



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:27 AM UTC

PDB ID : 4DUR / pdb_00004dur
Title : The X-ray Crystal Structure of Full-Length type II Human Plasminogen
Authors : Law, R.H.P.; Caradoc-Davies, T.; Whisstock, J.C.
Deposited on : 2012-02-22
Resolution : 2.45 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

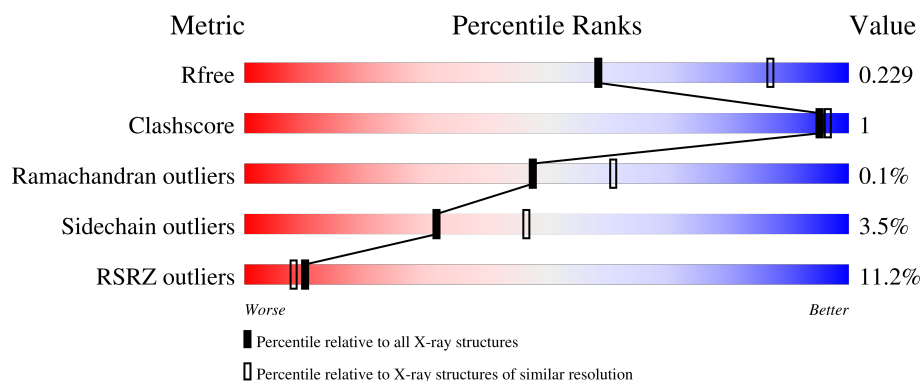
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	791	8% 88% 8% .
1	B	791	13% 90% 6% 5%
2	C	3	100%
2	D	3	100%

2 Entry composition [i](#)

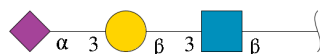
There are 7 unique types of molecules in this entry. The entry contains 13246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasminogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	4	0
			5894	3667	1042	1126	59			
1	B	754	Total	C	N	O	S	0	1	0
			5805	3623	1026	1099	57			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			45	25	2	18			
2	D	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	3	Total	Cl	0	0
			3	3		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

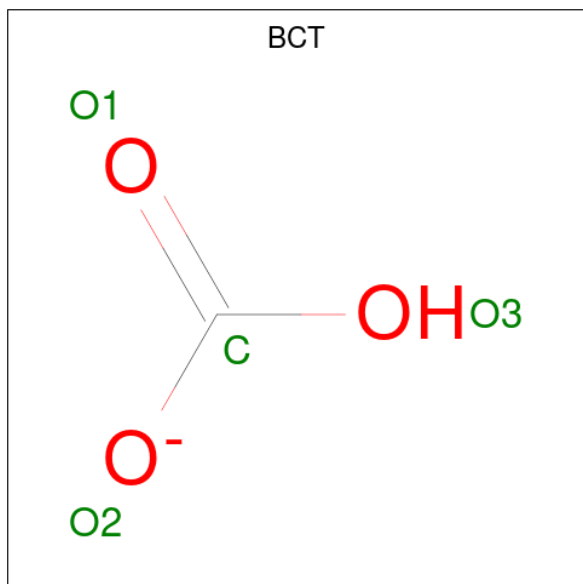
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

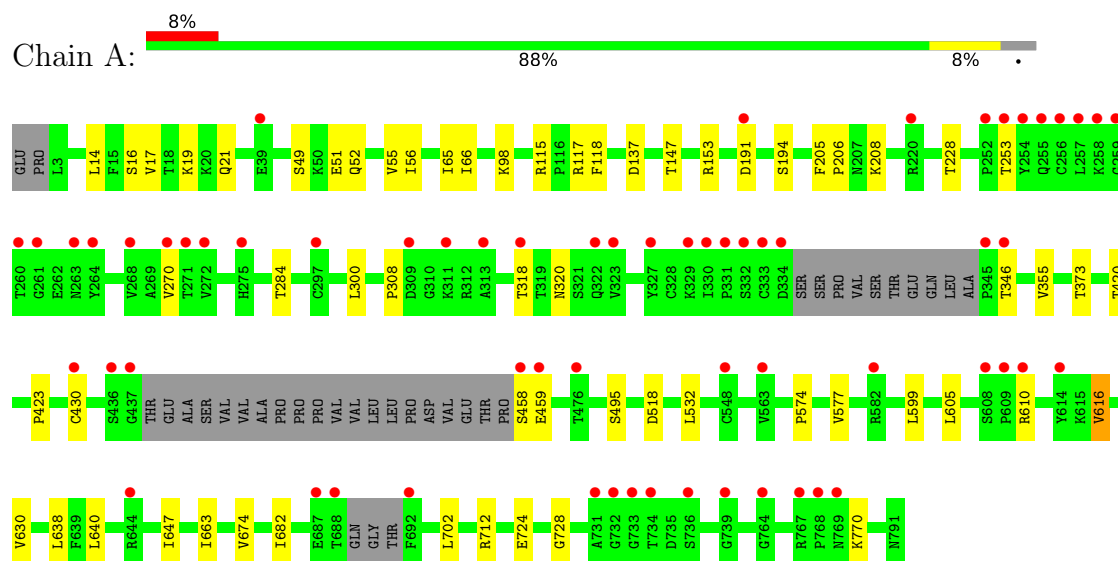
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	735	Total	O	0	0
			735	735		
7	B	701	Total	O	0	0
			701	701		

