



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:26 AM UTC

PDB ID : 4HMG / pdb_00004hmg
Title : REFINEMENT OF THE INFLUENZA VIRUS HEMAGGLUTININ BY SIMULATED ANNEALING
Authors : Weis, W.I.; Bruenger, A.T.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1989-09-11
Resolution : 3.00 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
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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

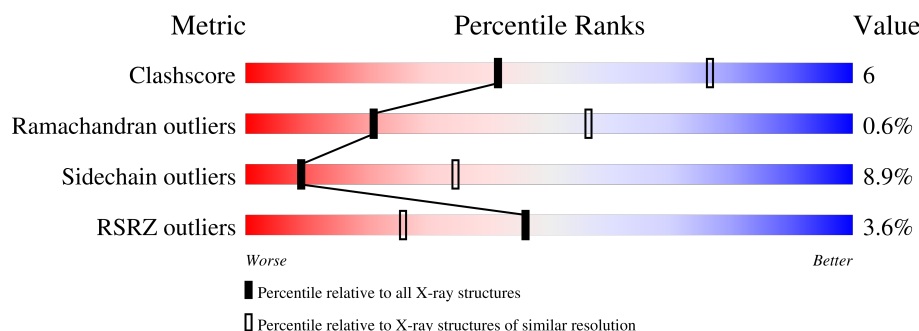
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	4% 72% 23% • •
1	C	328	4% 71% 25% • •
1	E	328	4% 73% 23% • •
2	B	175	3% 62% 31% 6% •
2	D	175	2% 65% 27% 7% •
2	F	175	2% 62% 31% 6% •

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Mol	Chain	Length	Quality of chain
3	G	3	 33% 67%
3	H	3	 100%
3	I	3	 33% 67%

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
3	MAN	G	3	X	-	-	-
3	MAN	H	3	X	-	-	-
3	MAN	I	3	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12243 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, CHAIN HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2533	1580	446	494	13			
1	C	328	Total	C	N	O	S	0	0	0
			2533	1580	446	494	13			
1	E	328	Total	C	N	O	S	0	0	0
			2533	1580	446	494	13			

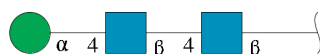
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLN	LEU	conflict	UNP P03437
C	226	GLN	LEU	conflict	UNP P03437
E	226	GLN	LEU	conflict	UNP P03437

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

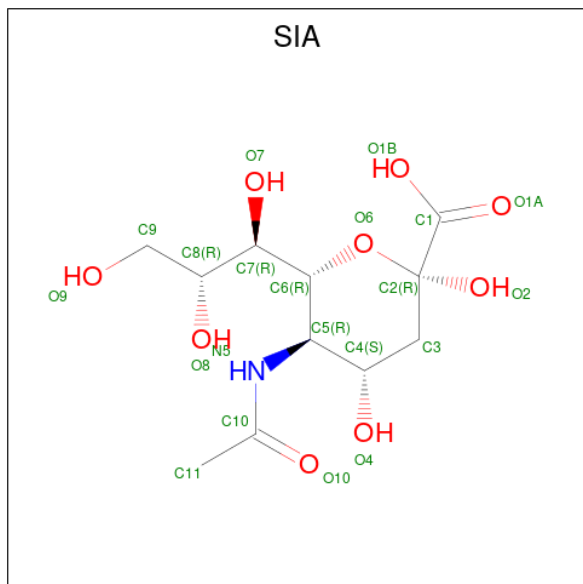
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	D	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	F	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

- Molecule 3 is an oligosaccharide called 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
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	11	1	9		
4	C	1	Total	C	N	O	0	0
			21	11	1	9		
4	E	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	B	5	Total 5	O 5	0	0
6	C	7	Total 7	O 7	0	0
6	D	4	Total 4	O 4	0	0
6	E	6	Total 6	O 6	0	0
6	F	5	Total 5	O 5	0	0

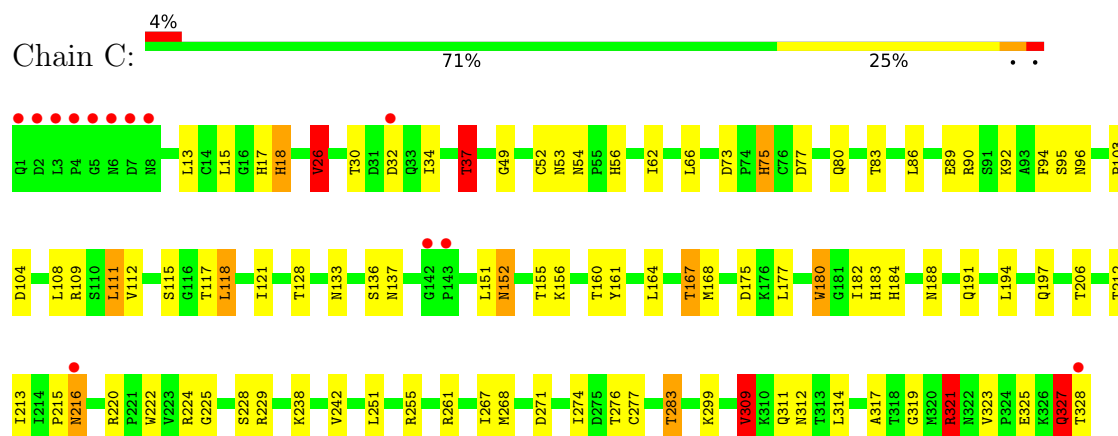
3 Residue-property plots [i](#)

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.

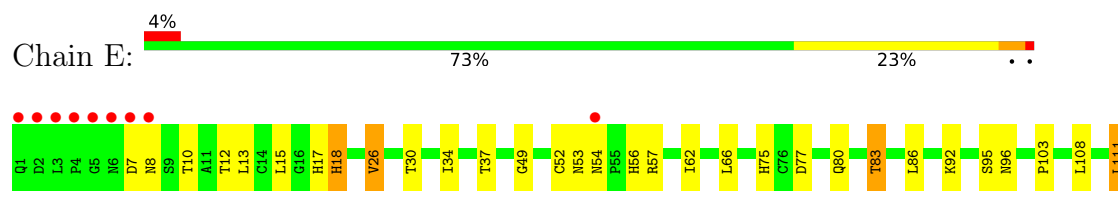
• Molecule 1: HEMAGGLUTININ, CHAIN HA1



• Molecule 1: HEMAGGLUTININ, CHAIN HA1



• Molecule 1: HEMAGGLUTININ, CHAIN HA1

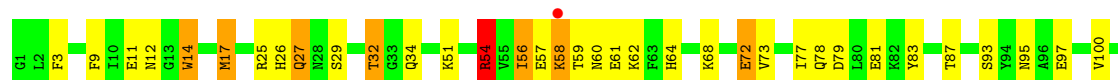




• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



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



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

Chain H:  100%

MAG1
MAG2
MAN3

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

Chain I:  33%  67%

MAG1
MAG2
MAN3

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 176.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 162.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 69.5 (162.80-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.231 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12243	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG, MAN

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	1.08	10/2590 (0.4%)	1.71	39/3528 (1.1%)
1	C	1.08	8/2590 (0.3%)	1.71	41/3528 (1.2%)
1	E	1.11	9/2590 (0.3%)	1.73	39/3528 (1.1%)
2	B	1.16	9/1445 (0.6%)	1.74	27/1939 (1.4%)
2	D	1.22	10/1445 (0.7%)	1.75	28/1939 (1.4%)
2	F	1.19	10/1445 (0.7%)	1.75	30/1939 (1.5%)
All	All	1.13	56/12105 (0.5%)	1.73	204/16401 (1.2%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	HIS	CD2-NE2	-7.12	1.30	1.37
2	F	159	HIS	CG-ND1	-7.06	1.30	1.38
1	E	184	HIS	CD2-NE2	-7.00	1.30	1.37
2	B	159	HIS	CG-ND1	-6.84	1.30	1.38
1	C	184	HIS	CD2-NE2	-6.76	1.30	1.37
2	B	64	HIS	CG-ND1	-6.75	1.30	1.38
2	D	106	HIS	CG-ND1	-6.71	1.30	1.38
2	D	159	HIS	CG-ND1	-6.71	1.30	1.38
1	A	75	HIS	CD2-NE2	-6.58	1.30	1.37
2	D	26	HIS	CD2-NE2	-6.57	1.30	1.37
2	B	106	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	75	HIS	CD2-NE2	-6.54	1.30	1.37
1	C	56	HIS	CD2-NE2	-6.54	1.30	1.37
2	B	64	HIS	CD2-NE2	-6.51	1.30	1.37
1	E	56	HIS	CD2-NE2	-6.46	1.30	1.37
2	D	159	HIS	CD2-NE2	-6.46	1.30	1.37
1	C	17	HIS	CD2-NE2	-6.46	1.30	1.37
2	F	26	HIS	CD2-NE2	-6.36	1.30	1.37
2	F	64	HIS	CD2-NE2	-6.33	1.30	1.37
2	B	159	HIS	CD2-NE2	-6.28	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	64	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	17	HIS	CD2-NE2	-6.16	1.31	1.37
1	E	17	HIS	CD2-NE2	-6.15	1.31	1.37
2	F	142	HIS	CD2-NE2	-6.14	1.31	1.37
2	D	142	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	56	HIS	CD2-NE2	-6.09	1.31	1.37
2	B	26	HIS	CD2-NE2	-6.07	1.31	1.37
2	F	64	HIS	CG-ND1	-6.05	1.31	1.38
2	F	106	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	184	HIS	CG-ND1	-5.96	1.31	1.38
1	C	18	HIS	CD2-NE2	-5.93	1.31	1.37
2	D	106	HIS	CD2-NE2	-5.91	1.31	1.37
2	F	159	HIS	CD2-NE2	-5.91	1.31	1.37
1	E	184	HIS	CG-ND1	-5.79	1.31	1.38
1	A	183	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	184	HIS	CD2-NE2	-5.74	1.31	1.37
1	E	56	HIS	CG-ND1	-5.69	1.31	1.38
1	E	183	HIS	CD2-NE2	-5.69	1.31	1.37
2	D	142	HIS	CG-ND1	-5.63	1.32	1.38
2	B	106	HIS	CG-ND1	-5.59	1.32	1.38
2	D	64	HIS	CG-ND1	-5.47	1.32	1.38
1	A	184	HIS	CG-ND1	-5.47	1.32	1.38
1	E	234	TRP	CG-CD2	-5.45	1.33	1.43
1	A	56	HIS	CG-ND1	-5.44	1.32	1.38
2	F	106	HIS	CG-ND1	-5.41	1.32	1.38
2	D	26	HIS	CG-ND1	-5.32	1.32	1.38
2	B	142	HIS	CG-ND1	-5.30	1.32	1.38
1	E	18	HIS	CD2-NE2	-5.27	1.32	1.37
1	C	56	HIS	CG-ND1	-5.24	1.32	1.38
2	F	142	HIS	CG-ND1	-5.24	1.32	1.38
1	A	284	PRO	CA-CB	-5.23	1.46	1.53
1	A	18	HIS	CG-ND1	-5.22	1.32	1.38
1	C	18	HIS	CG-ND1	-5.16	1.32	1.38
2	B	142	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	18	HIS	CD2-NE2	-5.13	1.32	1.37
2	F	26	HIS	CG-ND1	-5.02	1.32	1.38

