



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:42 PM UTC

PDB ID : 4CSY / pdb_00004csy
Title : E-selectin lectin, EGF-like and two SCR domains complexed with Sialyl Lewis X
Authors : Preston, R.C.; Jakob, R.P.; Binder, F.P.C.; Sager, C.P.; Ernst, B.; Maier, T.
Deposited on : 2014-03-11
Resolution : 2.41 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

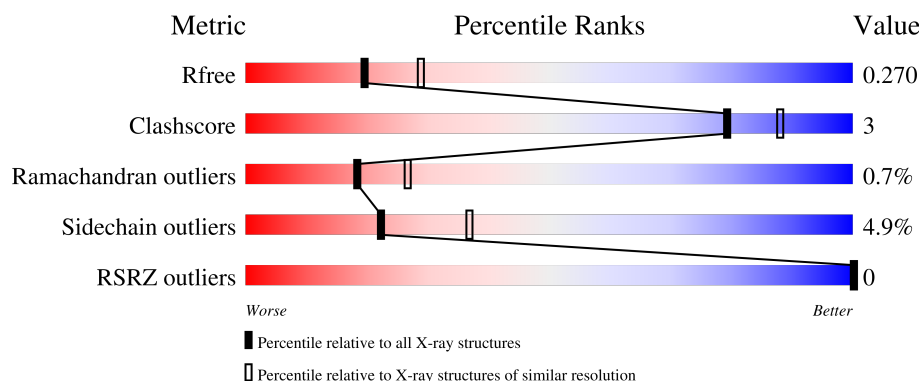
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	280	88% 10% .
1	B	280	88% 11% .
2	C	4	100%
2	D	4	100%

2 Entry composition [i](#)

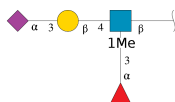
There are 5 unique types of molecules in this entry. The entry contains 4821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 E-SELECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	3	0
			2199	1361	363	447	28			
1	B	280	Total	C	N	O	S	0	1	0
			2183	1352	361	442	28			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			57	32	2	23			
2	D	4	Total	C	N	O	0	0	0
			57	32	2	23			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

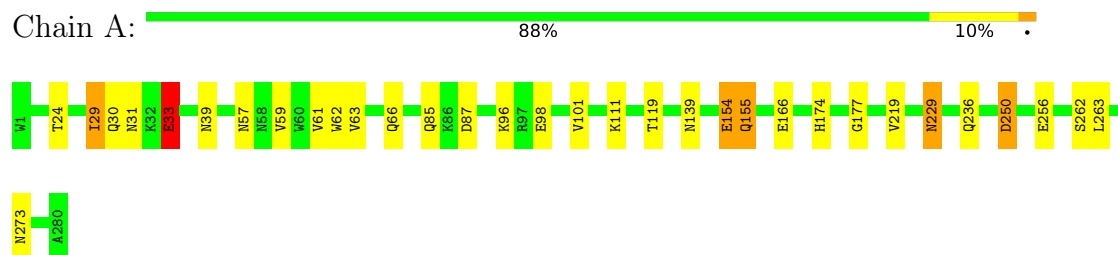
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	66	Total 66	O 66	0	0

