Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 10:40 AM EST

PDB ID	:	4WI2
Title	:	Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc (wild-type)
Authors	:	Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.
Deposited on	:	2014-09-25
Resolution	:	1.90 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:

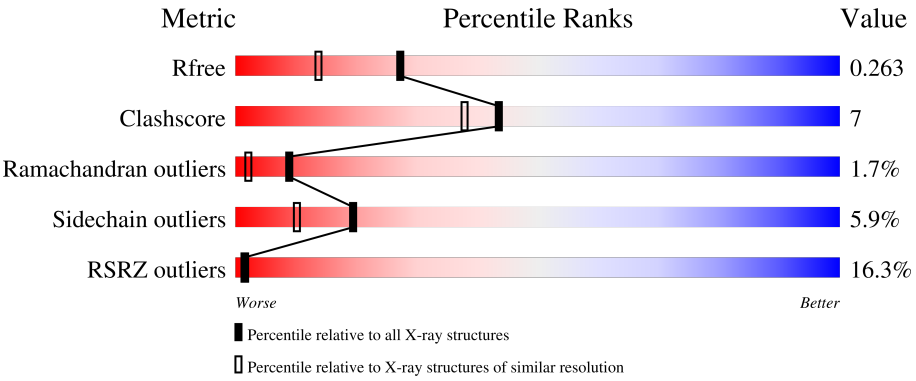
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	208	9% 82% 16%
1	B	208	24% 79% 15%
2	C	8	25% 75%
2	D	8	62% 38%

2 Entry composition (i)

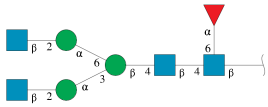
There are 4 unique types of molecules in this entry. The entry contains 3692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ig gamma-1 chain C region.

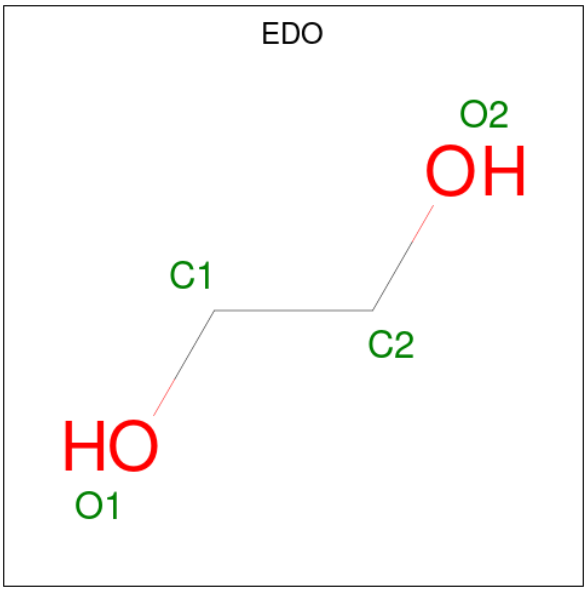
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			
2	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

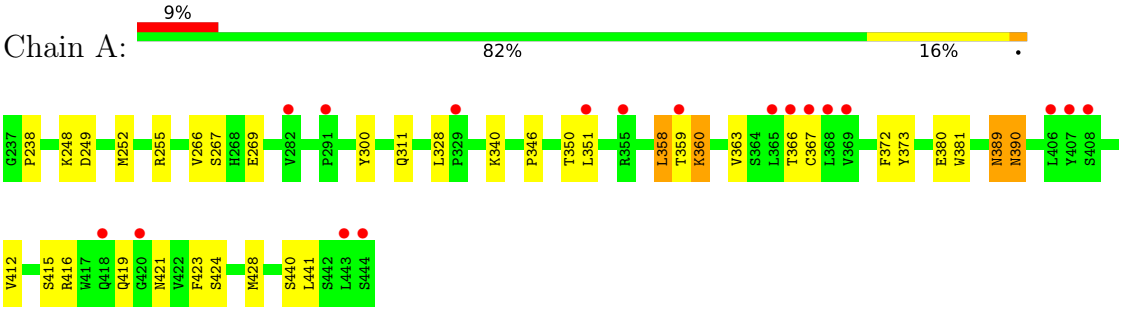
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	67	Total O 67 67	0	0

