Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2024 – 06:25 PM JST

PDB ID	:	8ZCM
Title	:	Cryogenic Temperature Crystal Structure of Fc Fragment of Human IgG1 from Biosimilar VEGF-Trap
Authors	:	Destan, E.; DeMirci, H.
Deposited on	:	2024-04-30
Resolution	:	2.64 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:

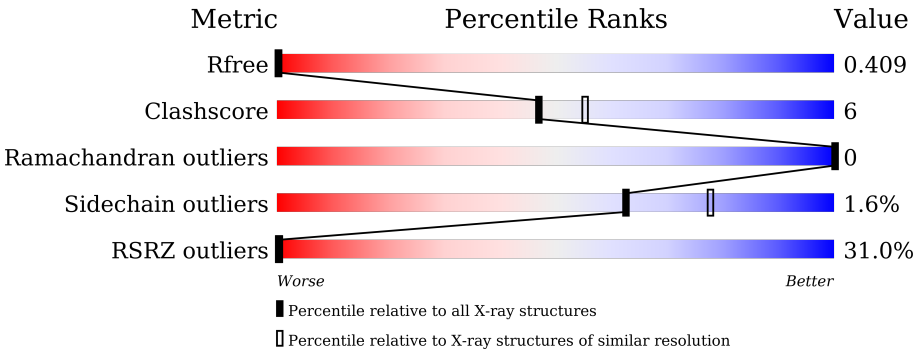
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	46% 80% 18%
1	B	208	16% 85% 14%
2	C	9	11% 44% 44%
3	D	7	57% 43%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	1	-	-	-	X

2 Entry composition

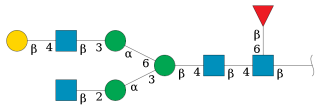
There are 5 unique types of molecules in this entry. The entry contains 3559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Immunoglobulin gamma-1 heavy chain.

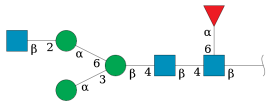
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	6	3	0
			1671	1064	282	319	6			
1	B	207	Total	C	N	O	S	0	0	0
			1658	1056	279	317	6			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



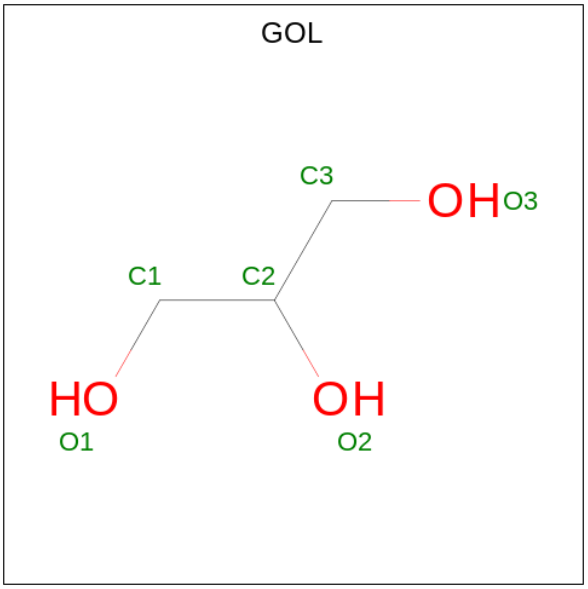
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
3	D	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

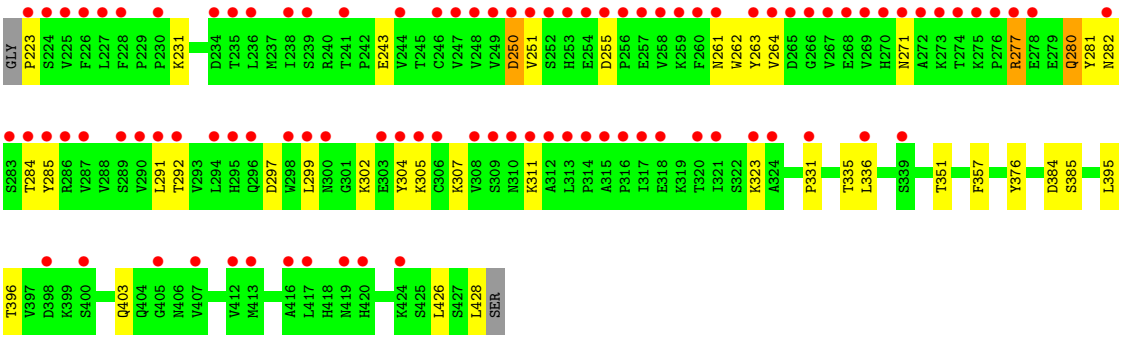
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total O 13 13	0	0
5	B	16	Total O 16 16	0	0

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.

