



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 10:05 PM EDT

PDB ID : 9NSF / pdb_00009nsf
Title : Crystal Structure of the Complex of Side-VI IG1 Domain and Beat-Vc IG1+2 Domains
Authors : Olechwier, A.M.; Ozkan, E.
Deposited on : 2025-03-16
Resolution : 3.93 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

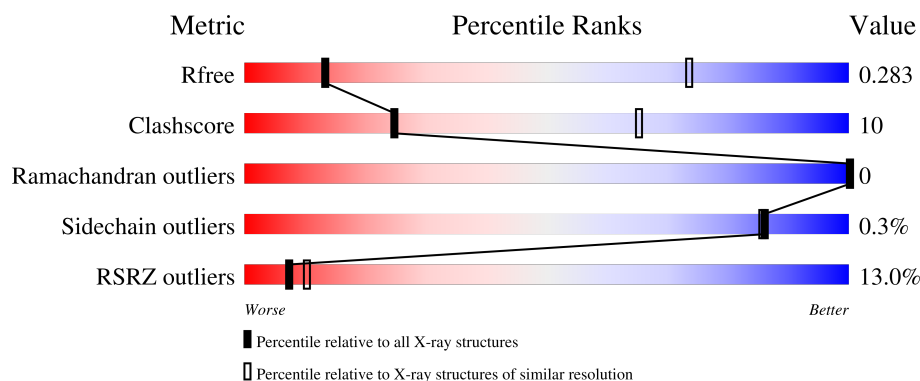
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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	240	<div> <div>8%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	C	240	<div> <div>15%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	B	142	<div> <div>13%</div> <div>64%</div> <div>17%</div> <div>19%</div> </div>
2	D	142	<div> <div>11%</div> <div>54%</div> <div>25%</div> <div>22%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	G	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5628 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 Beaten path Vc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1860	1181	329	338	12			
1	C	234	Total	C	N	O	S	0	0	0
			1855	1178	327	338	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	-	cloning artifact	UNP Q9VG28
A	24	ASP	-	cloning artifact	UNP Q9VG28
A	25	PRO	-	cloning artifact	UNP Q9VG28
A	257	HIS	-	expression tag	UNP Q9VG28
A	258	HIS	-	expression tag	UNP Q9VG28
A	259	HIS	-	expression tag	UNP Q9VG28
A	260	HIS	-	expression tag	UNP Q9VG28
A	261	HIS	-	expression tag	UNP Q9VG28
A	262	HIS	-	expression tag	UNP Q9VG28
C	23	ALA	-	cloning artifact	UNP Q9VG28
C	24	ASP	-	cloning artifact	UNP Q9VG28
C	25	PRO	-	cloning artifact	UNP Q9VG28
C	257	HIS	-	expression tag	UNP Q9VG28
C	258	HIS	-	expression tag	UNP Q9VG28
C	259	HIS	-	expression tag	UNP Q9VG28
C	260	HIS	-	expression tag	UNP Q9VG28
C	261	HIS	-	expression tag	UNP Q9VG28
C	262	HIS	-	expression tag	UNP Q9VG28

- Molecule 2 is a protein called Sidestep VI, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			915	573	165	175	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	111	Total	C	N	O	S	0	0	0
			886	554	161	169	2			

There are 18 discrepancies between the modelled and reference sequences:

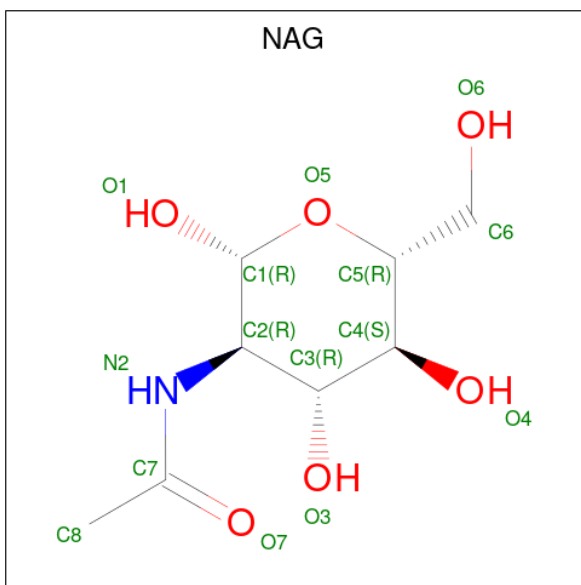
Chain	Residue	Modelled	Actual	Comment	Reference
B	17	ALA	-	cloning artifact	UNP Q0KI85
B	18	ASP	-	cloning artifact	UNP Q0KI85
B	19	PRO	-	cloning artifact	UNP Q0KI85
B	153	HIS	-	expression tag	UNP Q0KI85
B	154	HIS	-	expression tag	UNP Q0KI85
B	155	HIS	-	expression tag	UNP Q0KI85
B	156	HIS	-	expression tag	UNP Q0KI85
B	157	HIS	-	expression tag	UNP Q0KI85
B	158	HIS	-	expression tag	UNP Q0KI85
D	17	ALA	-	cloning artifact	UNP Q0KI85
D	18	ASP	-	cloning artifact	UNP Q0KI85
D	19	PRO	-	cloning artifact	UNP Q0KI85
D	153	HIS	-	expression tag	UNP Q0KI85
D	154	HIS	-	expression tag	UNP Q0KI85
D	155	HIS	-	expression tag	UNP Q0KI85
D	156	HIS	-	expression tag	UNP Q0KI85
D	157	HIS	-	expression tag	UNP Q0KI85
D	158	HIS	-	expression tag	UNP Q0KI85