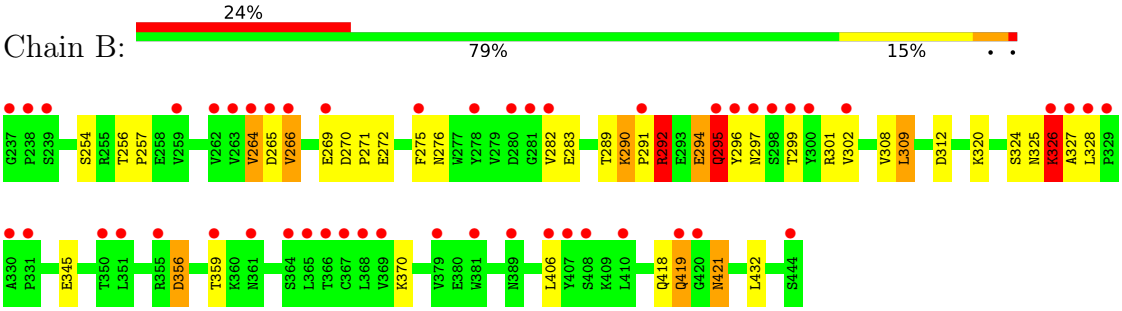
3 Residue-property plots (i)

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

• Molecule 1: Ig gamma-1 chain C region



• Molecule 1: Ig gamma-1 chain C region



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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


NAG1
NAG2
BMA3
MAN4
NAG5
MAN6
NAG7
FUC8

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.28Å 79.47Å 137.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.22 – 1.90 28.22 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.22-1.90) 97.0 (28.22-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.227 , 0.269 0.221 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3692	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/1710	0.75	0/2330
1	B	0.65	0/1710	0.76	1/2330 (0.0%)
All	All	0.67	0/3420	0.75	1/4660 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	292	ARG	N-CA-C	-5.61	95.86	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	326	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1630	20	0
1	B	1664	0	1630	26	0
2	C	99	0	85	0	0
2	D	99	0	85	4	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
4	A	87	0	0	1	0
4	B	67	0	0	1	0
All	All	3692	0	3448	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:HD3	1:B:326:LYS:H	1.53	0.73
1:B:264:VAL:HG21	2:D:1:NAG:O4	1.89	0.72
1:B:370:LYS:NZ	4:B:601:HOH:O	2.27	0.68
1:A:248:LYS:NZ	1:A:380:GLU:OE2	2.28	0.63
1:B:276:ASN:ND2	1:B:283:GLU:OE2	2.33	0.61
1:A:415:SER:O	1:A:419:GLN:HG2	2.02	0.59
1:B:266:VAL:HG11	1:B:302:VAL:HG23	1.83	0.59
1:B:294:GLU:O	1:B:295:GLN:HB2	2.04	0.57
1:A:415:SER:O	1:A:419:GLN:N	2.40	0.55
1:A:269:GLU:N	1:A:269:GLU:OE1	2.40	0.54
1:B:264:VAL:HG22	1:B:265:ASP:H	1.73	0.54
1:A:389:ASN:OD1	1:A:390:ASN:N	2.27	0.51
1:A:340:LYS:O	1:A:373:TYR:OH	2.20	0.50
1:A:249:ASP:OD1	1:A:255:ARG:NE	2.35	0.50
1:B:325:ASN:O	1:B:328:LEU:N	2.43	0.49
1:A:238:PRO:HD2	1:A:328:LEU:HD21	1.95	0.49
1:A:416:ARG:O	1:A:421:ASN:HB2	2.13	0.48
1:A:350:THR:HB	1:A:441:LEU:HD13	1.95	0.48
1:A:252:MET:SD	1:A:428:MET:HE1	2.54	0.47
2:D:1:NAG:H4	2:D:8:FUC:H2	1.96	0.47
1:A:267:SER:HB2	1:A:269:GLU:OE1	2.15	0.47
1:A:351:LEU:HB2	1:A:366:THR:HB	1.97	0.47
1:B:272:GLU:N	1:B:272:GLU:OE1	2.48	0.47
1:B:421:ASN:N	1:B:421:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:HD22	2:D:1:NAG:H83	1.79	0.46
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.99	0.45
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.99	0.44
1:A:358:LEU:C	1:A:360:LYS:H	2.21	0.44
1:A:311:GLN:HB2	4:A:652:HOH:O	2.17	0.44
1:B:257:PRO:O	1:B:308:VAL:HG12	2.18	0.43
1:B:309:LEU:HB2	1:B:312:ASP:OD1	2.19	0.43
1:A:412:VAL:HG11	1:A:423:PHE:CE2	2.53	0.43
1:B:271:PRO:HD2	1:B:272:GLU:OE1	2.19	0.42
1:B:301:ARG:NH2	2:D:6:MAN:O3	2.52	0.42
1:B:256:THR:HA	1:B:257:PRO:HD2	1.88	0.42
1:B:295:GLN:HB2	1:B:299:THR:O	2.20	0.42
1:B:289:THR:HG22	1:B:289:THR:O	2.20	0.42
1:B:290:LYS:HA	1:B:291:PRO:HD3	1.68	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.55	0.41
1:B:356:ASP:OD1	1:B:356:ASP:N	2.52	0.41
1:B:419:GLN:HG2	1:B:421:ASN:OD1	2.21	0.41
1:B:264:VAL:HG22	1:B:265:ASP:N	2.36	0.41
1:A:358:LEU:HA	1:A:358:LEU:HD13	1.57	0.40
1:B:275:PHE:CD1	1:B:289:THR:HG23	2.56	0.40
1:B:406:LEU:HD12	1:B:406:LEU:C	2.42	0.40
1:B:345:GLU:HG3	1:B:432:LEU:HD23	2.03	0.40
1:B:320:LYS:HB2	1:B:320:LYS:HE3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	206/208 (99%)	198 (96%)	6 (3%)	2 (1%)	15 6
1	B	206/208 (99%)	190 (92%)	11 (5%)	5 (2%)	6 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	412/416 (99%)	388 (94%)	17 (4%)	7 (2%)	9 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	B	294	GLU
1	B	292	ARG
1	B	295	GLN
1	B	327	ALA
1	A	389	ASN
1	B	326	LYS