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	PHE	CA-CB-CG	10.19	123.99	113.80
2	D	9	PHE	CA-CB-CG	9.88	123.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	PHE	CA-CB-CG	9.85	123.65	113.80
1	E	152	ASN	OD1-CG-ND2	-9.20	113.40	122.60
1	A	152	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	E	56	HIS	ND1-CG-CD2	8.69	114.79	106.10
1	C	152	ASN	OD1-CG-ND2	-8.34	114.26	122.60
2	D	172	GLN	OE1-CD-NE2	-8.33	114.27	122.60
2	B	159	HIS	ND1-CG-CD2	8.06	114.16	106.10
1	C	56	HIS	ND1-CG-CD2	8.01	114.11	106.10
2	F	106	HIS	ND1-CG-CD2	7.93	114.03	106.10
1	A	56	HIS	ND1-CG-CD2	7.74	113.84	106.10
2	F	159	HIS	ND1-CG-CD2	7.72	113.82	106.10
2	D	79	ASP	CA-CB-CG	7.63	120.23	112.60
2	D	159	HIS	ND1-CG-CD2	7.62	113.72	106.10
2	B	106	HIS	ND1-CG-CD2	7.55	113.65	106.10
1	C	184	HIS	ND1-CG-CD2	7.54	113.64	106.10
2	D	106	HIS	ND1-CG-CD2	7.43	113.53	106.10
1	A	96	ASN	CA-CB-CG	7.42	120.02	112.60
2	F	132	GLU	CA-CB-CG	-7.39	99.32	114.10
1	A	75	HIS	CA-CB-CG	7.37	121.17	113.80
1	C	75	HIS	CA-CB-CG	7.32	121.12	113.80
1	C	216	ASN	CA-CB-CG	7.27	119.87	112.60
2	B	95	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	E	184	HIS	ND1-CG-CD2	7.23	113.33	106.10
2	F	95	ASN	OD1-CG-ND2	-7.22	115.38	122.60
2	F	58	LYS	N-CA-C	7.21	121.31	110.64
1	A	184	HIS	ND1-CG-CD2	7.20	113.30	106.10
1	E	321	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	E	75	HIS	CA-CB-CG	7.16	120.96	113.80
2	D	132	GLU	CA-CB-CG	-7.13	99.85	114.10
1	A	137	ASN	OD1-CG-ND2	-7.12	115.48	122.60
2	F	79	ASP	CA-CB-CG	7.09	119.69	112.60
1	E	96	ASN	CA-CB-CG	7.09	119.69	112.60
1	C	321	ARG	NE-CZ-NH1	-7.05	114.44	121.50
2	B	132	GLU	CA-CB-CG	-7.03	100.04	114.10
1	A	216	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	321	ARG	NE-CZ-NH1	-6.92	114.58	121.50
1	E	216	ASN	CA-CB-CG	6.88	119.48	112.60
2	D	170	ARG	NE-CZ-NH1	-6.87	114.63	121.50
2	B	79	ASP	CA-CB-CG	6.80	119.40	112.60
1	C	321	ARG	CB-CG-CD	-6.79	95.69	111.30
2	B	58	LYS	N-CA-C	6.79	120.68	110.64
1	A	321	ARG	CB-CG-CD	-6.72	95.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	HIS	ND1-CG-CD2	6.72	112.82	106.10
2	F	28	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	E	321	ARG	CB-CG-CD	-6.69	95.92	111.30
1	C	137	ASN	OD1-CG-ND2	-6.69	115.91	122.60
2	D	58	LYS	N-CA-C	6.68	120.52	110.64
1	C	197	GLN	CA-CB-CG	-6.66	100.77	114.10
2	B	56	ILE	N-CA-CB	-6.65	100.25	111.23
1	E	197	GLN	CA-CB-CG	-6.64	100.83	114.10
1	A	111	LEU	CB-CA-C	-6.61	100.51	110.88
1	A	197	GLN	CA-CB-CG	-6.60	100.89	114.10
2	F	170	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	E	103	PRO	N-CA-C	-6.55	100.94	111.03
1	E	7	ASP	CA-CB-CG	6.46	119.06	112.60
2	F	56	ILE	N-CA-CB	-6.45	100.58	111.23
2	F	124	ARG	NE-CZ-NH1	-6.43	115.07	121.50
2	B	170	ARG	NE-CZ-NH1	-6.42	115.08	121.50
2	D	124	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	C	111	LEU	CB-CA-C	-6.36	100.63	110.81
1	E	111	LEU	CB-CA-C	-6.34	100.67	110.81
1	C	183	HIS	ND1-CG-CD2	6.33	112.43	106.10
1	C	96	ASN	CA-CB-CG	6.33	118.93	112.60
2	B	77	ILE	CB-CG1-CD1	-6.30	100.58	113.80
2	F	173	ILE	N-CA-C	6.28	116.54	108.12
1	E	171	ASN	OD1-CG-ND2	-6.27	116.33	122.60
2	D	77	ILE	CB-CG1-CD1	-6.18	100.81	113.80
1	C	321	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	E	191	GLN	OE1-CD-NE2	-6.17	116.43	122.60
2	D	56	ILE	N-CA-CB	-6.13	101.12	111.23
1	E	175	ASP	CA-CB-CG	6.11	118.71	112.60
2	B	173	ILE	N-CA-C	6.10	116.30	108.12
1	E	26	VAL	N-CA-CB	-6.10	101.07	112.36
1	C	26	VAL	N-CA-CB	-6.09	101.10	112.36
2	B	124	ARG	NE-CZ-NH1	-6.08	115.42	121.50
2	F	60	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	175	ASP	CA-CB-CG	6.04	118.64	112.60
2	F	77	ILE	CB-CG1-CD1	-6.04	101.12	113.80
1	C	103	PRO	N-CA-C	-6.01	101.77	111.03
1	A	103	PRO	N-CA-C	-6.01	101.78	111.03
2	D	95	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	E	56	HIS	CG-CD2-NE2	-5.98	101.22	107.20
2	D	60	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	E	180	TRP	CG-CD2-CE3	5.97	139.87	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	PHE	CA-CB-CG	-5.97	107.83	113.80
2	F	104	ASN	OD1-CG-ND2	-5.97	116.63	122.60
2	F	3	PHE	CA-CB-CG	-5.96	107.84	113.80
2	D	173	ILE	N-CA-C	5.94	116.08	108.12
2	B	3	PHE	CA-CB-CG	-5.93	107.86	113.80
2	B	60	ASN	OD1-CG-ND2	-5.91	116.69	122.60
2	F	25	ARG	CG-CD-NE	5.90	124.99	112.00
1	A	180	TRP	CG-CD2-CE3	5.89	139.79	133.90
2	B	104	ASN	OD1-CG-ND2	-5.86	116.75	122.60
2	D	104	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	C	175	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	255	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	A	183	HIS	ND1-CG-CD2	5.82	111.92	106.10
1	E	309	VAL	N-CA-CB	-5.81	101.61	112.36
1	C	26	VAL	CA-C-O	-5.80	115.88	121.63
2	B	153	ARG	CB-CG-CD	-5.80	97.97	111.30
1	E	324	PRO	O-C-N	5.79	130.07	123.00
1	C	191	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	C	327	GLN	OE1-CD-NE2	-5.74	116.86	122.60
2	F	95	ASN	CB-CG-ND2	5.73	124.99	116.40
1	C	188	ASN	CA-CB-CG	-5.72	106.88	112.60
2	F	153	ARG	CB-CG-CD	-5.72	98.15	111.30
1	E	321	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	C	180	TRP	CG-CD2-CE3	5.69	139.59	133.90
2	D	153	ARG	CB-CG-CD	-5.68	98.24	111.30
1	A	191	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	F	14	TRP	CG-CD2-CE3	5.66	139.56	133.90
2	B	95	ASN	CB-CG-ND2	5.66	124.89	116.40
2	F	106	HIS	CG-CD2-NE2	-5.60	101.60	107.20
2	D	160	ASP	CA-CB-CG	-5.60	107.00	112.60
2	D	32	THR	CA-C-O	-5.60	114.79	121.56
1	E	137	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	E	327	GLN	O-C-N	5.56	129.43	122.65
2	B	160	ASP	CA-CB-CG	-5.55	107.05	112.60
2	F	172	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	73	ASP	CA-CB-CG	5.54	118.14	112.60
2	D	14	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	C	323	VAL	CA-C-N	5.51	125.42	119.85
1	C	323	VAL	C-N-CA	5.51	125.42	119.85
1	A	26	VAL	N-CA-CB	-5.50	102.18	112.36
1	A	321	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	73	ASP	CA-C-N	5.49	124.95	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	C-N-CA	5.49	124.95	119.24
1	A	180	TRP	CE2-CD2-CG	-5.48	100.62	107.20
2	B	14	TRP	CG-CD2-CE3	5.48	139.38	133.90
2	D	135	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	C	56	HIS	CG-CD2-NE2	-5.43	101.77	107.20
1	C	309	VAL	N-CA-CB	-5.41	102.35	112.36
1	A	309	VAL	N-CA-CB	-5.41	102.36	112.36
1	A	188	ASN	CA-CB-CG	-5.40	107.20	112.60
1	C	128	THR	N-CA-C	5.38	117.48	109.25
2	F	127	ARG	CA-CB-CG	-5.38	103.35	114.10
1	E	8	ASN	OD1-CG-ND2	-5.36	117.25	122.60
2	B	159	HIS	CG-CD2-NE2	-5.34	101.86	107.20
2	B	169	ASN	CA-CB-CG	5.34	117.94	112.60
2	F	160	ASP	CA-CB-CG	-5.34	107.26	112.60
2	B	99	LEU	CA-C-O	-5.33	115.22	120.82
1	A	128	THR	N-CA-C	5.33	117.40	109.25
1	E	180	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	C	180	TRP	CE2-CD2-CG	-5.32	100.82	107.20
2	F	159	HIS	CG-CD2-NE2	-5.31	101.89	107.20
1	E	49	GLY	N-CA-C	-5.30	107.95	115.43
1	A	171	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	B	106	HIS	CG-CD2-NE2	-5.30	101.90	107.20
2	B	146	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	73	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	283	THR	CA-CB-OG1	-5.27	101.70	109.60
1	E	323	VAL	CA-C-N	5.27	125.24	120.03
1	E	323	VAL	C-N-CA	5.27	125.24	120.03
2	B	28	ASN	CA-C-N	5.26	127.64	120.54
2	B	28	ASN	C-N-CA	5.26	127.64	120.54
2	D	127	ARG	CA-CB-CG	-5.25	103.59	114.10
2	F	169	ASN	CA-CB-CG	5.25	117.85	112.60
1	E	255	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	D	113	SER	CA-C-O	-5.21	115.35	120.82
1	C	161	TYR	N-CA-C	-5.20	99.17	109.10
1	C	49	GLY	N-CA-C	-5.19	108.11	115.43
1	E	283	THR	CA-CB-OG1	-5.19	101.82	109.60
2	D	72	GLU	CA-CB-CG	-5.18	103.74	114.10
1	E	283	THR	O-C-N	-5.17	117.35	121.80
1	A	56	HIS	CG-CD2-NE2	-5.17	102.03	107.20
1	A	184	HIS	CA-C-N	5.17	125.10	119.78
1	A	184	HIS	C-N-CA	5.17	125.10	119.78
1	E	286	GLY	N-CA-C	-5.16	106.77	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	PRO	CA-C-N	-5.15	115.94	122.43
1	A	162	PRO	C-N-CA	-5.15	115.94	122.43
1	C	177	LEU	CA-C-O	-5.15	114.85	120.36
1	A	180	TRP	CG-CD1-NE1	-5.14	103.51	110.20
1	E	111	LEU	N-CA-CB	5.14	117.61	109.94
2	F	146	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	104	ASP	CA-C-O	5.13	127.65	121.65
1	E	26	VAL	CA-C-O	-5.12	116.56	121.63
1	A	137	ASN	CA-CB-CG	-5.11	107.49	112.60
2	D	106	HIS	CG-CD2-NE2	-5.10	102.10	107.20
2	F	76	ARG	N-CA-C	5.09	117.22	111.11
1	C	104	ASP	CA-C-O	5.09	127.60	121.65
1	C	168	MET	CA-C-N	5.08	124.99	119.85
1	C	168	MET	C-N-CA	5.08	124.99	119.85
1	E	137	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	49	GLY	N-CA-C	-5.08	108.27	115.43
2	D	169	ASN	CA-CB-CG	5.08	117.68	112.60
2	F	24	PHE	CA-CB-CG	5.07	118.87	113.80
1	C	283	THR	CA-CB-OG1	-5.07	101.99	109.60
2	B	72	GLU	CA-CB-CG	-5.07	103.96	114.10
1	C	121	ILE	N-CA-CB	-5.07	105.05	111.64
1	A	180	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	C	137	ASN	CA-CB-CG	-5.05	107.55	112.60
