



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 10:17 AM BST

PDB ID : 5FOB
Title : Crystal Structure of Human Complement C3b in complex with Smallpox Inhibitor of Complement (SPICE)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

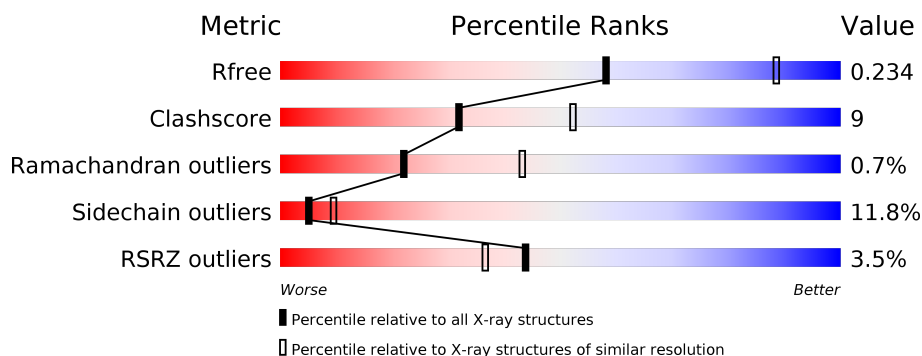
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 70% 25% . </div> </div>
2	B	915	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 75% 21% .. </div> </div>
3	C	245	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 15% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 64% 27% 7% . </div> </div>
4	D	4	<div> <div style="width: 100%; height: 10px; background-color: yellow; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 75% 25% </div> </div>
5	E	2	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	1	X	-	-	-
5	NAG	E	2	-	-	-	X
7	GOL	B	2673	-	-	-	X
9	IOD	B	2678	-	-	X	-
9	IOD	B	2679	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14474 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 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	3	0
			5011	3193	846	956	16			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7199	4563	1210	1388	38			

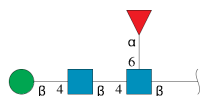
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	2	0
			1822	1138	309	356	19			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

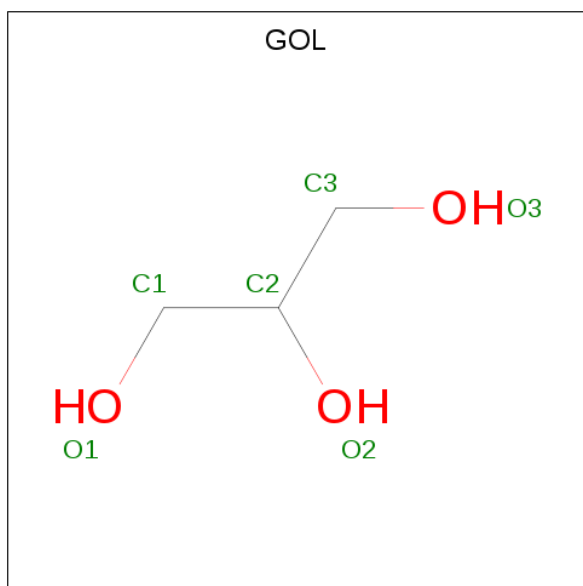


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	4	Total	I	0	0
			4	4		
9	A	3	Total	I	0	0
			3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total	O	0	0
			98	98		
10	B	92	Total	O	0	0
			92	92		
10	C	17	Total	O	0	0
			17	17		

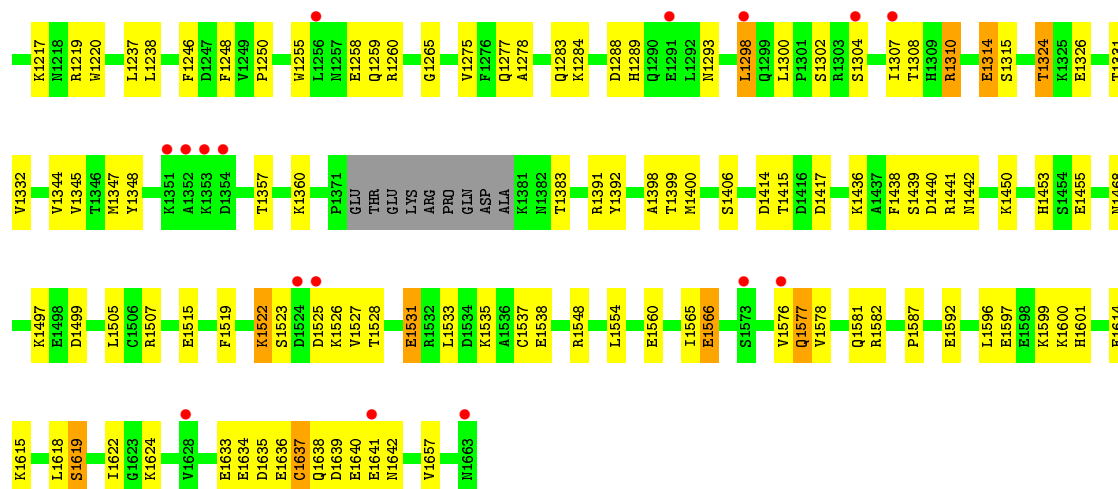
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A: ■ ■ ■

