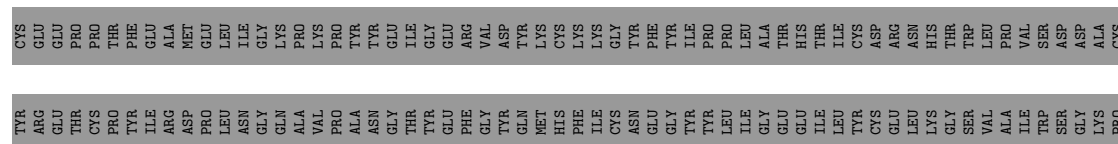


• Molecule 2: COMPLEMENT C3





• Molecule 3: MEMBRANE COFACTOR PROTEIN



• 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 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	82.83Å 130.63Å 233.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 2.40 57.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.02-2.40) 95.2 (57.02-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.219 0.193 , 0.223	Depositor DCC
R_{free} test set	4928 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	0.33	0/5079	0.76	4/6902 (0.1%)
2	B	0.36	0/7291	0.74	1/9872 (0.0%)
3	C	0.29	0/1029	0.72	0/1399
All	All	0.34	0/13399	0.75	5/18173 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	SER	CA-C-N	-5.92	113.84	119.76
1	A	23	SER	C-N-CA	-5.92	113.84	119.76
1	A	90	ILE	CA-C-N	5.52	126.30	120.11
1	A	90	ILE	C-N-CA	5.52	126.30	120.11
2	B	1440	ASP	N-CA-C	-5.20	106.89	113.18

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	57	0
2	B	7145	0	7070	83	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	19	1
7	C	27	0	0	0	0
All	All	13810	0	13320	141	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 (141) 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	0.96
2:B:873:CYS:HG	2:B:1513:CYS:HG	1.07	0.86
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	1.30	0.74
2:B:1313:TRP:O	7:B:2231:HOH:O	2.07	0.71
1:A:503:ALA:H	4:D:1:NAG:H81	1.55	0.70
2:B:822:GLU:OE1	7:B:2037:HOH:O	2.08	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:1483:TYR:OH	7:B:2238:HOH:O	2.12	0.67
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
1:A:42:MET:HE2	1:A:44:LEU:HD21	1.82	0.60
2:B:1339:GLN:HG2	6:B:2682:EDO:H11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1644:LYS:NZ	7:B:2281:HOH:O	2.37	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
1:A:503:ALA:N	4:D:1:NAG:H81	2.22	0.54
2:B:1141:MET:HG3	6:B:2678:EDO:H11	1.87	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
1:A:270:PHE:HD2	2:B:1400:MET:HE3	1.76	0.50
2:B:1438:PHE:C	2:B:1440:ASP:H	2.20	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
2:B:873:CYS:HG	2:B:1513:CYS:CB	2.24	0.49
1:A:573:ARG:HG2	1:A:575:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:860:LEU:HD22	2:B:916:VAL:HG21	1.96	0.47
2:B:1487:GLU:HG2	6:B:2671:EDO:H22	1.94	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
2:B:873:CYS:SG	2:B:1513:CYS:C	2.98	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
2:B:1181:MET:HB3	6:B:2677:EDO:H21	1.98	0.45
2:B:1632:PRO:O	6:B:2681:EDO:O1	2.28	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:HA	2:B:1113:LYS:HD3	1.83	0.44
2:B:1436:LYS:HD2	2:B:1436:LYS:HA	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
1:A:28:ILE:HB	1:A:42:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1399:THR:OG1	2:B:1400:MET:N	2.48	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:OD1	1:A:404:ASP:N	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
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:HD3	2:B:1522:LYS:HA	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
1:A:270:PHE:CD2	2:B:1400:MET:HE3	2.56	0.40
1:A:539:GLY:HA3	1:A:542:GLY:H	1.85	0.40
2:B:1367:ILE:HG12	2:B:1384:MET:HE2	2.04	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%)	43	58
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%)	48	64