1	C	167	THR	CA-CB-OG1	-5.05	102.03	109.60
1	E	312	ASN	CA-CB-CG	-5.05	107.55	112.60
2	D	172	GLN	CG-CD-NE2	5.04	123.96	116.40
1	A	296	ASN	N-CA-CB	-5.04	103.13	111.49
1	C	312	ASN	CA-CB-CG	-5.02	107.58	112.60
1	C	32	ASP	CA-C-O	5.02	124.66	119.14
1	E	128	THR	N-CA-C	5.02	116.93	109.25
1	E	83	THR	N-CA-CB	-5.02	102.05	111.13
2	F	172	GLN	CB-CG-CD	5.02	121.13	112.60
1	C	37	THR	CA-CB-OG1	-5.01	102.09	109.60
2	D	54	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	2533	0	2470	37	0
1	C	2533	0	2470	35	0
1	E	2533	0	2470	33	0
2	B	1421	0	1345	31	0
2	D	1421	0	1345	25	0
2	F	1421	0	1345	29	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
4	A	21	0	18	0	0
4	C	21	0	18	0	0
4	E	21	0	18	0	0
5	A	42	0	39	0	0
5	B	14	0	13	0	0
5	C	42	0	39	0	0
5	D	14	0	13	0	0
5	E	42	0	39	0	0
5	F	14	0	13	0	0
6	A	6	0	0	0	0
6	B	5	0	0	0	0
6	C	7	0	0	0	0
6	D	4	0	0	0	0
6	E	6	0	0	0	0
6	F	5	0	0	0	0
All	All	12243	0	11757	153	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 (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.62	0.81
1:A:12:THR:HG23	2:B:133:MET:HE1	1.66	0.76
1:E:321:ARG:HG2	1:E:321:ARG:HH21	1.57	0.70
1:E:156:LYS:HD2	1:E:196:VAL:HG23	1.73	0.69
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.75	0.69
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.75	0.69
1:A:321:ARG:HG2	1:A:321:ARG:HH21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ARG:HH21	1:C:321:ARG:HG2	1.58	0.68
2:D:27:GLN:HG2	2:D:32:THR:HG22	1.76	0.68
2:B:51:LYS:HG3	1:E:30:THR:HG22	1.76	0.67
1:A:133:ASN:H	1:A:152:ASN:ND2	1.93	0.67
1:C:133:ASN:H	1:C:152:ASN:ND2	1.93	0.66
1:C:77:ASP:O	1:C:80:GLN:HG3	1.97	0.65
1:E:156:LYS:HD2	1:E:196:VAL:CG2	2.28	0.64
2:B:83:TYR:O	2:B:87:THR:HG23	1.98	0.64
1:A:133:ASN:H	1:A:152:ASN:HD21	1.45	0.63
1:E:133:ASN:H	1:E:152:ASN:ND2	1.95	0.63
1:E:77:ASP:O	1:E:80:GLN:HG3	1.99	0.63
2:D:83:TYR:O	2:D:87:THR:HG23	1.99	0.63
1:C:133:ASN:H	1:C:152:ASN:HD21	1.45	0.62
2:F:83:TYR:O	2:F:87:THR:HG23	1.99	0.62
1:E:133:ASN:H	1:E:152:ASN:HD21	1.48	0.62
1:A:30:THR:HG22	2:D:51:LYS:HG3	1.80	0.61
1:C:220:ARG:HD3	1:C:229:ARG:HD3	1.82	0.61
1:E:66:LEU:HD21	1:E:112:VAL:HG23	1.82	0.61
1:A:66:LEU:HD21	1:A:112:VAL:HG23	1.82	0.61
2:D:14:TRP:HE3	2:D:17:MET:HG3	1.66	0.61
1:A:160:THR:HA	1:A:196:VAL:HG21	1.84	0.59
1:A:77:ASP:O	1:A:80:GLN:HG3	2.02	0.59
1:C:66:LEU:HD21	1:C:112:VAL:HG23	1.83	0.59
1:C:30:THR:HG22	2:F:51:LYS:HG3	1.83	0.59
2:B:14:TRP:HE3	2:B:17:MET:HG3	1.67	0.59
2:F:14:TRP:HE3	2:F:17:MET:HG3	1.67	0.59
1:E:220:ARG:HD3	1:E:229:ARG:HD3	1.83	0.59
1:A:220:ARG:HD3	1:A:229:ARG:HD3	1.84	0.58
1:A:117:THR:HG21	1:A:261:ARG:HH21	1.69	0.57
2:D:54:ARG:O	2:D:57:GLU:HB2	2.06	0.56
1:E:117:THR:HG21	1:E:261:ARG:HH21	1.70	0.55
1:E:325:GLU:HG2	2:F:13:GLY:O	2.07	0.54
2:B:54:ARG:O	2:B:57:GLU:HB2	2.07	0.54
1:C:117:THR:HG21	1:C:261:ARG:HH21	1.71	0.54
1:C:228:SER:O	1:C:229:ARG:HD2	2.07	0.54
1:A:52:CYS:HB3	1:A:277:CYS:O	2.07	0.54
2:F:54:ARG:O	2:F:57:GLU:HB2	2.07	0.54
1:A:228:SER:O	1:A:229:ARG:HD2	2.08	0.54
1:A:53:ASN:OD1	1:A:276:THR:HA	2.08	0.54
1:A:309:VAL:HG22	2:B:93:SER:HA	1.90	0.54
1:E:53:ASN:OD1	1:E:276:THR:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:GLN:HA	2:F:81:GLU:OE1	2.07	0.54
2:D:78:GLN:HA	2:D:81:GLU:OE1	2.08	0.53
1:C:53:ASN:OD1	1:C:276:THR:HA	2.08	0.53
2:B:68:LYS:HZ3	2:B:85:GLU:CD	2.16	0.53
1:E:52:CYS:HB3	1:E:277:CYS:O	2.09	0.52
1:E:228:SER:O	1:E:229:ARG:HD2	2.09	0.52
1:E:12:THR:HG23	2:F:133:MET:HE1	1.92	0.52
2:B:25:ARG:NH2	2:B:34:GLN:OE1	2.43	0.52
1:A:111:LEU:HD22	2:F:73:VAL:HG12	1.91	0.52
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.24	0.52
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.25	0.52
2:F:58:LYS:HE2	2:F:59:THR:O	2.11	0.51
2:B:58:LYS:HE2	2:B:59:THR:O	2.11	0.51
1:C:309:VAL:HG22	2:D:93:SER:HA	1.92	0.51
2:B:78:GLN:HA	2:B:81:GLU:OE1	2.11	0.51
2:D:58:LYS:HE2	2:D:59:THR:O	2.11	0.51
1:C:52:CYS:HB3	1:C:277:CYS:O	2.11	0.50
2:B:132:GLU:HG2	2:B:134:GLY:H	1.75	0.50
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.27	0.50
2:F:132:GLU:HG2	2:F:134:GLY:H	1.75	0.50
1:A:66:LEU:HD22	1:A:267:ILE:HD12	1.94	0.50
1:E:309:VAL:HG22	2:F:93:SER:HA	1.93	0.50
2:F:141:TYR:O	2:F:166:ALA:HA	2.12	0.50
2:B:141:TYR:O	2:B:166:ALA:HA	2.12	0.49
2:D:61:GLU:O	2:D:62:LYS:HD2	2.13	0.49
2:D:141:TYR:O	2:D:166:ALA:HA	2.12	0.49
2:D:132:GLU:HG2	2:D:134:GLY:H	1.78	0.49
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.48	0.49
1:C:66:LEU:HD22	1:C:267:ILE:HD12	1.95	0.48
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.49	0.48
2:D:25:ARG:HG2	2:D:34:GLN:HG3	1.96	0.48
2:D:25:ARG:CG	2:D:34:GLN:HG3	2.45	0.47
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.49	0.47
2:F:133:MET:HE2	2:F:139:LYS:HB2	1.95	0.47
2:B:61:GLU:O	2:B:62:LYS:HD2	2.15	0.47
1:A:57:ARG:HG2	1:A:57:ARG:HH21	1.80	0.47
1:A:326:LYS:HG2	1:A:327:GLN:H	1.80	0.46
2:B:173:ILE:HG21	2:D:167:LEU:HB3	1.96	0.46
1:C:86:LEU:HD11	1:C:268:MET:HB2	1.98	0.46
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.97	0.46
1:E:299:LYS:HE2	2:F:68:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD11	1:A:268:MET:HB2	1.98	0.45
1:A:299:LYS:HE2	2:B:68:LYS:HB3	1.98	0.45
2:B:88:LYS:HD2	2:F:87:THR:HB	1.98	0.45
1:E:66:LEU:HD22	1:E:267:ILE:HD12	1.97	0.45
2:B:167:LEU:HB3	2:F:173:ILE:HG21	1.99	0.45
1:C:15:LEU:HD23	2:D:118:LEU:HD13	1.98	0.45
1:C:299:LYS:HE2	2:D:68:LYS:HB3	1.99	0.45
2:F:61:GLU:O	2:F:62:LYS:HD2	2.16	0.45
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.99	0.44
1:E:206:THR:HA	1:E:242:VAL:O	2.18	0.44
2:F:26:HIS:O	2:F:32:THR:HA	2.17	0.44
2:B:174:LYS:HA	2:B:174:LYS:HD2	1.71	0.44
1:A:8:ASN:HB2	2:B:169:ASN:OD1	2.18	0.44
1:C:325:GLU:HB2	2:D:12:ASN:ND2	2.34	0.43
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.79	0.43
1:A:206:THR:HA	1:A:242:VAL:O	2.18	0.43
1:C:206:THR:HA	1:C:242:VAL:O	2.18	0.43
2:B:167:LEU:HD12	2:B:167:LEU:HA	1.84	0.43
1:C:37:THR:HG22	1:C:319:GLY:HA3	2.01	0.43
1:E:57:ARG:HG2	1:E:57:ARG:HH21	1.83	0.43
1:E:86:LEU:HD11	1:E:268:MET:HB2	2.01	0.43
1:A:15:LEU:HD23	2:B:118:LEU:HD13	1.99	0.43
2:D:87:THR:HB	2:F:88:LYS:HD2	2.01	0.43
1:A:37:THR:HG22	1:A:319:GLY:HA3	2.01	0.42
1:C:15:LEU:HD22	2:D:119:PHE:HA	2.00	0.42
2:D:73:VAL:HG12	1:E:111:LEU:HD22	2.02	0.42
1:A:180:TRP:CH2	1:A:213:ILE:HD13	2.55	0.42
2:B:174:LYS:HZ2	2:B:175:GLY:C	2.28	0.42
1:A:109:ARG:HH21	1:A:109:ARG:HD2	1.66	0.42
1:C:109:ARG:HH21	1:C:109:ARG:HD2	1.63	0.42
1:E:15:LEU:HD23	2:F:118:LEU:HD13	2.02	0.42
2:B:14:TRP:CD2	2:B:25:ARG:NH2	2.87	0.42
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.85	0.42
2:B:145:ASP:O	2:B:148:CYS:HB3	2.20	0.42
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.81	0.41
1:C:182:ILE:HD11	1:C:215:PRO:HD3	2.02	0.41
2:D:174:LYS:HA	2:D:174:LYS:HD2	1.71	0.41
1:C:89:GLU:OE2	1:C:109:ARG:NH2	2.53	0.41
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.84	0.41
1:A:230:ILE:HD13	1:A:230:ILE:HG21	1.91	0.41
2:D:167:LEU:HD12	2:D:167:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:TRP:CH2	1:E:213:ILE:HD13	2.55	0.41
2:F:120:GLU:OE2	2:F:123:ARG:NH2	2.54	0.41
1:A:325:GLU:O	1:A:326:LYS:HD3	2.20	0.41
2:B:127:ARG:NH2	2:F:131:GLU:OE1	2.53	0.41
2:F:174:LYS:HZ2	2:F:175:GLY:C	2.28	0.41
1:A:190:GLU:O	1:A:194:LEU:HB2	2.20	0.41
2:B:131:GLU:OE1	2:D:127:ARG:NH2	2.54	0.41
2:D:120:GLU:OE2	2:D:123:ARG:NH2	2.54	0.41
1:C:90:ARG:HH21	1:C:271:ASP:HA	1.86	0.41
1:E:190:GLU:O	1:E:194:LEU:HB2	2.21	0.41
1:C:115:SER:O	1:C:261:ARG:HB2	2.21	0.41
1:C:26:VAL:HG11	1:C:317:ALA:HB2	2.02	0.40
2:B:25:ARG:HH21	2:B:25:ARG:HG3	1.86	0.40
1:C:151:LEU:O	1:C:255:ARG:NH2	2.54	0.40
2:F:14:TRP:CH2	2:F:25:ARG:HB2	2.55	0.40
2:F:48:ILE:CD1	2:F:107:THR:HG23	2.51	0.40
1:A:89:GLU:OE2	1:A:109:ARG:NH2	2.54	0.40
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.56	0.40
1:C:75:HIS:HE1	1:C:94:PHE:O	2.04	0.40
1:C:180:TRP:CH2	1:C:213:ILE:HD13	2.56	0.40
1:E:10:THR:HG22	2:F:141:TYR:HA	2.03	0.40
1:E:10:THR:HG21	2:F:139:LYS:HE2	2.04	0.40
2:B:73:VAL:HG12	1:C:111:LEU:HD22	2.03	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%)	309 (95%)	14 (4%)	3 (1%)	14 48
1	C	326/328 (99%)	310 (95%)	14 (4%)	2 (1%)	21 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	326/328 (99%)	311 (95%)	14 (4%)	1 (0%)	36	70
2	B	173/175 (99%)	158 (91%)	14 (8%)	1 (1%)	21	56
2	D	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	21	56
2	F	173/175 (99%)	159 (92%)	13 (8%)	1 (1%)	21	56
All	All	1497/1509 (99%)	1407 (94%)	81 (5%)	9 (1%)	21	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	LYS
2	D	135	ASN
2	B	135	ASN
2	F	135	ASN
1	A	62	ILE
1	C	62	ILE
1	C	327	GLN
1	E	62	ILE
1	A	158	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/289 (100%)	263 (91%)	26 (9%)	9	34
1	C	289/289 (100%)	261 (90%)	28 (10%)	8	30
1	E	289/289 (100%)	263 (91%)	26 (9%)	9	34
2	B	149/149 (100%)	137 (92%)	12 (8%)	11	38
2	D	149/149 (100%)	135 (91%)	14 (9%)	8	32
2	F	149/149 (100%)	138 (93%)	11 (7%)	13	42
All	All	1314/1314 (100%)	1197 (91%)	117 (9%)	9	34

