



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:30 AM EDT

PDB ID : 5UK5 / pdb_00005uk5
Title : Complex of Notch1(EGF8-12) bound to Jagged1(N-EGF3)
Authors : Garcia, K.C.; Luca, V.C.
Deposited on : 2017-01-19
Resolution : 2.51 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

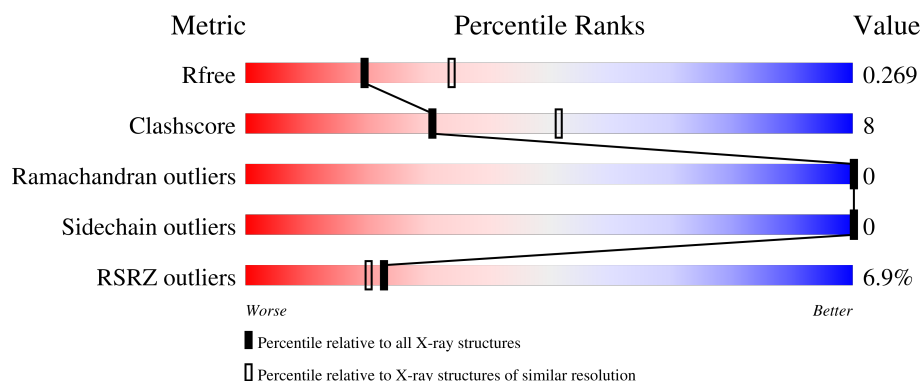
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	205	11% 79% 16% 5%
2	B	318	3% 82% 15% .
3	C	2	50% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4033 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 Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1389	819	247	292	31			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ASP	-	expression tag	UNP Q07008
A	294	PRO	-	expression tag	UNP Q07008
A	489	SER	-	expression tag	UNP Q07008
A	490	GLY	-	expression tag	UNP Q07008
A	491	ARG	-	expression tag	UNP Q07008
A	492	LEU	-	expression tag	UNP Q07008
A	493	GLU	-	expression tag	UNP Q07008
A	494	VAL	-	expression tag	UNP Q07008
A	495	LEU	-	expression tag	UNP Q07008
A	496	PHE	-	expression tag	UNP Q07008
A	497	GLN	-	expression tag	UNP Q07008

- Molecule 2 is a protein called Protein jagged-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2391	1469	433	455	34			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ALA	-	expression tag	UNP Q63722
B	29	ASP	-	expression tag	UNP Q63722
B	30	PRO	-	expression tag	UNP Q63722
B	31	ARG	-	expression tag	UNP Q63722
B	32	LEU	SER	engineered mutation	UNP Q63722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	68	GLY	ARG	engineered mutation	UNP Q63722
B	72	ASN	ASP	engineered mutation	UNP Q63722
B	87	ARG	THR	engineered mutation	UNP Q63722
B	182	ARG	GLN	engineered mutation	UNP Q63722
B	335	ALA	-	expression tag	UNP Q63722
B	336	ALA	-	expression tag	UNP Q63722
B	337	ALA	-	expression tag	UNP Q63722
B	338	HIS	-	expression tag	UNP Q63722
B	339	HIS	-	expression tag	UNP Q63722
B	340	HIS	-	expression tag	UNP Q63722
B	341	HIS	-	expression tag	UNP Q63722
B	342	HIS	-	expression tag	UNP Q63722
B	343	HIS	-	expression tag	UNP Q63722
B	344	HIS	-	expression tag	UNP Q63722
B	345	HIS	-	expression tag	UNP Q63722

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-3)-beta-D-glucopyranose.

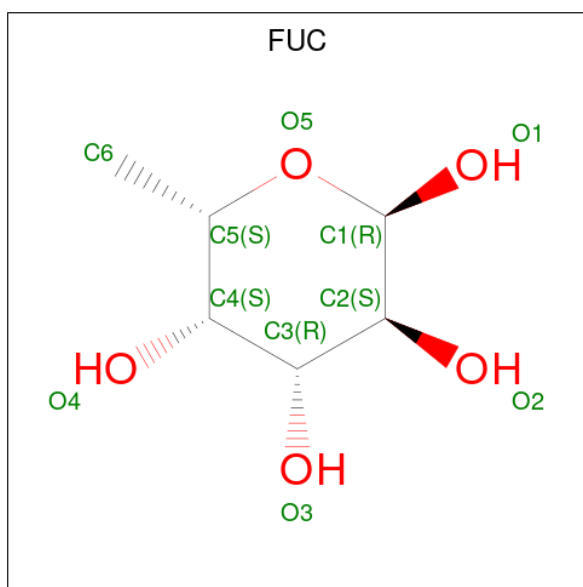


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			20	11	9			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

