



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:44 AM UTC

PDB ID : 6MYA / pdb_00006mya
Title : Crystal structure of InvbP.18715.a.KN11: Influenza hemagglutinin from strain A/Almaty/32/1998
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-11-01
Resolution : 2.05 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:

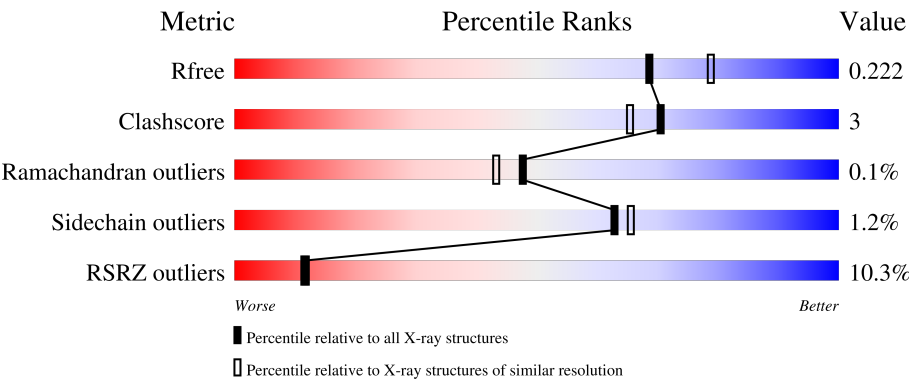
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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.



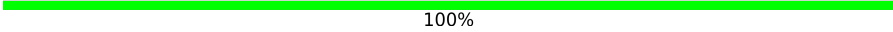
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	499	8% 89%8% ..
1	B	499	10% 86%10% .
1	C	499	2% 89%9% .
1	D	499	15% 87%9% .
1	E	499	12% 91%7% .

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Mol	Chain	Length	Quality of chain
1	F	499	 12% 88% 9%
2	G	2	 50% 50%
2	H	2	 50% 50%
2	I	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 24594 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	8	0
			3784	2384	651	730	19			
1	B	482	Total	C	N	O	S	0	4	0
			3715	2345	640	711	19			
1	C	486	Total	C	N	O	S	0	9	0
			3802	2395	647	741	19			
1	D	478	Total	C	N	O	S	0	7	0
			3650	2300	626	705	19			
1	E	489	Total	C	N	O	S	0	7	0
			3769	2377	647	725	20			
1	F	484	Total	C	N	O	S	0	5	0
			3698	2328	637	713	20			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	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	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		

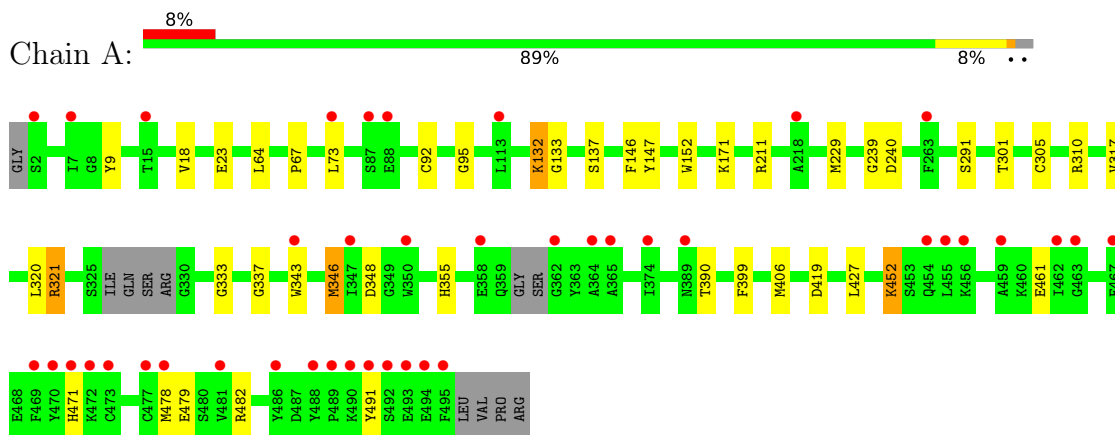
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	261	Total	O	0	3
			264	264		
6	B	295	Total	O	0	4
			299	299		
6	C	320	Total	O	0	3
			323	323		
6	D	309	Total	O	0	3
			312	312		
6	E	283	Total	O	0	1
			284	284		
6	F	289	Total	O	0	2
			291	291		

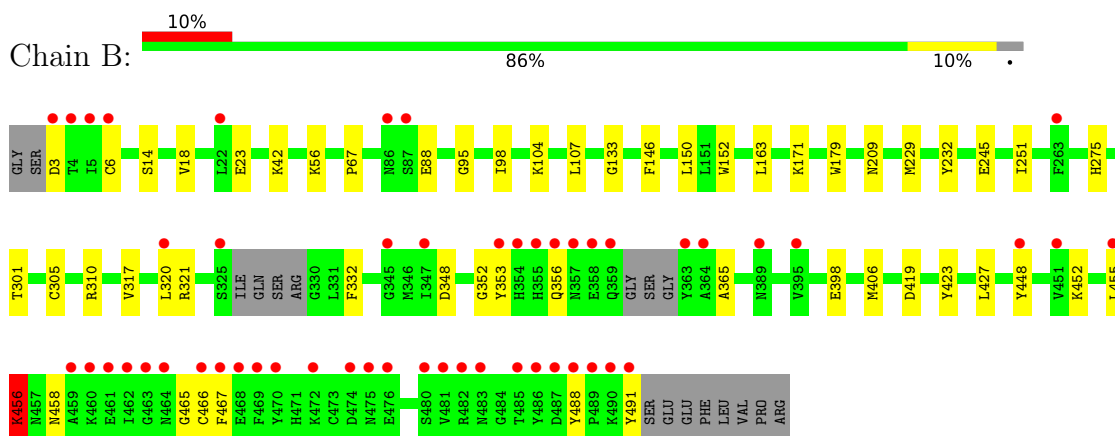
3 Residue-property plots [i](#)

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.

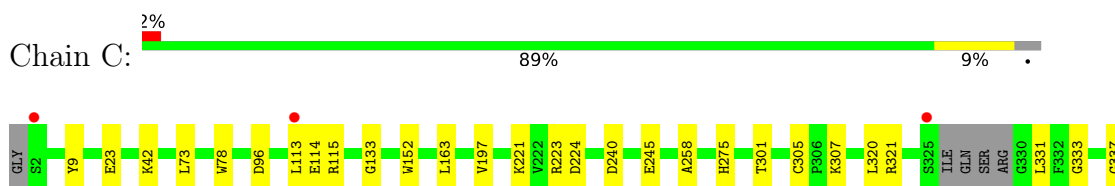
• Molecule 1: Hemagglutinin

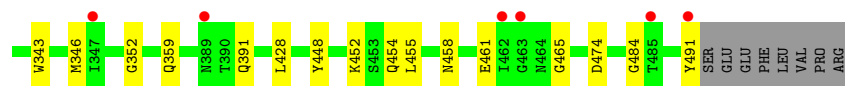


• Molecule 1: Hemagglutinin

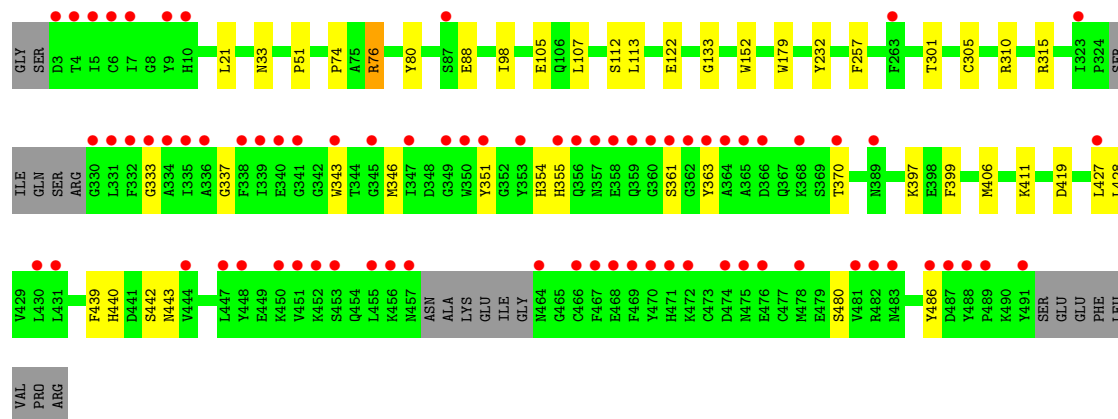
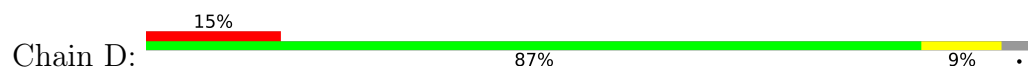


