Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 05:52 PM JST

PDB ID	:	4X83
Title	:	Crystal structure of Dscam1 isoform 7.44, N-terminal four Ig domains
Authors	:	Chen, Q.; Yu, Y.; Li, S.A.; Cheng, L.
Deposited on	:	2014-12-10
Resolution	:	1.90 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 (1)) were used in the production of this report:

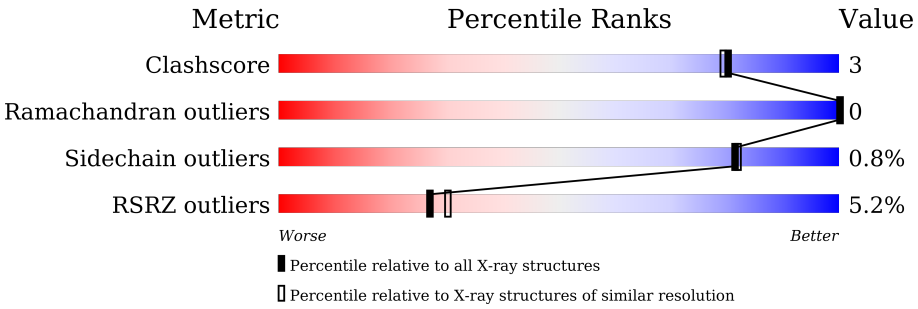
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	394	15% 95%
1	B	394	% 91% 8%
1	C	394	2% 91% 7%
1	D	394	3% 93% 6%
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25894 atoms, of which 12135 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.

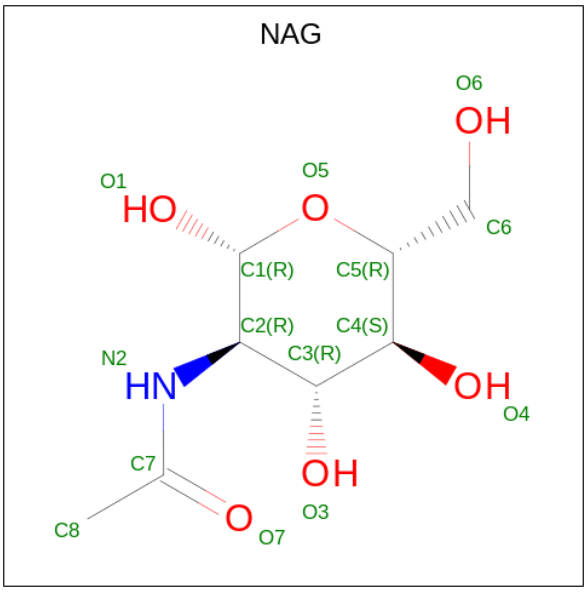
- Molecule 1 is a protein called Down syndrome cell adhesion molecule, isoform 7.44.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	389	Total	C	H	N	O	S	0	2	0
			5998	1902	2980	519	585	12			
1	B	389	Total	C	H	N	O	S	0	5	0
			6065	1925	3014	525	589	12			
1	C	389	Total	C	H	N	O	S	0	5	0
			6038	1913	3003	521	589	12			
1	D	391	Total	C	H	N	O	S	0	3	0
			6045	1916	3001	528	588	12			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			50	16	23	2	9			
2	G	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 27 8 13 1 5	0	0
3	B	1	Total C H N O 27 8 13 1 5	0	0
3	D	1	Total C H N O 27 8 13 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

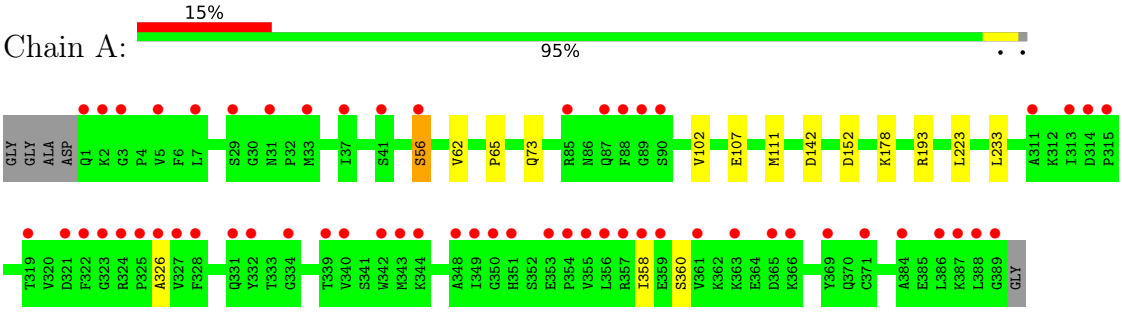
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	331	Total O 331 331	0	0
5	B	418	Total O 418 418	0	0
5	C	391	Total O 391 391	0	0
5	D	316	Total O 316 316	0	0

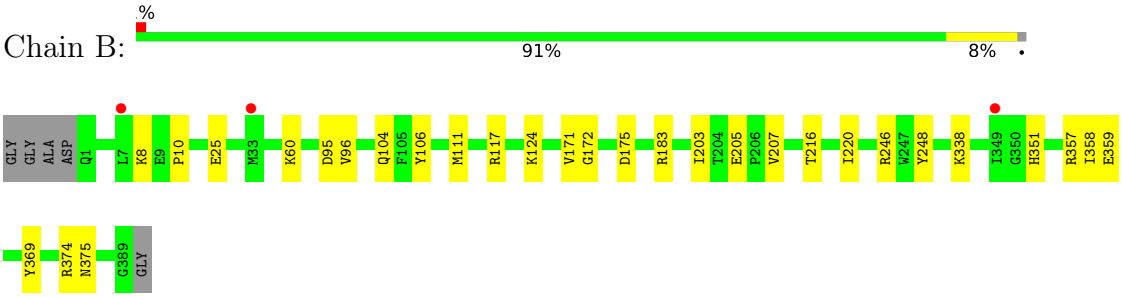
3 Residue-property plots (i)

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.

