



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 PM UTC

PDB ID : 1HGH / pdb_00001hgh
Title : BINDING OF INFLUENZA VIRUS HEMAGGLUTININ TO ANALOGS OF ITS CELL-SURFACE RECEPTOR, SIALIC ACID: ANALYSIS BY PROTON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND X-RAY CRYSTALLOGRAPHY
Authors : Sauter, N.K.; Hanson, J.E.; Glick, G.D.; Brown, J.H.; Crowther, R.L.; Park, S.-J.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1991-11-01
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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)

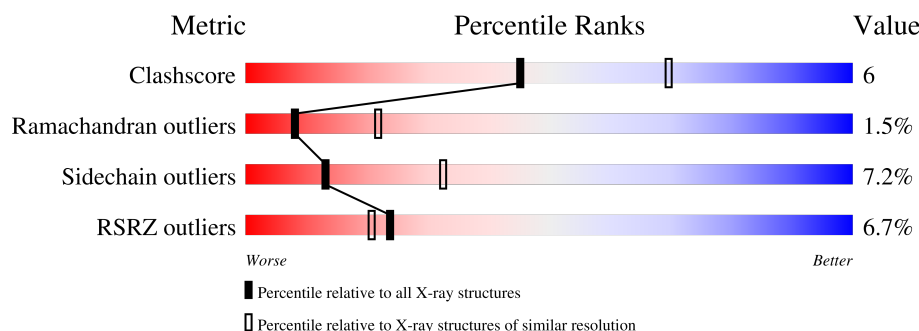
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

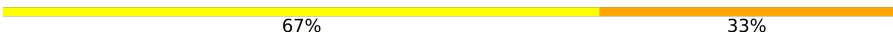
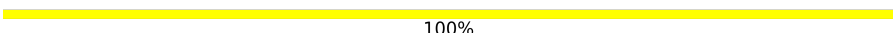
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	328	7% 73% 22% . .
1	C	328	7% 74% 20% . .
1	E	328	7% 73% 20% . .
2	B	175	7% 70% 26% . .
2	D	175	4% 70% 25% 5% .

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	F	175	 6% 70% 23% 7%
3	G	3	 33% 67%
3	H	3	 67% 33%
3	I	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15630 atoms, of which 3282 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.

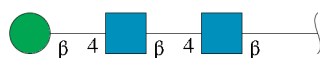
- Molecule 1 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			

- Molecule 3 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.



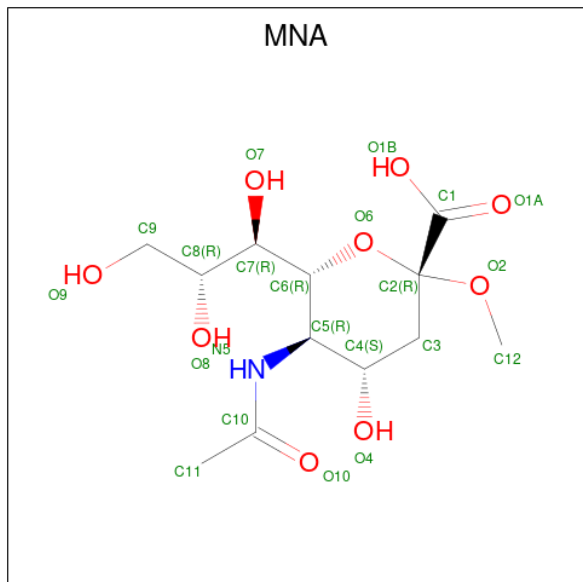
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O		0	0	0
			76	22	37	2	15				
3	H	3	Total	C	H	N	O		0	0	0
			76	22	37	2	15				
3	I	3	Total	C	H	N	O		0	0	0
			76	22	37	2	15				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	F	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is 2-O-methyl-5-N-acetyl-alpha-D-neuraminic acid (CCD ID: MNA) (formula: $C_{12}H_{21}NO_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	A	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	C	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	C	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	E	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	E	1	Total	C	H	N	O	0	0
			39	12	17	1	9		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	11	Total	H	O	0	0
			33	22	11		
6	B	13	Total	H	O	0	0
			39	26	13		
6	C	10	Total	H	O	0	0
			30	20	10		
6	D	14	Total	H	O	0	0
			42	28	14		

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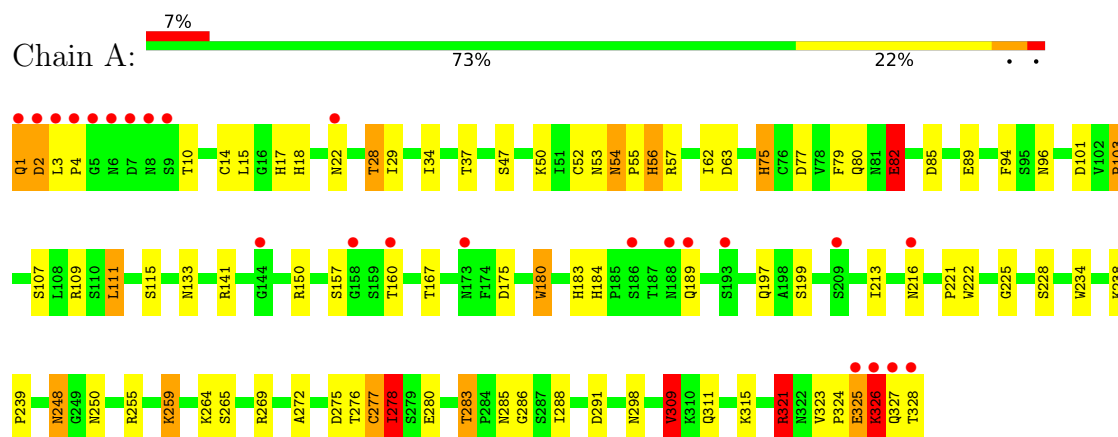
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	10	Total	H	O	0	0
			30	20	10		
6	F	14	Total	H	O	0	0
			42	28	14		

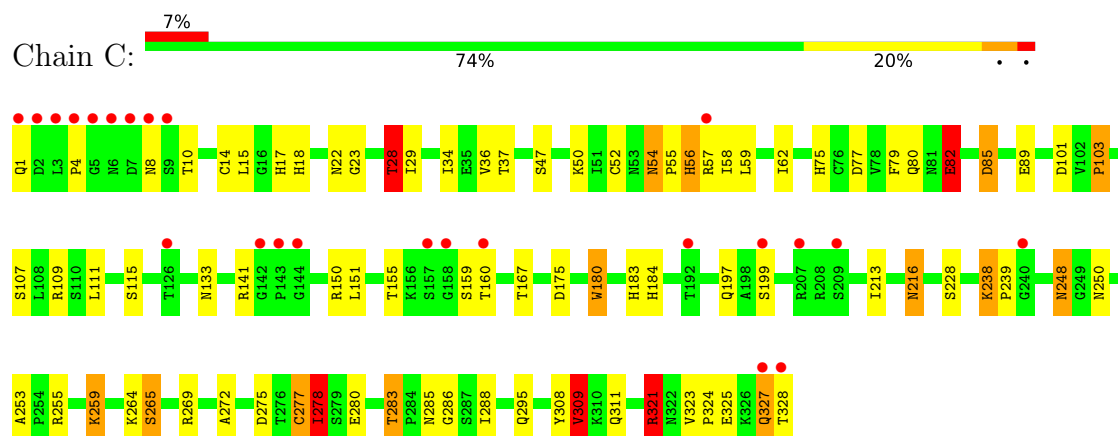
3 Residue-property plots [i](#)

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.

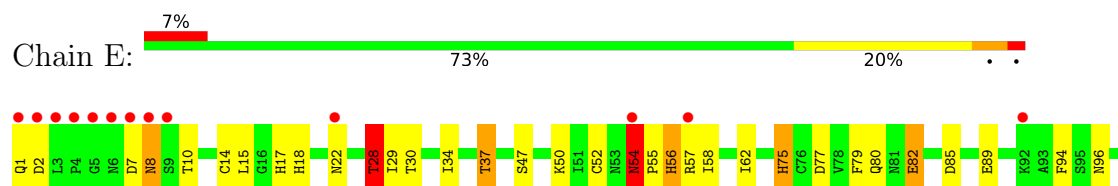
• Molecule 1: HEMAGGLUTININ, CHAIN HA1

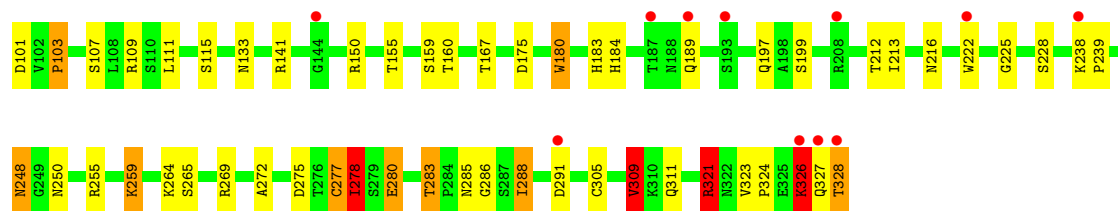


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

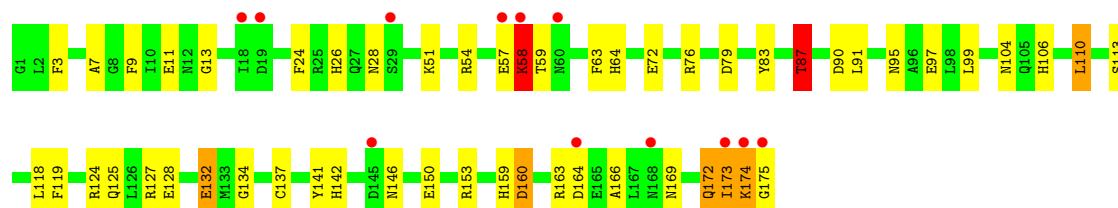


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

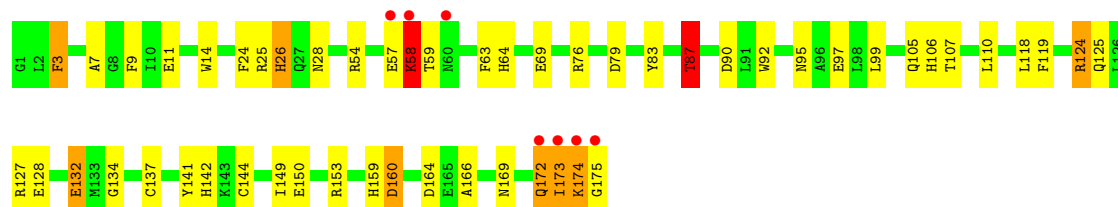




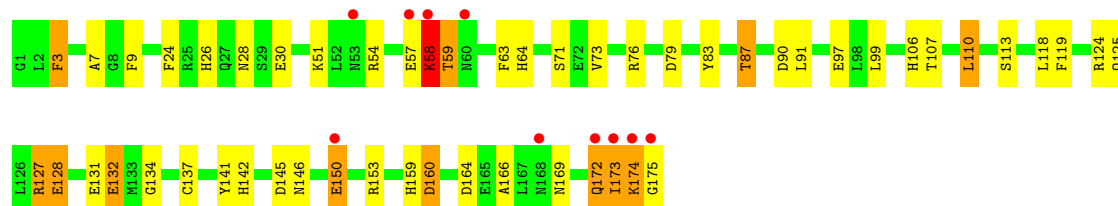
• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



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



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

Chain H:  67% 33%

MAG1
MAG2
BMA3

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

Chain I:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	162.80Å 162.80Å 178.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.70 7.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.70) 57.9 (7.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.72Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , (Not available) 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15630	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: BMA, MNA, 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	1.14	16/2589 (0.6%)	1.73	46/3527 (1.3%)
1	C	1.11	10/2589 (0.4%)	1.71	41/3527 (1.2%)
1	E	1.15	14/2589 (0.5%)	1.72	42/3527 (1.2%)
2	B	1.16	11/1445 (0.8%)	1.76	30/1939 (1.5%)
2	D	1.17	10/1445 (0.7%)	1.76	31/1939 (1.6%)
2	F	1.15	9/1445 (0.6%)	1.77	30/1939 (1.5%)
All	All	1.14	70/12102 (0.6%)	1.73	220/16398 (1.3%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	159	HIS	CG-ND1	-7.54	1.29	1.38
2	B	159	HIS	CG-ND1	-7.28	1.30	1.38
1	E	184	HIS	CG-ND1	-7.06	1.30	1.38
1	A	75	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	17	HIS	CD2-NE2	-6.82	1.30	1.37
1	E	56	HIS	CD2-NE2	-6.80	1.30	1.37
1	E	184	HIS	CD2-NE2	-6.79	1.30	1.37
1	E	18	HIS	CD2-NE2	-6.74	1.30	1.37
1	E	18	HIS	CG-ND1	-6.72	1.30	1.38
1	E	75	HIS	CD2-NE2	-6.72	1.30	1.37
2	B	159	HIS	CD2-NE2	-6.71	1.30	1.37
2	D	106	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	18	HIS	CG-ND1	-6.53	1.31	1.38
2	B	64	HIS	CG-ND1	-6.50	1.31	1.38
2	D	159	HIS	CD2-NE2	-6.50	1.30	1.37
1	C	75	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	183	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.36	1.30	1.37
2	B	106	HIS	CD2-NE2	-6.36	1.30	1.37
1	C	17	HIS	CD2-NE2	-6.36	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	142	HIS	CD2-NE2	-6.35	1.30	1.37
2	F	159	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	184	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	18	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	184	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	183	HIS	CG-ND1	-6.12	1.31	1.38
2	D	159	HIS	CG-ND1	-6.05	1.31	1.38
1	E	278	ILE	CA-CB	6.00	1.61	1.54
1	A	184	HIS	CG-ND1	-5.97	1.31	1.38
1	A	278	ILE	CA-CB	5.97	1.61	1.54
2	B	106	HIS	CG-ND1	-5.96	1.31	1.38
2	D	106	HIS	CG-ND1	-5.93	1.31	1.38
2	F	106	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	326	LYS	CA-CB	5.90	1.63	1.53
1	C	278	ILE	CA-CB	5.87	1.61	1.54
1	C	184	HIS	CG-ND1	-5.87	1.31	1.38
2	D	26	HIS	CD2-NE2	-5.86	1.31	1.37
1	E	96	ASN	CA-CB	-5.83	1.48	1.53
1	E	305	CYS	CA-CB	-5.80	1.46	1.54
2	B	26	HIS	CD2-NE2	-5.79	1.31	1.37
2	F	64	HIS	CD2-NE2	-5.77	1.31	1.37
1	C	56	HIS	CD2-NE2	-5.77	1.31	1.37
2	D	64	HIS	CD2-NE2	-5.77	1.31	1.37
2	B	142	HIS	CG-ND1	-5.76	1.31	1.38
1	E	17	HIS	CD2-NE2	-5.75	1.31	1.37
1	E	280	GLU	CA-CB	-5.67	1.44	1.53
2	B	87	THR	CA-CB	5.64	1.62	1.53
1	E	183	HIS	CG-ND1	-5.63	1.32	1.38
2	B	64	HIS	CD2-NE2	-5.61	1.31	1.37
1	C	18	HIS	CG-ND1	-5.60	1.32	1.38
2	D	26	HIS	CG-ND1	-5.59	1.32	1.38
2	F	26	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	17	HIS	CG-ND1	-5.56	1.32	1.38
1	E	56	HIS	CG-ND1	-5.54	1.32	1.38
1	A	17	HIS	CG-ND1	-5.50	1.32	1.38
2	B	142	HIS	CD2-NE2	-5.42	1.31	1.37
1	C	18	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	56	HIS	CG-ND1	-5.34	1.32	1.38
2	D	64	HIS	CG-ND1	-5.31	1.32	1.38
1	C	183	HIS	CG-ND1	-5.30	1.32	1.38
2	D	142	HIS	CD2-NE2	-5.29	1.32	1.37
2	F	64	HIS	CG-ND1	-5.28	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	87	THR	CA-CB	5.27	1.62	1.53
1	A	234	TRP	CG-CD2	-5.27	1.34	1.43
2	F	26	HIS	CG-ND1	-5.25	1.32	1.38
1	E	183	HIS	CD2-NE2	-5.20	1.32	1.37
2	B	26	HIS	CG-ND1	-5.15	1.32	1.38
2	F	106	HIS	CG-ND1	-5.15	1.32	1.38
1	A	96	ASN	CA-CB	-5.14	1.49	1.53
1	A	75	HIS	CG-ND1	-5.01	1.32	1.38