• Molecule 1: Hemagglutinin

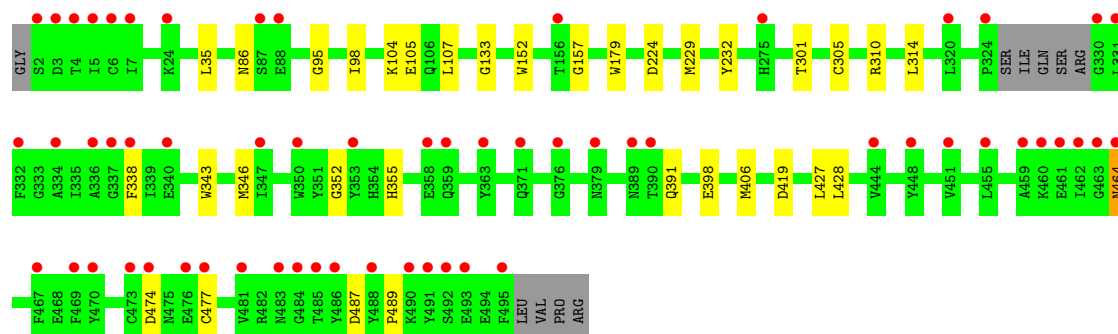
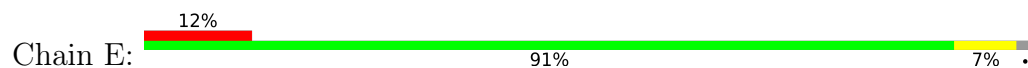




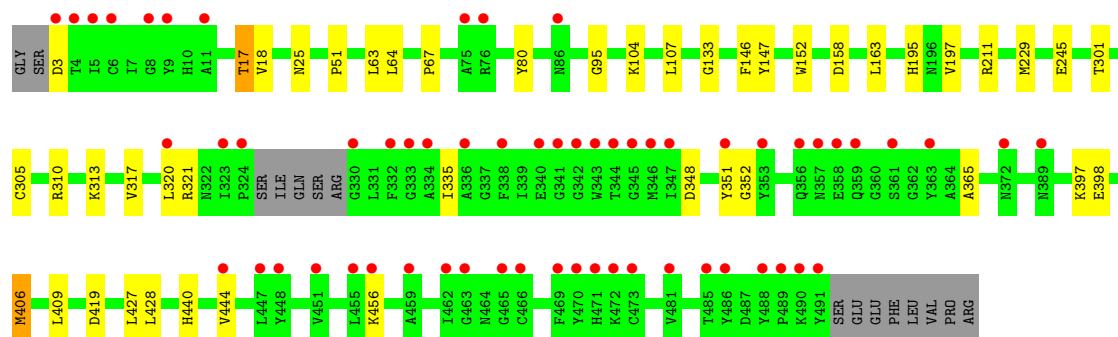
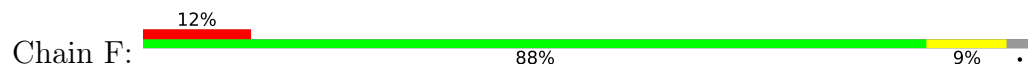
● Molecule 1: Hemagglutinin



● Molecule 1: Hemagglutinin



● Molecule 1: Hemagglutinin



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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.65Å 244.37Å 115.02Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	45.93 – 2.05 45.93 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.93-2.05) 96.5 (45.93-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_3283	Depositor
R, R_{free}	0.188 , 0.222 0.190 , 0.222	Depositor DCC
R_{free} test set	2003 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24594	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: EDO, NAG, PEG

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	0.31	0/3899	0.49	0/5310
1	B	0.33	0/3817	0.53	0/5195
1	C	0.34	0/3920	0.52	0/5332
1	D	0.36	0/3758	0.54	0/5118
1	E	0.33	0/3885	0.50	0/5294
1	F	0.35	0/3804	0.53	0/5186
All	All	0.34	0/23083	0.52	0/31435