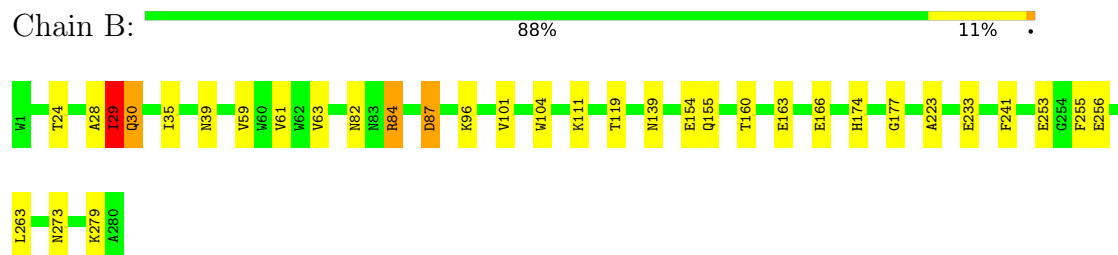
3 Residue-property plots

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: E-SELECTIN



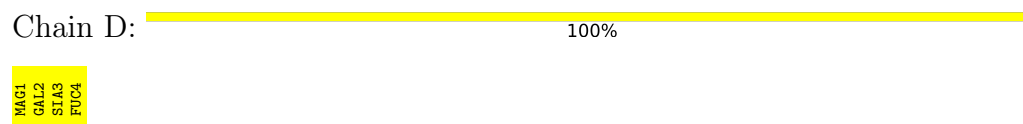
- Molecule 1: E-SELECTIN



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.29Å 58.67Å 58.87Å 76.03° 86.28° 86.31°	Depositor
Resolution (Å)	28.32 – 2.41 28.32 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (28.32-2.41) 95.8 (28.32-2.41)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.215 , 0.253 0.230 , 0.270	Depositor DCC
R_{free} test set	1298 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.440 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4821	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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: SIA, NAG, GAL, MAG, CA, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	1/2257 (0.0%)	1.23	9/3071 (0.3%)
1	B	0.84	0/2241	1.19	6/3049 (0.2%)
All	All	0.85	1/4498 (0.0%)	1.21	15/6120 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	VAL	CA-C	5.88	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ASP	CA-CB-CG	8.22	120.82	112.60
1	A	250	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	229	ASN	CA-CB-CG	7.53	120.13	112.60
1	A	87	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	63	VAL	N-CA-C	6.79	116.94	110.42
1	A	154	GLU	CB-CG-CD	6.56	123.75	112.60
1	B	63	VAL	N-CA-C	5.67	116.32	110.36
1	B	155	GLN	N-CA-C	5.54	117.76	108.73
1	A	98	GLU	CB-CG-CD	5.49	121.94	112.60
1	B	163	GLU	CB-CG-CD	5.42	121.81	112.60
1	B	84	ARG	N-CA-C	5.31	117.06	111.28
1	A	33	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	155	GLN	N-CA-C	5.29	117.15	108.52
1	A	57	ASN	CA-CB-CG	5.15	117.75	112.60
1	B	233	GLU	CB-CG-CD	5.04	121.16	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	2199	0	2009	12	0
1	B	2183	0	1998	14	0
2	C	57	0	49	0	0
2	D	57	0	49	0	0
3	A	98	0	91	1	0
3	B	98	0	91	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	61	0	0	1	0
5	B	66	0	0	0	0
All	All	4821	0	4287	24	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 3.

All (24) 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:30:GLN:HG2	1:A:62:TRP:HH2	1.46	0.81
1:A:39:ASN:HD21	1:A:96:LYS:H	1.29	0.80
1:B:39:ASN:HD21	1:B:96:LYS:H	1.29	0.79
1:A:31:ASN:OD1	1:A:33:GLU:HG2	1.87	0.73
1:B:255:PHE:HD1	1:B:279:LYS:O	1.73	0.71
1:A:263:LEU:HD22	1:A:273:ASN:HB2	1.75	0.67
1:B:263:LEU:HD22	1:B:273:ASN:HB2	1.75	0.67
1:A:154:GLU:HG3	1:B:160:THR:CG2	2.26	0.65
1:A:24:THR:HG22	1:A:119:THR:HB	1.81	0.62
1:A:30:GLN:HG2	1:A:62:TRP:CH2	2.34	0.59
1:B:24:THR:HG22	1:B:119:THR:HB	1.85	0.58
1:B:30:GLN:HG2	1:B:104:TRP:HZ2	1.68	0.57
1:B:255:PHE:CD1	1:B:279:LYS:O	2.56	0.55
1:A:154:GLU:HG3	1:B:160:THR:HG21	1.92	0.51
1:A:154:GLU:HG2	1:A:155:GLN:HG3	1.93	0.49
1:B:28:ALA:O	1:B:29:ILE:O	2.33	0.47
1:B:223:ALA:HA	1:B:241:PHE:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:HIS:HB3	1:B:177:GLY:O	2.17	0.44
1:A:174:HIS:HB3	1:A:177:GLY:O	2.17	0.43
1:B:82:ASN:CG	1:B:84:ARG:HG2	2.44	0.43
1:A:236:GLN:HB2	5:A:2048:HOH:O	2.19	0.42
1:B:28:ALA:O	1:B:29:ILE:C	2.62	0.42
1:B:30:GLN:HE21	1:B:35:ILE:HD11	1.83	0.42
1:A:155:GLN:HB3	3:A:283:NAG:H83	2.04	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	281/280 (100%)	269 (96%)	10 (4%)	2 (1%)	18	27
1	B	279/280 (100%)	268 (96%)	9 (3%)	2 (1%)	18	27
All	All	560/560 (100%)	537 (96%)	19 (3%)	4 (1%)	18	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	A	139	ASN
1	B	139	ASN
1	A	29	ILE