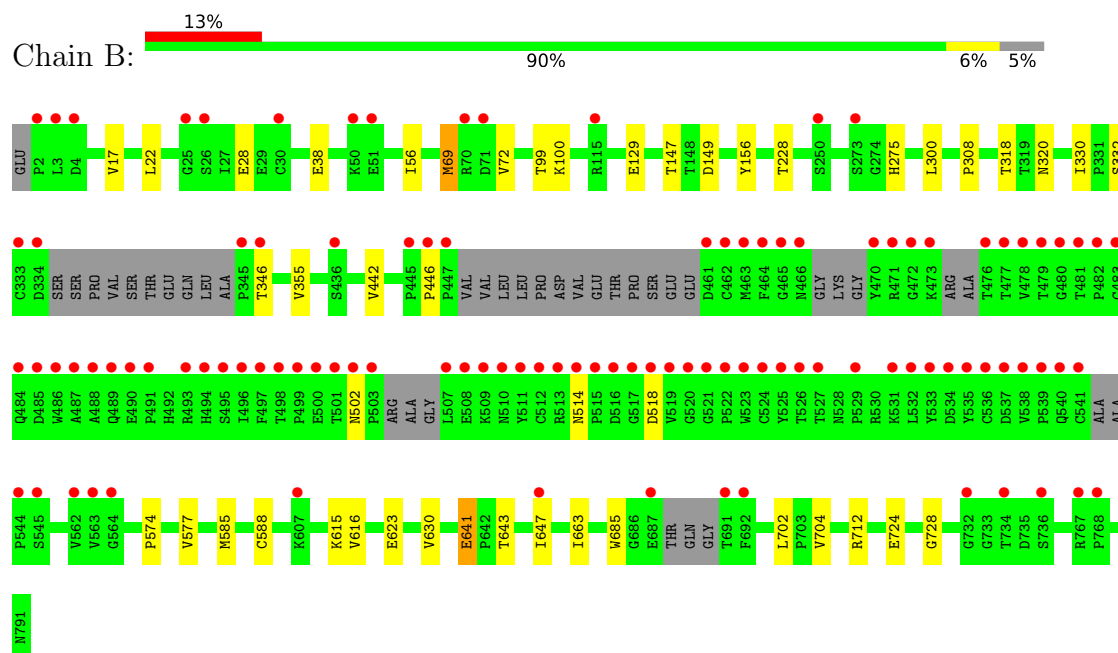
3 Residue-property plots [i](#)

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: Plasminogen



• Molecule 1: Plasminogen



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

NAG1
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

NAG1
GAL2
SIA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.62Å 144.62Å 233.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	125.25 – 2.45 125.25 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (125.25-2.45) 99.8 (125.25-2.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.215 0.200 , 0.229	Depositor DCC
R_{free} test set	5236 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13246	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA, ACT, BCT, K, GAL, CL