5.3.2 Protein sidechains (i)

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	194/194 (100%)	188 (97%)	6 (3%)	40 32
1	B	194/194 (100%)	177 (91%)	17 (9%)	10 4
All	All	388/388 (100%)	365 (94%)	23 (6%)	19 10

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LEU
1	A	359	THR
1	A	360	LYS
1	A	363	VAL
1	A	424	SER
1	A	440	SER
1	B	254	SER
1	B	264	VAL
1	B	266	VAL
1	B	269	GLU
1	B	270	ASP

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Mol	Chain	Res	Type
1	B	282	VAL
1	B	290	LYS
1	B	292	ARG
1	B	295	GLN
1	B	296	TYR
1	B	309	LEU
1	B	324	SER
1	B	356	ASP
1	B	359	THR
1	B	418	GLN
1	B	419	GLN
1	B	421	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.47	0	17,19,21	1.31	2 (11%)
2	NAG	C	2	2	14,14,15	0.93	1 (7%)	17,19,21	1.07	1 (5%)
2	BMA	C	3	2	11,11,12	0.72	0	15,15,17	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	C	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.47	2 (13%)
2	NAG	C	5	2	14,14,15	0.70	0	17,19,21	1.86	4 (23%)
2	MAN	C	6	2	11,11,12	0.54	0	15,15,17	1.24	1 (6%)
2	NAG	C	7	2	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
2	FUC	C	8	2	10,10,11	0.57	0	14,14,16	0.83	0
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	1.51	2 (11%)
2	NAG	D	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.57	3 (17%)
2	BMA	D	3	2	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
2	MAN	D	4	2	11,11,12	0.57	0	15,15,17	1.17	2 (13%)
2	NAG	D	5	2	14,14,15	0.47	0	17,19,21	1.15	1 (5%)
2	MAN	D	6	2	11,11,12	0.76	0	15,15,17	1.52	3 (20%)
2	NAG	D	7	2	14,14,15	0.57	0	17,19,21	1.72	2 (11%)
2	FUC	D	8	2	10,10,11	0.67	0	14,14,16	1.15	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	4/6/23/26	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	C	7	2	-	2/6/23/26	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	2/6/23/26	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	7	2	-	4/6/23/26	0/1/1/1