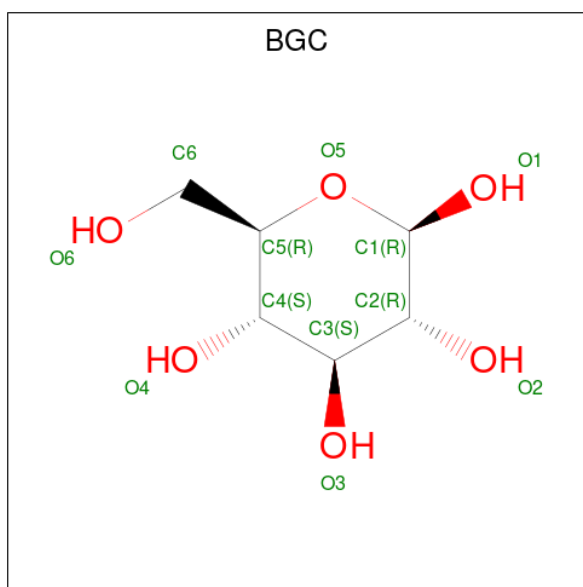
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



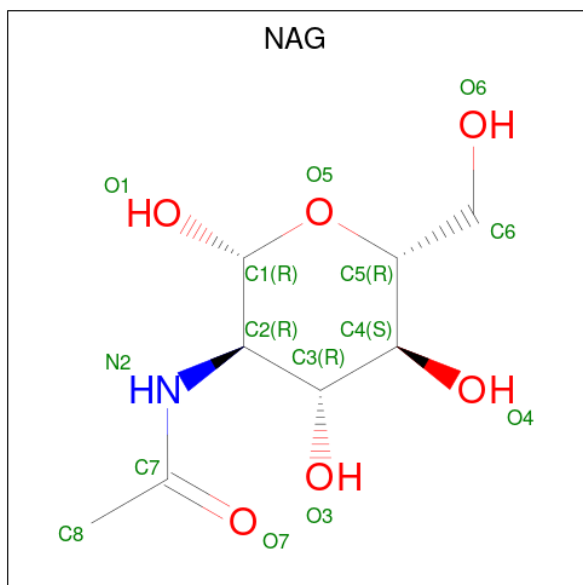
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

Continued on next page...

Continued from previous page...

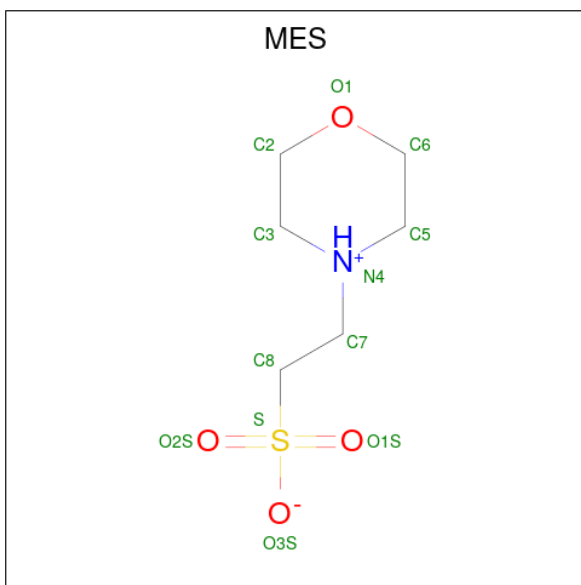
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

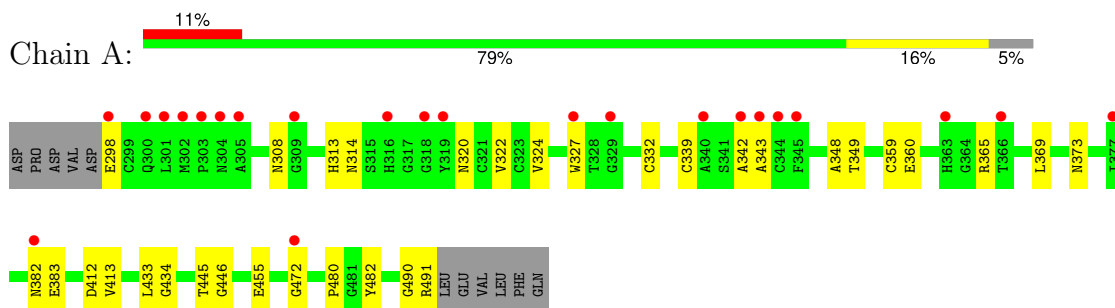
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	41	Total	O	0	0
			41	41		
9	B	97	Total	O	0	0
			97	97		

