



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:27 AM BST

PDB ID : 5HY9
Title : Glycosylated, disulfide-linked Knob-into-Hole Fc fragment
Authors : Kuglstatter, A.; Stihle, M.; Benz, J.
Deposited on : 2016-02-01
Resolution : 2.70 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

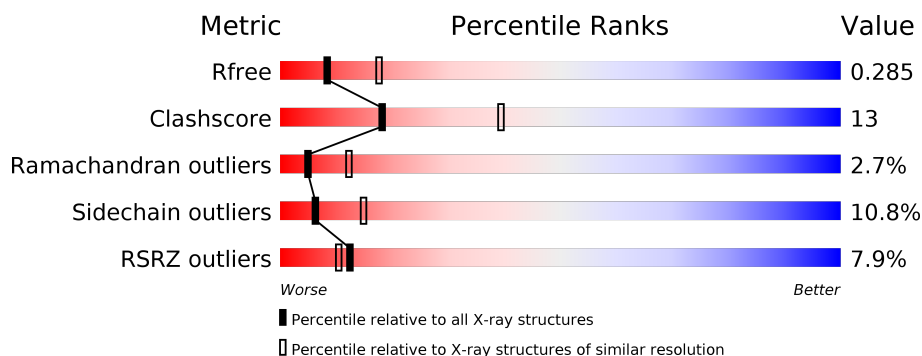
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	227	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 69% 17% 5% 9% </div> </div>
2	B	227	<div> <div style="width: 13%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 52% 28% 7% 12% </div> </div>
3	C	9	<div> <div style="width: 78%; height: 10px; background-color: yellow;"></div> <div style="width: 22%; height: 10px; background-color: orange;"></div> </div>
4	D	6	<div> <div style="width: 67%; height: 10px; background-color: yellow;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></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
4	BMA	D	4	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3470 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	207	Total	C	N	O	S	0	0	0
			1665	1063	280	315	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	CYS	SER	engineered mutation	UNP P01857
A	366	TRP	THR	engineered mutation	UNP P01857

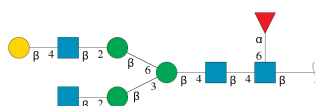
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	0	0
			1582	1005	268	302	7			

There are 4 discrepancies between the modelled and reference sequences:

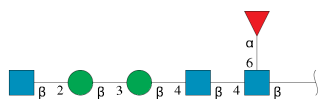
Chain	Residue	Modelled	Actual	Comment	Reference
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-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	C	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-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
4	D	6	Total	C	N	O	0	0	0
			74	42	3	29			

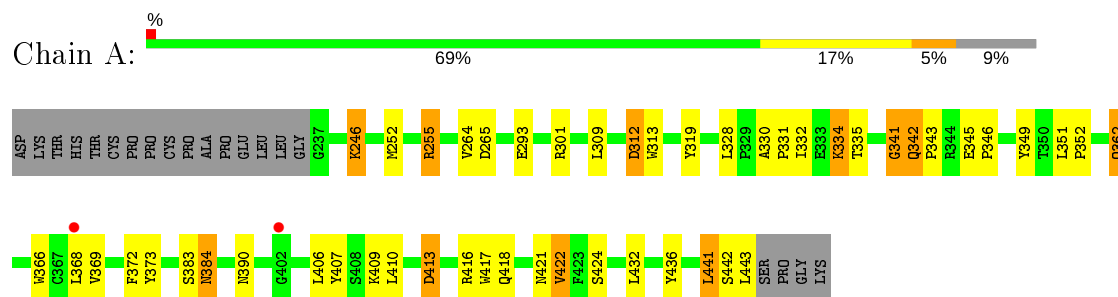
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	5	Total	O	0	0
			5	5		

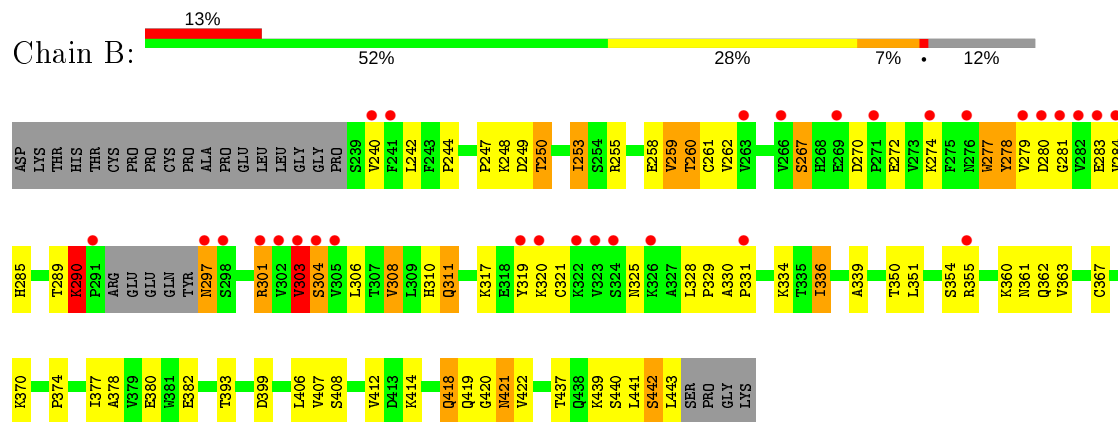
3 Residue-property plots [i](#)

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.

