



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:00 AM UTC

PDB ID : 5W42 / pdb_00005w42
Title : Crystal structure of human monoclonal antibody H3v-47 in complex with influenza virus hemagglutinin from A/Minnesota/11/2010 (H3N2)
Authors : Zhang, H.; Wilson, I.A.
Deposited on : 2017-06-08
Resolution : 3.57 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

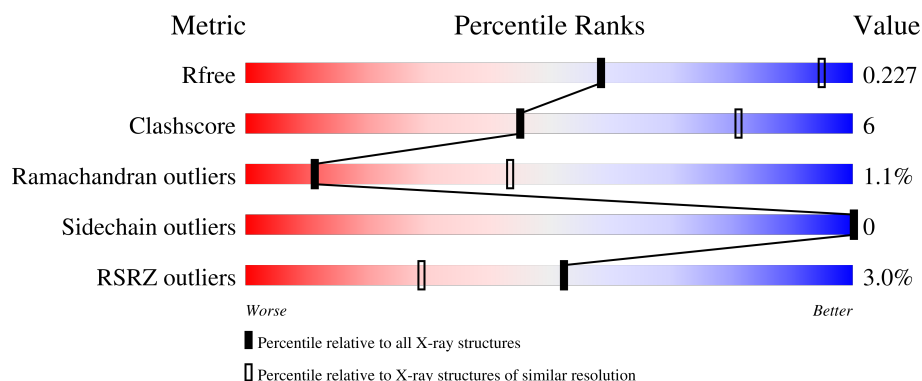
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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.



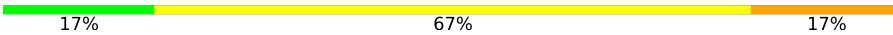
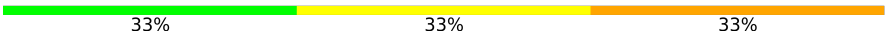
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	329	0% 85% 10% ..
2	B	174	3% 95% ..
3	H	236	4% 84% 11% ..
4	L	214	4% 87% 11% ..
5	C	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
5	G	5	 60%40%
6	D	4	 100%
7	E	6	 17%67%17%
8	F	3	 33%33%33%
9	I	2	 50%50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	1	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7573 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	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1409	876	252	275	6			

- Molecule 3 is a protein called Fab H3v-47 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	227	Total	C	N	O	S	0	0	0
			1701	1071	287	335	8			

There are 6 discrepancies between the modelled and reference sequences:

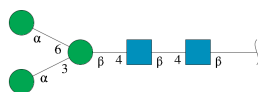
Chain	Residue	Modelled	Actual	Comment	Reference
H	217	HIS	-	expression tag	UNP Q6N089
H	218	HIS	-	expression tag	UNP Q6N089
H	219	HIS	-	expression tag	UNP Q6N089
H	220	HIS	-	expression tag	UNP Q6N089
H	221	HIS	-	expression tag	UNP Q6N089
H	222	HIS	-	expression tag	UNP Q6N089

- Molecule 4 is a protein called Fab H3v-47 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1617	1002	280	330	5			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



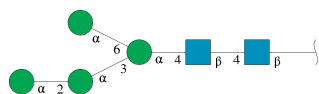
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



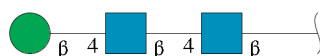
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



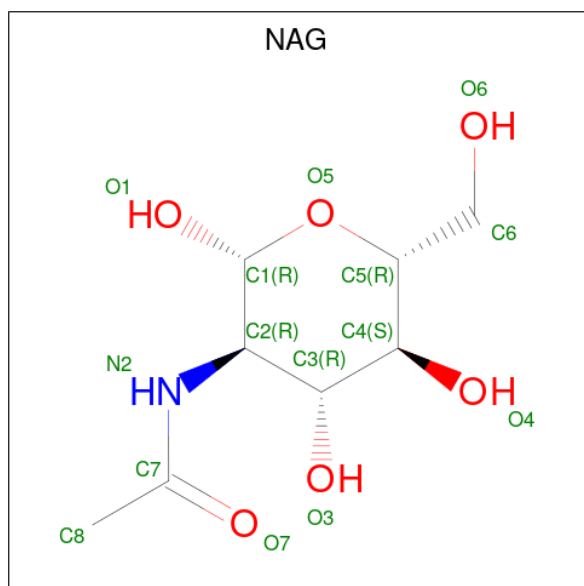
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 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
9	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

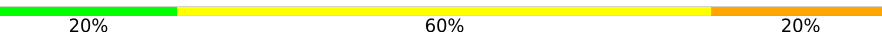


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

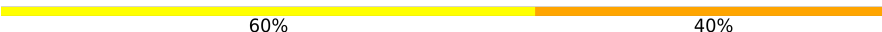
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	1	Total 1	Zn 1	0	0

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  20% 60% 20%

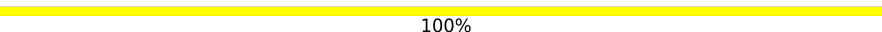


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  60% 40%

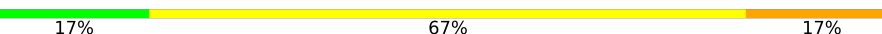


- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

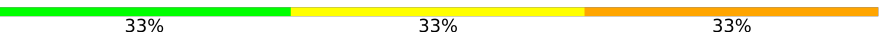


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  17% 67% 17%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 33% 33%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	194.62Å 194.62Å 194.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 3.57 38.92 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.92-3.57) 99.8 (38.92-3.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.196 , 0.228 0.193 , 0.227	Depositor DCC
R_{free} test set	1985 reflections (6.74%)	wwPDB-VP
Wilson B-factor (Å ²)	132.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.048 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7573	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: ZN, MAN, BMA, 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	0.83	4/2565 (0.2%)	1.25	31/3492 (0.9%)
2	B	0.76	0/1433	1.15	8/1924 (0.4%)
3	H	0.71	1/1743 (0.1%)	1.23	19/2376 (0.8%)
4	L	0.73	2/1650 (0.1%)	1.20	23/2239 (1.0%)
All	All	0.77	7/7391 (0.1%)	1.21	81/10031 (0.8%)