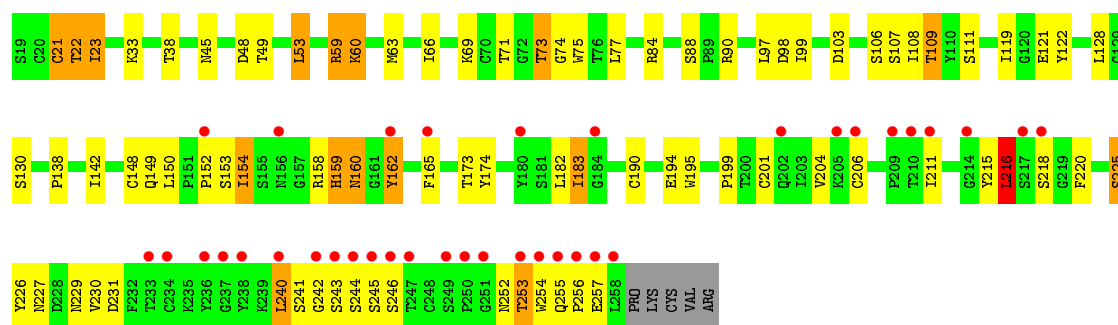
T582	N474	V387	K225	K104	S23
F475	P388	E233	E233	Q109	P24
V594	V389	A390	V236	A110	M25
K600	R478	V391	E248	T111	Y26
L605	R481	D395	K249	F112	I28
I616	E484	T396	K249	G113	I29
D634	R488	V397	R258	Q115	N32
G643	Y489	Q398	Y261	V116	L36
L644	Y490	S399	Y261	V117	E37
T645	L493	T401	G274	E118	M42
F646	L493	Q402	G274	K119	V43
T647	N496	G403	E279	V120	L44
S648	K497	K408	E280	L122	L44
S649	R498	L409	R281	V123	E45
T654	G499	S410	P292	S124	A46
Q664	L501	I411	P292	Q126	H47
PRO	K502	M412	S297	F131	Q50
ALA	A503	T413	G298	K136	D52
ALA	G504	S416	E299	R148	V53
	R505	L420	R304	V311	P54
	Q506	V424	V311	L319	V55
	V507	K427	Y325	V159	K65
	R508	K428	I331	G160	K66
	V515	Q429	E430	R161	L67
	L517	L431	S432	K176	S71
	I521	A434	E435	Q177	E72
	F525	S528	T448	D178	K73
	V534	Y534	V449	L186	T74
	Y535	T449	G450	L189	V75
	T536	M451	S452	L198	L76
	L537	M453	P547	N200	T77
	Q543	R544	L456	K205	T80
	R544	V551	S459	F357	N81
	V551	V555	V460	Y209	H82
	V555	Q569	R461	T360	V86
	Q569	S570	T463	K362	T87
	E571	D572	E464	K365	I90
	D572	R573	L465	P266	F91
	R573	Q580	T470	Y385	A92
	Q580	V581	L471	P385	N93
	V581			P385	R94
				P385	E95
				P385	F96
				P385	K97
				P385	S98
				P385	E99
				P385	K100
				P385	G101
				P385	R102
				P385	N102

Chain B:

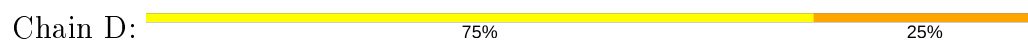
SER	ASU	ASU LEU	ASP	E753	D754	I755	A757	E758	F759	N760	R764	S765	E766	W773	E780	P781	K783	N784	G785	K789	D797	T800	T801	W802	E803	M826	F829	F830	I831	R834	R841	V845	E846	Y852	C873	S874	L875	K879	R880	H881	H882	V881
Q1033	W1034	E1035	L1039	E1040	K1041	R1042	Q1043	A1065	F1069	R1072	L1088	A1089	M1091	K1105	W1106	E1110	K1111	Q1112	K1113	Q1119	E1120	D1121	Q1127	E1128	M1129	I1130	L1133	M1136	L1148	Q1152	E1159	K1171	Y1194	M1199	L1206	L1211	T1212	T1213	T1214			