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	PHE	CA-CB-CG	9.39	123.19	113.80
2	B	169	ASN	CA-CB-CG	9.29	121.89	112.60
2	F	79	ASP	CA-CB-CG	8.86	121.46	112.60
2	F	169	ASN	CA-CB-CG	8.81	121.41	112.60
2	D	169	ASN	CA-CB-CG	8.79	121.39	112.60
2	F	9	PHE	CA-CB-CG	8.72	122.52	113.80
1	E	75	HIS	CA-CB-CG	8.49	122.29	113.80
1	E	326	LYS	CA-CB-CG	8.38	130.87	114.10
2	B	9	PHE	CA-CB-CG	8.38	122.18	113.80
2	B	79	ASP	CA-CB-CG	8.33	120.93	112.60
2	B	57	GLU	CA-CB-CG	8.29	130.68	114.10
2	D	57	GLU	CA-CB-CG	8.21	130.51	114.10
2	B	159	HIS	ND1-CG-CD2	8.16	114.26	106.10
2	F	57	GLU	CA-CB-CG	8.15	130.39	114.10
1	A	75	HIS	CA-CB-CG	8.06	121.86	113.80
1	C	75	HIS	CA-CB-CG	8.05	121.85	113.80
1	E	56	HIS	ND1-CG-CD2	8.01	114.11	106.10
1	A	56	HIS	ND1-CG-CD2	7.95	114.05	106.10
2	F	106	HIS	ND1-CG-CD2	7.78	113.88	106.10
2	D	64	HIS	ND1-CG-CD2	7.65	113.75	106.10
2	F	159	HIS	ND1-CG-CD2	7.60	113.70	106.10
2	D	79	ASP	CA-CB-CG	7.56	120.16	112.60
2	D	106	HIS	ND1-CG-CD2	7.55	113.65	106.10
2	F	64	HIS	ND1-CG-CD2	7.52	113.62	106.10
2	B	106	HIS	ND1-CG-CD2	7.51	113.61	106.10
2	D	159	HIS	ND1-CG-CD2	7.49	113.59	106.10
2	F	28	ASN	OD1-CG-ND2	-7.47	115.12	122.60
1	E	184	HIS	ND1-CG-CD2	7.43	113.53	106.10
1	C	56	HIS	ND1-CG-CD2	7.40	113.50	106.10
1	E	272	ALA	CA-C-N	7.22	126.98	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ALA	C-N-CA	7.22	126.98	119.76
1	C	272	ALA	CA-C-N	7.21	126.97	119.76
1	C	272	ALA	C-N-CA	7.21	126.97	119.76
2	B	64	HIS	ND1-CG-CD2	7.13	113.23	106.10
2	D	26	HIS	ND1-CG-CD2	7.03	113.13	106.10
1	A	272	ALA	CA-C-N	6.94	126.70	119.76
1	A	272	ALA	C-N-CA	6.94	126.70	119.76
1	A	111	LEU	N-CA-CB	-6.93	99.94	110.12
1	C	111	LEU	N-CA-CB	-6.91	99.96	110.12
1	C	184	HIS	ND1-CG-CD2	6.85	112.95	106.10
1	E	216	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	184	HIS	ND1-CG-CD2	6.76	112.86	106.10
1	A	324	PRO	O-C-N	6.76	131.37	123.06
1	A	1	GLN	N-CA-C	-6.75	92.11	111.00
2	F	26	HIS	ND1-CG-CD2	6.75	112.85	106.10
2	F	160	ASP	CA-CB-CG	-6.70	105.90	112.60
2	F	172	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	A	82	GLU	CB-CG-CD	6.66	123.92	112.60
1	C	183	HIS	ND1-CG-CD2	6.62	112.72	106.10
2	D	172	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	C	324	PRO	O-C-N	-6.57	114.72	122.86
2	B	90	ASP	CA-CB-CG	6.56	119.16	112.60
1	C	248	ASN	CB-CG-ND2	6.56	126.24	116.40
1	E	321	ARG	NE-CZ-NH2	-6.55	113.30	119.20
1	E	28	THR	CA-CB-CG2	6.54	121.61	110.50
1	C	321	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	E	111	LEU	N-CA-CB	-6.47	100.61	110.12
1	A	2	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	325	GLU	N-CA-C	-6.41	101.77	110.68
2	D	160	ASP	CA-CB-CG	-6.41	106.19	112.60
1	C	216	ASN	CA-CB-CG	6.37	118.97	112.60
1	E	28	THR	CA-CB-OG1	-6.36	100.06	109.60
1	A	325	GLU	CA-CB-CG	6.34	126.78	114.10
2	B	160	ASP	CA-CB-CG	-6.34	106.26	112.60
1	C	238	LYS	CA-CB-CG	-6.31	101.48	114.10
2	F	132	GLU	CA-CB-CG	-6.28	101.55	114.10
1	A	183	HIS	ND1-CG-CD2	6.27	112.37	106.10
2	B	172	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	E	183	HIS	ND1-CG-CD2	6.25	112.35	106.10
1	A	216	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	28	THR	CA-CB-CG2	6.22	121.07	110.50
1	A	238	LYS	CA-CB-CG	-6.21	101.68	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	GLU	CA-CB-CG	-6.20	101.70	114.10
2	D	132	GLU	CA-CB-CG	-6.20	101.71	114.10
1	C	58	ILE	N-CA-CB	-6.17	103.81	110.53
2	B	63	PHE	CA-CB-CG	-6.16	107.64	113.80
1	C	82	GLU	N-CA-CB	-6.15	101.96	110.38
1	C	248	ASN	N-CA-CB	-6.12	99.92	111.43
1	E	107	SER	CA-CB-OG	-6.12	98.86	111.10
2	D	125	GLN	CG-CD-NE2	6.10	125.55	116.40
1	C	18	HIS	ND1-CG-CD2	6.10	112.20	106.10
1	A	18	HIS	ND1-CG-CD2	6.09	112.19	106.10
1	E	180	TRP	CG-CD2-CE3	6.09	139.99	133.90
2	B	26	HIS	ND1-CG-CD2	6.07	112.17	106.10
1	E	238	LYS	CA-CB-CG	-6.06	101.98	114.10
1	E	248	ASN	CB-CG-ND2	6.05	125.47	116.40
1	E	56	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	C	28	THR	CA-CB-CG2	6.01	120.72	110.50
1	A	28	THR	CA-CB-OG1	-6.00	100.61	109.60
1	C	85	ASP	N-CA-C	-5.98	105.64	113.12
1	A	180	TRP	CG-CD2-CE3	5.97	139.87	133.90
1	A	248	ASN	CA-CB-CG	5.97	118.57	112.60
2	F	76	ARG	N-CA-C	5.93	118.23	111.11
1	A	56	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	E	1	GLN	N-CA-C	-5.93	94.41	111.00
1	C	1	GLN	N-CA-C	-5.92	94.42	111.00
1	C	29	ILE	N-CA-C	-5.91	104.97	110.53
1	E	275	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	248	ASN	CB-CG-ND2	5.90	125.25	116.40
2	B	99	LEU	CA-C-O	-5.90	114.62	120.82
1	C	115	SER	N-CA-C	-5.89	104.94	111.36
1	C	309	VAL	N-CA-CB	-5.88	100.93	111.92
1	C	103	PRO	CA-C-N	-5.87	115.10	123.20
1	C	103	PRO	C-N-CA	-5.87	115.10	123.20
1	E	309	VAL	N-CA-CB	-5.87	100.95	111.92
1	A	321	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	C	56	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	E	85	ASP	N-CA-C	-5.83	105.83	113.12
2	B	146	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	275	ASP	CA-CB-CG	5.80	118.40	112.60
2	F	54	ARG	N-CA-CB	-5.79	101.59	110.16
2	B	150	GLU	CB-CG-CD	5.78	122.43	112.60
1	E	56	HIS	CG-CD2-NE2	-5.78	101.42	107.20
1	E	115	SER	N-CA-C	-5.78	105.06	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASN	N-CA-CB	-5.75	100.63	111.43
2	F	125	GLN	CG-CD-NE2	5.74	125.01	116.40
1	E	18	HIS	ND1-CG-CD2	5.73	111.83	106.10
2	B	76	ARG	N-CA-C	5.72	117.98	111.11
1	E	248	ASN	CA-CB-CG	5.72	118.32	112.60
2	B	95	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	C	180	TRP	CG-CD2-CE3	5.70	139.60	133.90
1	C	107	SER	CA-CB-OG	-5.70	99.70	111.10
1	C	275	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	277	CYS	CA-C-N	-5.62	116.22	123.19
1	C	277	CYS	C-N-CA	-5.62	116.22	123.19
1	A	29	ILE	N-CA-C	-5.62	105.25	110.53
1	C	28	THR	CA-CB-OG1	-5.61	101.18	109.60
1	C	75	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	E	248	ASN	N-CA-CB	-5.58	100.95	111.43
2	B	125	GLN	CG-CD-NE2	5.57	124.76	116.40
1	E	54	ASN	O-C-N	-5.57	117.49	121.84
2	F	63	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	115	SER	N-CA-C	-5.55	105.31	111.36
1	A	85	ASP	N-CA-C	-5.54	106.20	113.12
1	C	36	VAL	CA-C-N	5.53	127.96	120.38
1	C	36	VAL	C-N-CA	5.53	127.96	120.38
2	D	64	HIS	CG-CD2-NE2	-5.53	101.67	107.20
1	A	103	PRO	CA-C-N	-5.51	115.59	123.20
1	A	103	PRO	C-N-CA	-5.51	115.59	123.20
1	E	37	THR	CA-CB-OG1	-5.48	101.38	109.60
2	D	76	ARG	N-CA-C	5.48	117.69	111.11
1	C	321	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	E	103	PRO	CA-C-N	-5.46	115.66	123.20
1	E	103	PRO	C-N-CA	-5.46	115.66	123.20
1	C	250	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	D	106	HIS	CG-CD2-NE2	-5.44	101.76	107.20
2	D	95	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	E	29	ILE	N-CA-C	-5.43	105.42	110.53
2	D	54	ARG	N-CA-CB	-5.41	102.16	110.16
1	E	291	ASP	CA-CB-CG	5.41	118.00	112.60
2	D	63	PHE	CA-CB-CG	-5.40	108.40	113.80
2	F	124	ARG	NE-CZ-NH2	-5.40	114.34	119.20
2	B	11	GLU	N-CA-C	5.39	117.58	111.11
1	A	321	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	E	101	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	321	ARG	NE-CZ-NH1	5.37	126.87	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	64	HIS	CG-CD2-NE2	-5.37	101.83	107.20
2	D	125	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	309	VAL	N-CA-CB	-5.36	101.91	111.92
1	A	298	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	C	28	THR	N-CA-CB	-5.35	102.37	111.31
2	D	125	GLN	N-CA-CB	-5.35	102.25	110.16
2	F	51	LYS	N-CA-CB	-5.32	102.30	110.12
2	F	58	LYS	N-CA-C	5.32	122.14	110.80
2	B	159	HIS	CG-CD2-NE2	-5.31	101.89	107.20
1	E	75	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	277	CYS	CA-C-N	-5.28	116.64	123.19
1	A	277	CYS	C-N-CA	-5.28	116.64	123.19
1	C	23	GLY	CA-C-O	-5.28	118.59	122.23
1	A	107	SER	CA-CB-OG	-5.25	100.59	111.10
2	B	58	LYS	N-CA-C	5.25	121.99	110.80
2	F	3	PHE	CA-CB-CG	-5.25	108.55	113.80
2	D	11	GLU	N-CA-C	5.25	117.68	111.33
1	E	288	ILE	O-C-N	-5.25	118.38	121.69
2	F	146	ASN	OD1-CG-ND2	-5.25	117.36	122.60
1	E	180	TRP	CB-CG-CD1	-5.24	119.04	126.90
2	B	125	GLN	N-CA-CB	-5.24	102.41	110.16
2	D	90	ASP	CA-CB-CG	5.24	117.83	112.60
1	E	8	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	28	THR	N-CA-CB	-5.22	102.60	111.31
1	A	291	ASP	CA-CB-CG	5.20	117.80	112.60
2	D	58	LYS	N-CA-C	5.20	121.87	110.80
2	B	28	ASN	CA-CB-CG	5.19	117.79	112.60
2	B	54	ARG	CA-CB-CG	5.19	124.48	114.10
2	D	26	HIS	CG-CD2-NE2	-5.19	102.01	107.20
1	A	180	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	D	107	THR	CA-CB-OG1	-5.18	101.83	109.60
2	F	125	GLN	OE1-CD-NE2	-5.17	117.44	122.60
2	D	69	GLU	CA-CB-CG	-5.15	103.79	114.10
2	B	3	PHE	CA-CB-CG	-5.15	108.65	113.80
2	F	90	ASP	CA-CB-CG	5.14	117.75	112.60
2	D	99	LEU	CA-C-O	-5.14	115.42	120.82
2	D	92	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	B	104	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	D	3	PHE	CA-CB-CG	-5.12	108.67	113.80
2	F	99	LEU	CA-C-O	-5.12	115.45	120.82
1	E	7	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	101	ASP	CA-CB-CG	5.10	117.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	HIS	CG-CD2-NE2	-5.09	102.11	107.20
2	F	159	HIS	CG-CD2-NE2	-5.08	102.12	107.20
1	C	248	ASN	CA-CB-CG	5.08	117.68	112.60
1	E	250	ASN	CB-CG-ND2	5.08	124.02	116.40
1	E	277	CYS	CA-C-N	-5.07	116.90	123.19
1	E	277	CYS	C-N-CA	-5.07	116.90	123.19
1	C	253	ALA	N-CA-C	5.06	117.63	110.24
2	F	107	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	250	ASN	OD1-CG-ND2	-5.05	117.55	122.60
2	B	26	HIS	CG-CD2-NE2	-5.05	102.15	107.20
2	D	159	HIS	CG-CD2-NE2	-5.05	102.15	107.20
2	F	125	GLN	N-CA-CB	-5.04	102.69	110.16
1	C	101	ASP	CA-CB-CG	5.04	117.64	112.60
2	F	71	SER	CA-CB-OG	-5.04	101.03	111.10
2	B	125	GLN	OE1-CD-NE2	-5.03	117.57	122.60
2	D	124	ARG	CG-CD-NE	-5.03	100.94	112.00
1	A	315	LYS	CA-CB-CG	-5.02	104.05	114.10
1	A	4	PRO	CA-N-CD	-5.01	104.98	112.00
2	B	64	HIS	CG-CD2-NE2	-5.01	102.19	107.20
2	F	59	THR	N-CA-C	-5.01	102.22	109.59
1	A	324	PRO	CA-C-N	5.00	129.59	122.08
1	A	324	PRO	C-N-CA	5.00	129.59	122.08