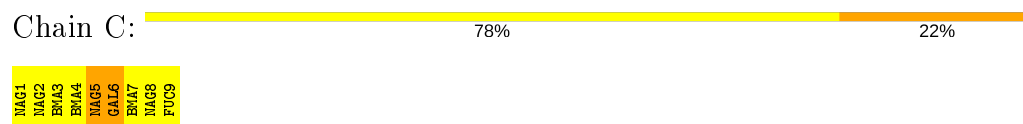
- Molecule 1: Ig gamma-1 chain C region



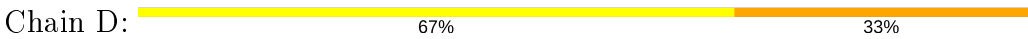
- Molecule 2: Ig gamma-1 chain C region



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



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-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



IMG1
IMG2
IMG3
IMG4
IMG5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.81Å 151.81Å 113.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.59 – 2.70 45.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.59-2.70) 99.8 (45.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.212 , 0.272 0.225 , 0.285	Depositor DCC
R_{free} test set	1109 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.5	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	3470	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: FUC, GAL, BMA, NAG

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	0.86	0/1713	0.98	4/2335 (0.2%)
2	B	0.66	0/1623	0.81	0/2210
All	All	0.77	0/3336	0.90	4/4545 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	312	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	312	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	A	334	LYS	CD-CE-NZ	-5.50	99.06	111.70

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	1665	0	1627	33	0
2	B	1582	0	1559	59	0
3	C	110	0	94	3	0
4	D	74	0	64	2	0
5	A	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
All	All	3470	0	3344	91	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 13.

All (91) 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:290:LYS:HE3	2:B:303:VAL:HG11	1.33	1.10
2:B:240:VAL:HG12	2:B:334:LYS:HG2	1.38	1.03
2:B:253:ILE:H	2:B:253:ILE:HD12	1.31	0.95
2:B:277:TRP:HZ2	2:B:304:SER:HG	1.18	0.87
2:B:267:SER:HB2	2:B:270:ASP:H	1.43	0.81
2:B:361:ASN:O	2:B:414:LYS:HB2	1.83	0.79
2:B:277:TRP:HZ2	2:B:304:SER:OG	1.67	0.78
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.66	0.76
2:B:290:LYS:CE	2:B:303:VAL:HG11	2.17	0.72
2:B:301:ARG:HH21	2:B:303:VAL:HG22	1.55	0.71
2:B:406:LEU:HD12	2:B:406:LEU:C	2.13	0.69
2:B:260:THR:HG22	2:B:262:VAL:HG23	1.76	0.68
2:B:308:VAL:HB	2:B:319:TYR:OH	1.96	0.66
2:B:319:TYR:HB2	2:B:336:ILE:HG22	1.86	0.58
1:A:407:TYR:CZ	2:B:407:VAL:HG11	2.39	0.57
2:B:289:THR:HG22	2:B:289:THR:O	2.05	0.57
1:A:383:SER:O	1:A:384:ASN:C	2.43	0.56
2:B:377:ILE:CG1	2:B:378:ALA:H	2.18	0.56
2:B:244:PRO:HD3	2:B:336:ILE:HD11	1.87	0.56
4:D:4:BMA:H4	4:D:5:NAG:C1	2.36	0.55
2:B:308:VAL:HB	2:B:319:TYR:CZ	2.41	0.55
2:B:260:THR:CG2	2:B:262:VAL:HG23	2.36	0.55
1:A:368:LEU:HD23	1:A:369:VAL:N	2.21	0.55
2:B:278:TYR:CD1	2:B:278:TYR:N	2.76	0.54
1:A:341:GLY:HA3	1:A:373:TYR:CE2	2.44	0.53
1:A:409:LYS:NZ	2:B:399:ASP:OD2	2.40	0.53
2:B:290:LYS:HB2	2:B:303:VAL:HB	1.91	0.53
2:B:281:GLY:HA2	2:B:320:LYS:HE3	1.91	0.52
2:B:297:ASN:N	2:B:297:ASN:OD1	2.41	0.52
2:B:253:ILE:CD1	2:B:253:ILE:H	2.02	0.52
2:B:367:CYS:O	2:B:407:VAL:HA	2.11	0.51
1:A:421:ASN:O	1:A:442:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:GLN:O	2:B:421:ASN:N	2.45	0.50
2:B:301:ARG:NE	2:B:301:ARG:O	2.44	0.49
2:B:377:ILE:CG1	2:B:378:ALA:N	2.76	0.49
1:A:345:GLU:HG2	1:A:432:LEU:HD23	1.95	0.49
2:B:242:LEU:HD21	2:B:319:TYR:O	2.12	0.49
2:B:262:VAL:HG11	2:B:301:ARG:NH1	2.29	0.48
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.13	0.48
2:B:350:THR:HB	2:B:441:LEU:HD22	1.95	0.48
2:B:249:ASP:HA	2:B:255:ARG:HD3	1.95	0.48
1:A:351:LEU:HB2	1:A:366:TRP:HB2	1.95	0.47
2:B:325:ASN:H	2:B:328:LEU:HD12	1.79	0.47
1:A:407:TYR:CE1	2:B:407:VAL:HG11	2.48	0.47
2:B:422:VAL:HA	2:B:442:SER:HB3	1.96	0.47
2:B:350:THR:O	2:B:351:LEU:HD23	2.15	0.47
2:B:377:ILE:HG12	2:B:378:ALA:H	1.79	0.47
1:A:246:LYS:CD	3:C:6:GAL:O4	2.63	0.47
2:B:259:VAL:O	2:B:260:THR:OG1	2.31	0.47
2:B:259:VAL:CG2	2:B:306:LEU:HB3	2.46	0.46
2:B:277:TRP:HA	2:B:320:LYS:O	2.16	0.46
1:A:417:TRP:CH2	1:A:442:SER:O	2.68	0.46
1:A:390:ASN:O	1:A:410:LEU:HD12	2.15	0.46
2:B:277:TRP:O	2:B:283:GLU:OE1	2.34	0.46
1:A:264:VAL:O	1:A:265:ASP:HB2	2.15	0.46
1:A:328:LEU:HD13	1:A:332:ILE:HG13	1.97	0.45
2:B:418:GLN:HA	2:B:443:LEU:HD13	1.96	0.45
1:A:422:VAL:HG12	1:A:422:VAL:O	2.16	0.45
1:A:436:TYR:C	1:A:436:TYR:CD1	2.89	0.45
1:A:362:GLN:HG3	1:A:413:ASP:HA	1.97	0.45
2:B:339:ALA:HB3	2:B:374:PRO:HB3	1.97	0.45
1:A:330:ALA:O	1:A:331:PRO:C	2.54	0.45
1:A:349:TYR:HB3	2:B:354:SER:CB	2.47	0.45
2:B:303:VAL:O	2:B:304:SER:CB	2.65	0.45
1:A:406:LEU:HD12	1:A:406:LEU:C	2.37	0.45
1:A:351:LEU:HA	1:A:352:PRO:HD3	1.79	0.44
1:A:312:ASP:O	1:A:313:TRP:C	2.54	0.44
2:B:334:LYS:HA	2:B:334:LYS:HD3	1.74	0.44
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.99	0.44
1:A:416:ARG:O	1:A:421:ASN:ND2	2.41	0.43
1:A:246:LYS:HD2	3:C:6:GAL:O4	2.19	0.43
2:B:393:THR:OG1	2:B:408:SER:OG	2.36	0.43
4:D:4:BMA:C4	4:D:5:NAG:C1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD23	1:A:309:LEU:N	2.35	0.42
1:A:441:LEU:HB2	5:A:630:HOH:O	2.19	0.42
2:B:311:GLN:HB3	2:B:311:GLN:HE21	1.59	0.42
2:B:301:ARG:NH2	2:B:303:VAL:HG22	2.27	0.42
2:B:279:VAL:O	2:B:280:ASP:HB2	2.19	0.42
2:B:303:VAL:O	2:B:304:SER:HB2	2.20	0.41
2:B:377:ILE:HG12	2:B:378:ALA:N	2.35	0.41
3:C:5:NAG:H61	3:C:6:GAL:C1	2.50	0.41
2:B:242:LEU:HD13	2:B:321:CYS:HB2	2.03	0.41
1:A:443:LEU:N	1:A:443:LEU:HD12	2.36	0.41
2:B:250:THR:O	2:B:310:HIS:HD2	2.04	0.41
2:B:360:LYS:HA	2:B:360:LYS:HD3	1.59	0.41
1:A:252:MET:CE	1:A:255:ARG:HD3	2.50	0.41
2:B:330:ALA:HB1	2:B:331:PRO:HD2	2.02	0.41
2:B:362:GLN:HB3	2:B:412:VAL:O	2.20	0.41
1:A:319:TYR:O	1:A:335:THR:HA	2.21	0.40
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.46	0.40
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