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

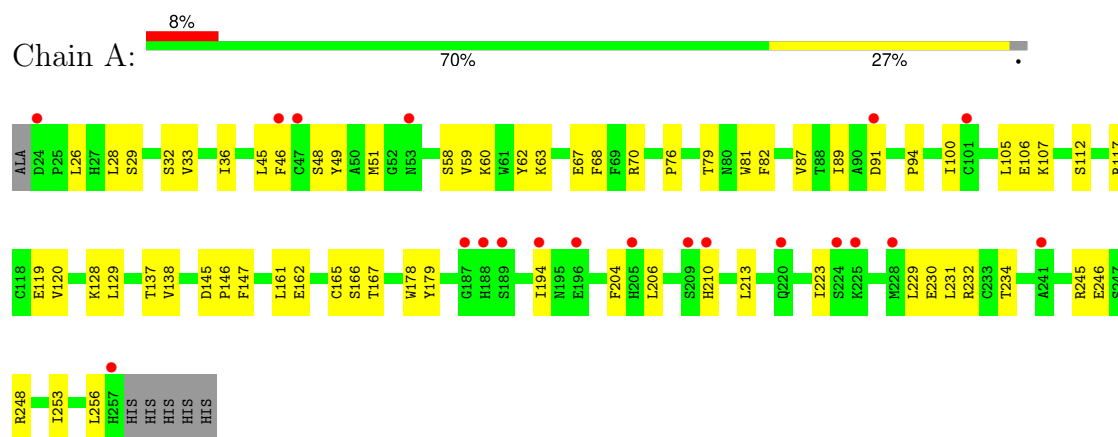


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

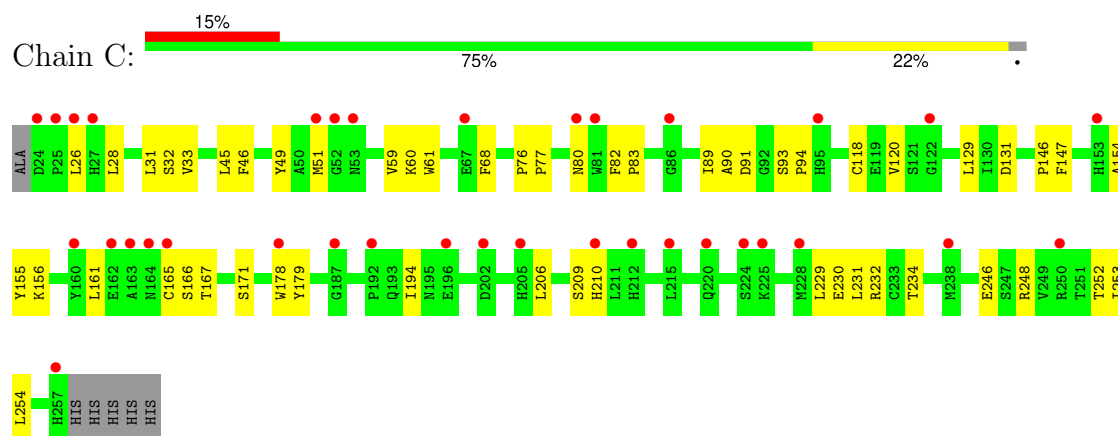
3 Residue-property plots [i](#)

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.

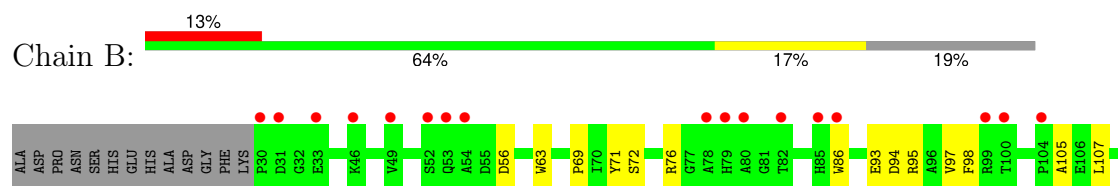
• Molecule 1: Beaten path Vc



• Molecule 1: Beaten path Vc



• Molecule 2: Sidestep VI, isoform B





- Molecule 2: Sidestep VI, isoform B



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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	P 61	Depositor
Cell constants a, b, c, α , β , γ	87.48Å 87.48Å 387.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.14 – 3.93 49.14 – 3.93	Depositor EDS
% Data completeness (in resolution range)	64.8 (49.14-3.93) 64.9 (49.14-3.93)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.88Å)	Xtriage
Refinement program	PHENIX dev_5533	Depositor
R, R_{free}	0.234 , 0.284 0.233 , 0.283	Depositor DCC
R_{free} test set	456 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 93.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.130 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	5628	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

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	0.16	0/1908	0.40	0/2589
1	C	0.15	0/1902	0.37	0/2581
2	B	0.17	0/934	0.43	0/1269
2	D	0.18	0/902	0.43	0/1223
All	All	0.17	0/5646	0.40	0/7662

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1860	0	1826	44	0
1	C	1855	0	1822	38	0
2	B	915	0	899	16	0
2	D	886	0	874	22	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
All	All	5628	0	5522	109	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 10.