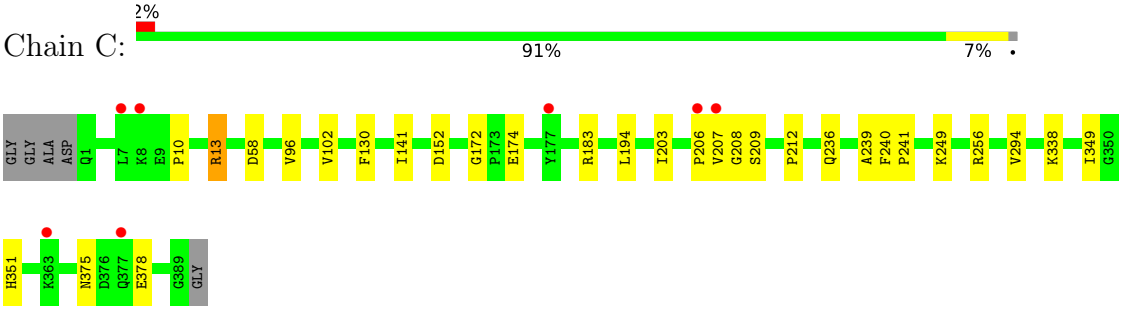
• Molecule 1: Down syndrome cell adhesion molecule, isoform 7.44



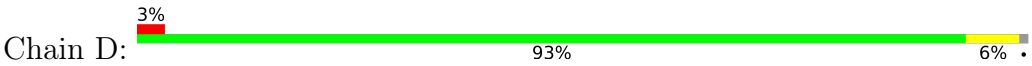
• Molecule 1: Down syndrome cell adhesion molecule, isoform 7.44

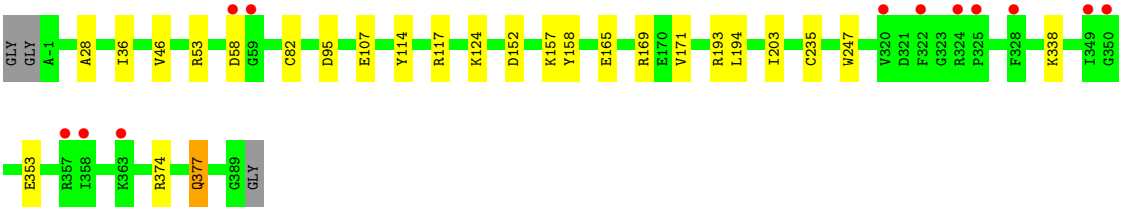


• Molecule 1: Down syndrome cell adhesion molecule, isoform 7.44



• Molecule 1: Down syndrome cell adhesion molecule, isoform 7.44





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.73Å 88.25Å 94.31Å 98.18° 98.79° 90.11°	Depositor
Resolution (Å)	49.44 – 1.90 49.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.44-1.90) 93.6 (49.44-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.193 , 0.235 0.196 , (Not available)	Depositor DCC
R_{free} test set	1000 reflections (0.70%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25894	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NAG

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	0.38	0/3082	0.54	0/4179
1	B	0.41	0/3117	0.59	0/4226
1	C	0.41	0/3107	0.58	0/4214
1	D	0.37	0/3108	0.53	0/4213
All	All	0.39	0/12414	0.56	0/16832

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

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	3018	2980	2993	8	0
1	B	3051	3014	3019	21	0
1	C	3035	3003	2999	21	0
1	D	3044	3001	3021	18	0
2	E	28	25	25	0	0
2	F	27	23	23	0	0
2	G	28	25	25	1	0
2	H	28	25	25	0	0
3	A	14	13	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	13	13	0	0
3	D	14	13	13	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	331	0	0	2	1
5	B	418	0	0	5	1
5	C	391	0	0	7	2
5	D	316	0	0	6	0
All	All	13759	12135	12169	66	2

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 (66) 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:95:ASP:OD2	1:B:374:ARG:NH1	2.12	0.80
1:C:183:ARG:NE	5:C:502:HOH:O	2.13	0.78
1:D:338:LYS:NZ	5:D:503:HOH:O	2.21	0.74
1:A:107:GLU:OE2	1:A:193:ARG:NH1	2.22	0.73
1:B:357:ARG:NH1	1:B:359:GLU:OE1	2.22	0.72
1:C:236:GLN:NE2	5:C:507:HOH:O	2.26	0.69
3:D:403:NAG:O7	5:D:501:HOH:O	2.10	0.68
1:C:249:LYS:O	5:C:501:HOH:O	2.10	0.68
1:D:117[A]:ARG:NH1	5:D:507:HOH:O	2.27	0.67
1:D:152:ASP:OD2	5:D:502:HOH:O	2.12	0.66
1:B:351:HIS:ND1	5:B:505:HOH:O	2.28	0.66
1:D:107:GLU:OE2	1:D:193:ARG:NH1	2.29	0.64
1:B:106[A]:TYR:OH	5:B:501:HOH:O	2.12	0.63
1:C:256:ARG:NH1	5:C:512:HOH:O	2.33	0.61
1:B:104:GLN:OE1	5:B:502:HOH:O	2.18	0.57
1:C:378:GLU:OE1	5:C:503:HOH:O	2.17	0.57
1:A:73:GLN:NE2	5:A:508:HOH:O	2.35	0.57
1:D:95:ASP:OD2	1:D:374:ARG:NH1	2.36	0.56
1:A:111:MET:HE3	1:B:111:MET:HB2	1.88	0.56
1:B:183:ARG:NH2	5:B:512:HOH:O	2.40	0.54
1:B:25:GLU:HB3	1:B:60:LYS:HG2	1.89	0.53
1:B:246:ARG:HG3	1:B:248:TYR:CE1	2.45	0.52
1:B:117[A]:ARG:NH1	1:B:205:GLU:HG2	2.25	0.52
1:C:206:PRO:HG3	1:C:240:PHE:CE1	2.45	0.52
3:A:403:NAG:O7	5:A:501:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:GLN:NE2	5:D:515:HOH:O	2.41	0.51
1:C:172:GLY:O	1:C:203:ILE:HD13	2.11	0.51
1:C:13:ARG:NE	5:C:524:HOH:O	2.43	0.50
1:B:10:PRO:HG2	1:B:96:VAL:HG21	1.93	0.49
1:C:209:SER:HB3	1:C:294:VAL:HG21	1.95	0.48
1:A:142:ASP:OD2	1:A:178:LYS:NZ	2.44	0.48
1:A:102:VAL:HG21	1:B:207:VAL:HG21	1.95	0.47
1:B:124:LYS:N	1:B:124:LYS:HD2	2.29	0.47
1:A:56:SER:HB2	1:A:62:VAL:HG21	1.97	0.47
1:D:169:ARG:NH2	5:D:522:HOH:O	2.47	0.46
1:C:10:PRO:HG2	1:C:96:VAL:HG21	1.97	0.46
1:C:130:PHE:HE2	1:D:114:TYR:CD2	2.34	0.46
1:D:171:VAL:HG12	1:D:203:ILE:HG12	1.98	0.46
1:B:172:GLY:O	1:B:203:ILE:HD13	2.16	0.46
1:B:8:LYS:HE3	1:B:25:GLU:HG3	1.99	0.45
1:D:124:LYS:HE2	1:D:165:GLU:HG2	1.97	0.44
1:B:358:ILE:HD11	1:B:369:TYR:CE2	2.53	0.44
1:C:102:VAL:HG13	2:G:1:NAG:O6	2.18	0.44
1:A:326:ALA:N	1:A:358:ILE:O	2.40	0.44
1:C:152:ASP:O	5:C:504:HOH:O	2.21	0.43
1:C:240:PHE:HA	1:C:241:PRO:C	2.39	0.43
1:D:46:VAL:HG13	1:D:53:ARG:CZ	2.49	0.43
1:B:171:VAL:HG13	1:B:175:ASP:HB2	2.00	0.43
1:B:117[A]:ARG:HH11	1:B:205:GLU:HG2	1.80	0.43
1:C:349:ILE:O	1:C:351:HIS:N	2.49	0.42
1:D:58:ASP:N	1:D:58:ASP:OD1	2.52	0.42
1:C:141:ILE:HD12	1:C:194:LEU:HD13	2.02	0.42
1:B:171:VAL:HG11	1:B:203:ILE:HG12	2.02	0.42
1:D:28:ALA:HB3	1:D:36:ILE:HD11	2.02	0.42
1:D:36:ILE:HG23	1:D:82:CYS:SG	2.60	0.41
1:D:235:CYS:HB2	1:D:247:TRP:CZ2	2.55	0.41
1:B:338:LYS:HB2	1:B:375:ASN:HA	2.03	0.41
1:B:216:THR:HG21	5:B:754:HOH:O	2.20	0.41
1:D:353:GLU:OE1	1:D:353:GLU:N	2.53	0.41
1:C:206:PRO:HB2	1:C:240:PHE:CD2	2.55	0.41
1:C:212:PRO:HA	1:C:239:ALA:HB2	2.03	0.41
1:A:223:LEU:HD23	1:A:233:LEU:CD2	2.51	0.40
1:C:130:PHE:CE2	1:D:114:TYR:CD2	3.09	0.40
1:C:207:VAL:CG2	1:C:208:GLY:N	2.85	0.40
1:C:338:LYS:HB2	1:C:375:ASN:HA	2.02	0.40
1:D:157:LYS:HG2	1:D:158:TYR:CE1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:867:HOH:O	5:C:824:HOH:O[1_455]	2.17	0.03
5:A:540:HOH:O	5:C:831:HOH:O[1_455]	2.19	0.01