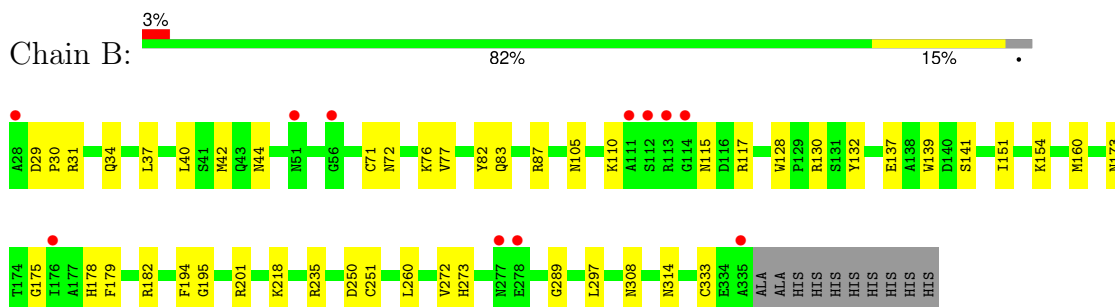
3 Residue-property plots [i](#)

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: Neurogenic locus notch homolog protein 1



- Molecule 2: Protein jagged-1



- Molecule 3: alpha-D-xylopyranose-(1-3)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.46Å 128.00Å 154.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 2.51 44.74 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.74-2.51) 99.2 (44.74-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.219 , 0.263 0.223 , 0.269	Depositor DCC
R_{free} test set	1179 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4033	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, MLY, NAG, CA, XYS, MES, BGC

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	0.23	0/1415	0.40	0/1924
2	B	0.29	0/2355	0.47	0/3199
All	All	0.27	0/3770	0.44	0/5123

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 [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	1389	0	1185	24	0
2	B	2391	0	2171	36	0
3	C	20	0	17	2	0
4	A	3	0	0	0	0
5	A	20	0	20	2	0
5	B	10	0	10	0	0
6	A	22	0	20	1	0
7	A	14	0	13	0	0
7	B	14	0	13	1	0
8	B	12	0	13	5	0
9	A	41	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	97	0	0	2	0
All	All	4033	0	3462	61	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 8.