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%)	539 (96%)	24 (4%)	26	44
2	B	792/810 (98%)	751 (95%)	41 (5%)	21	36
3	C	114/222 (51%)	109 (96%)	5 (4%)	25	43
All	All	1469/1599 (92%)	1399 (95%)	70 (5%)	23	40

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	199	VAL
1	A	201	MET
1	A	205	LYS
1	A	215	GLN
1	A	297	SER
1	A	312	GLN
1	A	333	HIS
1	A	396	THR
1	A	398	GLN
1	A	401	THR
1	A	411	ILE
1	A	418	LYS
1	A	459	SER
1	A	460	VAL
1	A	507	VAL
1	A	514	LEU
1	A	516	VAL
1	A	538	ILE
1	A	576	VAL
1	A	582	THR
1	A	588	ASP
1	A	660	LEU
2	B	793	ILE
2	B	811	ASP
2	B	828	ASP
2	B	850	VAL
2	B	878	THR
2	B	894	LEU
2	B	912	VAL
2	B	919	HIS
2	B	936	ILE
2	B	990	MET
2	B	1133	LEU
2	B	1153	GLU
2	B	1171	LYS
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

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Mol	Chain	Res	Type
2	B	1390	THR
2	B	1395	ASP
2	B	1426	ASP
2	B	1433	GLU
2	B	1438	PHE
2	B	1441	ARG
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	1588	ILE
2	B	1615	LYS
2	B	1619	SER
3	C	179	GLU
3	C	187	VAL
3	C	215	VAL
3	C	284	LEU
3	C	286	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	82	HIS
1	A	569	GLN
2	B	857	ASN
2	B	919	HIS
2	B	1014	ASN
2	B	1055	GLN
2	B	1127	GLN
2	B	1277	GLN
2	B	1355	GLN
3	C	170	ASN
3	C	238	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 ⓘ

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	0.53	0	17,19,21	1.04	1 (5%)
4	NAG	D	2	4	14,14,15	0.52	0	17,19,21	0.76	0
5	NAG	E	1	2,5	14,14,15	0.50	0	17,19,21	1.01	1 (5%)
5	NAG	E	2	5	14,14,15	0.56	0	17,19,21	1.13	2 (11%)
5	BMA	E	3	5	11,11,12	0.81	0	15,15,17	0.68	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	2.77	115.91	112.19
5	E	2	NAG	C3-C4-C5	2.64	115.03	110.23
5	E	2	NAG	C4-C3-C2	2.49	114.67	111.02
4	D	1	NAG	O5-C1-C2	-2.22	107.86	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