All (109) 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:32:SER:HB3	1:A:46:PHE:HB3	1.62	0.80
1:A:76:PRO:HG2	1:C:91:ASP:HB3	1.67	0.75
1:C:194:ILE:HB	1:C:210:HIS:HB2	1.72	0.70
1:A:68:PHE:HA	1:A:82:PHE:HB2	1.75	0.68
1:C:32:SER:HB3	1:C:46:PHE:HB3	1.75	0.68
1:A:107:LYS:HE2	2:D:78:ALA:HA	1.74	0.68
1:C:68:PHE:HA	1:C:82:PHE:HB2	1.76	0.68
1:C:59:VAL:HG13	1:C:120:VAL:HG22	1.79	0.65
1:C:178:TRP:HZ3	1:C:231:LEU:HB3	1.61	0.65
1:A:33:VAL:HG22	1:A:45:LEU:HD22	1.78	0.64
2:B:98:PHE:CZ	2:B:105:ALA:HB1	2.33	0.63
1:C:33:VAL:HG22	1:C:45:LEU:HD22	1.81	0.63
1:C:229:LEU:HD22	1:C:253:ILE:HD11	1.81	0.62
1:C:146:PRO:HB3	1:C:167:THR:HG22	1.81	0.61
1:C:165:CYS:HB2	1:C:178:TRP:CZ2	2.35	0.61
1:A:28:LEU:HD12	1:A:49:TYR:HB3	1.83	0.60
1:A:129:LEU:HD22	2:B:121:ARG:HH22	1.66	0.60
1:A:194:ILE:HB	1:A:210:HIS:HB2	1.84	0.60
1:C:77:PRO:HD2	1:C:80:ASN:HD21	1.68	0.59
1:A:26:LEU:HD13	1:A:51:MET:HA	1.85	0.58
1:A:179:TYR:HB2	1:A:232:ARG:HB3	1.85	0.58
1:A:145:ASP:HA	1:A:245:ARG:HB3	1.86	0.57
1:A:146:PRO:HB3	1:A:167:THR:HG22	1.87	0.57
2:B:63:TRP:HB2	2:B:71:TYR:HB3	1.87	0.56
1:C:129:LEU:HD22	2:D:121:ARG:HH22	1.70	0.56
1:A:59:VAL:HG13	1:A:120:VAL:HG22	1.87	0.55
2:D:95:ARG:HG2	2:D:111:PRO:HD2	1.88	0.55
1:A:81:TRP:CD2	1:C:77:PRO:HG3	2.41	0.55
1:A:81:TRP:CZ2	1:A:94:PRO:HG2	2.41	0.55
1:A:91:ASP:HB3	1:C:76:PRO:HG2	1.88	0.55
2:D:65:LYS:O	2:D:68:LEU:HB3	2.07	0.54
2:B:56:ASP:OD2	2:B:126:PHE:HB3	2.08	0.54
1:C:26:LEU:HD13	1:C:51:MET:HA	1.90	0.53
1:C:68:PHE:HD2	1:C:89:ILE:HD11	1.73	0.53
1:C:147:PHE:CE2	1:C:166:SER:HB2	2.43	0.53
1:C:230:GLU:OE2	1:C:248:ARG:HD3	2.09	0.53
1:A:62:TYR:HB2	1:A:117:ARG:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HG2	2:B:69:PRO:HG3	1.91	0.52
2:D:130:GLN:O	2:D:132:ARG:HG3	2.10	0.52
1:C:156:LYS:HG2	1:C:254:LEU:HD12	1.91	0.52
2:D:63:TRP:HB2	2:D:71:TYR:HB3	1.92	0.52
1:C:161:LEU:HD21	1:C:231:LEU:HD11	1.92	0.51
2:D:69:PRO:HB2	2:D:86:TRP:CZ3	2.45	0.51
1:A:119:GLU:HG3	1:A:129:LEU:HD21	1.92	0.51
1:C:179:TYR:HB2	1:C:232:ARG:HB3	1.94	0.50
1:A:161:LEU:HD21	1:A:231:LEU:HD11	1.93	0.50
1:A:223:ILE:HG23	1:A:256:LEU:HD12	1.94	0.49
2:D:56:ASP:OD2	2:D:126:PHE:HB3	2.11	0.49
2:B:130:GLN:O	2:B:132:ARG:HG3	2.12	0.49
1:C:155:TYR:CZ	1:C:161:LEU:HG	2.48	0.48
1:A:230:GLU:OE2	1:A:248:ARG:HD3	2.14	0.48
1:A:178:TRP:HZ3	1:A:231:LEU:HB3	1.78	0.48
1:A:79:THR:HB	1:A:81:TRP:HZ3	1.79	0.48
2:D:127:LYS:HG3	2:D:128:LEU:HG	1.96	0.48
1:C:171:SER:HB2	1:C:206:LEU:HD23	1.97	0.47
1:A:229:LEU:HD22	1:A:253:ILE:HD11	1.97	0.47
1:A:162:GLU:HA	1:A:213:LEU:O	2.14	0.47
1:A:112:SER:HB2	1:A:138:VAL:HG21	1.97	0.47
2:B:98:PHE:HZ	2:B:105:ALA:HB1	1.76	0.47
2:D:126:PHE:HE2	2:D:132:ARG:HD3	1.80	0.46
1:C:90:ALA:O	1:C:93:SER:HB3	2.15	0.46
1:C:60:LYS:HE2	2:D:131:THR:HG21	1.98	0.46
2:B:56:ASP:HB2	1:C:83:PRO:HB3	1.98	0.46
1:A:60:LYS:HD3	1:A:67:GLU:OE1	2.15	0.46
1:A:63:LYS:HD2	1:A:87:VAL:HG23	1.98	0.46
1:A:165:CYS:HB2	1:A:178:TRP:CZ2	2.50	0.46
1:C:166:SER:HA	1:C:209:SER:O	2.16	0.46
1:C:154:ALA:HA	1:C:252:THR:O	2.15	0.45
1:A:79:THR:HB	1:A:81:TRP:CZ3	2.51	0.45
2:B:113:LYS:HD2	2:B:115:LYS:HE2	1.99	0.45
2:D:100:THR:HG23	2:D:102:LYS:H	1.81	0.45
1:A:67:GLU:CD	2:B:131:THR:HB	2.42	0.45
1:A:81:TRP:CD1	1:A:89:ILE:HD12	2.52	0.44
1:A:147:PHE:CE2	1:A:166:SER:HB2	2.52	0.44
1:C:234:THR:HG22	1:C:246:GLU:HB2	1.99	0.44
1:A:87:VAL:HG13	1:A:105:LEU:HD21	2.00	0.44
1:A:48:SER:HA	1:A:100:ILE:HA	1.99	0.44
2:D:92:LEU:HA	2:D:95:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:NAG:H4	3:G:2:NAG:H2	1.61	0.43
2:B:97:VAL:O	2:B:107:LEU:HD12	2.18	0.43
2:D:52:SER:HB3	2:D:53:GLN:H	1.67	0.43
1:A:58:SER:OG	1:A:60:LYS:HE3	2.18	0.43
2:B:93:GLU:HB3	2:B:94:ASP:H	1.63	0.43
1:C:31:LEU:HD12	1:C:46:PHE:O	2.19	0.43
1:C:77:PRO:HD3	2:D:127:LYS:NZ	2.34	0.43
1:A:145:ASP:OD1	1:A:245:ARG:HD2	2.19	0.43
1:C:28:LEU:HD12	1:C:49:TYR:HB3	2.00	0.43
1:C:118:CYS:O	1:C:131:ASP:HA	2.19	0.43
2:D:36:ARG:HD3	2:D:139:GLU:OE1	2.20	0.42
1:C:77:PRO:HG2	1:C:80:ASN:OD1	2.19	0.42
1:A:36:ILE:HG13	1:A:137:THR:O	2.19	0.42
2:D:93:GLU:HB3	2:D:94:ASP:H	1.64	0.42
2:D:98:PHE:CZ	2:D:105:ALA:HB1	2.54	0.42
1:C:61:TRP:HB3	1:C:68:PHE:CZ	2.55	0.42
1:C:93:SER:N	1:C:94:PRO:HD2	2.35	0.42
2:D:44:GLN:HG2	2:D:46:LYS:HE3	2.01	0.42
1:A:60:LYS:HG2	1:A:70:ARG:HG3	2.01	0.41
1:A:234:THR:HG22	1:A:246:GLU:HB2	2.02	0.41
2:D:98:PHE:HZ	2:D:105:ALA:HB1	1.85	0.41
1:A:204:PHE:HB3	1:A:206:LEU:HD21	2.01	0.41
2:B:72:SER:HB3	2:B:86:TRP:HB3	2.01	0.41
2:B:76:ARG:HE	2:B:76:ARG:HB3	1.68	0.41
2:B:95:ARG:HG2	2:B:111:PRO:HD2	2.03	0.41
2:B:117:ALA:HB2	2:B:140:VAL:HG23	2.01	0.41
1:A:106:GLU:OE2	1:A:107:LYS:HE3	2.21	0.41
1:A:29:SER:H	1:A:49:TYR:HA	1.86	0.41
2:D:113:LYS:HD2	2:D:115:LYS:HE2	2.03	0.41
1:C:232:ARG:HG3	1:C:248:ARG:HG2	2.03	0.41
1:C:129:LEU:HD12	2:D:123:ARG:HH11	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	232/240 (97%)	220 (95%)	12 (5%)	0	100	100
1	C	232/240 (97%)	219 (94%)	13 (6%)	0	100	100
2	B	113/142 (80%)	102 (90%)	11 (10%)	0	100	100
2	D	109/142 (77%)	98 (90%)	11 (10%)	0	100	100
All	All	686/764 (90%)	639 (93%)	47 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	206/212 (97%)	206 (100%)	0	100	100
1	C	205/212 (97%)	205 (100%)	0	100	100
2	B	103/127 (81%)	103 (100%)	0	100	100
2	D	99/127 (78%)	97 (98%)	2 (2%)	48	66
All	All	613/678 (90%)	611 (100%)	2 (0%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	40	ASN
2	D	75	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	181	ASN
2	B	110	ASN