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	250/247 (101%)	237 (95%)	13 (5%)	21	34
1	B	248/247 (100%)	237 (96%)	11 (4%)	25	41
All	All	498/494 (101%)	474 (95%)	24 (5%)	22	38

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	33	GLU
1	A	59	VAL
1	A	61	VAL
1	A	66	GLN
1	A	85	GLN
1	A	101	VAL
1	A	111	LYS
1	A	166	GLU
1	A	229	ASN
1	A	250	ASP
1	A	256	GLU
1	A	262	SER
1	B	29	ILE
1	B	30	GLN
1	B	59	VAL
1	B	61	VAL
1	B	87	ASP
1	B	101	VAL
1	B	111	LYS
1	B	154	GLU
1	B	166	GLU
1	B	253	GLU
1	B	256	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	30	GLN
1	A	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	HIS
1	A	229	ASN
1	A	236	GLN
1	A	237	ASN
1	B	25	HIS
1	B	30	GLN
1	B	39	ASN
1	B	58	ASN
1	B	167	HIS
1	B	229	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 ⓘ

8 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	MAG	C	1	2	16,16,16	1.91	5 (31%)	22,22,22	1.42	5 (22%)
2	GAL	C	2	2	11,11,12	1.42	1 (9%)	15,15,17	0.89	0
2	SIA	C	3	2	20,20,21	2.25	7 (35%)	21,28,31	1.23	4 (19%)
2	FUC	C	4	4,2	10,10,11	1.21	1 (10%)	14,14,16	0.69	0
2	MAG	D	1	2	16,16,16	1.85	4 (25%)	22,22,22	1.47	5 (22%)
2	GAL	D	2	2	11,11,12	1.44	1 (9%)	15,15,17	0.85	0
2	SIA	D	3	2	20,20,21	2.20	7 (35%)	21,28,31	1.33	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	D	4	4,2	10,10,11	1.28	1 (10%)	14,14,16	0.74	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	MAG	C	1	2	-	2/8/28/28	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	SIA	C	3	2	-	5/18/34/38	0/1/1/1
2	FUC	C	4	4,2	-	-	0/1/1/1
2	MAG	D	1	2	-	2/8/28/28	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	FUC	D	4	4,2	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	SIA	O6-C6	4.88	1.51	1.44
2	D	3	SIA	O6-C6	4.25	1.50	1.44
2	C	1	MAG	C1-C2	4.06	1.59	1.53
2	C	1	MAG	O1-C1	3.92	1.46	1.40
2	D	1	MAG	C1-C2	3.91	1.59	1.53
2	D	1	MAG	O1-C1	3.89	1.46	1.40
2	D	3	SIA	C6-C5	3.83	1.59	1.53
2	D	3	SIA	O6-C2	3.82	1.50	1.43
2	C	3	SIA	C3-C2	3.72	1.58	1.52
2	C	3	SIA	O6-C2	3.60	1.50	1.43
2	D	3	SIA	C3-C2	3.53	1.58	1.52
2	C	3	SIA	C7-C6	3.20	1.56	1.52
2	C	3	SIA	C6-C5	3.18	1.58	1.53
2	C	2	GAL	C2-C3	3.16	1.57	1.52
2	D	2	GAL	C2-C3	3.14	1.57	1.52
2	D	3	SIA	C7-C6	3.09	1.56	1.52
2	C	3	SIA	C2-C1	2.74	1.55	1.52
2	C	3	SIA	C11-C10	2.73	1.56	1.50
2	C	1	MAG	O5-C1	2.44	1.48	1.41
2	C	1	MAG	C3-C2	2.43	1.57	1.53
2	D	1	MAG	O5-C1	2.43	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C2-C1	2.40	1.55	1.52
2	D	1	MAG	C3-C2	2.25	1.57	1.53
2	C	4	FUC	O5-C1	2.17	1.47	1.43
2	D	3	SIA	C4-C5	2.10	1.55	1.53
2	D	4	FUC	O5-C1	2.08	1.47	1.43
2	C	1	MAG	C4-C5	2.02	1.57	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SIA	O10-C10-N5	3.24	127.71	121.98
2	C	3	SIA	C11-C10-N5	3.06	121.19	116.12
2	D	3	SIA	C11-C10-N5	-2.67	111.68	116.12
2	D	1	MAG	O5-C1-C2	2.61	115.52	110.59
2	D	1	MAG	C4-C3-C2	2.55	114.12	110.40
2	C	1	MAG	C4-C3-C2	2.50	114.05	110.40
2	C	3	SIA	C5-N5-C10	2.48	128.91	123.11
2	C	1	MAG	O5-C1-C2	2.45	115.22	110.59
2	D	1	MAG	C3-C2-N2	-2.41	106.18	110.62
2	C	1	MAG	CM-O1-C1	2.39	116.90	113.26
2	D	1	MAG	CM-O1-C1	2.29	116.74	113.26
2	D	3	SIA	O1A-C1-C2	-2.22	118.05	122.85
2	D	1	MAG	O7-C7-N2	2.20	125.88	121.98
2	C	1	MAG	C3-C2-N2	-2.19	106.58	110.62
2	C	3	SIA	O1A-C1-C2	-2.15	118.21	122.85
2	C	3	SIA	O10-C10-C11	-2.06	118.38	122.05
2	C	1	MAG	O7-C7-N2	2.06	125.62	121.98
2	D	3	SIA	C5-N5-C10	2.02	127.84	123.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	MAG	C2-C1-O1-CM
2	C	1	MAG	O5-C1-O1-CM
2	D	1	MAG	C2-C1-O1-CM
2	D	1	MAG	O5-C1-O1-CM
2	C	2	GAL	O5-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	3	SIA	C11-C10-N5-C5
2	C	3	SIA	O10-C10-N5-C5
2	C	2	GAL	C4-C5-C6-O6

Continued on next page...

