Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 12:32 PM EDT

PDB ID	:	5UK5
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 (i) 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 (i)) were used in the production of this report:

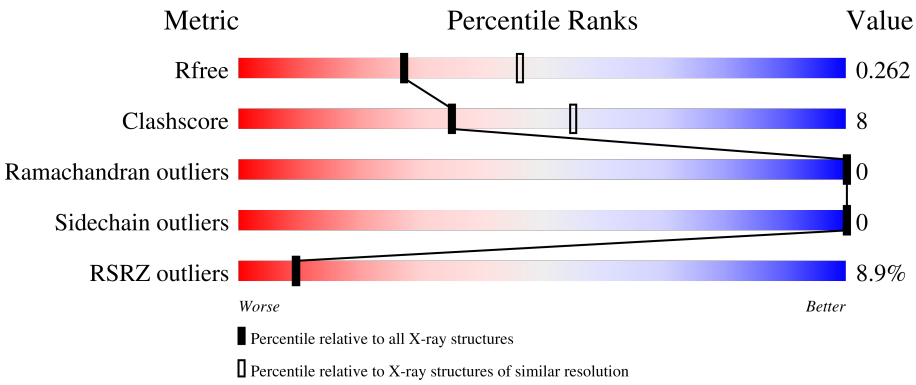
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.51 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	10% 79% 16% 5%
2	B	318	7% 82% 15% ·
3	C	2	50% 50%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	194	1389	819	247	292	31	0	0	0

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
			Total	C	N	O	S			
2	B	308	2391	1469	433	455	34	0	0	0

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

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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

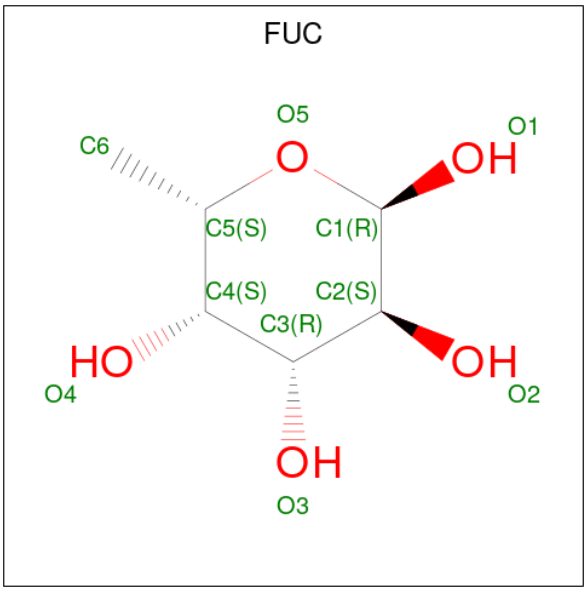
- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-3)-beta-D-glucopyranose.

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

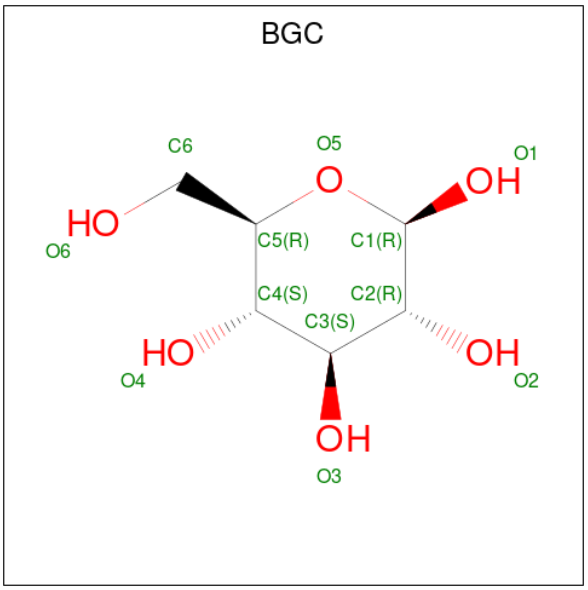
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	3	3	3	0	0

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 6 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