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	0.67	0/6069	1.12	6/8253 (0.1%)
1	B	0.68	0/5975	1.13	7/8133 (0.1%)
All	All	0.68	0/12044	1.13	13/16386 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	PRO	N-CA-C	8.34	120.88	110.70
1	A	17	VAL	N-CA-C	-6.05	105.92	111.67
1	A	117	ARG	N-CA-C	-5.92	106.21	113.50
1	B	643	THR	N-CA-C	5.83	117.32	110.97
1	B	17	VAL	N-CA-C	-5.62	106.73	111.56
1	B	355	VAL	N-CA-C	-5.22	98.47	109.34
1	B	99	THR	CA-C-N	5.21	127.26	120.28
1	B	99	THR	C-N-CA	5.21	127.26	120.28
1	A	518	ASP	CA-C-N	5.17	127.54	120.46
1	A	518	ASP	C-N-CA	5.17	127.54	120.46
1	A	49	SER	N-CA-C	5.09	116.83	111.28
1	A	355	VAL	N-CA-C	-5.05	99.23	106.55
1	B	149	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5894	0	5504	16	0
1	B	5805	0	5367	12	0
2	C	45	0	38	0	0
2	D	45	0	38	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	1	0	0
5	B	4	0	1	0	0
6	A	4	0	3	0	0
7	A	735	0	0	0	0
7	B	701	0	0	0	0
All	All	13246	0	10952	27	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 1.

All (27) 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:B:318:THR:HG22	1:B:320:ASN:H	1.62	0.64
1:B:100:LYS:HE2	1:B:156:TYR:HB2	1.88	0.56
1:B:702:LEU:HD22	1:B:728:GLY:HA2	1.87	0.56
1:A:638[A]:LEU:HD12	1:B:442:VAL:HG22	1.88	0.55
1:A:52:GLN:HE22	1:A:495:SER:HB2	1.74	0.53
1:A:300:LEU:HD21	1:A:308:PRO:HG3	1.94	0.50
1:A:373:THR:HA	1:A:430:CYS:HA	1.95	0.48
1:A:21:GLN:HG3	1:A:55:VAL:HG22	1.96	0.48
1:A:206:PRO:HB2	1:A:423:PRO:HD2	1.96	0.48
1:A:16:SER:HB3	1:A:19:LYS:HD3	1.95	0.47
1:A:51:GLU:HG3	1:A:532:LEU:HD13	1.97	0.47
1:A:318:THR:HG22	1:A:320:ASN:H	1.80	0.46
1:A:574:PRO:HB2	1:A:663:ILE:H	1.79	0.46
1:B:275:HIS:HB3	1:B:318:THR:HG23	1.98	0.46
1:A:702:LEU:HD22	1:A:728:GLY:HA2	1.98	0.45
1:A:115:ARG:O	1:A:153:ARG:NH2	2.49	0.45
1:B:69:MET:HB3	1:B:72:VAL:HG11	1.99	0.45
1:B:300:LEU:HD21	1:B:308:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:GLU:HG2	1:B:647:ILE:HG22	1.97	0.44
1:B:623:GLU:HB2	1:B:685:TRP:CD1	2.52	0.44
1:A:118:PHE:CZ	1:A:137:ASP:HB3	2.53	0.44
1:B:574:PRO:HB2	1:B:663:ILE:H	1.84	0.43
1:A:599:LEU:HD21	1:A:647:ILE:HD11	2.01	0.43
1:B:514:ASN:HD21	1:B:518:ASP:H	1.67	0.42
1:A:205:PHE:HB3	1:A:208:LYS:HG3	2.01	0.42
1:A:577:VAL:HG13	1:A:616:VAL:HG13	2.03	0.41
1:B:577:VAL:HG13	1:B:616:VAL:HG13	2.03	0.41

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	752/791 (95%)	727 (97%)	25 (3%)	0	100	100
1	B	739/791 (93%)	709 (96%)	28 (4%)	2 (0%)	36	45
All	All	1491/1582 (94%)	1436 (96%)	53 (4%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	ASN
1	B	38	GLU

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	647/694 (93%)	620 (96%)	27 (4%)	26	39
1	B	628/694 (90%)	610 (97%)	18 (3%)	37	52
All	All	1275/1388 (92%)	1230 (96%)	45 (4%)	32	46

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	56	ILE
1	A	65	ILE
1	A	66	ILE
1	A	98	LYS
1	A	147	THR
1	A	191[A]	ASP
1	A	191[B]	ASP
1	A	194	SER
1	A	228	THR
1	A	253	THR
1	A	270	VAL
1	A	284	THR
1	A	346	THR
1	A	420	THR
1	A	458	SER
1	A	459	GLU
1	A	605	LEU
1	A	610	ARG
1	A	616	VAL
1	A	630	VAL
1	A	640	LEU
1	A	674	VAL
1	A	682	ILE
1	A	712	ARG
1	A	724	GLU
1	A	770	LYS
1	B	22	LEU
1	B	28	GLU
1	B	56	ILE
1	B	69	MET
1	B	129	GLU
1	B	147	THR