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
4	L	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ASN	C-N	12.04	1.49	1.33
4	L	83	SER	CA-CB	-7.88	1.40	1.53
3	H	213	PRO	C-N	-7.37	1.24	1.33
1	A	21	PRO	C-N	-7.13	1.23	1.33
1	A	23	GLY	C-N	-6.64	1.24	1.33
4	L	83	SER	N-CA	6.55	1.54	1.46
1	A	24	THR	C-N	-6.42	1.24	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	PHE	N-CA-C	16.99	135.91	111.96
1	A	265	SER	N-CA-CB	12.00	132.23	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	213	PRO	O-C-N	11.39	138.01	122.64
1	A	21	PRO	CA-C-N	10.88	142.59	122.02
1	A	21	PRO	C-N-CA	10.88	142.59	122.02
1	A	21	PRO	O-C-N	-10.55	110.25	122.17
3	H	160	THR	CB-CA-C	-9.67	93.40	109.27
3	H	118	GLY	CA-C-N	9.67	129.60	120.03
3	H	118	GLY	C-N-CA	9.67	129.60	120.03
1	A	265	SER	N-CA-C	-9.04	93.91	108.55
3	H	125	ALA	CA-C-N	8.74	128.60	120.21
3	H	125	ALA	C-N-CA	8.74	128.60	120.21
3	H	19	ARG	N-CA-C	-8.47	93.96	107.93
1	A	201	ARG	N-CA-C	8.39	123.42	110.42
4	L	157	ASN	CB-CA-C	8.30	122.08	109.13
1	A	305	CYS	CA-C-N	8.29	128.24	120.03
1	A	305	CYS	C-N-CA	8.29	128.24	120.03
2	B	64	HIS	N-CA-C	-7.64	94.58	107.80
2	B	64	HIS	N-CA-CB	7.56	122.70	110.90
4	L	158	SER	N-CA-C	7.55	121.28	107.99
4	L	79	GLU	CA-C-N	7.40	127.11	119.56
4	L	79	GLU	C-N-CA	7.40	127.11	119.56
1	A	20	VAL	CA-C-N	7.40	126.67	118.97
1	A	20	VAL	C-N-CA	7.40	126.67	118.97
4	L	94	SER	CA-C-N	7.34	129.02	119.84
4	L	94	SER	C-N-CA	7.34	129.02	119.84
1	A	168	MET	CA-C-N	7.31	127.89	119.99
1	A	168	MET	C-N-CA	7.31	127.89	119.99
4	L	58	ILE	CA-C-N	7.22	127.20	119.76
4	L	58	ILE	C-N-CA	7.22	127.20	119.76
1	A	184	HIS	CA-C-N	7.18	127.18	119.78
1	A	184	HIS	C-N-CA	7.18	127.18	119.78
4	L	118	PRO	CA-C-N	7.00	126.76	119.76
4	L	118	PRO	C-N-CA	7.00	126.76	119.76
1	A	263	GLY	N-CA-C	6.99	120.31	110.74
4	L	117	PHE	CA-C-N	6.90	127.48	120.38
4	L	117	PHE	C-N-CA	6.90	127.48	120.38
1	A	161	TYR	CA-C-N	6.88	129.19	120.51
1	A	161	TYR	C-N-CA	6.88	129.19	120.51
3	H	22	CYS	N-CA-C	-6.81	97.16	108.32
2	B	56	ILE	N-CA-C	6.64	113.32	106.21
2	B	63	PHE	CB-CA-C	-6.61	99.18	110.88
1	A	201	ARG	N-CA-CB	-6.51	100.41	110.56
3	H	122	PHE	CA-C-N	6.48	126.44	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	122	PHE	C-N-CA	6.48	126.44	119.76
4	L	14	SER	CA-C-N	6.36	126.31	119.76
4	L	14	SER	C-N-CA	6.36	126.31	119.76
1	A	73	ASP	CA-C-N	6.36	127.79	119.84
1	A	73	ASP	C-N-CA	6.36	127.79	119.84
2	B	171	PHE	N-CA-C	6.31	120.83	112.25
4	L	202	SER	CA-C-N	6.29	126.26	119.78
4	L	202	SER	C-N-CA	6.29	126.26	119.78
3	H	19	ARG	CB-CA-C	6.23	119.06	110.34
3	H	144	ASP	N-CA-C	6.22	120.23	111.52
4	L	137	ASN	N-CA-C	6.20	119.79	111.24
3	H	22	CYS	CB-CA-C	6.13	120.24	109.89
3	H	20	VAL	N-CA-CB	6.08	120.09	111.82
1	A	253	ALA	CA-C-N	5.97	126.47	120.14
1	A	253	ALA	C-N-CA	5.97	126.47	120.14
3	H	166	PHE	CA-C-N	5.96	126.15	119.90
3	H	166	PHE	C-N-CA	5.96	126.15	119.90
1	A	264	LYS	N-CA-C	-5.84	98.36	110.80
4	L	158	SER	N-CA-CB	-5.82	101.68	110.35
4	L	111	ALA	CA-C-N	5.76	126.64	120.13
4	L	111	ALA	C-N-CA	5.76	126.64	120.13
1	A	22	ASN	O-C-N	-5.69	115.14	122.20
3	H	145	TYR	N-CA-C	5.66	118.47	109.81
1	A	264	LYS	CB-CA-C	-5.61	99.25	110.42
1	A	23	GLY	O-C-N	-5.56	117.16	123.61
2	B	63	PHE	CA-CB-CG	-5.44	108.36	113.80
2	B	76	ARG	N-CA-C	5.43	122.37	110.80
4	L	138	PHE	N-CA-C	5.24	117.82	109.81
1	A	220	ARG	CA-C-N	5.22	125.14	119.76
1	A	220	ARG	C-N-CA	5.22	125.14	119.76
3	H	184	VAL	CA-C-N	5.21	125.45	119.83
3	H	184	VAL	C-N-CA	5.21	125.45	119.83
1	A	245	ILE	O-C-N	5.18	128.54	122.99
4	L	39	LYS	CA-C-N	5.13	126.25	119.84
4	L	39	LYS	C-N-CA	5.13	126.25	119.84
1	A	244	LEU	CA-C-N	-5.12	116.28	123.13
1	A	244	LEU	C-N-CA	-5.12	116.28	123.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	210	ARG	Mainchain,Peptide

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	2506	0	2416	60	1
2	B	1409	0	1348	20	0
3	H	1701	0	1658	8	1
4	L	1617	0	1574	7	0
5	C	61	0	52	3	0
5	G	61	0	52	2	0
6	D	50	0	43	20	0
7	E	72	0	61	3	0
8	F	39	0	34	1	0
9	I	28	0	25	0	0
10	A	28	0	26	2	0
11	H	1	0	0	0	0
All	All	7573	0	7289	87	1

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 6.

All (87) 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:248:THR:HG22	6:D:1:NAG:C8	1.13	1.56
1:A:248:THR:CG2	6:D:1:NAG:H81	1.38	1.51
1:A:264:LYS:CD	2:B:63:PHE:CZ	2.11	1.32
1:A:248:THR:HG22	6:D:1:NAG:C7	1.72	1.19
1:A:264:LYS:HD3	2:B:63:PHE:CE2	1.77	1.18
1:A:248:THR:CG2	6:D:1:NAG:C8	2.09	1.14
1:A:264:LYS:HD2	2:B:63:PHE:CZ	1.82	1.13
1:A:163:GLU:CG	6:D:1:NAG:H4	1.80	1.11
1:A:264:LYS:HD3	2:B:63:PHE:CZ	1.82	1.07
1:A:163:GLU:HG3	6:D:1:NAG:C4	1.83	1.06
1:A:248:THR:CG2	6:D:1:NAG:C7	2.37	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:CG2	6:D:1:NAG:O7	2.11	0.96
1:A:163:GLU:HG3	6:D:1:NAG:H4	0.95	0.94
5:C:1:NAG:O6	5:C:2:NAG:N2	2.04	0.90
1:A:163:GLU:OE2	6:D:2:NAG:C1	2.21	0.89
1:A:248:THR:CB	6:D:1:NAG:H81	2.03	0.87
1:A:20:VAL:HG12	1:A:22:ASN:OD1	1.75	0.86
1:A:264:LYS:HD2	2:B:63:PHE:CE1	2.12	0.84
1:A:248:THR:HG21	6:D:1:NAG:O7	1.79	0.81
1:A:22:ASN:OD1	10:A:501:NAG:O7	2.00	0.80
1:A:114:SER:HA	1:A:265:SER:OG	1.81	0.80
1:A:264:LYS:CE	2:B:63:PHE:CZ	2.65	0.80
1:A:114:SER:C	1:A:265:SER:OG	2.28	0.77
1:A:264:LYS:CD	2:B:63:PHE:CE2	2.52	0.76
2:B:153:ARG:O	2:B:154:ASN:CB	2.34	0.76
1:A:20:VAL:CG1	1:A:22:ASN:OD1	2.33	0.75
1:A:264:LYS:HE2	2:B:63:PHE:CZ	2.24	0.72
1:A:114:SER:CA	1:A:265:SER:OG	2.38	0.71
8:F:1:NAG:O3	8:F:1:NAG:H83	1.92	0.70
3:H:217:HIS:O	3:H:218:HIS:HB2	1.92	0.67
1:A:195:TYR:O	1:A:196:VAL:C	2.35	0.66
2:B:153:ARG:O	2:B:154:ASN:HB3	1.99	0.63
1:A:264:LYS:HE2	2:B:63:PHE:HZ	1.63	0.62
5:C:1:NAG:O7	5:C:1:NAG:H3	1.99	0.62
5:C:1:NAG:O6	5:C:1:NAG:O4	2.18	0.60
1:A:163:GLU:HB2	6:D:1:NAG:C8	2.32	0.60
1:A:167:THR:CG2	7:E:1:NAG:H62	2.33	0.59
1:A:248:THR:HG22	6:D:1:NAG:H81	0.60	0.59
5:G:1:NAG:H83	5:G:1:NAG:H3	1.85	0.58
3:H:11:VAL:HG13	3:H:11:VAL:O	2.03	0.58
1:A:264:LYS:CE	2:B:63:PHE:HZ	2.15	0.57
1:A:200:GLY:O	1:A:215:PRO:HD2	2.05	0.56
1:A:326:LYS:HG2	1:A:326:LYS:O	2.04	0.56
1:A:266:SER:HB2	2:B:63:PHE:O	2.05	0.55
5:G:2:NAG:H3	5:G:5:MAN:H62	1.87	0.55
1:A:163:GLU:CD	6:D:2:NAG:C1	2.80	0.54
1:A:141:ARG:NH1	1:A:141:ARG:O	2.40	0.54
1:A:163:GLU:HG3	6:D:1:NAG:C3	2.37	0.54
2:B:56:ILE:HG22	2:B:56:ILE:O	2.06	0.54
1:A:163:GLU:HB2	6:D:1:NAG:H83	1.89	0.53
1:A:113:ALA:O	1:A:265:SER:OG	2.27	0.52
1:A:22:ASN:CG	10:A:501:NAG:O7	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LYS:CD	2:B:63:PHE:CE1	2.76	0.52
1:A:226:VAL:HG12	1:A:228:SER:H	1.75	0.51
3:H:44:GLY:O	3:H:45:LEU:HG	2.11	0.50
3:H:22:CYS:O	3:H:77:THR:HA	2.13	0.49
1:A:163:GLU:CB	6:D:1:NAG:H82	2.44	0.48
1:A:114:SER:C	1:A:265:SER:HG	2.20	0.48
1:A:264:LYS:CE	2:B:63:PHE:CE2	2.96	0.48
1:A:263:GLY:O	1:A:265:SER:N	2.46	0.48
1:A:244:LEU:C	1:A:244:LEU:HD23	2.40	0.47
2:B:110:LEU:C	2:B:110:LEU:HD12	2.41	0.46
1:A:114:SER:O	1:A:265:SER:OG	2.33	0.46
3:H:16:SER:O	3:H:82(C):LEU:HG	2.15	0.46
1:A:167:THR:HG23	7:E:1:NAG:H62	1.98	0.45
1:A:163:GLU:HB2	6:D:1:NAG:H82	1.99	0.45
1:A:170:ASN:OD1	1:A:170:ASN:C	2.60	0.44
1:A:114:SER:CA	1:A:265:SER:HG	2.28	0.44
1:A:264:LYS:HE2	2:B:63:PHE:CE2	2.52	0.44
1:A:167:THR:HG21	7:E:1:NAG:H62	1.98	0.44
3:H:178:LEU:C	3:H:178:LEU:HD23	2.43	0.43
1:A:248:THR:CA	6:D:1:NAG:H81	2.47	0.43
2:B:154:ASN:O	2:B:154:ASN:OD1	2.37	0.43
4:L:169:ASP:OD1	4:L:169:ASP:C	2.62	0.43
1:A:302:TYR:CD1	1:A:302:TYR:C	2.97	0.42
3:H:96:ALA:HA	3:H:101:ASP:HB2	2.01	0.42
2:B:153:ARG:O	2:B:154:ASN:HB2	2.15	0.42
1:A:184:HIS:O	1:A:228:SER:OG	2.29	0.41
4:L:209:ASN:O	4:L:210:ARG:HB2	2.20	0.41
1:A:126:ASN:OD1	1:A:126:ASN:C	2.62	0.41
4:L:65:SER:OG	4:L:66:GLY:N	2.54	0.41
1:A:174:PHE:CD1	1:A:174:PHE:C	2.98	0.41
4:L:66:GLY:HA3	4:L:71:PHE:HA	2.03	0.41
4:L:94:SER:HA	4:L:95:PRO:HD3	1.88	0.41
4:L:174:LEU:C	4:L:174:LEU:HD23	2.47	0.40
3:H:11:VAL:O	3:H:11:VAL:CG1	2.69	0.40
4:L:48:ILE:HG21	4:L:51:SER:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:CE1	3:H:216:CYS:SG[7_454]	2.10	0.10