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	205/227 (90%)	191 (93%)	12 (6%)	2 (1%)	15	37
2	B	196/227 (86%)	178 (91%)	9 (5%)	9 (5%)	2	4
All	All	401/454 (88%)	369 (92%)	21 (5%)	11 (3%)	5	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	259	VAL
2	B	290	LYS
2	B	304	SER
2	B	420	GLY
1	A	341	GLY
1	A	384	ASN
2	B	247	PRO
2	B	329	PRO
2	B	303	VAL
2	B	260	THR
2	B	253	ILE

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	193/210 (92%)	182 (94%)	11 (6%)	20	44
2	B	186/209 (89%)	156 (84%)	30 (16%)	2	6
All	All	379/419 (90%)	338 (89%)	41 (11%)	6	15

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	255	ARG
1	A	293	GLU
1	A	334	LYS
1	A	342	GLN
1	A	362	GLN
1	A	413	ASP
1	A	418	GLN
1	A	422	VAL
1	A	424	SER
1	A	441	LEU
2	B	248	LYS
2	B	250	THR

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Mol	Chain	Res	Type
2	B	258	GLU
2	B	261	CYS
2	B	267	SER
2	B	272	GLU
2	B	274	LYS
2	B	277	TRP
2	B	278	TYR
2	B	284	VAL
2	B	285	HIS
2	B	290	LYS
2	B	297	ASN
2	B	301	ARG
2	B	303	VAL
2	B	308	VAL
2	B	311	GLN
2	B	317	LYS
2	B	336	ILE
2	B	355	ARG
2	B	363	VAL
2	B	370	LYS
2	B	380	GLU
2	B	382	GLU
2	B	418	GLN
2	B	421	ASN
2	B	437	THR
2	B	439	LYS
2	B	440	SER
2	B	442	SER

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	362	GLN
2	B	285	HIS
2	B	310	HIS
2	B	311	GLN
2	B	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	8	3	14,14,15	0.73	0	17,19,21	1.88	4 (23%)
4	NAG	D	2	4	14,14,15	1.14	2 (14%)	17,19,21	2.69	6 (35%)
3	GAL	C	6	3	11,11,12	1.16	2 (18%)	15,15,17	1.78	4 (26%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	2.01	7 (41%)
3	NAG	C	1	1,3	14,14,15	0.65	0	17,19,21	1.46	2 (11%)
4	NAG	D	5	4	14,14,15	0.69	1 (7%)	17,19,21	1.70	3 (17%)
3	NAG	C	5	3	14,14,15	1.15	1 (7%)	17,19,21	2.55	5 (29%)
4	NAG	D	1	2,4	14,14,15	0.65	0	17,19,21	1.90	5 (29%)