• Molecule 3: SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 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 1	Depositor
Cell constants a, b, c, α , β , γ	68.89Å 83.31Å 127.38Å 75.03° 76.20° 68.50°	Depositor
Resolution (Å)	42.36 – 2.60 42.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.36-2.60) 97.3 (42.36-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.230 0.202 , 0.234	Depositor DCC
R_{free} test set	2251 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.7	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	14474	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: GOL, BMA, NAG, CL, NA, FUC, IOD

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	0.26	0/5121	0.47	0/6958
2	B	0.26	0/7343	0.47	2/9943 (0.0%)
3	C	0.29	0/1877	0.54	0/2550
All	All	0.27	0/14341	0.48	2/19451 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1009	GLY	C-N-CA	5.79	136.18	121.70
2	B	880	ARG	NE-CZ-NH1	-5.03	117.79	120.30

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	5011	0	5068	98	0
2	B	7199	0	7116	116	1
3	C	1822	0	1703	45	1
4	D	49	0	43	3	0
5	E	28	0	25	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	1	0
6	C	2	0	0	0	0
7	A	60	0	80	11	0
7	B	72	0	96	13	0
7	C	12	0	16	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	3	0	0	1	0
9	B	4	0	0	8	0
10	A	98	0	0	1	0
10	B	92	0	0	4	0
10	C	17	0	0	0	0
All	All	14474	0	14147	254	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 9.

The worst 5 of 254 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:760:ASN:ND2	9:B:2679:IOD:I	2.35	1.25
9:B:2679:IOD:I	10:B:2007:HOH:O	2.24	1.25
2:B:1032:GLU:HG3	9:B:2678:IOD:I	2.26	1.04
2:B:1010:CYS:HB3	2:B:1013:GLU:HB2	1.43	0.99
2:B:1105:LYS:HD2	9:B:2681:IOD:I	2.45	0.87

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)
2:B:1600:LYS:NZ	3:C:73:THR:O[1_545]	2.09	0.11

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	643/645 (100%)	625 (97%)	15 (2%)	3 (0%)	29	52
2	B	898/915 (98%)	875 (97%)	22 (2%)	1 (0%)	51	75
3	C	240/245 (98%)	218 (91%)	14 (6%)	8 (3%)	4	6
All	All	1781/1805 (99%)	1718 (96%)	51 (3%)	12 (1%)	22	43

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	21	CYS
3	C	240	LEU
3	C	256	PRO
1	A	82	HIS
3	C	22	THR

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	566/567 (100%)	491 (87%)	75 (13%)	4	7
2	B	797/810 (98%)	722 (91%)	75 (9%)	8	17
3	C	205/215 (95%)	169 (82%)	36 (18%)	2	3
All	All	1568/1592 (98%)	1382 (88%)	186 (12%)	5	9

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	891	LYS
2	B	1259	GLN
3	C	162	TYR
2	B	937	ARG
2	B	1043	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	82	HIS
1	A	216	GLN
1	A	580	GLN
2	B	1277	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	0.94	0
4	NAG	D	2	4	14,14,15	0.61	0	17,19,21	0.90	0
4	BMA	D	3	4	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
4	FUC	D	4	4	10,10,11	1.04	0	14,14,16	1.16	1 (7%)
5	NAG	E	1	2,5	14,14,15	0.72	0	17,19,21	0.84	0
5	NAG	E	2	5	14,14,15	0.55	0	17,19,21	0.67	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	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	O2-C2-C3	-2.30	105.53	110.14
4	D	4	FUC	O5-C5-C4	2.18	113.43	109.52

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1	NAG	C1

5 of 7 torsion outliers are listed below:

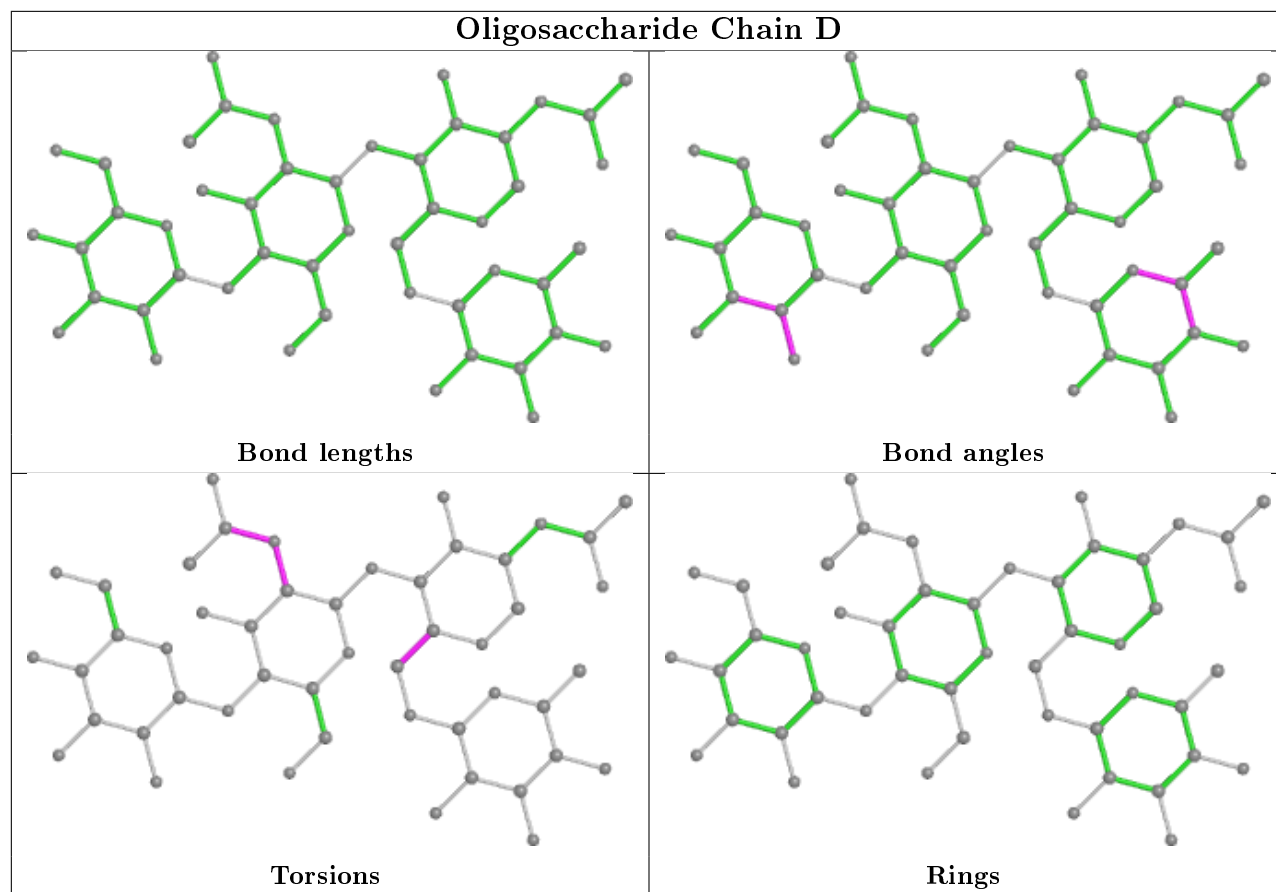
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

