



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:19 AM BST

PDB ID : 5LGJ
Title : THE CRYSTAL STRUCTURE OF IGE FC MUTANT - P333C
Authors : Dhaliwal, B.; Pang, M.O.Y.; Sutton, B.J.
Deposited on : 2016-07-07
Resolution : 2.60 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 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

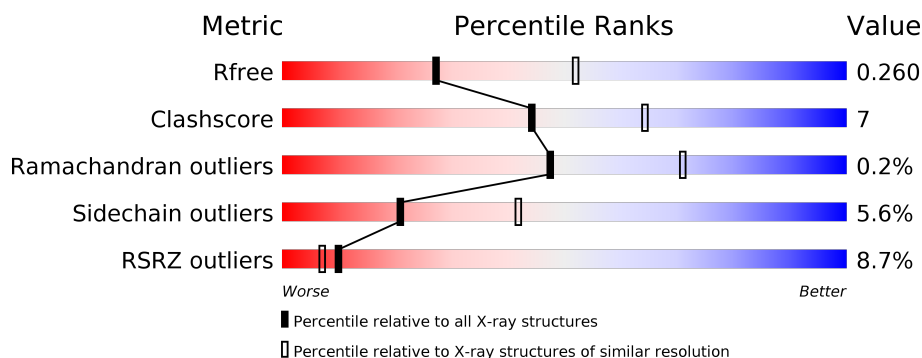
1 Overall quality at a glance

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	319	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
2	B	320	<div> <div>9%</div> <div>81%</div> <div>13%</div> <div>.</div> </div>
3	C	5	<div> <div>20%</div> <div>80%</div> </div>
4	D	7	<div> <div>57%</div> <div>29%</div> <div>14%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	-	-	-	X
6	PG4	A	609	-	-	-	X
6	PG4	A	610	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5305 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 epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2465	1539	438	476	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	conflict	UNP P01854
A	333	CYS	PRO	engineered mutation	UNP P01854
A	371	GLN	ASN	conflict	UNP P01854

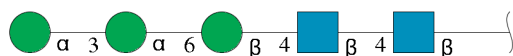
- Molecule 2 is a protein called Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2410	1506	428	465	11			

There are 3 discrepancies between the modelled and reference sequences:

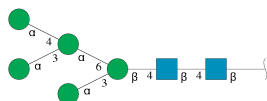
Chain	Residue	Modelled	Actual	Comment	Reference
B	265	GLN	ASN	conflict	UNP P01854
B	333	CYS	PRO	engineered mutation	UNP P01854
B	371	GLN	ASN	conflict	UNP P01854

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



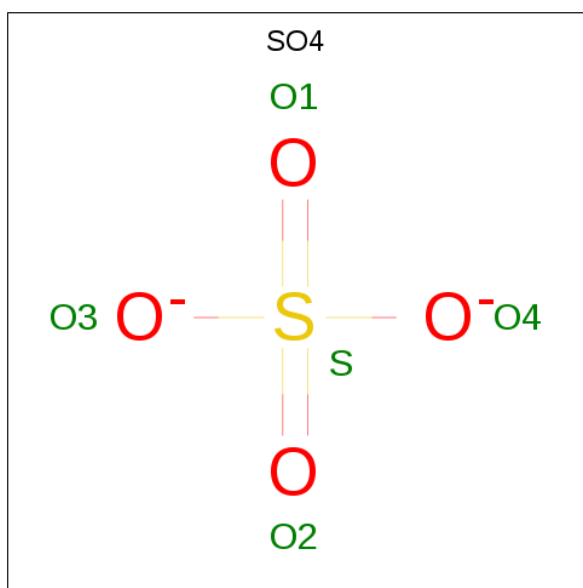
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



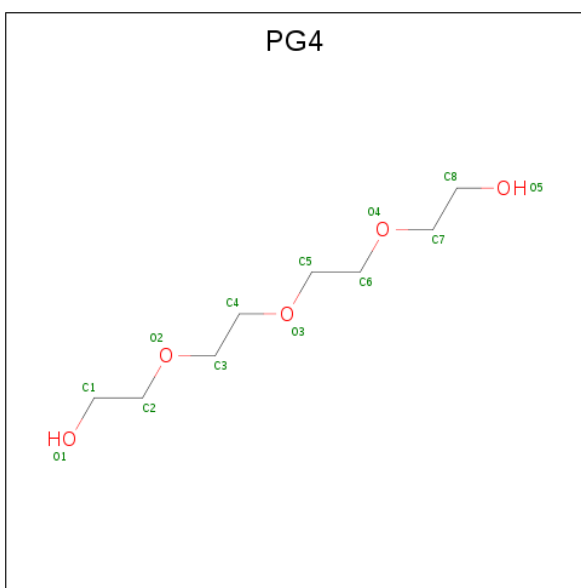
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