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	588	2473	34	0
1	C	2532	588	2473	35	0
1	E	2532	588	2473	37	0
2	B	1421	331	1345	23	0
2	D	1421	331	1345	21	0
2	F	1421	331	1345	24	0
3	G	39	37	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	39	37	34	2	0
3	I	39	37	34	1	0
4	A	42	42	39	0	0
4	B	14	14	13	0	0
4	C	42	42	39	0	0
4	D	14	14	13	0	0
4	E	42	42	39	0	0
4	F	14	14	13	0	0
5	A	44	34	40	1	0
5	C	44	34	40	1	0
5	E	44	34	40	1	0
6	A	11	22	0	0	0
6	B	13	26	0	1	0
6	C	10	20	0	0	0
6	D	14	28	0	1	0
6	E	10	20	0	0	0
6	F	14	28	0	1	0
All	All	12348	3282	11832	143	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 6.

All (143) 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:B:83:TYR:O	2:B:87:THR:HG23	1.85	0.76
2:D:83:TYR:O	2:D:87:THR:HG23	1.84	0.76
2:F:83:TYR:O	2:F:87:THR:HG23	1.85	0.76
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.51	0.75
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.54	0.73
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.55	0.71
1:A:325:GLU:HB2	2:B:13:GLY:O	1.94	0.68
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.79	0.64
2:F:58:LYS:HE2	2:F:59:THR:O	1.97	0.63
2:B:58:LYS:HE2	2:B:59:THR:O	1.99	0.62
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.15	0.62
2:D:58:LYS:HE2	2:D:59:THR:O	1.98	0.62
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.82	0.61
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.82	0.61
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.82	0.61
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.82	0.61
2:D:28:ASN:HB2	2:D:144:CYS:O	2.00	0.61
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.83	0.60
2:D:132:GLU:HG2	2:D:134:GLY:H	1.66	0.60
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.17	0.60
2:B:132:GLU:HG2	2:B:134:GLY:H	1.65	0.60
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.82	0.60
1:E:283:THR:HG22	1:E:285:ASN:H	1.68	0.59
2:F:132:GLU:HG2	2:F:134:GLY:H	1.67	0.59
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.85	0.58
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.19	0.58
1:E:77:ASP:O	1:E:80:GLN:HG3	2.05	0.56
1:C:77:ASP:O	1:C:80:GLN:HG3	2.05	0.55
1:A:77:ASP:O	1:A:80:GLN:HG3	2.06	0.55
1:C:283:THR:HG22	1:C:285:ASN:H	1.72	0.54
1:E:167:THR:HB	3:I:1:NAG:H62	1.88	0.54
1:A:283:THR:HG22	1:A:285:ASN:H	1.71	0.54
1:A:167:THR:HB	3:G:1:NAG:H62	1.89	0.54
1:C:167:THR:HB	3:H:1:NAG:H62	1.89	0.53
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.56	0.53
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.57	0.52
1:A:79:PHE:O	1:A:82:GLU:HB2	2.10	0.52
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.91	0.52
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.93	0.51
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.59	0.51
1:E:283:THR:HG22	1:E:285:ASN:N	2.26	0.51
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.93	0.51
1:E:326:LYS:HD2	1:E:327:GLN:H	1.76	0.51
2:F:30:GLU:OE1	2:F:145:ASP:HB2	2.12	0.49
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.13	0.49
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.28	0.48
1:A:221:PRO:HA	3:H:2:NAG:O7	2.13	0.48
1:C:52:CYS:HB3	1:C:277:CYS:O	2.14	0.48
1:E:15:LEU:HD23	2:F:118:LEU:HG	1.94	0.48
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.46	0.48
1:C:283:THR:HG22	1:C:285:ASN:N	2.28	0.48
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.13	0.48
1:A:283:THR:HG22	1:A:285:ASN:N	2.29	0.48
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.14	0.48
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.95	0.47
1:E:52:CYS:HB3	1:E:277:CYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.47	0.47
1:A:10:THR:HG22	2:B:141:TYR:HA	1.96	0.47
1:A:15:LEU:HD23	2:B:118:LEU:HG	1.96	0.47
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.48	0.47
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.47	0.47
1:C:269:ARG:NH1	5:C:350:MNA:H112	2.30	0.47
1:A:47:SER:HA	1:A:288:ILE:HG22	1.98	0.46
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.30	0.46
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.16	0.46
1:A:52:CYS:HB3	1:A:277:CYS:O	2.15	0.46
2:B:141:TYR:O	2:B:166:ALA:HA	2.16	0.46
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.16	0.46
1:E:10:THR:HG22	2:F:141:TYR:HA	1.97	0.46
1:E:321:ARG:HG2	1:E:321:ARG:NH1	2.26	0.46
1:E:324:PRO:HG3	1:E:328:THR:HG23	1.98	0.46
1:E:47:SER:HA	1:E:288:ILE:HG22	1.99	0.46
1:E:79:PHE:O	1:E:82:GLU:HB2	2.16	0.46
1:E:323:VAL:HG21	2:F:7:ALA:HB2	1.98	0.46
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.17	0.45
1:C:15:LEU:HD23	2:D:118:LEU:HG	1.98	0.45
1:A:14:CYS:HA	2:B:137:CYS:HA	1.98	0.45
1:C:283:THR:HB	1:C:286:GLY:O	2.17	0.45
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.49	0.45
1:C:259:LYS:NZ	1:C:259:LYS:HB2	2.31	0.45
1:A:326:LYS:HE2	1:A:328:THR:OG1	2.16	0.45
2:F:141:TYR:O	2:F:166:ALA:HA	2.16	0.45
2:B:51:LYS:HB2	1:E:30:THR:HG22	1.99	0.45
2:D:141:TYR:O	2:D:166:ALA:HA	2.16	0.45
1:C:10:THR:HG22	2:D:141:TYR:HA	1.98	0.44
1:C:14:CYS:HA	2:D:137:CYS:HA	1.99	0.44
1:A:111:LEU:HG	2:F:73:VAL:HG11	1.99	0.44
1:A:323:VAL:HG21	2:B:7:ALA:HB2	1.99	0.44
2:B:124:ARG:HE	2:F:132:GLU:CD	2.26	0.44
1:A:269:ARG:NH1	5:A:350:MNA:H112	2.33	0.44
6:B:414:HOH:O	2:F:87:THR:HG22	2.18	0.44
2:B:72:GLU:CD	1:C:238:LYS:HZ2	2.26	0.44
1:E:283:THR:HB	1:E:286:GLY:O	2.17	0.44
2:D:26:HIS:CD2	2:D:149:ILE:HG13	2.53	0.44
1:C:323:VAL:HG21	2:D:7:ALA:HB2	1.98	0.43
1:E:14:CYS:HA	2:F:137:CYS:HA	2.00	0.43
1:C:89:GLU:OE1	1:C:109:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ARG:HB3	2:F:128:GLU:H	1.71	0.43
1:A:283:THR:HB	1:A:286:GLY:O	2.18	0.43
1:C:47:SER:HA	1:C:288:ILE:HG22	2.00	0.43
2:F:110:LEU:O	2:F:113:SER:HB3	2.19	0.43
2:B:24:PHE:CD1	2:B:153:ARG:HD3	2.53	0.43
2:F:24:PHE:CD1	2:F:153:ARG:HD3	2.54	0.43
1:E:269:ARG:NH1	5:E:350:MNA:H112	2.34	0.42
1:E:54:ASN:O	1:E:278:ILE:HA	2.19	0.42
2:F:3:PHE:CD1	2:F:3:PHE:N	2.87	0.42
1:C:327:GLN:HG2	1:C:328:THR:N	2.34	0.42
1:A:54:ASN:O	1:A:278:ILE:HA	2.20	0.42
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.55	0.42
2:B:91:LEU:HD13	2:F:91:LEU:HD13	2.02	0.42
1:C:151:LEU:O	1:C:255:ARG:NH1	2.52	0.42
2:B:110:LEU:O	2:B:113:SER:HB3	2.20	0.42
1:C:59:LEU:CD2	1:C:82:GLU:HG3	2.50	0.42
2:D:87:THR:HG22	6:F:403:HOH:O	2.19	0.42
1:E:109:ARG:HH11	1:E:109:ARG:HD2	1.73	0.42
2:D:3:PHE:CD1	2:D:3:PHE:N	2.87	0.41
1:C:57:ARG:NH2	1:C:82:GLU:OE1	2.54	0.41
1:A:53:ASN:OD1	1:A:276:THR:HA	2.20	0.41
2:B:132:GLU:CD	2:D:124:ARG:HE	2.29	0.41
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.85	0.41
1:C:295:GLN:O	1:C:308:TYR:HA	2.20	0.41
1:C:54:ASN:O	1:C:278:ILE:HA	2.20	0.41
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.56	0.41
2:B:87:THR:HG22	6:D:402:HOH:O	2.21	0.41
1:C:79:PHE:O	1:C:82:GLU:HB2	2.21	0.41
1:C:325:GLU:O	1:C:325:GLU:HG2	2.21	0.41
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.54	0.41
2:B:163:ARG:NH2	2:F:131:GLU:OE2	2.54	0.41
2:D:24:PHE:CD1	2:D:153:ARG:HD3	2.55	0.41
1:E:57:ARG:NH2	1:E:82:GLU:OE1	2.54	0.41
1:C:28:THR:HG23	2:D:105:GLN:OE1	2.21	0.41
1:E:321:ARG:HH11	1:E:321:ARG:CG	2.28	0.41
2:D:14:TRP:CZ2	2:D:25:ARG:HD2	2.55	0.40
1:E:58:ILE:HD12	1:E:58:ILE:N	2.36	0.40
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.86	0.40
1:A:326:LYS:HG2	1:A:327:GLN:N	2.36	0.40
1:E:28:THR:HG22	1:E:30:THR:H	1.87	0.40
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:HE1	1:A:94:PHE:O	2.04	0.40
1:E:75:HIS:HE1	1:E:94:PHE:O	2.05	0.40
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.55	0.40
1:C:85:ASP:O	1:C:265:SER:HA	2.22	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	326/328 (99%)	304 (93%)	17 (5%)	5 (2%)	8	22
1	C	326/328 (99%)	307 (94%)	15 (5%)	4 (1%)	10	27
1	E	326/328 (99%)	310 (95%)	14 (4%)	2 (1%)	21	44
2	B	173/175 (99%)	161 (93%)	8 (5%)	4 (2%)	5	13
2	D	173/175 (99%)	160 (92%)	9 (5%)	4 (2%)	5	13
2	F	173/175 (99%)	161 (93%)	8 (5%)	4 (2%)	5	13
All	All	1497/1509 (99%)	1403 (94%)	71 (5%)	23 (2%)	8	22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
2	B	58	LYS
2	B	173	ILE
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	2	ASP

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Mol	Chain	Res	Type
1	A	326	LYS
1	C	327	GLN
2	B	172	GLN
2	D	172	GLN
2	F	172	GLN
1	A	22	ASN
1	A	62	ILE
2	B	174	LYS
1	C	22	ASN
1	C	62	ILE
2	D	174	LYS
1	E	22	ASN
1	E	62	ILE
2	F	174	LYS
1	C	4	PRO

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	289/289 (100%)	263 (91%)	26 (9%)	9	23
1	C	289/289 (100%)	265 (92%)	24 (8%)	10	26
1	E	289/289 (100%)	261 (90%)	28 (10%)	8	20
2	B	149/149 (100%)	144 (97%)	5 (3%)	32	62
2	D	149/149 (100%)	143 (96%)	6 (4%)	28	56
2	F	149/149 (100%)	143 (96%)	6 (4%)	28	56
All	All	1314/1314 (100%)	1219 (93%)	95 (7%)	13	32

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	28	THR
1	A	34	ILE

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Mol	Chain	Res	Type
1	A	37	THR
1	A	50	LYS
1	A	54	ASN
1	A	63	ASP
1	A	82	GLU
1	A	103	PRO
1	A	141	ARG
1	A	150	ARG
1	A	157	SER
1	A	160	THR
1	A	189	GLN
1	A	197	GLN
1	A	199	SER
1	A	228	SER
1	A	248	ASN
1	A	259	LYS
1	A	265	SER
1	A	278	ILE
1	A	280	GLU
1	A	283	THR
1	A	309	VAL
1	A	321	ARG
1	A	326	LYS
2	B	87	THR
2	B	110	LEU
2	B	127	ARG
2	B	128	GLU
2	B	160	ASP
1	C	8	ASN
1	C	28	THR
1	C	34	ILE
1	C	37	THR
1	C	50	LYS
1	C	54	ASN
1	C	82	GLU
1	C	103	PRO
1	C	141	ARG
1	C	150	ARG
1	C	155	THR
1	C	159	SER
1	C	160	THR
1	C	197	GLN

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Mol	Chain	Res	Type
1	C	199	SER
1	C	228	SER
1	C	248	ASN
1	C	259	LYS
1	C	265	SER
1	C	278	ILE
1	C	280	GLU
1	C	283	THR
1	C	309	VAL
1	C	321	ARG
2	D	87	THR
2	D	110	LEU
2	D	127	ARG
2	D	128	GLU
2	D	150	GLU
2	D	160	ASP
1	E	2	ASP
1	E	8	ASN
1	E	28	THR
1	E	34	ILE
1	E	37	THR
1	E	50	LYS
1	E	54	ASN
1	E	82	GLU
1	E	103	PRO
1	E	141	ARG
1	E	150	ARG
1	E	155	THR
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	197	GLN
1	E	199	SER
1	E	228	SER
1	E	248	ASN
1	E	259	LYS
1	E	265	SER
1	E	278	ILE
1	E	280	GLU
1	E	283	THR
1	E	309	VAL
1	E	321	ARG