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Mol	Chain	Res	Type
1	B	228	THR
1	B	330	ILE
1	B	332	SER
1	B	346	THR
1	B	585	MET
1	B	588	CYS
1	B	615	LYS
1	B	630	VAL
1	B	641	GLU
1	B	704	VAL
1	B	712	ARG
1	B	724	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	173	ASN
1	A	209	ASN
1	A	263	ASN
1	A	360	HIS
1	A	396	ASN
1	A	502	ASN
1	A	552	GLN
1	A	671	ASN
1	A	717	ASN
1	A	738	GLN
1	B	48	HIS
1	B	52	GLN
1	B	207	ASN
1	B	364	GLN
1	B	514	ASN
1	B	528	ASN
1	B	552	GLN
1	B	603	HIS
1	B	622	GLN
1	B	671	ASN
1	B	701	GLN
1	B	769	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	C	1	2,1	14,14,15	2.03	5 (35%)	17,19,21	1.61	4 (23%)
2	GAL	C	2	2	11,11,12	1.86	3 (27%)	15,15,17	2.58	4 (26%)
2	SIA	C	3	2	20,20,21	2.69	8 (40%)	21,28,31	1.52	3 (14%)
2	NAG	D	1	2,1	14,14,15	1.96	5 (35%)	17,19,21	1.63	4 (23%)
2	GAL	D	2	2	11,11,12	1.96	4 (36%)	15,15,17	1.90	5 (33%)
2	SIA	D	3	2	20,20,21	2.75	7 (35%)	21,28,31	1.37	2 (9%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	SIA	C	3	2	-	3/18/34/38	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	6/18/34/38	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C4-C5	5.97	1.58	1.53
2	C	3	SIA	C2-C1	5.87	1.59	1.52
2	D	3	SIA	C2-C1	5.73	1.59	1.52
2	C	1	NAG	C1-C2	5.62	1.60	1.52
2	C	3	SIA	C4-C5	5.27	1.57	1.53
2	D	1	NAG	C1-C2	5.11	1.59	1.52
2	D	3	SIA	C7-C6	5.09	1.59	1.52
2	C	3	SIA	C7-C6	4.82	1.58	1.52
2	D	2	GAL	C2-C3	4.06	1.58	1.52
2	C	2	GAL	C2-C3	3.76	1.58	1.52
2	D	3	SIA	C6-C5	3.63	1.58	1.53
2	C	3	SIA	C8-C7	3.55	1.59	1.53
2	D	3	SIA	C8-C7	3.50	1.59	1.53
2	C	3	SIA	C6-C5	3.26	1.58	1.53
2	C	3	SIA	C3-C2	3.15	1.57	1.52
2	D	2	GAL	C1-C2	2.98	1.59	1.52
2	C	2	GAL	C1-C2	2.97	1.59	1.52
2	D	3	SIA	C3-C2	2.73	1.56	1.52
2	C	3	SIA	C10-N5	2.58	1.42	1.34
2	D	1	NAG	C4-C5	2.55	1.58	1.53
2	D	1	NAG	C3-C2	2.52	1.57	1.52
2	C	1	NAG	C4-C5	2.47	1.58	1.53
2	D	3	SIA	C10-N5	2.42	1.42	1.34
2	C	1	NAG	C4-C3	2.39	1.58	1.52
2	D	2	GAL	C4-C3	2.39	1.58	1.52
2	C	1	NAG	C3-C2	2.35	1.57	1.52
2	D	1	NAG	C4-C3	2.23	1.58	1.52
2	D	1	NAG	C7-N2	2.16	1.41	1.34
2	D	2	GAL	C4-C5	2.13	1.57	1.53
2	C	2	GAL	C4-C3	2.10	1.57	1.52
2	C	1	NAG	C7-N2	2.08	1.41	1.34
2	C	3	SIA	C3-C4	2.00	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GAL	C3-C4-C5	-5.24	100.73	110.23
2	C	2	GAL	O3-C3-C2	5.10	120.47	110.05
2	C	2	GAL	C1-C2-C3	-4.33	103.34	109.64
2	C	2	GAL	C1-O5-C5	4.04	117.60	112.19
2	D	2	GAL	O3-C3-C2	4.01	118.24	110.05
2	D	2	GAL	C3-C4-C5	-3.92	103.12	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.81	117.29	112.19
2	C	1	NAG	C1-O5-C5	3.56	116.95	112.19
2	D	1	NAG	C3-C4-C5	-3.42	104.03	110.23
2	C	3	SIA	O6-C2-C3	3.18	114.83	110.56
2	C	3	SIA	O9-C9-C8	-3.10	104.65	111.16
2	C	1	NAG	C3-C4-C5	-2.94	104.91	110.23
2	D	3	SIA	O9-C9-C8	-2.90	105.07	111.16
2	C	3	SIA	O1B-C1-O1A	-2.77	117.78	124.08
2	D	2	GAL	C1-C2-C3	-2.70	105.71	109.64
2	C	1	NAG	O3-C3-C4	2.60	116.50	110.38
2	D	2	GAL	C1-O5-C5	2.53	115.57	112.19
2	C	1	NAG	O3-C3-C2	2.49	114.58	109.40
2	D	3	SIA	O1B-C1-O1A	-2.43	118.56	124.08
2	D	1	NAG	O3-C3-C4	2.41	116.06	110.38
2	D	2	GAL	O2-C2-C3	-2.06	105.88	110.15
2	D	1	NAG	O4-C4-C3	-2.03	105.59	110.38