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	317/329 (96%)	304 (96%)	11 (4%)	2 (1%)	21	54
2	B	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	21	54
3	H	223/236 (94%)	205 (92%)	12 (5%)	6 (3%)	4	27
4	L	210/214 (98%)	202 (96%)	7 (3%)	1 (0%)	24	57
All	All	922/953 (97%)	875 (95%)	37 (4%)	10 (1%)	11	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	2	VAL
3	H	215	SER
3	H	217	HIS
3	H	66	ARG
3	H	100(D)	PRO
4	L	40	PRO
1	A	264	LYS
3	H	213	PRO
1	A	74	PRO
2	B	8	GLY

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	284/293 (97%)	284 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	148/148 (100%)	148 (100%)	0	100	100
3	H	192/200 (96%)	192 (100%)	0	100	100
4	L	184/186 (99%)	184 (100%)	0	100	100
All	All	808/827 (98%)	808 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	12	ASN
3	H	43	HIS
3	H	164	HIS
3	H	192	GLN
3	H	217	HIS
4	L	209	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 ⓘ

25 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	$\# Z > 2$
5	NAG	C	1	1,5	14,14,15	0.53	0	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	2	5	14,14,15	0.40	0	17,19,21	0.56	0
5	BMA	C	3	5	11,11,12	0.94	0	15,15,17	0.92	0
5	MAN	C	4	5	11,11,12	0.92	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	C	5	5	11,11,12	0.81	1 (9%)	15,15,17	1.61	2 (13%)
6	NAG	D	1	1,6	14,14,15	0.36	0	17,19,21	0.67	0
6	NAG	D	2	6	14,14,15	0.30	0	17,19,21	0.45	0
6	BMA	D	3	6	11,11,12	1.03	1 (9%)	15,15,17	1.76	2 (13%)
6	MAN	D	4	6	11,11,12	0.92	1 (9%)	15,15,17	1.39	2 (13%)
7	NAG	E	1	1,7	14,14,15	0.38	0	17,19,21	1.37	1 (5%)
7	NAG	E	2	7	14,14,15	0.45	0	17,19,21	0.62	0
7	MAN	E	3	7	11,11,12	0.89	1 (9%)	15,15,17	1.01	2 (13%)
7	MAN	E	4	7	11,11,12	0.59	0	15,15,17	1.25	2 (13%)
7	MAN	E	5	7	11,11,12	0.54	0	15,15,17	1.03	2 (13%)
7	MAN	E	6	7	11,11,12	0.86	0	15,15,17	1.03	2 (13%)
8	NAG	F	1	8	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
8	NAG	F	2	8	14,14,15	0.47	0	17,19,21	1.72	3 (17%)
8	BMA	F	3	8	11,11,12	0.52	0	15,15,17	0.88	0
5	NAG	G	1	1,5	14,14,15	0.46	0	17,19,21	1.32	2 (11%)
5	NAG	G	2	5	14,14,15	0.16	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
5	MAN	G	4	5	11,11,12	0.91	0	15,15,17	1.22	2 (13%)
5	MAN	G	5	5	11,11,12	0.85	1 (9%)	15,15,17	1.25	2 (13%)
9	NAG	I	1	9,2	14,14,15	1.66	2 (14%)	17,19,21	1.26	2 (11%)
9	NAG	I	2	9	14,14,15	0.44	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
5	MAN	C	4	5	-	1/2/19/22	1/1/1/1
5	MAN	C	5	5	-	1/2/19/22	1/1/1/1
6	NAG	D	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	D	3	6	-	2/2/19/22	0/1/1/1
6	MAN	D	4	6	-	2/2/19/22	0/1/1/1
7	NAG	E	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	MAN	E	3	7	-	0/2/19/22	1/1/1/1
7	MAN	E	4	7	-	0/2/19/22	0/1/1/1
7	MAN	E	5	7	-	0/2/19/22	0/1/1/1
7	MAN	E	6	7	-	0/2/19/22	0/1/1/1
8	NAG	F	1	8	-	5/6/23/26	0/1/1/1
8	NAG	F	2	8	-	3/6/23/26	0/1/1/1
8	BMA	F	3	8	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	1/1/1/1
9	NAG	I	1	9,2	-	3/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	NAG	O5-C1	-4.68	1.35	1.43
9	I	1	NAG	C1-C2	-3.90	1.47	1.52
6	D	4	MAN	C1-C2	2.43	1.58	1.52
7	E	3	MAN	O5-C5	2.24	1.47	1.43
5	G	5	MAN	O5-C5	2.21	1.47	1.43
5	C	5	MAN	O5-C5	2.12	1.47	1.43
6	D	3	BMA	C4-C5	2.07	1.57	1.53
5	C	4	MAN	C1-C2	2.05	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5	MAN	C1-O5-C5	5.27	119.25	112.19
6	D	3	BMA	C1-O5-C5	5.25	119.22	112.19
7	E	1	NAG	C1-O5-C5	4.80	118.62	112.19
8	F	2	NAG	O5-C1-C2	-4.68	104.05	111.29
5	G	1	NAG	C2-N2-C7	4.58	129.04	122.90
7	E	4	MAN	C1-O5-C5	4.05	117.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-O5-C5	3.83	117.32	112.19
9	I	1	NAG	C3-C4-C5	3.83	117.17	110.23
5	C	4	MAN	C1-O5-C5	3.58	116.99	112.19
6	D	4	MAN	C1-O5-C5	3.58	116.98	112.19
8	F	2	NAG	C1-O5-C5	3.40	116.74	112.19
8	F	2	NAG	C2-N2-C7	-3.13	118.70	122.90
5	G	4	MAN	C1-O5-C5	3.00	116.21	112.19
7	E	5	MAN	C1-O5-C5	2.92	116.10	112.19
6	D	4	MAN	O2-C2-C3	-2.69	104.58	110.15
5	C	1	NAG	O5-C5-C6	2.68	112.88	107.66
7	E	3	MAN	C1-O5-C5	2.55	115.61	112.19
7	E	6	MAN	C1-O5-C5	2.48	115.51	112.19
8	F	1	NAG	O5-C1-C2	-2.47	107.47	111.29
6	D	3	BMA	C3-C4-C5	2.43	114.63	110.23
5	C	5	MAN	O2-C2-C3	-2.34	105.31	110.15
7	E	3	MAN	O2-C2-C3	-2.32	105.34	110.15
9	I	1	NAG	O4-C4-C5	-2.25	103.78	109.32
5	G	5	MAN	O2-C2-C3	-2.22	105.56	110.15
7	E	6	MAN	O2-C2-C3	-2.18	105.64	110.15
7	E	5	MAN	O2-C2-C3	-2.15	105.70	110.15
5	G	3	BMA	C1-O5-C5	2.12	115.03	112.19
5	G	4	MAN	O2-C2-C3	-2.12	105.77	110.15
5	C	4	MAN	O2-C2-C3	-2.11	105.77	110.15
7	E	4	MAN	O2-C2-C3	-2.11	105.78	110.15
5	G	1	NAG	C1-C2-N2	2.02	113.62	110.43