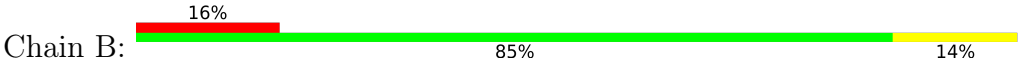
• Molecule 1: Immunoglobulin gamma-1 heavy chain

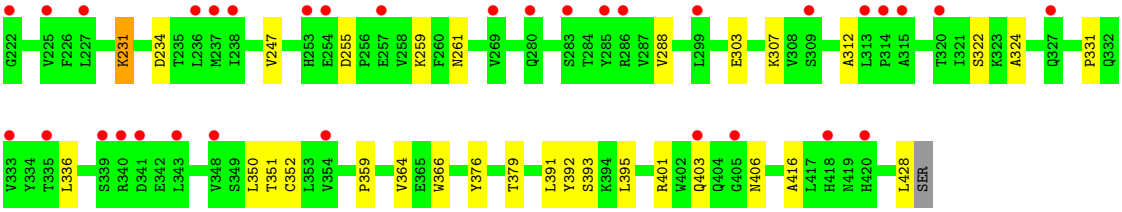
Chain A:



• Molecule 1: Immunoglobulin gamma-1 heavy chain

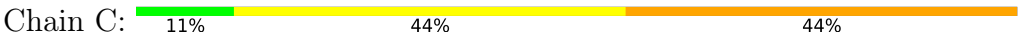
Chain B:





• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.45Å 79.62Å 125.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 2.64 46.01 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.01-2.64) 95.8 (46.01-2.64)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.354 , 0.409 0.354 , 0.409	Depositor DCC
R_{free} test set	1454 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	3559	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: GOL, NAG, GAL, BMA, FUL, MAN, FUC

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	0.24	0/1723	0.44	0/2346
1	B	0.23	0/1704	0.43	0/2322
All	All	0.23	0/3427	0.44	0/4668

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1671	0	1645	24	0
1	B	1658	0	1625	18	0
2	C	110	0	94	4	0
3	D	85	0	73	0	0
4	B	6	0	8	1	0
5	A	13	0	0	1	0
5	B	16	0	0	0	0
All	All	3559	0	3445	43	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 6.

All (43) 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:261:ASN:HB2	1:B:307:LYS:HB3	1.63	0.79
1:A:261:ASN:HB2	1:A:307:LYS:HB3	1.76	0.66
2:C:1:NAG:H61	2:C:2:NAG:HN2	1.60	0.66
1:A:396:THR:HG21	4:B:501:GOL:H12	1.80	0.64
1:A:282:ASN:OD1	1:A:284:THR:OG1	2.12	0.64
1:A:263:TYR:HB2	1:A:305:LYS:HB3	1.80	0.64
1:A:251:VAL:HB	1:A:285:TYR:HB2	1.79	0.63
1:B:401:ARG:O	1:B:406:ASN:ND2	2.32	0.63
1:A:336:LEU:HB2	1:A:351:THR:HB	1.81	0.61
1:A:351:THR:HG1	1:B:392:TYR:HH	1.49	0.61
1:B:364:VAL:HG21	1:B:391:LEU:HD11	1.83	0.61
1:B:336:LEU:HB2	1:B:351:THR:HB	1.83	0.59
1:A:223:PRO:HA	1:A:250:ASP:HB2	1.83	0.58
1:B:303:GLU:HA	1:B:322:SER:HB3	1.87	0.56
1:B:379:THR:HG1	1:B:392:TYR:H	1.54	0.56
1:B:231:LYS:HB2	1:B:234:ASP:OD2	2.06	0.56
1:A:277:ARG:H	1:A:277:ARG:HD2	1.74	0.53
1:A:271:ASN:HB2	1:A:291:LEU:HD12	1.90	0.52
1:A:331:PRO:HB3	1:A:357:PHE:HB3	1.90	0.52
1:A:403:GLN:HA	1:A:428:LEU:HD22	1.91	0.52
1:B:231:LYS:HZ2	1:B:231:LYS:H	1.58	0.52
2:C:2:NAG:H5	2:C:9:FUL:H61	1.91	0.51
1:B:324:ALA:HB3	1:B:359:PRO:HB3	1.97	0.47
1:B:403:GLN:HA	1:B:428:LEU:HD22	1.97	0.47
1:B:247:VAL:HG22	1:B:288:VAL:HG22	1.97	0.47
1:A:231:LYS:NZ	5:A:501:HOH:O	2.35	0.46
1:B:331:PRO:HD3	1:B:416:ALA:HB3	1.98	0.46
1:B:255:ASP:OD2	1:B:312:ALA:HB2	2.16	0.45
1:B:366:TRP:NE1	1:B:393:SER:OG	2.44	0.45
1:A:297:ASP:HB3	1:A:302:LYS:HD2	1.99	0.45
1:A:335:THR:HB	1:A:426:LEU:HD22	1.99	0.44
1:B:352:CYS:HB3	1:B:393:SER:HB3	1.99	0.43
1:B:350:LEU:HD12	1:B:395:LEU:HD23	2.01	0.43
1:A:280:GLN:HG3	2:C:1:NAG:C1	2.49	0.43
1:A:255:ASP:HB3	1:A:311:LYS:HB2	2.01	0.43
1:A:262:TRP:CE3	1:A:291:LEU:HD22	2.54	0.43
1:A:384:ASP:OD1	1:A:385:SER:N	2.44	0.43
1:B:376:TYR:HB3	1:B:395:LEU:HD13	2.00	0.43
1:A:231:LYS:HE2	2:C:6:GAL:H2	2.00	0.42
1:A:376:TYR:HB3	1:A:395:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG22	1:A:304:TYR:HD1	1.85	0.41
1:A:243:GLU:HA	1:A:292:THR:HA	2.02	0.40
1:A:299:LEU:O	1:A:323:LYS:NZ	2.48	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	207/208 (100%)	203 (98%)	4 (2%)	0	100	100
1	B	205/208 (99%)	204 (100%)	1 (0%)	0	100	100
All	All	412/416 (99%)	407 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	196/194 (101%)	192 (98%)	4 (2%)	55	72
1	B	193/194 (100%)	191 (99%)	2 (1%)	76	86
All	All	389/388 (100%)	383 (98%)	6 (2%)	62	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ASP
1	A	277	ARG
1	A	280	GLN
1	A	281	TYR
1	B	231	LYS
1	B	259	LYS