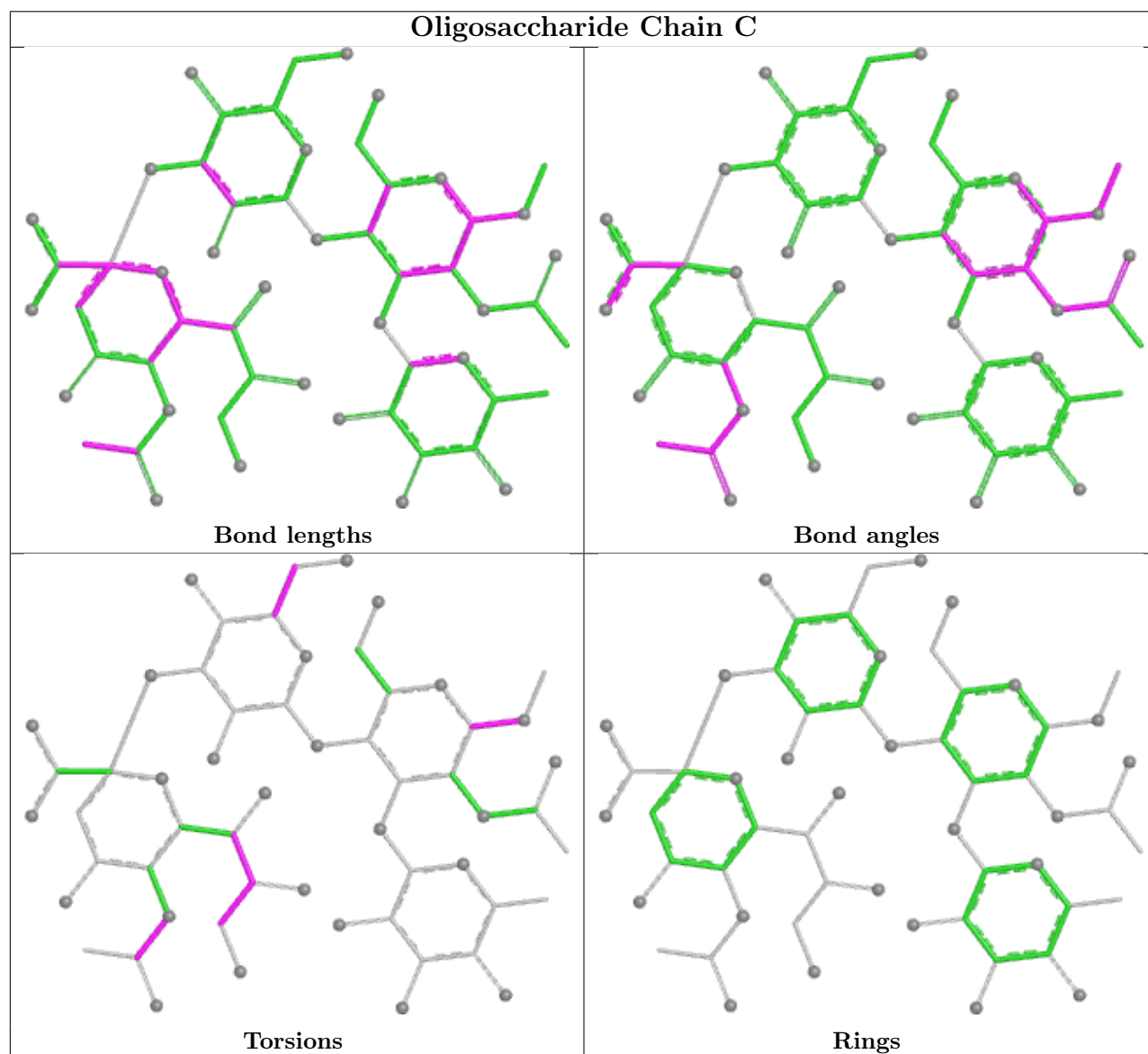
Continued from previous page...