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	1	NAG	C8-C7-N2-C2
8	F	1	NAG	O7-C7-N2-C2
6	D	3	BMA	O5-C5-C6-O6
6	D	4	MAN	C4-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
5	C	3	BMA	C4-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
6	D	3	BMA	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
6	D	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
5	C	5	MAN	O5-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
5	C	4	MAN	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
5	C	1	NAG	C3-C2-N2-C7
9	I	1	NAG	C4-C5-C6-O6
8	F	2	NAG	C8-C7-N2-C2
8	F	3	BMA	C4-C5-C6-O6
9	I	1	NAG	C3-C2-N2-C7
8	F	2	NAG	O7-C7-N2-C2
8	F	3	BMA	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
5	G	1	NAG	C3-C2-N2-C7
8	F	1	NAG	C3-C2-N2-C7

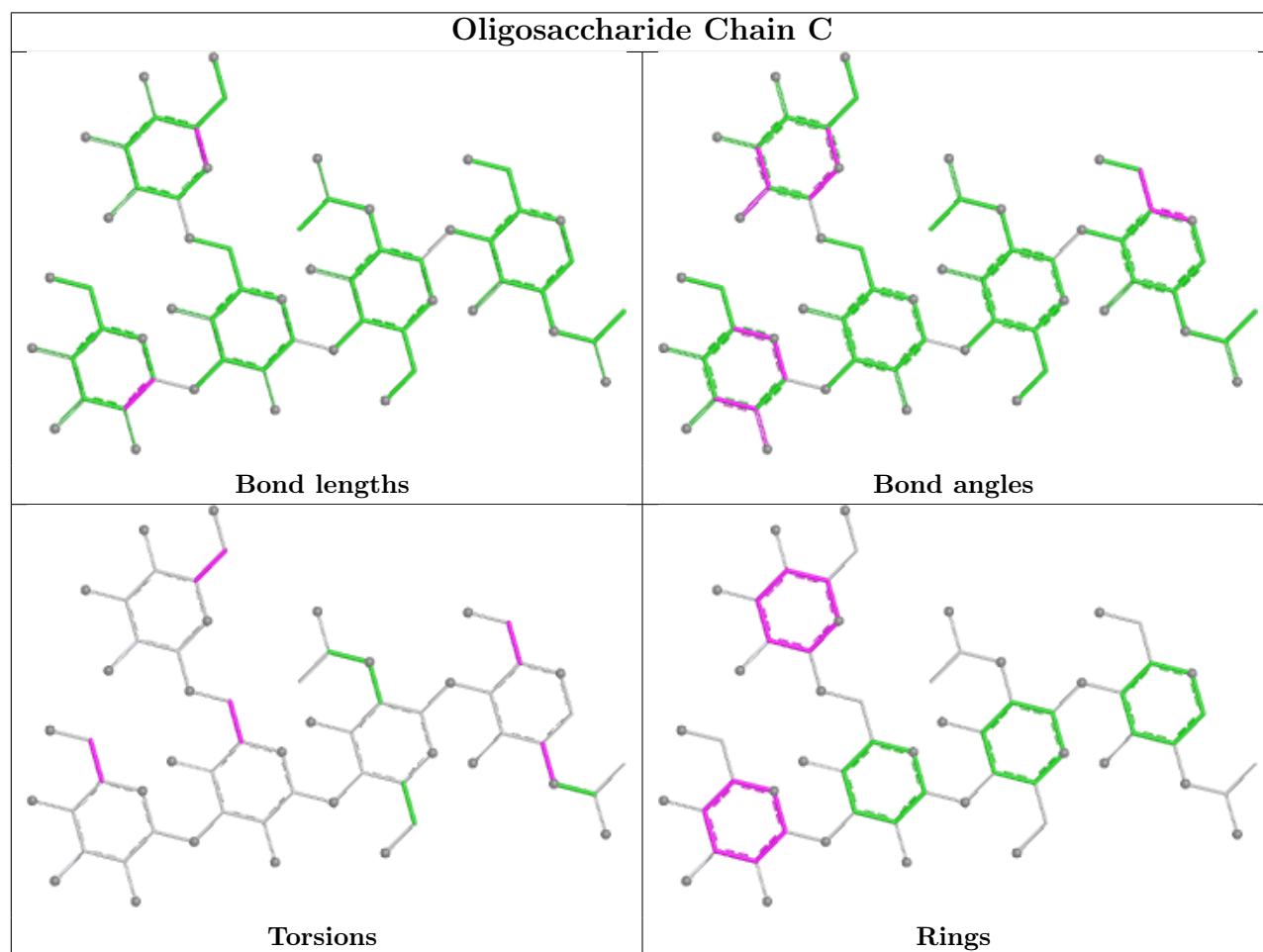
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	5	MAN	C1-C2-C3-C4-C5-O5
5	C	4	MAN	C1-C2-C3-C4-C5-O5
7	E	3	MAN	C1-C2-C3-C4-C5-O5
5	G	5	MAN	C1-C2-C3-C4-C5-O5