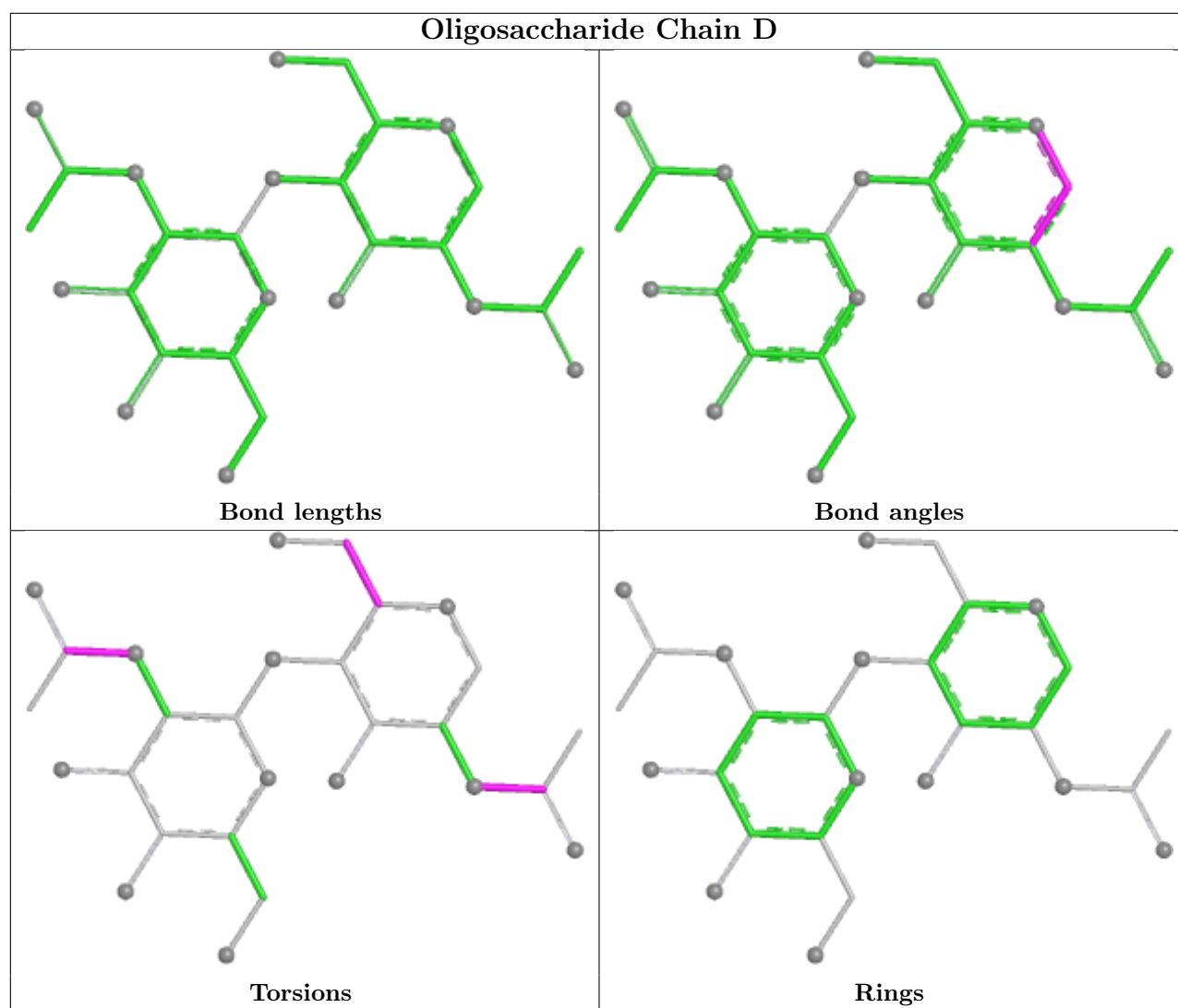
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6