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	1.74	1 (7%)	17,19,21	1.32	3 (17%)
2	NAG	C	2	2	14,14,15	0.78	1 (7%)	17,19,21	0.88	0
2	BMA	C	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.65	2 (13%)
2	MAN	C	4	2	11,11,12	1.16	1 (9%)	15,15,17	1.84	3 (20%)
2	NAG	C	5	2	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
2	GAL	C	6	2	11,11,12	0.43	0	15,15,17	1.03	1 (6%)
2	MAN	C	7	2	11,11,12	1.14	1 (9%)	15,15,17	1.20	1 (6%)
2	NAG	C	8	2	14,14,15	0.30	0	17,19,21	0.47	0
2	FUL	C	9	2	10,10,11	1.63	2 (20%)	14,14,16	2.59	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	D	1	3,1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.50	0
3	BMA	D	3	3	11,11,12	1.26	2 (18%)	15,15,17	1.44	3 (20%)
3	MAN	D	4	3	11,11,12	0.73	0	15,15,17	1.38	2 (13%)
3	NAG	D	5	3	14,14,15	0.24	0	17,19,21	0.42	0
3	MAN	D	6	3	11,11,12	0.83	0	15,15,17	1.25	2 (13%)
3	FUC	D	7	3	10,10,11	0.75	0	14,14,16	0.86	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
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	GAL	C	6	2	-	1/2/19/22	0/1/1/1
2	MAN	C	7	2	-	1/2/19/22	1/1/1/1
2	NAG	C	8	2	-	2/6/23/26	0/1/1/1
2	FUL	C	9	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	1/1/1/1
3	NAG	D	5	3	-	1/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	1/1/1/1
3	FUC	D	7	3	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	5.92	1.61	1.52
2	C	9	FUL	O5-C1	4.03	1.50	1.43
2	C	3	BMA	C2-C3	3.07	1.57	1.52
3	D	3	BMA	C2-C3	2.84	1.56	1.52
3	D	3	BMA	C1-C2	2.66	1.58	1.52
2	C	3	BMA	O3-C3	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	MAN	C1-C2	2.57	1.58	1.52
2	C	2	NAG	C1-C2	2.30	1.55	1.52
2	C	4	MAN	C1-C2	2.24	1.57	1.52
2	C	9	FUL	C2-C3	-2.00	1.49	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	5.29	119.35	112.19
2	C	3	BMA	O3-C3-C2	5.09	119.75	109.99
2	C	9	FUL	C3-C4-C5	4.91	117.42	109.77
2	C	9	FUL	C2-C3-C4	4.88	119.34	110.89
2	C	9	FUL	C1-C2-C3	4.73	115.48	109.67
2	C	5	NAG	C1-O5-C5	4.09	117.73	112.19
3	D	4	MAN	C1-O5-C5	3.96	117.55	112.19
3	D	3	BMA	C1-C2-C3	3.73	114.25	109.67
3	D	6	MAN	C1-O5-C5	3.64	117.12	112.19
2	C	7	MAN	C1-O5-C5	3.33	116.71	112.19
2	C	5	NAG	C3-C4-C5	3.09	115.75	110.24
2	C	1	NAG	O5-C5-C4	-2.90	103.77	110.83
2	C	4	MAN	C1-C2-C3	2.77	113.08	109.67
2	C	1	NAG	C4-C3-C2	2.76	115.07	111.02
3	D	4	MAN	O2-C2-C3	-2.59	104.95	110.14
2	C	9	FUL	C6-C5-C4	-2.54	108.39	113.07
2	C	6	GAL	C1-O5-C5	2.37	115.41	112.19
2	C	4	MAN	O2-C2-C3	-2.37	105.39	110.14
2	C	3	BMA	C1-O5-C5	2.37	115.40	112.19
2	C	1	NAG	C3-C4-C5	-2.36	106.03	110.24
2	C	9	FUL	O5-C5-C4	2.30	113.65	109.52
3	D	6	MAN	O2-C2-C3	-2.28	105.57	110.14
3	D	3	BMA	C1-O5-C5	2.13	115.08	112.19
3	D	3	BMA	O5-C1-C2	2.00	113.86	110.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6
2	C	8	NAG	O5-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
2	C	8	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
3	D	5	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

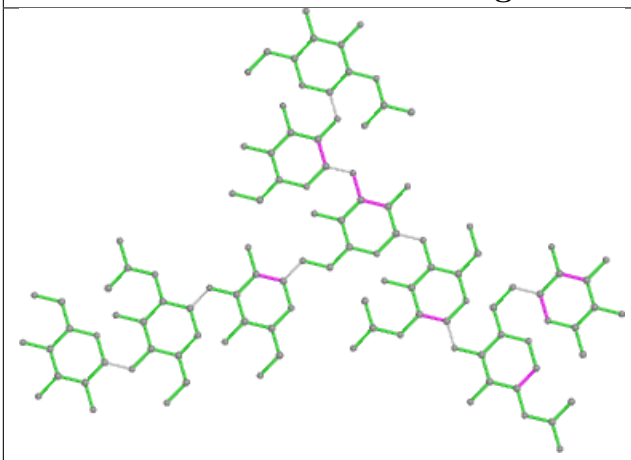
Mol	Chain	Res	Type	Atoms
2	C	7	MAN	C1-C2-C3-C4-C5-O5
3	D	6	MAN	C1-C2-C3-C4-C5-O5
3	D	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