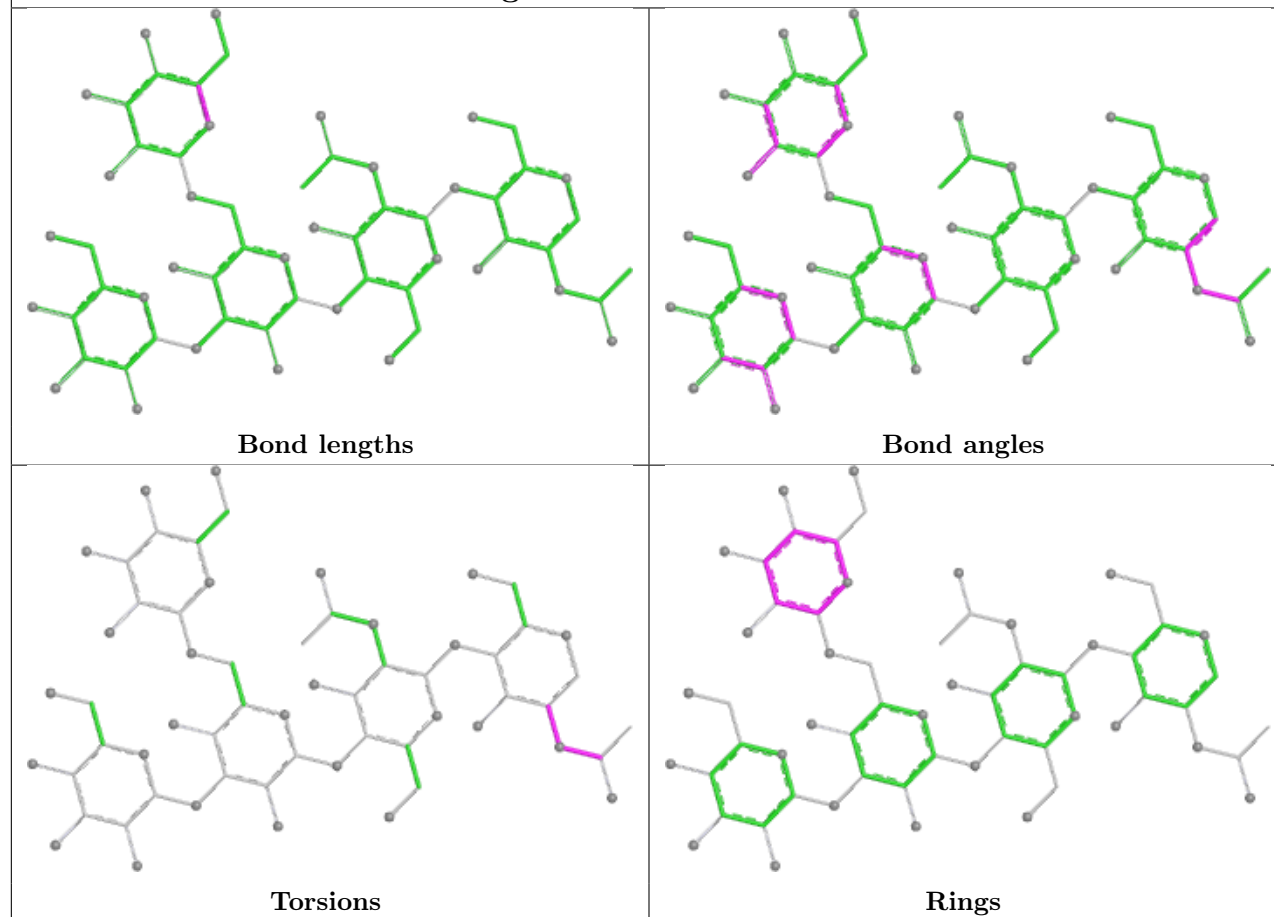
9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2	NAG	2	0
6	D	1	NAG	18	0
5	G	2	NAG	1	0
5	G	5	MAN	1	0
8	F	1	NAG	1	0
5	C	2	NAG	1	0
5	C	1	NAG	3	0
5	G	1	NAG	1	0
7	E	1	NAG	3	0

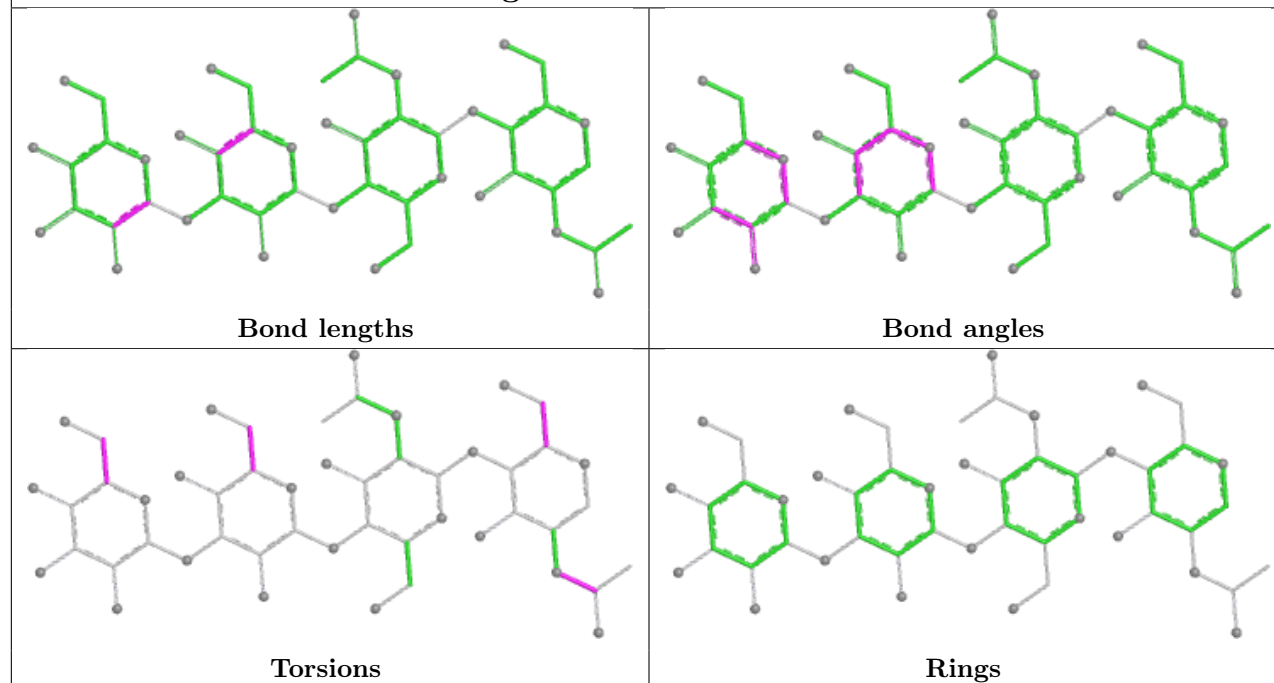
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