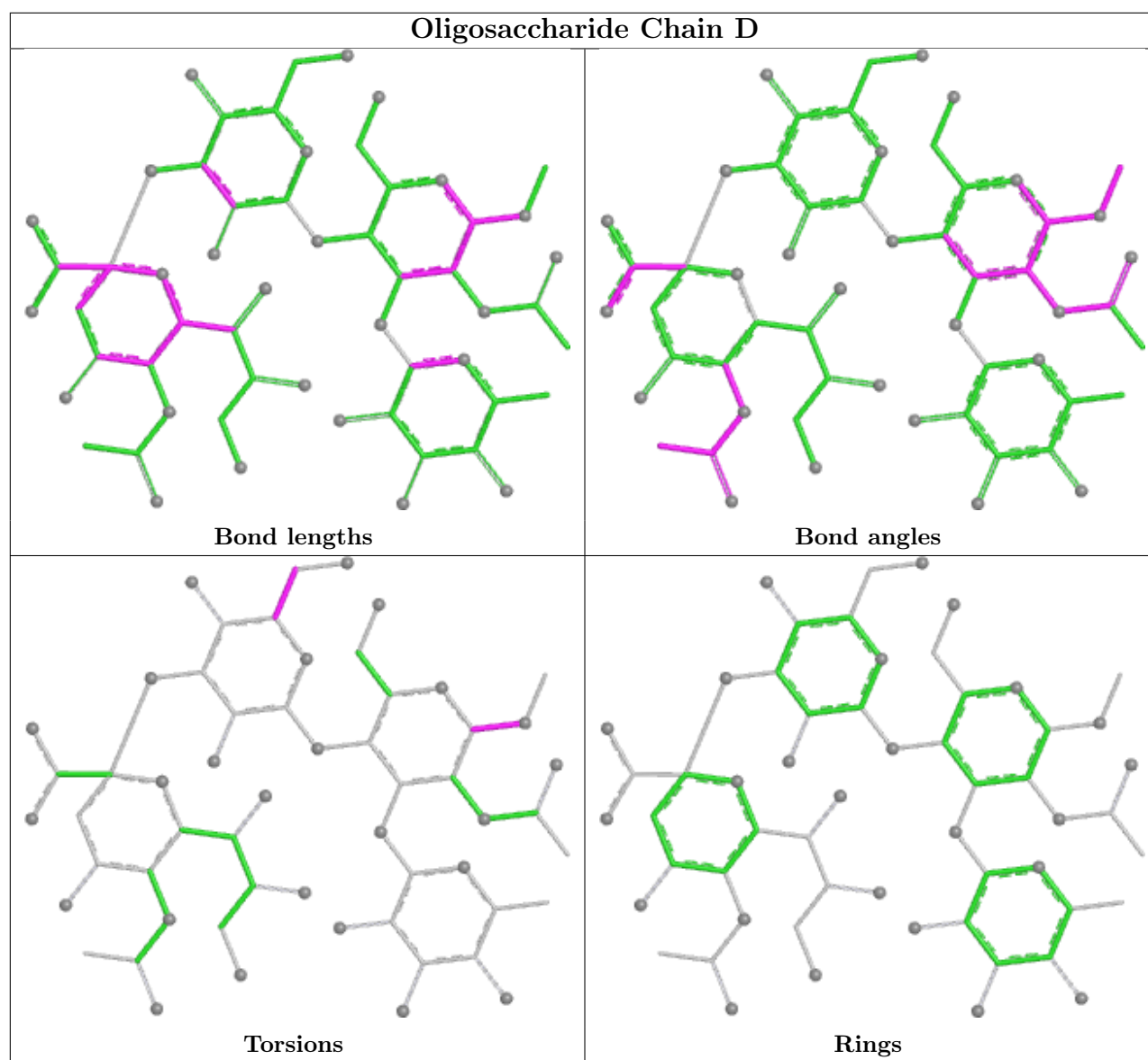
Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	C	3	SIA	C7-C8-C9-O9
2	C	3	SIA	O8-C8-C9-O9
2	C	3	SIA	C6-C7-C8-C9