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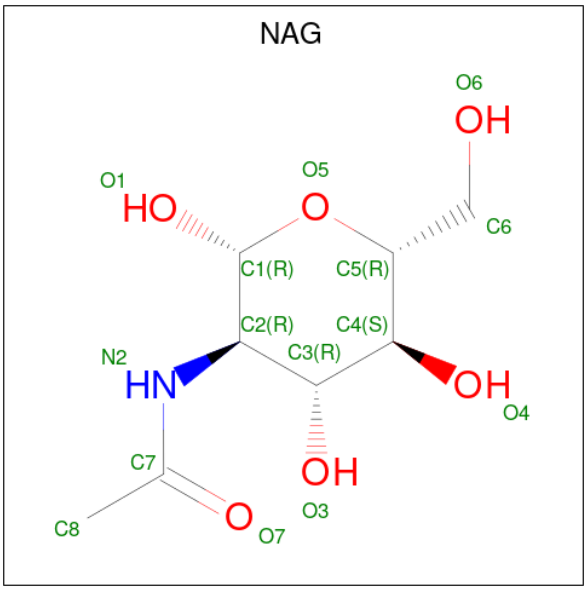
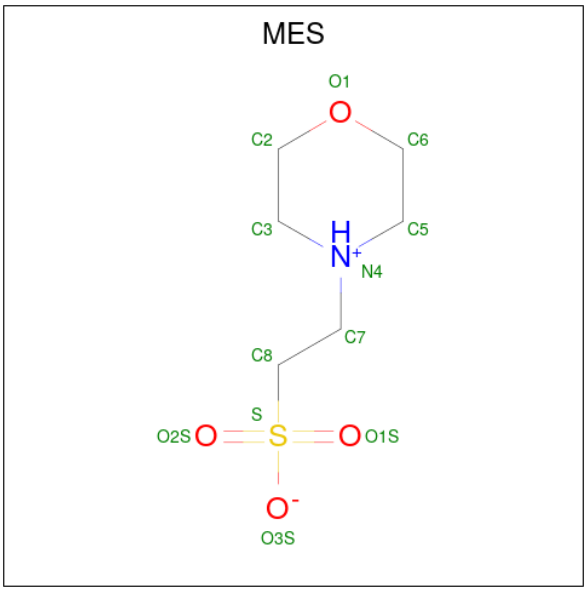
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	11	6	5	0	0

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



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

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



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

- Molecule 9 is water.

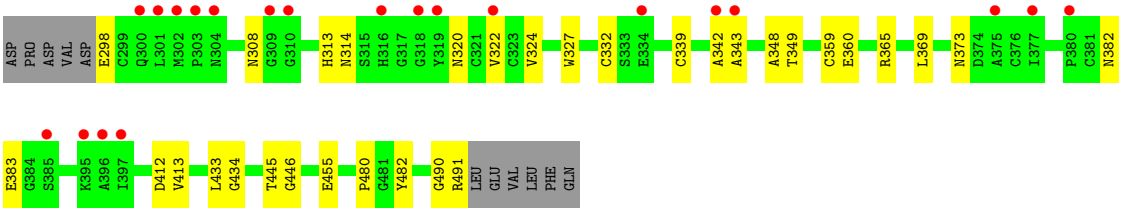
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	41	41	41	0	0
			Total	O		
9	B	97	97	97	0	0

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.

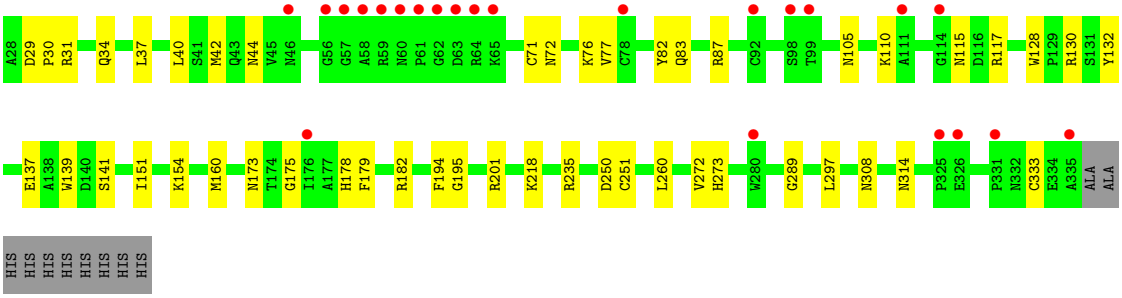
• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:



• Molecule 2: Protein jagged-1

Chain B:



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

Chain C:

4 Data and refinement statistics (i)

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) 99.3 (44.74-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.219 , 0.263 0.219 , 0.262	Depositor DCC
R_{free} test set	1178 reflections (5.00%)	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)	0.31 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, XYS, BGC, FUC, MLY, MES

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	0.35	0/1415	0.49	0/1924
2	B	0.39	0/2355	0.52	0/3199
All	All	0.37	0/3770	0.51	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	23	0
2	B	2391	0	2171	36	0
3	C	20	0	17	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	97	0	0	2	0
All	All	4033	0	3462	60	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 (60) 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
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
1:A:412:ASP:CG	1:A:434:GLY:H	2.12	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

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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
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 (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	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 (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	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. 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)

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	218	2	9,10,11	0.70	0	6,11,13	0.88	0
2	MLY	B	171	2	9,10,11	0.58	0	6,11,13	0.84	0
2	MLY	B	295	2	9,10,11	0.58	0	6,11,13	0.71	0
2	MLY	B	264	2	9,10,11	0.55	0	6,11,13	0.75	0
2	MLY	B	76	2	9,10,11	0.63	0	6,11,13	0.92	0
2	MLY	B	241	2	9,10,11	0.49	0	6,11,13	1.13	0
2	MLY	B	154	2	9,10,11	0.62	0	6,11,13	0.76	0
2	MLY	B	198	2	9,10,11	0.48	0	6,11,13	0.92	0
2	MLY	B	80	2	9,10,11	0.56	0	6,11,13	0.87	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	218	2	-	0/8/9/11	-
2	MLY	B	171	2	-	2/8/9/11	-
2	MLY	B	295	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	241	2	-	0/8/9/11	-
2	MLY	B	154	2	-	0/8/9/11	-
2	MLY	B	198	2	-	0/8/9/11	-
2	MLY	B	80	2	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	171	MLY	CG-CD-CE-NZ
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	218	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	MLY	1	0
2	B	154	MLY	2	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	3,1	11,11,12	0.23	0	15,15,17	0.67	0
3	XYS	C	2	3	9,9,10	0.21	0	10,12,14	0.45	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	3,1	-	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.

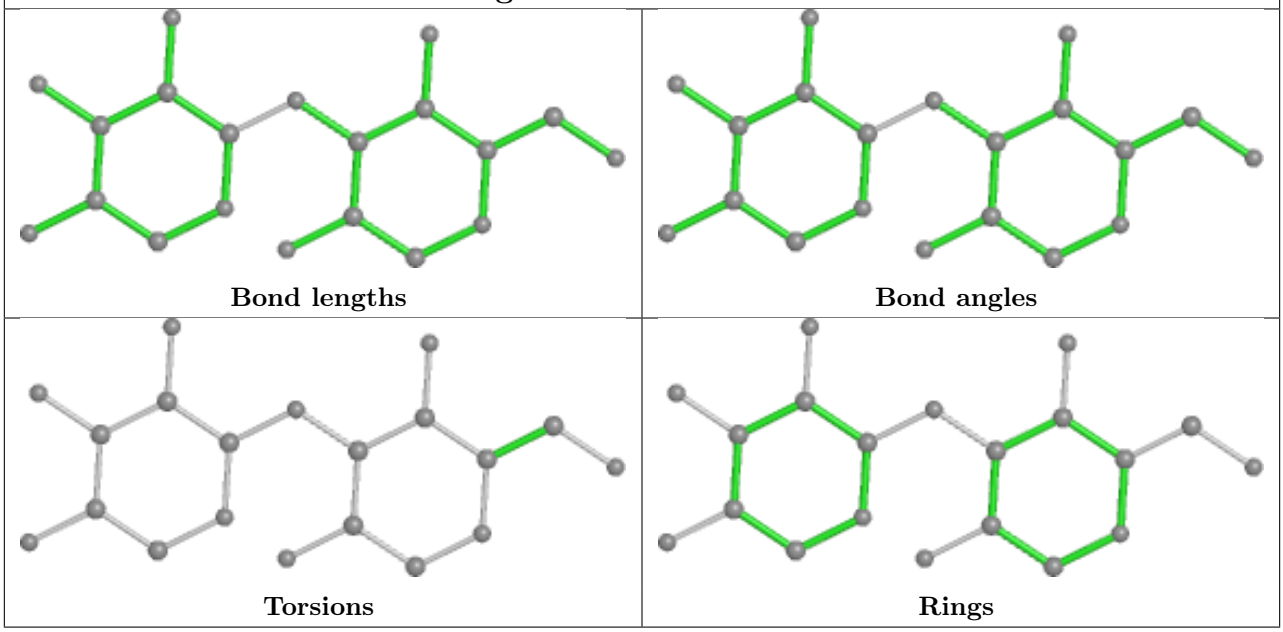
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	XYS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