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	8	3	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
3	GAL	C	6	3	-	2/2/19/22	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
4	NAG	D	5	4	-	2/6/23/26	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	NAG	O5-C1	-3.19	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	2.27	1.55	1.52
4	D	2	NAG	C3-C2	2.17	1.57	1.52
3	C	6	GAL	C1-C2	2.08	1.56	1.52
4	D	5	NAG	C1-C2	2.03	1.55	1.52
3	C	6	GAL	O4-C4	-2.02	1.38	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	-7.18	102.47	112.19
3	C	5	NAG	C1-O5-C5	5.33	119.41	112.19
3	C	5	NAG	O5-C5-C6	5.16	115.29	107.20
3	C	2	NAG	C1-O5-C5	5.12	119.13	112.19
4	D	2	NAG	C2-N2-C7	5.11	130.18	122.90
3	C	5	NAG	O5-C1-C2	-4.91	103.53	111.29
4	D	2	NAG	C4-C3-C2	4.24	117.23	111.02
3	C	8	NAG	C1-C2-N2	-4.01	103.63	110.49
3	C	1	NAG	C1-O5-C5	3.87	117.44	112.19
4	D	5	NAG	C1-O5-C5	3.80	117.34	112.19
3	C	8	NAG	O5-C1-C2	3.70	117.13	111.29
4	D	1	NAG	C4-C3-C2	3.66	116.38	111.02
3	C	6	GAL	O2-C2-C1	3.41	116.12	109.15
3	C	5	NAG	C3-C4-C5	-3.38	104.21	110.24
4	D	1	NAG	O4-C4-C3	-3.20	102.96	110.35
4	D	1	NAG	C3-C4-C5	3.17	115.90	110.24
4	D	5	NAG	C3-C4-C5	3.14	115.84	110.24
3	C	5	NAG	C6-C5-C4	-3.06	105.83	113.00
4	D	1	NAG	C2-N2-C7	2.81	126.90	122.90
3	C	6	GAL	C1-O5-C5	2.74	115.90	112.19
4	D	2	NAG	O5-C5-C6	2.59	111.26	107.20
3	C	6	GAL	C3-C4-C5	2.58	114.84	110.24
4	D	5	NAG	C4-C3-C2	2.55	114.76	111.02
3	C	2	NAG	O7-C7-C8	-2.54	117.33	122.06
3	C	2	NAG	O5-C1-C2	-2.52	107.30	111.29
4	D	1	NAG	O5-C5-C6	2.50	111.13	107.20
3	C	2	NAG	C2-N2-C7	2.50	126.46	122.90
3	C	6	GAL	C1-C2-C3	2.44	112.67	109.67
4	D	2	NAG	C1-C2-N2	-2.33	106.50	110.49
3	C	2	NAG	O4-C4-C5	-2.30	103.58	109.30
3	C	2	NAG	C3-C4-C5	-2.21	106.29	110.24
3	C	8	NAG	O3-C3-C2	2.12	113.85	109.47
4	D	2	NAG	C6-C5-C4	2.10	117.92	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	NAG	O5-C5-C6	2.08	110.47	107.20
3	C	1	NAG	C8-C7-N2	2.03	119.53	116.10
3	C	2	NAG	O7-C7-N2	2.01	125.64	121.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	5	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
3	C	6	GAL	O5-C5-C6-O6
3	C	6	GAL	C4-C5-C6-O6
3	C	5	NAG	O5-C5-C6-O6
3	C	8	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6	GAL	3	0
4	D	5	NAG	2	0
3	C	5	NAG	1	0

5.5 Carbohydrates [i](#)

15 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	0.65	0	17,19,21	1.46	2 (11%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	2.01	7 (41%)
3	BMA	C	3	3	11,11,12	0.47	0	15,15,17	2.75	7 (46%)
3	BMA	C	4	3	11,11,12	1.14	1 (9%)	15,15,17	4.72	6 (40%)
3	NAG	C	5	3	14,14,15	1.15	1 (7%)	17,19,21	2.55	5 (29%)
3	GAL	C	6	3	11,11,12	1.16	2 (18%)	15,15,17	1.78	4 (26%)
3	BMA	C	7	3	11,11,12	0.89	1 (9%)	15,15,17	2.13	3 (20%)
3	NAG	C	8	3	14,14,15	0.73	0	17,19,21	1.88	4 (23%)
3	FUC	C	9	3	10,10,11	1.08	1 (10%)	14,14,16	2.16	4 (28%)
4	NAG	D	1	2,4	14,14,15	0.65	0	17,19,21	1.90	5 (29%)
4	NAG	D	2	4	14,14,15	1.14	2 (14%)	17,19,21	2.69	6 (35%)
4	BMA	D	3	4	11,11,12	1.60	2 (18%)	15,15,17	2.61	6 (40%)
4	BMA	D	4	4	11,11,12	1.15	2 (18%)	15,15,17	2.10	7 (46%)
4	NAG	D	5	4	14,14,15	0.69	1 (7%)	17,19,21	1.70	3 (17%)
4	FUC	D	6	4	10,10,11	0.88	0	14,14,16	1.79	5 (35%)