There are no chirality outliers.

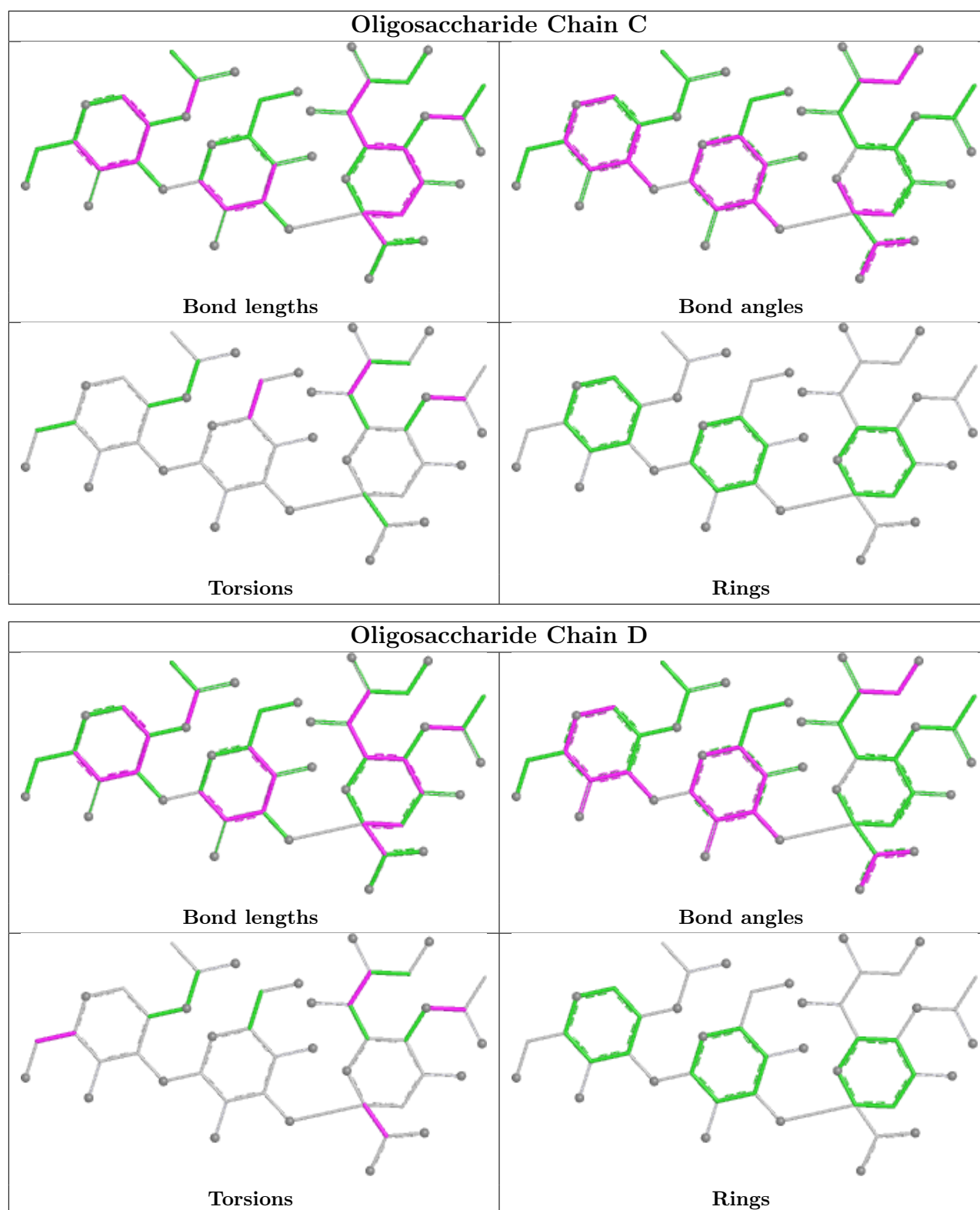
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	SIA	C6-C7-C8-O8
2	C	3	SIA	C11-C10-N5-C5
2	C	3	SIA	O10-C10-N5-C5
2	D	3	SIA	C11-C10-N5-C5
2	D	3	SIA	O10-C10-N5-C5
2	D	3	SIA	C6-C7-C8-C9
2	C	2	GAL	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	SIA	O7-C7-C8-O8
2	D	3	SIA	O1A-C1-C2-O6
2	C	3	SIA	C6-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
5	BCT	B	805	-	3,3,3	0.71	0	2,3,3	3.43	1 (50%)
6	ACT	A	807	-	3,3,3	1.10	0	3,3,3	0.89	0
5	BCT	A	806	-	3,3,3	0.71	0	2,3,3	3.36	1 (50%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805	BCT	O2-C-O1	4.53	131.26	119.68
5	A	806	BCT	O2-C-O1	4.42	130.99	119.68

