



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:13 AM UTC

PDB ID : 8UKV / pdb_00008ukv
Title : Crystal structure of nanobody/VHH domain of 34E5 in complex with the extracellular region of the epidermal growth factor variant III (EGFRvIII)
Authors : Stayrook, S.E.; Ferguson, K.M.; Bagchi, A.
Deposited on : 2023-10-15
Resolution : 2.94 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

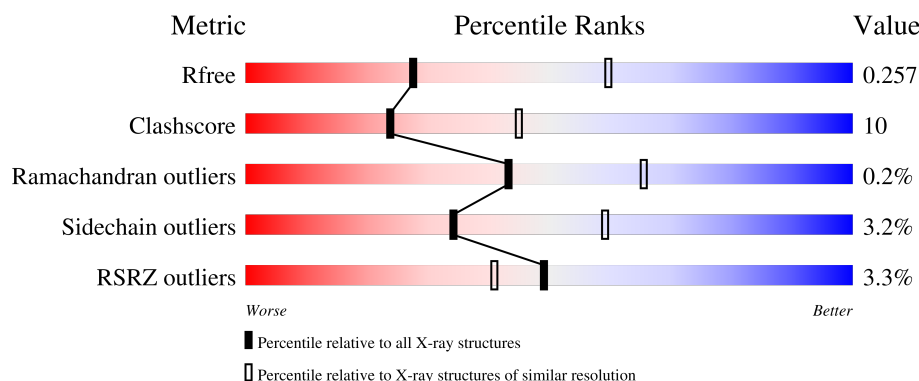
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	357	 3% 67% 22% 10%
1	B	357	 3% 71% 15% 13%
2	C	141	 3% 60% 25% 16%
2	D	141	 3% 53% 29% 16%
3	E	2	 100%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	G	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6739 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2446	1511	438	467	30			
1	B	310	Total	C	N	O	S	0	0	0
			2352	1453	424	447	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	VAL	engineered mutation	UNP P00533
A	619	HIS	-	expression tag	UNP P00533
A	620	HIS	-	expression tag	UNP P00533
A	621	HIS	-	expression tag	UNP P00533
A	622	HIS	-	expression tag	UNP P00533
A	623	HIS	-	expression tag	UNP P00533
A	624	HIS	-	expression tag	UNP P00533
B	273	GLY	VAL	engineered mutation	UNP P00533
B	619	HIS	-	expression tag	UNP P00533
B	620	HIS	-	expression tag	UNP P00533
B	621	HIS	-	expression tag	UNP P00533
B	622	HIS	-	expression tag	UNP P00533
B	623	HIS	-	expression tag	UNP P00533
B	624	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Nanobody/VHH domain 34E5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	119	Total	C	N	O	S	0	0	0
			924	574	163	182	5			
2	D	118	Total	C	N	O	S	0	0	0
			919	571	162	181	5			

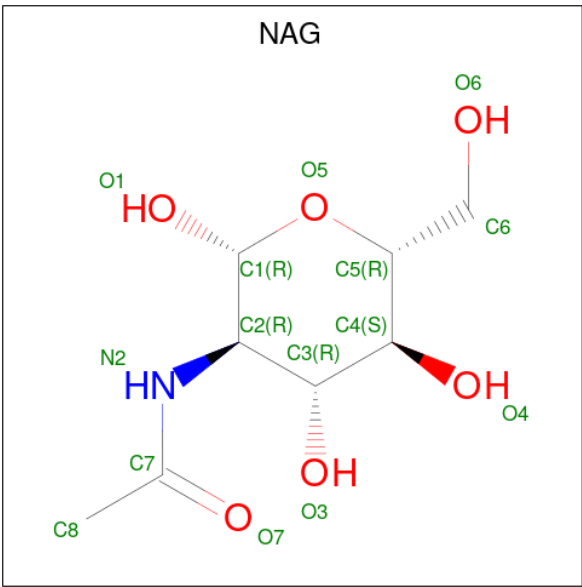
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-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).