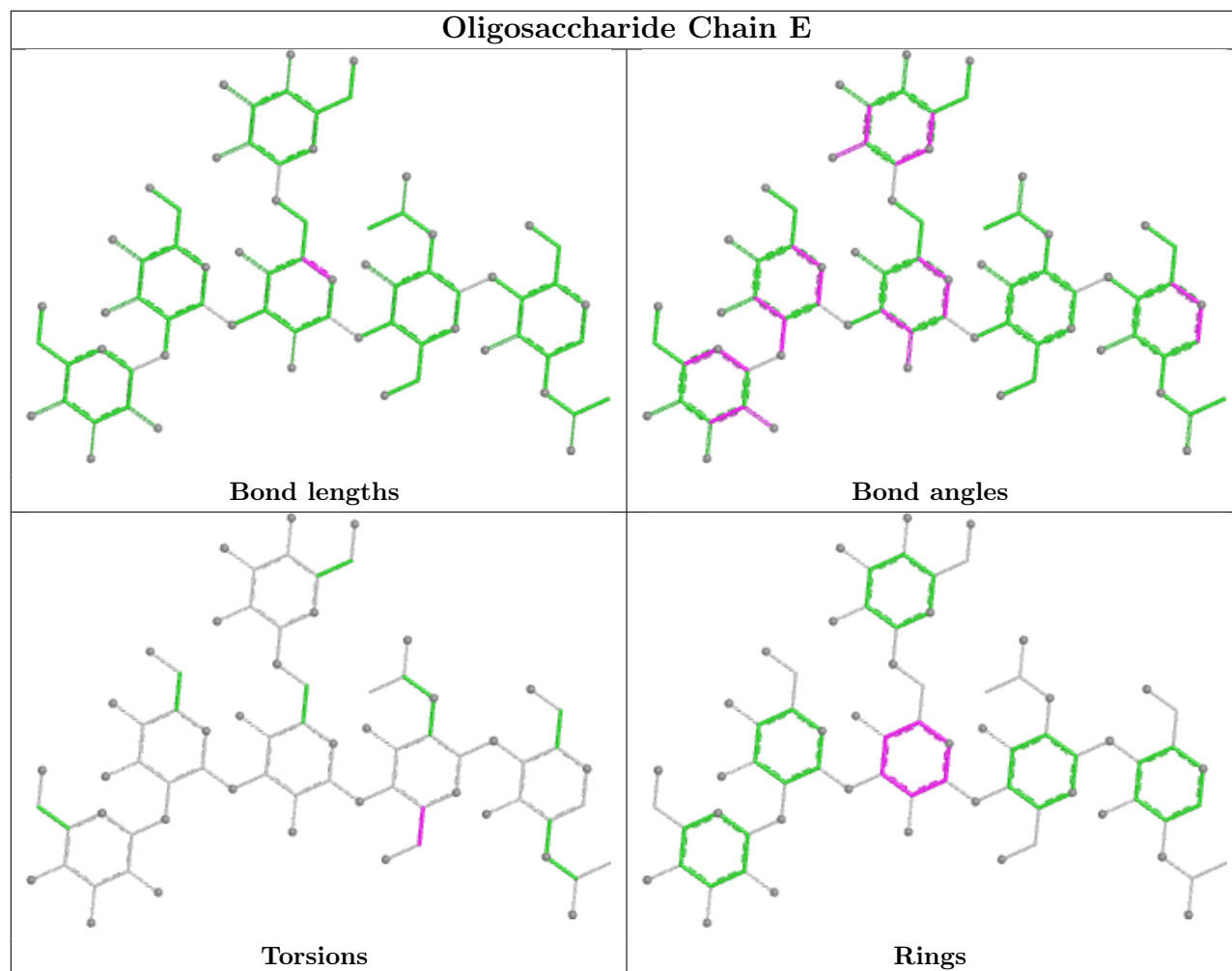


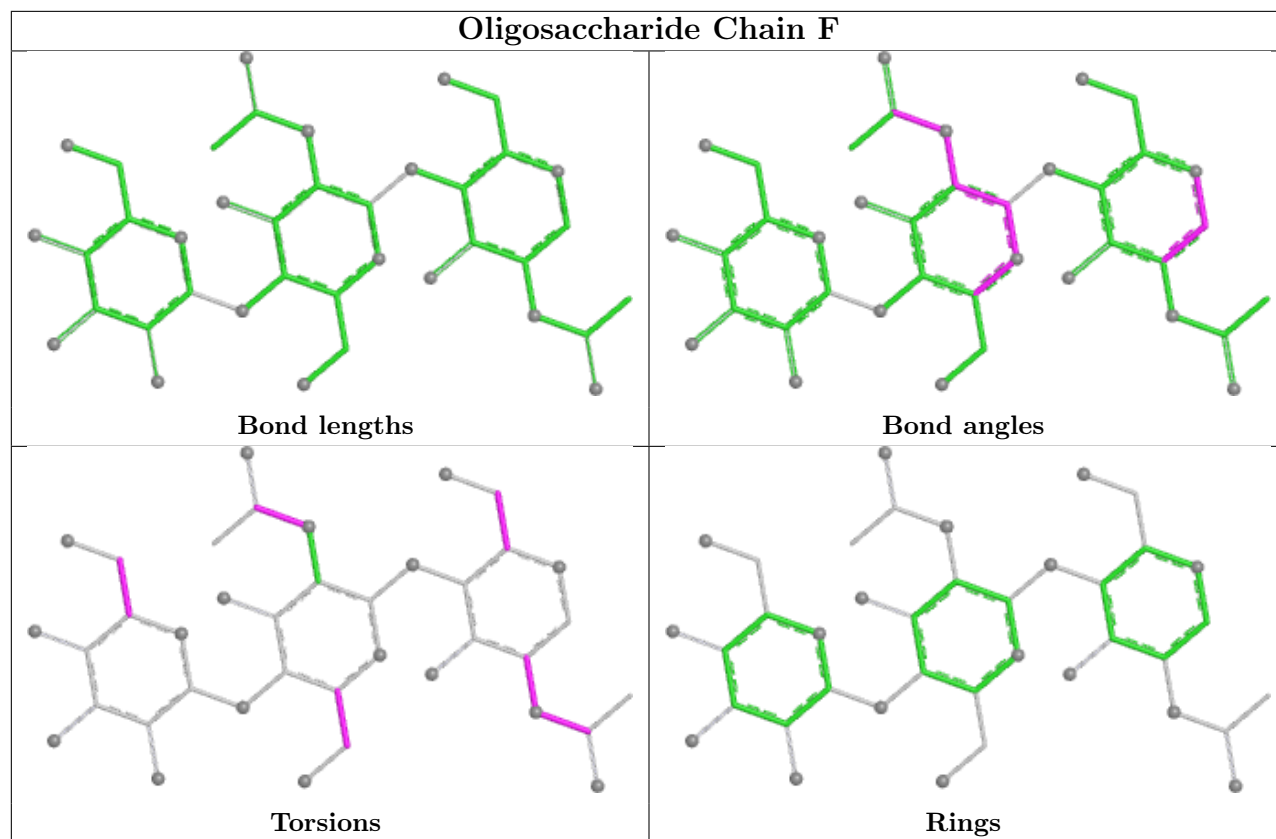
Oligosaccharide Chain G

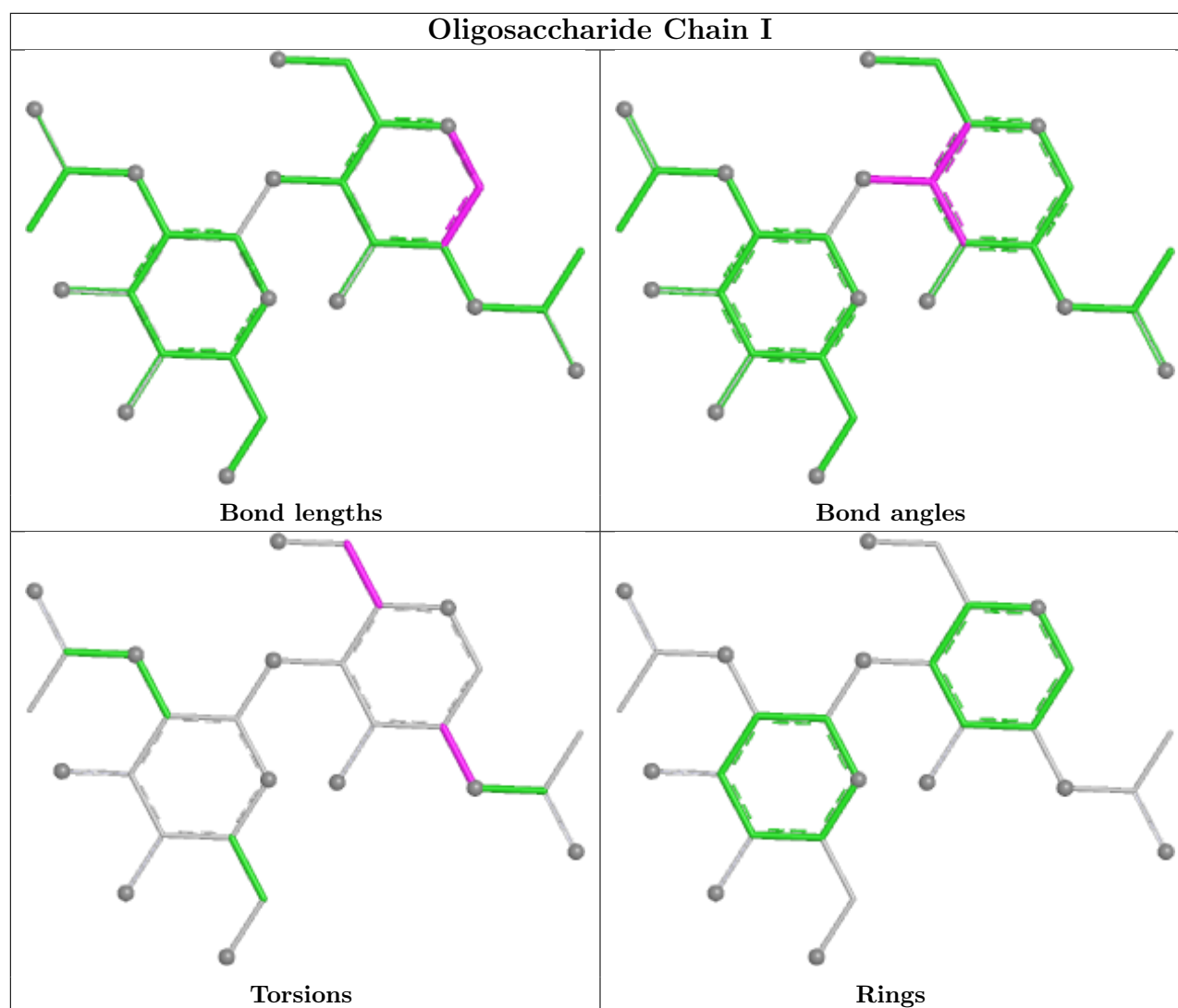


Oligosaccharide Chain D









5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	A	501	1	14,14,15	0.28	0	17,19,21	0.57	0
10	NAG	A	520	1	14,14,15	0.23	0	17,19,21	0.38	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
10	NAG	A	501	1	-	0/6/23/26	0/1/1/1
10	NAG	A	520	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	520	NAG	C8-C7-N2-C2
10	A	520	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	501	NAG	2	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	319/329 (96%)	-0.12	4 (1%) 75 47	72, 112, 165, 270	0
2	B	174/174 (100%)	0.12	6 (3%) 48 26	71, 141, 203, 244	0
3	H	227/236 (96%)	0.08	10 (4%) 39 21	94, 140, 186, 261	0
4	L	212/214 (99%)	-0.07	8 (3%) 44 24	101, 155, 217, 250	0
All	All	932/953 (97%)	-0.02	28 (3%) 52 29	71, 132, 201, 270	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	42	GLN	6.1
4	L	41	GLY	5.4
3	H	165	THR	4.0
3	H	218	HIS	3.8
4	L	40	PRO	3.8
3	H	65	ASP	3.4
3	H	166	PHE	3.4
1	A	326	LYS	3.2
2	B	22	TYR	3.0
4	L	196	THR	2.9
3	H	64	ASP	2.8
3	H	216	CYS	2.8
2	B	125	GLN	2.8
3	H	214	LYS	2.7
2	B	119	PHE	2.6
3	H	63	PHE	2.6
4	L	62	PHE	2.6
2	B	120	GLU	2.4
2	B	57	LYS	2.4
4	L	164	GLU	2.3
4	L	142	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	264	LYS	2.2
3	H	180	SER	2.1
1	A	119	GLU	2.1
1	A	312	ASN	2.1
2	B	132	ASP	2.1
4	L	210	ARG	2.0