2	FUC	D	8	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-2.46	1.39	1.43
2	C	4	MAN	O5-C1	-2.23	1.40	1.43
2	D	2	NAG	O5-C1	-2.13	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	NAG	C1-O5-C5	5.54	119.69	112.19
2	C	5	NAG	C3-C4-C5	4.67	118.57	110.24
2	D	2	NAG	C1-O5-C5	-4.45	106.16	112.19
2	D	1	NAG	C1-O5-C5	4.20	117.88	112.19
2	D	6	MAN	O5-C1-C2	-4.14	104.37	110.77
2	C	4	MAN	C2-C3-C4	-3.72	104.45	110.89
2	C	5	NAG	C2-N2-C7	-3.64	117.72	122.90
2	C	2	NAG	C2-N2-C7	-3.53	117.87	122.90
2	D	5	NAG	C1-O5-C5	3.45	116.86	112.19
2	C	1	NAG	C2-N2-C7	-3.32	118.18	122.90
2	C	7	NAG	C1-O5-C5	3.17	116.48	112.19
2	C	6	MAN	C1-C2-C3	2.90	113.23	109.67
2	C	5	NAG	O5-C1-C2	-2.73	106.98	111.29
2	C	1	NAG	O5-C5-C6	2.62	111.32	107.20
2	C	4	MAN	O5-C1-C2	-2.55	106.83	110.77
2	D	6	MAN	C1-C2-C3	2.51	112.76	109.67
2	D	1	NAG	O4-C4-C3	2.45	116.00	110.35
2	D	2	NAG	O5-C1-C2	-2.43	107.44	111.29
2	D	4	MAN	O5-C1-C2	-2.39	107.08	110.77
2	D	8	FUC	O2-C2-C1	2.31	113.87	109.15
2	D	2	NAG	O5-C5-C6	2.30	110.81	107.20
2	D	3	BMA	C1-C2-C3	2.05	112.19	109.67
2	D	4	MAN	O2-C2-C3	-2.05	106.03	110.14
2	C	5	NAG	C4-C3-C2	2.04	114.01	111.02
2	D	6	MAN	O2-C2-C3	-2.02	106.09	110.14
2	D	7	NAG	O7-C7-C8	-2.01	118.33	122.06

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	7	NAG	C8-C7-N2-C2
2	D	7	NAG	O7-C7-N2-C2
2	D	4	MAN	C4-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	D	7	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	C	7	NAG	C8-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	C	7	NAG	O7-C7-N2-C2
2	D	3	BMA	C4-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6

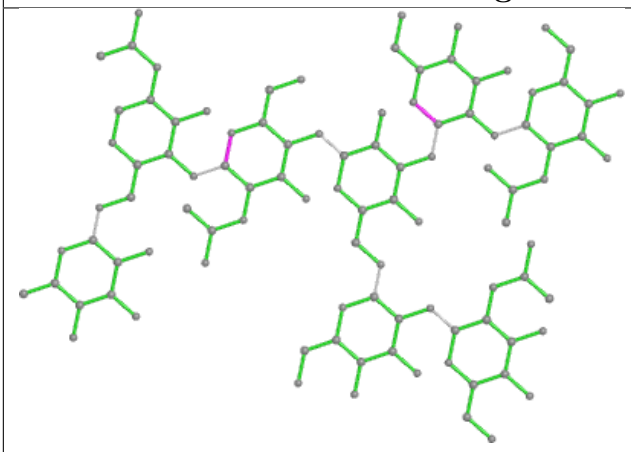
There are no ring outliers.

3 monomers are involved in 4 short contacts:

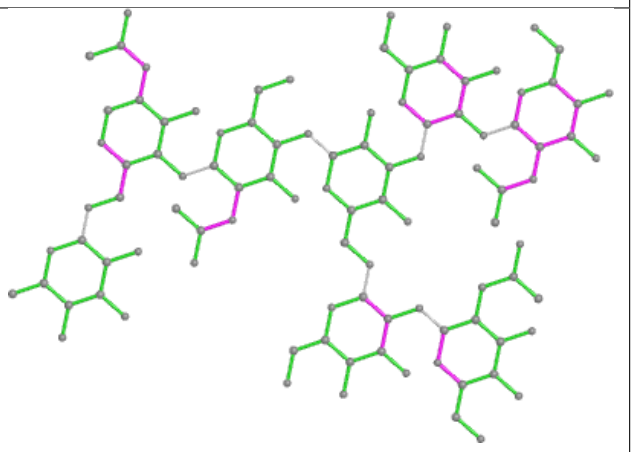
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	MAN	1	0
2	D	1	NAG	3	0
2	D	8	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