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	18	HIS
1	A	26	VAL
1	A	34	ILE
1	A	37	THR
1	A	54	ASN
1	A	83	THR
1	A	92	LYS
1	A	95	SER
1	A	108	LEU
1	A	118	LEU
1	A	155	THR
1	A	156	LYS
1	A	160	THR
1	A	164	LEU
1	A	167	THR
1	A	194	LEU
1	A	224	ARG
1	A	227	SER
1	A	238	LYS
1	A	251	LEU
1	A	283	THR
1	A	309	VAL
1	A	314	LEU
1	A	321	ARG
1	A	326	LYS
2	B	17	MET
2	B	32	THR
2	B	56	ILE
2	B	72	GLU
2	B	100	VAL
2	B	110	LEU
2	B	118	LEU
2	B	127	ARG
2	B	128	GLU
2	B	150	GLU
2	B	169	ASN
2	B	172	GLN
1	C	13	LEU
1	C	18	HIS
1	C	26	VAL
1	C	34	ILE
1	C	37	THR

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Mol	Chain	Res	Type
1	C	54	ASN
1	C	83	THR
1	C	92	LYS
1	C	95	SER
1	C	108	LEU
1	C	118	LEU
1	C	136	SER
1	C	155	THR
1	C	156	LYS
1	C	160	THR
1	C	164	LEU
1	C	167	THR
1	C	194	LEU
1	C	224	ARG
1	C	238	LYS
1	C	251	LEU
1	C	274	ILE
1	C	283	THR
1	C	309	VAL
1	C	314	LEU
1	C	321	ARG
1	C	327	GLN
1	C	328	THR
2	D	11	GLU
2	D	17	MET
2	D	27	GLN
2	D	29	SER
2	D	54	ARG
2	D	56	ILE
2	D	72	GLU
2	D	100	VAL
2	D	110	LEU
2	D	118	LEU
2	D	127	ARG
2	D	128	GLU
2	D	169	ASN
2	D	172	GLN
1	E	13	LEU
1	E	18	HIS
1	E	26	VAL
1	E	34	ILE
1	E	37	THR

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Mol	Chain	Res	Type
1	E	54	ASN
1	E	83	THR
1	E	92	LYS
1	E	95	SER
1	E	108	LEU
1	E	118	LEU
1	E	136	SER
1	E	155	THR
1	E	157	SER
1	E	160	THR
1	E	164	LEU
1	E	167	THR
1	E	194	LEU
1	E	224	ARG
1	E	227	SER
1	E	238	LYS
1	E	251	LEU
1	E	283	THR
1	E	309	VAL
1	E	314	LEU
1	E	321	ARG
2	F	17	MET
2	F	25	ARG
2	F	56	ILE
2	F	72	GLU
2	F	100	VAL
2	F	110	LEU
2	F	118	LEU
2	F	127	ARG
2	F	128	GLU
2	F	169	ASN
2	F	172	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	171	ASN
2	B	12	ASN
1	C	152	ASN
1	C	171	ASN
1	C	226	GLN

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Mol	Chain	Res	Type
2	D	172	GLN
1	E	152	ASN
1	E	171	ASN
2	F	12	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	0.54	0	17,19,21	0.97	1 (5%)
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	1.01	0
3	MAN	G	3	3	11,11,12	0.77	0	15,15,17	1.40	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.58	0	17,19,21	1.04	2 (11%)
3	NAG	H	2	3	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
3	MAN	H	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.23	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
3	NAG	I	2	3	14,14,15	0.39	0	17,19,21	1.05	1 (5%)
3	MAN	I	3	3	11,11,12	0.62	0	15,15,17	0.77	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	-	1/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	1/2/19/22	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	MAN	H	3	3	1/1/4/5	1/2/19/22	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	MAN	I	3	3	1/1/4/5	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	MAN	C2-C3	2.26	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	C1-C2-C3	-3.39	104.72	109.64
3	H	3	MAN	C1-O5-C5	2.81	115.95	112.19
3	H	3	MAN	O3-C3-C2	2.42	115.00	110.05
3	H	1	NAG	C1-C2-N2	2.35	114.13	110.43
3	G	3	MAN	C3-C4-C5	2.34	114.47	110.23
3	I	1	NAG	C1-O5-C5	2.30	115.27	112.19
3	I	2	NAG	C4-C3-C2	-2.23	107.76	111.02
3	G	1	NAG	C1-C2-N2	2.13	113.80	110.43
3	H	2	NAG	C4-C3-C2	-2.05	108.01	111.02
3	H	1	NAG	C1-O5-C5	2.02	114.89	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3	MAN	C1
3	H	3	MAN	C1
3	I	3	MAN	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	3	MAN	O5-C5-C6-O6
3	G	3	MAN	O5-C5-C6-O6