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:201:ARG:HH12	8:B:403:MES:H32	1.04	1.09
2:B:201:ARG:NH1	8:B:403:MES:H32	1.73	1.01
2:B:201:ARG:HH12	8:B:403:MES:C3	1.82	0.91
2:B:130:ARG:HD2	2:B:194:PHE:HB3	1.55	0.88
1:A:308:ASN:O	9:A:702:HOH:O	2.10	0.69
2:B:308:ASN:ND2	2:B:333:CYS:O	2.23	0.68
2:B:72:ASN:OD1	9:B:501:HOH:O	2.11	0.67
1:A:313:HIS:HB2	1:A:320:ASN:HB3	1.79	0.62
1:A:382:ASN:OD1	1:A:383:GLU:N	2.34	0.61
1:A:298:GLU:HA	1:A:314:ASN:ND2	2.15	0.60
2:B:151:ILE:HD11	2:B:154:MLY:HB3	1.83	0.60
1:A:412:ASP:HB2	1:A:433:LEU:HD12	1.84	0.60
1:A:327:TRP:HB3	1:A:332:CYS:HB3	1.85	0.59
1:A:412:ASP:CG	1:A:434:GLY:H	2.12	0.57
2:B:44:ASN:O	2:B:105:ASN:HB3	2.05	0.57
2:B:137:GLU:HG2	2:B:154:MLY:HG2	1.88	0.55
1:A:365:ARG:HA	1:A:373:ASN:HA	1.87	0.55
2:B:31:ARG:NH2	2:B:34:GLN:OE1	2.33	0.53
2:B:175:GLY:O	2:B:178:HIS:NE2	2.40	0.51
2:B:201:ARG:CZ	8:B:403:MES:H32	2.40	0.51
1:A:322:VAL:HG12	5:A:604:FUC:H61	1.91	0.51
1:A:349:THR:HB	1:A:360:GLU:HB3	1.93	0.51
5:A:610:FUC:H2	2:B:82:TYR:O	2.11	0.51
1:A:455:GLU:OE2	9:A:703:HOH:O	2.20	0.50
2:B:71:CYS:N	2:B:105:ASN:OD1	2.37	0.50
2:B:272:VAL:HG23	2:B:273:HIS:H	1.77	0.49
8:B:403:MES:H22	9:B:546:HOH:O	2.12	0.49
2:B:76:MLY:HH23	2:B:139:TRP:CZ2	2.48	0.49
2:B:289:GLY:HA3	2:B:297:LEU:HD21	1.95	0.49
1:A:359:CYS:SG	1:A:369:LEU:HA	2.53	0.48
2:B:250:ASP:OD1	2:B:251:CYS:N	2.47	0.48
2:B:173:ASN:HA	2:B:178:HIS:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:VAL:HG23	2:B:273:HIS:N	2.30	0.47
2:B:128:TRP:HB3	2:B:195:GLY:HA2	1.98	0.46
1:A:480:PRO:HG3	2:B:87:ARG:HD2	1.98	0.45
1:A:472:GLY:C	3:C:2:XYS:HO4	2.23	0.45
2:B:29:ASP:N	2:B:30:PRO:HD3	2.32	0.45
2:B:37:LEU:HD22	2:B:77:VAL:HG21	2.00	0.44
2:B:235:ARG:NH1	2:B:260:LEU:HD12	2.32	0.44
1:A:339:CYS:HA	1:A:342:ALA:HB2	1.98	0.44
2:B:83:GLN:NE2	2:B:87:ARG:H	2.16	0.44
7:B:401:NAG:O7	7:B:401:NAG:O3	2.29	0.43
2:B:40:LEU:HD21	2:B:182:ARG:HG2	2.01	0.43
1:A:324:VAL:HA	2:B:314:ASN:HD22	1.84	0.43
2:B:115:ASN:HD21	2:B:117:ARG:HH11	1.67	0.43
1:A:343:ALA:HB3	1:A:369:LEU:HD22	2.00	0.42
2:B:130:ARG:O	2:B:160:MET:HA	2.20	0.42
2:B:40:LEU:HB3	2:B:110:LYS:HG2	2.01	0.42
1:A:491:ARG:HE	1:A:491:ARG:HB3	1.57	0.42
2:B:173:ASN:HA	2:B:178:HIS:CG	2.55	0.41
1:A:482:TYR:CD1	1:A:490:GLY:HA2	2.55	0.41
1:A:412:ASP:OD1	1:A:413:VAL:N	2.53	0.41
6:A:606:BGC:H6C1	9:A:736:HOH:O	2.19	0.41
2:B:42:MET:SD	2:B:179:PHE:HB3	2.60	0.41
2:B:218:MLY:HH22	2:B:218:MLY:HD3	1.84	0.41
2:B:82:TYR:HB2	2:B:132:TYR:N	2.36	0.41
1:A:348:ALA:HB2	9:A:732:HOH:O	2.20	0.41
1:A:482:TYR:HD1	1:A:490:GLY:HA2	1.85	0.41
2:B:72:ASN:HB2	2:B:141:SER:HB3	2.03	0.41
1:A:455:GLU:HG2	3:C:2:XYS:O4	2.21	0.40
1:A:445:THR:OG1	1:A:446:GLY:N	2.54	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	192/205 (94%)	185 (96%)	7 (4%)	0	100	100
2	B	297/318 (93%)	288 (97%)	9 (3%)	0	100	100
All	All	489/523 (94%)	473 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	155/170 (91%)	155 (100%)	0	100	100
2	B	250/260 (96%)	250 (100%)	0	100	100
All	All	405/430 (94%)	405 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	351	HIS
1	A	462	GLN
2	B	72	ASN
2	B	83	GLN
2	B	172	GLN
2	B	254	GLN
2	B	273	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	$\# Z > 2$
2	MLY	B	241	2	9,10,11	0.50	0	6,11,13	1.13	0
2	MLY	B	264	2	9,10,11	0.54	0	6,11,13	0.75	0
2	MLY	B	76	2	9,10,11	0.63	0	6,11,13	0.91	0
2	MLY	B	198	2	9,10,11	0.48	0	6,11,13	0.92	0
2	MLY	B	154	2	9,10,11	0.63	0	6,11,13	0.77	0
2	MLY	B	171	2	9,10,11	0.59	0	6,11,13	0.84	0
2	MLY	B	80	2	9,10,11	0.57	0	6,11,13	0.87	0
2	MLY	B	218	2	9,10,11	0.69	0	6,11,13	0.89	0
2	MLY	B	295	2	9,10,11	0.58	0	6,11,13	0.70	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	MLY	B	241	2	-	0/8/9/11	-
2	MLY	B	264	2	-	0/8/9/11	-
2	MLY	B	76	2	-	0/8/9/11	-
2	MLY	B	198	2	-	1/8/9/11	-
2	MLY	B	154	2	-	0/8/9/11	-
2	MLY	B	171	2	-	2/8/9/11	-
2	MLY	B	80	2	-	0/8/9/11	-
2	MLY	B	218	2	-	0/8/9/11	-
2	MLY	B	295	2	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	171	MLY	CG-CD-CE-NZ
2	B	198	MLY	C-CA-CB-CG
2	B	171	MLY	CD-CE-NZ-CH2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	MLY	1	0
2	B	154	MLY	2	0
2	B	218	MLY	1	0