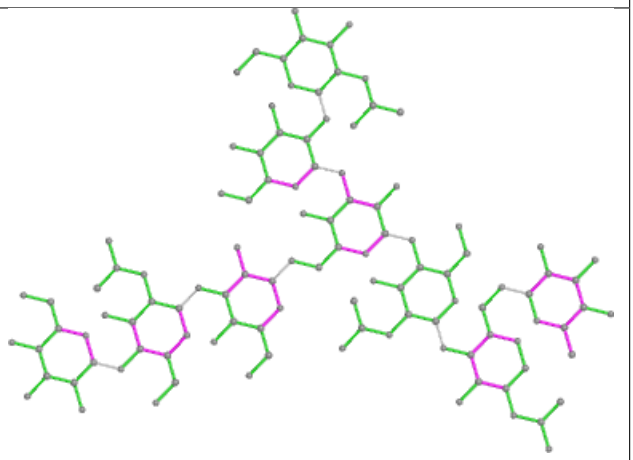
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	GAL	1	0
2	C	2	NAG	2	0
2	C	9	FUL	1	0
2	C	1	NAG	2	0

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

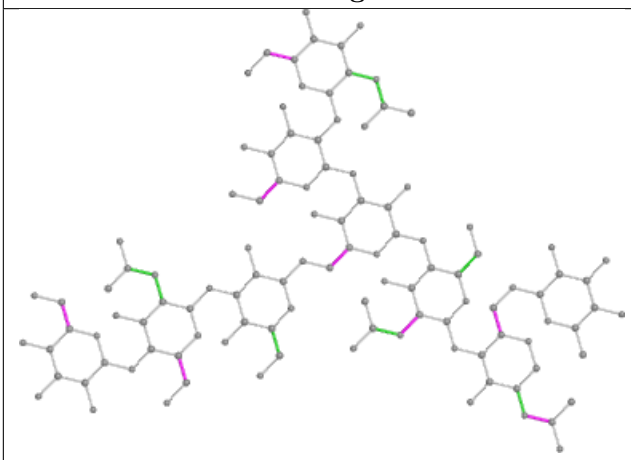
Oligosaccharide Chain C



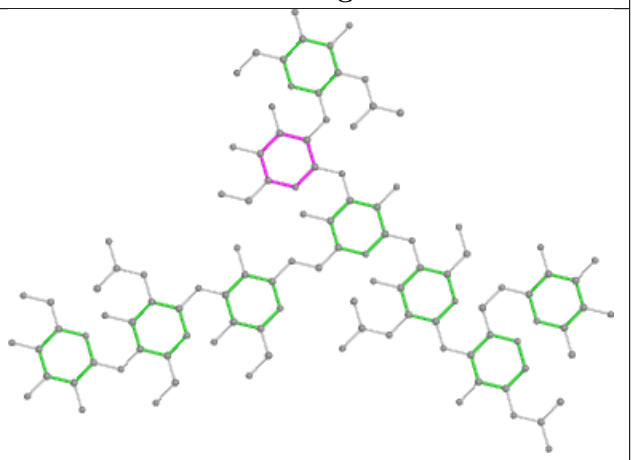
Bond lengths



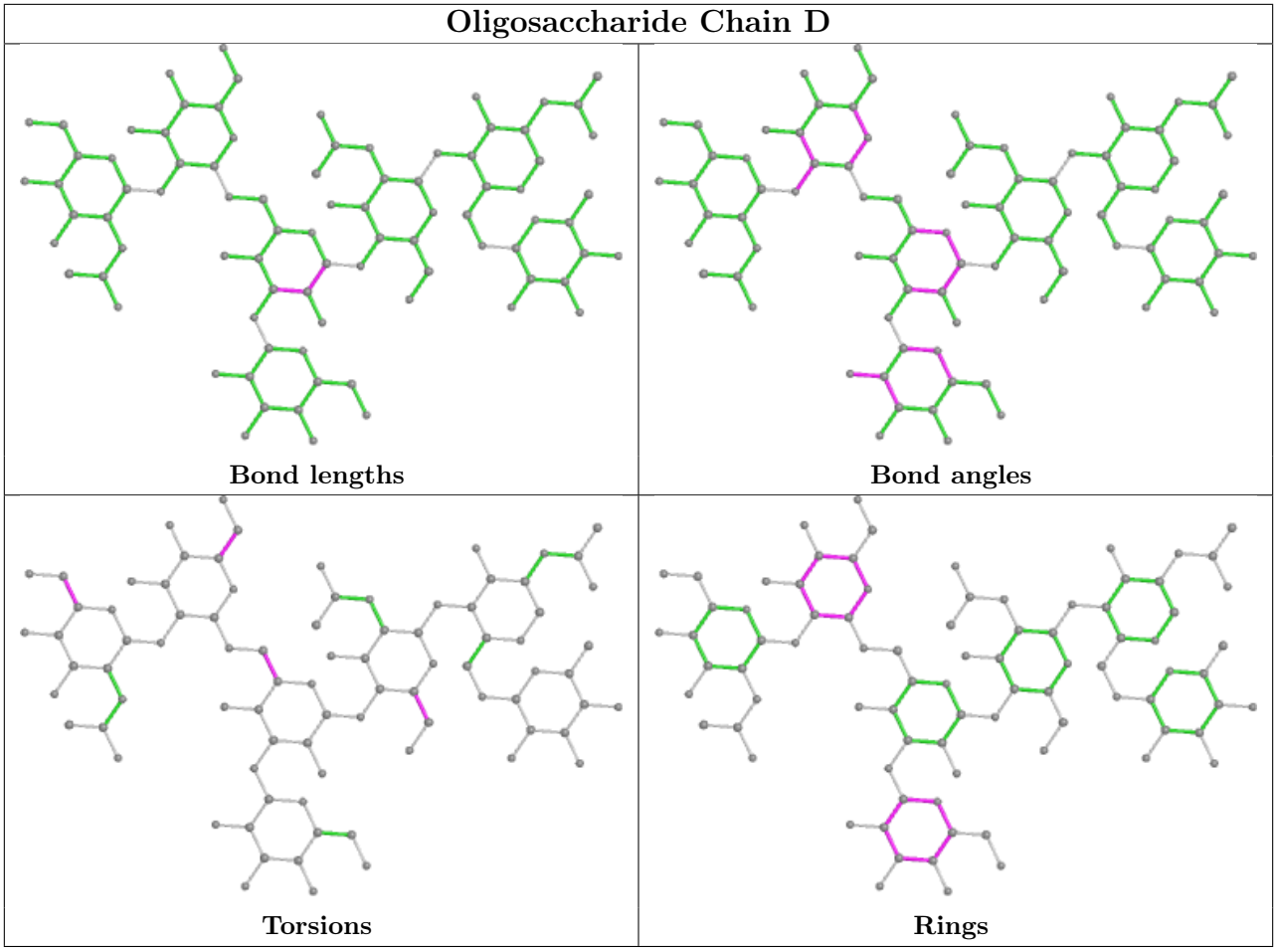
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

1 ligand is 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	GOL	B	501	-	5,5,5	0.91	0	5,5,5	0.99	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	GOL	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

