



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 PM UTC

PDB ID : 1HGD / pdb_00001hgd
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
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)

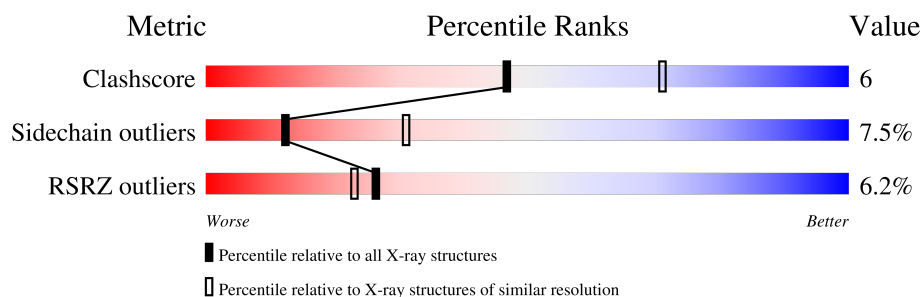
1 Overall quality at a glance

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)
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	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15432 atoms, of which 3195 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
			3132	1585	593	448	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3132	1585	593	448	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3132	1585	593	448	493	13			

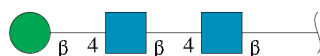
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ARG	GLY	conflict	UNP P03437
C	135	ARG	GLY	conflict	UNP P03437
E	135	ARG	GLY	conflict	UNP P03437

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

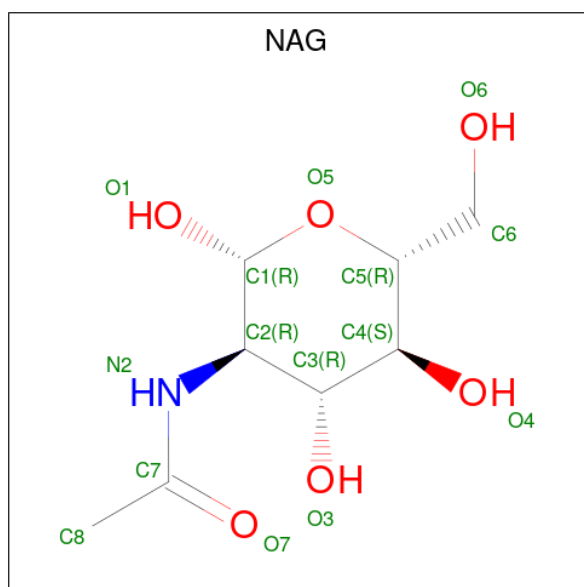
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

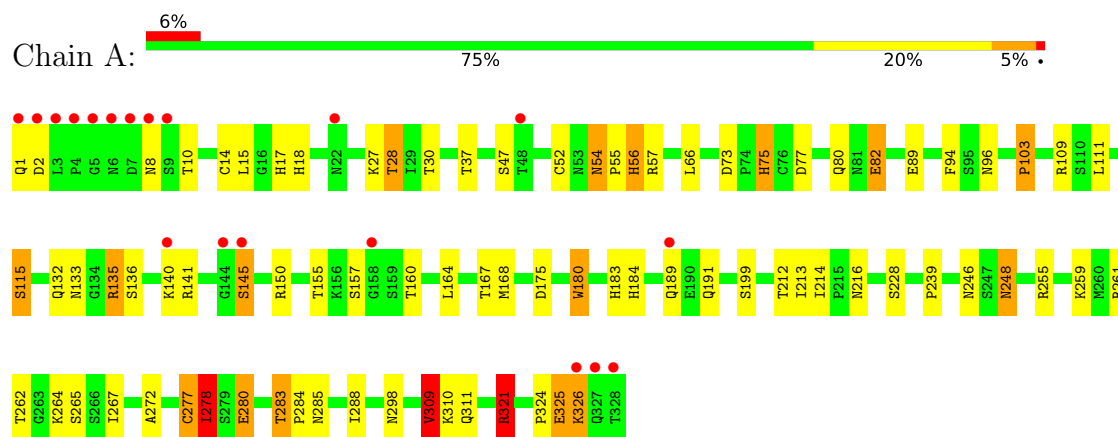
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	12	Total	H	O	0	0
			36	24	12		
5	B	12	Total	H	O	0	0
			36	24	12		
5	C	11	Total	H	O	0	0
			33	22	11		
5	D	13	Total	H	O	0	0
			39	26	13		
5	E	12	Total	H	O	0	0
			36	24	12		
5	F	12	Total	H	O	0	0
			36	24	12		