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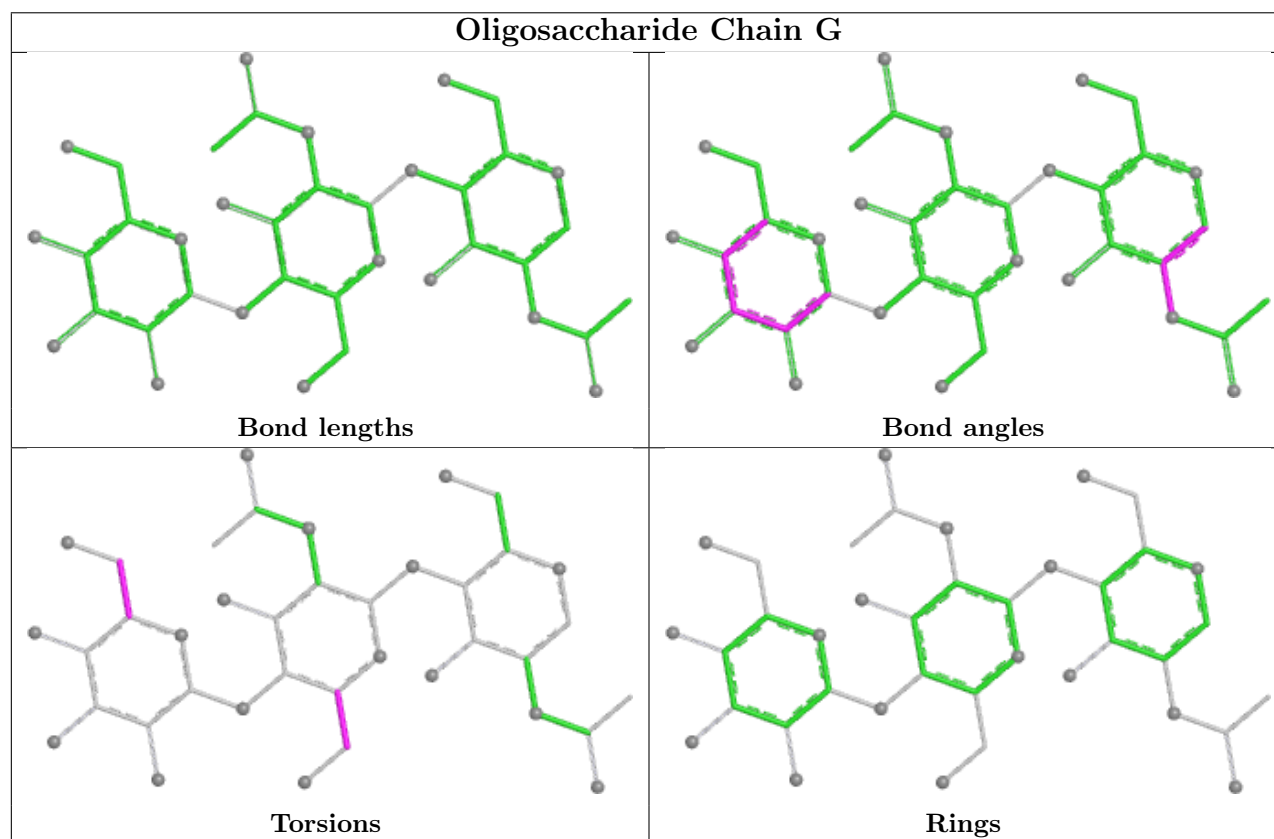
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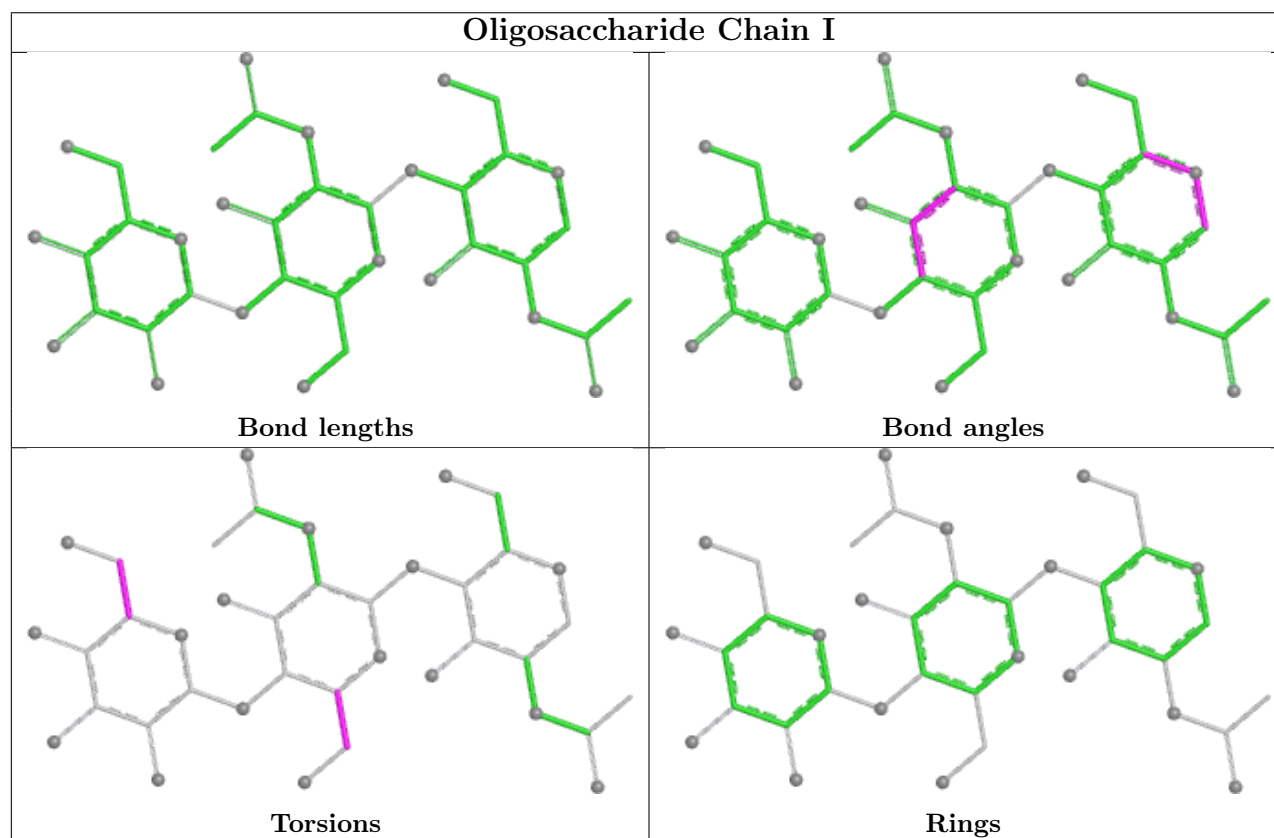
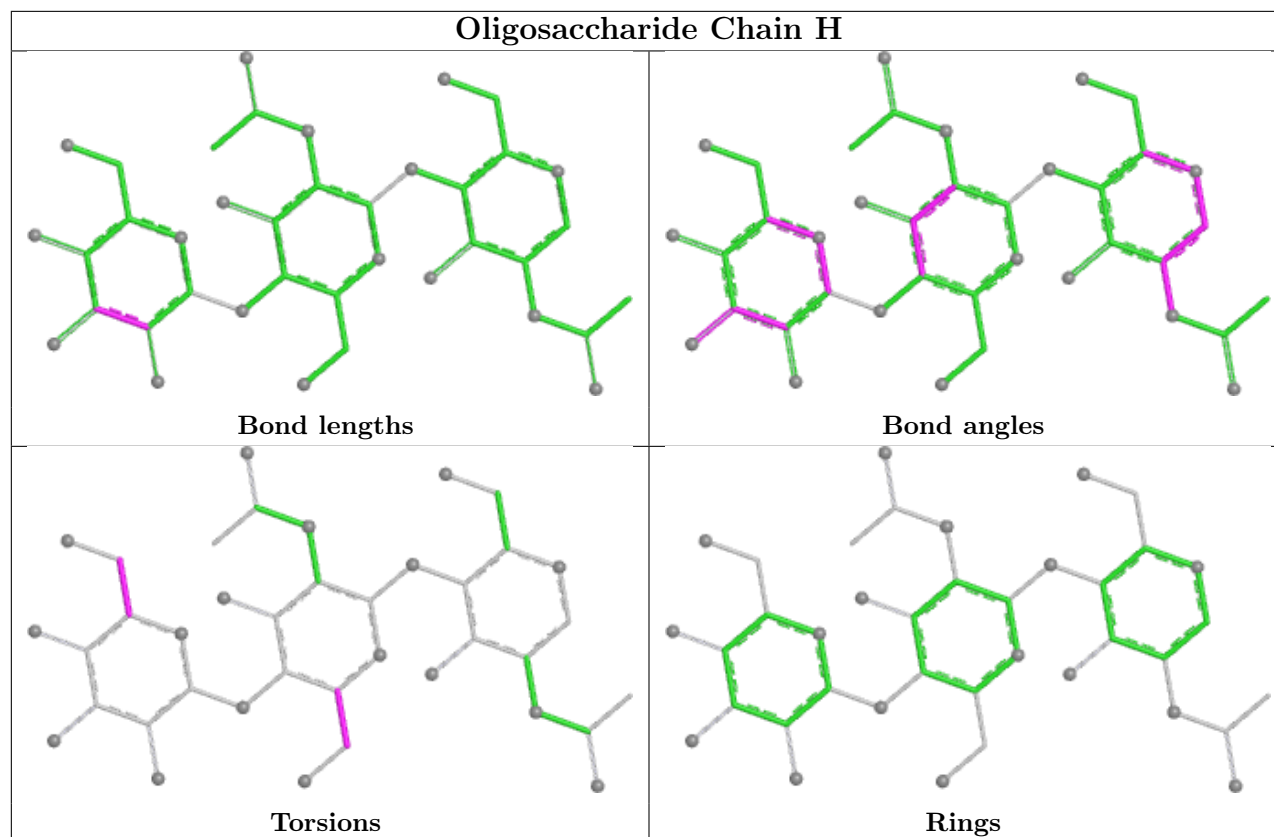
Mol	Chain	Res	Type	Atoms
3	I	3	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry

15 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
5	NAG	E	348	1	14,14,15	0.66	0	17,19,21	1.05	1 (5%)
5	NAG	F	401	2	14,14,15	0.52	0	17,19,21	1.21	1 (5%)
5	NAG	A	348	1	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
5	NAG	C	348	1	14,14,15	0.65	0	17,19,21	1.07	1 (5%)
5	NAG	E	330	1	14,14,15	0.92	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	330	1	14,14,15	0.86	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	B	401	2	14,14,15	0.65	0	17,19,21	1.24	2 (11%)
4	SIA	E	329	-	21,21,21	0.96	1 (4%)	24,31,31	1.23	2 (8%)
5	NAG	C	330	1	14,14,15	1.00	1 (7%)	17,19,21	1.13	2 (11%)
5	NAG	C	334	1	14,14,15	0.81	0	17,19,21	1.39	2 (11%)
5	NAG	A	334	1	14,14,15	0.91	0	17,19,21	1.28	2 (11%)
5	NAG	E	334	1	14,14,15	0.70	0	17,19,21	1.34	1 (5%)
4	SIA	C	329	-	21,21,21	0.96	1 (4%)	24,31,31	1.24	4 (16%)
4	SIA	A	329	-	21,21,21	0.92	1 (4%)	24,31,31	1.27	3 (12%)
5	NAG	D	401	2	14,14,15	0.55	0	17,19,21	1.23	2 (11%)