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Mol	Chain	Res	Type
2	B	119	ASN
1	C	111	HIS
2	D	110	ASN
2	D	119	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$
3	NAG	E	1	3,1	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
3	NAG	E	2	3	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	F	1	2,3	14,14,15	0.60	0	17,19,21	0.84	0
3	NAG	F	2	3	14,14,15	0.84	0	17,19,21	0.89	1 (5%)
3	NAG	G	1	2,3	14,14,15	1.12	2 (14%)	17,19,21	2.52	7 (41%)
3	NAG	G	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.29	4 (23%)

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	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-2.61	1.39	1.43
3	G	2	NAG	C1-C2	2.35	1.55	1.52
3	G	1	NAG	C1-C2	2.02	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	5.58	119.67	112.19
3	G	1	NAG	O6-C6-C5	-4.21	96.99	111.33
3	G	1	NAG	C3-C4-C5	-3.71	103.50	110.23
3	G	1	NAG	C2-N2-C7	3.55	127.66	122.90
3	G	1	NAG	O5-C1-C2	-3.44	105.97	111.29
3	G	1	NAG	O5-C5-C6	-3.27	101.29	107.66
3	G	2	NAG	C1-O5-C5	2.39	115.39	112.19
3	F	2	NAG	C1-O5-C5	2.32	115.30	112.19
3	G	2	NAG	O6-C6-C5	-2.30	103.50	111.33
3	G	2	NAG	O5-C1-C2	-2.21	107.88	111.29
3	G	2	NAG	C3-C4-C5	-2.10	106.42	110.23
3	G	1	NAG	C6-C5-C4	2.08	118.13	113.02
3	E	1	NAG	O3-C3-C4	2.08	115.27	110.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