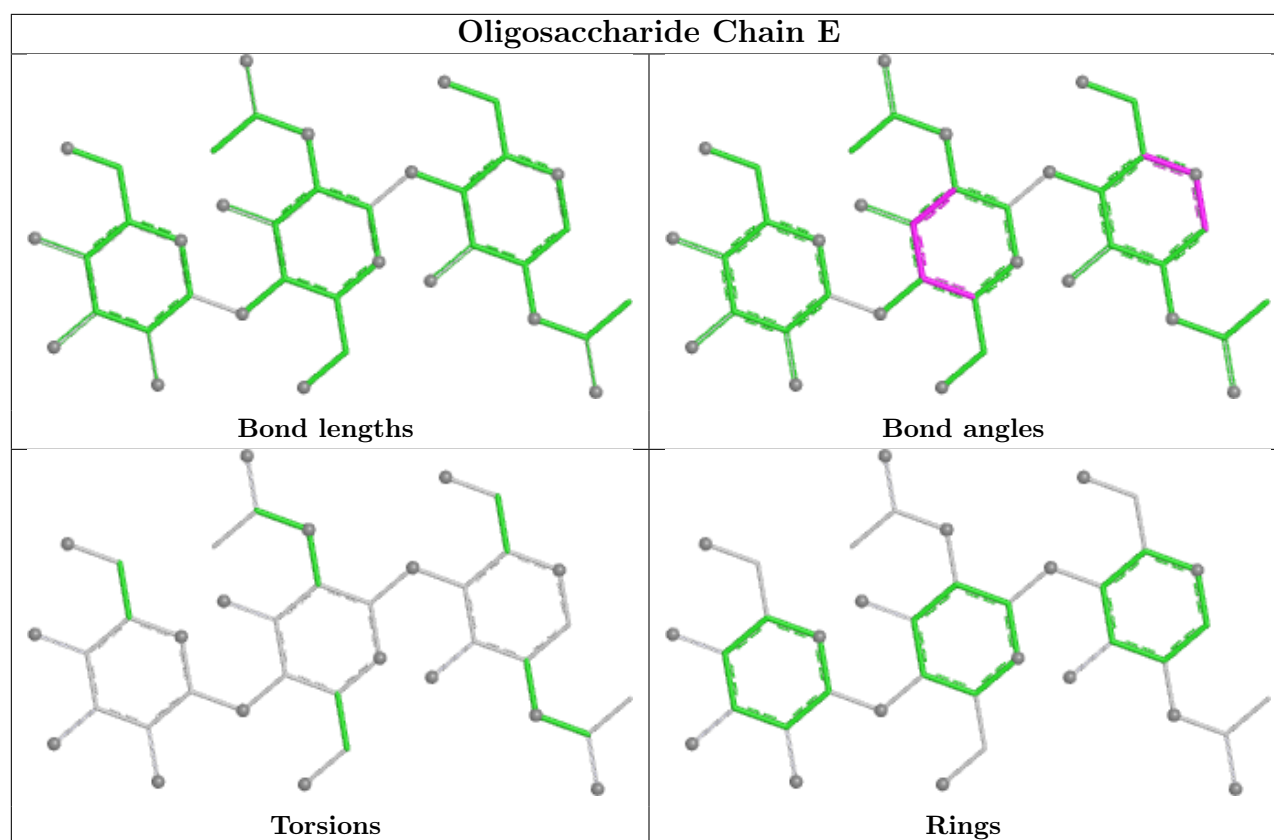
There are no ring outliers.