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	389/394 (99%)	377 (97%)	12 (3%)	0	100	100
1	B	392/394 (100%)	383 (98%)	9 (2%)	0	100	100
1	C	392/394 (100%)	380 (97%)	12 (3%)	0	100	100
1	D	392/394 (100%)	380 (97%)	12 (3%)	0	100	100
All	All	1565/1576 (99%)	1520 (97%)	45 (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	335/334 (100%)	331 (99%)	4 (1%)	71	70
1	B	338/334 (101%)	337 (100%)	1 (0%)	92	93
1	C	338/334 (101%)	335 (99%)	3 (1%)	78	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	337/334 (101%)	335 (99%)	2 (1%)	86 87
All	All	1348/1336 (101%)	1338 (99%)	10 (1%)	81 84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	65	PRO
1	A	152	ASP
1	A	360	SER
1	B	220	ILE
1	C	13	ARG
1	C	58	ASP
1	C	174	GLU
1	D	194	LEU
1	D	377	GLN

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)

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

5.5 Carbohydrates (i)

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	NAG	E	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	1.20	2 (11%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	0.41	0
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	F	2	2	13,13,15	0.66	1 (7%)	16,17,21	0.52	0
2	NAG	G	1	2,1	14,14,15	0.48	0	17,19,21	0.76	1 (5%)
2	NAG	G	2	2	14,14,15	0.24	0	17,19,21	0.61	0
2	NAG	H	1	2,1	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
2	NAG	H	2	2	14,14,15	0.49	0	17,19,21	0.43	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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/19/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.17	1.40	1.43
2	F	2	NAG	C1-C2	2.03	1.53	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAG	C1-O5-C5	3.28	116.64	112.19
2	H	1	NAG	C3-C4-C5	2.80	115.23	110.24
2	E	1	NAG	C3-C4-C5	2.73	115.11	110.24
2	E	1	NAG	C1-O5-C5	2.71	115.86	112.19
2	G	1	NAG	O4-C4-C5	-2.04	104.22	109.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