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	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	GAL	C	6	3	-	2/2/19/22	0/1/1/1
3	BMA	C	7	3	-	1/2/19/22	0/1/1/1
3	NAG	C	8	3	-	1/6/23/26	0/1/1/1
3	FUC	C	9	3	-	-	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1
4	NAG	D	5	4	-	2/6/23/26	0/1/1/1
4	FUC	D	6	4	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C2-C3	3.20	1.57	1.52
3	C	5	NAG	O5-C1	-3.19	1.38	1.43
4	D	3	BMA	O3-C3	3.11	1.50	1.43
3	C	9	FUC	C2-C3	-3.09	1.48	1.52
4	D	4	BMA	C2-C3	2.79	1.56	1.52
3	C	4	BMA	O5-C1	-2.62	1.39	1.43
4	D	2	NAG	C1-C2	2.27	1.55	1.52
4	D	2	NAG	C3-C2	2.17	1.57	1.52
3	C	6	GAL	C1-C2	2.08	1.56	1.52
3	C	7	BMA	O5-C1	-2.05	1.40	1.43
4	D	5	NAG	C1-C2	2.03	1.55	1.52
4	D	4	BMA	C1-C2	2.02	1.56	1.52
3	C	6	GAL	O4-C4	-2.02	1.38	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	BMA	C1-O5-C5	-14.02	93.19	112.19
3	C	4	BMA	C1-C2-C3	-10.33	96.97	109.67
4	D	2	NAG	C1-O5-C5	-7.18	102.47	112.19
3	C	3	BMA	C1-O5-C5	6.40	120.86	112.19
4	D	3	BMA	O3-C3-C2	6.13	121.73	109.99
3	C	7	BMA	C1-O5-C5	-5.86	104.25	112.19
3	C	9	FUC	O2-C2-C3	-5.35	99.43	110.14
3	C	5	NAG	C1-O5-C5	5.33	119.41	112.19
3	C	5	NAG	O5-C5-C6	5.16	115.29	107.20
3	C	2	NAG	C1-O5-C5	5.12	119.13	112.19
4	D	2	NAG	C2-N2-C7	5.11	130.18	122.90
3	C	5	NAG	O5-C1-C2	-4.91	103.53	111.29
3	C	3	BMA	O3-C3-C2	4.88	119.35	109.99
4	D	3	BMA	C1-C2-C3	4.84	115.61	109.67
3	C	9	FUC	O3-C3-C2	-4.25	101.86	109.99
4	D	2	NAG	C4-C3-C2	4.24	117.23	111.02
4	D	3	BMA	C3-C4-C5	4.05	117.46	110.24
3	C	8	NAG	C1-C2-N2	-4.01	103.63	110.49
4	D	4	BMA	C1-C2-C3	-3.93	104.83	109.67
3	C	1	NAG	C1-O5-C5	3.87	117.44	112.19
4	D	5	NAG	C1-O5-C5	3.80	117.34	112.19
3	C	8	NAG	O5-C1-C2	3.70	117.13	111.29
4	D	1	NAG	C4-C3-C2	3.66	116.38	111.02
3	C	3	BMA	O6-C6-C5	-3.60	98.94	111.29
3	C	6	GAL	O2-C2-C1	3.41	116.12	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	NAG	C3-C4-C5	-3.38	104.21	110.24
4	D	6	FUC	C2-C3-C4	3.35	116.69	110.89
3	C	7	BMA	O2-C2-C3	3.29	116.73	110.14
3	C	7	BMA	O4-C4-C3	-3.24	102.86	110.35
4	D	1	NAG	O4-C4-C3	-3.20	102.96	110.35
4	D	1	NAG	C3-C4-C5	3.17	115.90	110.24
4	D	4	BMA	O3-C3-C2	3.16	116.04	109.99
4	D	4	BMA	O2-C2-C3	3.15	116.46	110.14
4	D	5	NAG	C3-C4-C5	3.14	115.84	110.24
3	C	5	NAG	C6-C5-C4	-3.06	105.83	113.00
4	D	1	NAG	C2-N2-C7	2.81	126.90	122.90
4	D	6	FUC	C3-C4-C5	2.75	114.05	109.77
3	C	4	BMA	O6-C6-C5	-2.74	101.89	111.29
3	C	6	GAL	C1-O5-C5	2.74	115.90	112.19
3	C	3	BMA	C1-C2-C3	-2.73	106.31	109.67
4	D	4	BMA	O5-C1-C2	-2.71	106.58	110.77
4	D	4	BMA	O5-C5-C6	2.66	111.38	107.20
3	C	4	BMA	O5-C5-C6	2.66	111.38	107.20
4	D	6	FUC	C1-O5-C5	2.61	118.70	112.78
4	D	2	NAG	O5-C5-C6	2.59	111.26	107.20
3	C	6	GAL	C3-C4-C5	2.58	114.84	110.24
3	C	3	BMA	O4-C4-C3	-2.58	104.39	110.35
4	D	5	NAG	C4-C3-C2	2.55	114.76	111.02
3	C	2	NAG	O7-C7-C8	-2.54	117.33	122.06
3	C	2	NAG	O5-C1-C2	-2.52	107.30	111.29
4	D	1	NAG	O5-C5-C6	2.50	111.13	107.20
3	C	2	NAG	C2-N2-C7	2.50	126.46	122.90
3	C	9	FUC	O5-C1-C2	-2.47	106.96	110.77
3	C	3	BMA	O2-C2-C3	-2.45	105.22	110.14
4	D	6	FUC	O5-C5-C6	2.45	112.60	107.33
3	C	6	GAL	C1-C2-C3	2.44	112.67	109.67
4	D	6	FUC	C1-C2-C3	2.41	112.63	109.67
3	C	3	BMA	O5-C5-C4	2.41	116.68	110.83
4	D	4	BMA	O2-C2-C1	2.40	114.07	109.15
4	D	3	BMA	C1-O5-C5	-2.37	108.99	112.19
4	D	2	NAG	C1-C2-N2	-2.33	106.50	110.49
3	C	2	NAG	O4-C4-C5	-2.30	103.58	109.30
3	C	9	FUC	C1-O5-C5	2.28	117.94	112.78
3	C	2	NAG	C3-C4-C5	-2.21	106.29	110.24
3	C	4	BMA	C6-C5-C4	2.20	118.15	113.00
4	D	3	BMA	O5-C5-C6	2.18	110.62	107.20
3	C	4	BMA	O5-C5-C4	-2.15	105.59	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	NAG	O3-C3-C2	2.12	113.85	109.47
4	D	2	NAG	C6-C5-C4	2.10	117.92	113.00
3	C	8	NAG	O5-C5-C6	2.08	110.47	107.20
4	D	4	BMA	O6-C6-C5	-2.06	104.21	111.29
4	D	3	BMA	O2-C2-C3	2.06	114.27	110.14
3	C	1	NAG	C8-C7-N2	2.03	119.53	116.10
3	C	2	NAG	O7-C7-N2	2.01	125.64	121.95