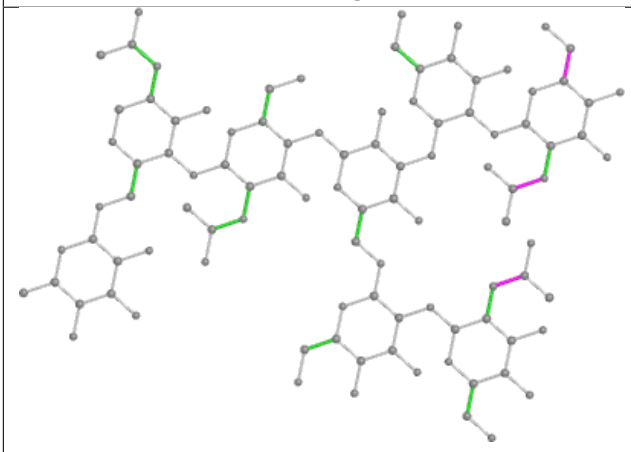
Oligosaccharide Chain C



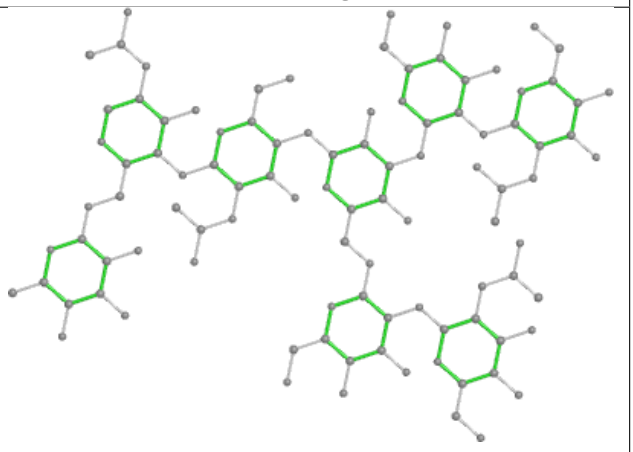
Bond lengths



Bond angles

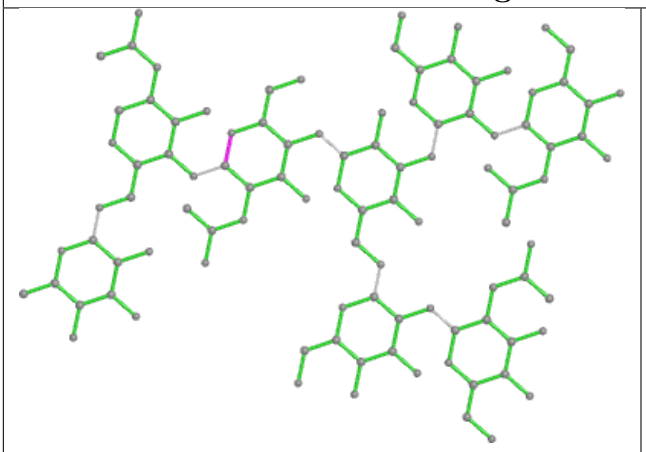


Torsions

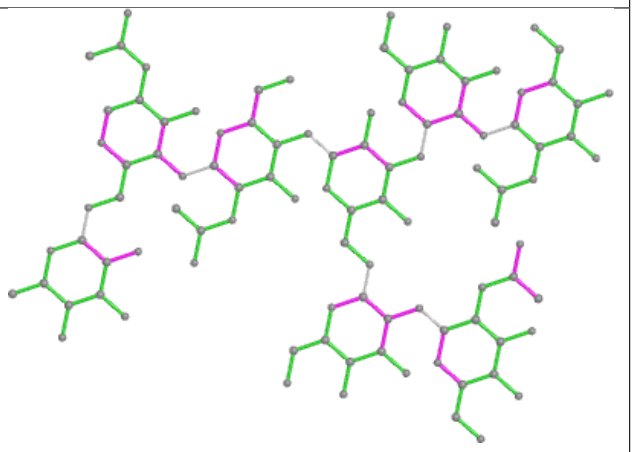


Rings

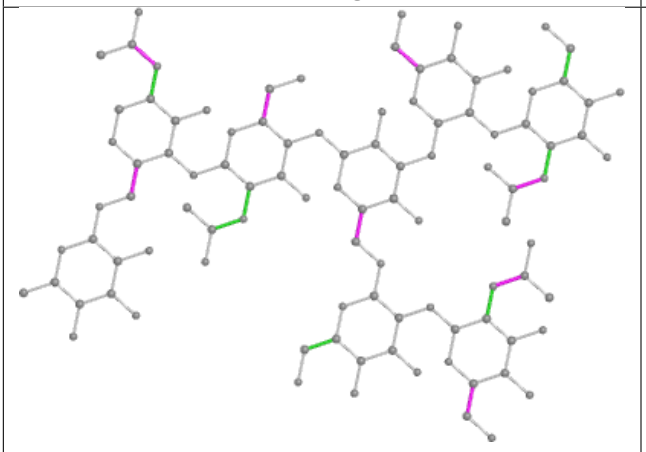
Oligosaccharide Chain D



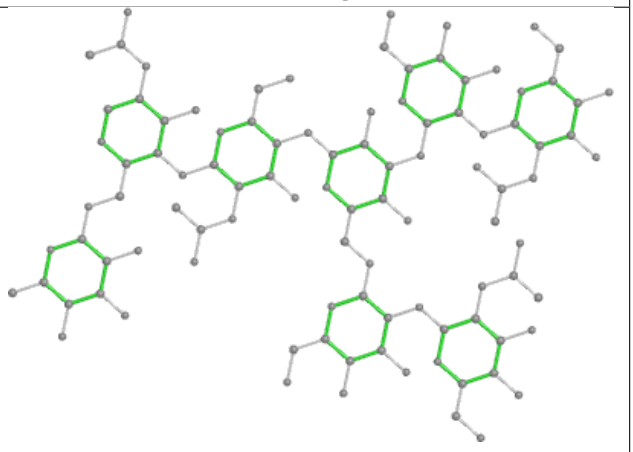
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	EDO	B	510	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	A	509	-	3,3,3	0.56	0	2,2,2	0.35	0
3	EDO	B	509	-	3,3,3	0.48	0	2,2,2	0.40	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
3	EDO	B	510	-	-	0/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	B	509	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	509	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	208/208 (100%)	0.48	18 (8%)	10	11	34, 58, 103, 120	0
1	B	208/208 (100%)	1.22	50 (24%)	0	0	33, 69, 120, 150	0
All	All	416/416 (100%)	0.85	68 (16%)	1	1	33, 62, 113, 150	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	10.1
1	B	237	GLY	6.7
1	B	281	GLY	6.6
1	B	300	TYR	6.2
1	B	329	PRO	5.8
1	B	330	ALA	5.5