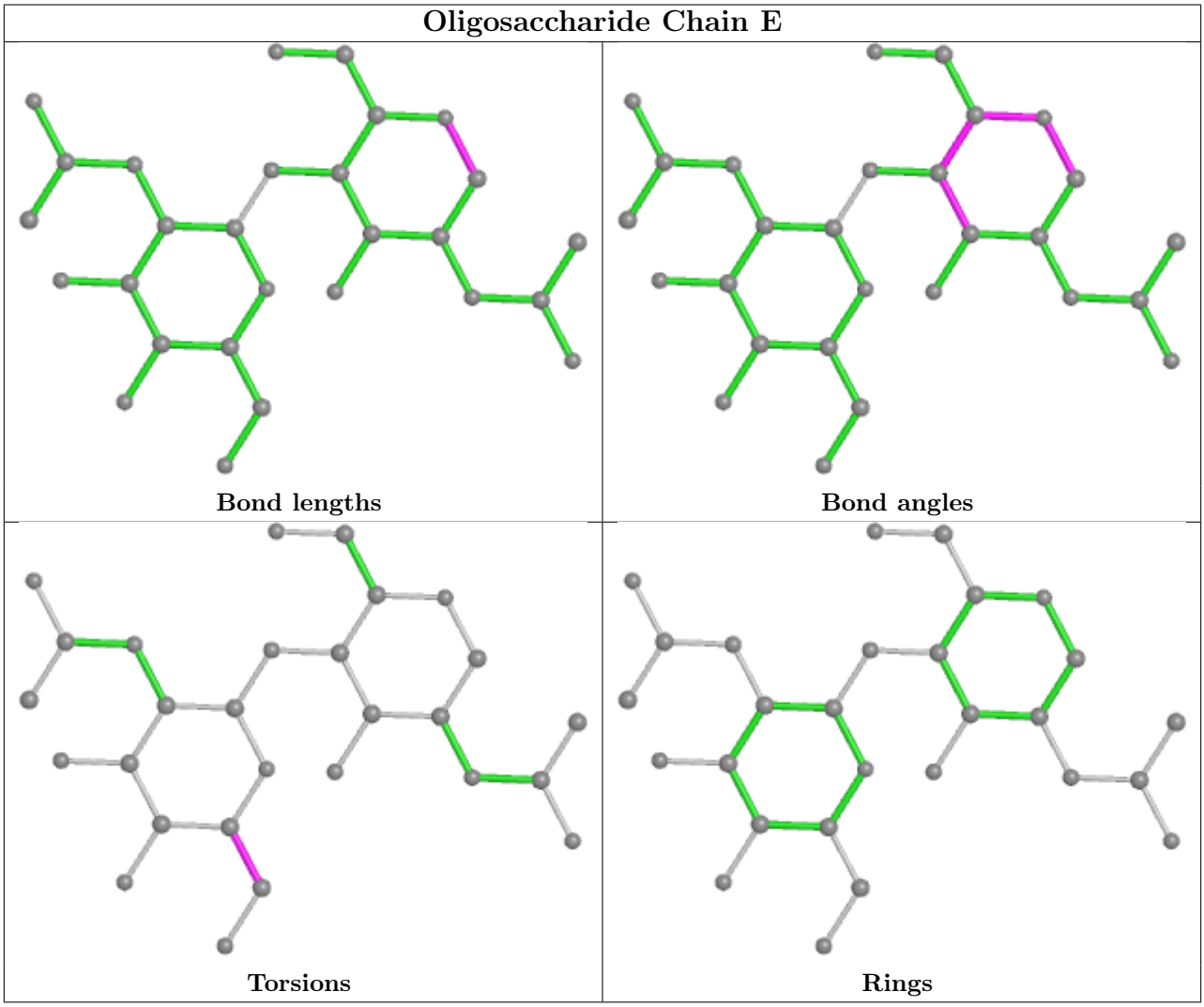
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

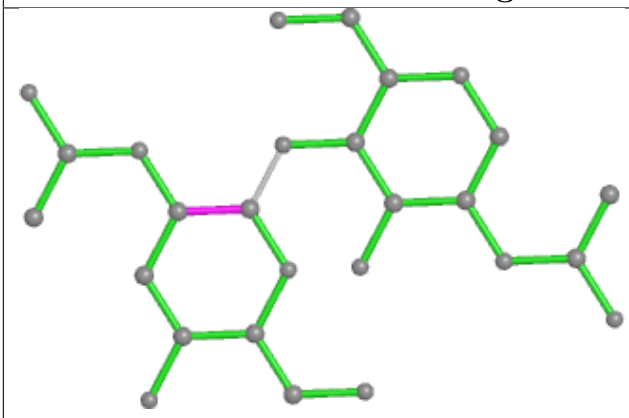
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0

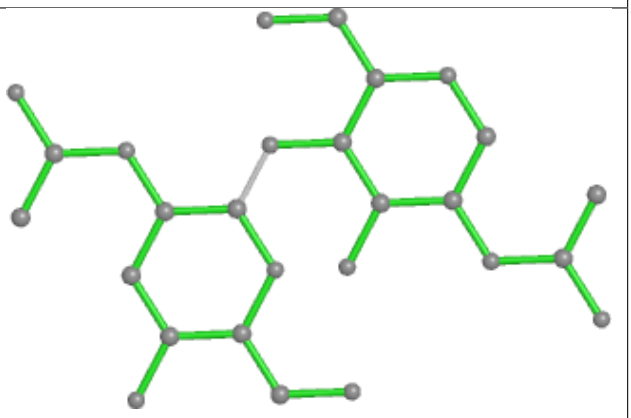
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