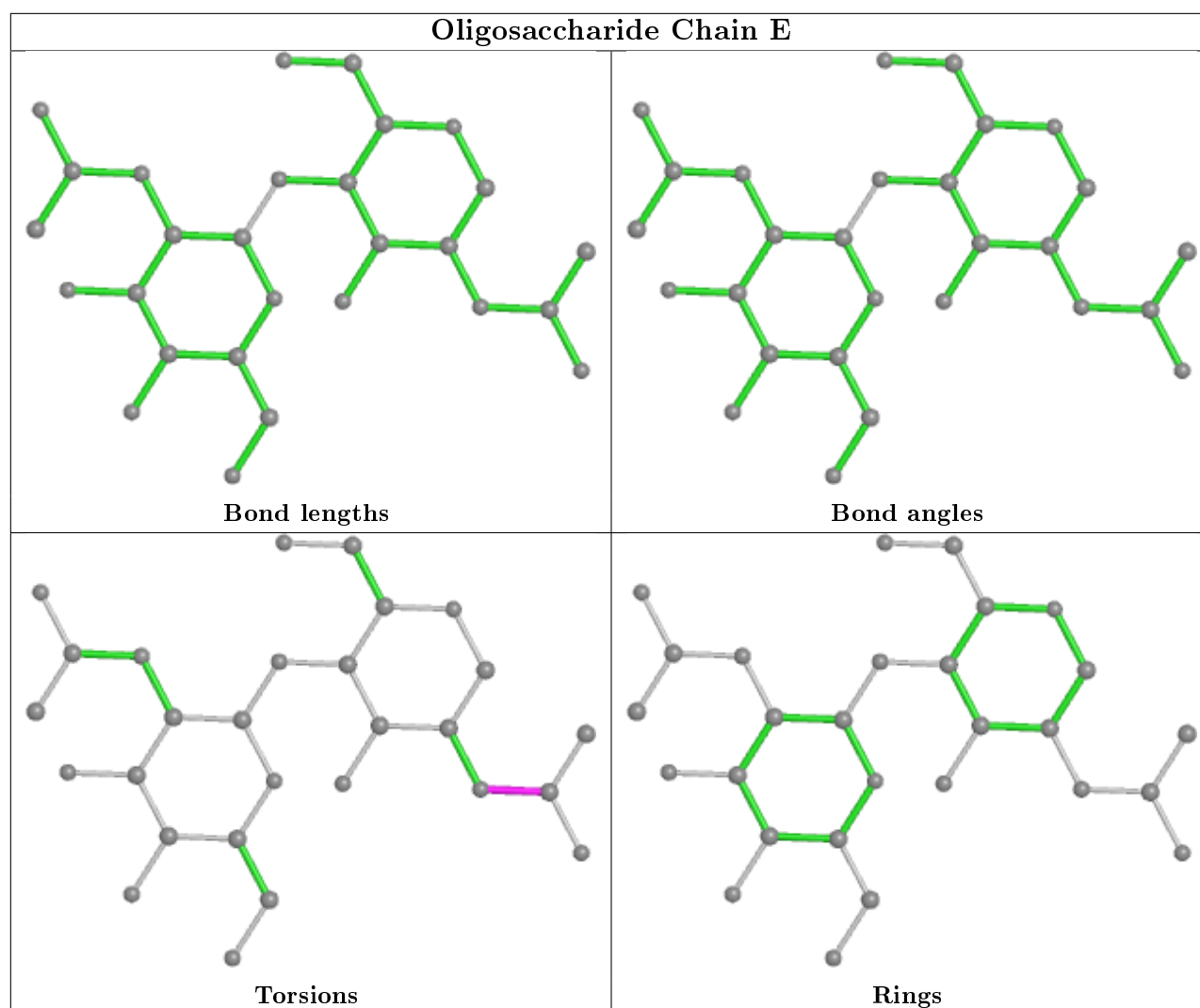
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	FUC	2	0
4	D	2	NAG	1	0
4	D	1	NAG	1	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](#)