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	5	NAG	O5-C5-C6-O6
4	D	4	BMA	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	4	BMA	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
4	D	5	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
3	C	7	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	6	GAL	O5-C5-C6-O6
3	C	6	GAL	C4-C5-C6-O6
3	C	5	NAG	O5-C5-C6-O6
3	C	8	NAG	O5-C5-C6-O6

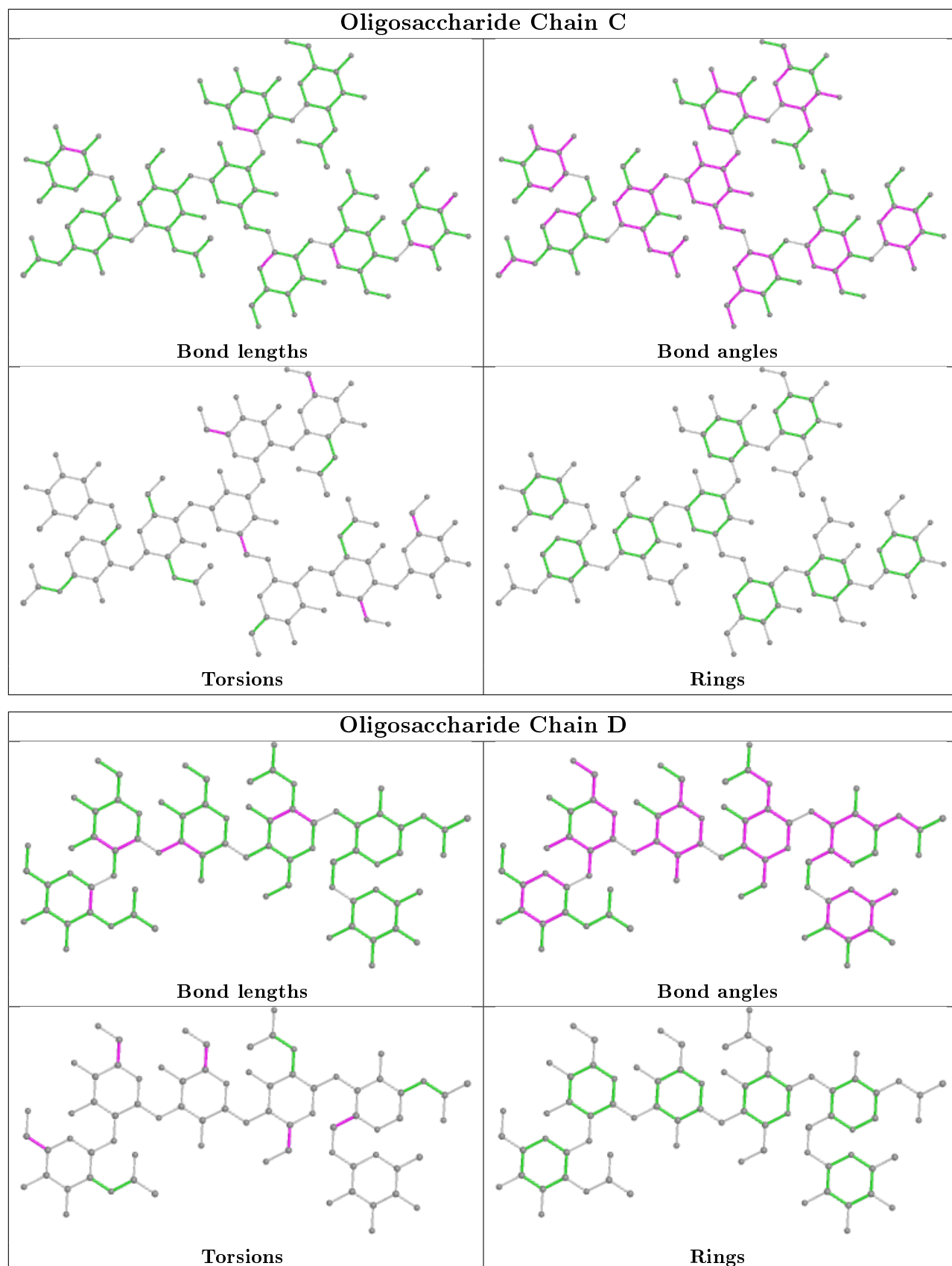
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	BMA	2	0
3	C	6	GAL	3	0
4	D	5	NAG	2	0
3	C	5	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

There are no ligands in this entry.