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
3	NAG	A	287	1	14,14,15	0.27	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	282	1	14,14,15	0.36	0	17,19,21	0.51	0
3	NAG	B	281	1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
3	NAG	A	285	1	14,14,15	0.35	0	17,19,21	1.23	2 (11%)
3	NAG	A	286	1	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	A	283	1	14,14,15	0.38	0	17,19,21	0.81	0
3	NAG	B	285	1	14,14,15	0.37	0	17,19,21	1.22	2 (11%)
3	NAG	A	282	1	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	B	284	1	14,14,15	0.39	0	17,19,21	1.15	2 (11%)
3	NAG	B	287	1	14,14,15	0.29	0	17,19,21	0.49	0
3	NAG	A	284	1	14,14,15	0.35	0	17,19,21	0.97	1 (5%)
3	NAG	B	286	1	14,14,15	0.30	0	17,19,21	2.05	3 (17%)
3	NAG	B	283	1	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	A	281	1	14,14,15	0.26	0	17,19,21	0.89	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	287	1	-	0/6/23/26	0/1/1/1
3	NAG	B	282	1	-	2/6/23/26	0/1/1/1
3	NAG	B	281	1	-	0/6/23/26	0/1/1/1
3	NAG	A	285	1	-	2/6/23/26	0/1/1/1
3	NAG	A	286	1	-	0/6/23/26	0/1/1/1
3	NAG	A	283	1	-	0/6/23/26	0/1/1/1
3	NAG	B	285	1	-	1/6/23/26	0/1/1/1
3	NAG	A	282	1	-	0/6/23/26	0/1/1/1
3	NAG	B	284	1	-	0/6/23/26	0/1/1/1
3	NAG	B	287	1	-	0/6/23/26	0/1/1/1
3	NAG	A	284	1	-	0/6/23/26	0/1/1/1
3	NAG	B	286	1	-	1/6/23/26	0/1/1/1
3	NAG	B	283	1	-	0/6/23/26	0/1/1/1
3	NAG	A	281	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	286	NAG	C1-C2-N2	7.35	122.01	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	285	NAG	C1-C2-N2	4.37	117.32	110.43