Of 38 ligands modelled in this entry, 14 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	A	1675	-	5,5,5	0.36	0	5,5,5	0.37	0
7	GOL	B	2664	-	5,5,5	0.38	0	5,5,5	0.30	0
7	GOL	B	2672	-	5,5,5	0.38	0	5,5,5	0.29	0
7	GOL	A	1669	-	5,5,5	0.35	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	2665	-	5,5,5	0.35	0	5,5,5	0.34	0
7	GOL	A	1673	-	5,5,5	0.37	0	5,5,5	0.26	0
7	GOL	B	2670	-	5,5,5	0.37	0	5,5,5	0.25	0
7	GOL	A	1668	-	5,5,5	0.37	0	5,5,5	0.28	0
7	GOL	B	2674	-	5,5,5	0.39	0	5,5,5	0.27	0
7	GOL	A	1667	-	5,5,5	0.35	0	5,5,5	0.34	0
7	GOL	B	2671	-	5,5,5	0.35	0	5,5,5	0.33	0
7	GOL	C	1259	-	5,5,5	0.37	0	5,5,5	0.29	0
7	GOL	B	2669	-	5,5,5	0.38	0	5,5,5	0.33	0
7	GOL	A	1666	-	5,5,5	0.37	0	5,5,5	0.26	0
7	GOL	B	2673	-	5,5,5	0.36	0	5,5,5	0.27	0
7	GOL	A	1671	-	5,5,5	0.38	0	5,5,5	0.26	0
7	GOL	B	2675	-	5,5,5	0.39	0	5,5,5	0.33	0
7	GOL	B	2667	-	5,5,5	0.36	0	5,5,5	0.32	0
7	GOL	A	1672	-	5,5,5	0.35	0	5,5,5	0.30	0
7	GOL	C	1260	-	5,5,5	0.37	0	5,5,5	0.30	0
7	GOL	A	1674	-	5,5,5	0.36	0	5,5,5	0.29	0
7	GOL	B	2668	-	5,5,5	0.34	0	5,5,5	0.29	0
7	GOL	B	2666	-	5,5,5	0.37	0	5,5,5	0.39	0
7	GOL	A	1670	-	5,5,5	0.34	0	5,5,5	0.33	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
7	GOL	A	1675	-	-	2/4/4/4	-
7	GOL	B	2664	-	-	4/4/4/4	-
7	GOL	B	2672	-	-	2/4/4/4	-
7	GOL	A	1669	-	-	2/4/4/4	-
7	GOL	B	2665	-	-	2/4/4/4	-
7	GOL	A	1673	-	-	2/4/4/4	-
7	GOL	B	2670	-	-	2/4/4/4	-
7	GOL	A	1668	-	-	2/4/4/4	-
7	GOL	B	2674	-	-	2/4/4/4	-
7	GOL	A	1667	-	-	2/4/4/4	-
7	GOL	B	2671	-	-	2/4/4/4	-
7	GOL	C	1259	-	-	2/4/4/4	-
7	GOL	B	2669	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1666	-	-	2/4/4/4	-
7	GOL	B	2673	-	-	2/4/4/4	-
7	GOL	A	1671	-	-	2/4/4/4	-
7	GOL	B	2675	-	-	2/4/4/4	-
7	GOL	B	2667	-	-	2/4/4/4	-
7	GOL	A	1672	-	-	2/4/4/4	-
7	GOL	C	1260	-	-	0/4/4/4	-
7	GOL	A	1674	-	-	1/4/4/4	-
7	GOL	B	2668	-	-	2/4/4/4	-
7	GOL	B	2666	-	-	4/4/4/4	-
7	GOL	A	1670	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1675	GOL	C1-C2-C3-O3
7	B	2664	GOL	C1-C2-C3-O3
7	A	1669	GOL	O2-C2-C3-O3
7	B	2665	GOL	O1-C1-C2-C3
7	B	2670	GOL	C1-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1675	GOL	2	0
7	B	2664	GOL	2	0
7	A	1669	GOL	1	0
7	B	2665	GOL	1	0
7	A	1673	GOL	2	0
7	A	1668	GOL	2	0
7	B	2674	GOL	3	0
7	A	1667	GOL	2	0
7	A	1671	GOL	1	0
7	B	2675	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2667	GOL	1	0
7	C	1260	GOL	2	0
7	A	1674	GOL	1	0
7	B	2668	GOL	2	0
7	B	2666	GOL	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	642/645 (99%)	-0.10	8 (1%) 79 76	29, 73, 140, 195	0
2	B	902/915 (98%)	-0.08	19 (2%) 63 58	28, 74, 121, 174	0
3	C	240/245 (97%)	0.52	36 (15%) 2 1	44, 91, 171, 207	0
All	All	1784/1805 (98%)	-0.00	63 (3%) 44 36	28, 75, 142, 207	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	209	PRO	6.6
3	C	217	SER	6.0
3	C	243	SER	6.0
3	C	250	PRO	5.3
3	C	242	GLY	5.2

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.