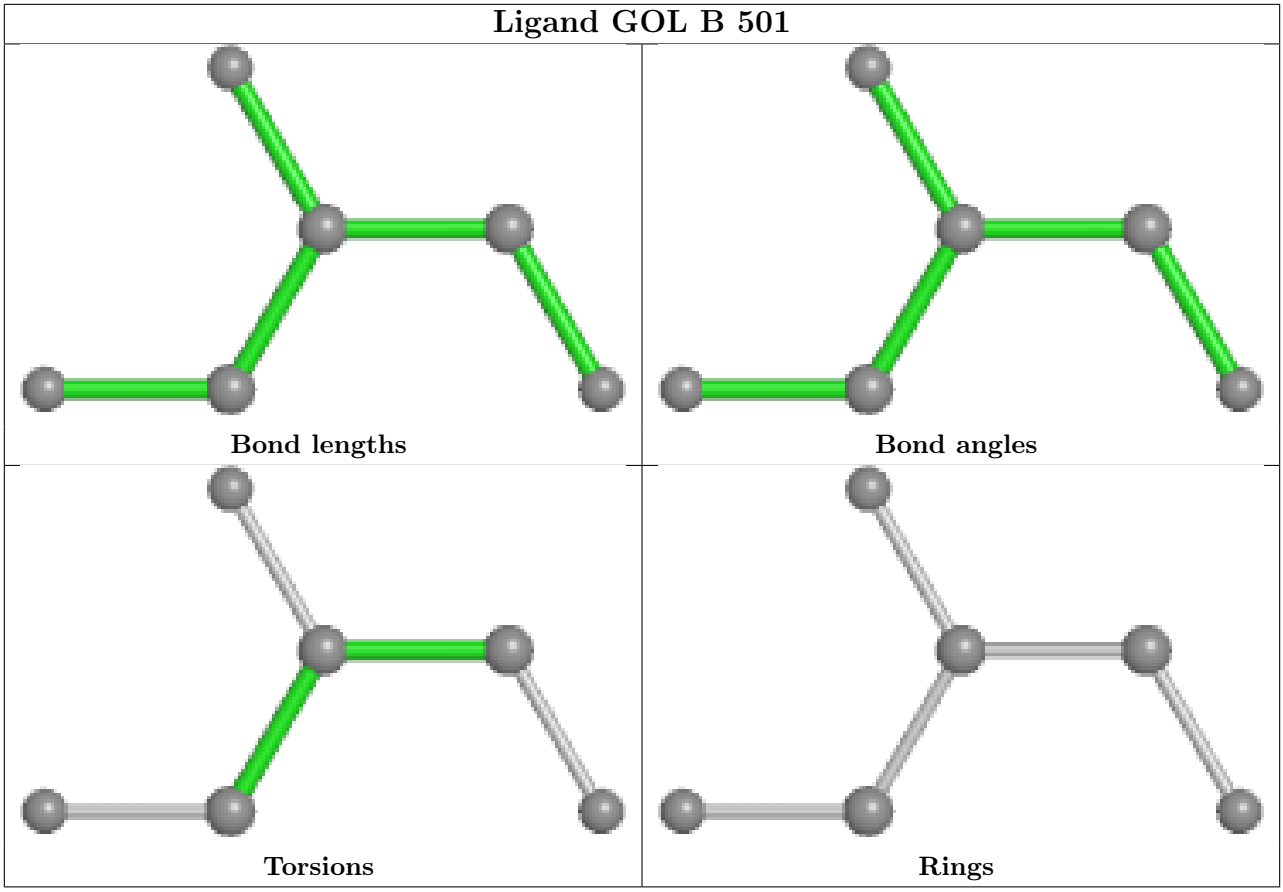
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	GOL	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	206/208 (99%)	2.66	95 (46%)	0	0	39, 108, 189, 213	0
1	B	207/208 (99%)	1.00	33 (15%)	1	1	40, 67, 102, 124	0
All	All	413/416 (99%)	1.83	128 (30%)	0	0	39, 73, 180, 213	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	16.9
1	A	224	SER	15.5
1	A	311	LYS	14.6
1	A	244	VAL	9.7
1	A	324	ALA	9.7
1	A	268	GLU	9.6
1	A	285	TYR	9.3
1	A	272	ALA	9.0
1	A	266	GLY	8.5
1	A	248	VAL	8.5
1	A	306	CYS	8.5
1	A	292	THR	7.7
1	A	310	ASN	7.7
1	A	228	PHE	7.3
1	A	249	VAL	7.2
1	A	271	ASN	7.1
1	A	287	VAL	6.8
1	A	239	SER	6.6
1	A	267	VAL	6.5
1	A	405	GLY	6.5
1	A	275	LYS	6.5
1	A	223	PRO	6.4
1	A	251	VAL	6.4
1	A	320	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	PHE	6.4
1	A	318	GLU	6.4
1	A	227	LEU	6.3
1	A	309	SER	6.2
1	A	255	ASP	6.1
1	A	314	PRO	5.8
1	A	424	LYS	5.7
1	A	250	ASP	5.6
1	A	305	LYS	5.2
1	A	316	PRO	5.1
1	A	234	ASP	5.0
1	A	258	VAL	5.0
1	A	236	LEU	4.9
1	B	314	PRO	4.7
1	A	284	THR	4.6
1	A	263	TYR	4.6
1	A	264	VAL	4.6
1	A	419	ASN	4.5
1	A	282	ASN	4.4
1	A	295	HIS	4.3
1	A	296	GLN	4.3
1	A	294	LEU	4.3
1	B	340	ARG	4.3
1	A	317	ILE	4.2
1	A	312	ALA	4.0
1	A	300	ASN	4.0
1	A	304	TYR	3.9
1	A	407	VAL	3.9
1	A	257	GLU	3.9
1	B	280	GLN	3.9
1	A	299	LEU	3.8
1	A	256	PRO	3.8
1	A	412	VAL	3.7
1	A	400	SER	3.7
1	A	252	SER	3.6
1	A	315	ALA	3.5
1	B	299	LEU	3.5
1	A	253	HIS	3.4
1	B	225	VAL	3.4
1	B	283	SER	3.4
1	B	405	GLY	3.4
1	A	254	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	3.3