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	3784	0	3511	26	0
1	B	3715	0	3462	31	0
1	C	3802	0	3580	29	0
1	D	3650	0	3355	25	0
1	E	3769	0	3480	19	0
1	F	3698	0	3399	26	0
2	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	56	0	52	0	0
3	B	42	0	39	0	0
3	C	56	0	52	0	0
3	D	14	0	13	0	0
3	E	28	0	26	0	0
3	F	28	0	26	0	0
4	A	12	0	18	2	0
4	C	36	0	54	4	0
4	D	16	0	24	0	0
4	E	16	0	24	2	0
4	F	8	0	12	1	0
5	E	7	0	10	0	0
6	A	264	0	0	2	0
6	B	299	0	0	1	0
6	C	323	0	0	2	0
6	D	312	0	0	2	0
6	E	284	0	0	1	0
6	F	291	0	0	2	0
All	All	24594	0	21212	149	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 (149) 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:C:23:GLU:OE1	1:C:321:ARG:NH2	2.13	0.77
1:A:399:PHE:CE1	1:A:406:MET:HG2	2.23	0.74
1:A:406:MET:HE1	1:B:406:MET:HG3	1.73	0.69
1:C:343:TRP:HE3	1:C:346:MET:HE2	1.58	0.69
1:B:104:LYS:NZ	1:B:398:GLU:OE1	2.26	0.68
1:E:98[A]:ILE:HG13	1:E:232:TYR:CE2	2.31	0.65
1:F:335:ILE:HG13	1:F:444:VAL:HG21	1.79	0.64
1:F:351:TYR:OH	1:F:440:HIS:ND1	2.25	0.64
1:E:104:LYS:HB3	4:E:508:EDO:H12	1.78	0.64
1:F:63:LEU:HD11	1:F:107:LEU:HD11	1.80	0.64
1:E:310:ARG:NH1	1:E:419:ASP:OD1	2.29	0.62
1:C:454:GLN:HE22	1:C:484:GLY:HA2	1.65	0.62
1:D:343:TRP:CE3	1:D:346:MET:HE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:TRP:HE3	1:D:346:MET:HE2	1.65	0.61
1:B:458:ASN:ND2	1:B:491:TYR:HB2	2.16	0.61
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.82	0.60
1:E:343:TRP:HE3	1:E:346:MET:HE2	1.66	0.60
1:B:56:LYS:NZ	1:B:88:GLU:OE2	2.35	0.59
1:B:310:ARG:NH1	1:B:419:ASP:OD1	2.25	0.59
1:E:133:GLY:HA3	1:E:152:TRP:HB3	1.85	0.58
1:A:427:LEU:HD21	1:C:428:LEU:HD13	1.84	0.58
1:B:98[A]:ILE:HG13	1:B:232:TYR:CE2	2.39	0.58
1:C:223:ARG:HH12	4:C:510:EDO:H22	1.70	0.56
1:B:23:GLU:OE1	1:B:321[B]:ARG:NH2	2.31	0.56
1:D:105:GLU:OE1	1:D:397:LYS:HE2	2.05	0.56
1:F:17:THR:OG1	1:F:25:ASN:HA	2.06	0.56
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.88	0.55
1:B:171:LYS:HE2	6:B:624:HOH:O	2.07	0.55
1:E:301:THR:HB	1:E:305:CYS:SG	2.47	0.55
1:B:3:ASP:N	1:B:356:GLN:O	2.40	0.54
1:A:343:TRP:HE3	1:A:346:MET:HE2	1.73	0.54
1:D:480:SER:OG	1:D:486:TYR:HA	2.07	0.54
1:D:133:GLY:HA3	1:D:152:TRP:HB3	1.90	0.53
1:E:105:GLU:HA	4:E:508:EDO:H21	1.91	0.53
1:F:197:VAL:HG12	6:F:812:HOH:O	2.08	0.53
1:B:423:TYR:CZ	1:B:427:LEU:HD12	2.44	0.53
1:D:301:THR:HB	1:D:305:CYS:SG	2.49	0.53
1:D:439:PHE:O	1:D:443:ASN:ND2	2.42	0.53
1:C:240:ASP:HB2	4:C:513:EDO:H11	1.91	0.53
1:D:33:ASN:HB2	1:D:315:ARG:NH2	2.24	0.53
1:B:67:PRO:HG3	1:B:146:PHE:O	2.10	0.52
1:C:454:GLN:NE2	1:C:484:GLY:HA2	2.23	0.52
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.90	0.52
1:F:440:HIS:O	1:F:444:VAL:HG22	2.10	0.52
1:E:338:PHE:O	1:E:464:ASN:HA	2.09	0.51
1:C:301:THR:HB	1:C:305:CYS:SG	2.51	0.51
1:D:98[A]:ILE:HG13	1:D:232:TYR:CE2	2.45	0.51
1:D:427:LEU:HD21	1:F:428:LEU:HD13	1.91	0.51
1:B:95:GLY:HA3	1:B:229:MET:O	2.09	0.51
1:C:114:GLU:HG3	1:C:258:ALA:HB3	1.92	0.51
1:C:96:ASP:HB2	4:C:511:EDO:H21	1.92	0.50
1:C:197:VAL:HG12	6:C:771:HOH:O	2.10	0.50
1:A:301:THR:HB	1:A:305:CYS:SG	2.51	0.50
1:F:3:ASP:N	1:F:3:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:HG21	1:B:317:VAL:HB	1.94	0.49
1:F:17:THR:HG23	1:F:313:LYS:NZ	2.28	0.49
1:A:310:ARG:NH1	1:A:419:ASP:OD1	2.30	0.48
1:F:301:THR:HB	1:F:305:CYS:SG	2.53	0.48
1:F:133:GLY:HA3	1:F:152:TRP:HB3	1.95	0.48
1:A:348:ASP:OD1	1:A:348:ASP:N	2.47	0.48
1:B:42:LYS:HE2	1:B:275:HIS:ND1	2.29	0.48
1:A:67:PRO:HG3	1:A:146:PHE:O	2.14	0.48
1:A:479:GLU:HA	1:A:482:ARG:HD2	1.94	0.48
1:D:411:LYS:NZ	6:D:608:HOH:O	2.44	0.48
1:D:354:HIS:HB2	1:D:363:TYR:CD1	2.48	0.48
1:C:452:LYS:HE3	1:C:461:GLU:OE1	2.13	0.48
1:C:221:LYS:NZ	6:C:619:HOH:O	2.45	0.48
1:D:399:PHE:HE1	1:D:406:MET:HE2	1.79	0.47
1:F:348:ASP:OD1	1:F:348:ASP:N	2.45	0.47
1:F:67:PRO:HG3	1:F:146:PHE:O	2.14	0.47
1:E:95:GLY:HA3	1:E:229:MET:O	2.14	0.47
1:F:95:GLY:HA3	1:F:229:MET:O	2.14	0.47
1:F:406[A]:MET:HE2	1:F:409:LEU:HD23	1.97	0.47
1:A:95:GLY:HA3	1:A:229:MET:O	2.15	0.47
1:A:211[B]:ARG:HD2	6:A:627:HOH:O	2.14	0.47
1:B:352:GLY:HA3	1:B:365:ALA:HA	1.95	0.47
1:F:104:LYS:NZ	1:F:398:GLU:OE1	2.39	0.47
1:B:301:THR:HB	1:B:305:CYS:SG	2.55	0.47
1:C:346:MET:SD	1:C:352:GLY:HA3	2.56	0.46
1:D:351:TYR:OH	1:D:440:HIS:ND1	2.37	0.46
1:E:474:ASP:N	1:E:477:CYS:HB3	2.30	0.46
1:F:211[B]:ARG:NH1	4:F:503:EDO:O1	2.49	0.46
1:A:171:LYS:HE2	6:A:666:HOH:O	2.15	0.45
1:C:343:TRP:CE3	1:C:346:MET:HE2	2.45	0.45
1:F:18:VAL:HG21	1:F:317:VAL:HB	1.98	0.45
1:F:352:GLY:HA3	1:F:365:ALA:HA	1.98	0.45
1:C:42:LYS:HD2	1:C:275:HIS:CD2	2.52	0.45
1:F:17:THR:HG22	6:F:603:HOH:O	2.16	0.45
1:E:104:LYS:NZ	1:E:398:GLU:OE2	2.49	0.45
1:F:310:ARG:NH1	1:F:419:ASP:OD1	2.38	0.45
1:B:209:ASN:HB3	4:C:505:EDO:H12	1.97	0.45
1:A:18:VAL:HG21	1:A:317:VAL:HB	1.98	0.45
1:D:113:LEU:HD22	1:D:257:PHE:HB3	1.98	0.44
1:A:132:LYS:HB2	1:A:132:LYS:HE2	1.77	0.44
1:D:355:HIS:O	1:D:361:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HE2	1:B:275:HIS:CE1	2.53	0.44
1:C:333:GLY:O	1:C:337:GLY:HA3	2.18	0.44
1:D:310:ARG:NH1	1:D:419:ASP:OD1	2.34	0.44
1:F:163:LEU:O	1:F:245:GLU:HA	2.17	0.44
1:A:240:ASP:HB2	4:A:506:EDO:H12	2.00	0.44
1:F:64:LEU:O	1:F:147:TYR:HB3	2.18	0.43
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.53	0.43
1:A:23:GLU:OE2	1:A:321[B]:ARG:NH1	2.52	0.43
1:A:343:TRP:CE3	1:A:346:MET:HE2	2.54	0.43
1:B:150:LEU:HB3	1:B:251:ILE:HG22	2.00	0.43
1:B:6:CYS:HA	1:B:466:CYS:HA	1.99	0.43
1:C:307:LYS:HD2	1:C:391:GLN:HB2	2.00	0.43
1:E:487:ASP:OD2	1:E:489:PRO:HD2	2.19	0.43
1:E:35:LEU:HB2	1:E:314:LEU:HB2	2.01	0.42
1:A:333:GLY:O	1:A:337:GLY:HA3	2.20	0.42
1:D:179:TRP:CE2	1:D:232:TYR:HB2	2.55	0.42
1:C:448:TYR:CE1	1:C:465:GLY:HA2	2.55	0.42
1:E:355:HIS:HD2	6:E:798:HOH:O	2.01	0.42
1:A:64:LEU:O	1:A:147:TYR:HB3	2.19	0.42
1:A:452:LYS:NZ	1:A:461:GLU:OE1	2.49	0.42
1:B:348:ASP:OD1	1:B:348:ASP:N	2.51	0.42
1:C:458:ASN:ND2	1:C:491:TYR:HB2	2.35	0.42
1:B:456:LYS:HB2	1:B:488:TYR:CE2	2.55	0.42
1:A:9:TYR:HB2	1:A:320:LEU:HD22	2.02	0.42
1:C:9:TYR:HB2	1:C:320:LEU:CD2	2.50	0.41
1:B:42:LYS:HG2	1:B:275:HIS:CD2	2.56	0.41
1:B:179:TRP:CE2	1:B:232:TYR:HB2	2.55	0.41
1:D:406:MET:HE3	1:E:406[B]:MET:HG2	2.01	0.41
1:F:158:ASP:OD1	1:F:195:HIS:ND1	2.50	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.90	0.41
1:D:88:GLU:HB3	6:D:863:HOH:O	2.21	0.41
1:D:333:GLY:O	1:D:337:GLY:HA3	2.20	0.41
1:B:332:PHE:CZ	1:C:331:LEU:HG	2.56	0.41
1:A:239:GLY:C	4:A:506:EDO:H21	2.45	0.41
1:A:471:HIS:CD2	1:A:491:TYR:HB3	2.56	0.41
1:C:73:LEU:HD22	1:C:115:ARG:CZ	2.50	0.41
1:B:6:CYS:O	1:B:353:TYR:HA	2.20	0.41
1:B:455:LEU:HD21	1:B:467:PHE:CG	2.56	0.41
1:C:359:GLN:OE1	1:C:474:ASP:HB2	2.21	0.41
1:E:346:MET:SD	1:E:352:GLY:HA3	2.61	0.41
1:E:428:LEU:HD13	1:F:427:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LEU:HD13	1:E:427:LEU:HD21	2.03	0.41
1:C:114:GLU:CG	1:C:258:ALA:HB3	2.51	0.40
1:E:179:TRP:CE2	1:E:232:TYR:HB2	2.56	0.40
1:C:78:TRP:HH2	1:C:113:LEU:HG	1.86	0.40
1:C:455:LEU:O	1:C:458:ASN:HB2	2.21	0.40
1:A:92:CYS:HB2	1:A:137:SER:O	2.21	0.40
1:D:51:PRO:HB3	1:D:80:TYR:CZ	2.56	0.40
1:A:355:HIS:HB2	1:A:478:MET:HE3	2.03	0.40
1:B:163:LEU:O	1:B:245:GLU:HA	2.22	0.40
1:B:320:LEU:N	1:B:320:LEU:HD12	2.36	0.40
1:C:163:LEU:O	1:C:245:GLU:HA	2.21	0.40
1:D:74:PRO:O	1:D:76:ARG:HG2	2.22	0.40
1:F:51:PRO:HB3	1:F:80:TYR:CZ	2.57	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	490/499 (98%)	480 (98%)	10 (2%)	0	100	100
1	B	480/499 (96%)	468 (98%)	11 (2%)	1 (0%)	43	37
1	C	491/499 (98%)	482 (98%)	9 (2%)	0	100	100
1	D	479/499 (96%)	468 (98%)	11 (2%)	0	100	100
1	E	492/499 (99%)	479 (97%)	11 (2%)	2 (0%)	30	22
1	F	485/499 (97%)	473 (98%)	11 (2%)	1 (0%)	43	37
All	All	2917/2994 (97%)	2850 (98%)	63 (2%)	4 (0%)	48	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	456	LYS
1	F	456	LYS
1	E	86	ASN
1	E	157	GLY