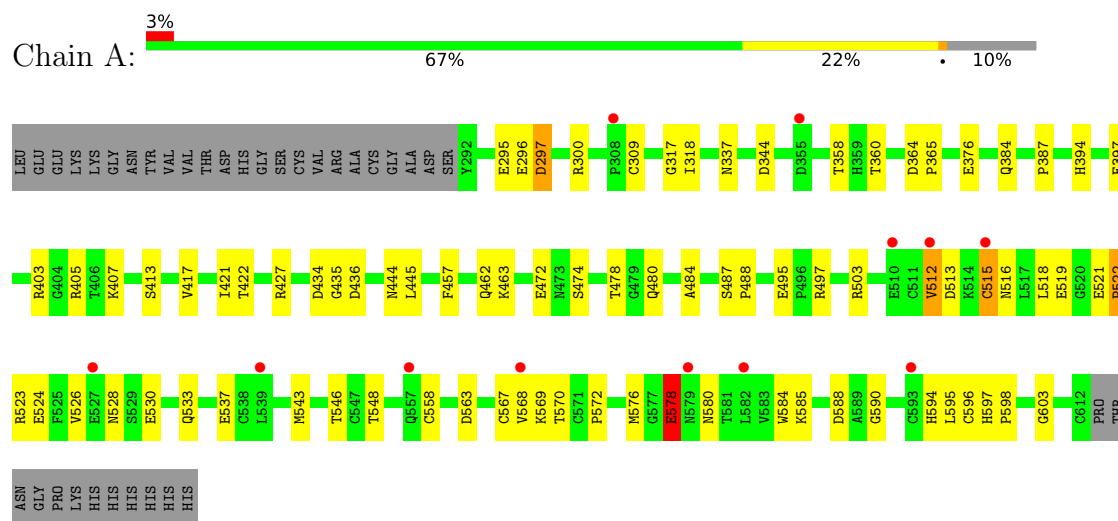


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

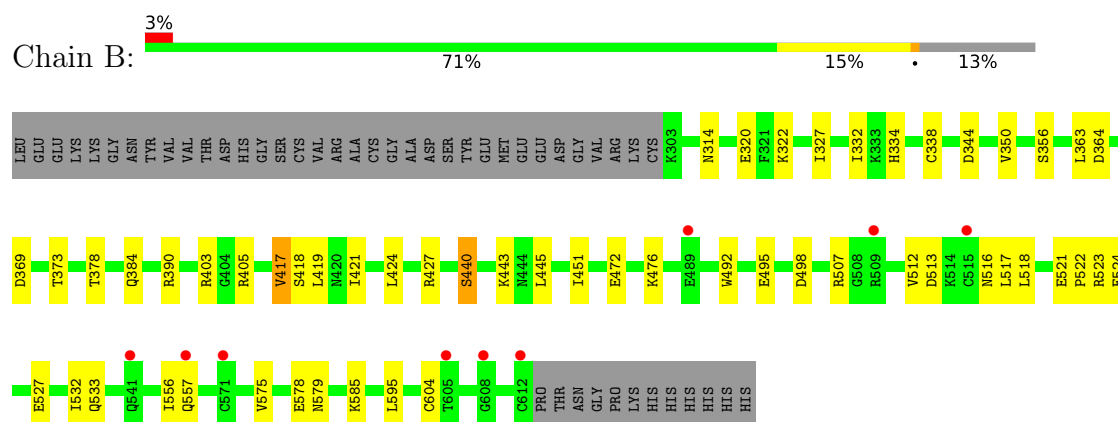
3 Residue-property plots [i](#)

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.

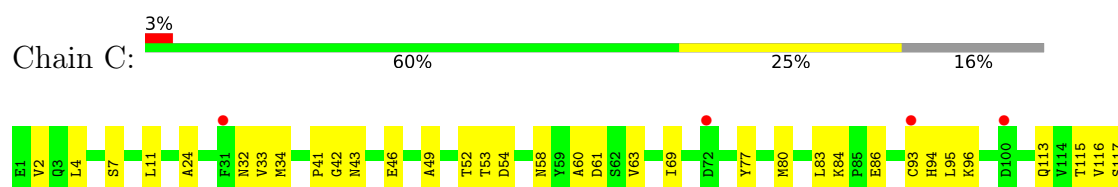
- Molecule 1: Epidermal growth factor receptor

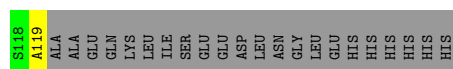


- Molecule 1: Epidermal growth factor receptor

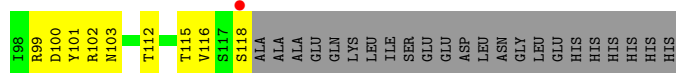


- Molecule 2: Nanobody/VHH domain 34E5





- Molecule 2: Nanobody/VHH domain 34E5



- 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 1	Depositor
Cell constants a, b, c, α , β , γ	66.29Å 80.36Å 91.84Å 106.92° 103.50° 104.56°	Depositor
Resolution (Å)	46.55 – 2.94 46.55 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.55-2.94) 98.2 (46.55-2.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.215 , 0.252 0.228 , 0.257	Depositor DCC
R_{free} test set	1682 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6739	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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

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	0.27	0/2496	0.53	1/3377 (0.0%)
1	B	0.26	0/2401	0.52	0/3253
2	C	0.28	0/942	0.51	0/1276
2	D	0.23	0/937	0.53	0/1269
All	All	0.26	0/6776	0.52	1/9175 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CA-CB-CG	5.70	118.30	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	GLU	Peptide
1	B	523	ARG	Sidechain