1	A	225	VAL	3.2
1	A	339	SER	3.2
1	B	339	SER	3.2
1	A	277	ARG	3.2
1	A	276	PRO	3.2
1	A	270	HIS	3.2
1	A	265	ASP	3.1
1	B	309	SER	3.1
1	A	298	TRP	3.0
1	A	416	ALA	3.0
1	A	278	GLU	3.0
1	B	238	ILE	3.0
1	A	286	ARG	3.0
1	A	336	LEU	2.9
1	B	313	LEU	2.9
1	A	261	ASN	2.9
1	B	222	GLY	2.8
1	B	227	LEU	2.8
1	B	286	ARG	2.8
1	A	283	SER	2.8
1	A	308	VAL	2.7
1	B	348	VAL	2.7
1	A	417	LEU	2.7
1	A	259	LYS	2.6
1	B	285	TYR	2.6
1	A	273	LYS	2.6
1	A	241	THR	2.6
1	A	398	ASP	2.6
1	B	341	ASP	2.5
1	B	420	HIS	2.5
1	A	246	CYS	2.5
1	B	403	GLN	2.5
1	A	230	PRO	2.4
1	A	420	HIS	2.4
1	A	238	ILE	2.4
1	B	320	THR	2.4
1	A	290	VAL	2.3
1	B	333	VAL	2.3
1	B	236	LEU	2.3
1	A	323	LYS	2.3
1	B	335	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	2.3
1	A	291	LEU	2.3
1	B	253	HIS	2.3
1	A	289	SER	2.2
1	A	331	PRO	2.2
1	A	274	THR	2.2
1	B	327	GLN	2.2
1	B	257	GLU	2.2
1	B	343	LEU	2.2
1	A	235	THR	2.2
1	A	313	LEU	2.2
1	B	254	GLU	2.2
1	B	354	VAL	2.1
1	A	413	MET	2.1
1	B	237	MET	2.1
1	A	303	GLU	2.1
1	A	226	PHE	2.1
1	B	418	HIS	2.0
1	B	315	ALA	2.0
1	B	269	VAL	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^{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	C	1	14/15	0.25	0.50	139,157,166,170	0
2	NAG	C	2	14/15	0.39	0.40	91,118,125,133	0
3	FUC	D	7	10/11	0.61	0.33	75,80,89,100	0
2	FUL	C	9	10/11	0.63	0.23	112,124,130,133	0
2	MAN	C	7	11/12	0.65	0.18	67,87,98,99	0
2	MAN	C	4	11/12	0.66	0.18	71,79,92,96	0
3	MAN	D	6	11/12	0.71	0.16	42,59,75,75	0
2	BMA	C	3	11/12	0.75	0.17	83,89,94,96	0