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	402/438 (92%)	394 (98%)	8 (2%)	48	48
1	B	392/438 (90%)	388 (99%)	4 (1%)	68	72
1	C	414/438 (94%)	412 (100%)	2 (0%)	81	85
1	D	378/438 (86%)	371 (98%)	7 (2%)	50	50
1	E	398/438 (91%)	394 (99%)	4 (1%)	68	72
1	F	386/438 (88%)	380 (98%)	6 (2%)	55	56
All	All	2370/2628 (90%)	2339 (99%)	31 (1%)	63	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	132	LYS
1	A	291	SER
1	A	321[A]	ARG
1	A	321[B]	ARG
1	A	346	MET
1	A	390	THR
1	A	452	LYS
1	B	14	SER
1	B	107	LEU
1	B	452	LYS
1	B	456	LYS
1	C	224[A]	ASP
1	C	224[B]	ASP
1	D	76	ARG

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Mol	Chain	Res	Type
1	D	107	LEU
1	D	112	SER
1	D	122[A]	GLU
1	D	122[B]	GLU
1	D	370	THR
1	D	442	SER
1	E	107	LEU
1	E	224	ASP
1	E	391	GLN
1	E	464	ASN
1	F	17	THR
1	F	320	LEU
1	F	321	ARG
1	F	397	LYS
1	F	406[A]	MET
1	F	406[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	89	ASN
1	C	356	GLN
1	C	371	GLN
1	D	140	HIS
1	D	454	GLN
1	E	443	ASN
1	F	354	HIS
1	F	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.41	0	17,19,21	0.42	0
2	NAG	G	2	2	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.30	0	17,19,21	0.59	0
2	NAG	H	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.74	0
2	NAG	I	1	1,2	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	I	2	2	14,14,15	0.34	0	17,19,21	0.85	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	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	C1-C2	2.16	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	2.52	115.56	112.19

There are no chirality outliers.

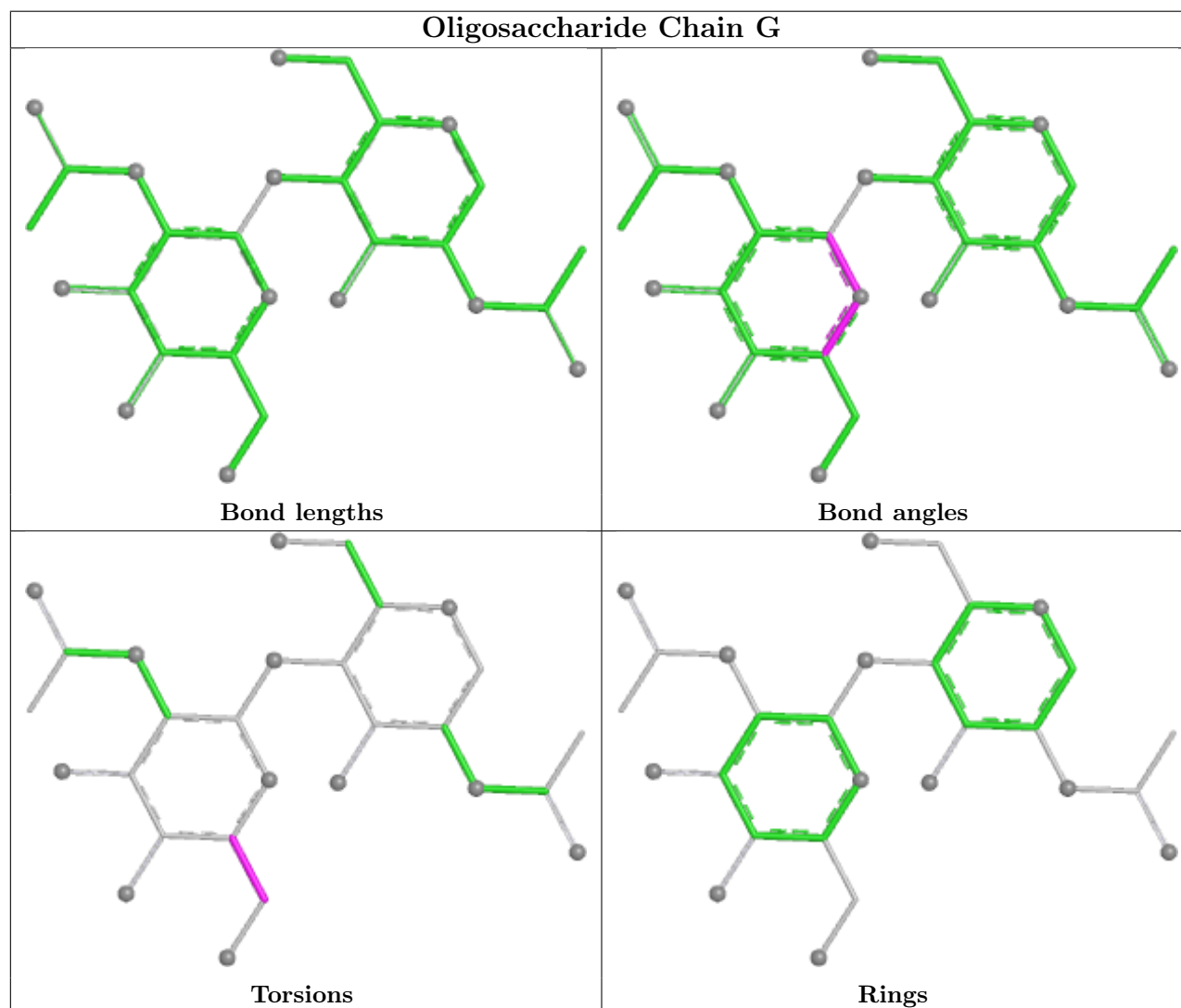
All (9) torsion outliers are listed below:

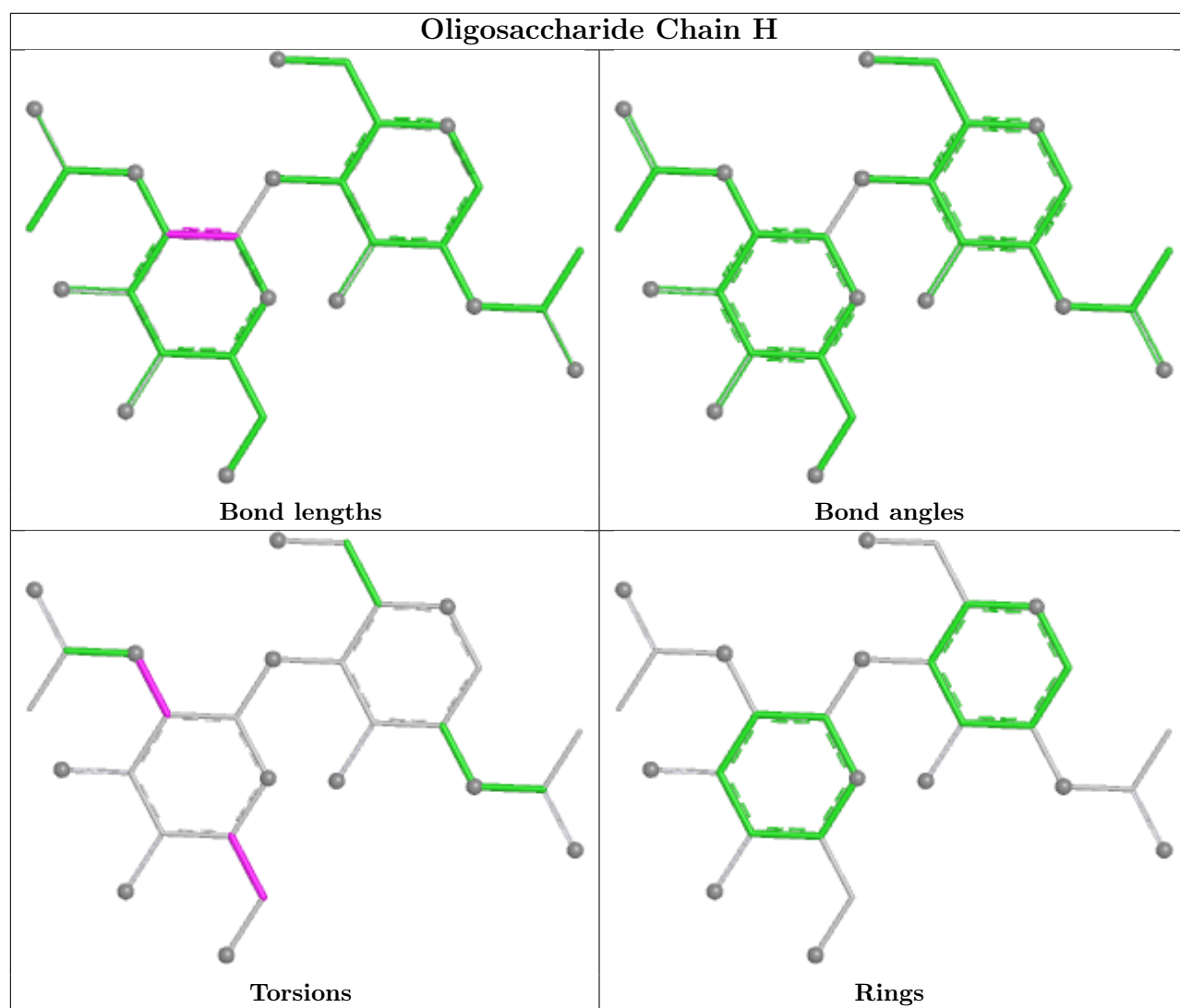
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	C1-C2-N2-C7
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
2	I	1	NAG	O5-C5-C6-O6

