



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 07:31 AM EDT

PDB ID : 3POY
Title : Crystal Structure of the alpha-Neurexin-1 ectodomain, LNS 2-6
Authors : Miller, M.T.; Mileni, M.; Comoletti, D.; Stevens, R.C.; Harel, M.; Taylor, P.
Deposited on : 2010-11-23
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

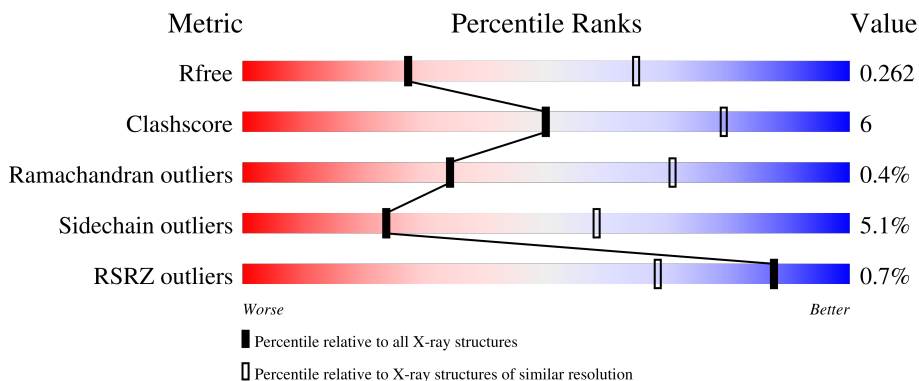
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	1019	 82% 15% ..
2	B	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7878 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1005	7795	4900	1341	1511	43	0	2	0

There are 57 discrepancies between the modelled and reference sequences:

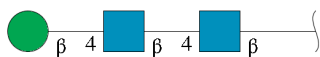
Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	expression tag	UNP Q28146
A	293	ALA	-	expression tag	UNP Q28146
A	294	ALA	-	expression tag	UNP Q28146
A	295	ALA	-	expression tag	UNP Q28146
A	?	-	THR	deletion	UNP Q28146
A	?	-	SER	deletion	UNP Q28146
A	?	-	GLY	deletion	UNP Q28146
A	?	-	ILE	deletion	UNP Q28146
A	?	-	GLY	deletion	UNP Q28146
A	?	-	HIS	deletion	UNP Q28146
A	?	-	ALA	deletion	UNP Q28146
A	?	-	MET	deletion	UNP Q28146
A	?	-	VAL	deletion	UNP Q28146
A	?	-	ASN	deletion	UNP Q28146
A	?	-	LYS	deletion	UNP Q28146
A	?	-	LEU	deletion	UNP Q28146
A	?	-	HIS	deletion	UNP Q28146
A	?	-	CYS	deletion	UNP Q28146
A	?	-	SER	deletion	UNP Q28146
A	628	GLU	GLN	engineered mutation	UNP Q28146
A	1128	PHE	ILE	engineered mutation	UNP Q28146
A	?	-	GLY	deletion	UNP Q28146
A	?	-	ASN	deletion	UNP Q28146
A	?	-	ASN	deletion	UNP Q28146
A	?	-	ASP	deletion	UNP Q28146
A	?	-	ASN	deletion	UNP Q28146
A	?	-	GLU	deletion	UNP Q28146