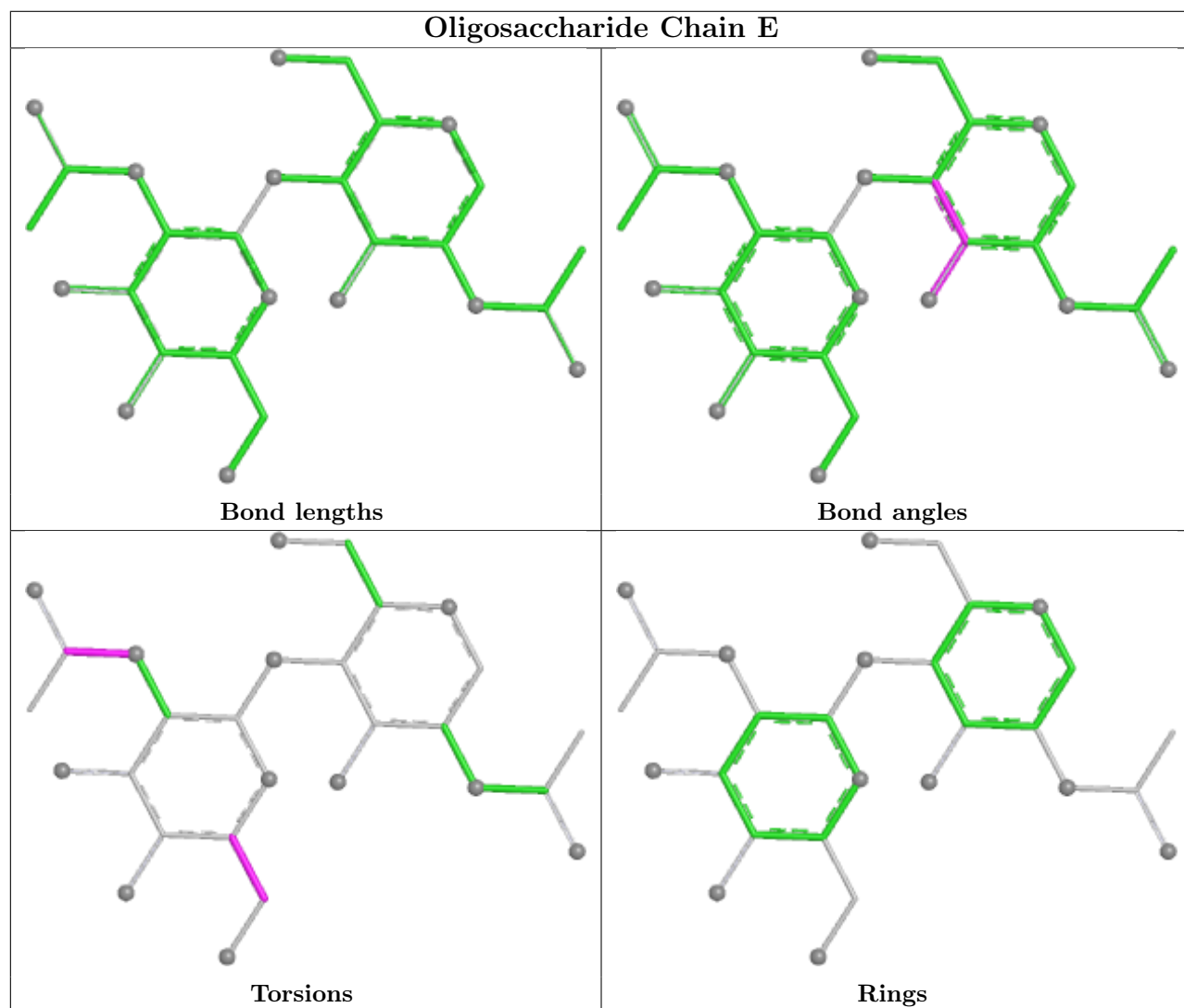
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6

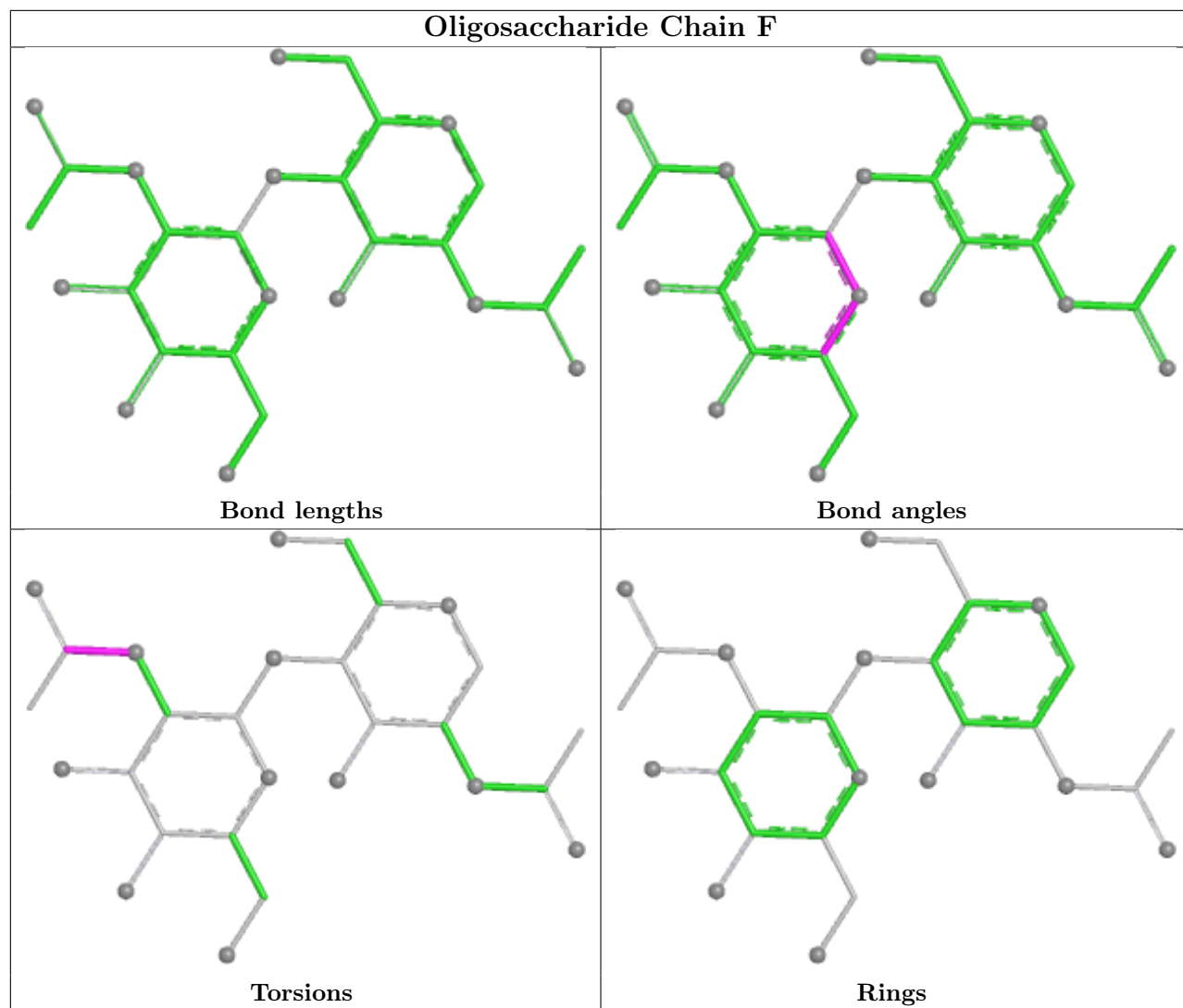
There are no ring outliers.