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Mol	Chain	Res	Type
1	E	326	LYS
1	E	328	THR
2	F	87	THR
2	F	110	LEU
2	F	127	ARG
2	F	128	GLU
2	F	150	GLU
2	F	160	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	8	ASN
1	A	132	GLN
1	A	171	ASN
2	B	27	GLN
2	B	28	ASN
2	B	49	ASN
1	C	132	GLN
1	C	171	ASN
2	D	12	ASN
2	D	172	GLN
1	E	8	ASN
1	E	132	GLN
1	E	171	ASN
2	F	26	HIS
2	F	49	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 ⓘ

9 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	G	1	1,3	14,14,15	0.48	0	17,19,21	0.82	0
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	1.06	1 (5%)
3	BMA	G	3	3	11,11,12	0.67	0	15,15,17	0.93	0
3	NAG	H	1	1,3	14,14,15	0.65	0	17,19,21	0.88	0
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
3	BMA	H	3	3	11,11,12	0.77	0	15,15,17	1.09	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.55	0	17,19,21	0.80	0
3	NAG	I	2	3	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
3	BMA	I	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.00	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	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	BMA	C2-C3	-2.36	1.48	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C4-C3-C2	-2.60	107.21	111.02
3	G	2	NAG	C4-C3-C2	-2.55	107.28	111.02
3	H	3	BMA	C6-C5-C4	-2.36	107.23	113.02
3	H	2	NAG	C4-C3-C2	-2.31	107.63	111.02
3	H	3	BMA	C1-O5-C5	2.18	115.11	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

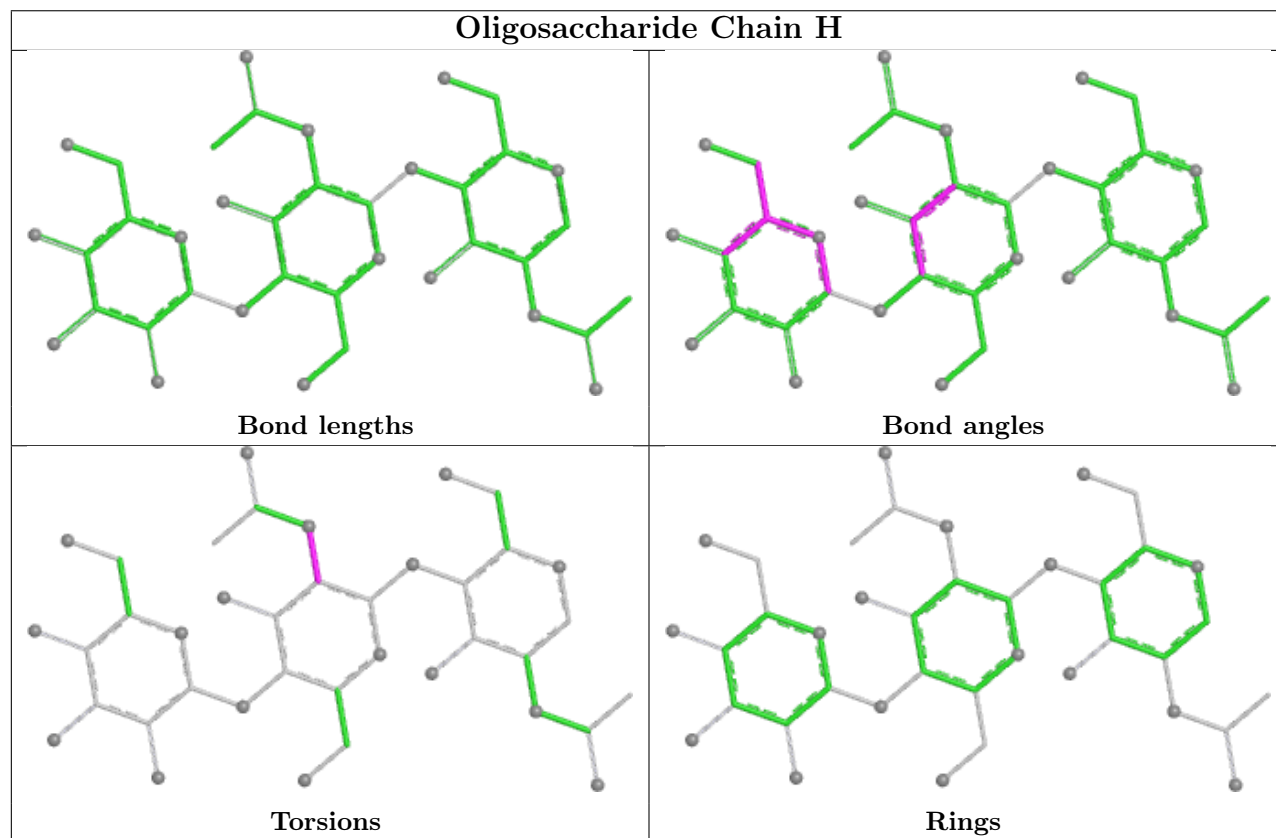
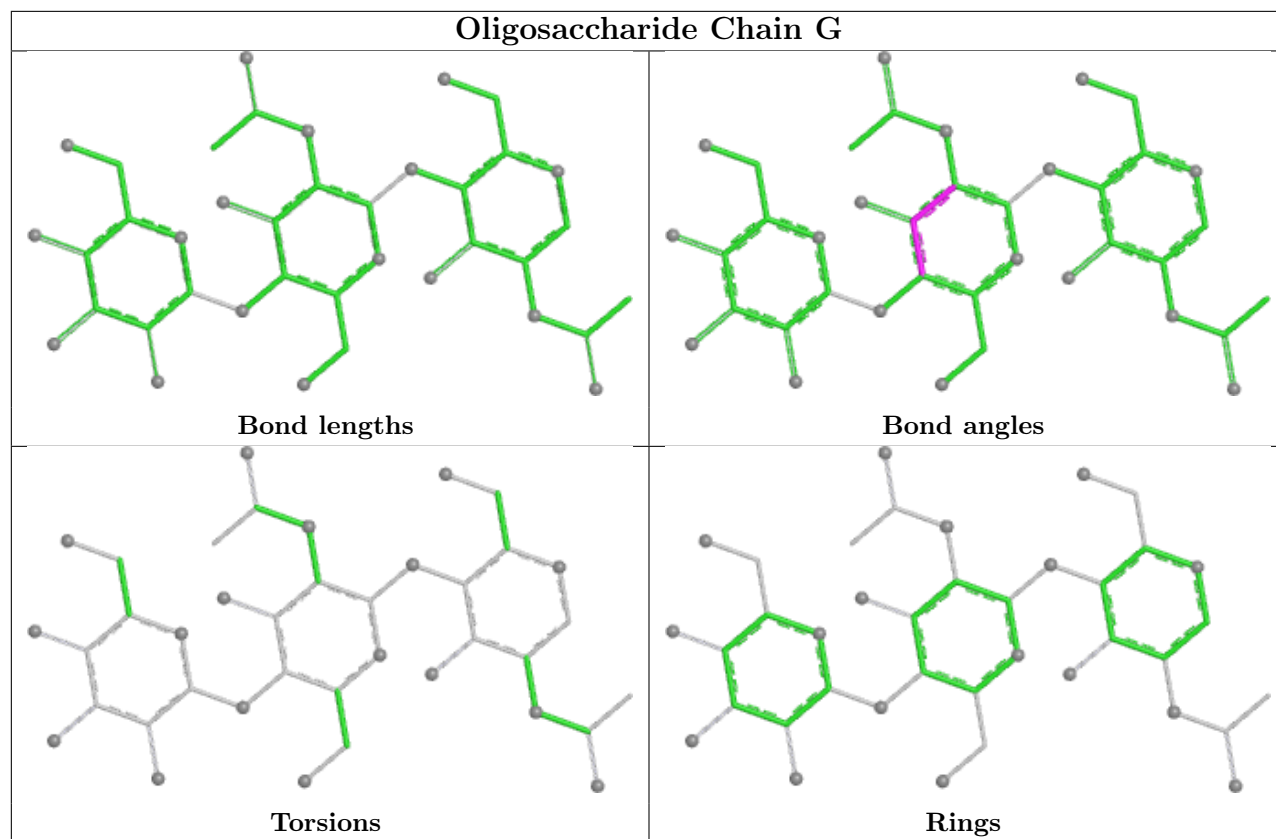
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7

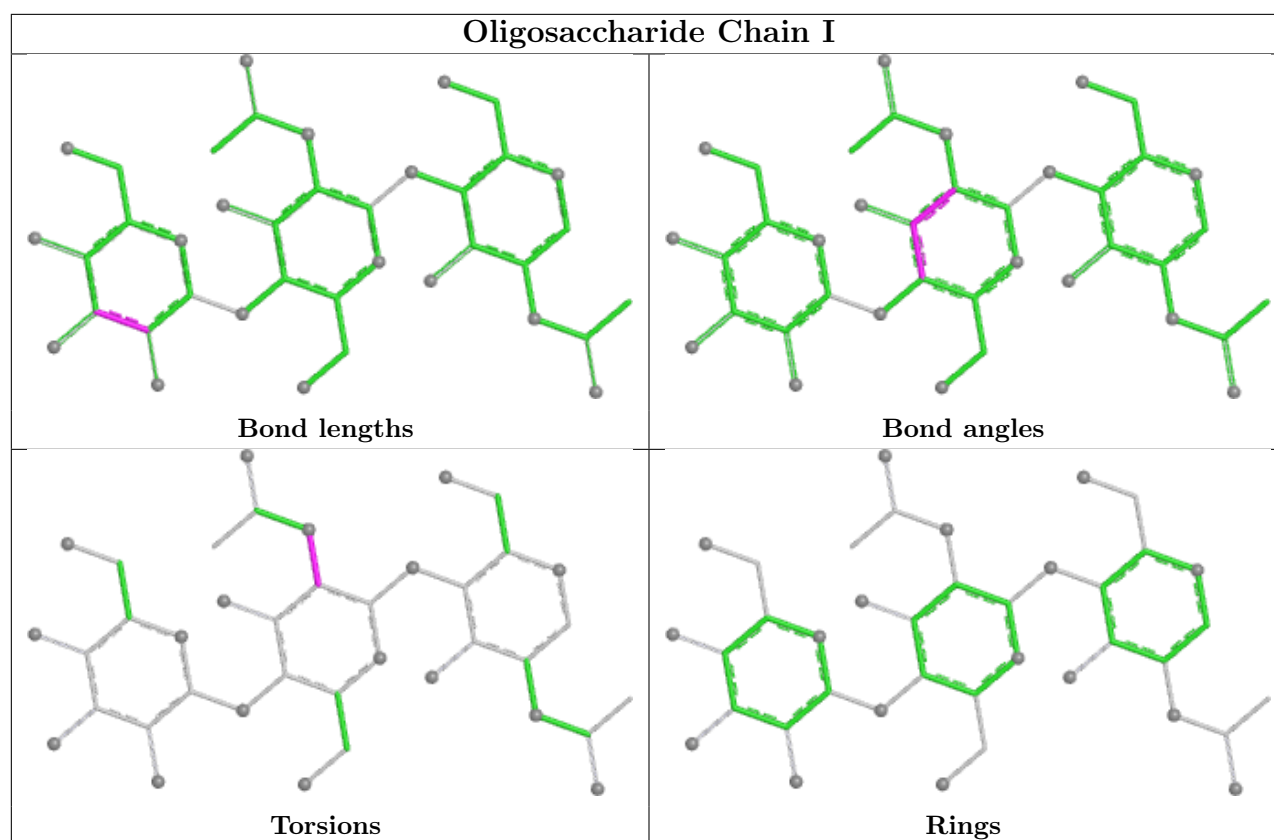
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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