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	$\#\|Z\| > 2$
7	NAG	B	401	2	14,14,15	0.54	0	17,19,21	0.46	0
5	FUC	A	610	1	10,10,11	0.53	0	14,14,16	0.94	1 (7%)
5	FUC	A	604	1	10,10,11	0.53	0	14,14,16	0.95	1 (7%)
8	MES	B	403	-	12,12,12	0.96	1 (8%)	14,16,16	1.17	1 (7%)
6	BGC	A	606	1	11,11,12	0.23	0	15,15,17	0.68	0
5	FUC	B	402	2	10,10,11	0.53	0	14,14,16	0.97	1 (7%)
6	BGC	A	605	1	11,11,12	0.24	0	15,15,17	0.68	0
7	NAG	A	607	1	14,14,15	0.31	0	17,19,21	0.48	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
7	NAG	B	401	2	-	4/6/23/26	0/1/1/1
5	FUC	A	610	1	-	-	0/1/1/1
5	FUC	A	604	1	-	-	0/1/1/1
8	MES	B	403	-	-	0/6/14/14	0/1/1/1
6	BGC	A	606	1	-	0/2/19/22	0/1/1/1
5	FUC	B	402	2	-	-	0/1/1/1
6	BGC	A	605	1	-	0/2/19/22	0/1/1/1
7	NAG	A	607	1	-	2/6/23/26	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	3.02	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	402	FUC	C1-O5-C5	-2.27	107.62	112.78
5	A	604	FUC	C1-O5-C5	-2.22	107.74	112.78
8	B	403	MES	O3S-S-C8	2.22	109.36	105.77
5	A	610	FUC	C1-O5-C5	-2.18	107.83	112.78

There are no chirality outliers.

All (6) 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	C1-C2-N2-C7
7	B	401	NAG	C4-C5-C6-O6
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
7	B	401	NAG	1	0
5	A	610	FUC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	FUC	1	0
8	B	403	MES	5	0
6	A	606	BGC	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.76	21 (10%) 5 5	60, 102, 160, 176	0
2	B	299/318 (94%)	0.67	23 (7%) 13 13	50, 83, 135, 189	0
All	All	493/523 (94%)	0.70	44 (8%) 9 9	50, 91, 149, 189	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	PRO	10.7
1	A	318	GLY	9.4
2	B	335	ALA	8.8
2	B	63	ASP	6.4
1	A	304	ASN	6.1
2	B	176	ILE	5.6
1	A	397	ILE	5.1
2	B	62	GLY	5.1
1	A	385	SER	4.8
2	B	64	ARG	4.7
2	B	114	GLY	4.4
2	B	56	GLY	4.3
1	A	309	GLY	4.1
2	B	61	PRO	4.1
1	A	301	LEU	3.7
2	B	326	GLU	3.6
1	A	302	MET	3.5
1	A	310	GLY	3.4
1	A	396	ALA	3.3
2	B	280	TRP	3.1
1	A	375	ALA	3.1
2	B	57	GLY	3.1
2	B	65	LYS	3.0
1	A	342	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	377	ILE	2.9
2	B	325	PRO	2.7
2	B	99	THR	2.7
1	A	319	TYR	2.6
1	A	322	VAL	2.6
2	B	59	ARG	2.5
1	A	395	LYS	2.5
2	B	331	PRO	2.5
1	A	316	HIS	2.4
1	A	300	GLN	2.3
2	B	60	ASN	2.3
1	A	380	PRO	2.3
2	B	111	ALA	2.2
2	B	46	ASN	2.2
2	B	92	CYS	2.2
1	A	334	GLU	2.1
1	A	343	ALA	2.1
2	B	58	ALA	2.1
2	B	98	SER	2.1
2	B	78	CYS	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	0.91	0.25	92,99,123,134	0
2	MLY	B	171	11/12	0.92	0.21	79,86,111,112	0
2	MLY	B	154	11/12	0.92	0.24	75,84,126,127	0
2	MLY	B	76	11/12	0.94	0.30	47,57,68,76	0
2	MLY	B	295	11/12	0.94	0.21	72,91,112,112	0
2	MLY	B	264	11/12	0.95	0.33	74,82,104,115	0
2	MLY	B	198	11/12	0.95	0.23	54,65,92,92	0
2	MLY	B	218	11/12	0.97	0.18	59,67,75,91	0
2	MLY	B	80	11/12	0.97	0.25	51,62,74,76	0