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	2672	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	B	2665	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	B	2687	-	3,3,3	0.42	0	2,2,2	0.41	0
6	EDO	B	2675	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	B	2683	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	B	2668	-	3,3,3	0.44	0	2,2,2	0.27	0
6	EDO	B	2690	-	3,3,3	0.45	0	2,2,2	0.44	0
6	EDO	B	2688	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	B	2666	-	3,3,3	0.42	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	2664	-	3,3,3	0.42	0	2,2,2	0.46	0
6	EDO	A	1669	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	B	2671	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	B	2681	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	B	2678	-	3,3,3	0.41	0	2,2,2	0.41	0
6	EDO	B	2673	-	3,3,3	0.44	0	2,2,2	0.43	0
6	EDO	B	2667	-	3,3,3	0.41	0	2,2,2	0.37	0
6	EDO	B	2682	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	A	1667	-	3,3,3	0.42	0	2,2,2	0.37	0
6	EDO	B	2686	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	B	2685	-	3,3,3	0.40	0	2,2,2	0.44	0
6	EDO	B	2677	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	B	2670	-	3,3,3	0.42	0	2,2,2	0.42	0
6	EDO	A	1666	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	B	2689	-	3,3,3	0.41	0	2,2,2	0.37	0
6	EDO	B	2691	-	3,3,3	0.40	0	2,2,2	0.48	0
6	EDO	A	1668	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	B	2676	-	3,3,3	0.44	0	2,2,2	0.31	0
6	EDO	B	2679	-	3,3,3	0.42	0	2,2,2	0.41	0
6	EDO	B	2669	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	B	2674	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	B	2680	-	3,3,3	0.40	0	2,2,2	0.40	0
6	EDO	B	2684	-	3,3,3	0.44	0	2,2,2	0.18	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	2672	-	-	0/1/1/1	-
6	EDO	B	2665	-	-	0/1/1/1	-
6	EDO	B	2687	-	-	1/1/1/1	-
6	EDO	B	2675	-	-	0/1/1/1	-
6	EDO	B	2683	-	-	0/1/1/1	-
6	EDO	B	2668	-	-	0/1/1/1	-
6	EDO	B	2690	-	-	0/1/1/1	-
6	EDO	B	2688	-	-	0/1/1/1	-
6	EDO	B	2666	-	-	0/1/1/1	-
6	EDO	B	2664	-	-	0/1/1/1	-
6	EDO	A	1669	-	-	1/1/1/1	-
6	EDO	B	2671	-	-	0/1/1/1	-
6	EDO	B	2681	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	2678	-	-	0/1/1/1	-
6	EDO	B	2673	-	-	0/1/1/1	-
6	EDO	B	2667	-	-	1/1/1/1	-
6	EDO	B	2682	-	-	0/1/1/1	-
6	EDO	A	1667	-	-	0/1/1/1	-
6	EDO	B	2686	-	-	0/1/1/1	-
6	EDO	B	2685	-	-	0/1/1/1	-
6	EDO	B	2677	-	-	0/1/1/1	-
6	EDO	B	2670	-	-	0/1/1/1	-
6	EDO	A	1666	-	-	0/1/1/1	-
6	EDO	B	2689	-	-	0/1/1/1	-
6	EDO	B	2691	-	-	0/1/1/1	-
6	EDO	A	1668	-	-	0/1/1/1	-
6	EDO	B	2676	-	-	0/1/1/1	-
6	EDO	B	2679	-	-	1/1/1/1	-
6	EDO	B	2669	-	-	0/1/1/1	-
6	EDO	B	2674	-	-	0/1/1/1	-
6	EDO	B	2680	-	-	0/1/1/1	-
6	EDO	B	2684	-	-	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	A	1669	EDO	O1-C1-C2-O2
6	B	2687	EDO	O1-C1-C2-O2
6	B	2679	EDO	O1-C1-C2-O2
6	B	2667	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	2687	EDO	1	0
6	B	2675	EDO	1	0
6	B	2666	EDO	2	0
6	B	2671	EDO	1	0
6	B	2681	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2678	EDO	1	0
6	B	2673	EDO	1	0
6	B	2682	EDO	1	0
6	B	2677	EDO	1	0
6	A	1666	EDO	1	0
6	B	2691	EDO	1	0
6	B	2680	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, 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	639/645 (99%)	0.37	23 (3%)	46 42	38, 64, 99, 164	0
2	B	894/915 (97%)	0.35	61 (6%)	23 20	25, 64, 118, 157	1 (0%)
3	C	129/252 (51%)	0.58	10 (7%)	19 15	43, 71, 101, 122	0
All	All	1662/1812 (91%)	0.38	94 (5%)	29 25	25, 65, 110, 164	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	ALA	5.6
2	B	1506	CYS	4.1
1	A	461	LEU	4.1
1	A	665	PRO	3.9
2	B	1466	TYR	3.8
2	B	1437	ALA	3.7
2	B	1471	LEU	3.6
2	B	1454	SER	3.5
2	B	1472	ILE	3.5
2	B	1438	PHE	3.5
3	C	177	GLU	3.4
2	B	1511	CYS	3.4
2	B	1362	ASP	3.3
2	B	1467	PHE	3.3
2	B	1496	GLU	3.2
2	B	1523	SER	3.2
3	C	286	VAL	3.2
3	C	271	ASP	3.2
2	B	1371	PRO	3.2
2	B	1497	LYS	3.2
1	A	462	ARG	3.1
1	A	557	ASP	3.1
2	B	1383	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	658	ALA	3.1
3	C	158	GLU	3.0
2	B	1355	GLN	3.0
1	A	100	LYS	3.0
2	B	950	GLU	3.0
2	B	1616	PRO	3.0
2	B	790	LEU	3.0
1	A	588	ASP	3.0
2	B	966	ASP	2.8
3	C	159	LYS	2.8
2	B	785	GLY	2.8
2	B	954	ARG	2.8
2	B	1538	GLU	2.8
2	B	1611	PHE	2.8
2	B	792	ASN	2.7
2	B	1439	SER	2.7
3	C	160	VAL	2.6
2	B	1494	HIS	2.6
1	A	94	ARG	2.6
2	B	1425	VAL	2.6
2	B	1526	LYS	2.6
1	A	659	GLU	2.5
1	A	485	ALA	2.5
1	A	481	ARG	2.5
2	B	1291	GLU	2.5
2	B	916	VAL	2.5
1	A	463	THR	2.5
2	B	1525	ASP	2.5
2	B	1436	LYS	2.5
2	B	1410	GLY	2.5
2	B	1432	TYR	2.4
2	B	1433	GLU	2.4
2	B	1510	LEU	2.4
1	A	464	GLU	2.4
2	B	873	CYS	2.4
1	A	333	HIS	2.4
3	C	213	ASN	2.3
1	A	542	GLY	2.3
2	B	794	PHE	2.3
2	B	920	PHE	2.3
2	B	1662	PRO	2.3
2	B	882	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	582	THR	2.3
3	C	161	LEU	2.3
2	B	1394	GLY	2.2
1	A	583	LEU	2.2
2	B	872	PHE	2.2
2	B	762	VAL	2.2
1	A	385	TYR	2.2
2	B	1298	LEU	2.2
2	B	1313	TRP	2.2
2	B	957	VAL	2.2
2	B	1137	ASN	2.2
3	C	182	GLU	2.2
3	C	180	VAL	2.2
2	B	915	ALA	2.2
1	A	543	GLN	2.1
1	A	99	GLU	2.1
2	B	955	GLU	2.1
2	B	1612	TRP	2.1
2	B	775	VAL	2.1
2	B	1663	ASN	2.1
2	B	755	ILE	2.1
2	B	880	ARG	2.0
2	B	1554	LEU	2.0
1	A	585	ILE	2.0
2	B	1367	ILE	2.0
1	A	410	SER	2.0
2	B	1469	VAL	2.0
2	B	1507	ARG	2.0
2	B	990	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