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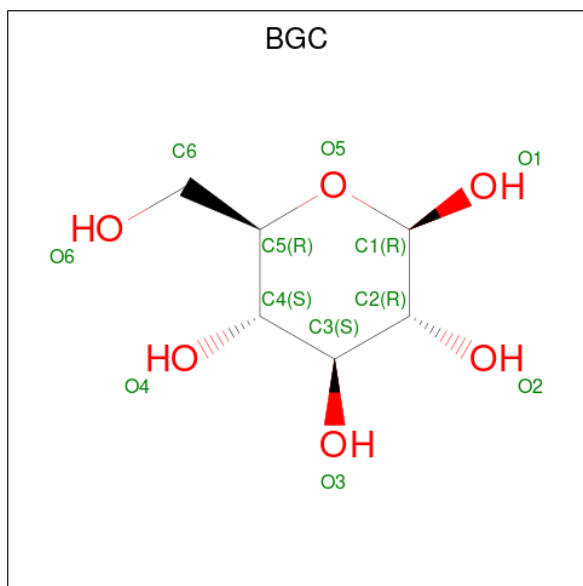
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q28146
A	?	-	LEU	deletion	UNP Q28146
A	?	-	ALA	deletion	UNP Q28146
A	?	-	ILE	deletion	UNP Q28146
A	?	-	ALA	deletion	UNP Q28146
A	?	-	ARG	deletion	UNP Q28146
A	?	-	GLN	deletion	UNP Q28146
A	?	-	ARG	deletion	UNP Q28146
A	?	-	ILE	deletion	UNP Q28146
A	?	-	PRO	deletion	UNP Q28146
A	?	-	TYR	deletion	UNP Q28146
A	?	-	ARG	deletion	UNP Q28146
A	?	-	LEU	deletion	UNP Q28146
A	?	-	GLY	deletion	UNP Q28146
A	?	-	ARG	deletion	UNP Q28146
A	?	-	VAL	deletion	UNP Q28146
A	?	-	VAL	deletion	UNP Q28146
A	?	-	ASP	deletion	UNP Q28146
A	?	-	GLU	deletion	UNP Q28146
A	?	-	TRP	deletion	UNP Q28146
A	?	-	LEU	deletion	UNP Q28146
A	?	-	LEU	deletion	UNP Q28146
A	?	-	ASP	deletion	UNP Q28146
A	?	-	LYS	deletion	UNP Q28146
A	1350	LEU	-	expression tag	UNP Q28146
A	1351	GLU	-	expression tag	UNP Q28146
A	1352	VAL	-	expression tag	UNP Q28146
A	1353	LEU	-	expression tag	UNP Q28146
A	1354	PHE	-	expression tag	UNP Q28146
A	1355	GLN	-	expression tag	UNP Q28146

- Molecule 2 is an oligosaccharide called 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	
			Total	C	N				O
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



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

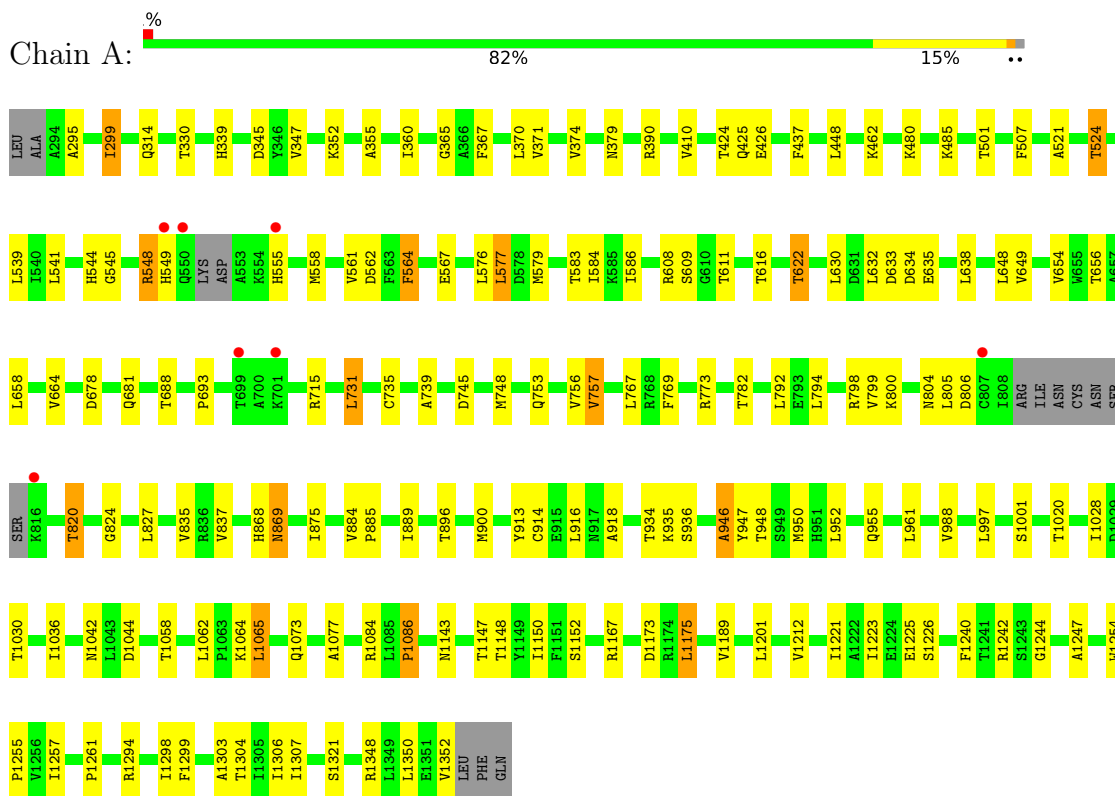
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total	0	0
			O		
			33	33	