There are no chirality outliers.

There are no torsion outliers.

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

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	756/791 (95%)	0.33	63 (8%) 17 15	12, 28, 57, 99	4 (0%)
1	B	754/791 (95%)	0.57	106 (14%) 6 5	12, 27, 99, 123	1 (0%)
All	All	1510/1582 (95%)	0.45	169 (11%) 10 8	12, 28, 75, 123	5 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASP	8.1
1	B	478	VAL	7.7
1	B	473	LYS	7.2
1	B	687	GLU	7.0
1	B	470	TYR	6.9
1	B	466	ASN	6.9
1	A	688	THR	6.8
1	B	479	THR	6.7
1	B	520	GLY	6.6
1	B	477	THR	6.5
1	B	537	ASP	6.5
1	A	437	GLY	6.4
1	B	496	ILE	6.1
1	B	476	THR	6.1
1	B	507	LEU	5.9
1	B	519	VAL	5.9
1	B	540	GLN	5.9
1	B	481	THR	5.9
1	B	503	PRO	5.7
1	B	527	THR	5.7
1	B	539	PRO	5.6
1	B	447	PRO	5.6
1	B	541	CYS	5.5
1	A	609	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	461	ASP	5.5
1	B	538	VAL	5.4
1	B	691	THR	5.3
1	B	563	VAL	5.2
1	B	510	ASN	5.1
1	B	480	GLY	5.0
1	A	345	PRO	4.9
1	B	500	GLU	4.8
1	B	482	PRO	4.8
1	B	534	ASP	4.8
1	B	512	CYS	4.7
1	B	502	ASN	4.7
1	B	522	PRO	4.6
1	B	497	PHE	4.6
1	B	501	THR	4.6
1	B	511	TYR	4.5
1	B	463	MET	4.5
1	B	509	LYS	4.5
1	B	536	CYS	4.4
1	B	508	GLU	4.4
1	B	2	PRO	4.4
1	B	464	PHE	4.4
1	B	513	ARG	4.3
1	B	532	LEU	4.3
1	B	535	TYR	4.3
1	A	330	ILE	4.1
1	B	471	ARG	4.1
1	B	495	SER	3.9
1	B	525	TYR	3.9
1	A	333	CYS	3.9
1	A	767	ARG	3.8
1	B	521	GLY	3.7
1	B	487	ALA	3.7
1	B	533	TYR	3.7
1	B	517	GLY	3.6
1	B	734	THR	3.6
1	A	687	GLU	3.6
1	B	768	PRO	3.6
1	B	345	PRO	3.5
1	B	516	ASP	3.5
1	A	257	LEU	3.5
1	B	493	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	563	VAL	3.4
1	B	472	GLY	3.4
1	A	430	CYS	3.4
1	B	490	GLU	3.4
1	B	499	PRO	3.4
1	A	692	PHE	3.3
1	B	51	GLU	3.3
1	B	446	PRO	3.3