3	A	285	NAG	C1-C2-N2	4.37	117.32	110.43
3	B	284	NAG	C1-O5-C5	3.38	116.71	112.19
3	A	281	NAG	C1-O5-C5	3.07	116.31	112.19
3	B	281	NAG	C1-O5-C5	2.85	116.00	112.19
3	B	286	NAG	C2-N2-C7	2.58	126.36	122.90
3	B	286	NAG	O5-C1-C2	-2.49	107.44	111.29
3	A	284	NAG	C1-O5-C5	2.25	115.20	112.19
3	B	285	NAG	C2-N2-C7	2.14	125.77	122.90
3	A	285	NAG	C2-N2-C7	2.08	125.69	122.90
3	B	284	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	285	NAG	C1-C2-N2-C7
3	B	285	NAG	C1-C2-N2-C7
3	B	286	NAG	C1-C2-N2-C7
3	B	282	NAG	C4-C5-C6-O6
3	A	285	NAG	C3-C2-N2-C7
3	B	282	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
3	A	283	NAG	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	280/280 (100%)	-0.69	0 100 100	30, 73, 115, 137	3 (1%)
1	B	280/280 (100%)	-0.70	0 100 100	35, 73, 119, 143	2 (0%)
All	All	560/560 (100%)	-0.70	0 100 100	30, 73, 116, 143	5 (0%)

There are no RSRZ outliers to report.

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](#)

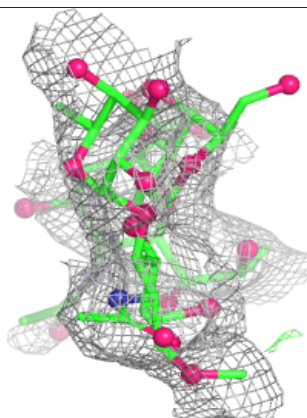
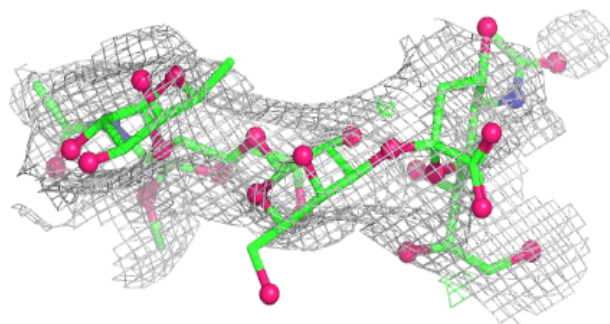
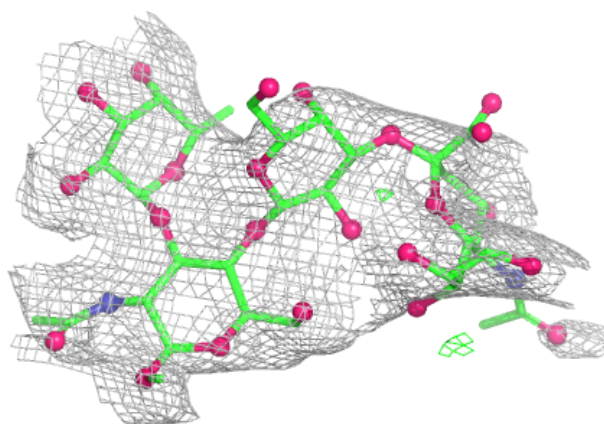
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	MAG	C	1	16/16	0.95	0.05	109,114,127,129	0
2	SIA	C	3	20/21	0.95	0.07	105,124,135,136	0
2	GAL	D	2	11/12	0.95	0.09	103,106,111,113	0
2	MAG	D	1	16/16	0.96	0.07	105,107,121,121	0
2	SIA	D	3	20/21	0.96	0.07	112,122,131,132	0
2	FUC	C	4	10/11	0.98	0.05	93,102,105,106	0
2	GAL	C	2	11/12	0.98	0.08	104,107,111,115	0
2	FUC	D	4	10/11	0.99	0.06	99,104,106,107	0