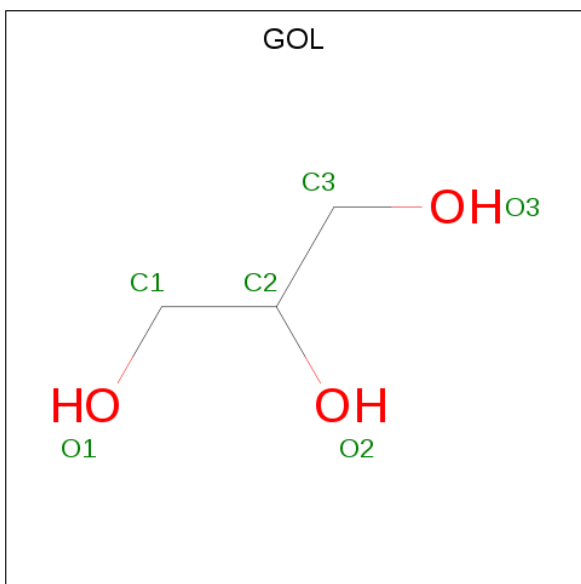
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

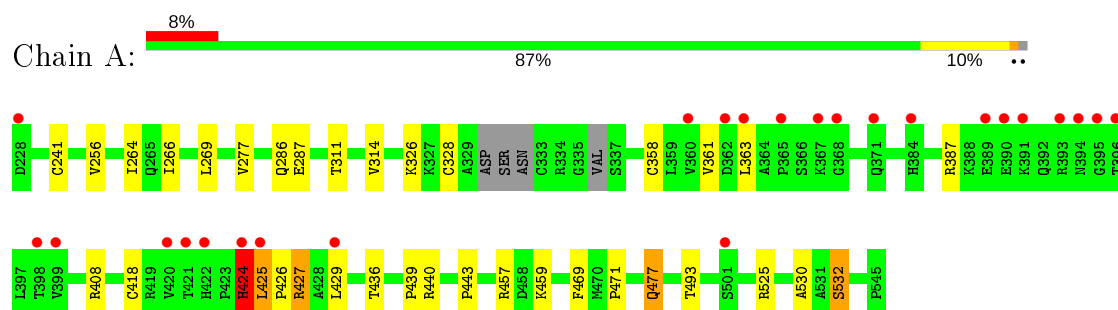
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total 113	O 113	0	0
8	B	122	Total 122	O 122	0	0

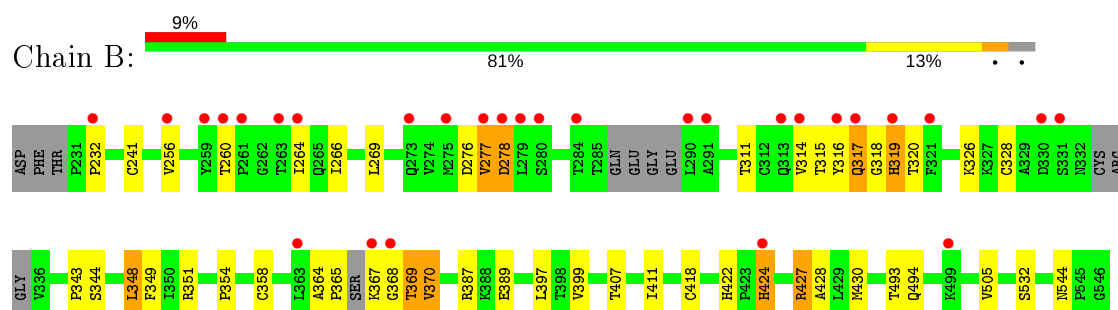
3 Residue-property plots [i](#)

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 epsilon chain C region



- Molecule 2: Ig epsilon chain C region



- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.45Å 74.91Å 79.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.60 67.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.49-2.60) 98.9 (67.47-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.62Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.188 , 0.248 0.202 , 0.260	Depositor DCC
R_{free} test set	1223 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5305	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, PG4, SO4, 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	0.61	2/2524 (0.1%)	0.75	6/3436 (0.2%)
2	B	0.42	0/2467	0.69	0/3360
All	All	0.52	2/4991 (0.0%)	0.72	6/6796 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	LEU	C-N	-20.94	0.94	1.34
1	A	424	HIS	C-N	10.63	1.58	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	LEU	O-C-N	12.25	144.38	121.10
1	A	425	LEU	C-N-CD	11.72	153.01	128.40
1	A	424	HIS	O-C-N	-8.96	108.36	122.70
1	A	425	LEU	CA-C-N	-8.79	92.48	117.10
1	A	425	LEU	C-N-CA	-7.33	91.20	122.00
1	A	424	HIS	C-N-CA	5.68	135.90	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	HIS	Mainchain