5.5 Carbohydrates [i](#)

2 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	BGC	C	1	1,3	11,11,12	0.23	0	15,15,17	0.58	0
3	XYS	C	2	3	9,9,10	0.20	0	10,12,14	0.41	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	BGC	C	1	1,3	-	0/2/19/22	0/1/1/1
3	XYS	C	2	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

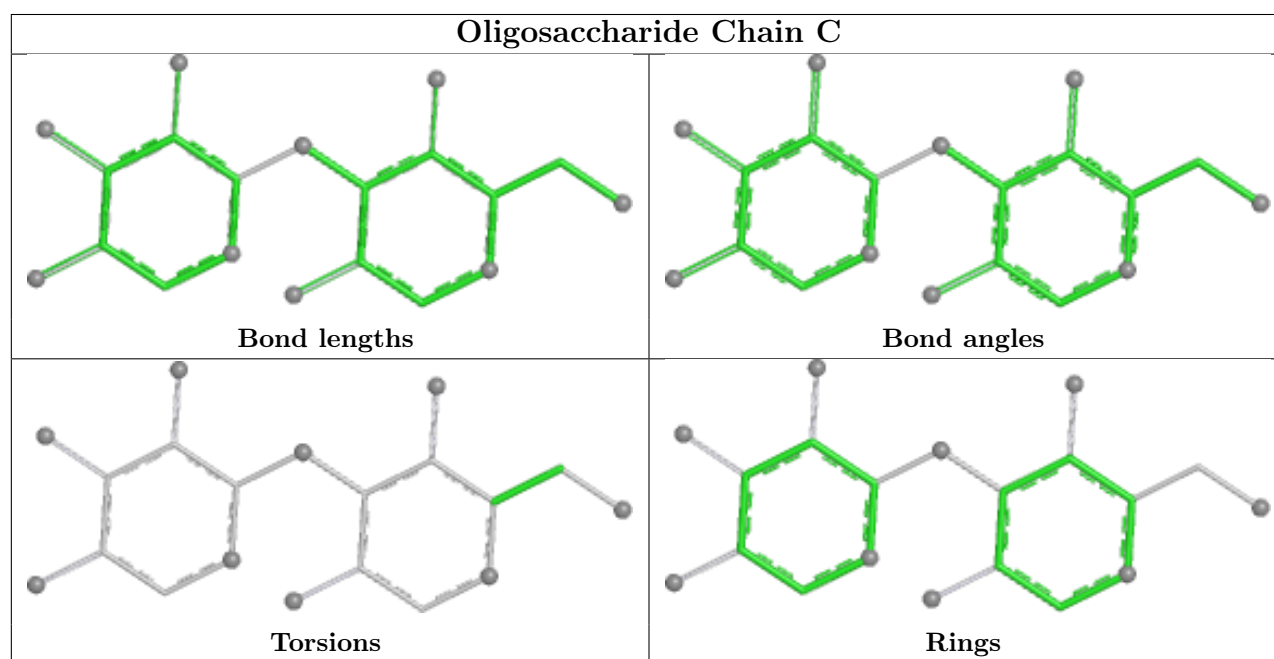
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	XYS	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.