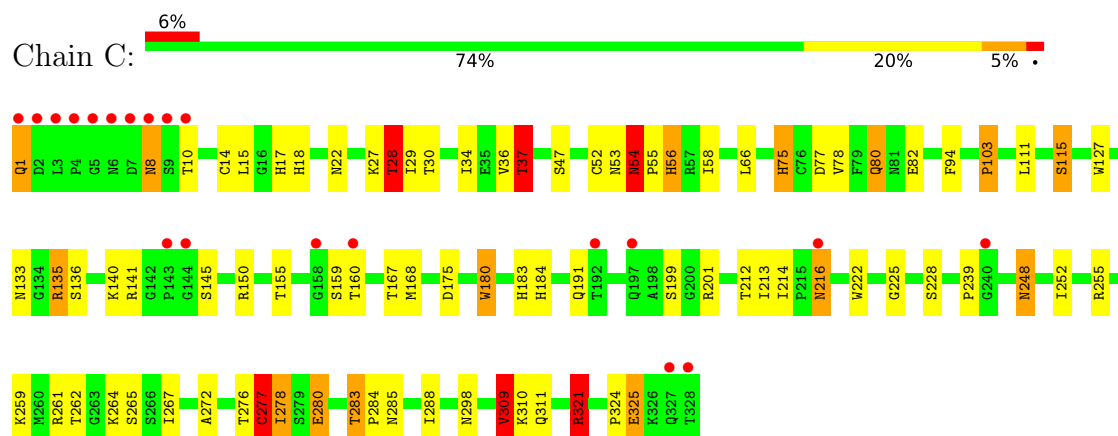
3 Residue-property plots [i](#)

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.