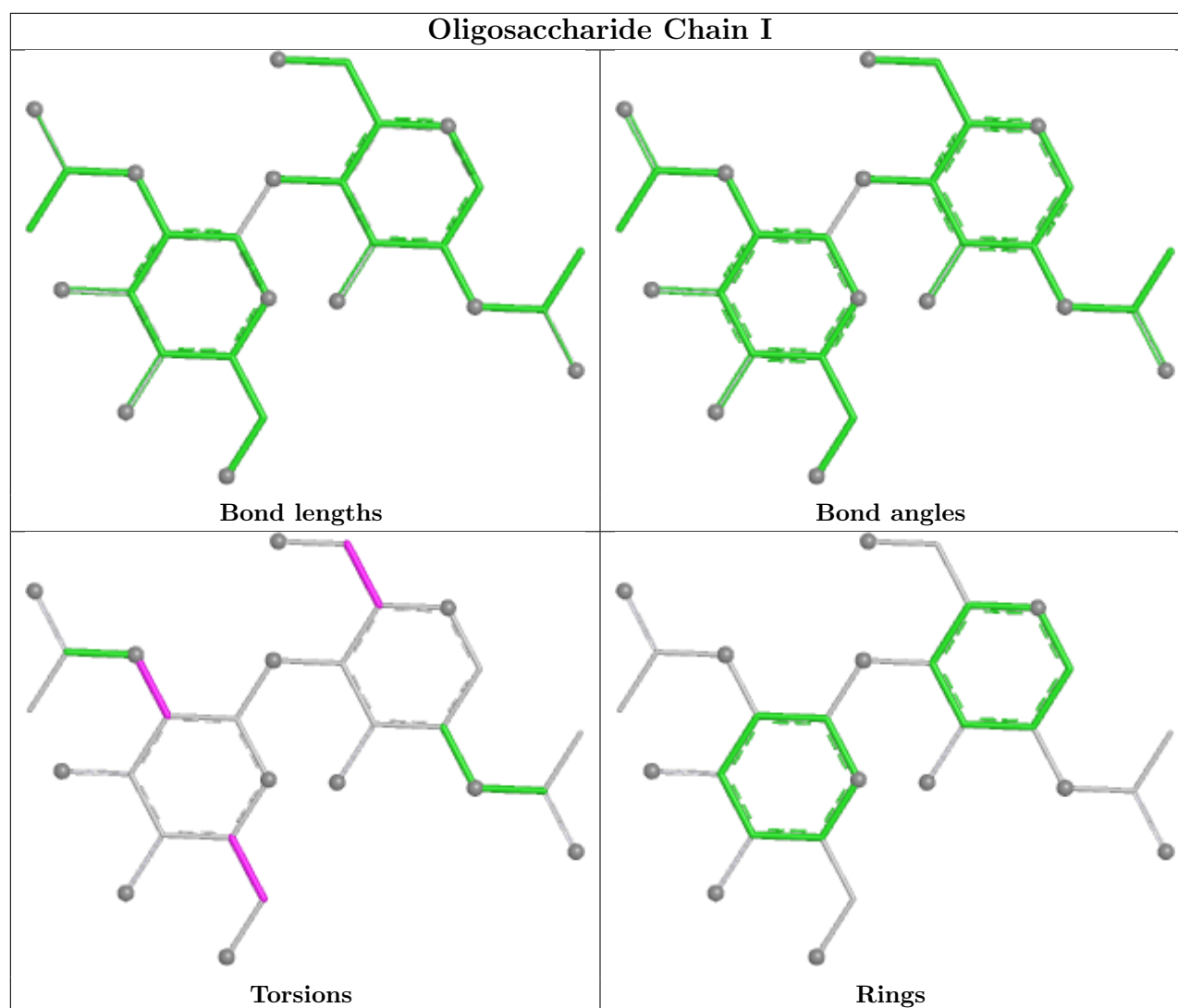
There are no ring outliers.

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](#)

39 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	EDO	D	506	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	C	510	-	3,3,3	0.45	0	2,2,2	0.18	0
3	NAG	C	501	1	14,14,15	0.34	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	504	-	3,3,3	0.41	0	2,2,2	0.36	0
3	NAG	B	505	1	14,14,15	0.35	0	17,19,21	0.55	0
4	EDO	C	512	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	D	507	-	3,3,3	0.59	0	2,2,2	0.13	0
4	EDO	C	511	-	3,3,3	0.52	0	2,2,2	0.23	0
4	EDO	E	508	-	3,3,3	0.41	0	2,2,2	0.25	0
4	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.30	0
3	NAG	D	501	1	14,14,15	0.73	0	17,19,21	0.62	1 (5%)
3	NAG	C	502	1	14,14,15	0.37	0	17,19,21	0.41	0
3	NAG	F	502	1	14,14,15	0.49	0	17,19,21	0.51	0
4	EDO	C	506	-	3,3,3	0.51	0	2,2,2	0.42	0
3	NAG	E	504	1	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	A	504	1	14,14,15	0.48	0	17,19,21	0.52	0
4	EDO	C	509	-	3,3,3	0.48	0	2,2,2	0.25	0
4	EDO	C	513	-	3,3,3	0.51	0	2,2,2	0.29	0
3	NAG	A	502	1	14,14,15	0.47	0	17,19,21	0.57	0
4	EDO	F	504	-	3,3,3	0.33	0	2,2,2	0.69	0
4	EDO	E	505	-	3,3,3	0.48	0	2,2,2	0.28	0
3	NAG	E	503	1	14,14,15	0.54	0	17,19,21	0.73	1 (5%)
4	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.20	0
3	NAG	B	501	1	14,14,15	0.65	0	17,19,21	0.62	1 (5%)
3	NAG	C	504	1	14,14,15	0.44	0	17,19,21	0.61	0
4	EDO	D	505	-	3,3,3	0.37	0	2,2,2	0.54	0
3	NAG	B	504	1	14,14,15	0.49	0	17,19,21	0.48	0
4	EDO	E	506	-	3,3,3	0.37	0	2,2,2	0.41	0
4	EDO	E	509	-	3,3,3	0.51	0	2,2,2	0.16	0
3	NAG	A	503	1	14,14,15	0.45	0	17,19,21	0.48	0
4	EDO	C	508	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	C	505	-	3,3,3	0.79	0	2,2,2	0.48	0
5	PEG	E	507	-	6,6,6	0.25	0	5,5,5	0.10	0
3	NAG	F	501	1	14,14,15	0.51	0	17,19,21	0.49	0
3	NAG	C	503	1	14,14,15	0.65	1 (7%)	17,19,21	0.58	0
4	EDO	A	507	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	C	507	-	3,3,3	0.33	0	2,2,2	0.63	0
3	NAG	A	501	1	14,14,15	0.55	0	17,19,21	0.65	0
4	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.28	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	EDO	D	506	-	-	1/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	EDO	D	504	-	-	0/1/1/1	-
3	NAG	B	505	1	-	1/6/23/26	0/1/1/1
4	EDO	C	512	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
4	EDO	E	508	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	NAG	F	502	1	-	1/6/23/26	0/1/1/1
4	EDO	C	506	-	-	0/1/1/1	-
3	NAG	E	504	1	-	1/6/23/26	0/1/1/1
3	NAG	A	504	1	-	4/6/23/26	0/1/1/1
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	EDO	F	504	-	-	0/1/1/1	-
4	EDO	E	505	-	-	1/1/1/1	-
3	NAG	E	503	1	-	0/6/23/26	0/1/1/1
4	EDO	A	505	-	-	1/1/1/1	-
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	NAG	C	504	1	-	2/6/23/26	0/1/1/1
4	EDO	D	505	-	-	0/1/1/1	-
3	NAG	B	504	1	-	1/6/23/26	0/1/1/1
4	EDO	E	506	-	-	0/1/1/1	-
4	EDO	E	509	-	-	0/1/1/1	-
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
5	PEG	E	507	-	-	1/4/4/4	-
3	NAG	F	501	1	-	3/6/23/26	0/1/1/1
3	NAG	C	503	1	-	0/6/23/26	0/1/1/1
4	EDO	A	507	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
3	NAG	A	501	1	-	4/6/23/26	0/1/1/1
4	EDO	F	503	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	NAG	O5-C1	2.07	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	NAG	C1-O5-C5	2.61	115.68	112.19
3	B	501	NAG	C1-O5-C5	2.14	115.05	112.19
3	D	501	NAG	C1-O5-C5	2.10	115.01	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	C	502	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6
3	F	501	NAG	C4-C5-C6-O6
3	A	504	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	F	501	NAG	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	B	504	NAG	O5-C5-C6-O6
4	C	505	EDO	O1-C1-C2-O2
4	C	508	EDO	O1-C1-C2-O2
4	E	508	EDO	O1-C1-C2-O2
4	F	503	EDO	O1-C1-C2-O2
3	A	504	NAG	C4-C5-C6-O6
3	E	504	NAG	O5-C5-C6-O6
4	A	505	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	E	505	EDO	O1-C1-C2-O2
3	C	504	NAG	C4-C5-C6-O6
4	A	506	EDO	O1-C1-C2-O2
3	A	501	NAG	C3-C2-N2-C7
3	A	504	NAG	C3-C2-N2-C7
5	E	507	PEG	C1-C2-O2-C3
3	B	505	NAG	O5-C5-C6-O6
3	C	504	NAG	O5-C5-C6-O6
4	C	509	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C1-C2-N2-C7
3	A	504	NAG	C1-C2-N2-C7
4	C	511	EDO	O1-C1-C2-O2
4	C	512	EDO	O1-C1-C2-O2
3	F	501	NAG	C3-C2-N2-C7
3	F	502	NAG	C3-C2-N2-C7
4	D	506	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	510	EDO	1	0
4	C	511	EDO	1	0
4	E	508	EDO	2	0
4	A	506	EDO	2	0
4	C	513	EDO	1	0
4	C	505	EDO	1	0
4	F	503	EDO	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	488/499 (97%)	0.50	42 (8%)	16 16	19, 47, 91, 110	8 (1%)
1	B	482/499 (96%)	0.43	52 (10%)	11 10	14, 42, 96, 124	4 (0%)
1	C	486/499 (97%)	0.08	9 (1%)	66 68	19, 38, 70, 101	9 (1%)
1	D	478/499 (95%)	0.57	76 (15%)	5 4	11, 42, 122, 154	7 (1%)
1	E	489/499 (97%)	0.62	60 (12%)	8 7	14, 46, 96, 123	7 (1%)
1	F	484/499 (96%)	0.50	60 (12%)	8 7	15, 43, 104, 130	5 (1%)
All	All	2907/2994 (97%)	0.45	299 (10%)	12 11	11, 43, 99, 154	40 (1%)