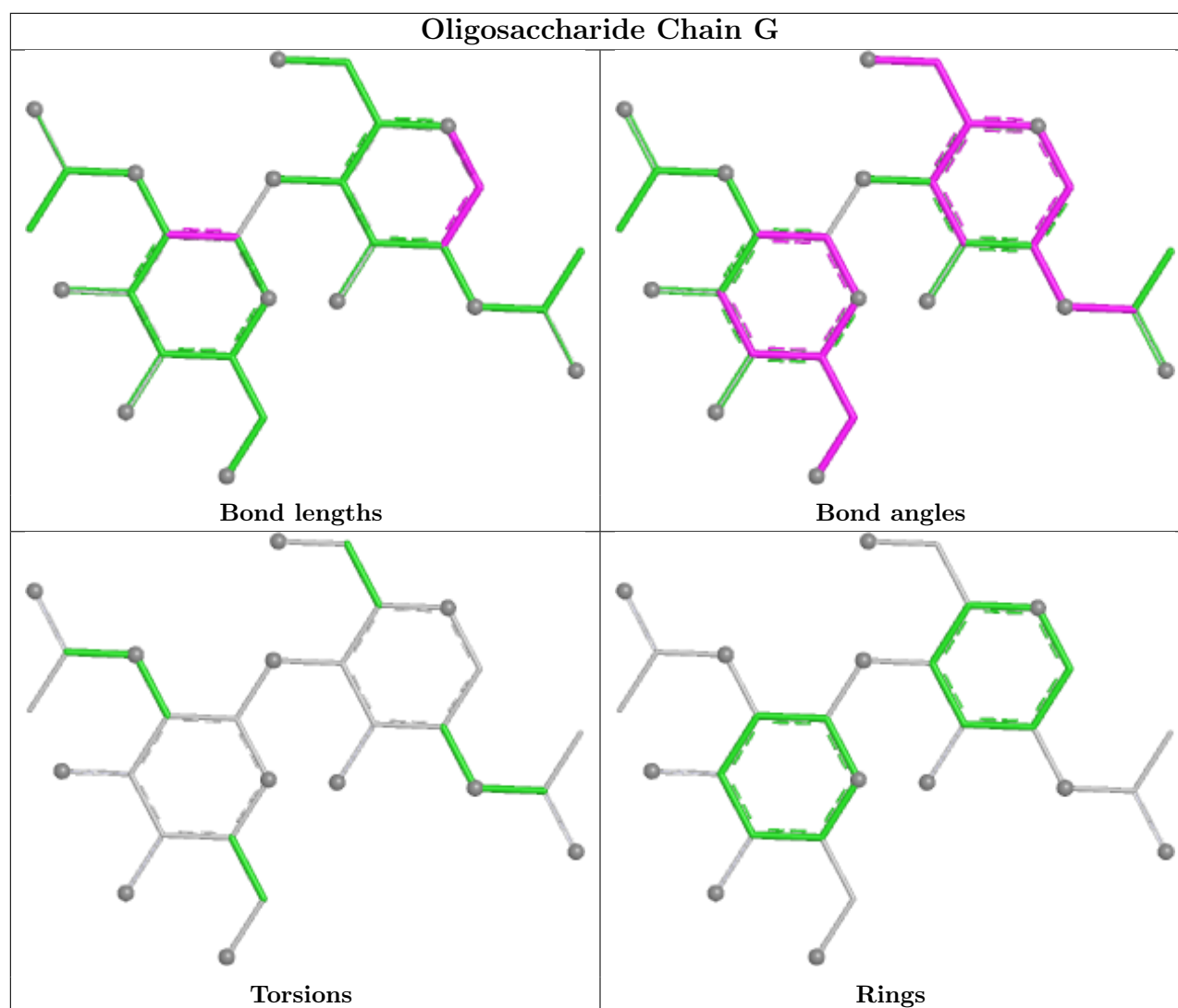
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	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.







5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
4	NAG	C	901	1	14,14,15	0.69	0	17,19,21	1.09	1 (5%)
4	NAG	A	301	1	14,14,15	0.67	0	17,19,21	1.03	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
4	NAG	C	901	1	-	0/6/23/26	0/1/1/1
4	NAG	A	301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	NAG	C1-O5-C5	2.29	115.25	112.19
4	C	901	NAG	O5-C1-C2	-2.04	108.13	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	NAG	C8-C7-N2-C2
4	A	301	NAG	O7-C7-N2-C2

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	234/240 (97%)	0.79	20 (8%) 16 17	44, 75, 104, 126	0
1	C	234/240 (97%)	0.95	35 (14%) 5 8	45, 81, 125, 147	0
2	B	115/142 (80%)	1.00	19 (16%) 4 7	45, 76, 131, 154	0
2	D	111/142 (78%)	1.09	16 (14%) 6 9	52, 76, 118, 135	0
All	All	694/764 (90%)	0.93	90 (12%) 7 10	44, 79, 120, 154	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	ASP	6.9
2	B	85	HIS	4.9
2	D	81	GLY	4.6
2	D	32	GLY	4.5
2	B	30	PRO	4.3
2	D	78	ALA	4.1
1	C	210	HIS	4.0
2	D	36	ARG	3.9
1	A	257	HIS	3.9
1	A	24	ASP	3.8
2	D	80	ALA	3.7
2	D	142	VAL	3.5
1	A	224	SER	3.5
1	C	205	HIS	3.4
1	A	209	SER	3.2
1	A	187	GLY	3.2
2	B	49	VAL	3.2
2	B	80	ALA	3.2
1	A	53	ASN	3.2
1	A	46	PHE	3.2
2	D	86	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	225	LYS	3.1
2	D	106	GLU	3.1
2	D	90	GLU	3.1
2	D	79	HIS	3.0
1	C	153	HIS	3.0
2	D	101	HIS	3.0
1	C	165	CYS	2.9
1	A	241	ALA	2.9
2	D	54	ALA	2.9
1	A	188	HIS	2.9
1	C	257	HIS	2.8
1	C	178	TRP	2.8
1	C	202	ASP	2.8
1	A	91	ASP	2.8
1	C	160	TYR	2.8
1	C	187	GLY	2.8
2	B	78	ALA	2.8
2	B	104	PRO	2.8
2	B	144	PRO	2.7
1	C	162	GLU	2.7
1	A	210	HIS	2.7
2	D	49	VAL	2.7
2	B	52	SER	2.7
1	A	205	HIS	2.6
2	B	141	VAL	2.6
1	C	52	GLY	2.6
1	C	51	MET	2.6
1	C	27	HIS	2.6
1	A	225	LYS	2.5
1	C	228	MET	2.5
2	B	100	THR	2.5
2	B	79	HIS	2.4
2	D	85	HIS	2.4
2	D	39	VAL	2.4
2	B	53	GLN	2.4
2	B	86	TRP	2.4
1	A	194	ILE	2.4
2	B	31	ASP	2.4
1	C	67	GLU	2.4
2	D	51	SER	2.3
1	C	81	TRP	2.3
1	C	238	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	163	ALA	2.3
1	C	196	GLU	2.3
1	C	212	HIS	2.3
1	A	101	CYS	2.3
1	C	53	ASN	2.3
1	C	80	ASN	2.3
1	C	86	GLY	2.3
1	C	26	LEU	2.2
2	B	33	GLU	2.2
1	C	192	PRO	2.2
2	B	54	ALA	2.2
1	A	189	SER	2.2
2	B	46	LYS	2.2
1	C	220	GLN	2.1
1	C	224	SER	2.1
1	A	228	MET	2.1
1	C	215	LEU	2.1
1	A	220	GLN	2.1
1	A	196	GLU	2.1
2	B	82	THR	2.1
1	C	25	PRO	2.1
1	C	164	ASN	2.1
2	B	99	ARG	2.1
1	A	47	CYS	2.1
1	C	122	GLY	2.0
1	C	250	ARG	2.0
1	C	95	HIS	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.