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: Neurexin-1-alpha



- Molecule 2: 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.74Å 61.24Å 155.58Å 90.00° 121.21° 90.00°	Depositor
Resolution (Å)	38.56 – 3.02 38.56 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.56-3.02) 98.2 (38.56-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.269 0.216 , 0.262	Depositor DCC
R_{free} test set	1586 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7878	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: NAG, BGC, BMA

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	0.53	0/7955	0.68	3/10769 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	CYS	CA-CB-SG	-5.49	104.13	114.00
1	A	426	GLU	N-CA-CB	5.22	120.00	110.60
1	A	1028	ILE	CB-CA-C	-5.13	101.34	111.60

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	7795	0	7628	90	0
2	B	39	0	34	1	0
3	A	11	0	10	0	0
4	A	33	0	0	0	0
All	All	7878	0	7672	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:THR:HG23	1:A:1321:SER:HB3	1.67	0.76
1:A:352:LYS:HE2	1:A:616:THR:HG23	1.71	0.73
1:A:948:THR:HG22	1:A:1020:THR:CG2	2.19	0.72
1:A:579:MET:HE3	1:A:608:ARG:HA	1.74	0.70
1:A:948:THR:HG22	1:A:1020:THR:HG22	1.74	0.70
1:A:875:ILE:HD12	1:A:884:VAL:HG13	1.78	0.65
1:A:1244:GLY:HA3	2:B:1:NAG:H82	1.78	0.64
1:A:946:ALA:CB	1:A:947:TYR:HA	2.27	0.64
1:A:745:ASP:OD1	1:A:748:MET:HG3	2.01	0.60
1:A:352:LYS:CE	1:A:616:THR:HG23	2.32	0.59
1:A:577:LEU:CD2	1:A:579:MET:HE2	2.31	0.59
1:A:792:LEU:HD21	1:A:837:VAL:CG2	2.32	0.59
1:A:548:ARG:H	1:A:548:ARG:HD3	1.69	0.58
1:A:539:LEU:HD13	1:A:656:THR:OG1	2.04	0.58
1:A:792:LEU:HD21	1:A:837:VAL:HG21	1.86	0.57
1:A:1084:ARG:O	1:A:1086:PRO:HD3	2.05	0.56
1:A:1225:GLU:OE2	1:A:1257:ILE:HD11	2.05	0.55
1:A:634:ASP:OD2	1:A:635:GLU:HG2	2.06	0.54
1:A:1306:ILE:HD12	1:A:1306:ILE:N	2.23	0.54
1:A:753:GLN:HA	1:A:869:ASN:HB3	1.88	0.54
1:A:767:LEU:HD12	1:A:767:LEU:C	2.29	0.54
1:A:884:VAL:HG12	1:A:885:PRO:O	2.09	0.53
1:A:1167:ARG:HD3	1:A:1303:ALA:HA	1.90	0.53
1:A:567:GLU:HB2	1:A:656:THR:HG21	1.92	0.52
1:A:1304:THR:OG1	1:A:1306:ILE:HD11	2.08	0.52
1:A:544:HIS:CD2	1:A:649:VAL:HG12	2.45	0.52
1:A:1058:THR:HG22	1:A:1062:LEU:HD21	1.91	0.51
1:A:584:ILE:HD13	1:A:622:THR:O	2.10	0.51
1:A:355:ALA:HB1	1:A:371:VAL:O	2.10	0.51
1:A:1221:ILE:HD13	1:A:1261:PRO:HG3	1.93	0.51
1:A:630:LEU:CD2	1:A:632:LEU:HD13	2.41	0.51
1:A:946:ALA:HB3	1:A:947:TYR:HA	1.92	0.50
1:A:630:LEU:HD23	1:A:632:LEU:HD13	1.93	0.50
1:A:800:LYS:HE2	1:A:820:THR:HG21	1.92	0.50
1:A:1212:VAL:HG11	1:A:1240:PHE:CE1	2.47	0.50
1:A:934:THR:HG22	1:A:935:LYS:N	2.27	0.50