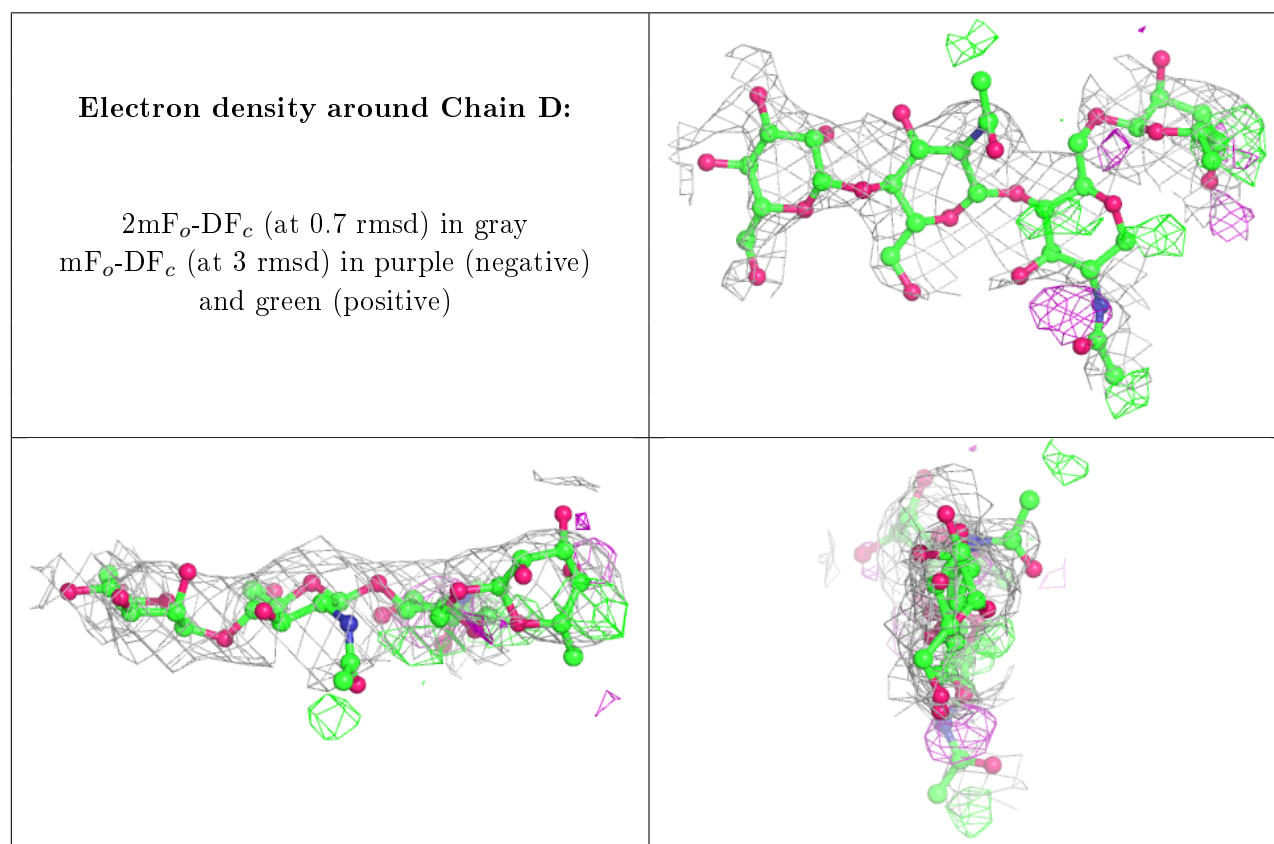
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	D	3	11/12	0.53	0.29	148,156,159,161	0
4	NAG	D	1	14/15	0.71	0.26	98,124,145,149	0
5	NAG	E	2	14/15	0.71	0.55	153,160,164,164	0

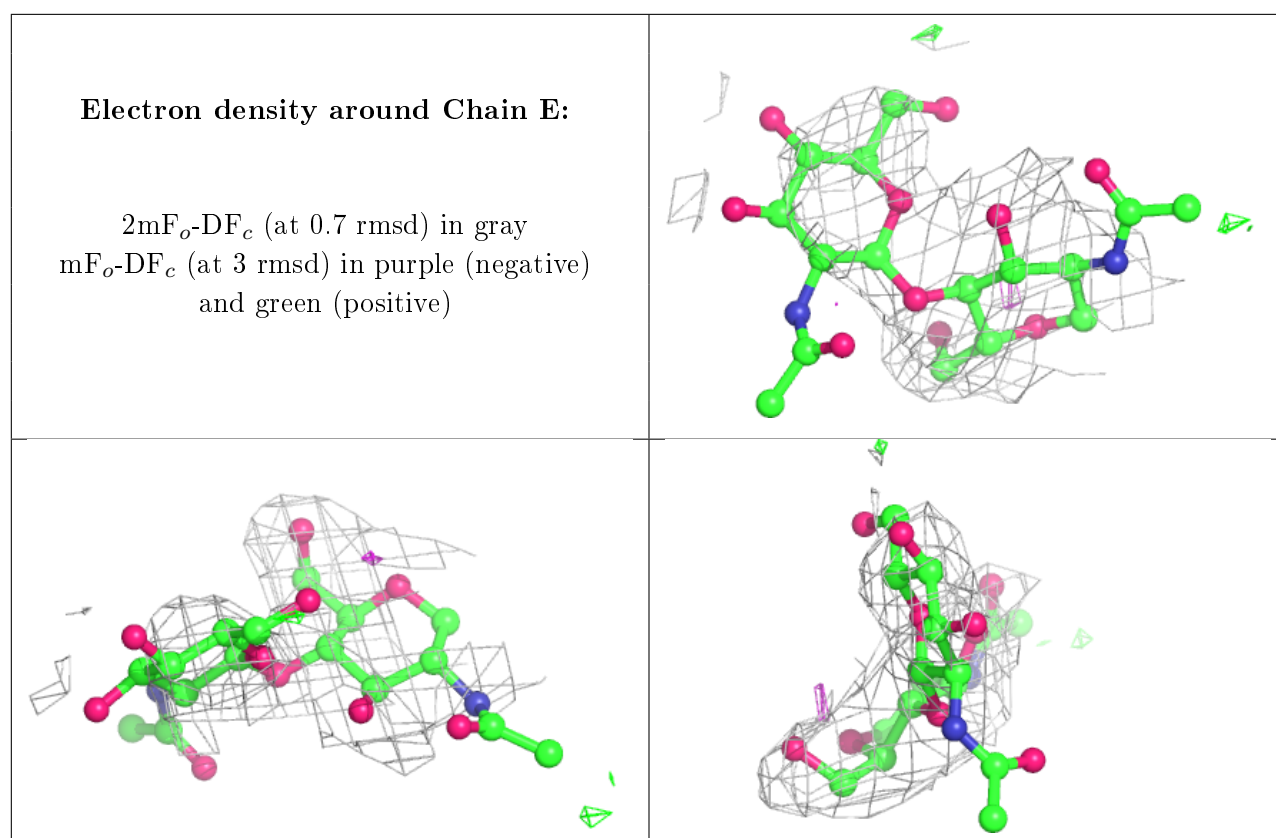
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FUC	D	4	10/11	0.81	0.32	67,116,142,148	0
5	NAG	E	1	14/15	0.83	0.26	103,130,146,146	0
4	NAG	D	2	14/15	0.89	0.17	137,141,147,152	0