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	455	LEU	6.1
1	E	5	ILE	5.8
1	D	451	VAL	5.7
1	B	469	PHE	5.5
1	D	481	VAL	5.5
1	D	338	PHE	5.3
1	D	3	ASP	5.0
1	F	75	ALA	5.0
1	D	464	ASN	4.7
1	D	469	PHE	4.7
1	F	4	THR	4.7
1	D	5	ILE	4.7
1	D	6	CYS	4.6
1	E	320	LEU	4.6
1	D	457	ASN	4.6
1	E	462	ILE	4.5
1	A	2	SER	4.5
1	D	489	PRO	4.5
1	E	483	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	447	LEU	4.4
1	E	459	ALA	4.3
1	F	333	GLY	4.3
1	D	323	ILE	4.2
1	B	487	ASP	4.1
1	D	453	SER	4.1
1	B	470	TYR	4.1
1	E	2	SER	4.1
1	D	431	LEU	4.0
1	E	493	GLU	4.0
1	D	361	SER	4.0
1	D	360	GLY	4.0
1	B	4	THR	4.0
1	D	353	TYR	4.0
1	D	491	TYR	4.0
1	B	359	GLN	4.0
1	A	263	PHE	3.9
1	A	495	PHE	3.9
1	D	339	ILE	3.9
1	D	355	HIS	3.9
1	E	4	THR	3.9
1	F	491	TYR	3.8
1	F	5	ILE	3.8
1	D	475	ASN	3.8
1	B	481	VAL	3.8
1	F	341	GLY	3.8
1	D	7	ILE	3.8
1	D	335	ILE	3.8
1	E	467	PHE	3.8
1	D	366	ASP	3.7
1	D	341	GLY	3.7
1	F	338	PHE	3.6
1	E	455	LEU	3.6
1	A	389	ASN	3.6
1	D	347	ILE	3.6
1	F	356	GLN	3.6
1	D	370	THR	3.6
1	E	334	ALA	3.6
1	B	472	LYS	3.6
1	E	463	GLY	3.6
1	E	390	THR	3.5
1	B	358	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	474	ASP	3.5
1	D	343	TRP	3.5
1	D	4	THR	3.5
1	F	8	GLY	3.5
1	F	345	GLY	3.5
1	E	389	ASN	3.5
1	F	343	TRP	3.4
1	E	448	TYR	3.4
1	D	357	ASN	3.4
1	B	455	LEU	3.4
1	F	357	ASN	3.4
1	D	358	GLU	3.4
1	D	471	HIS	3.4
1	C	325	SER	3.4
1	D	263	PHE	3.4
1	E	470	TYR	3.3
1	D	359	GLN	3.3
1	B	491	TYR	3.3
1	F	323	ILE	3.3
1	B	389	ASN	3.3
1	B	475	ASN	3.3
1	D	356	GLN	3.3
1	B	345	GLY	3.2
1	E	460	LYS	3.2
1	F	451	VAL	3.2
1	E	336	ALA	3.2
1	A	486	TYR	3.2
1	D	351	TYR	3.2
1	E	486	TYR	3.2
1	F	462	ILE	3.2
1	D	467	PHE	3.2
1	D	330	GLY	3.2
1	D	345	GLY	3.2
1	B	364	ALA	3.2
1	B	356	GLN	3.2
1	A	462	ILE	3.2
1	B	490	LYS	3.2
1	A	481	VAL	3.1
1	A	469	PHE	3.1
1	F	359	GLN	3.1
1	A	364	ALA	3.1
1	D	448	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	349	GLY	3.1
1	E	376	GLY	3.1
1	F	76	ARG	3.1
1	F	447	LEU	3.1
1	F	472	LYS	3.1
1	D	488	TYR	3.1
1	E	338	PHE	3.1
1	E	324	PRO	3.1
1	E	347	ILE	3.1
1	B	486	TYR	3.0
1	A	350	TRP	3.0
1	E	88	GLU	3.0
1	D	444	VAL	3.0
1	B	86	ASN	3.0
1	F	481	VAL	3.0
1	F	465	GLY	3.0
1	D	470	TYR	3.0
1	E	488	TYR	3.0
1	F	332	PHE	3.0
1	A	493	GLU	2.9
1	D	365	ALA	2.9
1	C	113	LEU	2.9
1	C	463	GLY	2.9
1	F	330	GLY	2.9
1	B	485	THR	2.9
1	D	487	ASP	2.9
1	E	3	ASP	2.9
1	E	485	THR	2.9
1	F	9	TYR	2.9
1	B	461	GLU	2.9
1	D	363	TYR	2.9
1	F	448	TYR	2.9
1	C	389	ASN	2.9
1	D	486	TYR	2.9
1	E	379	ASN	2.9
1	D	468	GLU	2.8
1	F	358	GLU	2.8
1	F	86	ASN	2.8
1	D	362	GLY	2.8
1	F	469	PHE	2.8
1	A	494	GLU	2.8
1	F	324	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	490	LYS	2.8
1	A	73	LEU	2.8
1	F	320	LEU	2.8
1	B	451	VAL	2.8
1	E	481	VAL	2.8
1	B	357	ASN	2.7
1	F	463	GLY	2.7
1	B	467	PHE	2.7
1	F	334	ALA	2.7
1	F	363	TYR	2.7
1	C	347	ILE	2.7
1	B	474	ASP	2.7
1	F	351	TYR	2.7
1	E	358	GLU	2.7
1	E	444	VAL	2.7
1	F	471	HIS	2.7
1	C	2	SER	2.7
1	E	491	TYR	2.7
1	F	456	LYS	2.7
1	E	484	GLY	2.7
1	B	355	HIS	2.6
1	E	6	CYS	2.6
1	F	372	ASN	2.6
1	E	331	LEU	2.6
1	D	478	MET	2.6
1	F	459	ALA	2.6
1	A	455	LEU	2.6
1	A	472	LYS	2.6
1	D	368	LYS	2.6
1	A	218	ALA	2.6
1	E	350	TRP	2.6
1	B	462	ILE	2.5
1	F	444	VAL	2.5
1	A	470	TYR	2.5
1	B	6	CYS	2.5
1	E	477	CYS	2.5
1	D	483	ASN	2.5
1	A	467	PHE	2.5
1	B	87	SER	2.5
1	B	489	PRO	2.5
1	B	347	ILE	2.5
1	E	7	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	456	LYS	2.5
1	E	461	GLU	2.4
1	B	363	TYR	2.4
1	B	488	TYR	2.4
1	D	87	SER	2.4
1	E	371	GLN	2.4
1	A	473	CYS	2.4
1	F	470	TYR	2.4
1	F	488	TYR	2.4
1	F	342	GLY	2.4
1	B	464	ASN	2.4
1	B	476	GLU	2.4
1	D	340	GLU	2.4
1	E	451	VAL	2.4
1	D	472	LYS	2.4
1	E	490	LYS	2.4
1	D	334	ALA	2.4
1	F	3	ASP	2.4
1	A	459	ALA	2.3
1	E	476	GLU	2.3
1	A	113	LEU	2.3
1	D	389	ASN	2.3
1	F	455	LEU	2.3
1	F	344	THR	2.3
1	F	485	THR	2.3
1	A	358	GLU	2.3
1	F	6	CYS	2.3
1	A	488	TYR	2.3
1	D	336	ALA	2.3
1	B	463	GLY	2.3
1	D	333	GLY	2.3
1	D	474	ASP	2.3
1	D	450	LYS	2.3
1	E	492	SER	2.3
1	C	462	ILE	2.3
1	A	15	THR	2.3
1	B	483	ASN	2.3
1	A	490	LYS	2.3
1	B	354	HIS	2.3
1	F	361	SER	2.3
1	B	395	VAL	2.3
1	E	464	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	466	CYS	2.3
1	F	466	CYS	2.3
1	B	459	ALA	2.3
1	F	336	ALA	2.3
1	D	332	PHE	2.2
1	F	489	PRO	2.2
1	A	365	ALA	2.2
1	D	466	CYS	2.2
1	E	330	GLY	2.2
1	E	87	SER	2.2
1	B	263	PHE	2.2
1	A	347	ILE	2.2
1	B	5	ILE	2.2
1	F	389	ASN	2.2
1	E	473	CYS	2.2
1	B	22	LEU	2.2
1	E	363	TYR	2.2
1	B	460	LYS	2.2
1	A	374	ILE	2.2
1	E	332	PHE	2.2
1	E	495	PHE	2.2
1	A	478	MET	2.2
1	B	3	ASP	2.2
1	A	88	GLU	2.2
1	A	463	GLY	2.2
1	A	471	HIS	2.2
1	D	331	LEU	2.2
1	D	482	ARG	2.2
1	A	491	TYR	2.2
1	B	353	TYR	2.2
1	B	468	GLU	2.1
1	F	340	GLU	2.1
1	F	347	ILE	2.1
1	F	473	CYS	2.1
1	D	9	TYR	2.1
1	D	364	ALA	2.1
1	B	480	SER	2.1
1	F	346	MET	2.1
1	E	340	GLU	2.1
1	C	491	TYR	2.1
1	F	353	TYR	2.1
1	F	486	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	454	GLN	2.1
1	C	485	THR	2.1
1	A	362	GLY	2.1
1	A	343	TRP	2.1
1	A	87	SER	2.1
1	D	430	LEU	2.1
1	A	477	CYS	2.1
1	D	10	HIS	2.1
1	E	156	THR	2.1
1	E	337	GLY	2.1
1	A	7	ILE	2.1
1	E	469	PHE	2.1
1	D	350	TRP	2.1
1	A	492	SER	2.1
1	B	325	SER	2.1
1	D	476	GLU	2.0
1	D	427	LEU	2.0
1	B	482	ARG	2.0
1	A	456	LYS	2.0
1	E	24	LYS	2.0
1	F	11	ALA	2.0
1	B	320	LEU	2.0
1	E	359	GLN	2.0
1	E	275	HIS	2.0
1	D	452	LYS	2.0
1	A	489	PRO	2.0
1	B	448	TYR	2.0
1	E	353	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