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, 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	207/227 (91%)	0.10	2 (0%) 82 83	41, 63, 132, 176	0
2	B	200/227 (88%)	0.71	30 (15%) 2 1	59, 111, 161, 190	0
All	All	407/454 (89%)	0.40	32 (7%) 12 10	41, 90, 154, 190	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	7.0
2	B	324	SER	6.1
2	B	301	ARG	5.9
2	B	263	VAL	4.6
2	B	279	VAL	4.6
2	B	297	ASN	4.2
2	B	291	PRO	4.2
2	B	241	PHE	4.0
2	B	266	VAL	3.6
2	B	319	TYR	3.6
2	B	269	GLU	3.5
2	B	322	LYS	3.4
2	B	331	PRO	3.2
2	B	271	PRO	3.1
2	B	276	ASN	3.1
2	B	326	LYS	2.9
2	B	298	SER	2.8
2	B	274	LYS	2.8
2	B	303	VAL	2.5
2	B	281	GLY	2.5
2	B	323	VAL	2.5
2	B	304	SER	2.5
2	B	283	GLU	2.4
1	A	402	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	368	LEU	2.2
2	B	240	VAL	2.2
2	B	282	VAL	2.2
2	B	320	LYS	2.1
2	B	280	ASP	2.1
2	B	355	ARG	2.0
2	B	284	VAL	2.0
2	B	305	VAL	2.0

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

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	NAG	D	5	14/15	0.63	0.30	77,92,107,112	0
4	NAG	D	1	14/15	0.76	0.37	73,79,83,84	0
4	NAG	D	2	14/15	0.78	0.38	87,102,107,107	0
3	NAG	C	8	14/15	0.85	0.16	62,73,90,91	0
3	GAL	C	6	11/12	0.94	0.14	45,56,64,65	0
3	NAG	C	2	14/15	0.96	0.11	30,33,39,40	0
3	NAG	C	5	14/15	0.96	0.14	38,44,50,52	0
3	NAG	C	1	14/15	0.96	0.12	28,31,36,43	0

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.

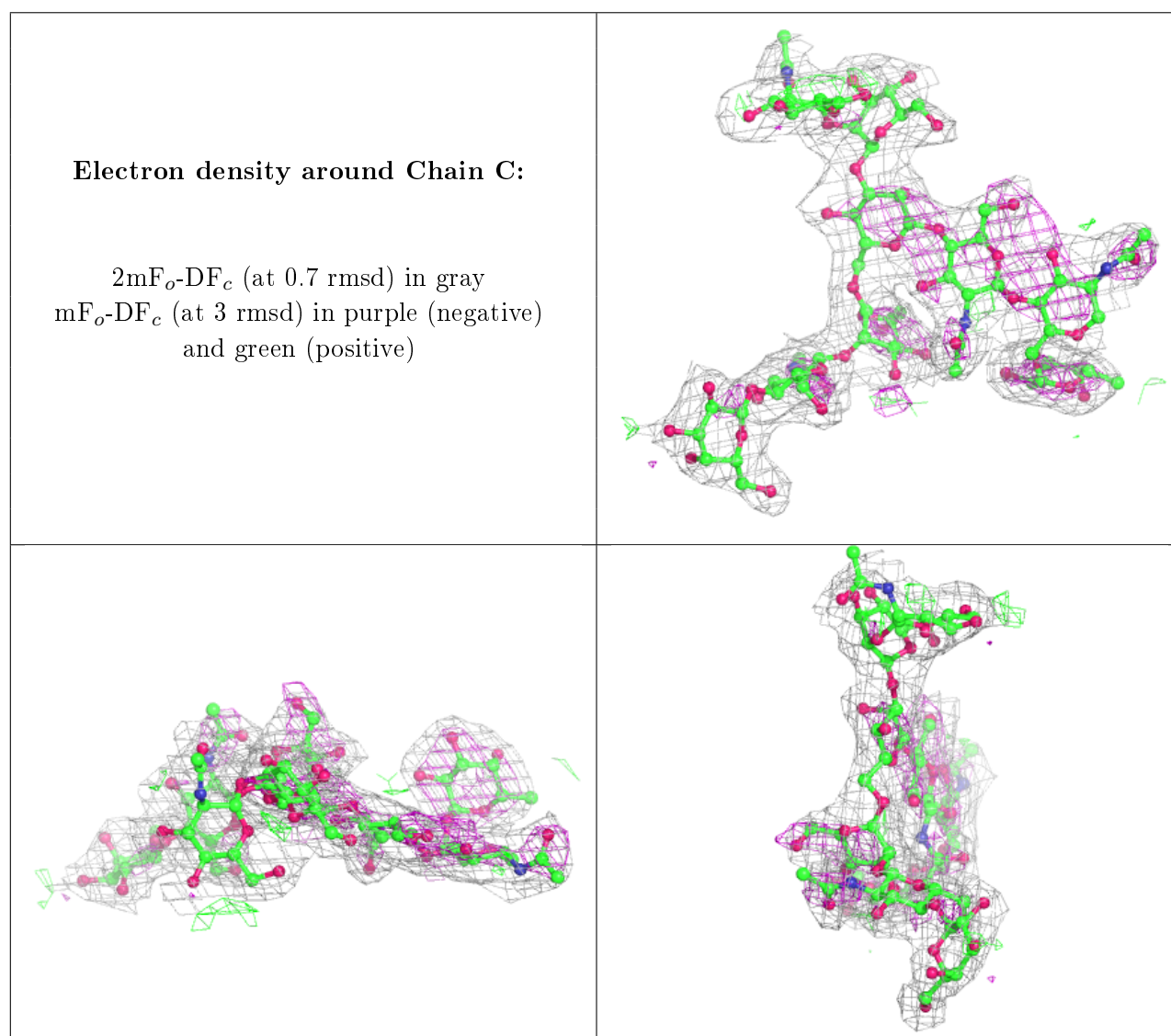
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	D	4	11/12	0.54	0.41	88,101,115,115	0
4	BMA	D	3	11/12	0.57	0.31	73,93,105,115	0
4	NAG	D	5	14/15	0.63	0.30	77,92,107,112	0
4	NAG	D	1	14/15	0.76	0.37	73,79,83,84	0
4	NAG	D	2	14/15	0.78	0.38	87,102,107,107	0
3	NAG	C	8	14/15	0.85	0.16	62,73,90,91	0
4	FUC	D	6	10/11	0.85	0.33	73,78,79,82	0