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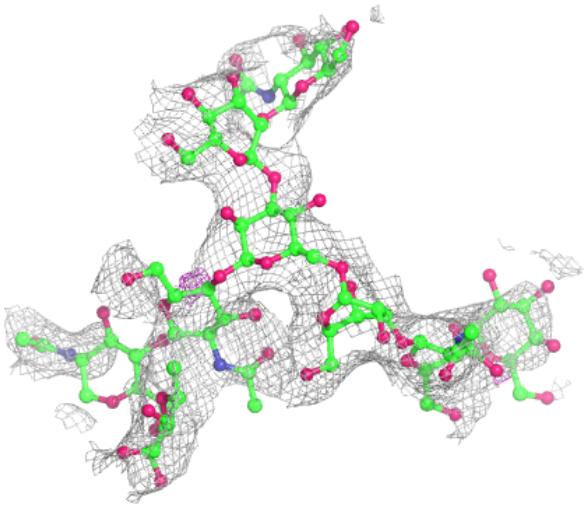
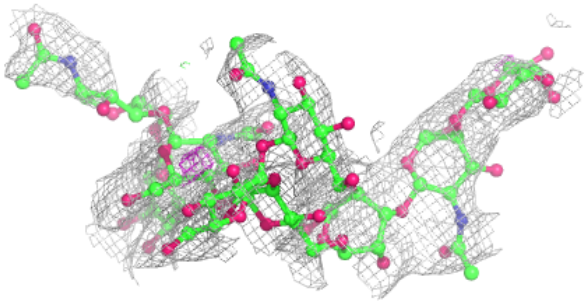
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	1	14/15	0.75	0.24	55,82,92,99	0
2	NAG	C	8	14/15	0.76	0.20	96,102,105,111	0
2	GAL	C	6	11/12	0.82	0.60	106,117,123,132	0
3	MAN	D	4	11/12	0.83	0.18	47,50,66,74	0
2	NAG	C	5	14/15	0.85	0.22	66,94,104,105	0
3	NAG	D	2	14/15	0.87	0.15	48,58,67,73	0
3	BMA	D	3	11/12	0.88	0.13	54,59,69,75	0
3	NAG	D	5	14/15	0.89	0.18	37,49,77,82	0

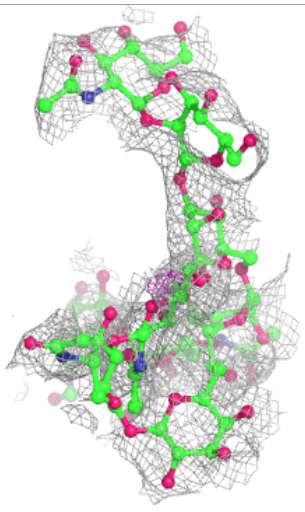
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