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	2446	0	2358	56	0
1	B	2352	0	2262	31	0
2	C	924	0	889	22	0
2	D	919	0	886	28	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
4	A	14	0	13	1	0
All	All	6739	0	6483	134	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 (134) 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)
2:D:99:ARG:HD2	2:D:103:ASN:HB3	1.28	1.08
1:A:484:ALA:O	1:A:503:ARG:NH1	2.06	0.88
1:B:521:GLU:HB3	1:B:522:PRO:HD3	1.64	0.79
2:D:28:ILE:HA	2:D:97:ASN:HD21	1.47	0.78
1:A:521:GLU:HB3	1:A:522:PRO:HD3	1.67	0.77
2:D:66:ARG:NH2	2:D:87:ASP:OD2	2.18	0.77
1:B:522:PRO:HB2	1:B:533:GLN:HG2	1.69	0.73
1:B:320:GLU:OE1	1:B:334:HIS:ND1	2.23	0.69
1:A:568:VAL:HG12	1:A:570:THR:H	1.58	0.69
1:B:338:CYS:O	1:B:373:THR:OG1	2.14	0.66
1:A:436:ASP:OD1	1:A:463:LYS:N	2.25	0.66
1:A:478:THR:HG23	1:A:480:GLN:HG3	1.76	0.65
1:A:512:VAL:HG12	1:A:513:ASP:H	1.61	0.65
2:C:2:VAL:HG11	2:C:95:LEU:HD13	1.78	0.65
2:D:2:VAL:HG11	2:D:95:LEU:HD13	1.78	0.64
1:A:407:LYS:NZ	1:A:434:ASP:OD2	2.30	0.64
1:A:576:MET:HG3	1:A:580:ASN:HB3	1.80	0.63
2:D:11:LEU:HD22	2:D:118:SER:HB3	1.80	0.63
1:A:472:GLU:H	1:A:472:GLU:CD	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLY:O	2:D:112:THR:HG21	2.01	0.61
1:A:397:GLU:OE1	1:A:427:ARG:NH2	2.35	0.60
1:A:572:PRO:HD2	1:A:585:LYS:HD3	1.83	0.60
2:D:11:LEU:HD23	2:D:115:THR:HB	1.85	0.59
1:B:585:LYS:HE2	1:B:595:LEU:HD23	1.84	0.58
2:C:113:GLN:HE21	2:C:113:GLN:HA	1.68	0.57
2:C:52:THR:HG23	2:C:54:ASP:H	1.68	0.57
2:D:6:GLU:HB3	2:D:93:CYS:SG	2.44	0.57
1:B:421:ILE:HG13	1:B:445:LEU:HD13	1.88	0.56
1:A:519:GLU:HA	1:A:523:ARG:HH21	1.70	0.56
1:A:384:GLN:HG2	1:A:417:VAL:HG23	1.87	0.56
2:D:33:VAL:HG22	2:D:52:THR:HG22	1.88	0.55
1:A:337:ASN:HD22	4:A:701:NAG:H83	1.71	0.55
1:A:584:TRP:CE3	1:A:603:GLY:HA2	2.42	0.55
1:A:519:GLU:N	1:A:519:GLU:OE2	2.40	0.54
1:B:344:ASP:N	1:B:344:ASP:OD1	2.40	0.53
1:A:457:PHE:CD2	1:A:462:GLN:HB3	2.44	0.53
1:A:487:SER:HB2	1:A:488:PRO:HD2	1.91	0.52
1:B:527:GLU:HB3	1:B:532:ILE:HD13	1.92	0.52
2:D:67:PHE:CE1	2:D:80:MET:HG2	2.45	0.52
1:A:515:CYS:SG	1:A:526:VAL:HG12	2.50	0.52
1:B:403:ARG:HD3	1:B:405:ARG:NH2	2.25	0.52
1:B:513:ASP:OD1	1:B:513:ASP:N	2.36	0.51
2:C:32:ASN:O	2:C:53:THR:HG23	2.11	0.51
1:A:405:ARG:NH1	2:D:41:PRO:HB3	2.26	0.51
2:C:52:THR:HG23	2:C:54:ASP:N	2.26	0.49
1:B:378:THR:HA	1:B:403:ARG:HB2	1.93	0.49
1:A:444:ASN:N	1:A:444:ASN:OD1	2.46	0.49
1:B:557:GLN:HB2	2:D:102:ARG:HA	1.94	0.49
2:C:33:VAL:HG13	2:C:96:LYS:HB3	1.95	0.49
2:D:69:ILE:HD12	2:D:77:TYR:O	2.13	0.49
1:B:517:LEU:HB2	1:B:518:LEU:HD22	1.95	0.48
1:A:537:GLU:OE1	1:A:569:LYS:HG3	2.13	0.48
1:A:518:LEU:HB2	1:A:519:GLU:OE2	2.13	0.48
2:D:85:PRO:HA	2:D:116:VAL:CG2	2.44	0.48
1:B:527:GLU:HB3	1:B:532:ILE:CD1	2.44	0.48
2:D:99:ARG:HH11	2:D:103:ASN:C	2.22	0.48
1:B:556:ILE:HD12	1:B:557:GLN:N	2.29	0.47
1:A:585:LYS:HG2	1:A:595:LEU:HA	1.94	0.47
2:C:80:MET:HB3	2:C:83:LEU:HD21	1.95	0.47
1:B:369:ASP:OD1	1:B:390:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ARG:HA	1:B:492:TRP:CD1	2.49	0.47
2:D:29:PHE:N	2:D:29:PHE:CD1	2.82	0.47
2:D:30:SER:O	2:D:53:THR:HG21	2.15	0.47
1:B:363:LEU:HD12	1:B:364:ASP:N	2.29	0.47
1:B:417:VAL:HA	1:B:440:SER:O	2.15	0.47
2:D:67:PHE:CZ	2:D:80:MET:HG2	2.50	0.47
1:A:578:GLU:HA	1:A:580:ASN:ND2	2.30	0.46
2:C:43:ASN:HD22	2:C:43:ASN:N	2.13	0.46
2:C:60:ALA:HB3	2:C:63:VAL:HG22	1.97	0.46
1:A:317:GLY:O	1:A:318:ILE:HD12	2.16	0.46
1:A:576:MET:CG	1:A:580:ASN:HB3	2.44	0.46
1:B:472:GLU:O	1:B:476:LYS:HG2	2.16	0.46
1:B:314:ASN:HD21	2:C:11:LEU:H	1.62	0.46
1:A:568:VAL:HG12	1:A:569:LYS:N	2.31	0.46
1:B:418:SER:C	1:B:419:LEU:HD12	2.41	0.46
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.81	0.46
2:C:33:VAL:CG1	2:C:96:LYS:HB3	2.45	0.46
1:A:364:ASP:OD1	1:A:365:PRO:HD2	2.15	0.45
2:C:11:LEU:HA	2:C:115:THR:O	2.16	0.45
1:A:422:THR:HA	1:A:444:ASN:O	2.16	0.45
2:D:12:VAL:O	2:D:116:VAL:HA	2.16	0.45
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.81	0.45
1:A:474:SER:O	1:A:478:THR:HG22	2.17	0.45
1:A:584:TRP:CD2	1:A:603:GLY:HA2	2.52	0.45
1:A:295:GLU:HA	1:A:300:ARG:HA	1.99	0.44
1:A:515:CYS:O	1:A:524:GLU:HG3	2.16	0.44
2:C:41:PRO:HA	2:C:42:GLY:HA2	1.72	0.44
1:A:576:MET:HE3	1:A:580:ASN:CB	2.47	0.44
1:A:528:ASN:O	1:A:530:GLU:HG3	2.17	0.44
2:D:36:TRP:CZ3	2:D:76:VAL:HG23	2.53	0.44
1:A:588:ASP:OD1	1:A:590:GLY:N	2.51	0.44
2:D:43:ASN:N	2:D:43:ASN:OD1	2.50	0.44
1:A:376:GLU:OE1	1:A:403:ARG:NE	2.38	0.44
1:A:296:GLU:O	1:A:297:ASP:C	2.61	0.43
1:B:384:GLN:HG2	1:B:417:VAL:HG22	2.00	0.43
2:C:61:ASP:N	2:C:61:ASP:OD1	2.49	0.43
1:A:519:GLU:HA	1:A:523:ARG:NH2	2.33	0.43
2:C:117:SER:C	2:C:119:ALA:H	2.26	0.43
2:D:100:ASP:OD1	2:D:100:ASP:C	2.61	0.43
1:B:327:ILE:CG2	1:B:332:ILE:HD12	2.48	0.43
2:C:4:LEU:HD21	2:C:95:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:HIS:ND1	1:A:598:PRO:HD2	2.34	0.43
1:B:516:ASN:HD22	1:B:522:PRO:HD2	1.83	0.43
1:A:588:ASP:OD2	1:A:594:HIS:HE1	2.01	0.43
2:C:34:MET:HE3	2:C:34:MET:HB2	1.84	0.43
1:A:523:ARG:HD2	1:A:546:THR:OG1	2.19	0.43
1:A:365:PRO:HB3	1:A:387:PRO:CG	2.49	0.42
1:B:578:GLU:O	1:B:579:ASN:C	2.62	0.42
1:A:495:GLU:OE2	1:A:497:ARG:NH1	2.52	0.42
1:A:558:CYS:HB3	1:A:567:CYS:HB3	1.87	0.42
2:C:84:LYS:HB3	2:C:86:GLU:OE2	2.19	0.42
2:D:90:VAL:HG12	2:D:92:TYR:CE2	2.54	0.42
2:C:93:CYS:SG	2:C:94:HIS:N	2.92	0.42
1:A:413:SER:HB3	1:A:435:GLY:HA3	2.02	0.42
1:A:516:ASN:O	1:A:523:ARG:HB2	2.19	0.42
1:B:507:ARG:NH1	1:B:524:GLU:OE2	2.52	0.42
1:B:495:GLU:HB2	1:B:498:ASP:OD2	2.19	0.42
1:B:585:LYS:HE2	1:B:595:LEU:CD2	2.50	0.42
2:D:32:ASN:OD1	2:D:71:ARG:NH2	2.37	0.42
2:D:61:ASP:OD1	2:D:61:ASP:N	2.53	0.42
1:A:512:VAL:HG12	1:A:513:ASP:OD1	2.20	0.42
1:A:524:GLU:HB3	1:A:533:GLN:HA	2.02	0.42
1:A:344:ASP:OD1	1:A:344:ASP:N	2.53	0.41
1:A:358:THR:OG1	1:A:360:THR:HG23	2.20	0.41
1:A:563:ASP:OD1	1:A:563:ASP:C	2.63	0.41
1:B:512:VAL:HG12	1:B:513:ASP:N	2.35	0.41
2:D:69:ILE:HD12	2:D:69:ILE:HA	1.89	0.41
1:A:317:GLY:C	1:A:318:ILE:HD12	2.46	0.41
2:D:20:LEU:HB2	2:D:78:LEU:HB3	2.01	0.41
1:A:421:ILE:HG13	1:A:445:LEU:HD13	2.02	0.41
2:C:4:LEU:HD23	2:C:24:ALA:HB2	2.02	0.41
2:C:69:ILE:HD12	2:C:77:TYR:O	2.20	0.41
2:C:49:ALA:HA	2:C:58:ASN:O	2.21	0.40
2:D:12:VAL:CG1	2:D:116:VAL:HG12	2.52	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	319/357 (89%)	288 (90%)	30 (9%)	1 (0%)	36	59
1	B	308/357 (86%)	274 (89%)	33 (11%)	1 (0%)	36	59
2	C	117/141 (83%)	111 (95%)	6 (5%)	0	100	100
2	D	116/141 (82%)	108 (93%)	8 (7%)	0	100	100
All	All	860/996 (86%)	781 (91%)	77 (9%)	2 (0%)	43	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	443	LYS
1	A	522	PRO