5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	C	334	1	14,14,15	0.91	0	17,19,21	1.18	2 (11%)
5	MNA	A	350	-	22,22,22	0.89	0	26,32,32	1.70	7 (26%)
4	NAG	C	329	1	14,14,15	0.83	1 (7%)	17,19,21	0.87	1 (5%)
5	MNA	E	349	-	22,22,22	0.90	1 (4%)	26,32,32	1.20	2 (7%)
4	NAG	D	401	2	14,14,15	0.83	1 (7%)	17,19,21	1.48	1 (5%)
4	NAG	E	329	1	14,14,15	0.79	0	17,19,21	0.89	1 (5%)
4	NAG	E	348	1	14,14,15	0.74	0	17,19,21	1.53	4 (23%)
4	NAG	B	401	2	14,14,15	0.72	1 (7%)	17,19,21	1.46	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	334	1	14,14,15	0.90	0	17,19,21	1.21	2 (11%)
4	NAG	E	334	1	14,14,15	0.87	0	17,19,21	1.11	2 (11%)
4	NAG	A	348	1	14,14,15	0.61	0	17,19,21	1.62	4 (23%)
5	MNA	A	349	-	22,22,22	0.97	1 (4%)	26,32,32	1.27	3 (11%)
5	MNA	C	349	-	22,22,22	0.77	0	26,32,32	1.26	2 (7%)
5	MNA	C	350	-	22,22,22	1.14	1 (4%)	26,32,32	1.73	8 (30%)
5	MNA	E	350	-	22,22,22	1.17	2 (9%)	26,32,32	1.72	7 (26%)
4	NAG	A	329	1	14,14,15	0.90	0	17,19,21	0.93	1 (5%)
4	NAG	F	401	2	14,14,15	0.84	1 (7%)	17,19,21	1.48	1 (5%)
4	NAG	C	348	1	14,14,15	0.60	0	17,19,21	1.58	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
5	MNA	A	350	-	-	5/23/41/41	0/1/1/1
4	NAG	C	329	1	-	0/6/23/26	0/1/1/1
5	MNA	E	349	-	-	5/23/41/41	0/1/1/1
4	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	NAG	E	329	1	-	0/6/23/26	0/1/1/1
4	NAG	E	348	1	-	2/6/23/26	0/1/1/1
4	NAG	B	401	2	-	0/6/23/26	0/1/1/1
4	NAG	A	334	1	-	0/6/23/26	0/1/1/1
4	NAG	E	334	1	-	0/6/23/26	0/1/1/1
4	NAG	A	348	1	-	2/6/23/26	0/1/1/1
5	MNA	A	349	-	-	5/23/41/41	0/1/1/1
5	MNA	C	349	-	-	5/23/41/41	0/1/1/1
5	MNA	C	350	-	-	5/23/41/41	0/1/1/1
5	MNA	E	350	-	-	4/23/41/41	0/1/1/1
4	NAG	A	329	1	-	0/6/23/26	0/1/1/1
4	NAG	F	401	2	-	0/6/23/26	0/1/1/1
4	NAG	C	348	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	350	MNA	C3-C2	3.52	1.57	1.52
5	E	350	MNA	C3-C2	3.31	1.56	1.52
4	C	329	NAG	C4-C5	2.56	1.58	1.53
5	E	350	MNA	C4-C5	2.36	1.55	1.53
4	F	401	NAG	C4-C5	2.35	1.58	1.53
4	D	401	NAG	C4-C5	2.23	1.57	1.53
5	A	349	MNA	O1B-C1	-2.18	1.22	1.30
4	B	401	NAG	C4-C5	2.14	1.57	1.53
5	E	349	MNA	O1B-C1	-2.05	1.23	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	350	MNA	O6-C2-C3	-4.74	104.98	111.35
4	D	401	NAG	C1-O5-C5	4.31	117.96	112.19
4	B	401	NAG	C1-O5-C5	4.24	117.87	112.19
4	A	348	NAG	C1-O5-C5	4.21	117.83	112.19
5	C	350	MNA	O6-C2-C3	-4.21	105.69	111.35
4	F	401	NAG	C1-O5-C5	4.19	117.80	112.19
5	A	350	MNA	O6-C2-C3	-4.01	105.97	111.35
4	C	348	NAG	C1-O5-C5	3.85	117.35	112.19
4	E	348	NAG	C1-O5-C5	3.46	116.82	112.19
5	C	350	MNA	O6-C6-C5	3.24	112.81	109.84
5	A	350	MNA	C12-O2-C2	3.14	119.53	115.46
5	C	350	MNA	O9-C9-C8	-2.84	105.20	111.16
5	C	349	MNA	O6-C2-C3	-2.76	107.64	111.35
5	A	350	MNA	O9-C9-C8	-2.75	105.38	111.16
4	C	348	NAG	C8-C7-N2	2.74	120.65	116.12
4	E	348	NAG	C3-C4-C5	-2.71	105.32	110.23
5	E	350	MNA	O9-C9-C8	-2.71	105.47	111.16
5	A	349	MNA	O6-C2-C3	-2.69	107.73	111.35
5	E	350	MNA	O6-C6-C5	2.68	112.30	109.84
4	A	348	NAG	C3-C4-C5	-2.65	105.43	110.23
4	A	334	NAG	C1-O5-C5	2.63	115.71	112.19
5	E	349	MNA	O6-C2-C3	-2.62	107.82	111.35
4	A	329	NAG	C1-O5-C5	2.59	115.66	112.19
4	C	334	NAG	C1-O5-C5	2.51	115.55	112.19
4	E	334	NAG	C1-C2-N2	2.51	114.38	110.43
4	E	329	NAG	C1-O5-C5	2.46	115.48	112.19
5	A	350	MNA	C11-C10-N5	2.46	120.20	116.12
4	E	348	NAG	O4-C4-C5	2.44	115.33	109.32
4	A	348	NAG	O4-C4-C5	2.42	115.29	109.32
4	E	348	NAG	C8-C7-N2	2.42	120.13	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	348	NAG	C3-C4-C5	-2.36	105.95	110.23
5	E	350	MNA	C12-O2-C2	2.35	118.52	115.46
5	E	350	MNA	C2-O6-C6	2.35	119.89	114.36
4	A	334	NAG	C1-C2-N2	2.33	114.11	110.43
4	C	348	NAG	O4-C4-C5	2.26	114.88	109.32
5	C	350	MNA	C12-O2-C2	2.25	118.38	115.46
4	A	348	NAG	C8-C7-N2	2.23	119.82	116.12
5	C	350	MNA	C2-O6-C6	2.22	119.57	114.36
4	C	329	NAG	C1-O5-C5	2.20	115.13	112.19
5	C	350	MNA	C6-C5-N5	2.19	114.40	110.91
5	A	350	MNA	C2-O6-C6	2.18	119.48	114.36
5	A	350	MNA	O6-C6-C7	-2.17	103.27	106.65
5	E	350	MNA	C2-C3-C4	2.15	115.07	110.73
5	C	350	MNA	O10-C10-C11	-2.14	118.24	122.05
5	C	350	MNA	O6-C6-C7	-2.14	103.32	106.65
4	E	334	NAG	C1-O5-C5	2.14	115.05	112.19
5	C	349	MNA	C4-C5-N5	-2.13	106.24	110.44
5	A	350	MNA	C2-C3-C4	2.10	114.98	110.73
4	C	334	NAG	C1-C2-N2	2.05	113.67	110.43
5	E	350	MNA	C6-C5-N5	2.02	114.14	110.91
5	E	349	MNA	O9-C9-C8	-2.02	106.91	111.16
5	A	349	MNA	O9-C9-C8	-2.02	106.92	111.16
5	A	349	MNA	C4-C5-N5	-2.01	106.47	110.44

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	349	MNA	O1B-C1-C2-O2
5	A	349	MNA	O1B-C1-C2-O6
5	A	350	MNA	O1B-C1-C2-O2
5	A	350	MNA	O1B-C1-C2-O6
5	C	349	MNA	O1B-C1-C2-O2
5	C	349	MNA	O1B-C1-C2-O6
5	C	350	MNA	O1B-C1-C2-O2
5	C	350	MNA	O1B-C1-C2-O6
5	E	349	MNA	O1B-C1-C2-O2
5	E	349	MNA	O1B-C1-C2-O6
5	E	350	MNA	O1B-C1-C2-O2
5	E	350	MNA	O1B-C1-C2-O6
4	C	348	NAG	O5-C5-C6-O6
4	E	348	NAG	O5-C5-C6-O6

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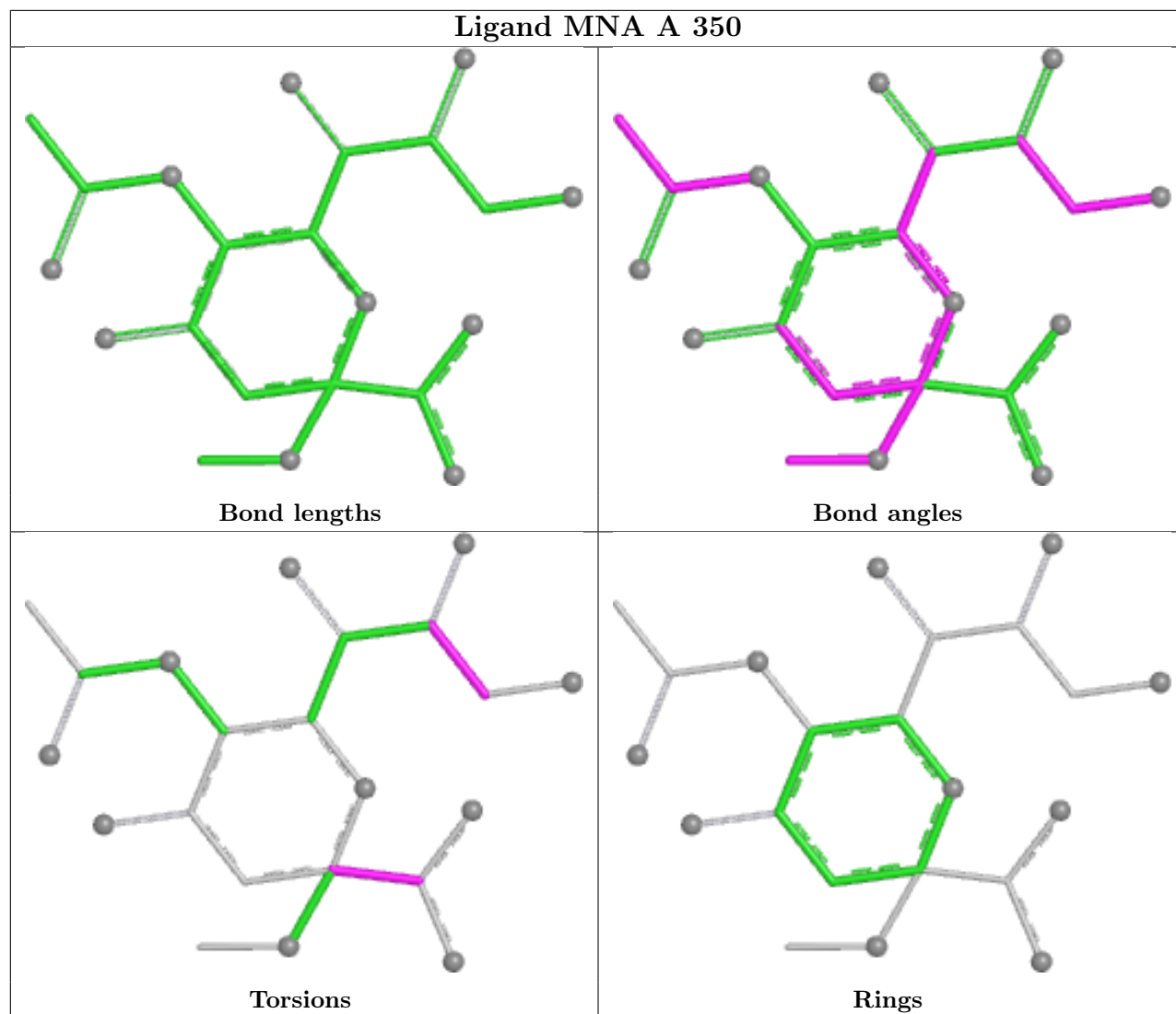
Mol	Chain	Res	Type	Atoms
4	A	348	NAG	O5-C5-C6-O6
4	C	348	NAG	C4-C5-C6-O6
4	E	348	NAG	C4-C5-C6-O6
4	A	348	NAG	C4-C5-C6-O6
5	A	349	MNA	O1A-C1-C2-O2
5	C	349	MNA	O1A-C1-C2-O2
5	E	349	MNA	O1A-C1-C2-O2
5	E	350	MNA	O8-C8-C9-O9
5	A	350	MNA	O1A-C1-C2-O2
5	A	350	MNA	O1A-C1-C2-O6
5	C	350	MNA	O1A-C1-C2-O2
5	C	350	MNA	O1A-C1-C2-O6
5	E	350	MNA	O1A-C1-C2-O6
5	A	350	MNA	O8-C8-C9-O9
5	C	350	MNA	O8-C8-C9-O9
5	E	349	MNA	O8-C8-C9-O9
5	A	349	MNA	O1A-C1-C2-C3
5	C	349	MNA	O1A-C1-C2-C3
5	E	349	MNA	O1A-C1-C2-C3
5	A	349	MNA	O8-C8-C9-O9
5	C	349	MNA	O8-C8-C9-O9

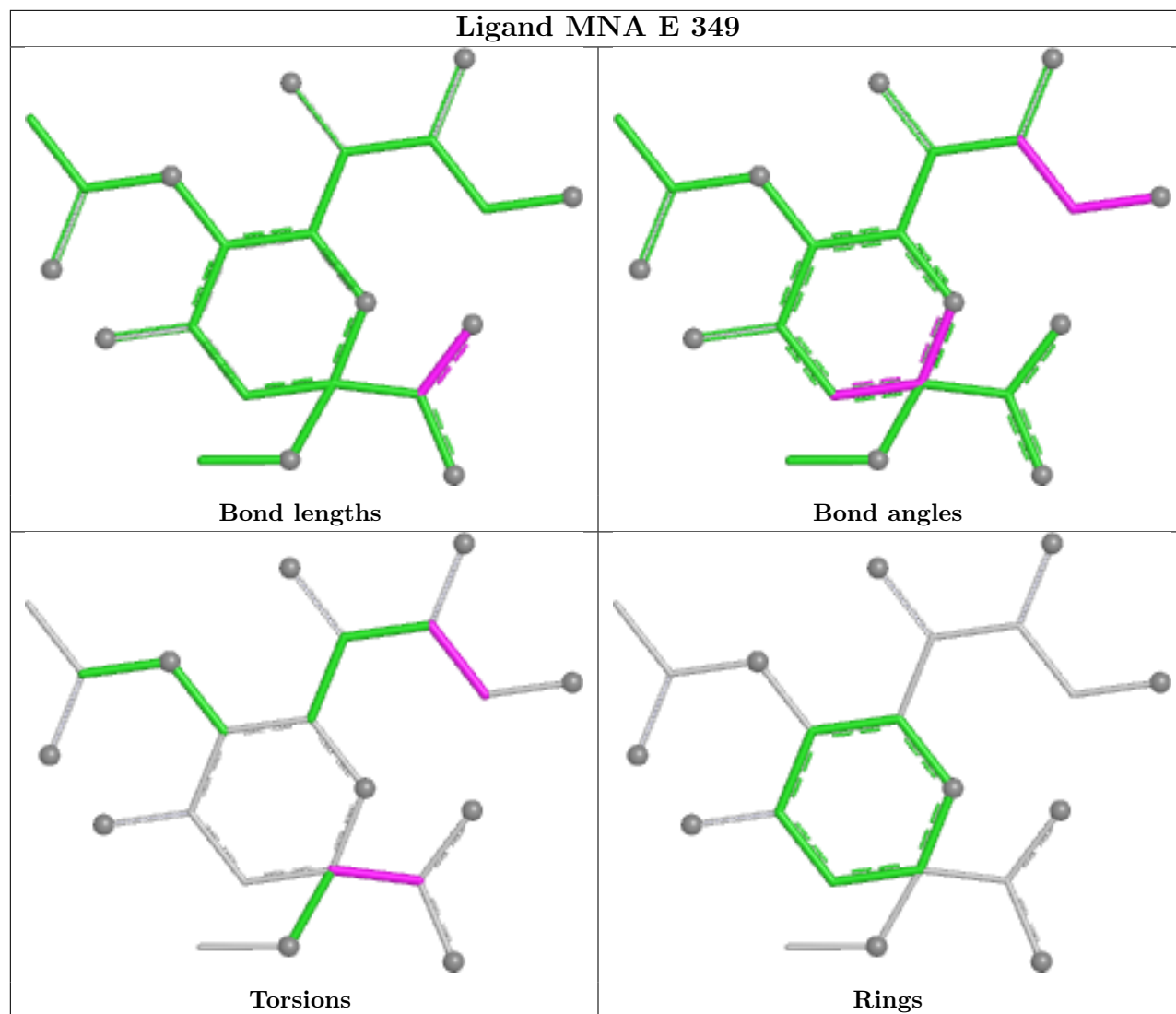
There are no ring outliers.