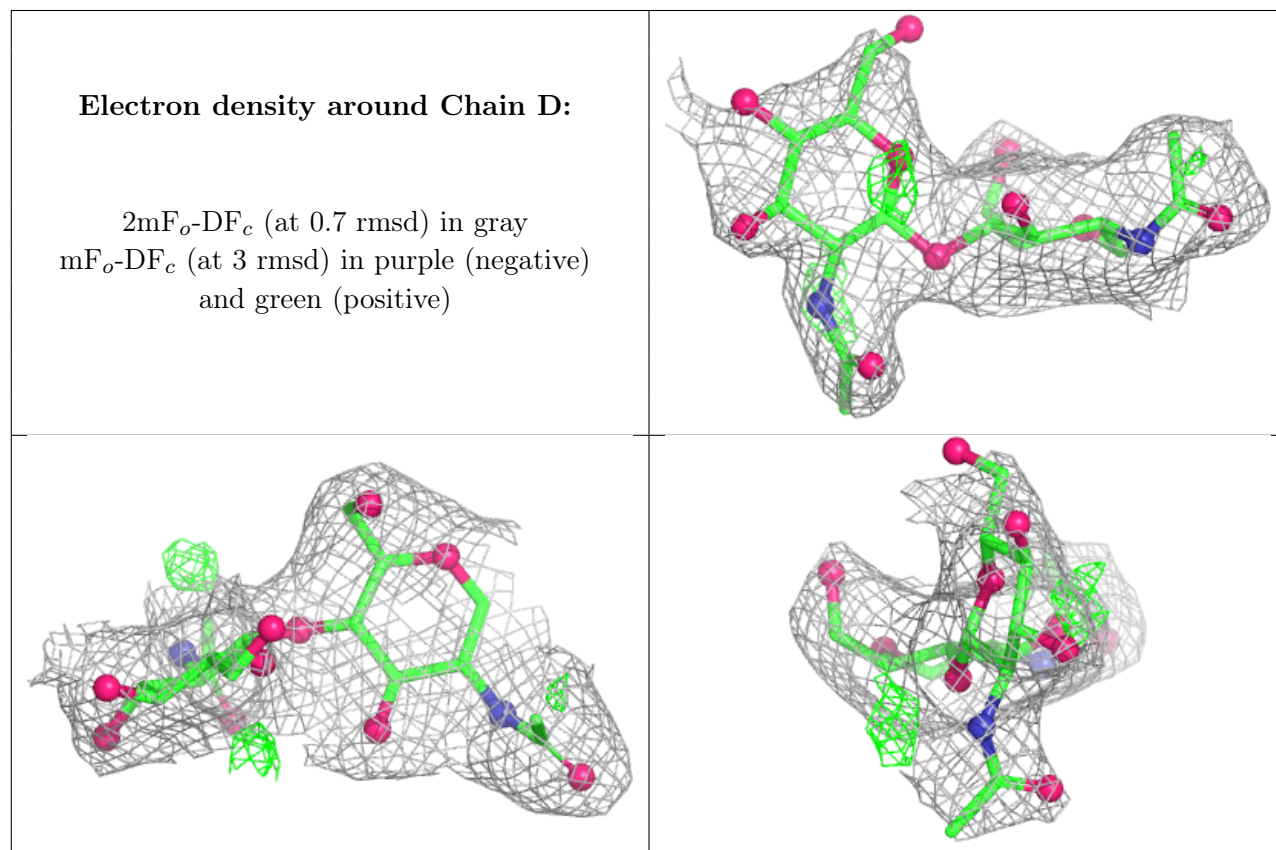
There are no non-standard protein/DNA/RNA residues in this entry.