1:A:299:ILE:HG23	1:A:462:LYS:HB3	1.94	0.49
1:A:314:GLN:HB2	1:A:485:LYS:NZ	2.27	0.49
1:A:609:SER:OG	1:A:622:THR:HG23	2.12	0.49
1:A:804:ASN:O	1:A:805:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ARG:HG3	1:A:410:VAL:HG22	1.94	0.47
1:A:955:GLN:HG3	1:A:1077:ALA:HB3	1.96	0.47
1:A:583:THR:HG22	1:A:584:ILE:N	2.29	0.47
1:A:792:LEU:HD22	1:A:835:VAL:HG11	1.97	0.47
1:A:1148:THR:CG2	1:A:1321:SER:HB3	2.41	0.47
1:A:1175:LEU:O	1:A:1175:LEU:HD23	2.15	0.47
1:A:1150:ILE:HD11	1:A:1350:LEU:HD12	1.97	0.47
1:A:896:THR:HA	1:A:900:MET:O	2.15	0.46
1:A:521:ALA:HB1	1:A:524:THR:O	2.16	0.46
1:A:757:VAL:HG22	1:A:868:HIS:CE1	2.51	0.46
1:A:1201:LEU:HD11	1:A:1240:PHE:CE2	2.50	0.46
1:A:1212:VAL:HG11	1:A:1240:PHE:CD1	2.51	0.45
1:A:1254:TRP:HB3	1:A:1255:PRO:HD2	1.98	0.45
1:A:367:PHE:HB2	1:A:424:THR:HG22	1.99	0.45
1:A:564:PHE:HB2	1:A:577:LEU:HD12	1.99	0.45
1:A:1298:ILE:N	1:A:1298:ILE:HD12	2.31	0.44
1:A:946:ALA:CB	1:A:947:TYR:CA	2.95	0.44
1:A:347:VAL:HG13	1:A:360:ILE:HG12	1.99	0.44
1:A:295:ALA:H	1:A:480:LYS:NZ	2.15	0.44
1:A:330:THR:O	1:A:379:ASN:HA	2.17	0.43
1:A:731:LEU:HD23	1:A:739:ALA:HB2	1.99	0.43
1:A:782:THR:OG1	1:A:869:ASN:ND2	2.52	0.43
1:A:1189:VAL:HG22	1:A:1307:ILE:HG13	2.01	0.43
1:A:950:MET:HE3	1:A:952:LEU:HG	2.01	0.43
1:A:507:PHE:O	1:A:664:VAL:HA	2.19	0.42
1:A:630:LEU:CD2	1:A:632:LEU:CD1	2.97	0.42
1:A:541:LEU:HD21	1:A:638:LEU:HD13	2.01	0.42
1:A:773:ARG:HD2	1:A:889:ILE:HD12	2.01	0.42
1:A:545:GLY:N	1:A:562:ASP:O	2.51	0.42
1:A:1173:ASP:OD2	1:A:1242:ARG:NE	2.51	0.42
1:A:1064:LYS:O	1:A:1065:LEU:HB2	2.20	0.42
1:A:916:LEU:HD13	1:A:918:ALA:O	2.20	0.42
1:A:1223:ILE:HD11	1:A:1247:ALA:HB3	2.02	0.42
1:A:365:GLY:HA3	1:A:425:GLN:HB2	2.02	0.41
1:A:753:GLN:O	1:A:913:TYR:HB2	2.21	0.41
1:A:988:VAL:HG22	1:A:997:LEU:HD13	2.03	0.41
1:A:769:PHE:CE1	1:A:794:LEU:HD21	2.55	0.41
1:A:544:HIS:CD2	1:A:649:VAL:CG1	3.04	0.41
1:A:314:GLN:HB2	1:A:485:LYS:HZ2	1.86	0.41
1:A:339:HIS:CD2	1:A:448:LEU:HD13	2.55	0.41
1:A:544:HIS:CE1	1:A:648:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HD3	1:A:548:ARG:N	2.34	0.41
1:A:576:LEU:HD22	1:A:654:VAL:HG22	2.03	0.41
1:A:798:ARG:HG2	1:A:824:GLY:O	2.21	0.41
1:A:934:THR:HG21	1:A:936:SER:OG	2.21	0.41
1:A:1064:LYS:O	1:A:1065:LEU:CB	2.68	0.41
1:A:678:ASP:O	1:A:681:GLN:HB3	2.21	0.41
1:A:731:LEU:CD2	1:A:739:ALA:HB2	2.51	0.41
1:A:630:LEU:HD21	1:A:632:LEU:HD11	2.03	0.40
1:A:799:VAL:HG23	1:A:827:LEU:CD1	2.51	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	1001/1019 (98%)	929 (93%)	68 (7%)	4 (0%)	34 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	ALA
1	A	1065	LEU
1	A	693	PRO
1	A	757	VAL