3	H	178	LEU	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.

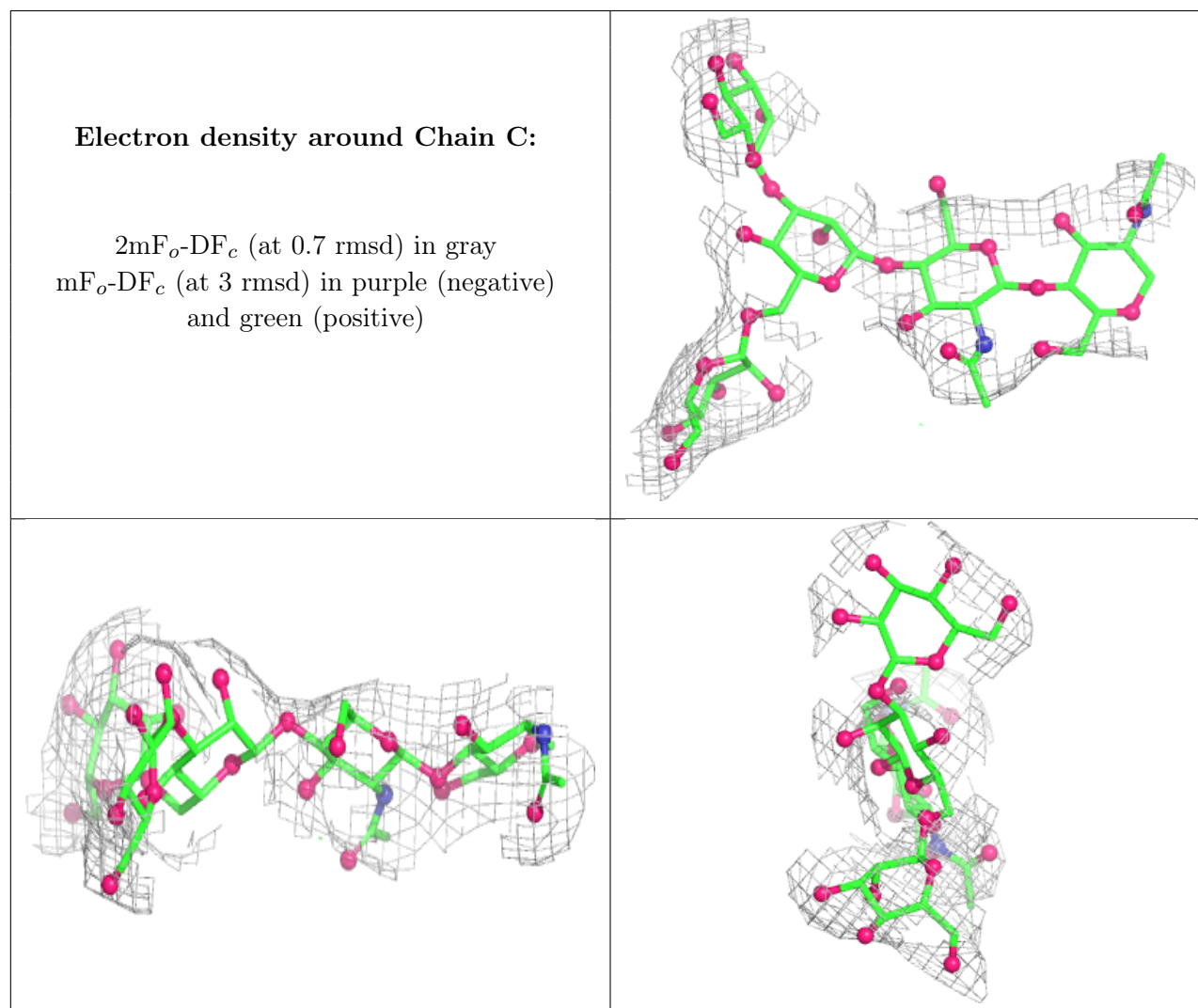
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	151,189,228,233	0
5	NAG	C	2	14/15	-	-	174,213,222,231	0
5	BMA	C	3	11/12	-	-	202,212,217,228	0
5	MAN	C	4	11/12	-	-	172,220,229,236	0
5	MAN	C	5	11/12	-	-	191,221,235,237	0
8	BMA	F	3	11/12	-0.07	0.11	216,285,291,297	0
5	MAN	G	5	11/12	0.46	0.14	242,262,278,280	0
5	BMA	G	3	11/12	-	-	268,284,290,293	0
7	MAN	E	4	11/12	0.48	0.10	237,249,300,311	0
7	MAN	E	5	11/12	0.63	0.11	178,217,263,279	0
6	NAG	D	1	14/15	-	-	169,201,241,244	0
6	NAG	D	2	14/15	-	-	146,187,205,237	0
6	BMA	D	3	11/12	-	-	259,274,282,294	0
6	MAN	D	4	11/12	-	-	220,275,288,291	0
7	NAG	E	2	14/15	0.63	0.17	114,159,213,233	0
9	NAG	I	1	14/15	0.68	0.12	187,257,286,304	0
7	MAN	E	3	11/12	-	-	166,214,228,230	0
9	NAG	I	2	14/15	0.71	0.09	224,292,313,315	0
5	MAN	G	4	11/12	0.79	0.18	183,238,278,282	0
7	MAN	E	6	11/12	-	-	201,241,279,291	0
8	NAG	F	2	14/15	0.81	0.13	148,227,271,279	0

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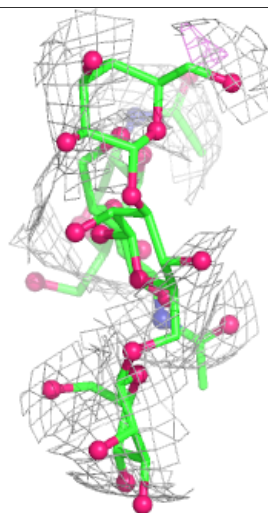
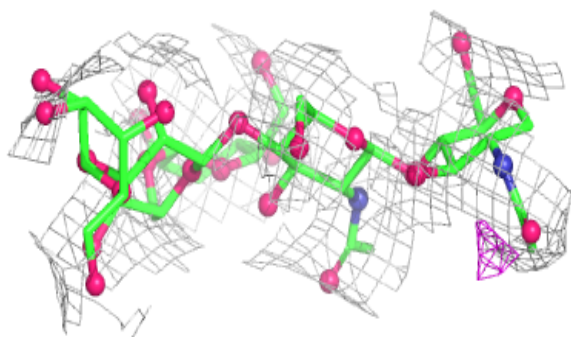
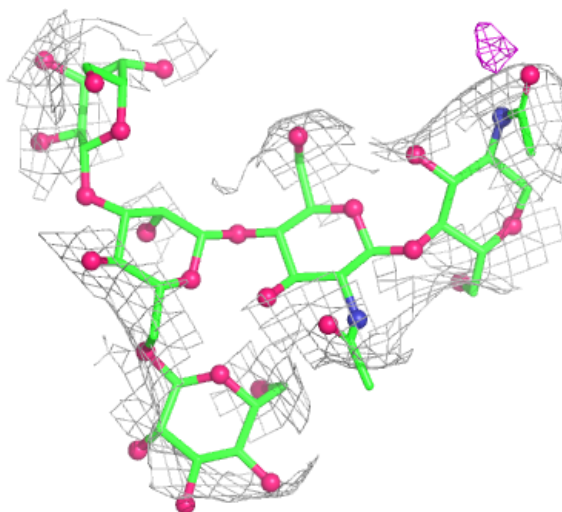
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	F	1	14/15	0.86	0.15	131,168,201,205	0
7	NAG	E	1	14/15	0.87	0.10	123,134,156,164	0
5	NAG	G	2	14/15	0.88	0.16	148,234,272,276	0
5	NAG	G	1	14/15	0.90	0.12	127,173,211,232	0

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.