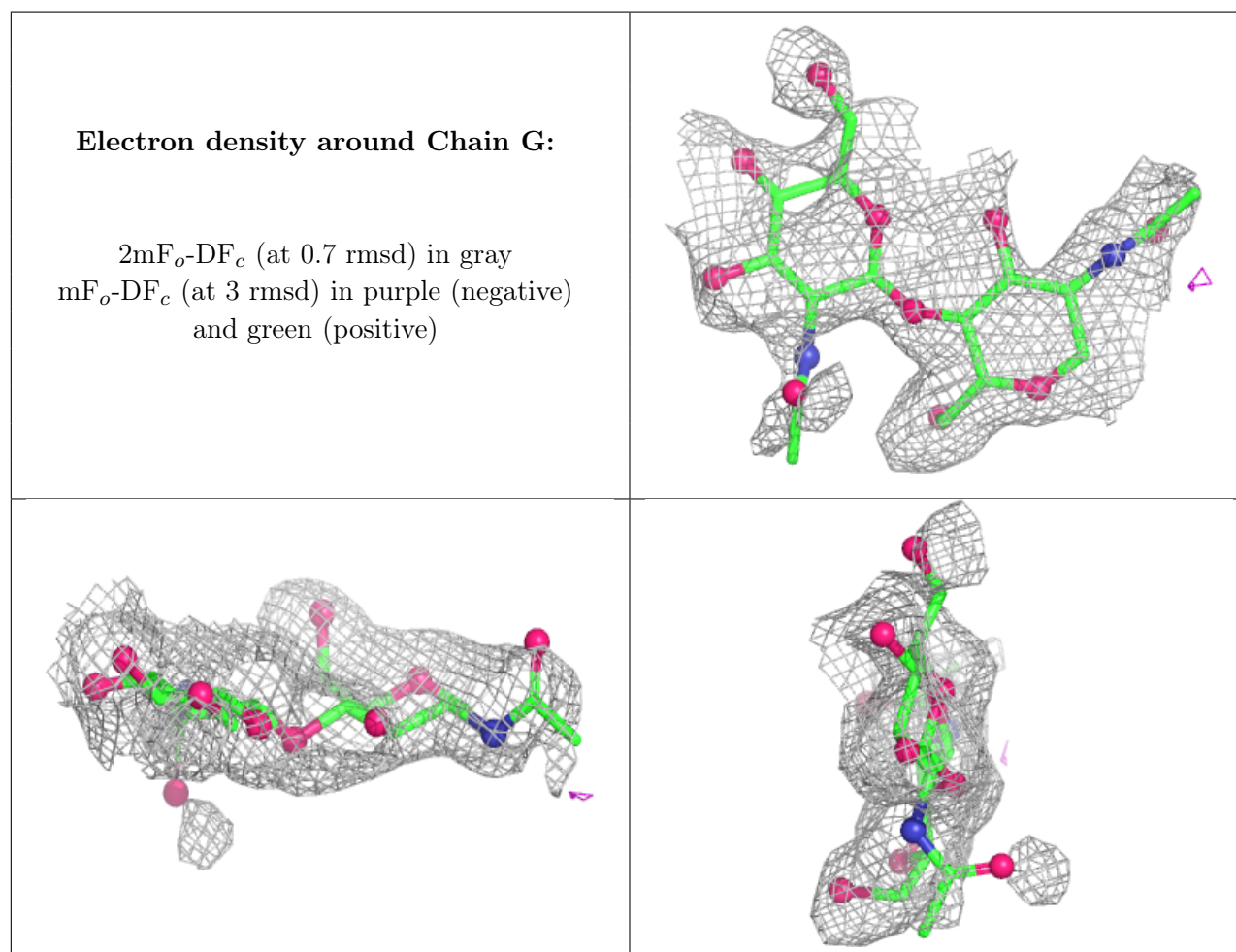
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