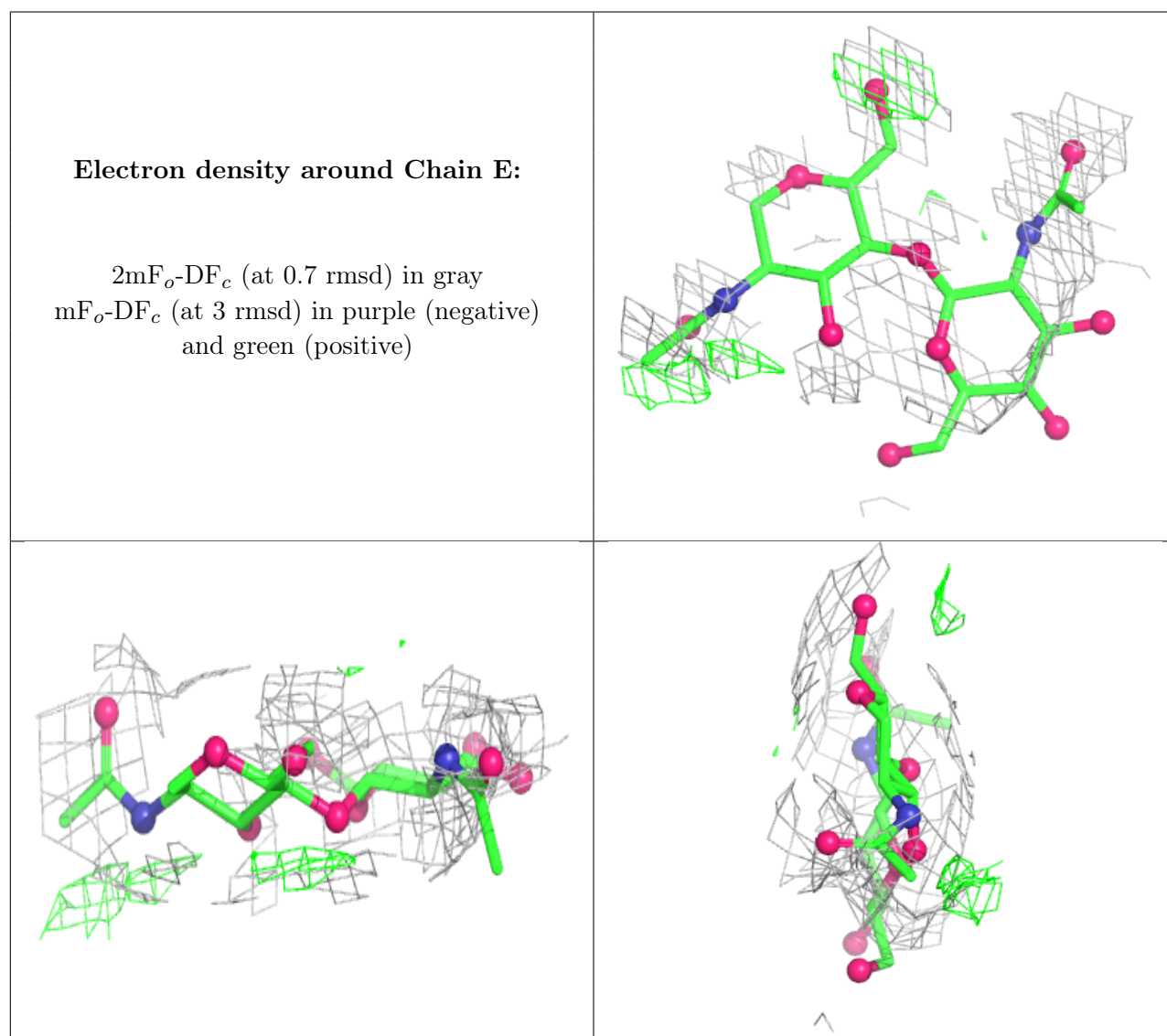
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	2	14/15	0.57	0.26	101,155,173,178	0