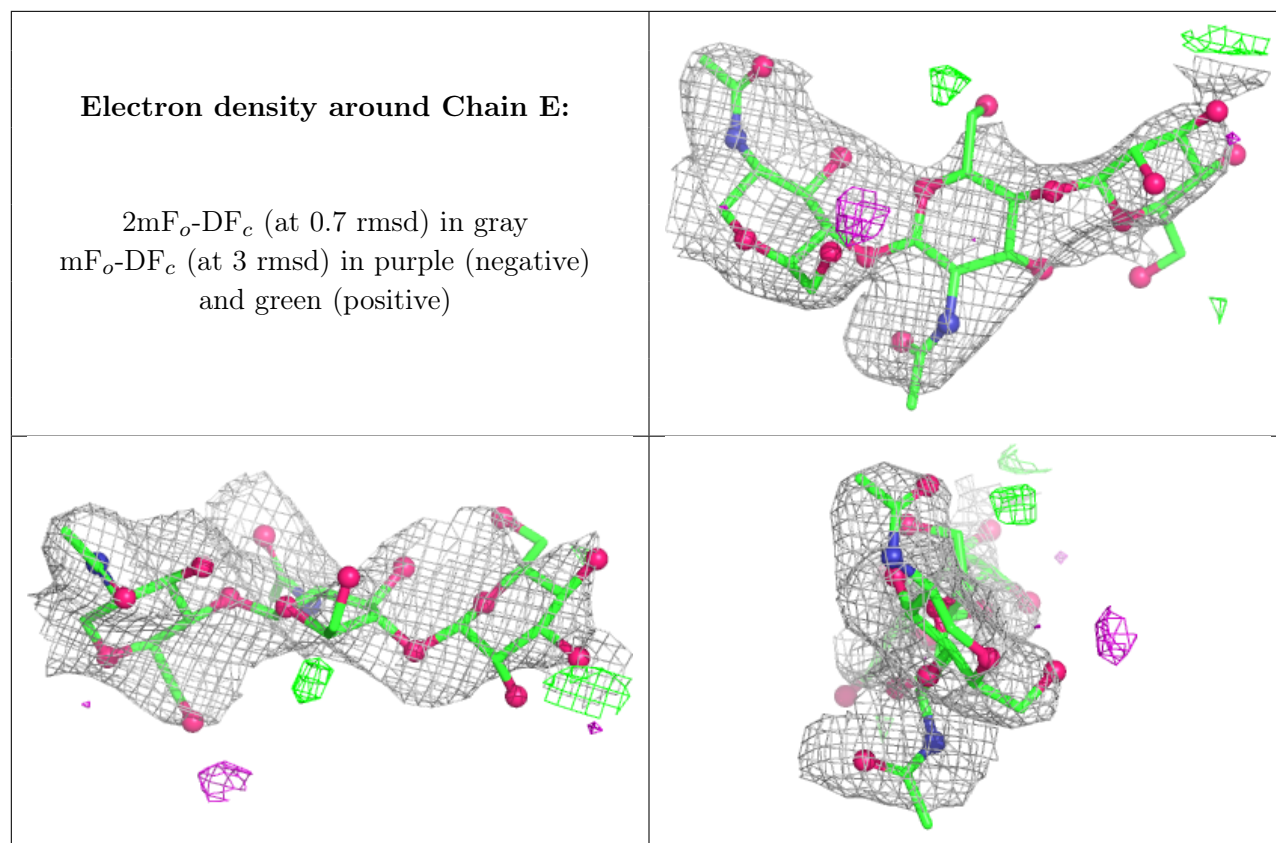
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	E	3	11/12	0.29	0.17	122,143,153,153	0
5	NAG	E	2	14/15	0.60	0.15	102,132,138,142	0
4	NAG	D	2	14/15	0.67	0.18	94,112,117,117	0
5	NAG	E	1	14/15	0.77	0.14	94,100,108,121	0
4	NAG	D	1	14/15	0.91	0.11	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.