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	2465	0	2414	26	2
2	B	2410	0	2360	41	0
3	C	61	0	52	1	0
4	D	83	0	70	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	25	0	33	0	0
7	B	6	0	8	1	0
8	A	113	0	0	0	0
8	B	122	0	0	0	0
All	All	5305	0	4937	61	2

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 (61) 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:260:THR:O	2:B:316:TYR:OH	1.53	1.27
1:A:424:HIS:CD2	1:A:425:LEU:CD2	2.35	1.08
2:B:317:GLN:HG3	2:B:318:GLY:N	1.65	1.08
2:B:364:ALA:O	2:B:367:LYS:HA	1.55	1.06
1:A:439:PRO:HG2	2:B:278:ASP:HB3	1.34	1.04
2:B:318:GLY:O	2:B:319:HIS:HB3	1.64	0.96
2:B:317:GLN:CG	2:B:318:GLY:H	1.79	0.95
2:B:317:GLN:CG	2:B:318:GLY:N	2.30	0.93
1:A:424:HIS:CD2	1:A:425:LEU:HD21	2.06	0.89
2:B:358:CYS:HG	2:B:418:CYS:HG	0.85	0.85
2:B:368:GLY:HA3	2:B:422:HIS:NE2	1.94	0.81
2:B:369:THR:O	2:B:370:VAL:HB	1.82	0.78
1:A:424:HIS:CD2	1:A:425:LEU:HD22	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:THR:HG22	2:B:319:HIS:C	2.05	0.77
1:A:328:CYS:HG	2:B:241:CYS:HG	0.78	0.77
1:A:439:PRO:HG2	2:B:278:ASP:CB	2.12	0.76
1:A:424:HIS:NE2	1:A:425:LEU:HD21	2.05	0.72
2:B:318:GLY:O	2:B:319:HIS:CB	2.35	0.72
2:B:427:ARG:HD2	2:B:428:ALA:H	1.59	0.68
2:B:348:LEU:HD13	2:B:354:PRO:HB3	1.79	0.65
2:B:364:ALA:O	2:B:367:LYS:CA	2.42	0.61
1:A:477:GLN:HG2	1:A:525:ARG:HB3	1.85	0.59
1:A:425:LEU:O	1:A:426:PRO:C	2.27	0.59
2:B:422:HIS:HD1	2:B:424:HIS:H	1.51	0.58
2:B:315:THR:HG22	2:B:320:THR:N	2.19	0.57
2:B:407:THR:H	7:B:608:GOL:H32	1.72	0.55
2:B:317:GLN:HG2	2:B:318:GLY:H	1.68	0.53
2:B:343:PRO:HB2	2:B:348:LEU:HD22	1.90	0.53
2:B:369:THR:O	2:B:370:VAL:CB	2.49	0.53
1:A:241:CYS:SG	2:B:328:CYS:SG	3.04	0.51
2:B:358:CYS:CB	2:B:418:CYS:HG	2.23	0.50
1:A:425:LEU:N	1:A:425:LEU:HD22	2.25	0.50
2:B:370:VAL:HG22	2:B:422:HIS:HB2	1.94	0.50
2:B:368:GLY:CA	2:B:422:HIS:NE2	2.71	0.49
1:A:425:LEU:HD13	1:A:426:PRO:HD2	1.95	0.49
1:A:424:HIS:CD2	1:A:425:LEU:HD23	2.43	0.48
1:A:443:PRO:HB3	1:A:469:PHE:HB3	1.96	0.48
2:B:277:VAL:O	2:B:277:VAL:CG2	2.61	0.48
2:B:266:ILE:HG12	2:B:314:VAL:HG22	1.95	0.48
2:B:365:PRO:HG3	2:B:397:LEU:HB2	1.95	0.47
1:A:241:CYS:HG	2:B:328:CYS:HG	1.49	0.47
1:A:425:LEU:CD1	1:A:426:PRO:HD2	2.45	0.47
1:A:436:THR:HG21	1:A:471:PRO:HG3	1.96	0.46
2:B:232:PRO:HD3	2:B:316:TYR:CD2	2.51	0.46
2:B:232:PRO:HD3	2:B:316:TYR:HD2	1.82	0.45
1:A:493:THR:HG21	2:B:493:THR:HG21	1.98	0.45
2:B:344:SER:HB3	4:D:6:MAN:H61	1.98	0.45
2:B:349:PHE:HE1	2:B:411:ILE:HD11	1.83	0.43
1:A:425:LEU:HD13	1:A:425:LEU:HA	1.84	0.43
1:A:256:VAL:HG11	1:A:264:ILE:HD11	2.00	0.43
1:A:266:ILE:HG12	1:A:314:VAL:HG22	2.00	0.43
2:B:256:VAL:HG11	2:B:264:ILE:HD11	2.01	0.42
2:B:269:LEU:HB2	2:B:311:THR:HB	2.01	0.42
1:A:424:HIS:C	1:A:425:LEU:HD22	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HB2	1:A:311:THR:HB	2.03	0.40
1:A:358:CYS:CB	1:A:418:CYS:HG	2.35	0.40
2:B:389:GLU:HG2	2:B:399:VAL:HG22	2.03	0.40
1:A:361:VAL:HG11	3:C:2:NAG:H2	2.03	0.40
2:B:260:THR:O	2:B:316:TYR:CZ	2.61	0.40
2:B:348:LEU:HD13	2:B:354:PRO:CB	2.50	0.40
1:A:440:ARG:HB3	1:A:530:ALA:HB2	2.03	0.40