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	276/307 (90%)	268 (97%)	8 (3%)	37	62
1	B	265/307 (86%)	257 (97%)	8 (3%)	36	61
2	C	100/119 (84%)	97 (97%)	3 (3%)	36	61
2	D	100/119 (84%)	95 (95%)	5 (5%)	22	46
All	All	741/852 (87%)	717 (97%)	24 (3%)	34	59

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

Mol	Chain	Res	Type
1	A	309	CYS
1	A	394	HIS
1	A	512	VAL
1	A	515	CYS
1	A	543	MET
1	A	548	THR
1	A	578	GLU
1	A	596	CYS
1	B	322	LYS
1	B	350	VAL
1	B	356	SER
1	B	417	VAL
1	B	440	SER
1	B	451	ILE
1	B	575	VAL
1	B	604	CYS
2	C	7	SER
2	C	46	GLU
2	C	116	VAL
2	D	7	SER
2	D	25	SER
2	D	66	ARG
2	D	93	CYS
2	D	101	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	566	HIS
1	A	594	HIS
1	B	314	ASN
1	B	346	HIS
1	B	408	GLN
1	B	504	ASN
1	B	579	ASN
2	C	43	ASN
2	C	79	GLN
2	D	39	GLN
2	D	97	ASN
2	D	110	GLN