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	E	348	1	-	2/6/23/26	0/1/1/1
5	NAG	F	401	2	-	0/6/23/26	0/1/1/1
5	NAG	A	348	1	-	2/6/23/26	0/1/1/1
5	NAG	C	348	1	-	2/6/23/26	0/1/1/1
5	NAG	E	330	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	330	1	-	0/6/23/26	0/1/1/1
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1
4	SIA	E	329	-	-	2/20/38/38	0/1/1/1
5	NAG	C	330	1	-	0/6/23/26	0/1/1/1
5	NAG	C	334	1	-	0/6/23/26	0/1/1/1
5	NAG	A	334	1	-	0/6/23/26	0/1/1/1
5	NAG	E	334	1	-	0/6/23/26	0/1/1/1
4	SIA	C	329	-	-	3/20/38/38	0/1/1/1
4	SIA	A	329	-	-	3/20/38/38	0/1/1/1
5	NAG	D	401	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	330	NAG	C4-C5	3.00	1.59	1.53
5	E	330	NAG	C4-C5	2.55	1.58	1.53
5	A	330	NAG	C4-C5	2.48	1.58	1.53
4	E	329	SIA	C3-C2	2.40	1.55	1.51
4	A	329	SIA	O1B-C1	-2.06	1.23	1.30
4	C	329	SIA	O1B-C1	-2.00	1.23	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	NAG	C1-C2-N2	-3.97	104.18	110.43
5	B	401	NAG	C1-C2-N2	-3.92	104.25	110.43
5	F	401	NAG	C1-C2-N2	-3.85	104.37	110.43
5	E	334	NAG	C1-O5-C5	3.44	116.79	112.19
5	C	334	NAG	C1-O5-C5	3.12	116.36	112.19
5	A	334	NAG	C1-O5-C5	2.98	116.18	112.19
5	A	330	NAG	C1-O5-C5	2.78	115.91	112.19
4	C	329	SIA	C4-C5-N5	-2.65	105.22	110.44
5	C	330	NAG	C1-O5-C5	2.64	115.73	112.19
4	C	329	SIA	C6-C5-N5	2.61	115.06	110.91
4	A	329	SIA	C4-C5-N5	-2.60	105.31	110.44
4	E	329	SIA	C4-C5-N5	-2.56	105.39	110.44
5	E	330	NAG	C1-O5-C5	2.55	115.61	112.19
5	E	348	NAG	C8-C7-N2	2.52	120.29	116.12
5	C	334	NAG	C1-C2-N2	2.46	114.31	110.43
5	A	334	NAG	C1-C2-N2	2.46	114.31	110.43
5	A	348	NAG	C8-C7-N2	2.42	120.12	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	329	SIA	C6-C5-N5	2.39	114.72	110.91
4	E	329	SIA	C6-C5-N5	2.35	114.65	110.91
5	C	348	NAG	C8-C7-N2	2.34	120.01	116.12
5	D	401	NAG	C1-O5-C5	2.10	115.00	112.19
5	B	401	NAG	C1-O5-C5	2.05	114.93	112.19
4	C	329	SIA	C8-C7-C6	-2.04	109.21	113.05
5	C	330	NAG	O7-C7-C8	-2.03	118.44	122.05
4	A	329	SIA	C8-C7-C6	-2.02	109.26	113.05
4	C	329	SIA	C3-C2-C1	-2.01	109.10	112.84

There are no chirality outliers.

All (14) torsion outliers are listed below:

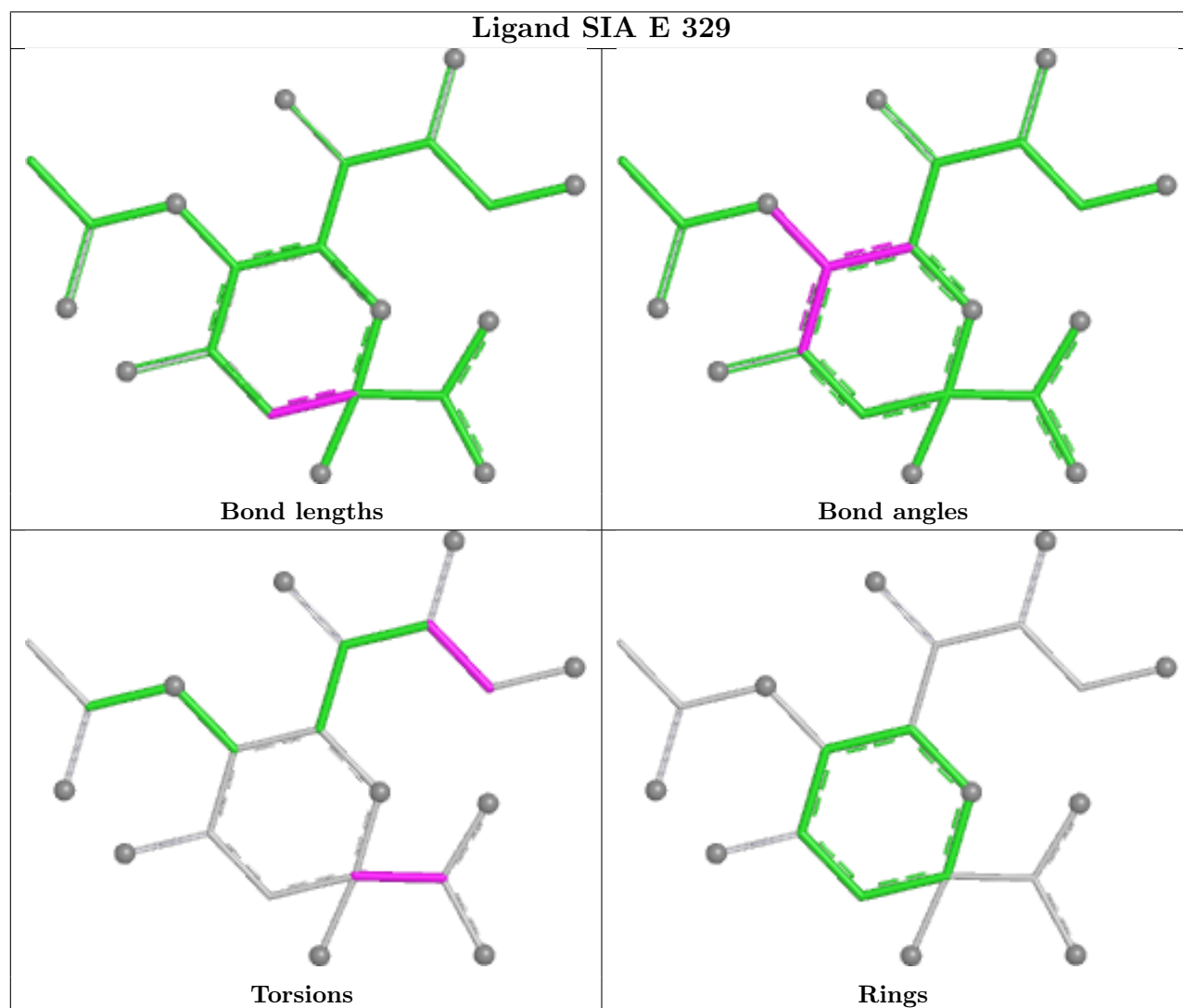
Mol	Chain	Res	Type	Atoms
4	A	329	SIA	O1B-C1-C2-O2
5	E	348	NAG	O5-C5-C6-O6
5	A	348	NAG	O5-C5-C6-O6
5	C	348	NAG	O5-C5-C6-O6
5	C	348	NAG	C4-C5-C6-O6
5	E	348	NAG	C4-C5-C6-O6
5	A	348	NAG	C4-C5-C6-O6
4	A	329	SIA	O8-C8-C9-O9
4	E	329	SIA	O8-C8-C9-O9
4	C	329	SIA	O8-C8-C9-O9
4	C	329	SIA	O1B-C1-C2-O2
4	E	329	SIA	O1B-C1-C2-O2
4	A	329	SIA	O1A-C1-C2-C3
4	C	329	SIA	O1A-C1-C2-C3

There are no ring outliers.

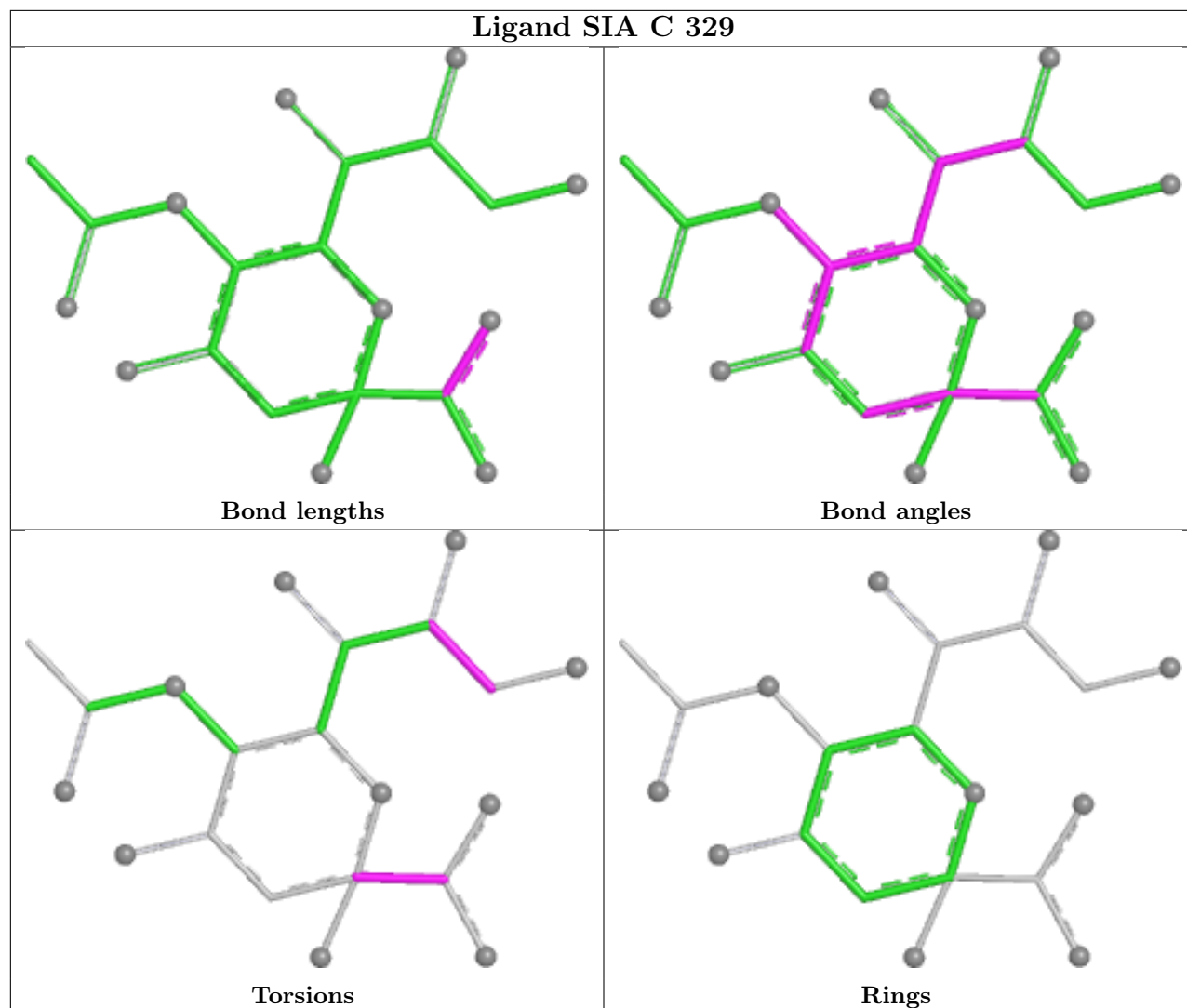
No monomer is involved in short contacts.