6.3 Carbohydrates (i)

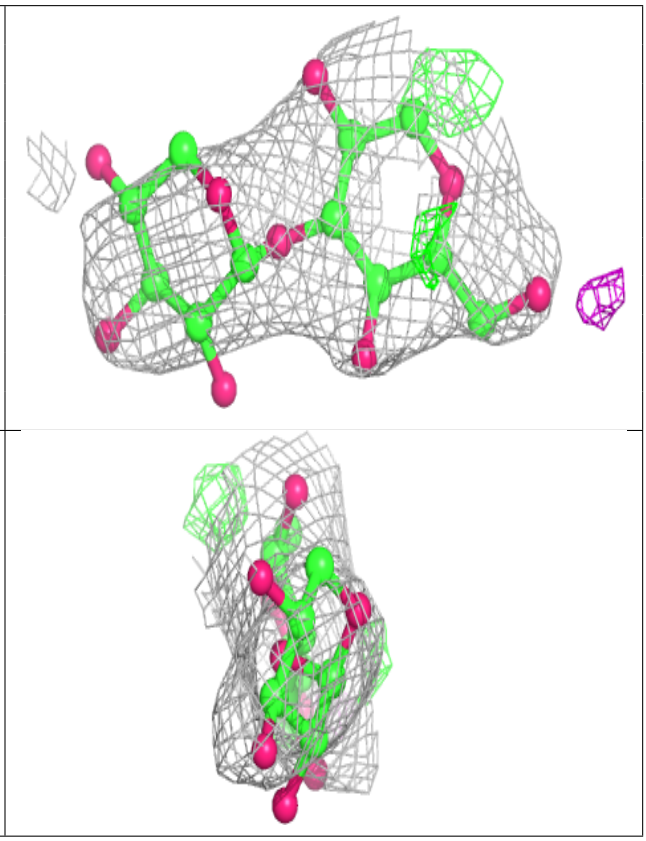
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

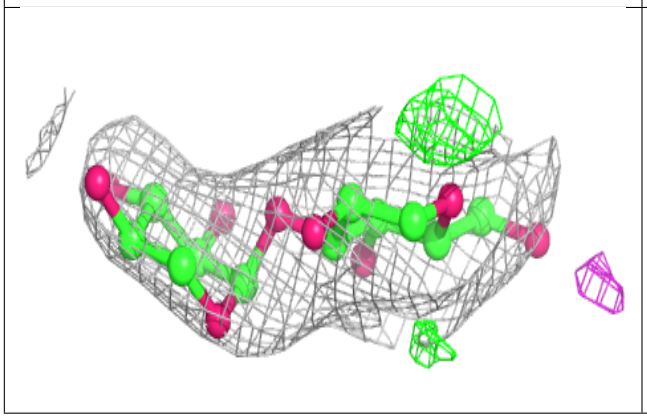
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XYS	C	2	9/10	0.89	0.29	88,96,99,108	9
3	BGC	C	1	11/12	0.94	0.19	73,87,102,104	0

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)





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	0.60	0.21	100,125,179,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BGC	A	606	11/12	0.76	0.32	73,91,105,107	11
7	NAG	B	401	14/15	0.79	0.33	95,126,134,138	0
7	NAG	A	607	14/15	0.85	0.20	92,121,137,137	0
5	FUC	B	402	10/11	0.88	0.19	82,91,103,105	0
6	BGC	A	605	11/12	0.89	0.30	79,104,116,121	11
5	FUC	A	604	10/11	0.94	0.15	75,79,85,86	0
4	CA	A	601	1/1	0.95	0.18	88,88,88,88	1
5	FUC	A	610	10/11	0.95	0.14	54,78,86,96	0
4	CA	A	602	1/1	0.96	0.13	68,68,68,68	1
4	CA	A	603	1/1	0.99	0.12	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.