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	1,3	14,14,15	0.46	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.55	0
3	NAG	F	1	1,3	14,14,15	0.51	0	17,19,21	0.63	0
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	G	1	1,3	14,14,15	0.33	0	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.46	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	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	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

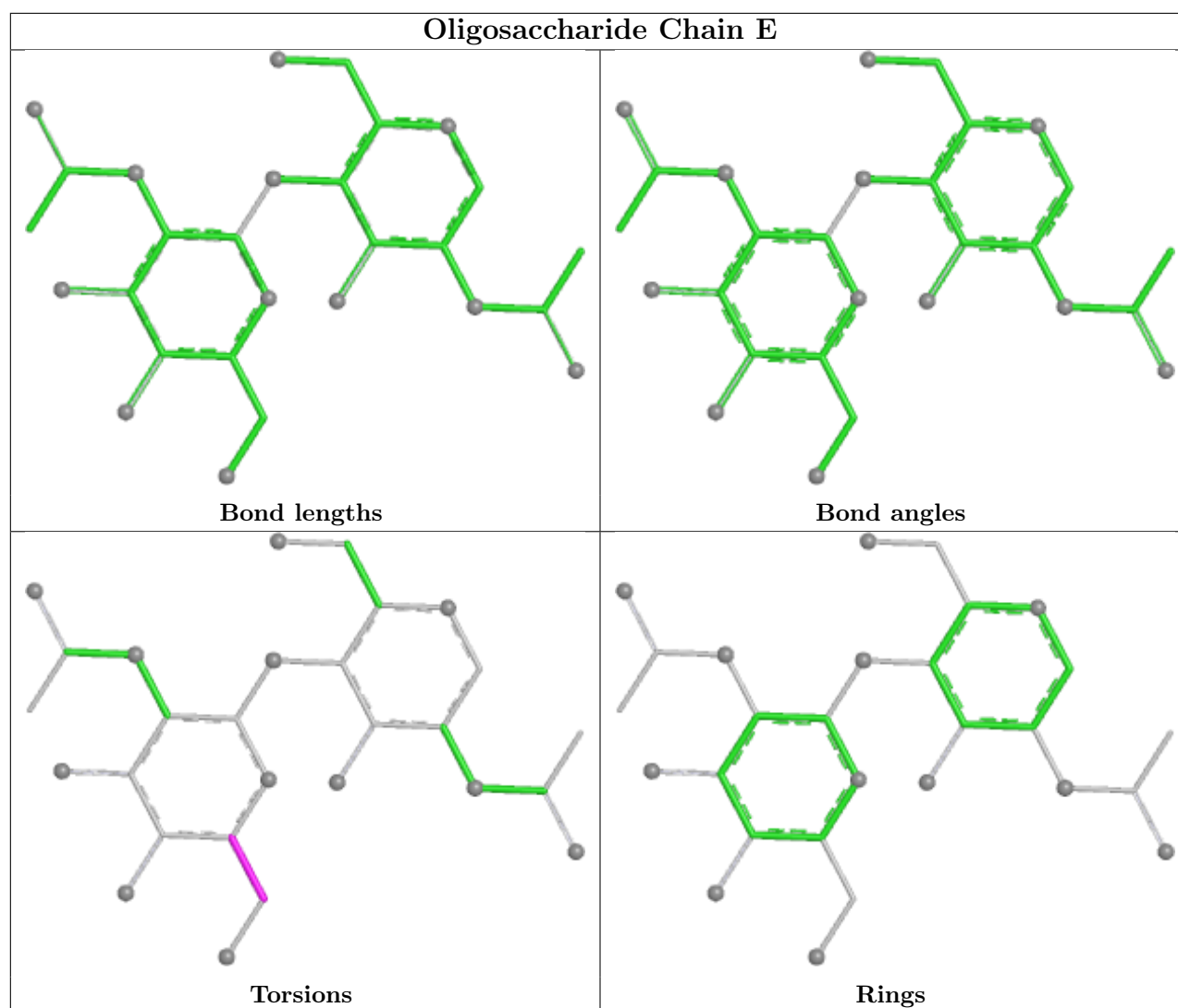
All (10) torsion outliers are listed below:

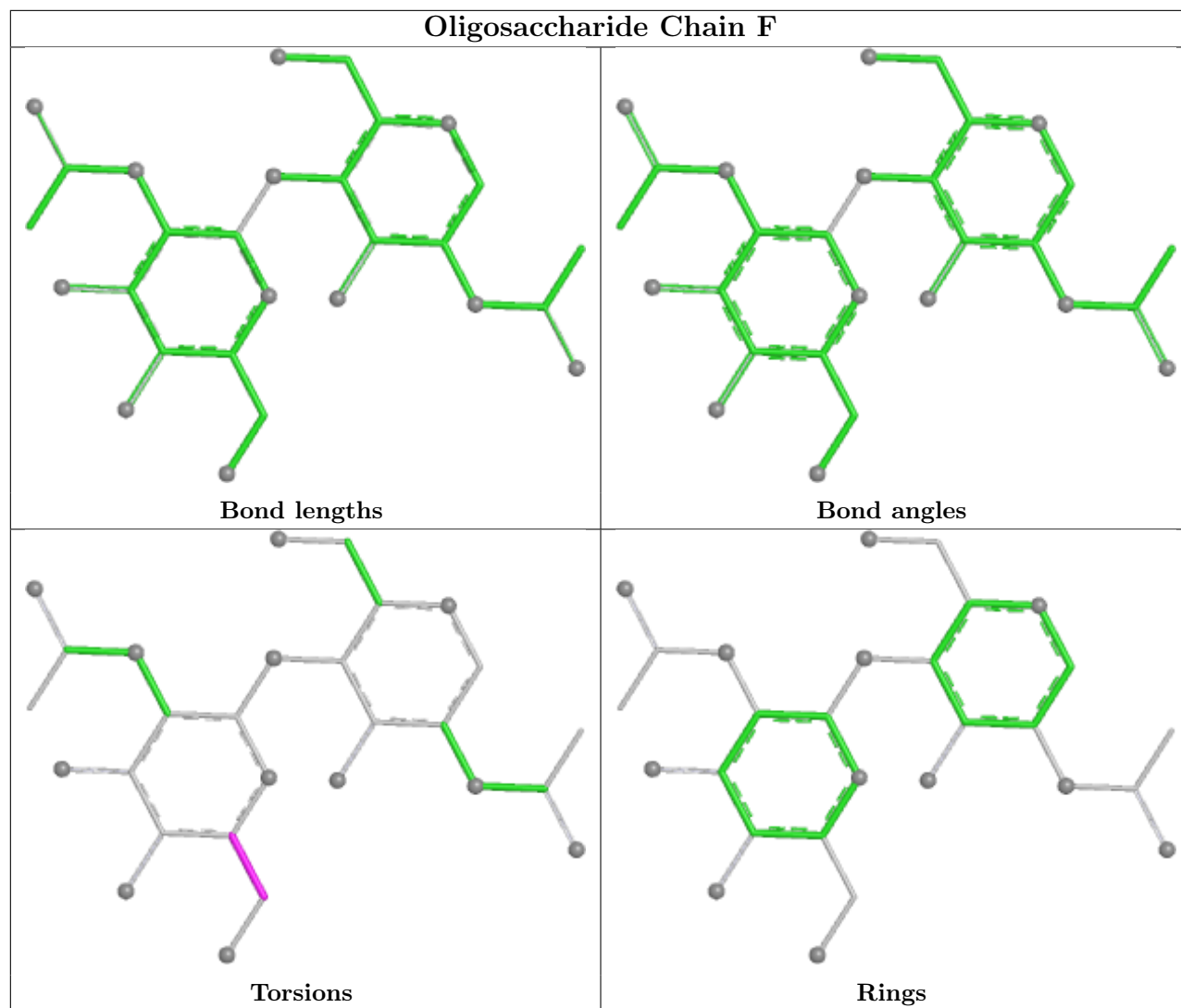
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

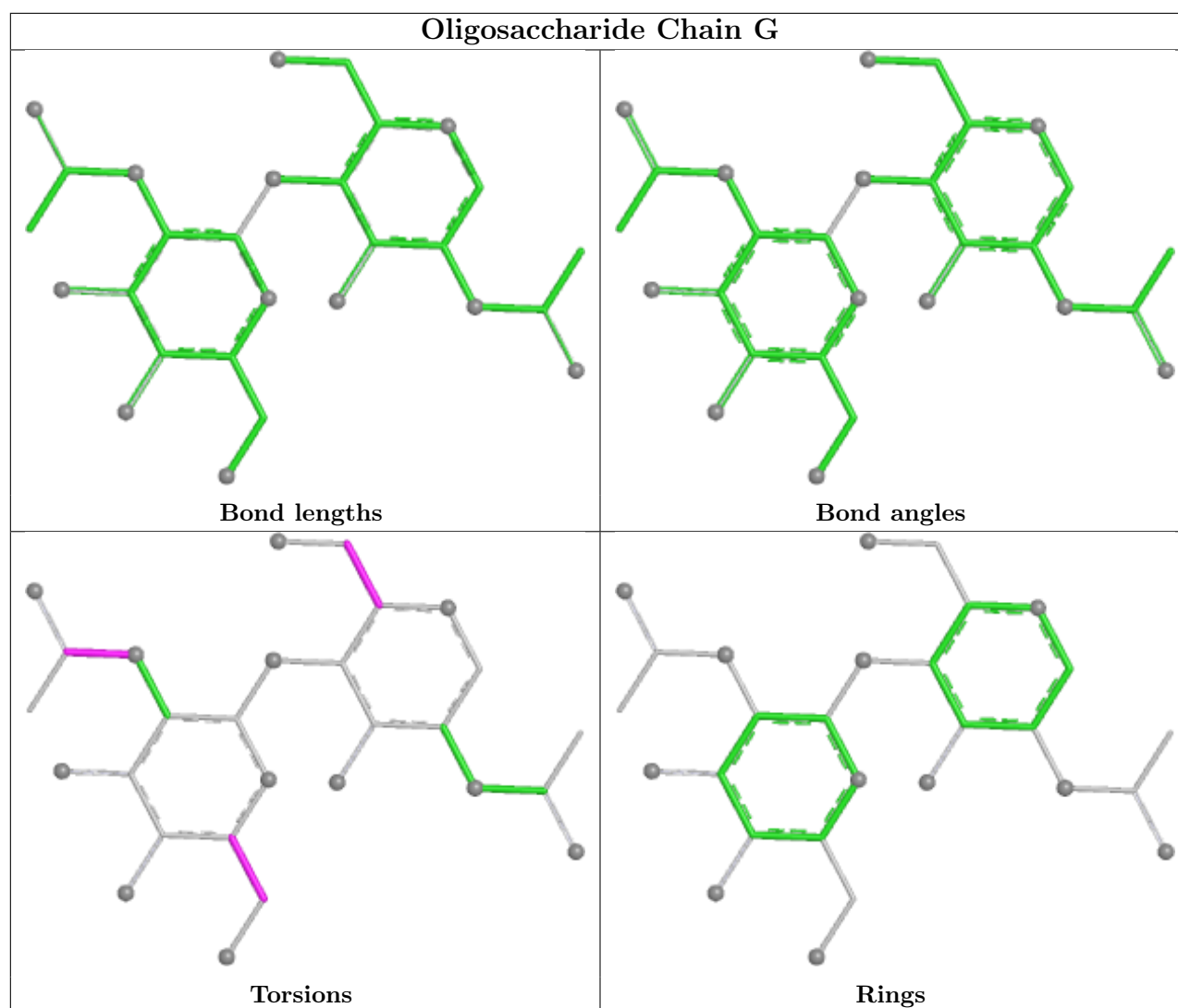
There are no ring outliers.