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	859/870 (99%)	815 (95%)	44 (5%)	24	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ILE
1	A	345	ASP
1	A	370	LEU
1	A	374	VAL
1	A	437	PHE
1	A	501	THR
1	A	524	THR
1	A	548	ARG
1	A	549	HIS
1	A	555	HIS
1	A	558	MET
1	A	561	VAL
1	A	564	PHE
1	A	577	LEU
1	A	586	ILE
1	A	611	THR
1	A	622	THR
1	A	633	ASP
1	A	658	LEU
1	A	688	THR
1	A	715	ARG
1	A	731	LEU
1	A	756	VAL
1	A	806	ASP
1	A	820	THR
1	A	869	ASN
1	A	914	CYS
1	A	961	LEU
1	A	1001	SER
1	A	1030	THR
1	A	1036	ILE
1	A	1042	ASN
1	A	1044	ASP
1	A	1073	GLN
1	A	1086	PRO
1	A	1143	ASN

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Mol	Chain	Res	Type
1	A	1147	THR
1	A	1152	SER
1	A	1175	LEU
1	A	1226	SER
1	A	1294	ARG
1	A	1299	PHE
1	A	1348	ARG
1	A	1352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	456	ASN
1	A	469	ASN
1	A	544	HIS
1	A	660	ASN
1	A	719	ASN
1	A	772	GLN
1	A	869	ASN
1	A	891	HIS
1	A	908	ASN
1	A	924	ASN
1	A	955	GLN
1	A	996	ASN
1	A	1013	ASN
1	A	1035	GLN
1	A	1143	ASN
1	A	1300	ASN
1	A	1302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates i

3 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	0.88	0	17,19,21	1.14	1 (5%)
2	NAG	B	2	2	14,14,15	1.65	5 (35%)	17,19,21	1.23	2 (11%)
2	BMA	B	3	2	11,11,12	1.71	3 (27%)	15,15,17	1.58	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	O5-C1	4.22	1.50	1.43
2	B	2	NAG	O4-C4	3.20	1.50	1.43
2	B	3	BMA	O5-C5	2.58	1.48	1.43
2	B	2	NAG	C8-C7	2.45	1.55	1.50
2	B	3	BMA	C1-C2	2.18	1.57	1.52
2	B	2	NAG	C1-C2	2.10	1.55	1.52
2	B	2	NAG	O5-C5	2.07	1.47	1.43
2	B	2	NAG	C4-C5	2.00	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	O5-C5-C6	4.04	113.54	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C5-C6	-3.01	102.49	107.20
2	B	3	BMA	O5-C1-C2	2.55	114.70	110.77
2	B	3	BMA	C1-C2-C3	2.18	112.35	109.67
2	B	2	NAG	O5-C5-C6	2.11	110.51	107.20
2	B	2	NAG	C4-C3-C2	2.06	114.03	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