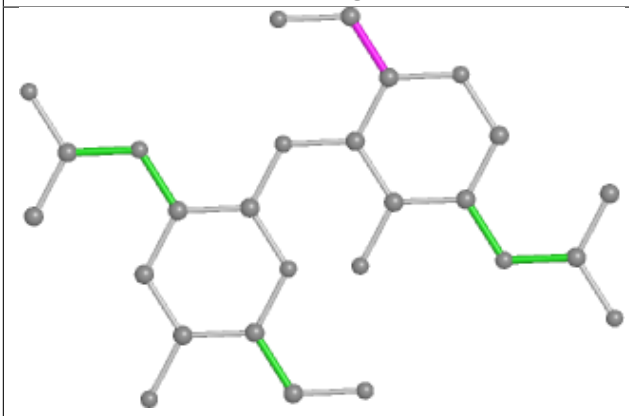
Oligosaccharide Chain F



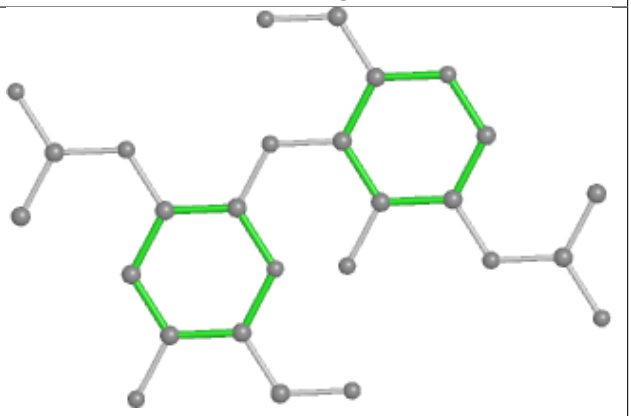
Bond lengths



Bond angles

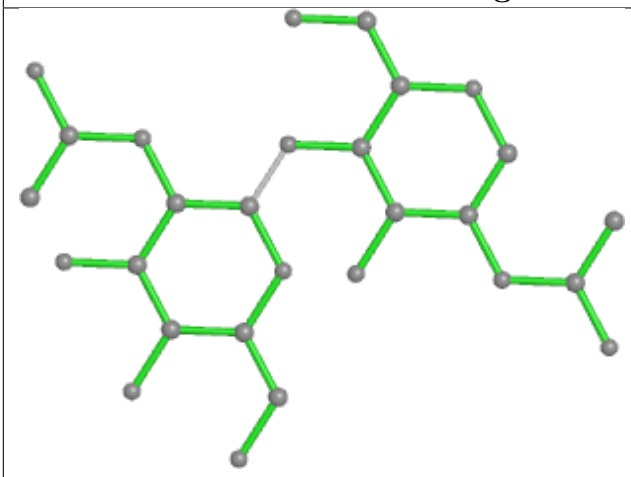


Torsions

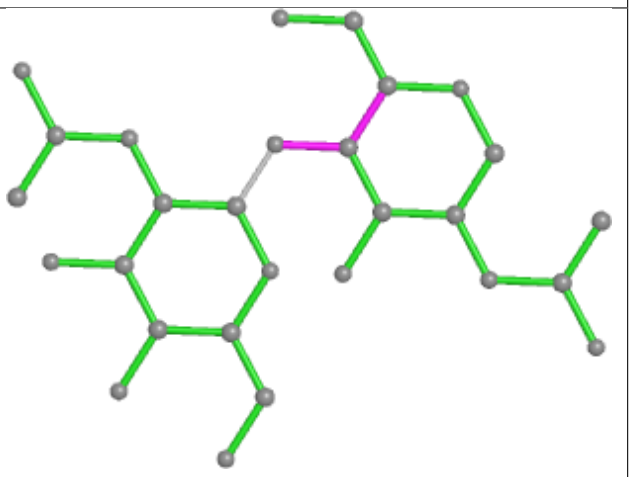


Rings

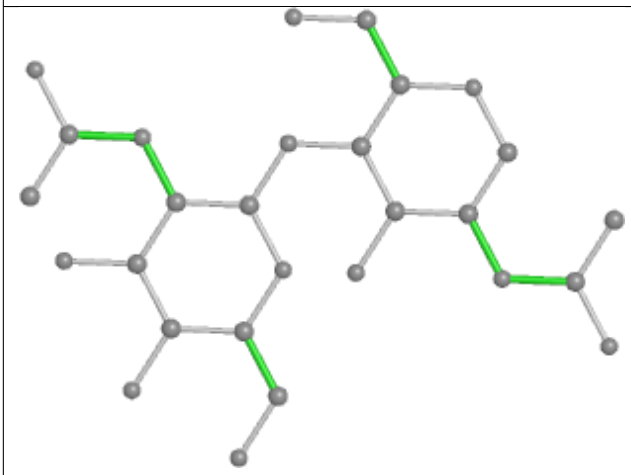
Oligosaccharide Chain G



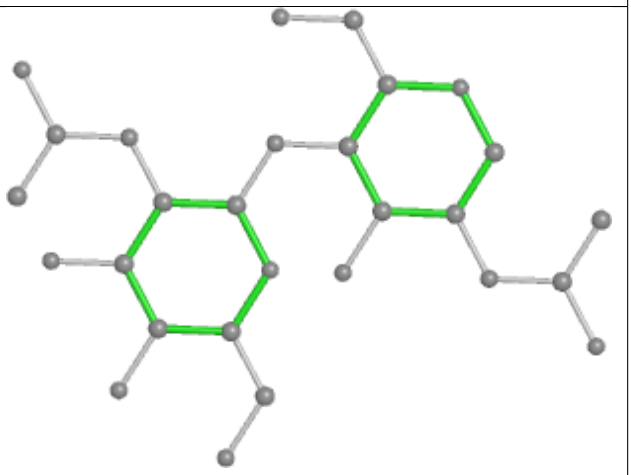
Bond lengths



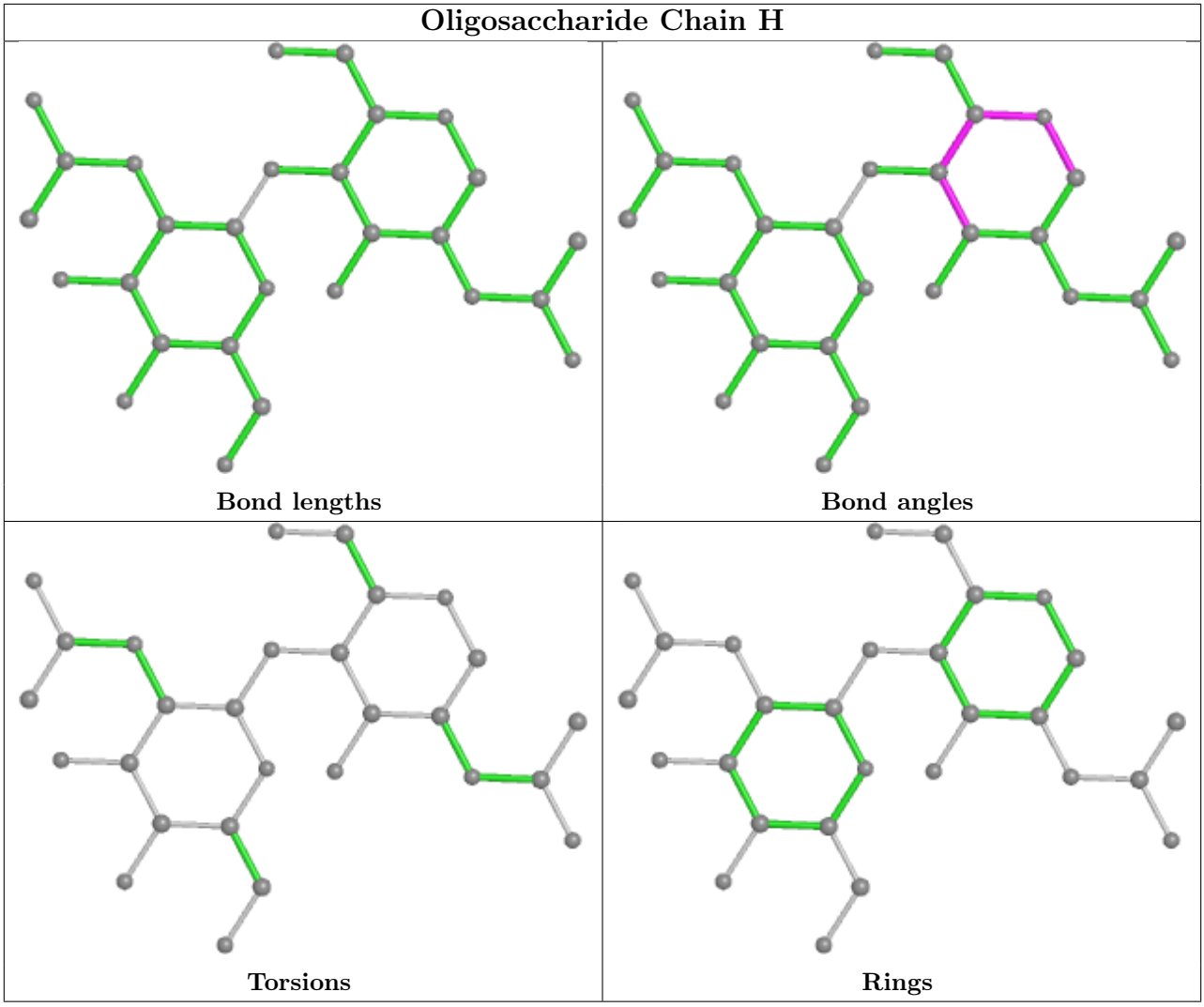
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
3	NAG	A	403	1	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	D	403	1	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	B	403	1	14,14,15	0.20	0	17,19,21	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	NAG	A	403	1	-	0/6/23/26	0/1/1/1
3	NAG	D	403	1	-	0/6/23/26	0/1/1/1
3	NAG	B	403	1	-	0/6/23/26	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	NAG	1	0
3	D	403	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