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	701	1	14,14,15	0.31	0	17,19,21	0.59	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
4	NAG	A	701	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	O5-C5-C6-O6
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	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, 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	321/357 (89%)	0.44	12 (3%) 45 36	53, 95, 180, 219	0
1	B	310/357 (86%)	0.25	9 (2%) 53 44	47, 82, 137, 190	0
2	C	119/141 (84%)	0.41	4 (3%) 48 40	57, 79, 117, 176	0
2	D	118/141 (83%)	0.32	4 (3%) 48 40	55, 86, 116, 155	0
All	All	868/996 (87%)	0.35	29 (3%) 49 41	47, 87, 161, 219	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	118	SER	5.5
1	A	557	GLN	4.4
2	D	54	ASP	4.0
1	A	579	ASN	4.0
1	A	515	CYS	4.0
1	A	593	CYS	3.8
2	C	100	ASP	3.5
1	B	541	GLN	3.2
2	C	72	ASP	2.8
1	A	308	PRO	2.7
1	B	571	CYS	2.7
1	A	510	GLU	2.6
1	A	527	GLU	2.6
1	B	557	GLN	2.6
1	A	539	LEU	2.5
1	A	355	ASP	2.4
1	B	608	GLY	2.4
1	B	509	ARG	2.4
1	B	489	GLU	2.3
1	B	605	THR	2.3
1	A	568	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	612	CYS	2.2
1	A	582	LEU	2.2
2	D	1	GLU	2.2
2	D	46	GLU	2.2
2	C	31	PHE	2.1
2	C	93	CYS	2.1
1	A	512	VAL	2.1
1	B	515	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

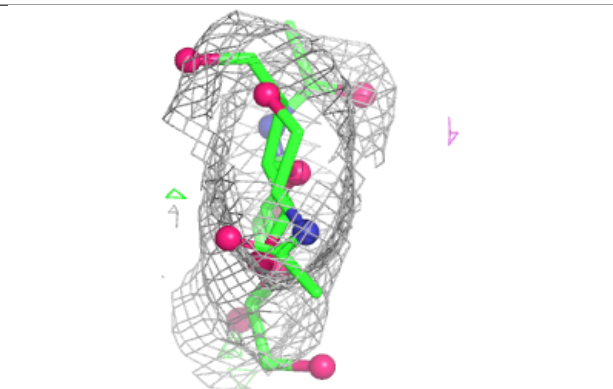
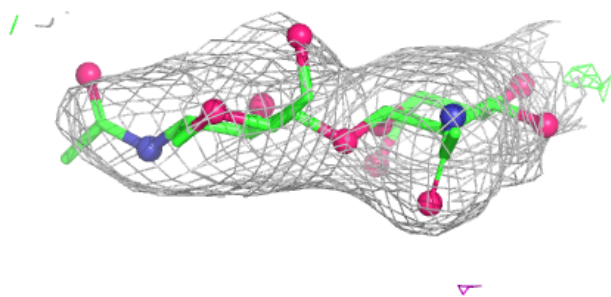
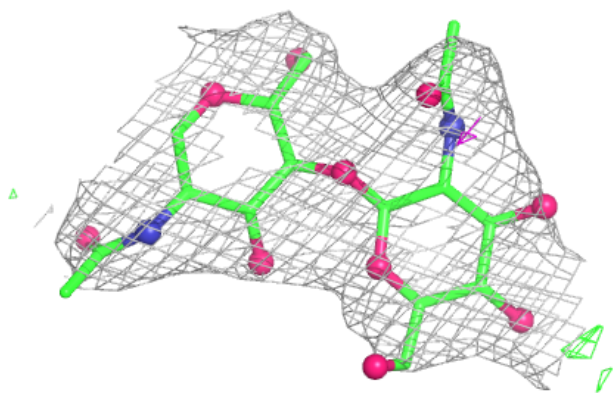
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	G	2	14/15	0.64	0.08	129,131,132,132	0
3	NAG	G	1	14/15	0.87	0.08	117,117,124,127	0
3	NAG	E	2	14/15	0.87	0.13	121,127,129,130	0
3	NAG	F	2	14/15	0.88	0.15	123,127,129,130	0
3	NAG	F	1	14/15	0.96	0.12	117,117,117,123	0
3	NAG	E	1	14/15	0.96	0.13	117,117,117,123	0