1	A	258	LYS	3.3
1	A	329	LYS	3.2
1	A	644	ARG	3.2
1	A	768	PRO	3.2
1	B	445	PRO	3.2
1	B	531	LYS	3.2
1	A	268	VAL	3.2
1	A	734	THR	3.2
1	A	253	THR	3.1
1	B	514	ASN	3.1
1	B	523	TRP	3.1
1	B	465	GLY	3.1
1	B	485	ASP	3.0
1	B	498	THR	3.0
1	A	614	TYR	3.0
1	A	733	GLY	2.9
1	A	256	CYS	2.9
1	B	70	ARG	2.9
1	A	331	PRO	2.9
1	B	484	GLN	2.9
1	A	259	GLY	2.9
1	B	529	PRO	2.8
1	B	518	ASP	2.8
1	A	436	SER	2.8
1	B	736	SER	2.8
1	B	544	PRO	2.8
1	B	767	ARG	2.8
1	B	526	THR	2.8
1	A	732	GLY	2.8
1	A	608	SER	2.8
1	B	489	GLN	2.8
1	A	264	TYR	2.7
1	A	731	ALA	2.7
1	A	322	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	483	CYS	2.7
1	A	252	PRO	2.7
1	A	255	GLN	2.7
1	B	564	GLY	2.7
1	A	254	TYR	2.7
1	B	25	GLY	2.6
1	B	524	CYS	2.6
1	A	769	ASN	2.6
1	B	545	SER	2.6
1	A	271	THR	2.6
1	A	476	THR	2.6
1	B	250	SER	2.6
1	A	458	SER	2.5
1	B	333	CYS	2.5
1	A	739	GLY	2.5
1	B	647	ILE	2.5
1	B	692	PHE	2.5
1	A	323	VAL	2.5
1	A	459	GLU	2.5
1	B	50	LYS	2.5
1	B	462	CYS	2.5
1	B	515	PRO	2.5
1	A	39	GLU	2.5
1	A	327	TYR	2.4
1	B	486	TRP	2.4
1	A	346	THR	2.4
1	A	313	ALA	2.4
1	A	332	SER	2.4
1	B	491	PRO	2.4
1	A	610	ARG	2.4
1	B	488	ALA	2.4
1	A	736	SER	2.3
1	B	436	SER	2.3
1	B	3	LEU	2.3
1	B	334	ASP	2.3
1	B	562	VAL	2.3
1	A	191[A]	ASP	2.3
1	A	275	HIS	2.3
1	B	494	HIS	2.2
1	A	270	VAL	2.2
1	A	318	THR	2.2
1	A	764	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	115	ARG	2.2
1	A	272	VAL	2.2
1	B	26	SER	2.2
1	A	220	ARG	2.1
1	A	297	CYS	2.1
1	B	30	CYS	2.1
1	A	311	LYS	2.1
1	A	260	THR	2.1
1	B	346	THR	2.1
1	B	273	SER	2.1
1	A	263	ASN	2.1
1	A	261	GLY	2.0
1	B	607	LYS	2.0
1	B	71	ASP	2.0
1	A	548	CYS	2.0
1	A	582	ARG	2.0
1	B	732	GLY	2.0
1	A	309	ASP	2.0
1	B	4	ASP	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](#)