All (2) 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)
1:A:427:ARG:NH1	1:A:532:SER:OG[3_556]	1.25	0.95
1:A:427:ARG:NH1	1:A:532:SER:CB[3_556]	1.81	0.39

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	309/319 (97%)	300 (97%)	9 (3%)	0	100	100
2	B	301/320 (94%)	287 (95%)	13 (4%)	1 (0%)	41	64
All	All	610/639 (96%)	587 (96%)	22 (4%)	1 (0%)	47	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	370	VAL

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	279/283 (99%)	265 (95%)	14 (5%)	24	47
2	B	273/283 (96%)	256 (94%)	17 (6%)	18	37
All	All	552/566 (98%)	521 (94%)	31 (6%)	21	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	VAL
1	A	286	GLN
1	A	287	GLU
1	A	326	LYS
1	A	363	LEU
1	A	387	ARG
1	A	408	ARG
1	A	424	HIS
1	A	427	ARG
1	A	429	LEU
1	A	457	ARG
1	A	459	LYS
1	A	477	GLN
1	A	532	SER
2	B	276	ASP
2	B	277	VAL
2	B	278	ASP
2	B	317	GLN
2	B	319	HIS
2	B	326	LYS
2	B	348	LEU
2	B	351	ARG
2	B	369	THR
2	B	387	ARG
2	B	424	HIS
2	B	427	ARG
2	B	430	MET

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Mol	Chain	Res	Type
2	B	494	GLN
2	B	505	VAL
2	B	532	SER
2	B	544	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
1	A	424	HIS
1	A	468	ASN
2	B	317	GLN
2	B	468	ASN
2	B	481	ASN
2	B	538	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 ⓘ

12 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	C	3	3	11,11,12	0.33	0	15,15,17	0.62	0
3	MAN	C	4	3	11,11,12	0.38	0	15,15,17	0.82	1 (6%)
3	MAN	C	5	3	11,11,12	0.43	0	15,15,17	1.08	2 (13%)
4	NAG	D	1	2,4	14,14,15	0.24	0	17,19,21	0.74	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.58	0
4	BMA	D	3	4	11,11,12	0.29	0	15,15,17	0.55	0
4	MAN	D	4	4	11,11,12	0.37	0	15,15,17	0.93	1 (6%)
4	MAN	D	5	4	11,11,12	0.38	0	15,15,17	0.94	1 (6%)
4	MAN	D	6	4	11,11,12	0.35	0	15,15,17	0.94	2 (13%)
4	MAN	D	7	4	11,11,12	0.37	0	15,15,17	0.63	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	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	1/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O5-C1-C2	-3.49	105.78	111.29
4	D	5	MAN	C1-O5-C5	3.23	116.56	112.19
4	D	4	MAN	C1-O5-C5	3.08	116.36	112.19
3	C	4	MAN	C1-O5-C5	2.75	115.92	112.19
4	D	6	MAN	C1-O5-C5	2.75	115.92	112.19
3	C	5	MAN	C1-O5-C5	2.73	115.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	MAN	C1-C2-C3	2.71	113.00	109.67
4	D	6	MAN	C1-C2-C3	2.05	112.19	109.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6