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, 95^{th} 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	389/394 (98%)	0.80	59 (15%) 2 2	20, 37, 79, 95	0
1	B	389/394 (98%)	0.11	3 (0%) 86 87	18, 31, 58, 78	0
1	C	389/394 (98%)	0.15	7 (1%) 68 71	17, 31, 59, 86	0
1	D	391/394 (99%)	0.30	12 (3%) 49 51	23, 37, 63, 91	0
All	All	1558/1576 (98%)	0.34	81 (5%) 27 30	17, 34, 67, 95	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	GLY	8.2
1	A	361	VAL	7.6
1	A	56	SER	6.7
1	D	59	GLY	6.6
1	A	7	LEU	5.5
1	A	328	PHE	5.5
1	A	349	ILE	5.3
1	A	388	LEU	5.2
1	B	7	LEU	4.6
1	A	322	PHE	4.4
1	C	207	VAL	4.3
1	A	355	VAL	4.2
1	A	371	CYS	4.1
1	A	88	PHE	4.1
1	A	313	ILE	3.9
1	A	369	TYR	3.8
1	C	7	LEU	3.8
1	A	363	LYS	3.7
1	A	327	VAL	3.7
1	A	33	MET	3.6
1	A	358	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	3.6
1	A	386	LEU	3.5
1	A	323	GLY	3.5
1	A	3	GLY	3.5
1	A	384	ALA	3.5
1	A	326	ALA	3.4
1	A	348	ALA	3.4
1	D	349	ILE	3.4
1	D	320	VAL	3.4
1	A	321	ASP	3.3
1	A	357	ARG	3.3
1	A	314	ASP	3.2
1	A	342	TRP	3.1
1	A	351	HIS	3.1
1	A	87	GLN	3.0
1	B	349	ILE	3.0
1	A	315	PRO	2.9
1	A	387	LYS	2.8
1	A	85	ARG	2.8
1	A	359	GLU	2.8
1	A	37	ILE	2.8
1	A	366	LYS	2.8
1	A	332	TYR	2.8
1	A	353	GLU	2.7
1	A	1	GLN	2.7
1	A	325	PRO	2.7
1	D	58	ASP	2.6
1	A	89	GLY	2.6
1	C	177	TYR	2.5
1	D	350	GLY	2.5
1	A	354	PRO	2.5
1	A	29	SER	2.5
1	A	334	GLY	2.4
1	A	340	VAL	2.4
1	A	339	THR	2.4
1	A	365	ASP	2.4
1	A	350	GLY	2.4
1	A	2	LYS	2.3
1	C	377	GLN	2.3
1	A	31	ASN	2.2
1	A	311	ALA	2.2
1	D	324	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	357	ARG	2.2
1	A	41	SER	2.2
1	C	363	LYS	2.2
1	A	343	MET	2.1
1	B	33	MET	2.1
1	A	5	VAL	2.1
1	C	206	PRO	2.1
1	A	319	THR	2.1
1	C	8	LYS	2.1
1	D	363	LYS	2.1
1	A	324	ARG	2.1
1	A	344	LYS	2.1
1	D	322	PHE	2.1
1	A	90	SER	2.1
1	D	328	PHE	2.0
1	D	358	ILE	2.0
1	A	331	GLN	2.0
1	D	325	PRO	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, 95^{th} 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.