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 ⓘ

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	CL	B	2682	1/1	0.53	0.31	66,66,66,66	0
7	GOL	B	2673	6/6	0.55	0.50	104,108,113,114	0
7	GOL	A	1669	6/6	0.61	0.39	95,100,101,102	0
7	GOL	A	1668	6/6	0.71	0.35	98,106,111,118	0
7	GOL	B	2669	6/6	0.73	0.39	116,118,119,119	0
7	GOL	A	1675	6/6	0.74	0.29	121,124,125,128	0
8	NA	A	1676	1/1	0.75	0.17	55,55,55,55	0
7	GOL	B	2670	6/6	0.78	0.19	87,99,105,107	0
7	GOL	A	1672	6/6	0.79	0.18	81,86,89,94	0
7	GOL	B	2668	6/6	0.81	0.18	56,77,84,88	0
7	GOL	A	1671	6/6	0.82	0.24	75,92,96,98	0
7	GOL	B	2672	6/6	0.82	0.32	105,110,115,116	0
8	NA	B	2677	1/1	0.84	0.38	85,85,85,85	0
7	GOL	A	1674	6/6	0.84	0.27	74,100,109,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	B	2674	6/6	0.85	0.15	72,77,85,87	0
7	GOL	B	2667	6/6	0.87	0.20	75,80,86,91	0
7	GOL	B	2671	6/6	0.88	0.21	77,79,80,82	0
7	GOL	B	2675	6/6	0.88	0.17	76,84,85,88	0
7	GOL	C	1259	6/6	0.89	0.21	77,94,98,101	0
6	CL	B	2676	1/1	0.90	0.18	72,72,72,72	0
7	GOL	A	1666	6/6	0.90	0.16	76,92,95,99	0
7	GOL	B	2664	6/6	0.91	0.27	79,83,87,90	0
7	GOL	C	1260	6/6	0.91	0.27	54,83,89,90	0
6	CL	A	1665	1/1	0.91	0.09	87,87,87,87	0
7	GOL	B	2665	6/6	0.91	0.18	59,64,71,77	0
7	GOL	A	1670	6/6	0.91	0.17	57,64,69,76	0
7	GOL	B	2666	6/6	0.95	0.13	52,55,64,70	0
7	GOL	A	1673	6/6	0.95	0.34	75,77,87,88	0
9	IOD	B	2680	1/1	0.96	0.14	68,68,68,68	1
7	GOL	A	1667	6/6	0.97	0.28	76,78,91,105	0
9	IOD	A	1678	1/1	0.97	0.16	64,64,64,64	1
9	IOD	A	1677	1/1	0.97	0.20	55,55,55,55	1
6	CL	C	1262	1/1	0.98	0.12	60,60,60,60	0
6	CL	C	1261	1/1	0.98	0.27	49,49,49,49	0
9	IOD	B	2681	1/1	0.99	0.17	75,75,75,75	1
9	IOD	B	2678	1/1	0.99	0.12	83,83,83,83	1
9	IOD	A	1679	1/1	0.99	0.14	65,65,65,65	1
9	IOD	B	2679	1/1	0.99	0.10	67,67,67,67	1

6.5 Other polymers

There are no such residues in this entry.