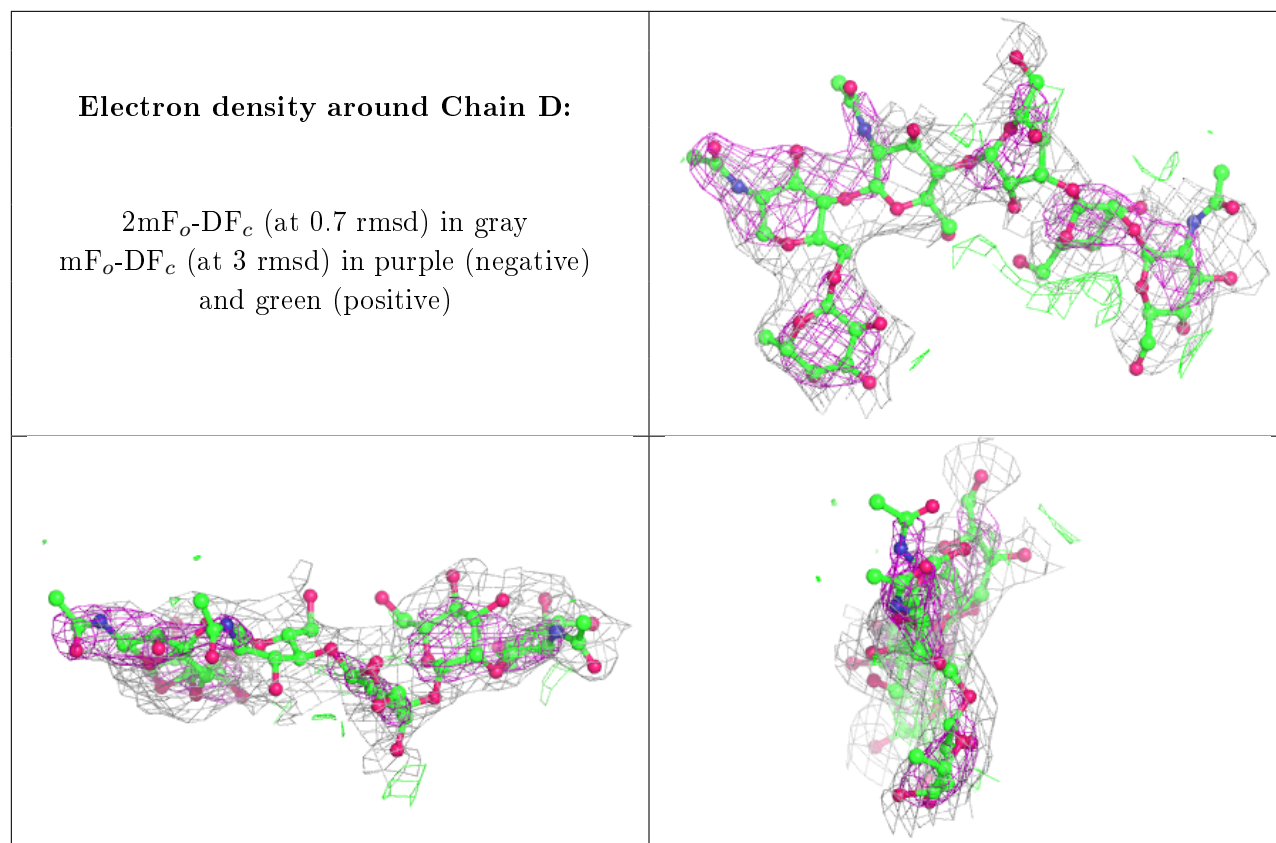
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	C	7	11/12	0.93	0.10	62,70,78,80	0
3	GAL	C	6	11/12	0.94	0.14	45,56,64,65	0
3	NAG	C	1	14/15	0.96	0.12	28,31,36,43	0
3	BMA	C	4	11/12	0.96	0.10	36,39,47,49	0
3	NAG	C	5	14/15	0.96	0.14	38,44,50,52	0
3	NAG	C	2	14/15	0.96	0.11	30,33,39,40	0
3	BMA	C	3	11/12	0.97	0.07	35,39,44,47	0
3	FUC	C	9	10/11	0.97	0.11	31,35,40,46	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.