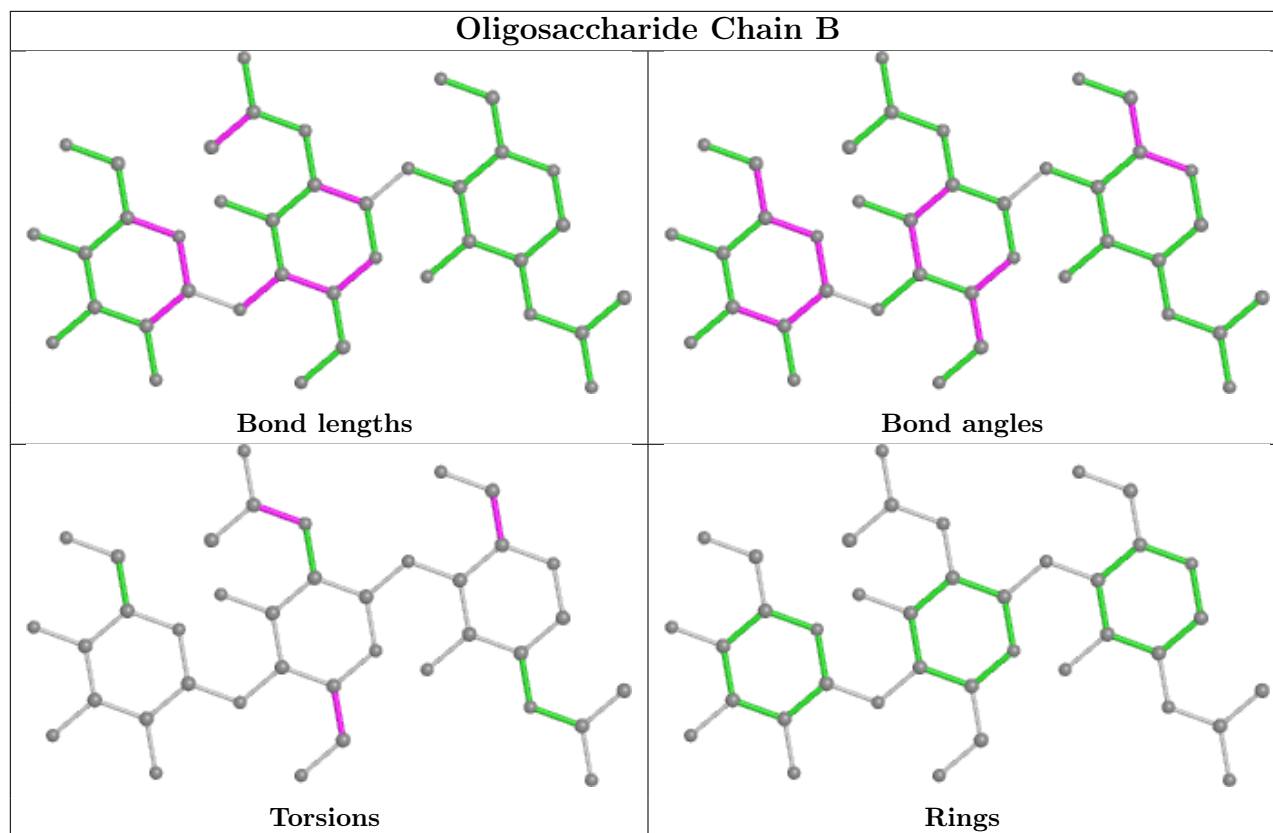
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	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 [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	BGC	A	2000	1	11,11,12	1.88	3 (27%)	15,15,17	2.59	8 (53%)

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	A	2000	1	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	BGC	O5-C1	3.53	1.49	1.43
3	A	2000	BGC	O5-C5	3.18	1.49	1.43
3	A	2000	BGC	C6-C5	2.48	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	BGC	O5-C5-C6	4.28	113.91	107.20
3	A	2000	BGC	C6-C5-C4	-3.85	103.98	113.00
3	A	2000	BGC	O2-C2-C3	-3.85	102.43	110.14
3	A	2000	BGC	C2-C3-C4	3.40	116.77	110.89
3	A	2000	BGC	O5-C1-C2	3.30	115.86	110.77
3	A	2000	BGC	C3-C4-C5	2.85	115.32	110.24
3	A	2000	BGC	C1-C2-C3	2.83	113.14	109.67
3	A	2000	BGC	C1-O5-C5	2.71	115.86	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	BGC	C4-C5-C6-O6
3	A	2000	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	1005/1019 (98%)	-0.43	7 (0%) 87 68	23, 47, 71, 104	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	THR	5.2
1	A	555	HIS	3.7
1	A	816	LYS	3.3
1	A	549	HIS	2.7
1	A	550	GLN	2.2
1	A	807	CYS	2.2
1	A	701	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