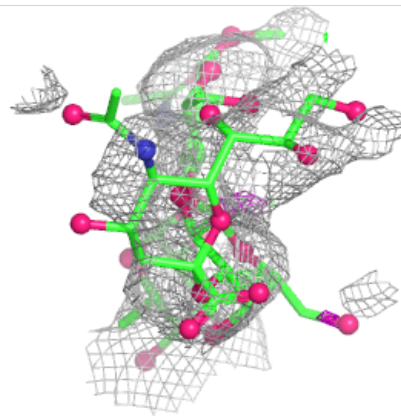
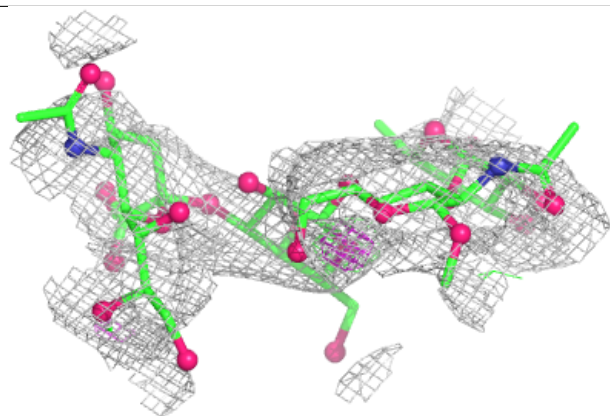
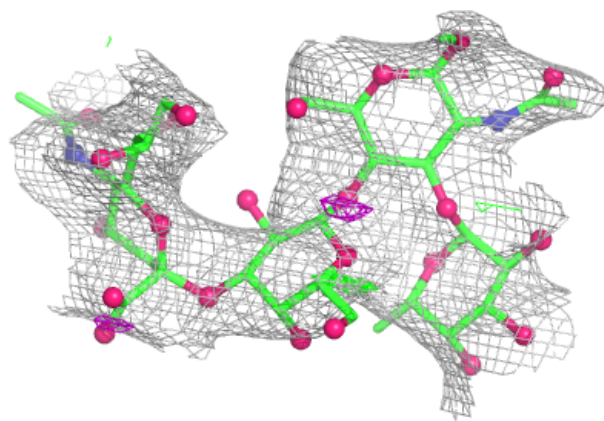
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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

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	NAG	A	282	14/15	0.95	0.06	101,107,112,112	0
3	NAG	A	285	14/15	0.95	0.07	105,110,113,115	0
3	NAG	B	281	14/15	0.95	0.07	66,76,84,85	0
3	NAG	B	285	14/15	0.95	0.09	124,128,130,130	0
3	NAG	B	286	14/15	0.96	0.09	118,127,133,134	0
3	NAG	A	281	14/15	0.97	0.05	71,82,90,91	0
3	NAG	B	282	14/15	0.97	0.07	106,109,115,116	0
3	NAG	B	284	14/15	0.97	0.07	68,78,89,90	0
3	NAG	A	286	14/15	0.97	0.05	107,116,121,122	0
3	NAG	A	287	14/15	0.97	0.08	89,94,106,112	0
3	NAG	B	287	14/15	0.97	0.06	89,95,109,112	0
3	NAG	A	283	14/15	0.98	0.05	36,53,57,64	0
3	NAG	B	283	14/15	0.98	0.05	36,49,54,63	0
3	NAG	A	284	14/15	0.98	0.06	69,81,100,103	0
4	CA	B	306	1/1	0.98	0.03	82,82,82,82	0
4	CA	A	306	1/1	0.99	0.03	82,82,82,82	0

6.5 Other polymers

There are no such residues in this entry.