5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	BGC	A	606	1	11,11,12	0.23	0	15,15,17	0.59	0
5	FUC	B	402	2	10,10,11	0.52	0	14,14,16	0.95	1 (7%)
8	MES	B	403	-	12,12,12	0.95	1 (8%)	15,16,16	1.03	0
6	BGC	A	605	1	11,11,12	0.23	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	A	604	1	10,10,11	0.52	0	14,14,16	0.93	2 (14%)
7	NAG	A	607	1	14,14,15	0.30	0	17,19,21	0.50	0
7	NAG	B	401	2	14,14,15	0.58	0	17,19,21	0.48	0
5	FUC	A	610	1	10,10,11	0.52	0	14,14,16	0.93	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BGC	A	606	1	-	0/2/19/22	0/1/1/1
5	FUC	B	402	2	-	-	0/1/1/1
8	MES	B	403	-	-	0/6/14/14	0/1/1/1
6	BGC	A	605	1	-	0/2/19/22	0/1/1/1
5	FUC	A	604	1	-	-	0/1/1/1
7	NAG	B	401	2	-	3/6/23/26	0/1/1/1
7	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	FUC	A	610	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	MES	C8-S	3.00	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	FUC	C1-O5-C5	-2.26	107.62	112.97
5	A	604	FUC	C1-O5-C5	-2.22	107.74	112.97
5	A	610	FUC	C1-O5-C5	-2.18	107.83	112.97
5	A	604	FUC	C6-C5-C4	-2.01	109.40	113.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	607	NAG	O5-C5-C6-O6
7	A	607	NAG	C4-C5-C6-O6
7	B	401	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	401	NAG	O5-C5-C6-O6
7	B	401	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	BGC	1	0
8	B	403	MES	5	0
5	A	604	FUC	1	0
7	B	401	NAG	1	0
5	A	610	FUC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	194/205 (94%)	0.80	23 (11%) 9 7	60, 102, 160, 176	0
2	B	299/318 (94%)	0.33	11 (3%) 45 40	50, 83, 135, 189	0
All	All	493/523 (94%)	0.51	34 (6%) 23 20	50, 91, 149, 189	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	114	GLY	6.2
2	B	335	ALA	5.7
1	A	302	MET	4.9
1	A	301	LEU	4.0
1	A	303	PRO	4.0
1	A	300	GLN	3.4
1	A	345	PHE	3.1
1	A	309	GLY	2.7
1	A	342	ALA	2.6
1	A	305	ALA	2.6
1	A	343	ALA	2.6
1	A	366	THR	2.6
1	A	298	GLU	2.6
2	B	28	ALA	2.6
2	B	176	ILE	2.5
2	B	111	ALA	2.5
1	A	377	ILE	2.4
1	A	363	HIS	2.4
1	A	344	CYS	2.4
2	B	56	GLY	2.3
1	A	319	TYR	2.3
1	A	316	HIS	2.3
1	A	304	ASN	2.3
1	A	382	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	112	SER	2.3
2	B	277	ASN	2.2
1	A	472	GLY	2.2
1	A	329	GLY	2.2
2	B	278	GLU	2.2
2	B	113	ARG	2.2
1	A	340	ALA	2.1
2	B	51	ASN	2.0
1	A	318	GLY	2.0
1	A	327	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MLY	B	241	11/12	0.70	0.21	92,99,123,134	0
2	MLY	B	154	11/12	0.84	0.19	75,84,126,127	0
2	MLY	B	171	11/12	0.89	0.13	79,86,111,112	0
2	MLY	B	295	11/12	0.90	0.13	72,91,112,112	0
2	MLY	B	198	11/12	0.91	0.13	54,65,92,92	0
2	MLY	B	264	11/12	0.92	0.15	74,82,104,115	0
2	MLY	B	218	11/12	0.93	0.12	59,67,75,91	0
2	MLY	B	76	11/12	0.93	0.12	47,57,68,76	0
2	MLY	B	80	11/12	0.97	0.08	51,62,74,76	0