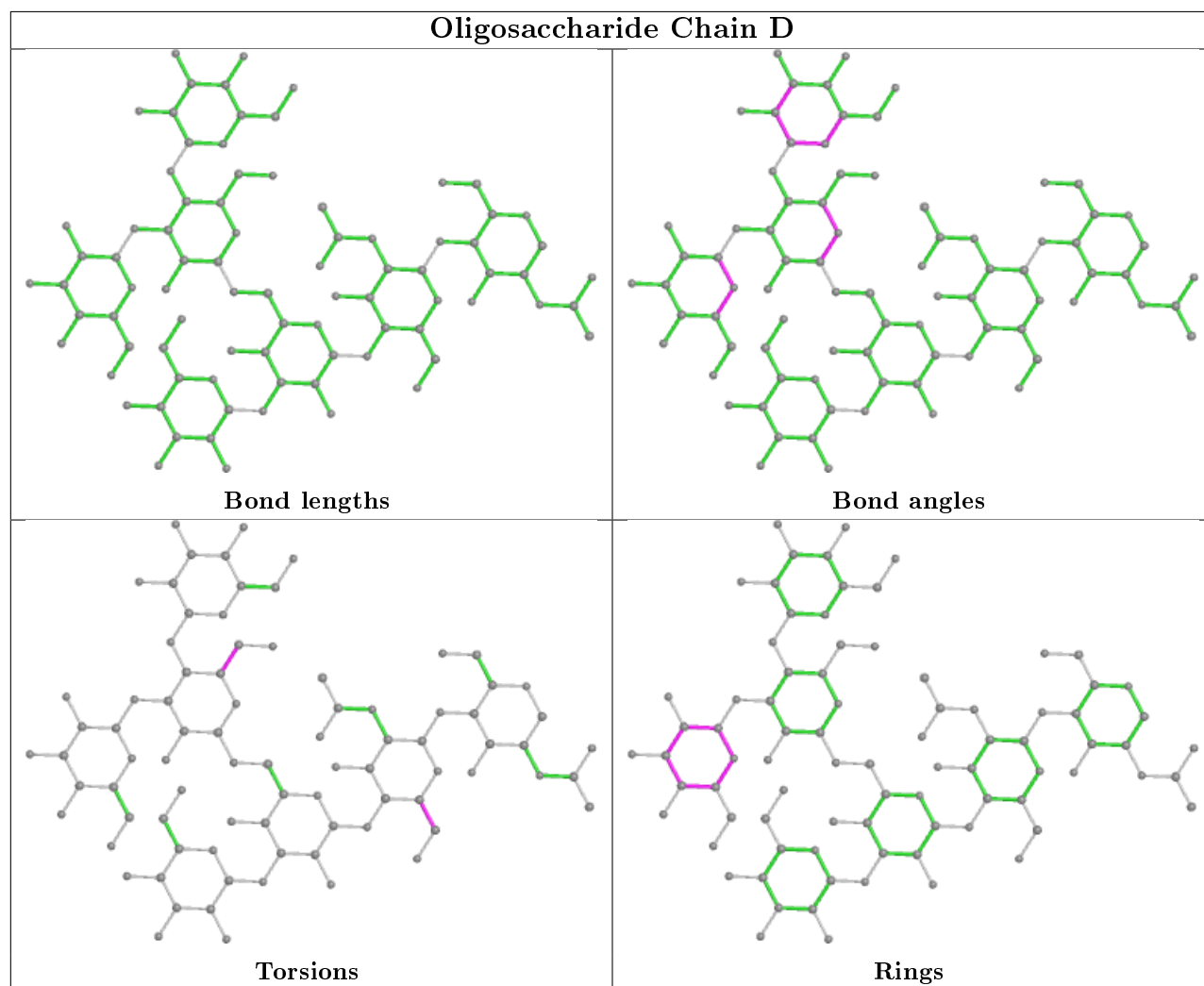
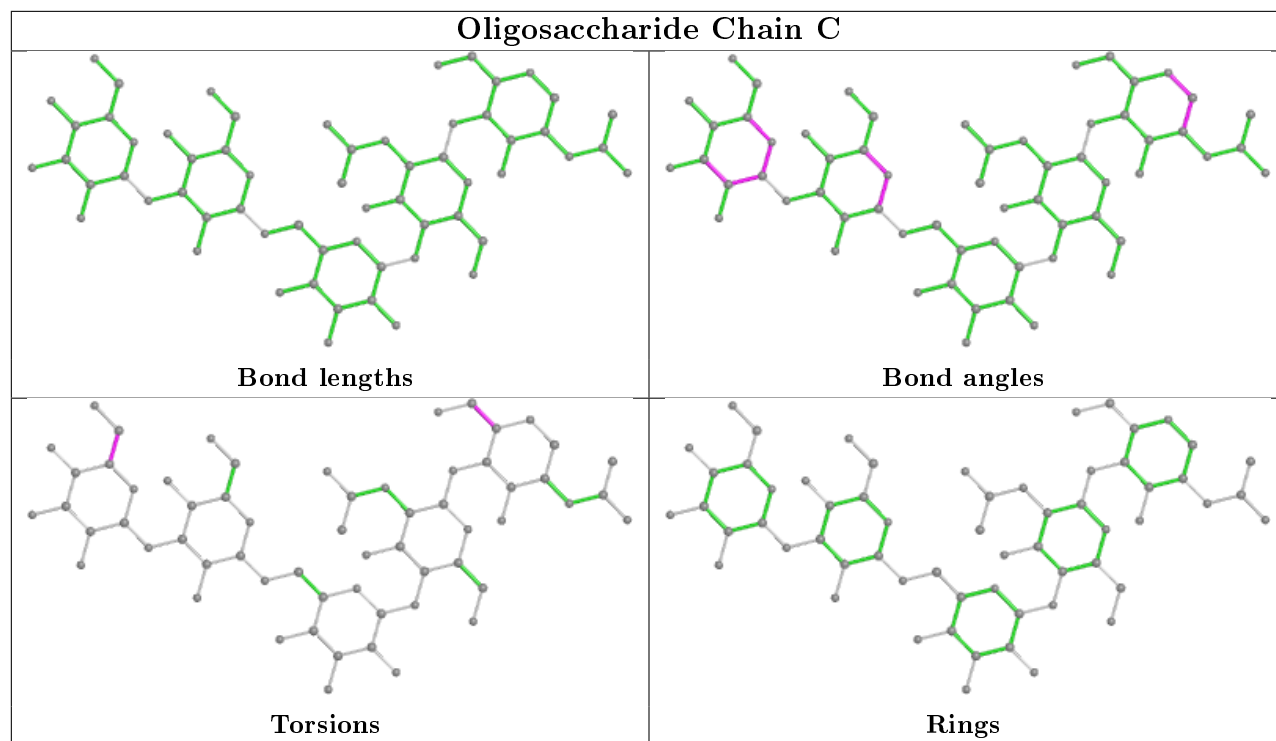
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6	MAN	1	0
3	C	2	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