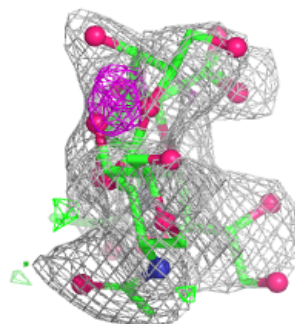
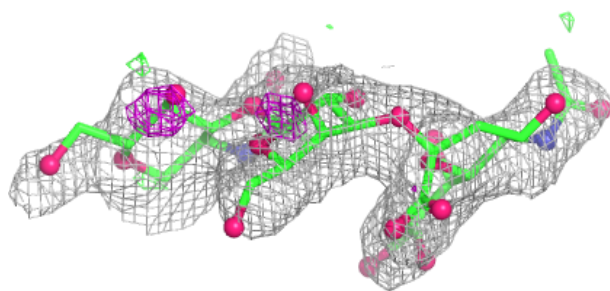
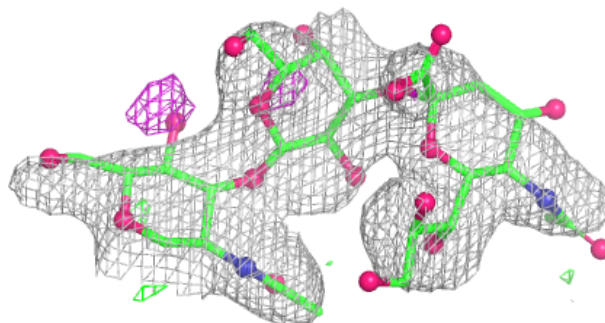
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	D	2	11/12	0.66	0.19	83,85,86,88	0
2	GAL	C	2	11/12	0.72	0.17	81,83,84,87	0
2	NAG	D	1	14/15	0.76	0.21	76,78,79,82	0
2	SIA	C	3	20/21	0.76	0.19	87,89,90,90	0
2	SIA	D	3	20/21	0.77	0.21	88,89,89,89	0
2	NAG	C	1	14/15	0.78	0.20	71,73,76,79	0

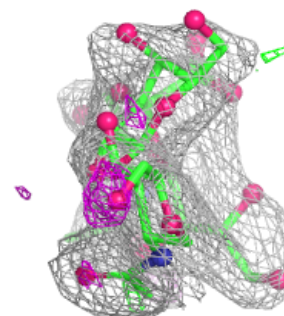
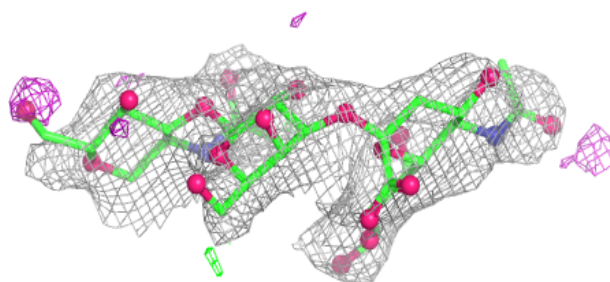
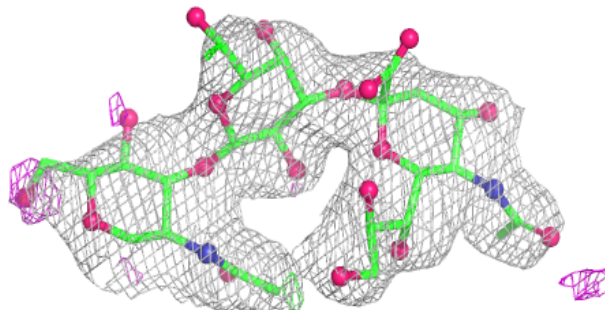
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

**Electron density around Chain D:**

$2mF_o-DF_c$ (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
5	BCT	A	806	4/4	0.81	0.20	66,66,67,67	0
5	BCT	B	805	4/4	0.81	0.26	79,80,80,80	0
6	ACT	A	807	4/4	0.96	0.09	34,35,35,36	0
4	K	A	805	1/1	0.98	0.07	42,42,42,42	0
4	K	B	804	1/1	0.98	0.07	36,36,36,36	0
3	CL	A	802	1/1	0.98	0.09	35,35,35,35	0
3	CL	A	803	1/1	0.98	0.03	26,26,26,26	0
3	CL	B	803	1/1	0.98	0.06	28,28,28,28	0
3	CL	B	801	1/1	0.99	0.03	24,24,24,24	0
3	CL	B	802	1/1	0.99	0.02	25,25,25,25	0
3	CL	A	801	1/1	0.99	0.04	25,25,25,25	0
3	CL	A	804	1/1	0.99	0.06	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.