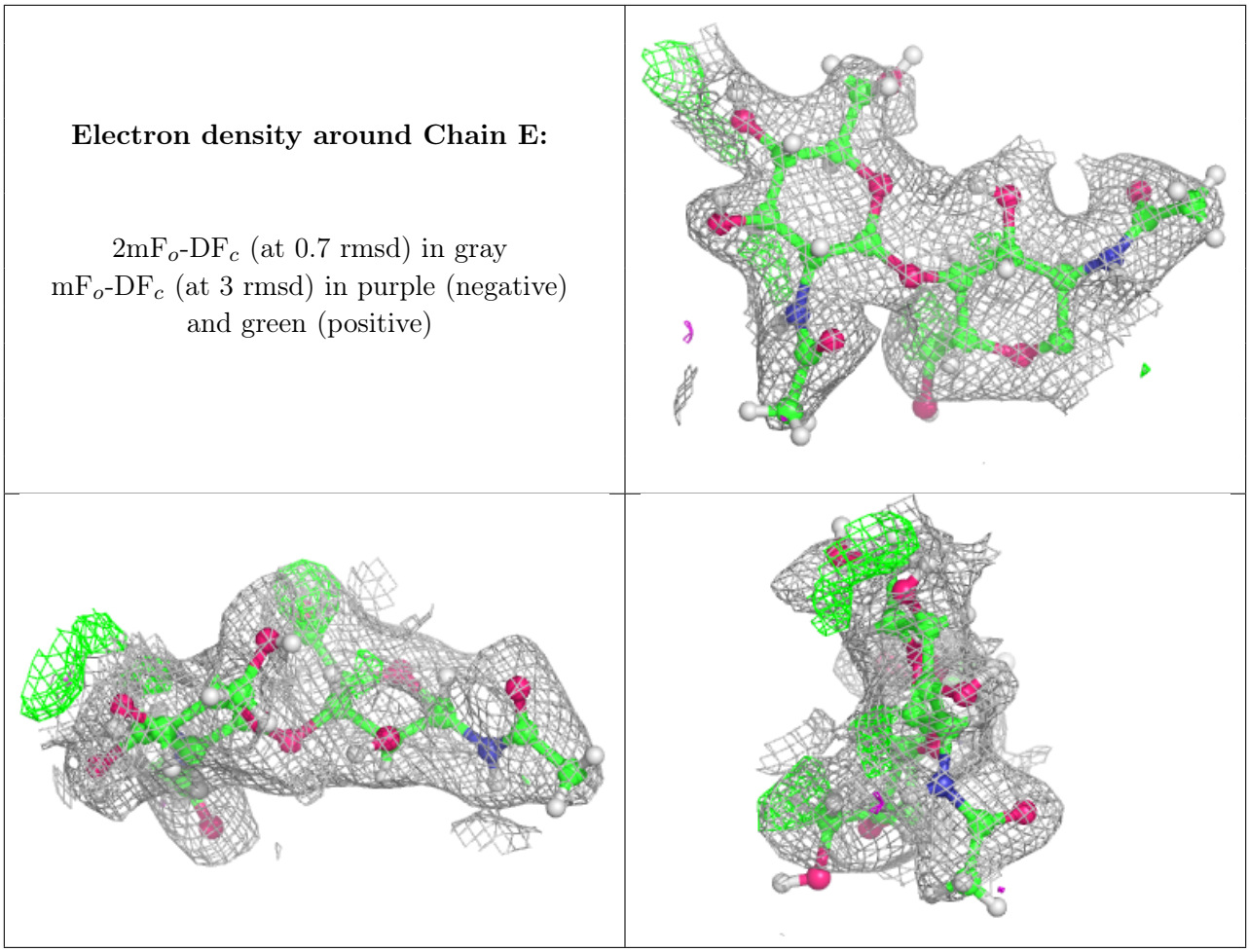
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.78	0.16	41,60,72,75	0
2	NAG	E	2	14/15	0.80	0.14	42,62,81,89	0
2	NAG	F	2	13/15	0.81	0.21	46,67,86,93	0
2	NAG	G	2	14/15	0.83	0.16	45,64,84,90	0
2	NAG	H	1	14/15	0.93	0.10	32,48,57,64	0
2	NAG	E	1	14/15	0.94	0.10	34,44,56,80	0
2	NAG	G	1	14/15	0.95	0.09	24,35,42,45	0
2	NAG	F	1	14/15	0.95	0.09	26,38,51,54	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.

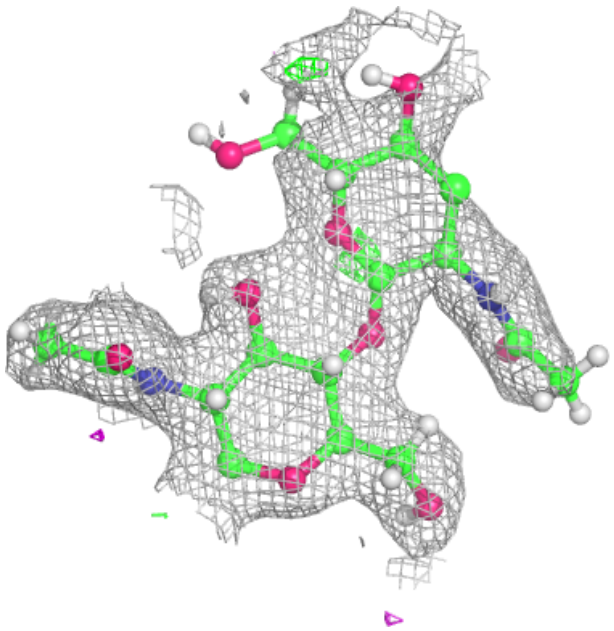
Electron density around Chain E:

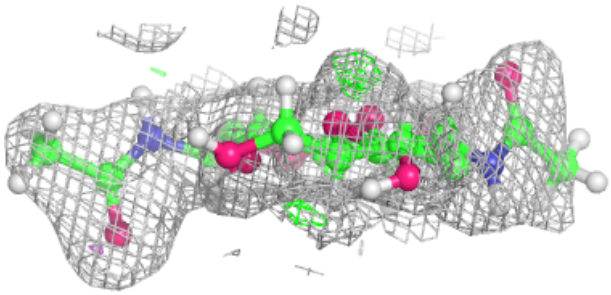
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