7 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
5	SO4	A	608	-	4,4,4	0.20	0	6,6,6	0.48	0
6	PG4	A	610	-	11,11,12	0.24	0	10,10,11	0.28	0
5	SO4	A	607	-	4,4,4	0.19	0	6,6,6	0.11	0
6	PG4	A	609	-	12,12,12	0.18	0	11,11,11	0.16	0
7	GOL	B	608	-	5,5,5	0.04	0	5,5,5	0.21	0
5	SO4	A	606	-	4,4,4	0.23	0	6,6,6	0.22	0
5	SO4	B	609	-	4,4,4	0.10	0	6,6,6	0.20	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	PG4	A	610	-	-	3/9/9/10	-
7	GOL	B	608	-	-	2/4/4/4	-
6	PG4	A	609	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	608	GOL	O1-C1-C2-C3
7	B	608	GOL	O1-C1-C2-O2
6	A	609	PG4	O3-C5-C6-O4
6	A	610	PG4	C1-C2-O2-C3
6	A	610	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
6	A	609	PG4	C3-C4-O3-C5
6	A	609	PG4	C4-C3-O2-C2
6	A	609	PG4	C5-C6-O4-C7
6	A	610	PG4	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	608	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	425:LEU	C	426:PRO	N	0.94

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	315/319 (98%)	0.30	25 (7%) 12 9	20, 49, 127, 187	0
2	B	309/320 (96%)	0.42	29 (9%) 8 5	17, 46, 117, 161	0
All	All	624/639 (97%)	0.36	54 (8%) 10 7	17, 48, 125, 187	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	284	THR	9.6
1	A	362	ASP	8.4
2	B	291	ALA	7.6
2	B	263	THR	6.0
2	B	278	ASP	5.9
1	A	363	LEU	5.6
2	B	290	LEU	5.2
1	A	429	LEU	4.9
1	A	424	HIS	4.7
1	A	396	THR	4.7
1	A	393	ARG	4.5
1	A	399	VAL	4.4
1	A	422	HIS	4.4
2	B	316	TYR	4.2
1	A	425	LEU	4.2
2	B	277	VAL	4.1
1	A	365	PRO	4.0
1	A	394	ASN	4.0
1	A	367	LYS	3.8
1	A	420	VAL	3.8
1	A	389	GLU	3.7
2	B	232	PRO	3.7
1	A	421	THR	3.6
2	B	317	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	280	SER	3.5
1	A	395	GLY	3.5
2	B	259	TYR	3.4
2	B	264	ILE	3.3
2	B	260	THR	3.2
2	B	321	PHE	3.0
1	A	360	VAL	3.0
1	A	501	SER	2.9
2	B	314	VAL	2.9
2	B	313	GLN	2.8
2	B	261	PRO	2.7
1	A	368	GLY	2.7
2	B	331	SER	2.7
2	B	368	GLY	2.5
1	A	398	THR	2.5
2	B	424	HIS	2.5
2	B	363	LEU	2.5
1	A	390	GLU	2.4
1	A	391	LYS	2.4
1	A	228	ASP	2.4
2	B	319	HIS	2.4
2	B	279	LEU	2.4
2	B	367	LYS	2.4
2	B	275	MET	2.2
1	A	371	GLN	2.2
2	B	273	GLN	2.1
1	A	384	HIS	2.1
2	B	499	LYS	2.1
2	B	330	ASP	2.1
2	B	256	VAL	2.0