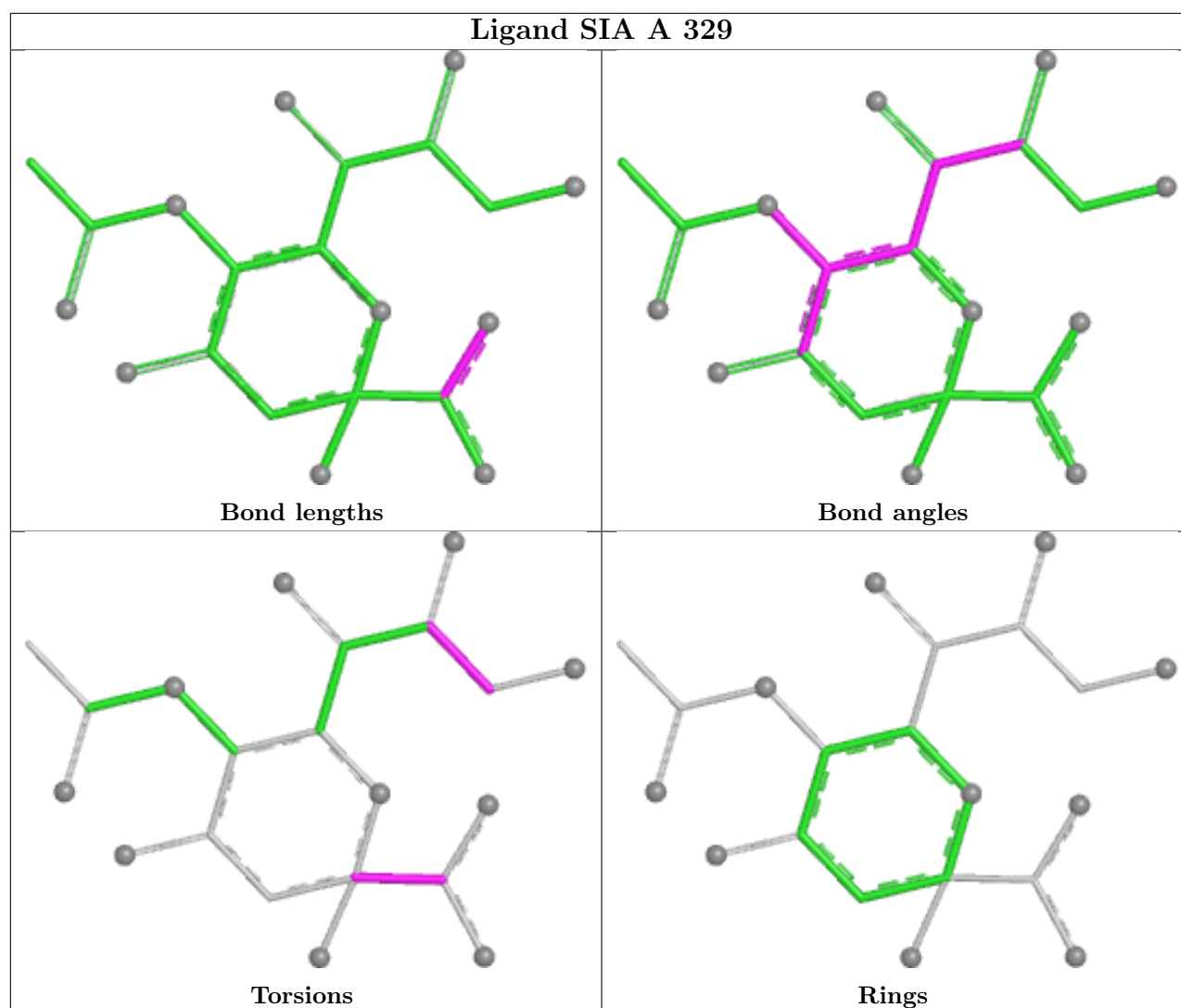
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand SIA C 329





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%)	-0.21	14 (4%)	40	21	4, 26, 56, 143	0
1	C	328/328 (100%)	-0.25	13 (3%)	42	23	4, 26, 54, 142	0
1	E	328/328 (100%)	-0.26	14 (4%)	40	21	4, 26, 54, 146	0
2	B	175/175 (100%)	-0.33	6 (3%)	48	27	3, 21, 53, 101	0
2	D	175/175 (100%)	-0.37	4 (2%)	61	38	2, 20, 50, 101	0
2	F	175/175 (100%)	-0.34	4 (2%)	61	38	2, 20, 51, 101	0
All	All	1509/1509 (100%)	-0.28	55 (3%)	46	26	2, 24, 54, 146	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	GLY	8.1
2	F	174	LYS	7.7
1	A	6	ASN	7.5
1	E	3	LEU	6.2
1	A	5	GLY	5.4
1	E	1	GLN	5.4
1	A	4	PRO	5.3
1	E	5	GLY	5.2
1	E	2	ASP	4.9
1	A	326	LYS	4.7
1	C	6	ASN	4.7
2	F	175	GLY	4.4
1	A	1	GLN	4.3
1	E	7	ASP	4.3
1	A	7	ASP	4.2
2	B	175	GLY	4.0
1	A	8	ASN	4.0
1	A	327	GLN	3.9
1	A	328	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	8	ASN	3.9
2	F	58	LYS	3.9
2	D	173	ILE	3.8
1	A	2	ASP	3.8
2	D	58	LYS	3.8
1	E	4	PRO	3.5
1	C	5	GLY	3.5
1	C	2	ASP	3.4
1	C	216	ASN	3.3
1	E	6	ASN	3.3
1	C	8	ASN	3.1
1	E	137	ASN	3.1
2	D	174	LYS	3.1
1	C	143	PRO	3.0
1	C	328	THR	2.9
1	E	54	ASN	2.9
2	B	174	LYS	2.7
1	C	142	GLY	2.6
2	F	168	ASN	2.6
2	B	72	GLU	2.6
1	E	327	GLN	2.6
1	C	4	PRO	2.5
1	A	189	GLN	2.5
1	C	32	ASP	2.5
2	B	29	SER	2.4
1	E	291	ASP	2.3
1	C	3	LEU	2.3
1	C	7	ASP	2.3
1	A	3	LEU	2.2
1	A	222	TRP	2.2
2	B	164	ASP	2.2
1	C	1	GLN	2.1
1	E	328	THR	2.1
1	A	144	GLY	2.1
1	E	143	PRO	2.1
2	B	58	LYS	2.0

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

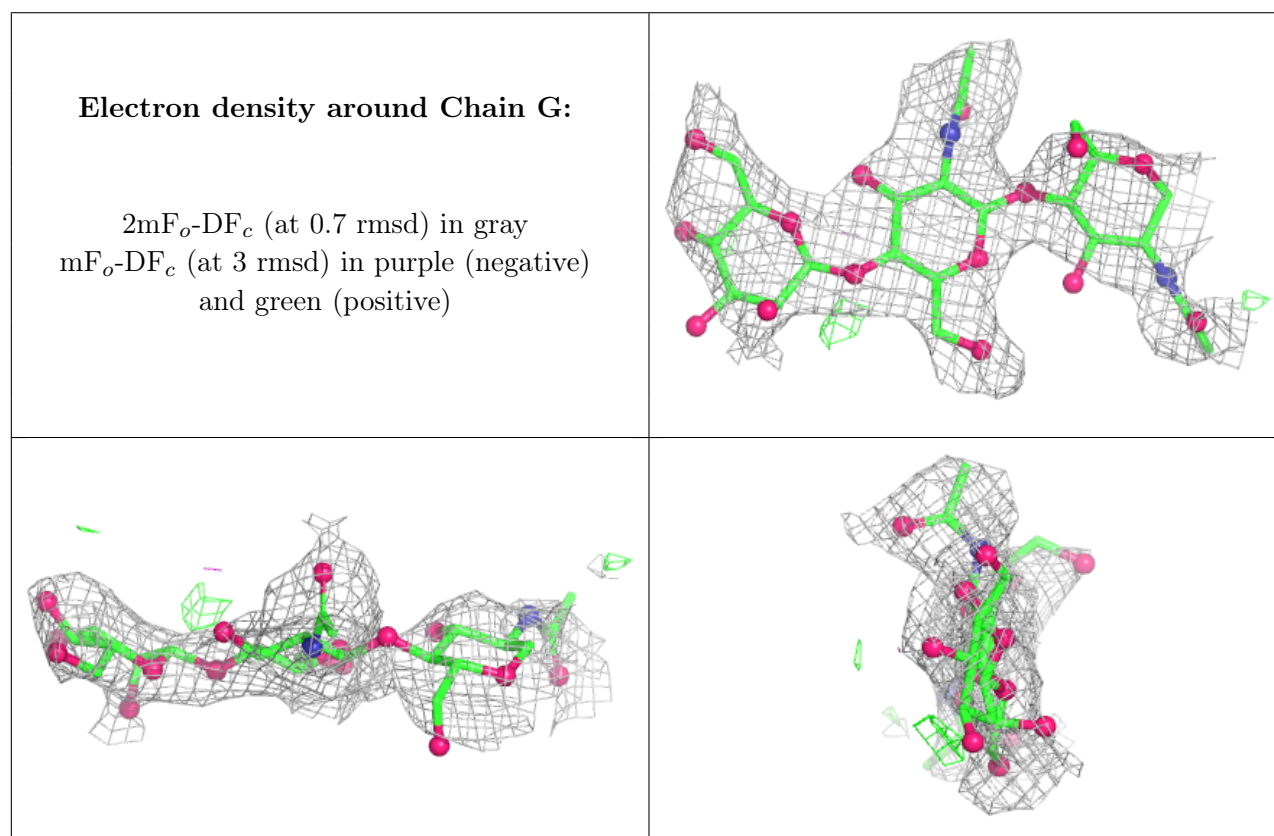
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

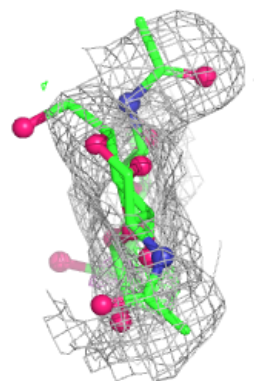
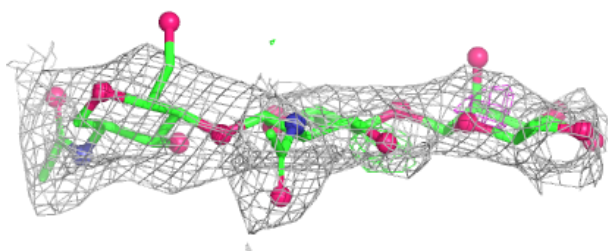
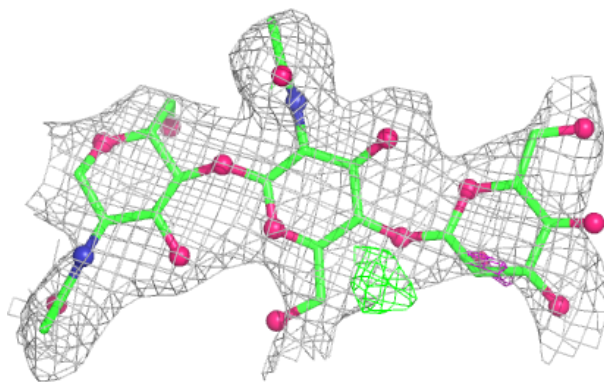
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	H	2	14/15	0.77	0.13	60,61,65,66	0
3	MAN	H	3	11/12	0.84	0.14	69,71,71,71	0
3	NAG	G	2	14/15	0.86	0.10	60,61,64,66	0
3	MAN	G	3	11/12	0.86	0.12	68,69,70,71	0
3	NAG	H	1	14/15	0.89	0.12	51,54,57,57	0
3	MAN	I	3	11/12	0.90	0.12	68,70,71,71	0
3	NAG	G	1	14/15	0.92	0.11	51,55,56,58	0
3	NAG	I	2	14/15	0.94	0.07	60,61,64,66	0
3	NAG	I	1	14/15	0.95	0.09	51,53,55,57	0