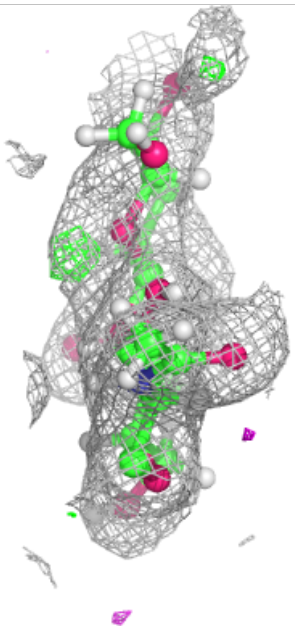


Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

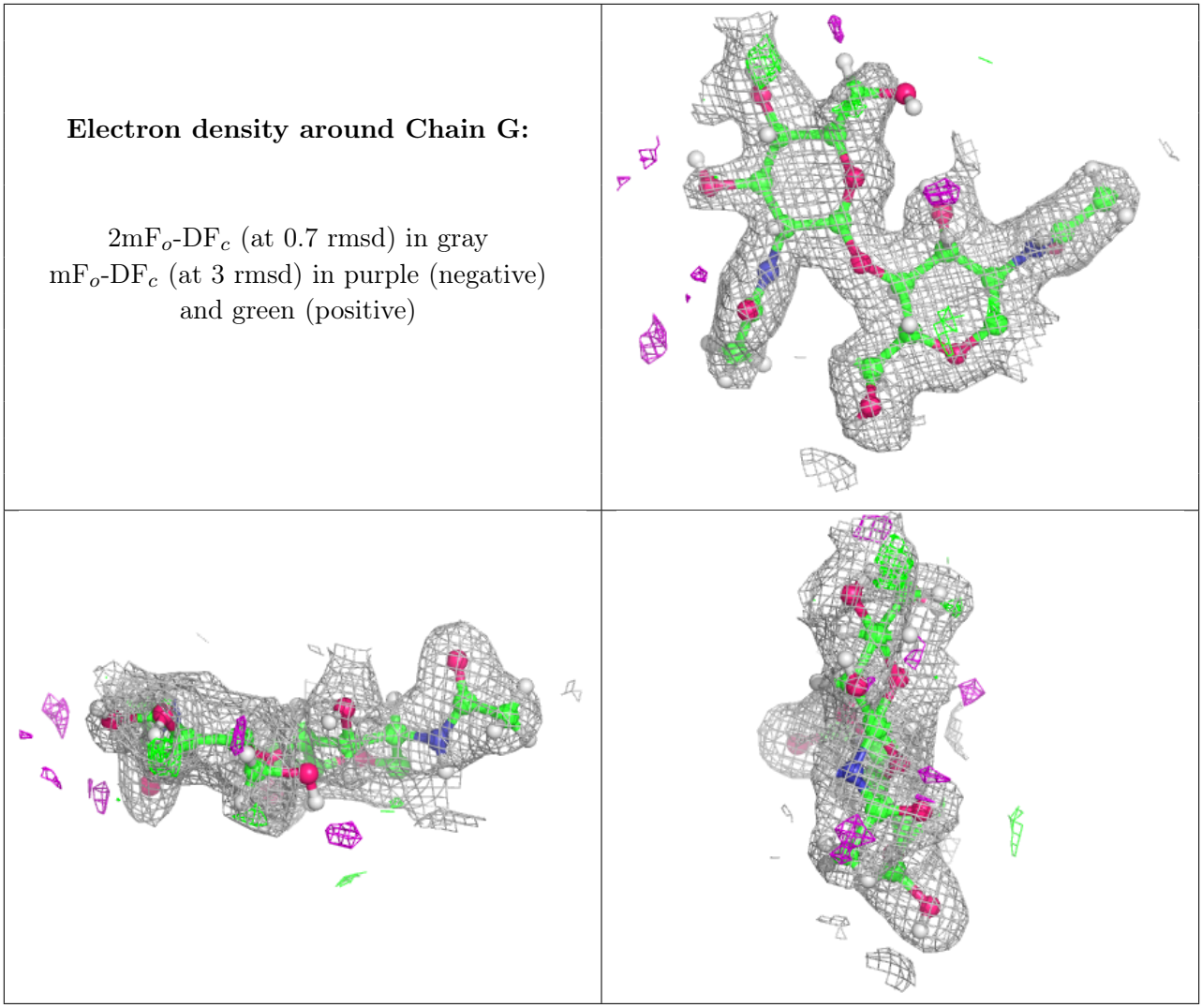






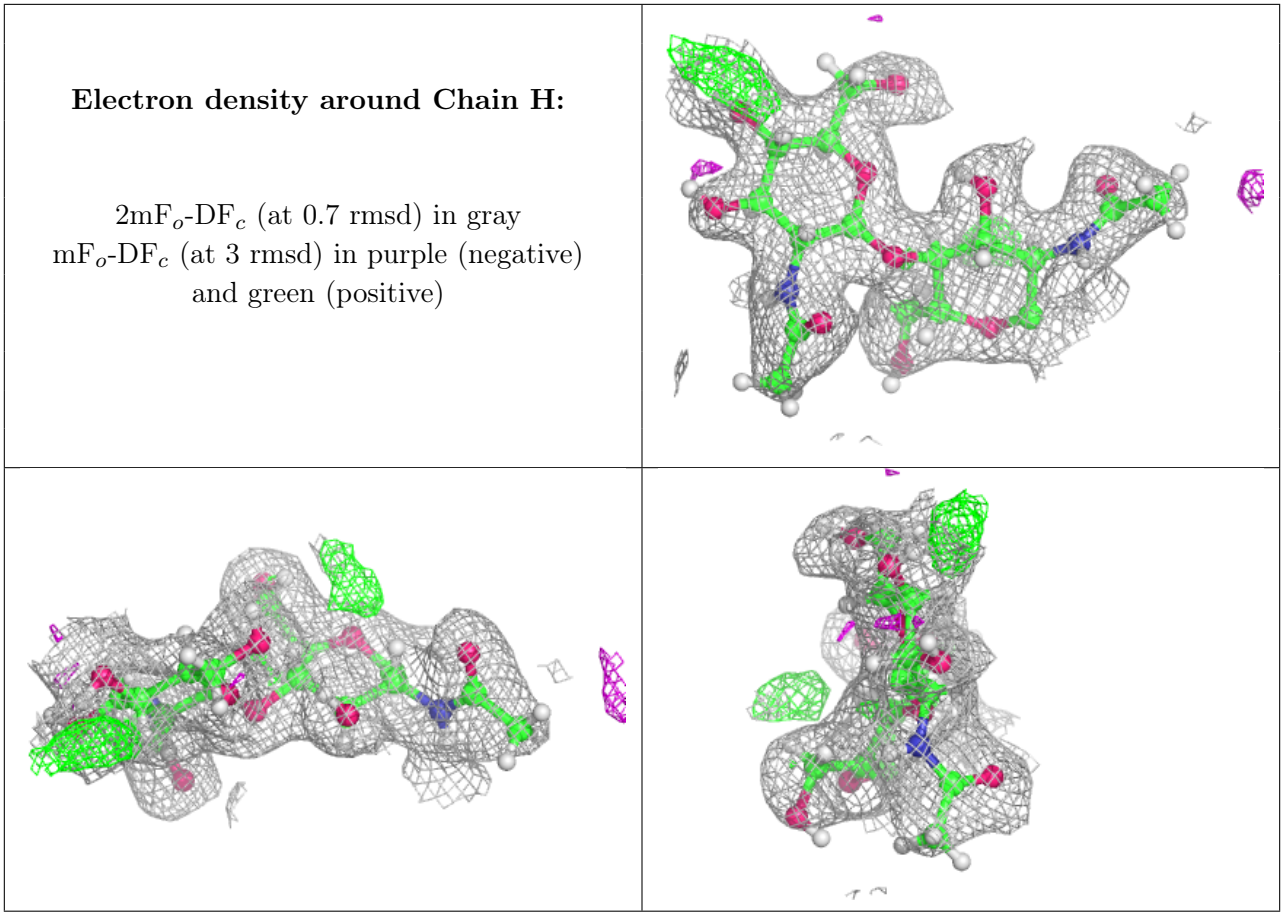
Electron density around Chain G:

$2mF_o$-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 H:

$2mF_o$-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, 95^{th} 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	B	403	14/15	0.74	0.21	58,82,102,106	0
3	NAG	D	403	14/15	0.84	0.19	36,60,73,79	0
3	NAG	A	403	14/15	0.88	0.13	38,55,73,80	0
4	CL	B	404	1/1	1.00	0.16	22,22,22,22	0
4	CL	C	403	1/1	1.00	0.10	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.