1	B	351	LEU	5.1
1	B	368	LEU	5.0
1	B	366	THR	5.0
1	B	367	CYS	4.9
1	B	328	LEU	4.7
1	B	407	TYR	4.6
1	A	368	LEU	4.2
1	A	407	TYR	4.2
1	B	359	THR	4.1
1	A	444	SER	4.1
1	B	238	PRO	4.0
1	B	298	SER	4.0
1	B	266	VAL	3.9
1	B	291	PRO	3.8
1	A	355	ARG	3.8
1	A	366	THR	3.5
1	B	263	VAL	3.5
1	B	327	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	331	PRO	3.4
1	B	365	LEU	3.4
1	B	444	SER	3.3
1	B	295	GLN	3.3
1	B	419	GLN	3.3
1	A	329	PRO	3.2
1	A	367	CYS	3.2
1	B	408	SER	3.1
1	A	443	LEU	3.1
1	B	297	ASN	3.0
1	B	369	VAL	2.9
1	B	379	VAL	2.9
1	B	302	VAL	2.9
1	B	326	LYS	2.9
1	B	265	ASP	2.8
1	A	369	VAL	2.8
1	B	420	GLY	2.8
1	B	406	LEU	2.6
1	B	410	LEU	2.6
1	B	278	TYR	2.5
1	B	282	VAL	2.5
1	A	365	LEU	2.5
1	A	420	GLY	2.4
1	B	269	GLU	2.4
1	B	361	ASN	2.4
1	B	264	VAL	2.4
1	B	364	SER	2.4
1	A	282	VAL	2.4
1	B	275	PHE	2.4
1	B	389	ASN	2.4
1	B	299	THR	2.4
1	B	239	SER	2.3
1	B	350	THR	2.3
1	B	262	VAL	2.2
1	A	406	LEU	2.2
1	A	351	LEU	2.2
1	B	355	ARG	2.1
1	A	408	SER	2.1
1	A	359	THR	2.1
1	A	418	GLN	2.1
1	B	381	TRP	2.1
1	B	259	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	280	ASP	2.1
1	A	291	PRO	2.1