6.4 Ligands [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
6	EDO	A	1669	4/4	0.46	0.25	99,99,100,101	0
6	EDO	B	2686	4/4	0.73	0.17	70,75,86,92	0
6	EDO	B	2688	4/4	0.74	0.24	76,78,82,85	0
6	EDO	B	2665	4/4	0.76	0.26	88,90,92,93	0
6	EDO	A	1666	4/4	0.78	0.26	79,82,83,85	0
6	EDO	B	2682	4/4	0.79	0.23	77,81,86,91	0
6	EDO	B	2666	4/4	0.80	0.20	59,60,62,63	2
6	EDO	B	2668	4/4	0.81	0.22	82,82,84,84	0
6	EDO	A	1668	4/4	0.82	0.20	92,92,95,96	0
6	EDO	B	2674	4/4	0.84	0.22	82,87,93,96	0
6	EDO	B	2673	4/4	0.85	0.24	70,70,75,77	1
6	EDO	B	2671	4/4	0.85	0.18	76,76,76,85	1
6	EDO	B	2677	4/4	0.85	0.17	85,87,88,88	0
6	EDO	B	2676	4/4	0.86	0.24	65,66,77,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	2669	4/4	0.86	0.17	87,87,88,88	0
6	EDO	B	2681	4/4	0.86	0.20	91,92,92,98	0
6	EDO	B	2678	4/4	0.88	0.28	62,63,64,65	0
6	EDO	A	1667	4/4	0.89	0.21	90,90,92,93	0
6	EDO	B	2685	4/4	0.90	0.19	48,58,61,64	0
6	EDO	B	2667	4/4	0.90	0.20	64,65,68,76	1
6	EDO	B	2679	4/4	0.90	0.18	68,73,77,82	0
6	EDO	B	2675	4/4	0.91	0.14	48,50,51,55	3
6	EDO	B	2672	4/4	0.92	0.16	74,74,76,78	0
6	EDO	B	2691	4/4	0.92	0.16	47,54,66,77	0
6	EDO	B	2689	4/4	0.93	0.14	62,65,71,73	0
6	EDO	B	2684	4/4	0.94	0.15	36,43,55,66	0
6	EDO	B	2664	4/4	0.94	0.12	42,56,63,72	0
6	EDO	B	2680	4/4	0.94	0.12	78,86,89,91	0
6	EDO	B	2683	4/4	0.95	0.11	55,56,56,57	0
6	EDO	B	2687	4/4	0.96	0.12	51,53,55,59	0
6	EDO	B	2690	4/4	0.96	0.11	33,38,48,54	0
6	EDO	B	2670	4/4	0.96	0.12	45,47,48,49	3

6.5 Other polymers [i](#)

There are no such residues in this entry.