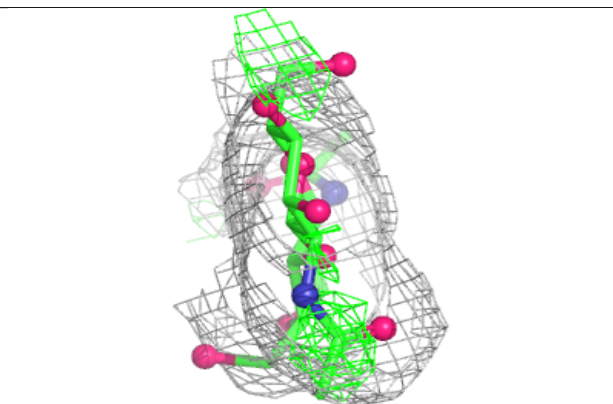
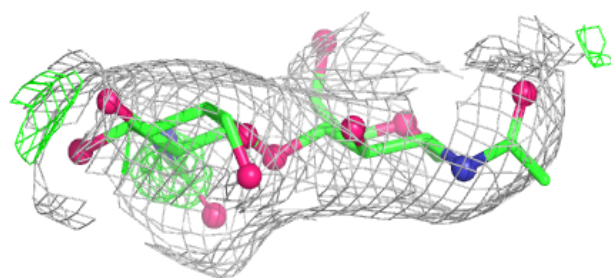
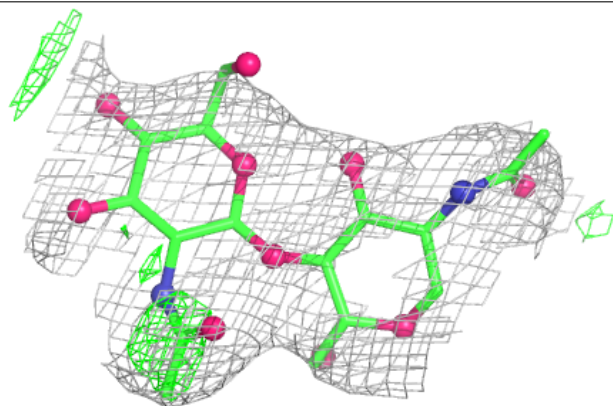
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

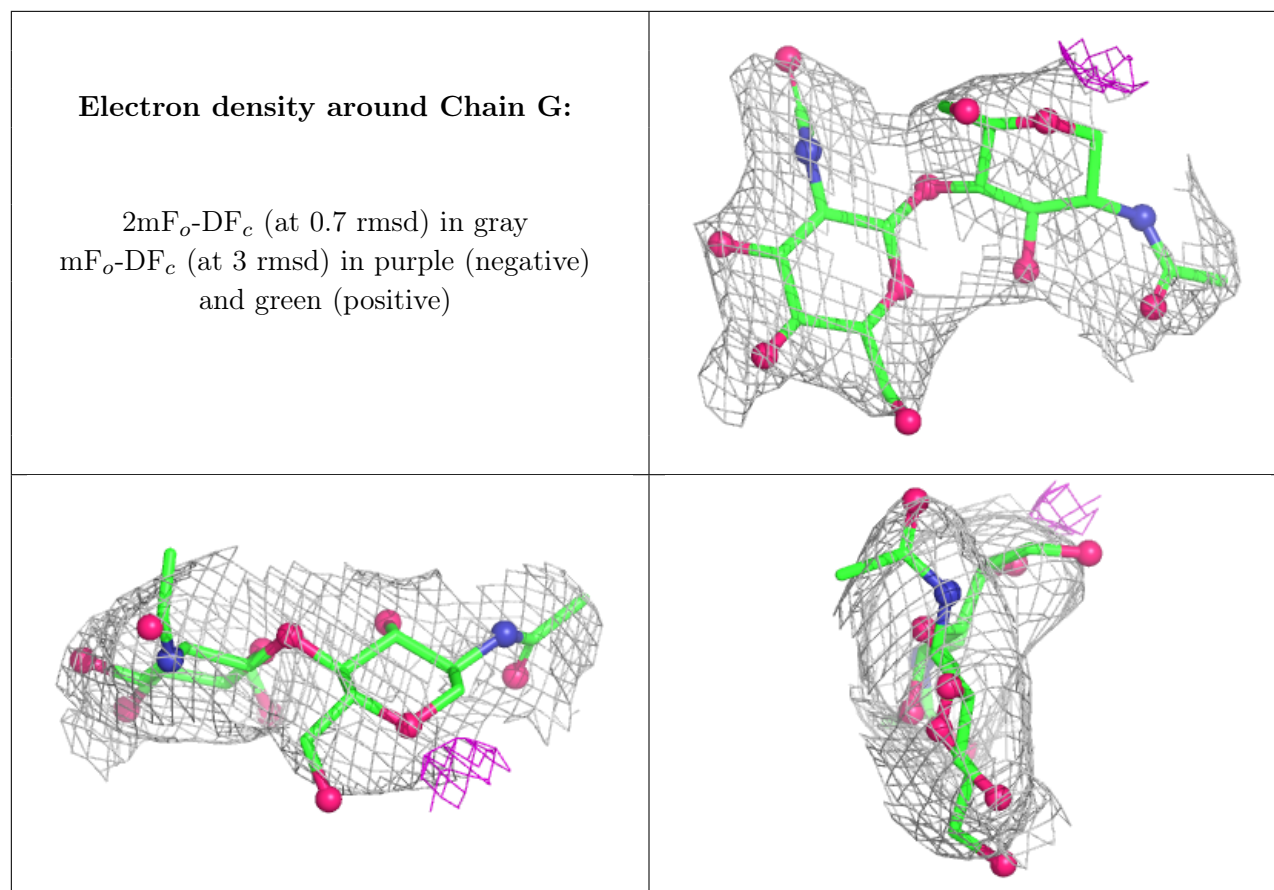
Electron density around Chain E:

$2mF_o-DF_c$ (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)





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	701	14/15	0.57	0.11	120,124,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.