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

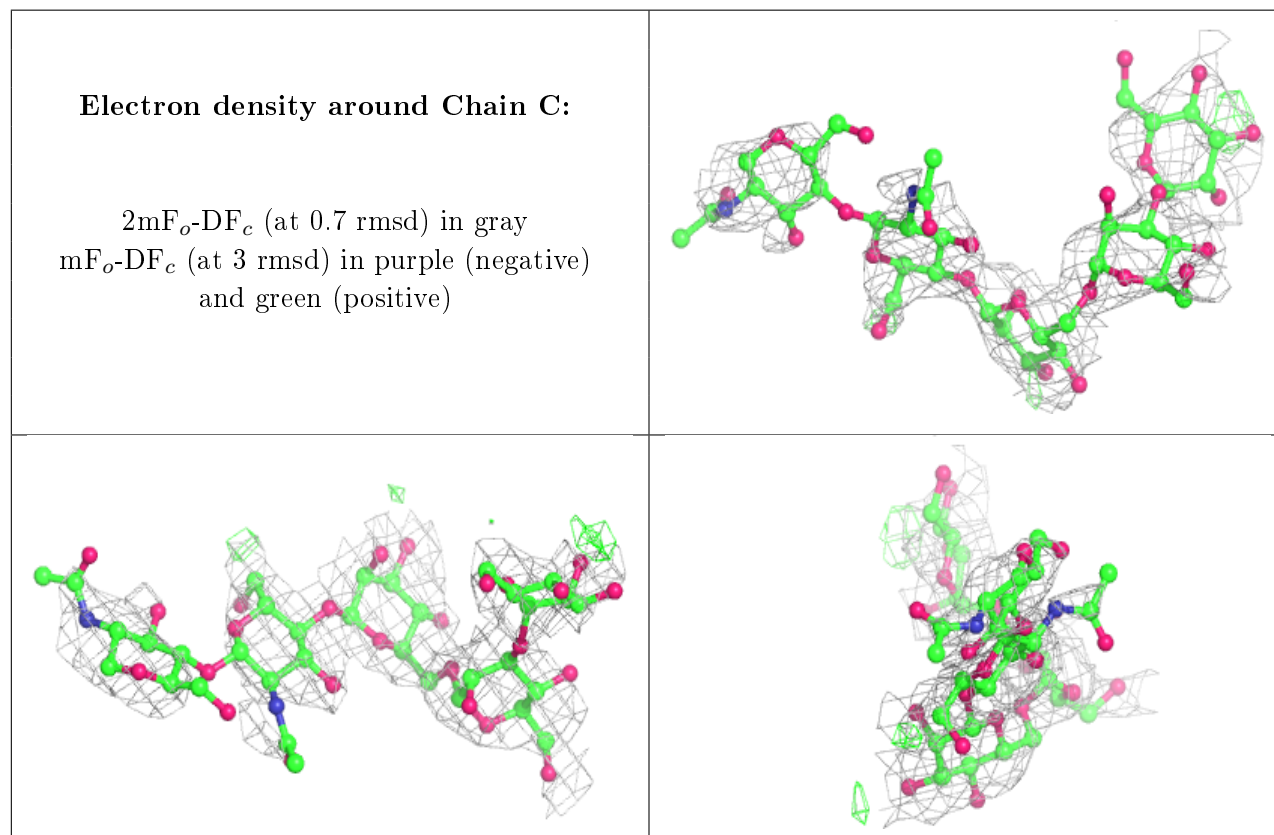
There are no non-standard protein/DNA/RNA residues in this entry.