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

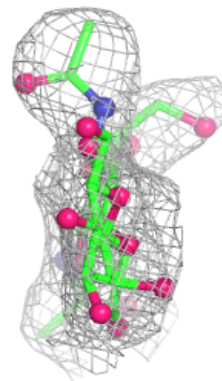
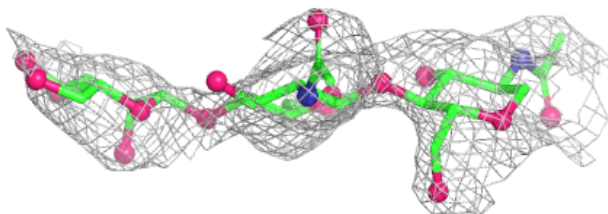
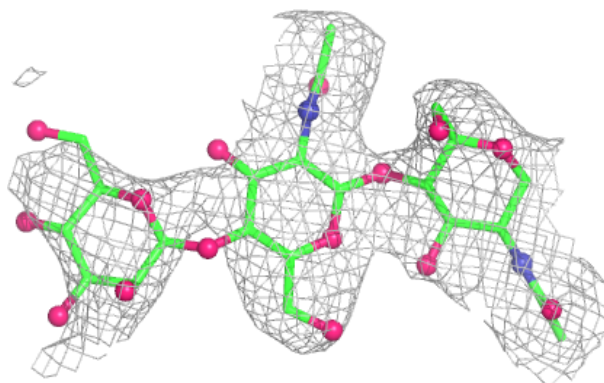


Electron density around Chain H:

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

**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

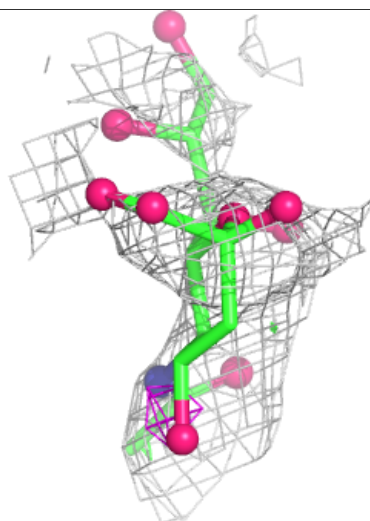
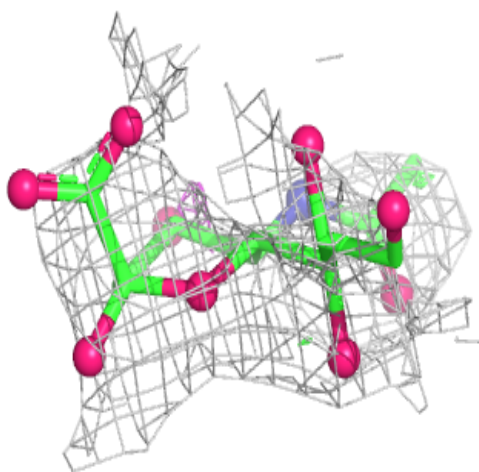
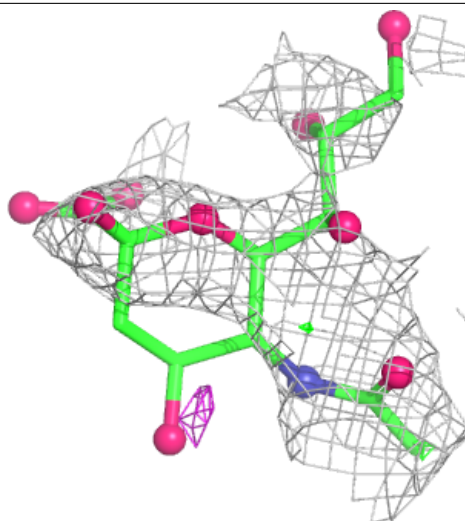
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	330	14/15	0.76	0.20	42,46,47,47	0
5	NAG	B	401	14/15	0.77	0.21	55,58,59,60	0
4	SIA	C	329	21/21	0.78	0.22	35,36,37,38	21
4	SIA	E	329	21/21	0.81	0.17	34,35,36,36	21
5	NAG	E	348	14/15	0.81	0.17	40,43,46,46	0
5	NAG	C	330	14/15	0.82	0.14	42,45,46,46	0
5	NAG	C	334	14/15	0.82	0.13	39,42,43,45	0
5	NAG	F	401	14/15	0.85	0.13	54,57,59,59	0
5	NAG	C	348	14/15	0.86	0.16	40,44,45,46	0
5	NAG	A	348	14/15	0.86	0.12	39,43,45,46	0
5	NAG	A	330	14/15	0.87	0.13	41,45,46,46	0
5	NAG	A	334	14/15	0.87	0.09	39,42,43,44	0
5	NAG	D	401	14/15	0.88	0.16	55,58,59,60	0
4	SIA	A	329	21/21	0.89	0.12	35,36,36,37	21
5	NAG	E	334	14/15	0.92	0.07	39,41,42,44	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.

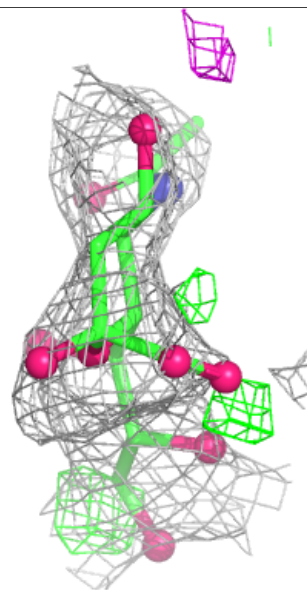
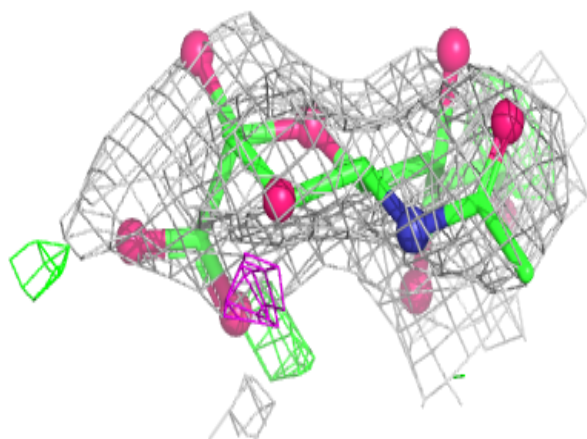
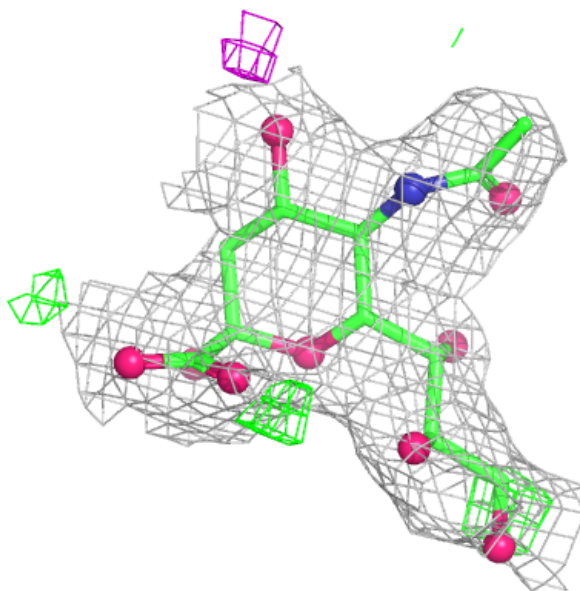
Electron density around SIA C 329:

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



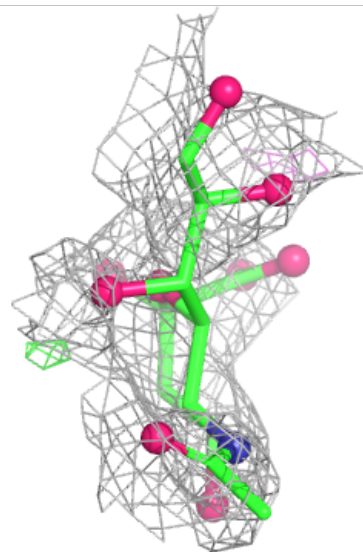
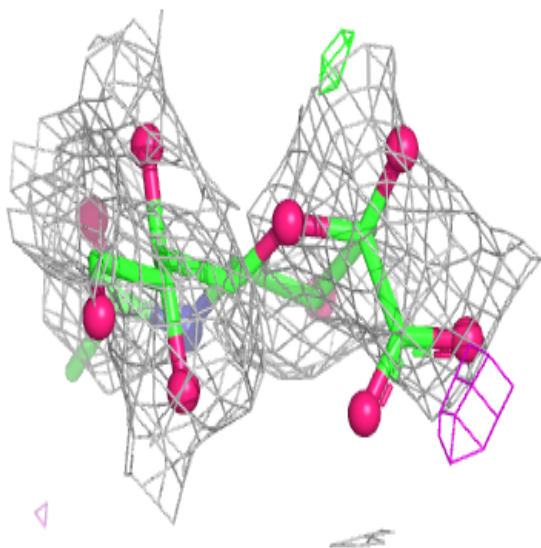
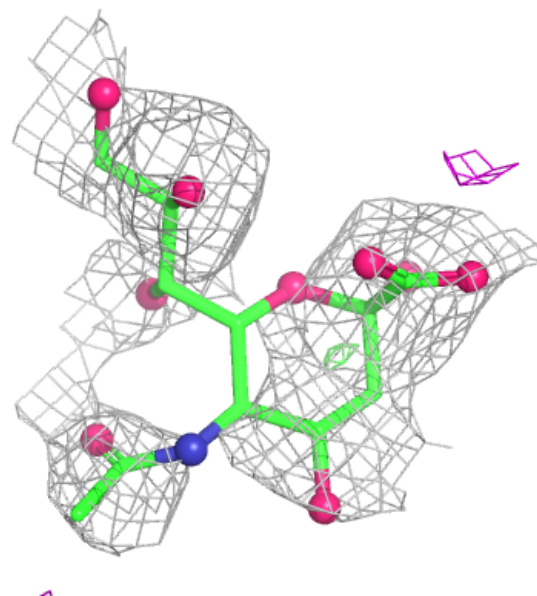
Electron density around SIA E 329:

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



Electron density around SIA A 329:

$2mF_o-DF_c$ (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.