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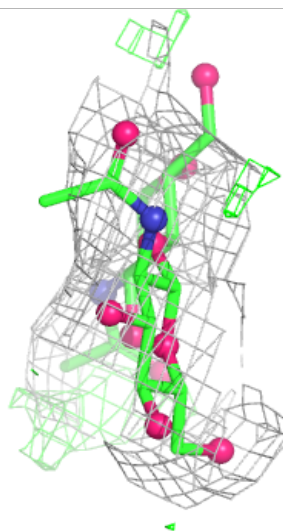
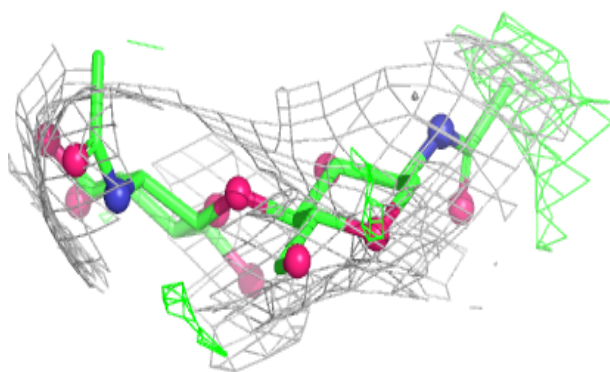
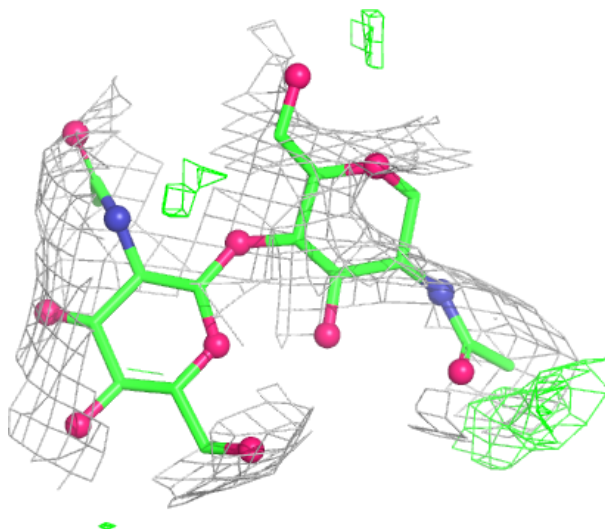
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	2	14/15	0.60	0.29	93,136,144,157	0
3	NAG	F	1	14/15	0.73	0.23	46,121,147,151	0
3	NAG	F	2	14/15	0.80	0.18	71,135,154,160	0
3	NAG	G	1	14/15	0.83	0.18	73,130,158,160	0
3	NAG	E	1	14/15	0.83	0.15	59,79,120,140	0

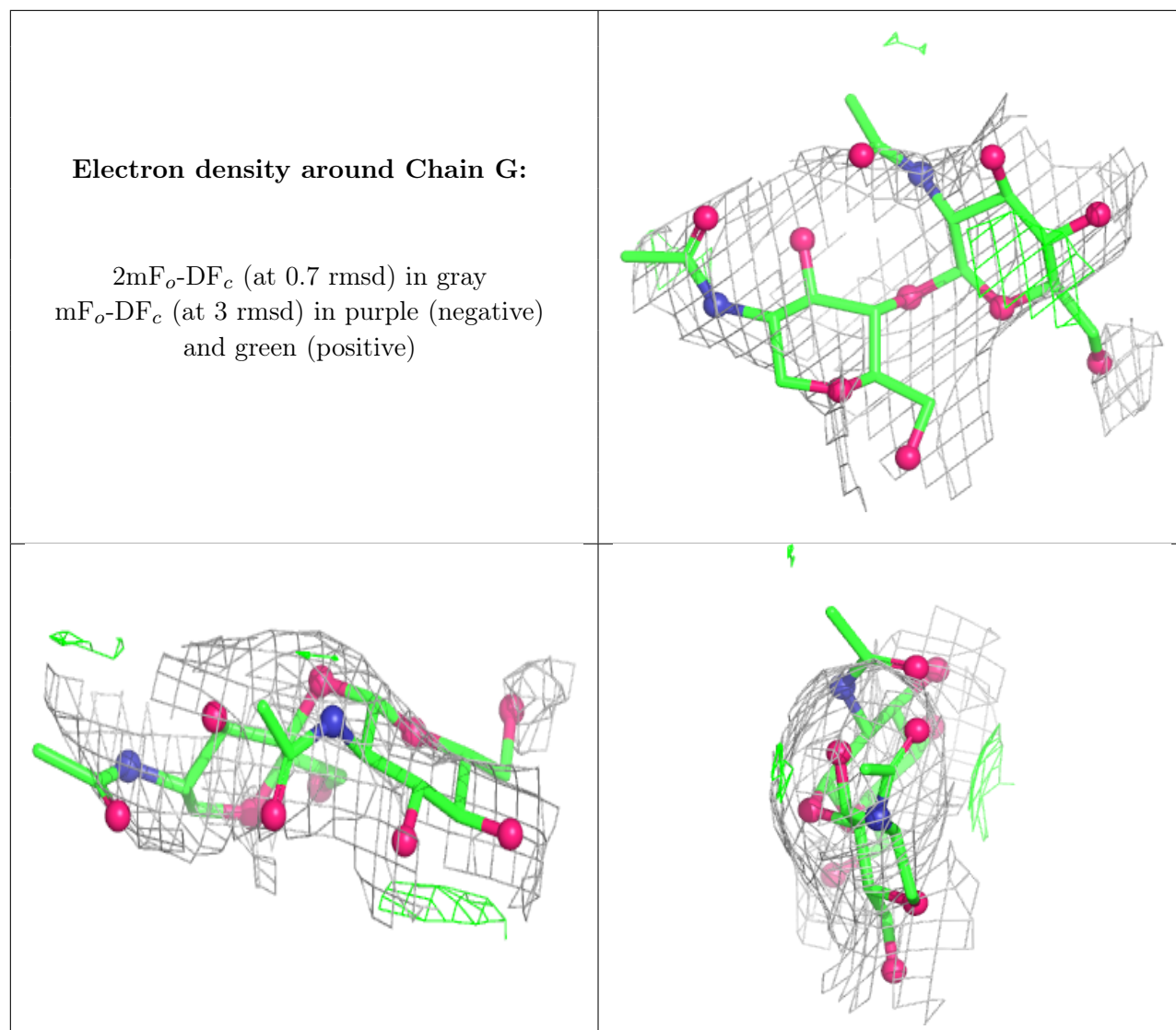
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

$2mF_o-DF_c$ (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
4	NAG	A	301	14/15	0.67	0.17	60,120,146,151	0
4	NAG	C	901	14/15	0.74	0.21	46,92,114,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.