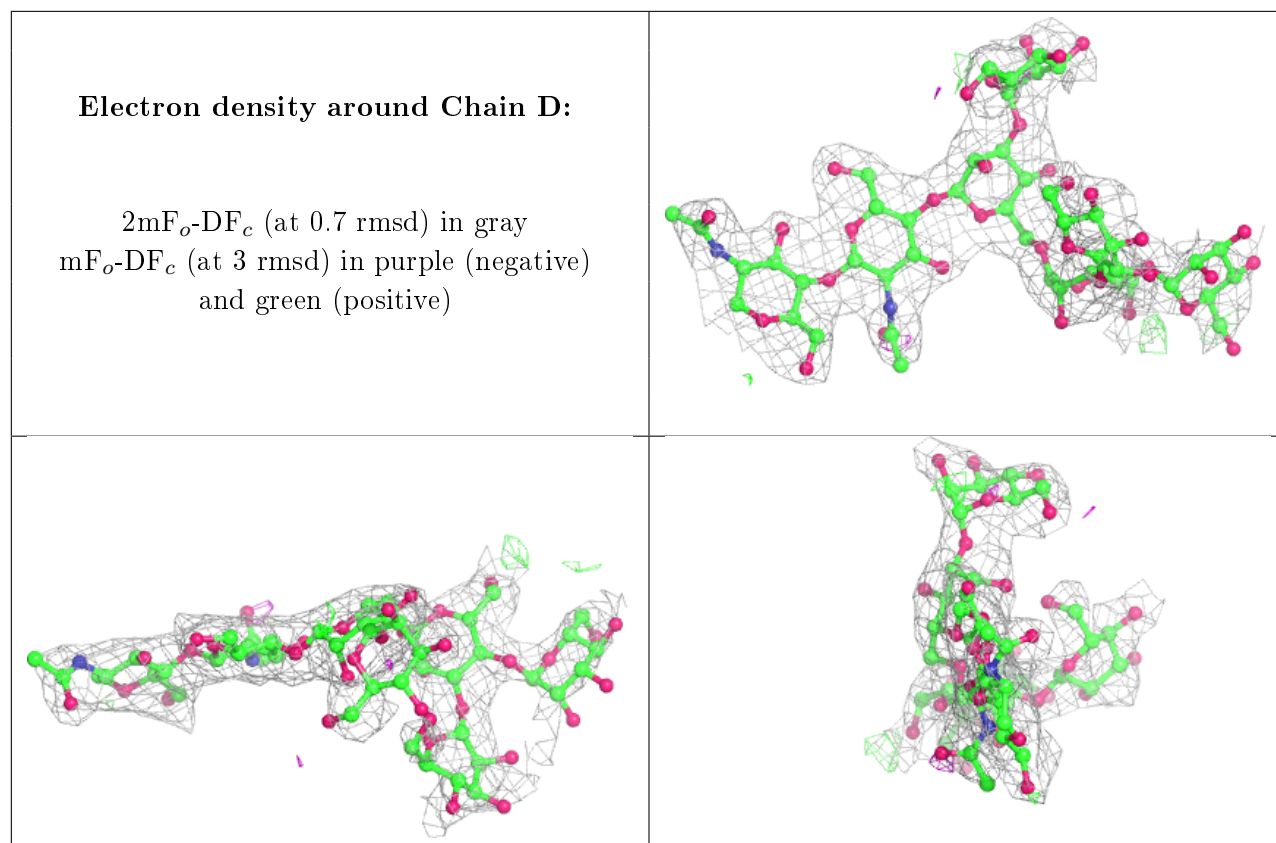
6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
3	MAN	C	5	11/12	0.61	0.29	126,127,128,128	0
3	NAG	C	2	14/15	0.66	0.34	117,119,120,120	0
4	MAN	D	5	11/12	0.67	0.26	105,106,107,107	0
4	MAN	D	7	11/12	0.70	0.25	88,90,92,92	0
4	MAN	D	6	11/12	0.72	0.38	110,112,113,114	0
3	MAN	C	4	11/12	0.74	0.28	120,121,123,125	0
3	NAG	C	1	14/15	0.77	0.45	113,116,118,119	0
3	BMA	C	3	11/12	0.80	0.21	113,115,117,119	0
4	MAN	D	4	11/12	0.81	0.19	96,100,103,107	0
4	NAG	D	1	14/15	0.92	0.17	52,54,55,56	0
4	BMA	D	3	11/12	0.93	0.13	76,83,87,91	0
4	NAG	D	2	14/15	0.94	0.17	55,58,61,68	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	PG4	A	609	13/13	0.58	0.42	79,81,82,83	0
6	PG4	A	610	12/13	0.69	0.41	63,65,69,70	0
5	SO4	B	609	5/5	0.72	0.28	109,110,111,111	0
7	GOL	B	608	6/6	0.91	0.16	67,68,69,70	0
5	SO4	A	607	5/5	0.94	0.20	91,93,93,94	0
5	SO4	A	608	5/5	0.94	0.19	61,64,64,65	0
5	SO4	A	606	5/5	0.95	0.27	63,64,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.