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)

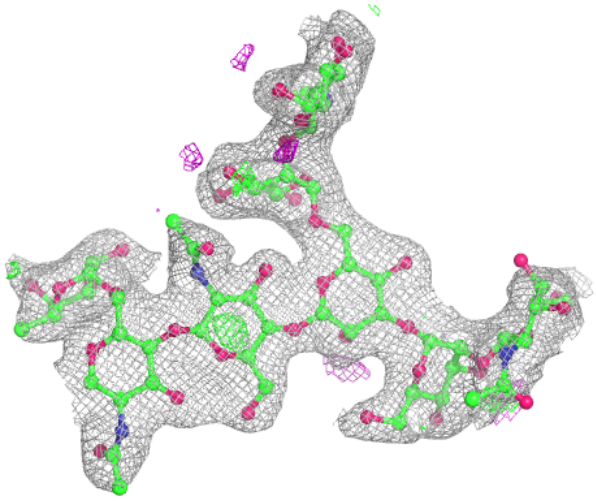
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

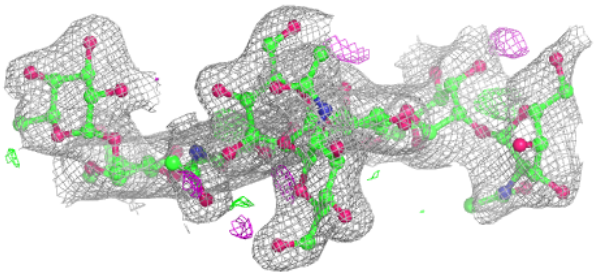
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	1	14/15	0.60	0.34	101,105,110,113	0
2	NAG	D	2	14/15	0.72	0.35	92,100,103,103	0
2	FUC	D	8	10/11	0.81	0.39	115,116,118,119	0
2	BMA	D	3	11/12	0.84	0.12	79,80,84,86	0
2	NAG	D	5	14/15	0.87	0.23	93,96,98,99	0
2	NAG	C	5	14/15	0.88	0.28	94,102,106,107	0
2	NAG	C	7	14/15	0.90	0.12	52,59,69,70	0
2	MAN	D	4	11/12	0.90	0.18	76,80,83,87	0
2	NAG	D	7	14/15	0.91	0.12	70,73,77,77	0
2	MAN	C	4	11/12	0.92	0.10	63,68,73,83	0
2	NAG	C	1	14/15	0.93	0.09	51,60,68,69	0
2	FUC	C	8	10/11	0.93	0.13	64,67,69,70	0
2	MAN	C	6	11/12	0.93	0.12	50,54,57,59	0
2	NAG	C	2	14/15	0.94	0.10	50,54,57,59	0
2	BMA	C	3	11/12	0.95	0.07	50,53,56,56	0
2	MAN	D	6	11/12	0.95	0.14	76,77,77,78	0

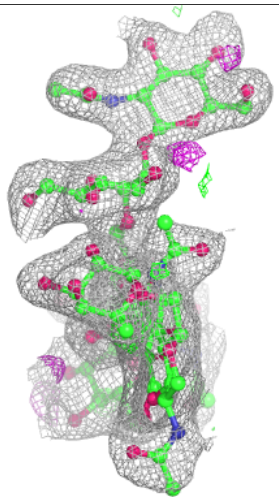
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