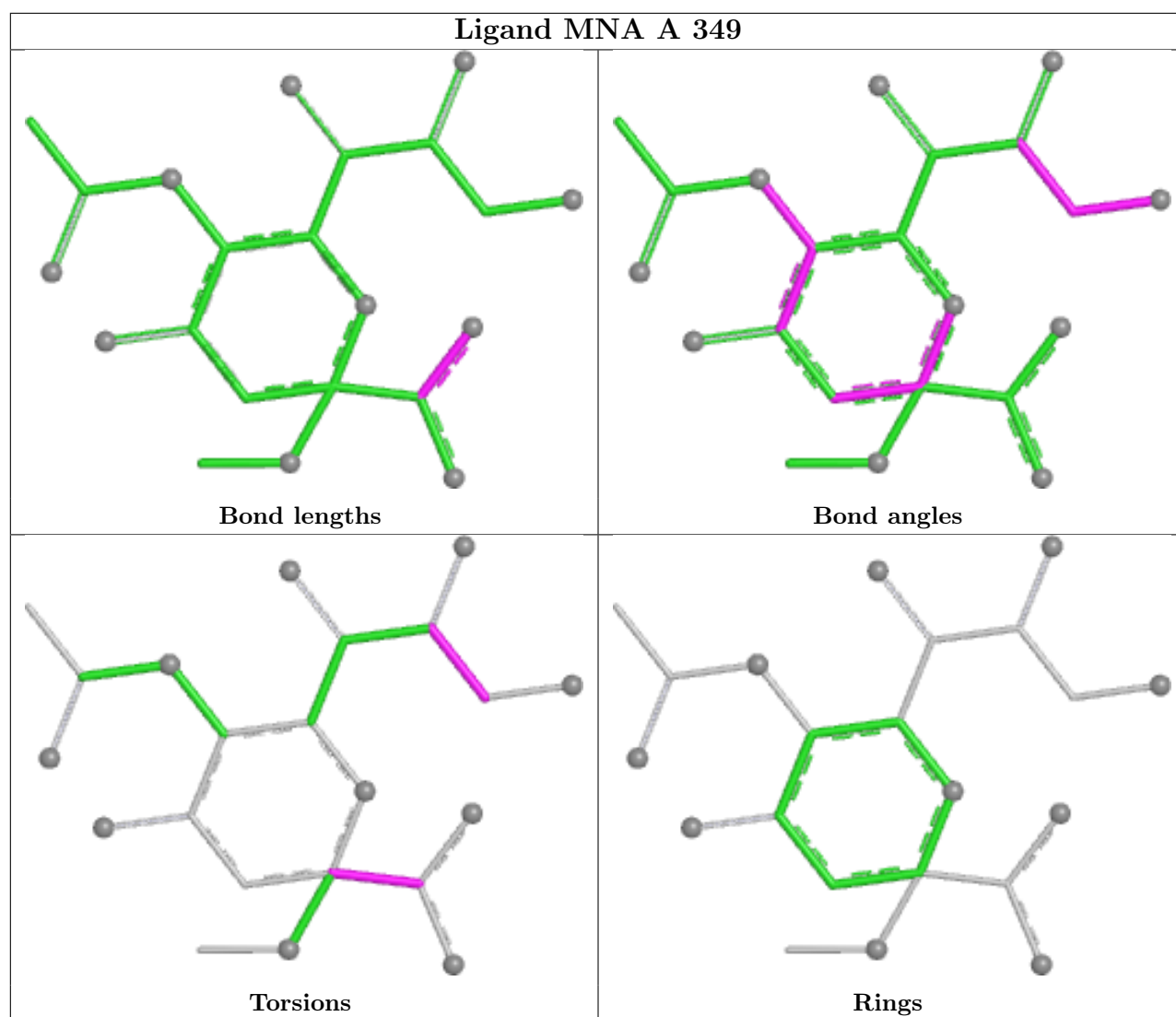
3 monomers are involved in 3 short contacts:

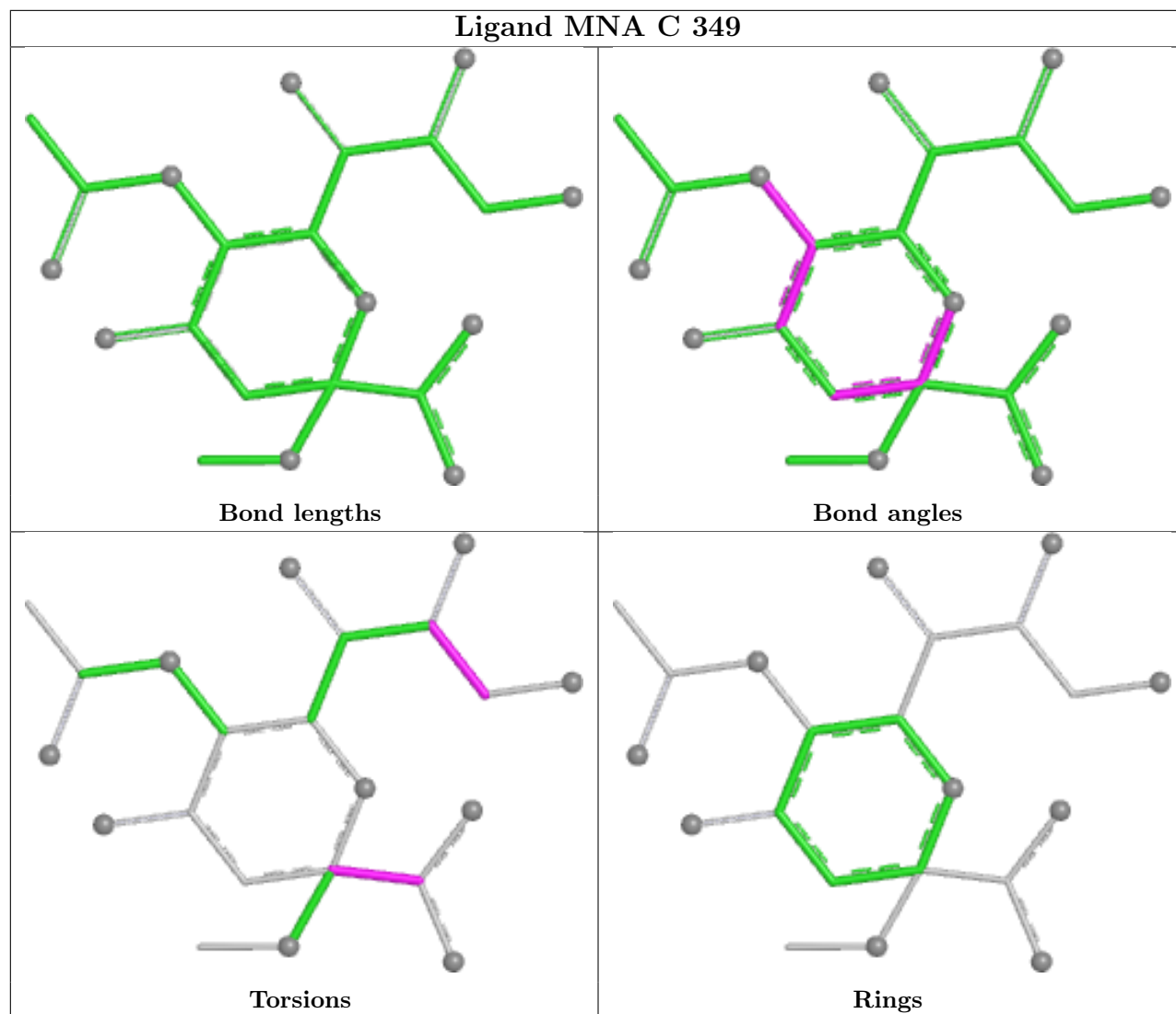
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	350	MNA	1	0
5	C	350	MNA	1	0
5	E	350	MNA	1	0

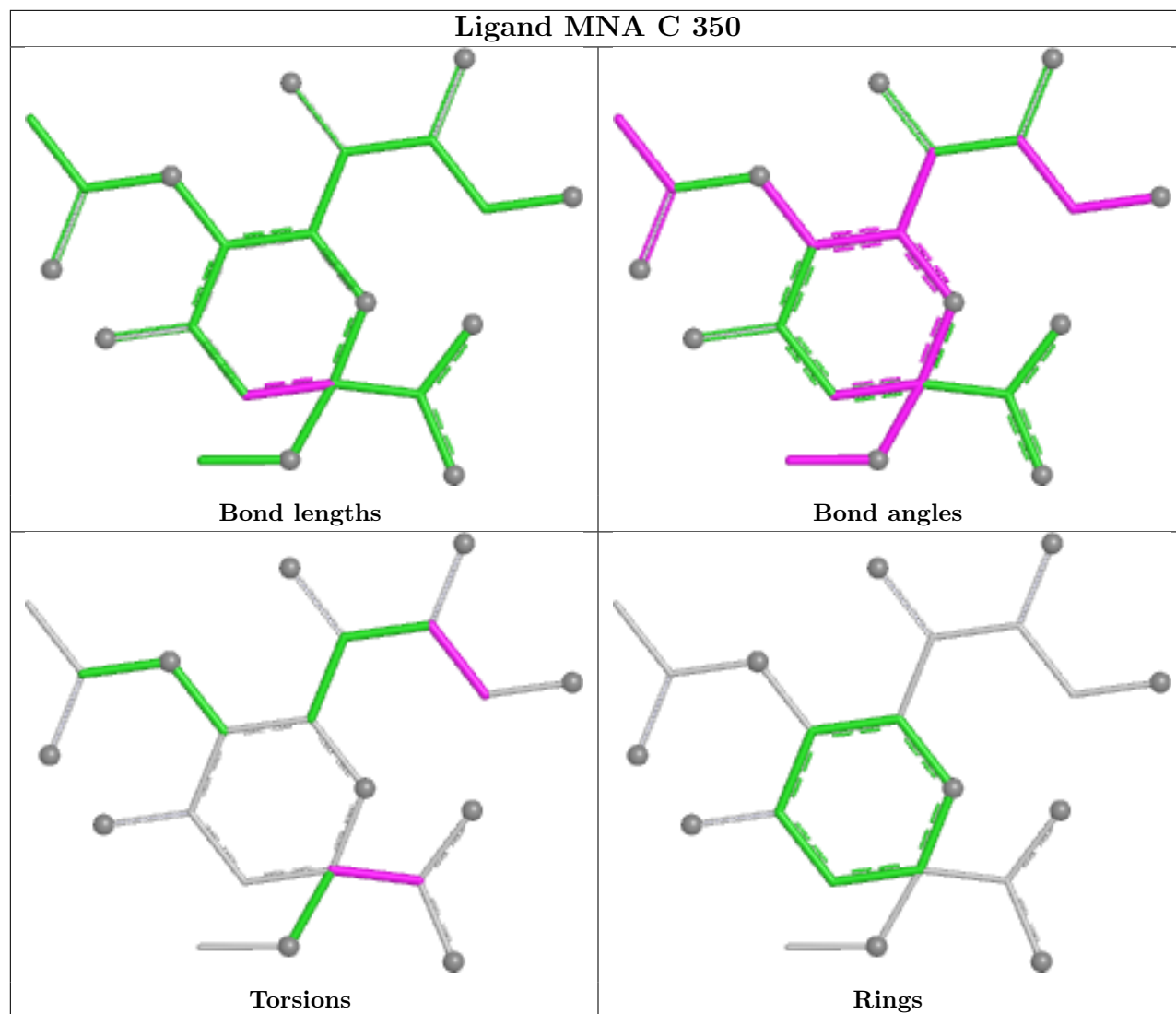
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