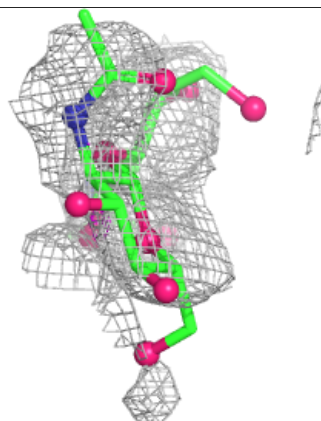
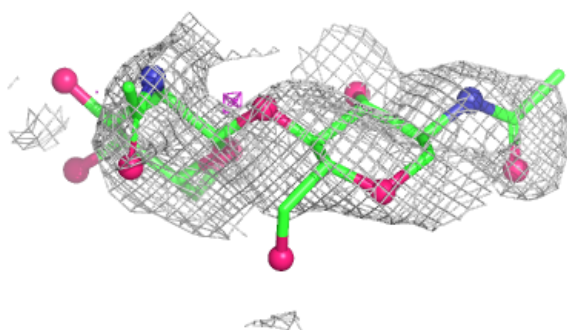
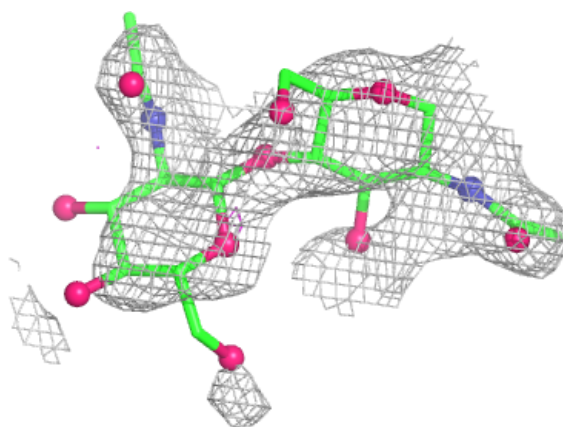
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	2	14/15	0.45	0.13	107,114,122,125	0
2	NAG	H	2	14/15	0.46	0.15	97,121,126,127	0
2	NAG	I	1	14/15	0.57	0.14	71,91,98,105	0
2	NAG	G	2	14/15	0.57	0.15	106,112,117,119	0
2	NAG	H	1	14/15	0.75	0.12	78,92,108,112	0
2	NAG	G	1	14/15	0.79	0.12	66,86,95,102	0

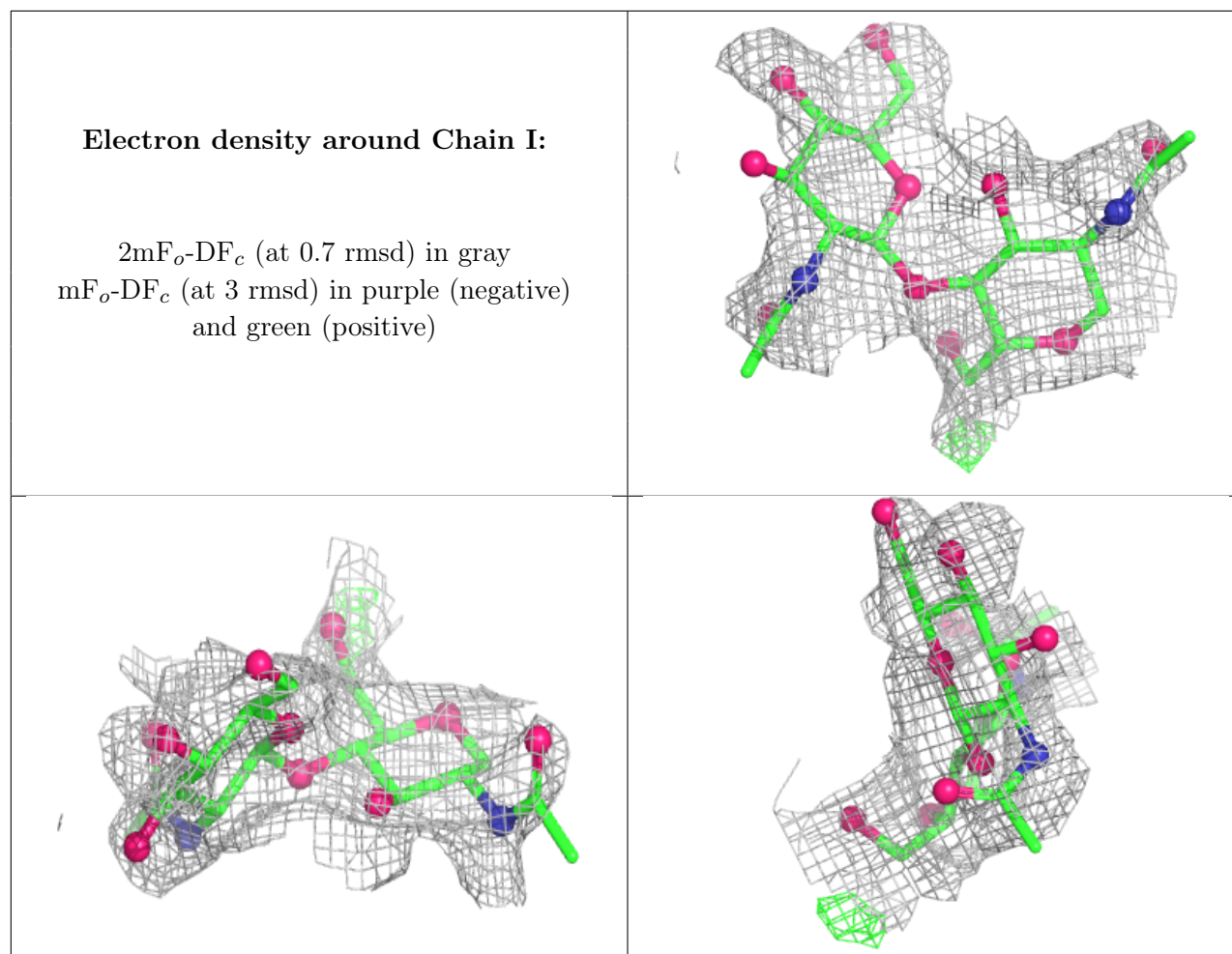
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	504	14/15	0.45	0.16	76,100,106,111	0
3	NAG	A	503	14/15	0.49	0.17	95,111,120,122	0
3	NAG	D	501	14/15	0.52	0.15	87,102,109,112	0
3	NAG	E	504	14/15	0.55	0.16	77,99,104,105	0
3	NAG	F	501	14/15	0.57	0.14	82,100,109,109	0
3	NAG	B	501	14/15	0.59	0.14	84,100,106,110	0
3	NAG	C	503	14/15	0.61	0.14	77,86,92,94	0
3	NAG	A	502	14/15	0.61	0.15	87,102,107,109	0
3	NAG	F	502	14/15	0.63	0.15	85,100,111,112	0
3	NAG	C	501	14/15	0.64	0.13	79,99,104,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	504	14/15	0.67	0.13	82,95,104,104	0
4	EDO	E	509	4/4	0.70	0.17	63,67,69,70	0
3	NAG	C	502	14/15	0.71	0.14	69,88,99,99	0
3	NAG	E	503	14/15	0.74	0.14	78,91,101,101	0
3	NAG	B	505	14/15	0.75	0.14	74,87,96,97	0
3	NAG	C	504	14/15	0.75	0.13	67,78,91,92	0
4	EDO	A	506	4/4	0.76	0.19	71,74,75,75	0
3	NAG	A	501	14/15	0.76	0.13	65,81,96,101	0
4	EDO	D	505	4/4	0.78	0.23	61,66,69,71	0
4	EDO	D	507	4/4	0.81	0.20	46,54,57,58	0
5	PEG	E	507	7/7	0.81	0.18	51,58,63,69	0
4	EDO	C	505	4/4	0.82	0.22	33,43,46,50	0
4	EDO	C	506	4/4	0.82	0.20	44,46,52,55	0
4	EDO	C	508	4/4	0.84	0.15	64,66,69,74	0
4	EDO	E	505	4/4	0.84	0.19	47,48,52,60	0
4	EDO	A	507	4/4	0.85	0.15	65,65,68,69	0
4	EDO	D	506	4/4	0.85	0.14	57,59,62,62	0
4	EDO	A	505	4/4	0.87	0.14	60,62,62,64	0
4	EDO	C	512	4/4	0.87	0.16	65,67,67,70	0
4	EDO	F	504	4/4	0.88	0.12	46,48,56,57	0
4	EDO	C	513	4/4	0.88	0.16	54,56,59,61	0
4	EDO	C	509	4/4	0.89	0.14	52,52,54,55	0
4	EDO	C	507	4/4	0.90	0.12	40,45,47,52	0
4	EDO	F	503	4/4	0.90	0.16	64,70,70,72	0
4	EDO	D	504	4/4	0.90	0.12	50,54,57,67	0
4	EDO	E	506	4/4	0.90	0.14	60,61,63,63	0
4	EDO	C	511	4/4	0.91	0.14	38,46,57,60	0
4	EDO	C	510	4/4	0.93	0.20	47,59,64,66	0
4	EDO	E	508	4/4	0.93	0.14	37,39,42,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.