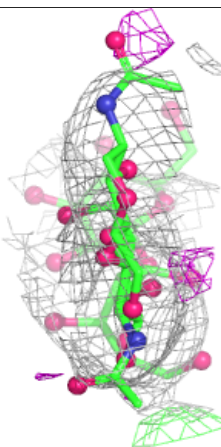
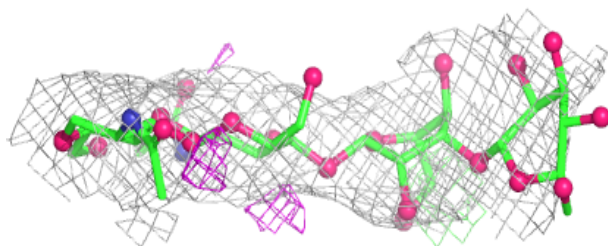
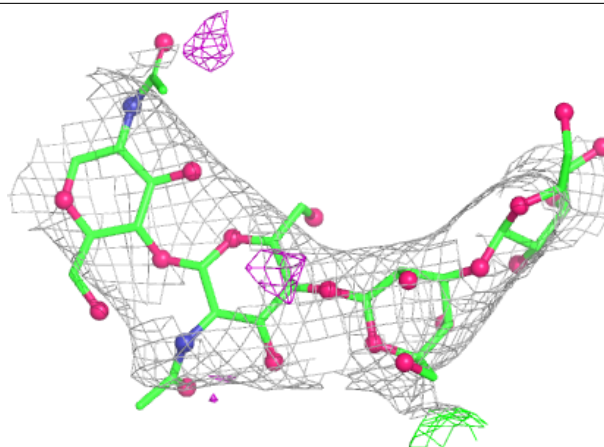
Electron density around Chain G:

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



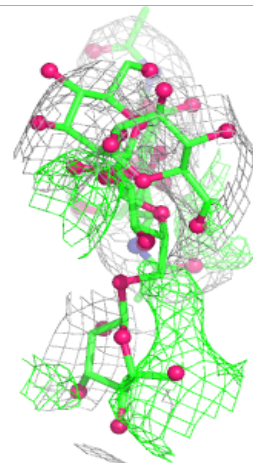
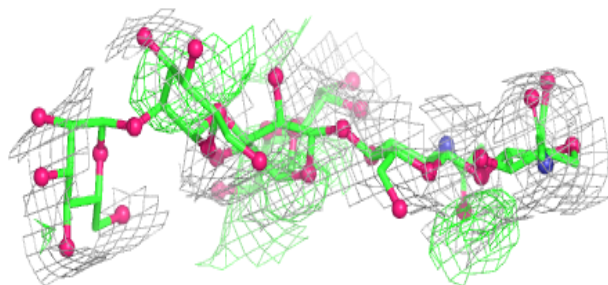
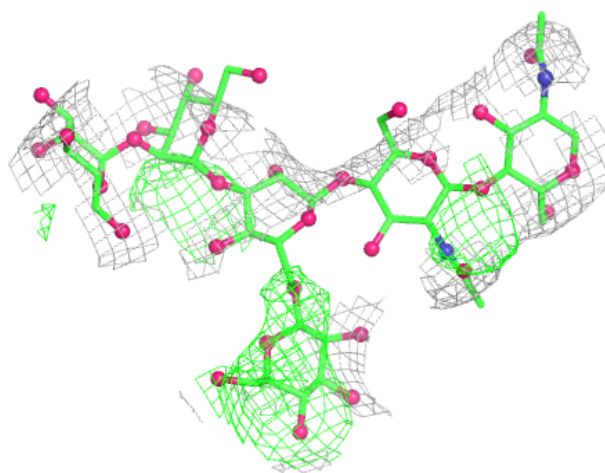
Electron density around Chain D:

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



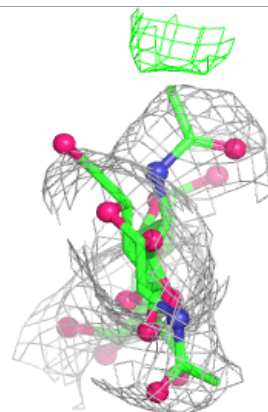
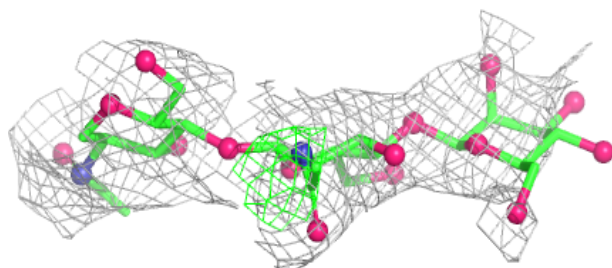
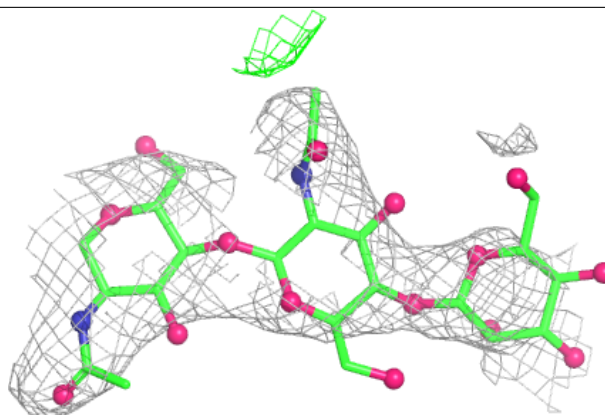
Electron density around Chain E:

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

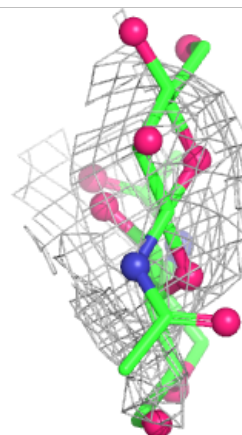
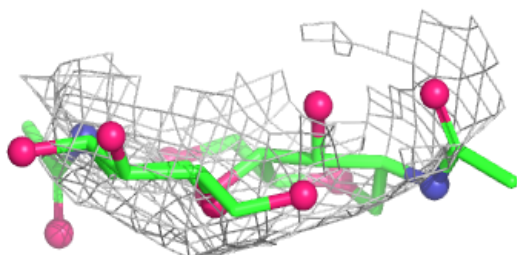
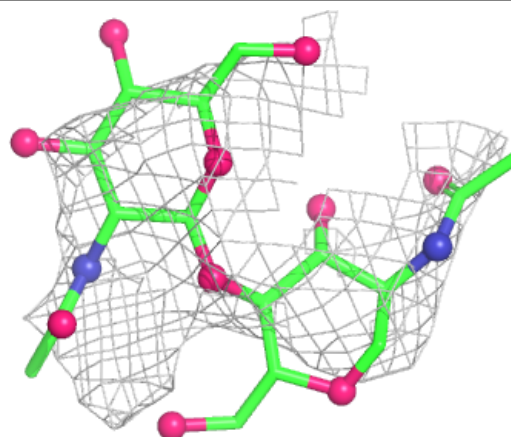


Electron density around Chain F:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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
10	NAG	A	520	14/15	0.50	0.21	181,267,296,297	0
10	NAG	A	501	14/15	0.54	0.11	207,244,252,269	0
11	ZN	H	301	1/1	0.89	0.17	187,187,187,187	0

6.5 Other polymers [i](#)

There are no such residues in this entry.