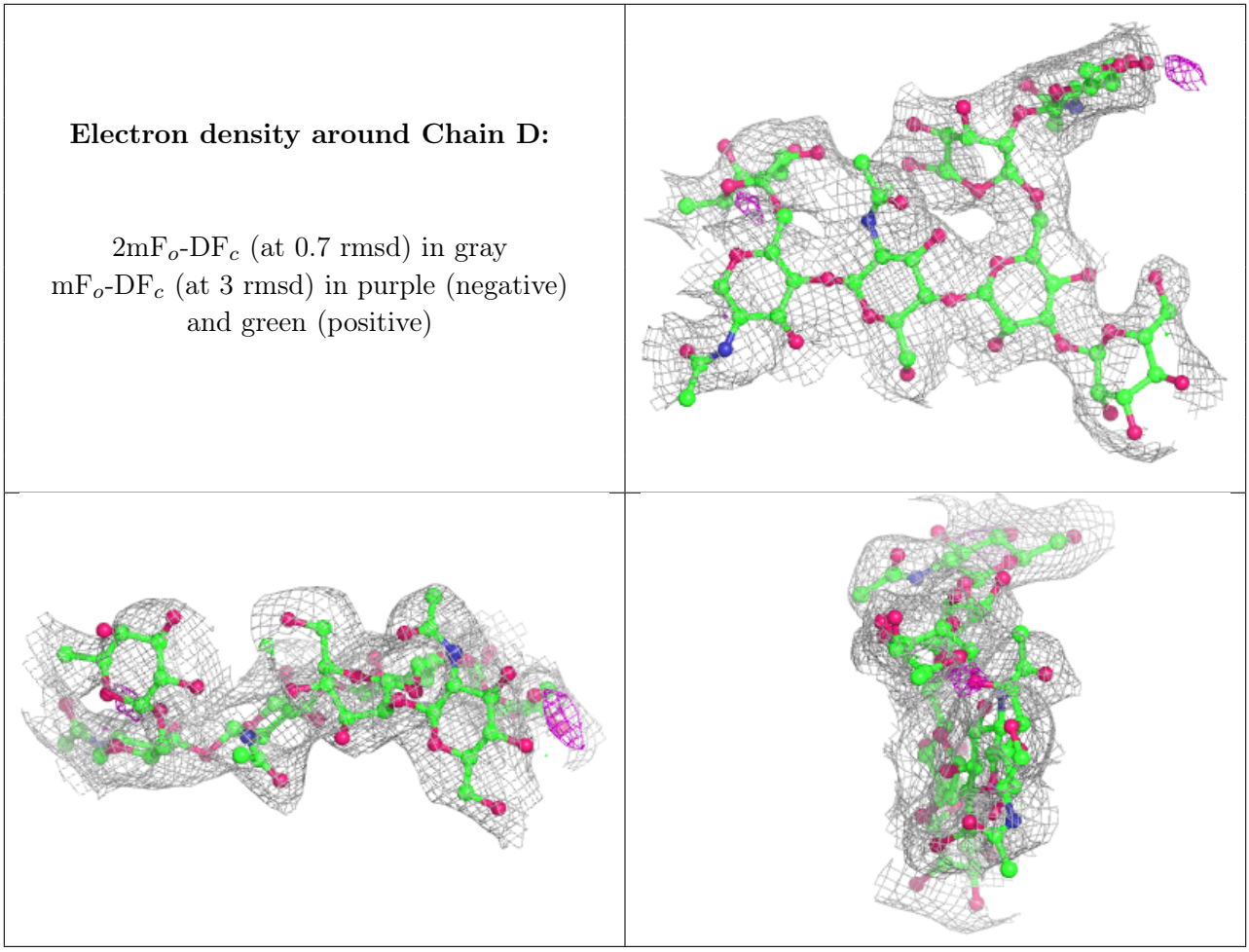






Electron density around Chain D:

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



6.4 Ligands

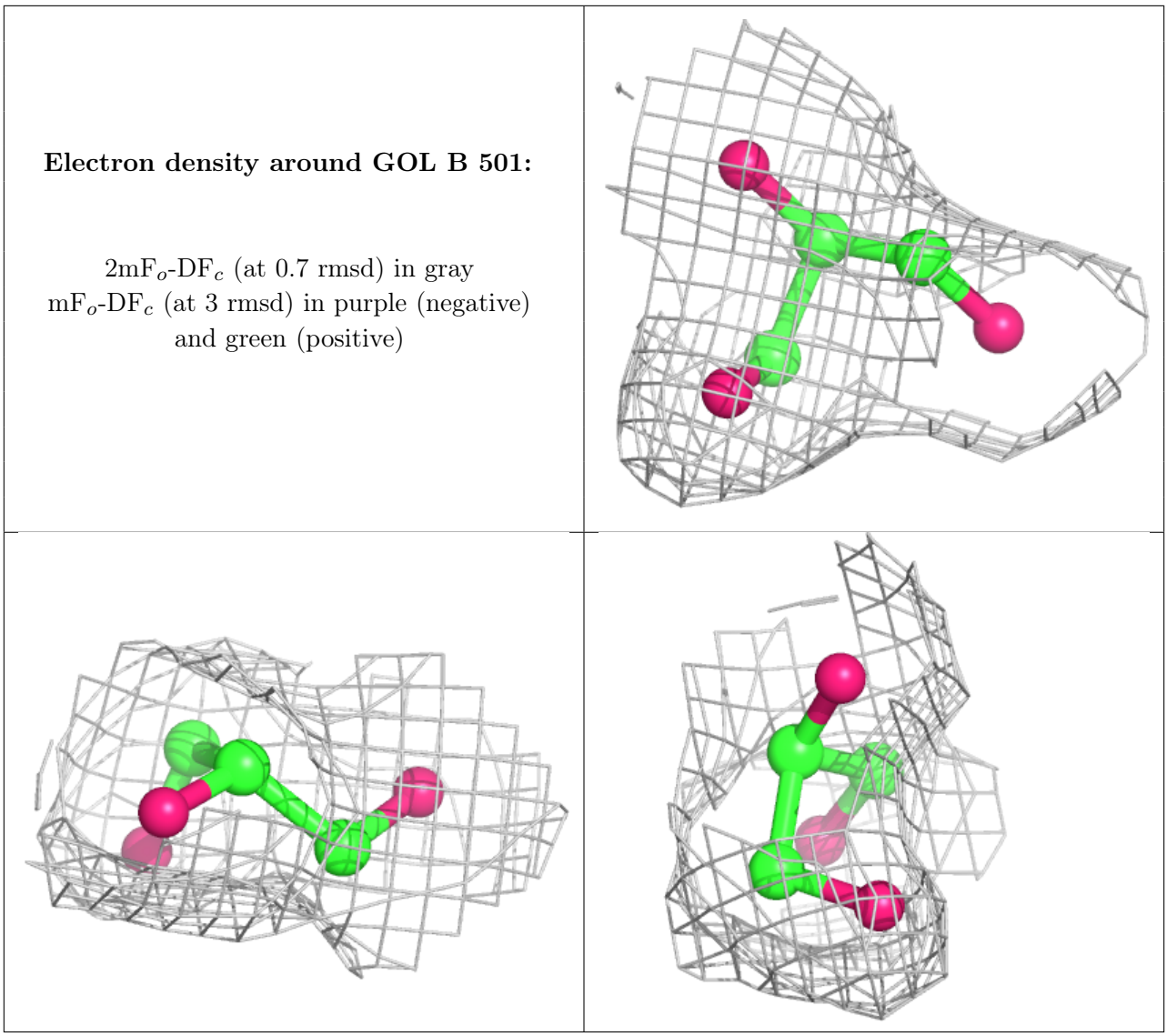
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	B	501	6/6	0.61	0.20	58,59,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GOL B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.