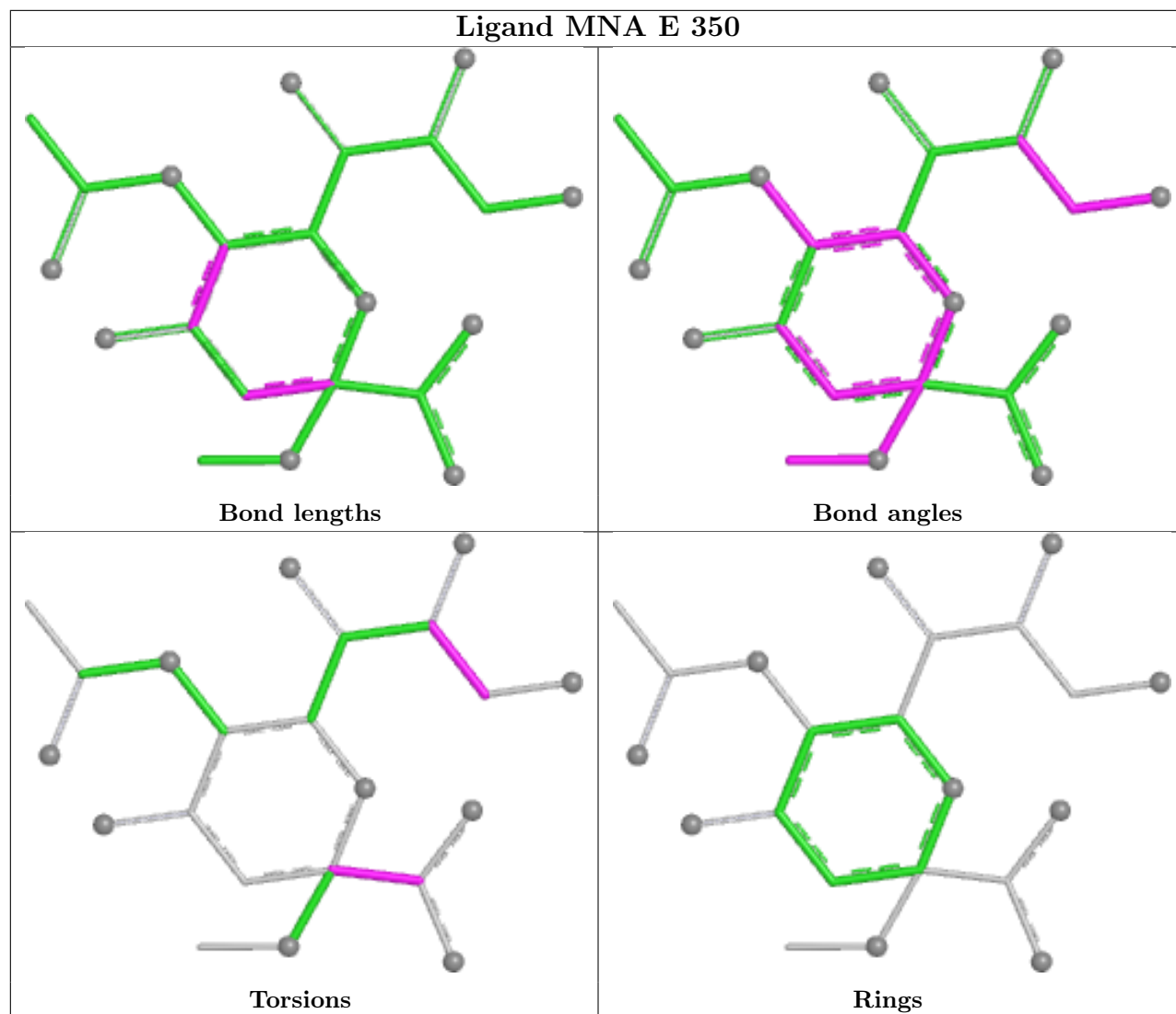












5.7 Other polymers [i](#)

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	328/328 (100%)	0.17	24 (7%)	21	18	7, 23, 43, 138	0
1	C	328/328 (100%)	0.16	24 (7%)	21	18	8, 23, 42, 143	0
1	E	328/328 (100%)	0.11	24 (7%)	21	18	8, 22, 42, 139	0
2	B	175/175 (100%)	-0.03	12 (6%)	23	20	4, 17, 39, 88	0
2	D	175/175 (100%)	-0.10	7 (4%)	42	38	4, 17, 39, 88	0
2	F	175/175 (100%)	-0.11	10 (5%)	29	26	3, 17, 39, 88	0
All	All	1509/1509 (100%)	0.07	101 (6%)	24	21	3, 21, 43, 143	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	9.7
1	E	5	GLY	9.3
1	E	4	PRO	9.1
1	A	2	ASP	8.8
1	E	3	LEU	8.2
2	B	173	ILE	7.6
1	E	8	ASN	7.0
2	D	173	ILE	6.9
1	A	328	THR	6.5
1	A	6	ASN	6.5
1	A	326	LYS	6.5
1	E	1	GLN	6.4
1	E	327	GLN	6.4
1	E	6	ASN	6.1
1	C	3	LEU	5.9
2	F	58	LYS	5.6
2	F	172	GLN	5.6
1	C	5	GLY	5.5
1	A	327	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	8	ASN	5.3
1	A	1	GLN	4.9
1	E	328	THR	4.9
1	E	2	ASP	4.9
1	C	2	ASP	4.6
1	C	6	ASN	4.5
1	C	209	SER	4.5
1	C	8	ASN	4.5
2	F	175	GLY	4.5
1	C	4	PRO	4.5
1	C	327	GLN	4.5
1	A	3	LEU	4.4
2	F	57	GLU	4.4
2	D	58	LYS	4.2
2	F	173	ILE	4.2
1	C	328	THR	4.2
1	C	192	THR	4.0
1	C	143	PRO	4.0
1	E	92	LYS	4.0
1	C	142	GLY	3.9
1	C	7	ASP	3.9
1	E	7	ASP	3.9
2	B	175	GLY	3.8
2	B	19	ASP	3.8
1	A	158	GLY	3.7
1	A	7	ASP	3.6
1	A	189	GLN	3.6
2	D	60	ASN	3.6
1	E	189	GLN	3.5
1	C	1	GLN	3.5
2	B	58	LYS	3.5
1	A	144	GLY	3.4
1	A	22	ASN	3.4
2	B	168	ASN	3.4
2	B	174	LYS	3.3
2	D	174	LYS	3.3
1	E	326	LYS	3.2
2	B	164	ASP	3.2
2	B	145	ASP	3.1
1	C	9	SER	3.1
2	B	57	GLU	2.9
1	C	157	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	57	GLU	2.9
2	F	60	ASN	2.9
1	A	4	PRO	2.9
2	D	175	GLY	2.9
2	B	18	ILE	2.8
1	C	240	GLY	2.8
1	E	222	TRP	2.7
1	E	291	ASP	2.7
1	C	158	GLY	2.7
1	E	22	ASN	2.7
1	E	193	SER	2.7
2	F	174	LYS	2.7
1	A	216	ASN	2.6
1	E	9	SER	2.6
1	A	193	SER	2.6
1	E	187	THR	2.6
1	A	209	SER	2.5
1	C	160	THR	2.5
1	C	57	ARG	2.4
2	B	60	ASN	2.4
1	A	9	SER	2.4
1	C	144	GLY	2.4
2	D	172	GLN	2.4
1	A	186	SER	2.3
1	E	208	ARG	2.3
1	A	160	THR	2.2
2	B	29	SER	2.2
1	A	325	GLU	2.2
1	C	126	THR	2.2
1	E	238	LYS	2.2
1	C	199	SER	2.2
2	F	168	ASN	2.1
1	A	188	ASN	2.1
1	E	54	ASN	2.1
2	F	150	GLU	2.1
2	F	53	ASN	2.1
1	A	173	ASN	2.0
1	E	144	GLY	2.0
1	E	57	ARG	2.0
1	C	207	ARG	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](#)

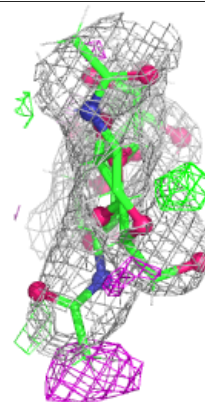
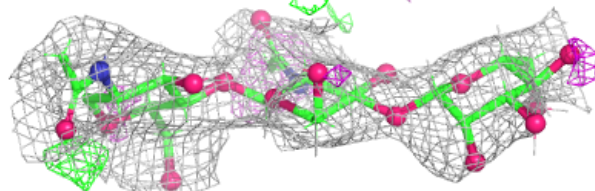
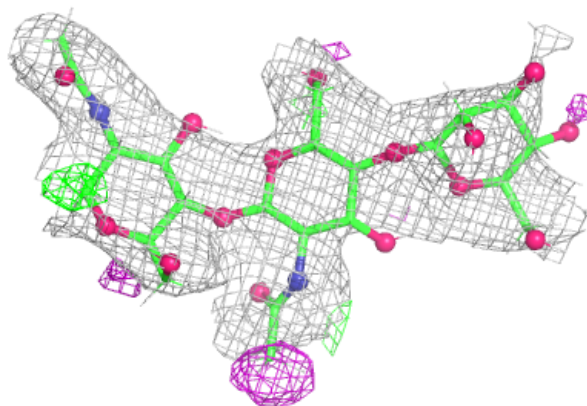
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	BMA	H	3	11/12	0.64	0.18	0,0,71,71	0
3	NAG	I	2	14/15	0.78	0.13	0,0,60,63	0
3	BMA	I	3	11/12	0.78	0.14	0,0,69,70	0
3	NAG	H	1	14/15	0.82	0.14	0,0,50,53	0
3	NAG	G	2	14/15	0.83	0.14	0,0,60,62	0
3	NAG	G	1	14/15	0.84	0.10	0,0,51,53	0
3	BMA	G	3	11/12	0.84	0.13	0,0,68,70	0
3	NAG	H	2	14/15	0.85	0.10	0,0,60,63	0
3	NAG	I	1	14/15	0.88	0.10	0,0,50,53	0

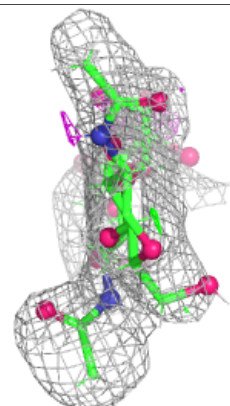
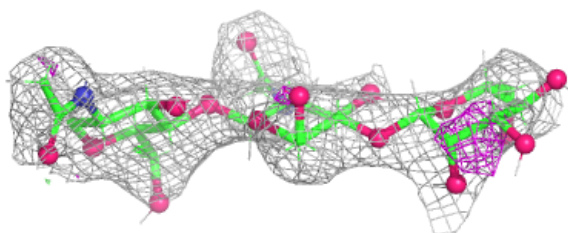
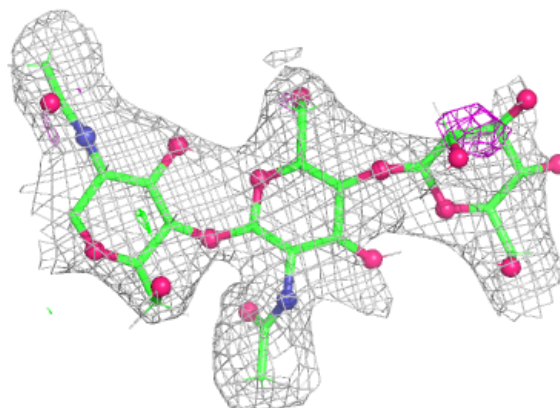
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

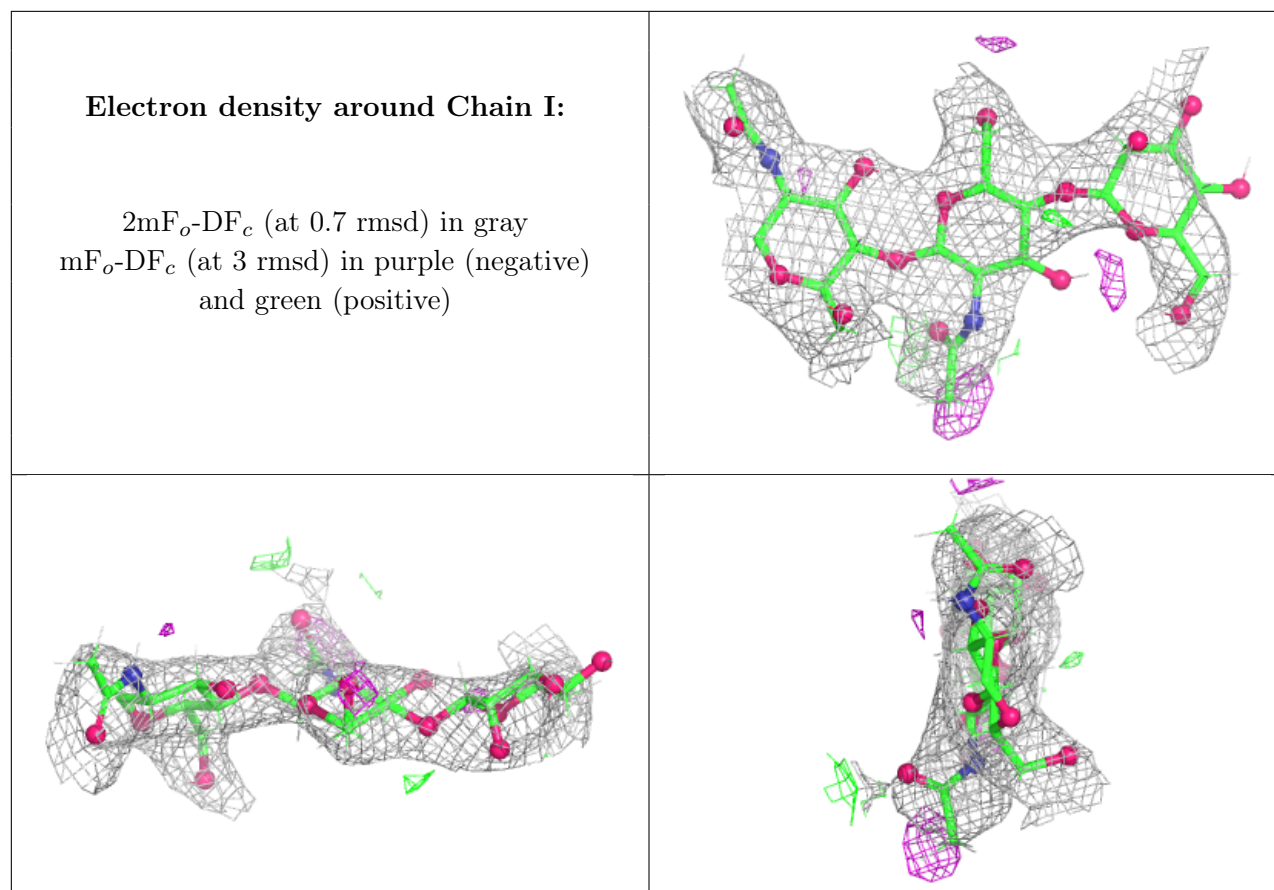
Electron density around Chain G:

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

**Electron density around Chain H:**

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	F	401	14/15	0.76	0.17	0,0,64,65	0
4	NAG	C	334	14/15	0.78	0.16	0,0,46,48	0
4	NAG	A	329	14/15	0.78	0.17	0,0,54,54	0
4	NAG	B	401	14/15	0.80	0.18	0,0,64,64	0
4	NAG	D	401	14/15	0.81	0.16	0,0,64,65	0
4	NAG	C	329	14/15	0.82	0.14	0,0,54,54	0
5	MNA	A	350	22/22	0.84	0.18	0,26,29,32	39
4	NAG	C	348	14/15	0.85	0.12	0,0,43,46	0
4	NAG	A	334	14/15	0.86	0.12	0,0,46,48	0
4	NAG	E	329	14/15	0.86	0.17	0,0,54,55	0
5	MNA	C	350	22/22	0.86	0.15	0,26,30,32	39
5	MNA	E	350	22/22	0.86	0.17	0,25,29,32	39
4	NAG	E	334	14/15	0.87	0.11	0,0,46,48	0

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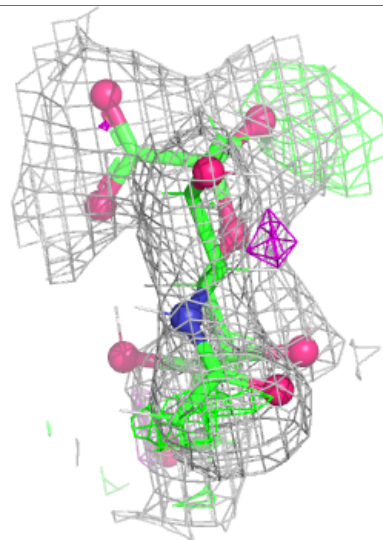
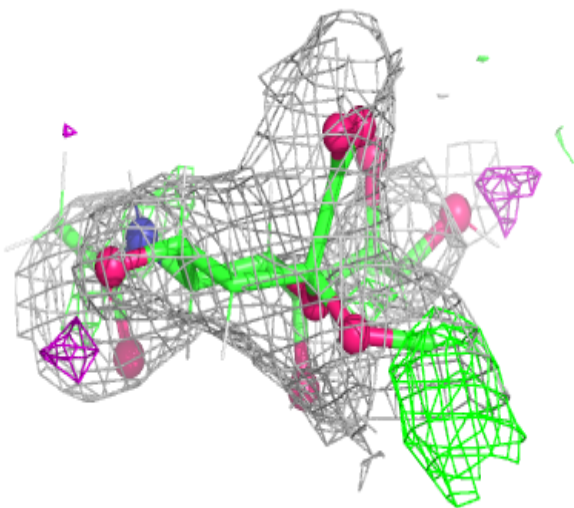
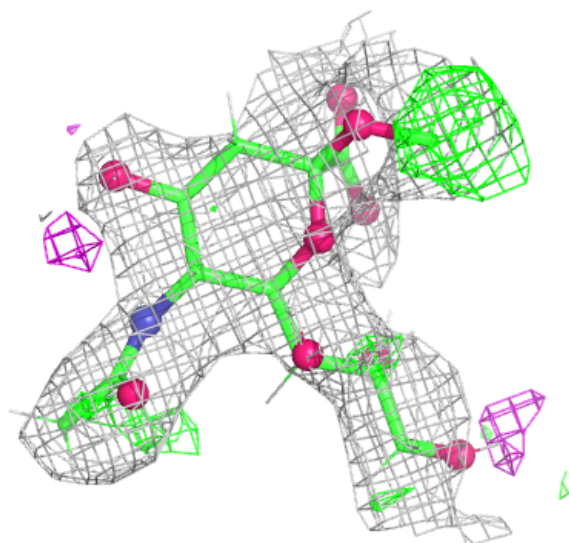
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	348	14/15	0.88	0.11	0,0,44,47	0
4	NAG	E	348	14/15	0.88	0.14	0,0,44,46	0
5	MNA	C	349	22/22	0.90	0.09	0,28,32,33	0
5	MNA	E	349	22/22	0.92	0.10	0,26,31,32	0
5	MNA	A	349	22/22	0.92	0.09	0,28,31,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