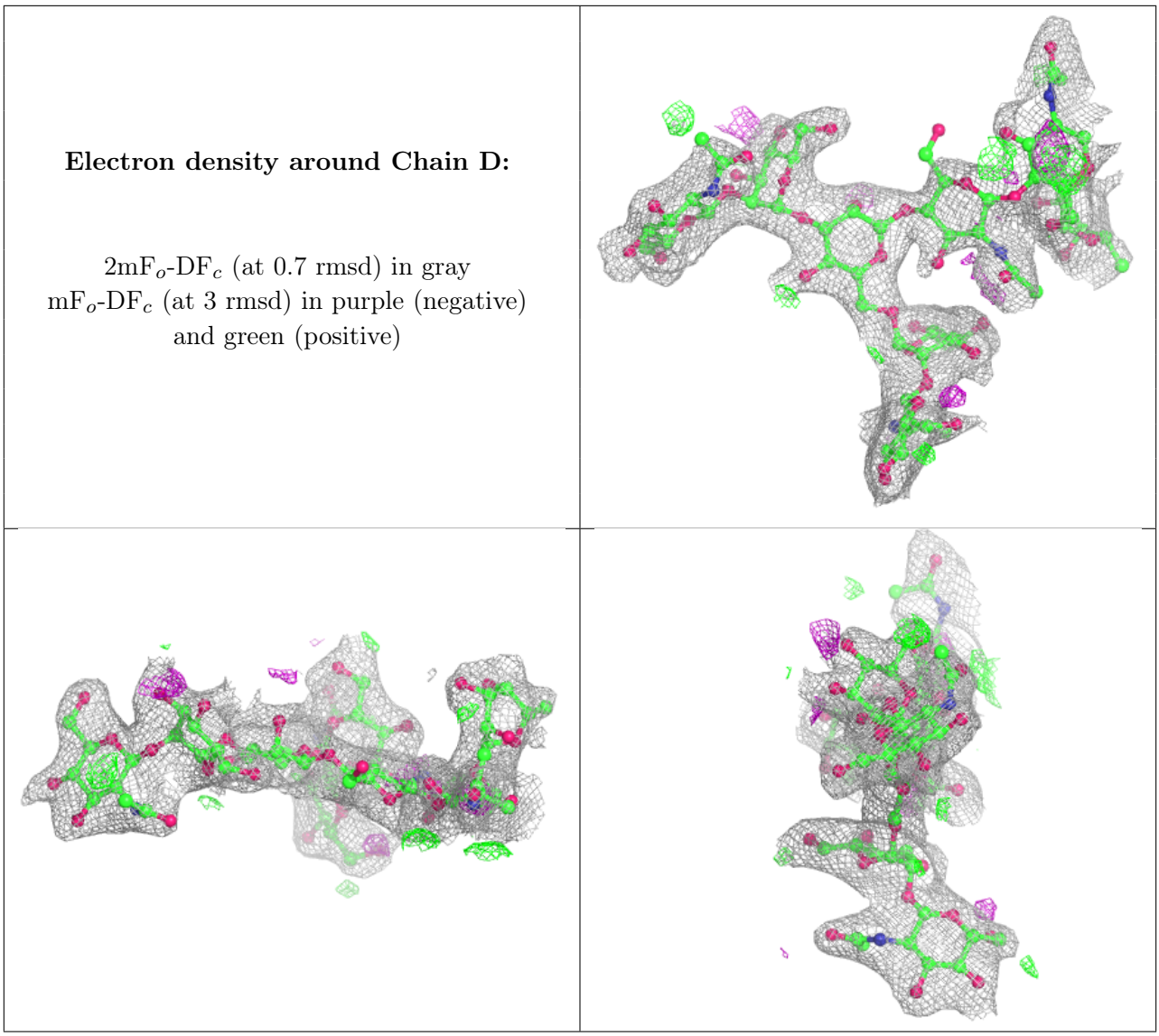






Electron density around Chain D:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	EDO	A	509	4/4	0.86	0.16	57,61,64,65	0
3	EDO	B	510	4/4	0.91	0.12	88,88,89,89	0
3	EDO	B	509	4/4	0.97	0.08	40,43,45,47	0

6.5 Other polymers (i)

There are no such residues in this entry.