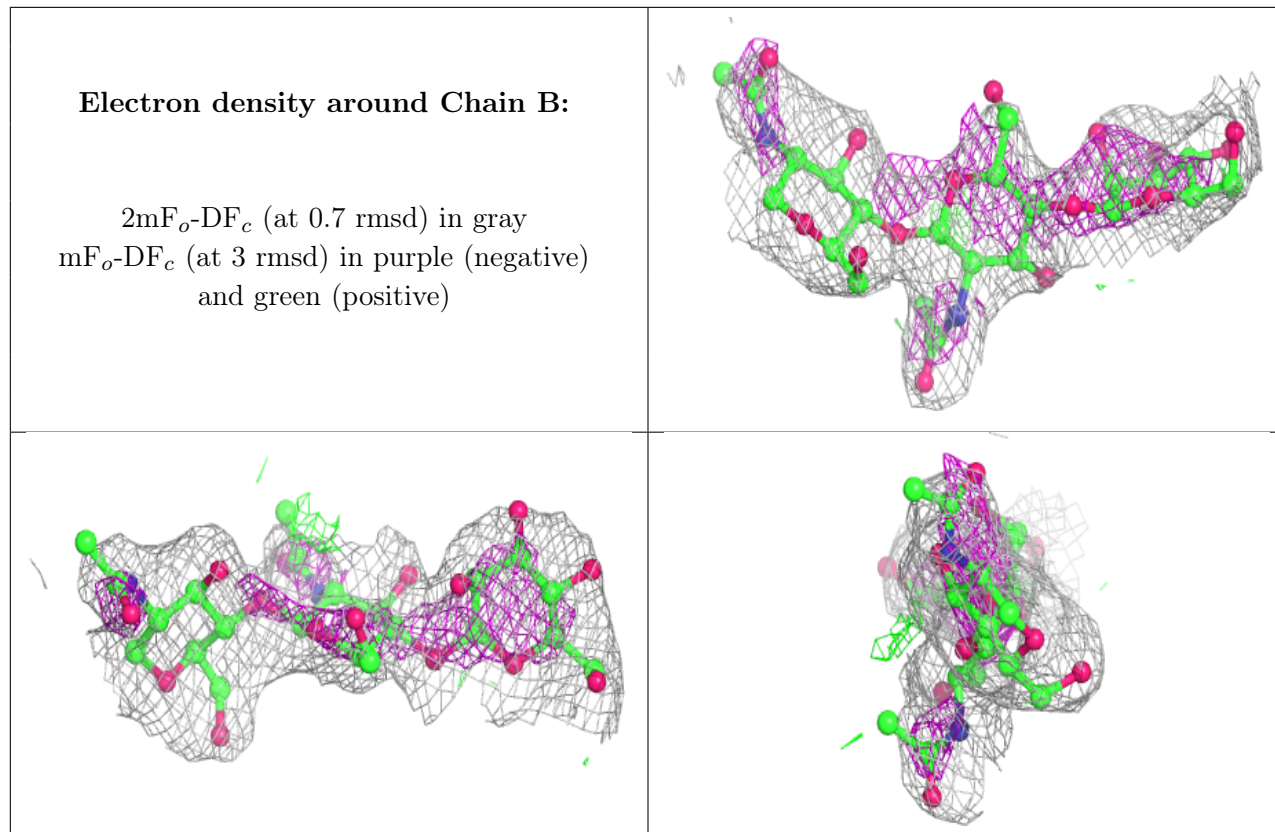
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	B	2	14/15	0.82	0.47	49,49,50,50	0
2	BMA	B	3	11/12	0.82	0.49	48,49,49,49	0
2	NAG	B	1	14/15	0.92	0.31	46,47,47,48	0

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
3	BGC	A	2000	11/12	0.85	0.38	45,45,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.