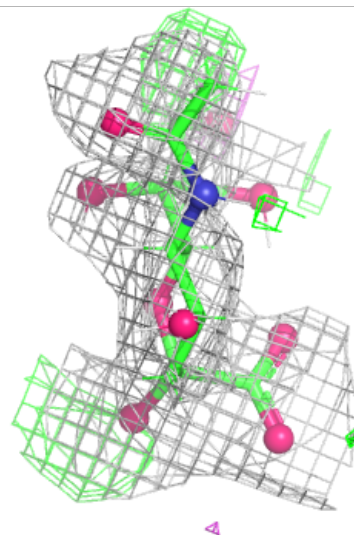
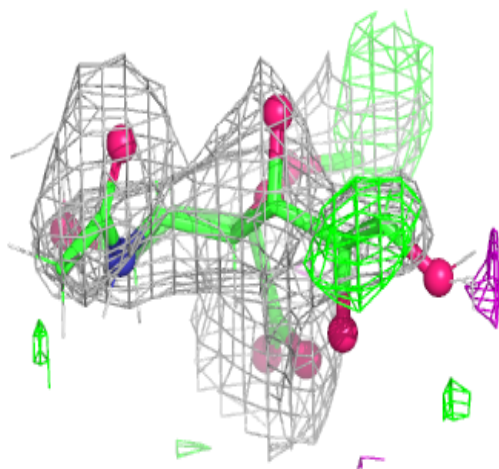
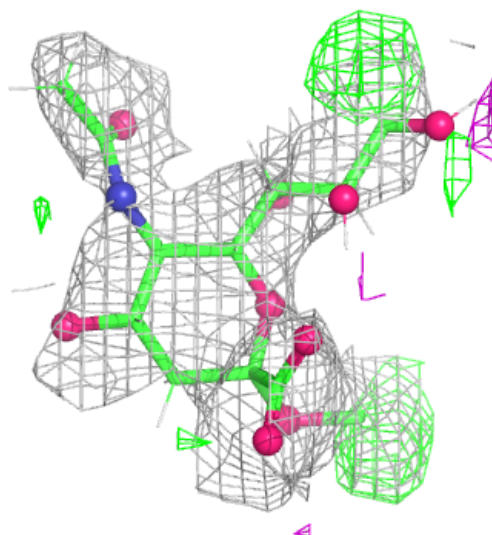
Electron density around MNA A 350:

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



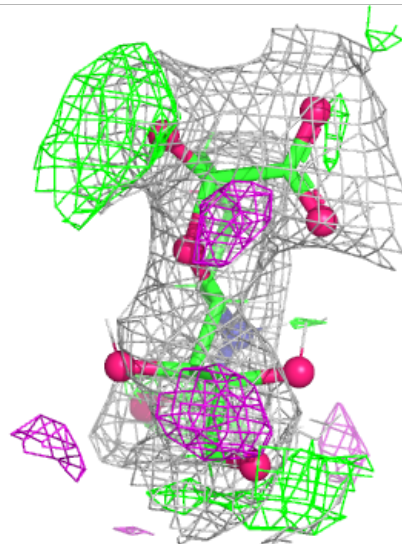
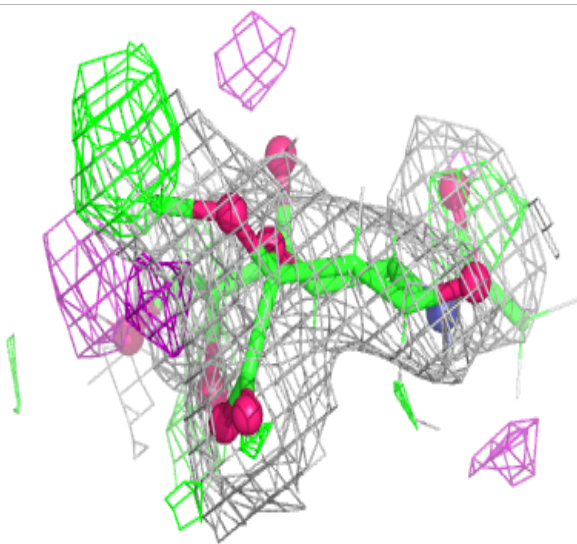
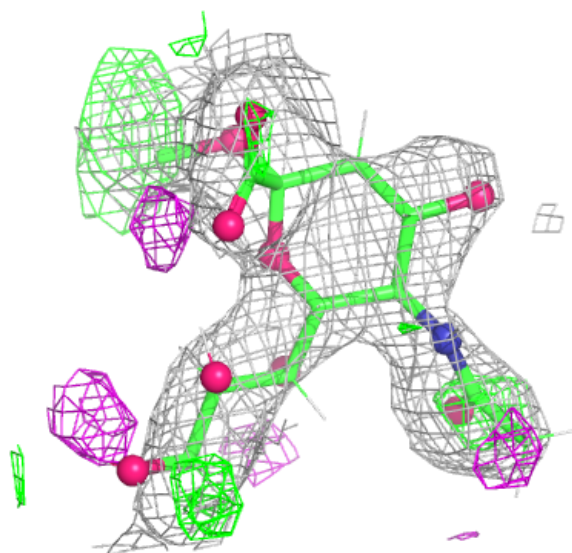
Electron density around MNA C 350:

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



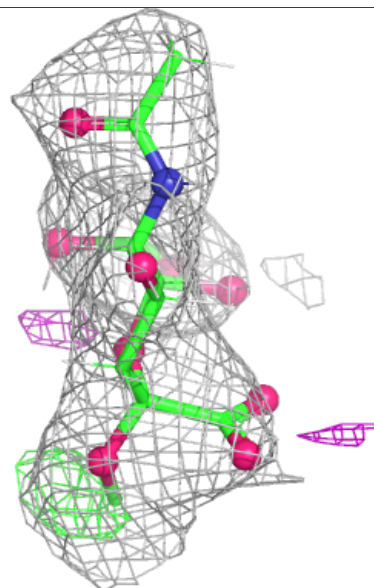
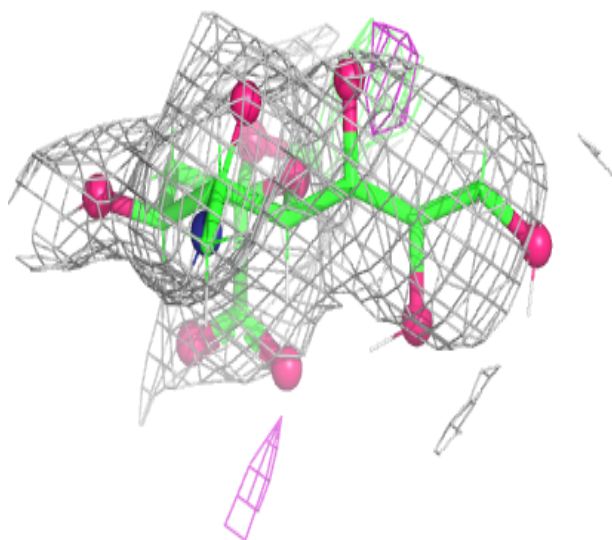
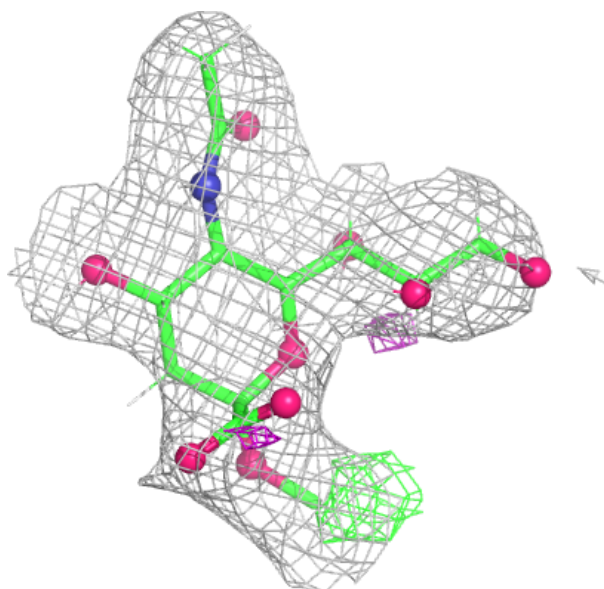
Electron density around MNA E 350:

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



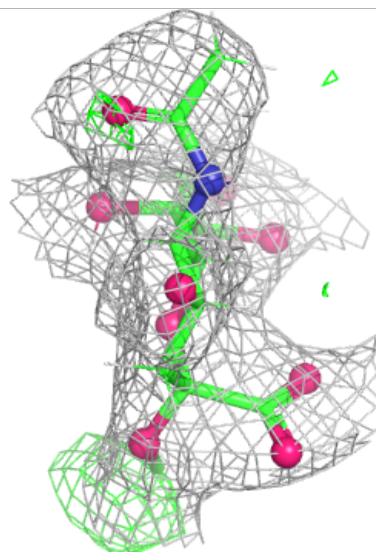
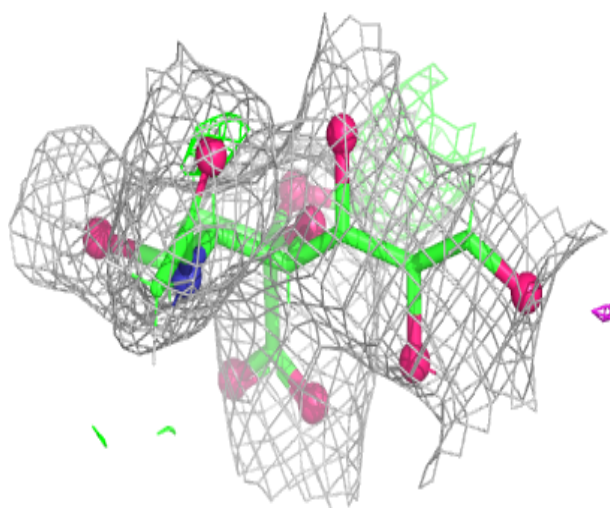
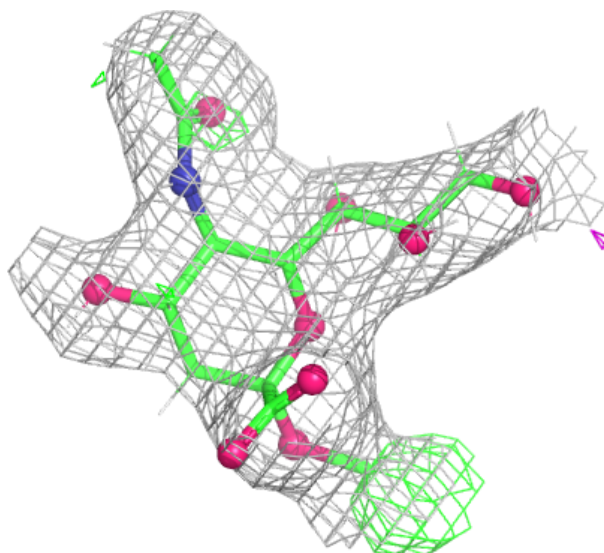
Electron density around MNA C 349:

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



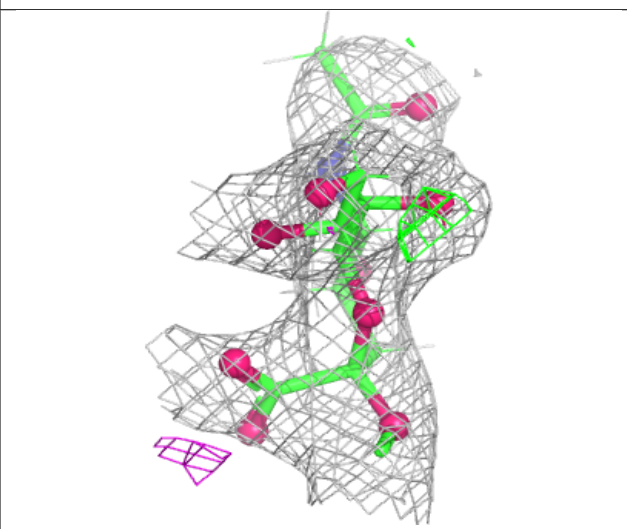
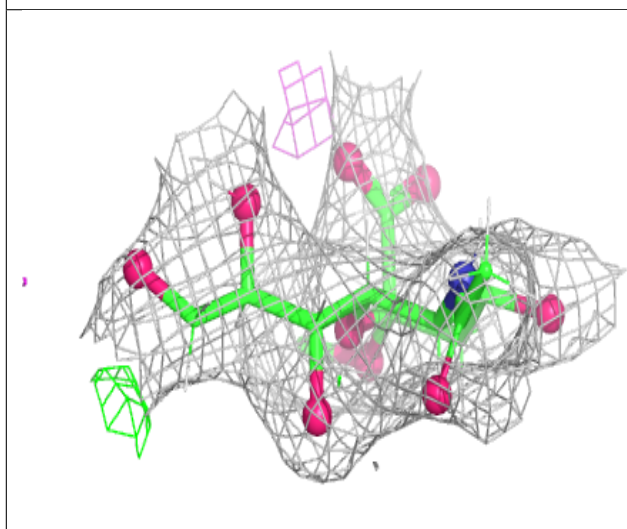
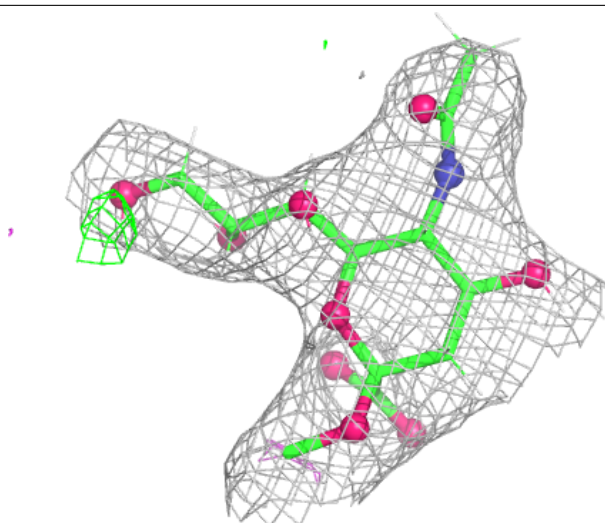
Electron density around MNA E 349:

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



Electron density around MNA A 349:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.