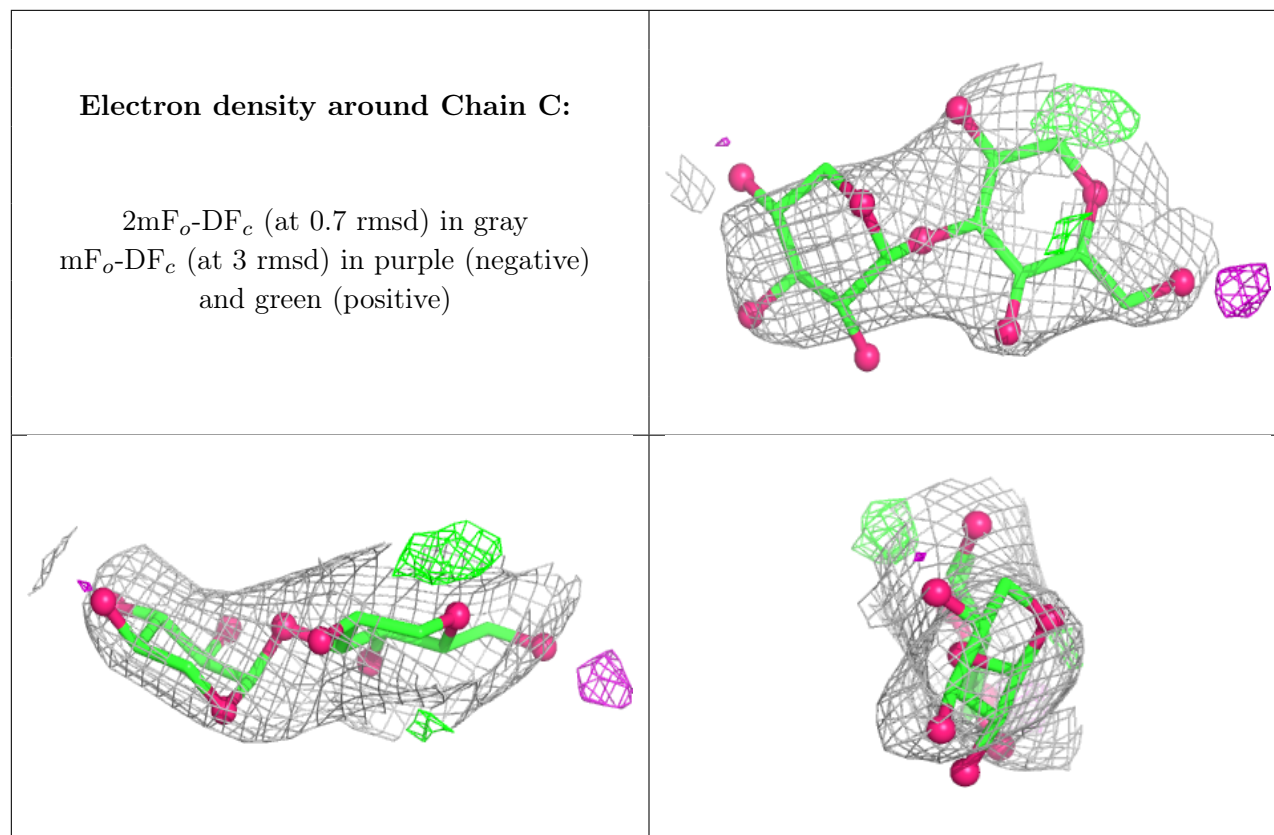
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	C	1	11/12	0.79	0.13	73,87,102,104	0
3	XYS	C	2	9/10	0.86	0.15	88,96,99,108	9

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. 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
8	MES	B	403	12/12	0.34	0.18	100,125,179,180	0
7	NAG	B	401	14/15	0.58	0.16	95,126,134,138	0
6	BGC	A	606	11/12	0.66	0.21	73,91,105,107	11
6	BGC	A	605	11/12	0.73	0.12	79,104,116,121	11
7	NAG	A	607	14/15	0.78	0.15	92,121,137,137	0
5	FUC	B	402	10/11	0.79	0.12	82,91,103,105	0
5	FUC	A	604	10/11	0.90	0.09	75,79,85,86	0
5	FUC	A	610	10/11	0.92	0.09	54,78,86,96	0
4	CA	A	601	1/1	0.98	0.08	88,88,88,88	1
4	CA	A	602	1/1	0.98	0.05	68,68,68,68	1
4	CA	A	603	1/1	1.00	0.03	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.