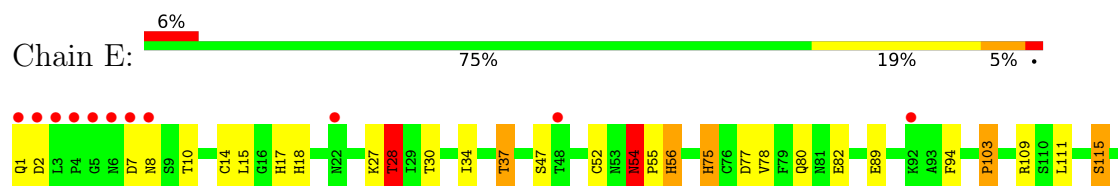
• Molecule 1: HEMAGGLUTININ, CHAIN HA1

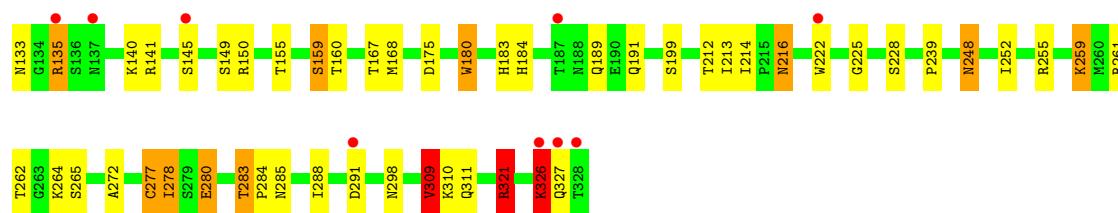


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

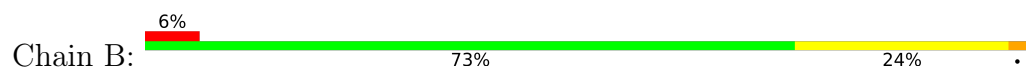


• Molecule 1: HEMAGGLUTININ, CHAIN HA1





• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



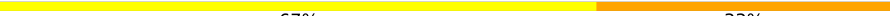
• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• 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:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	163.30Å 163.30Å 176.70Å 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) 58.6 (7.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.70Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , (Not available) 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15432	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 2.53% 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, 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	1.13	14/2596 (0.5%)	1.73	47/3536 (1.3%)
1	C	1.13	12/2596 (0.5%)	1.70	45/3536 (1.3%)
1	E	1.17	13/2596 (0.5%)	1.71	41/3536 (1.2%)
2	B	1.13	9/1445 (0.6%)	1.75	26/1939 (1.3%)
2	D	1.18	10/1445 (0.7%)	1.76	24/1939 (1.2%)
2	F	1.15	8/1445 (0.6%)	1.74	22/1939 (1.1%)
All	All	1.15	66/12123 (0.5%)	1.73	205/16425 (1.2%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	135	ARG	NE-CZ	8.40	1.42	1.33
1	E	56	HIS	CD2-NE2	-7.75	1.29	1.37
1	A	75	HIS	CD2-NE2	-7.37	1.29	1.37
2	F	26	HIS	CD2-NE2	-7.25	1.29	1.37
1	C	56	HIS	CD2-NE2	-7.23	1.29	1.37
1	C	184	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	56	HIS	CD2-NE2	-6.98	1.30	1.37
1	E	183	HIS	CG-ND1	-6.97	1.30	1.38
2	F	159	HIS	CG-ND1	-6.96	1.30	1.38
1	C	18	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.89	1.30	1.37
1	E	184	HIS	CD2-NE2	-6.70	1.30	1.37
1	E	18	HIS	CD2-NE2	-6.65	1.30	1.37
2	B	64	HIS	CG-ND1	-6.60	1.30	1.38
2	B	159	HIS	CG-ND1	-6.56	1.31	1.38
2	B	64	HIS	CD2-NE2	-6.55	1.30	1.37
2	B	26	HIS	CD2-NE2	-6.51	1.30	1.37
2	F	64	HIS	CD2-NE2	-6.50	1.30	1.37
1	E	75	HIS	CD2-NE2	-6.49	1.30	1.37
2	B	159	HIS	CD2-NE2	-6.42	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	HIS	CG-ND1	-6.41	1.31	1.38
1	C	75	HIS	CD2-NE2	-6.29	1.30	1.37
1	E	184	HIS	CG-ND1	-6.19	1.31	1.38
2	D	106	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	18	HIS	CG-ND1	-6.15	1.31	1.38
2	D	64	HIS	CG-ND1	-6.14	1.31	1.38
1	E	183	HIS	CD2-NE2	-6.11	1.31	1.37
1	C	18	HIS	CG-ND1	-6.08	1.31	1.38
1	A	18	HIS	CD2-NE2	-6.05	1.31	1.37
2	D	159	HIS	CG-ND1	-6.05	1.31	1.38
2	D	26	HIS	CD2-NE2	-6.01	1.31	1.37
1	E	280	GLU	CA-CB	-5.99	1.43	1.53
2	F	106	HIS	CD2-NE2	-5.93	1.31	1.37
2	B	106	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	183	HIS	CD2-NE2	-5.90	1.31	1.37
2	F	142	HIS	CD2-NE2	-5.83	1.31	1.37
2	D	159	HIS	CD2-NE2	-5.80	1.31	1.37
2	F	64	HIS	CG-ND1	-5.74	1.31	1.38
2	D	106	HIS	CG-ND1	-5.71	1.31	1.38
1	A	17	HIS	CD2-NE2	-5.68	1.31	1.37
2	F	26	HIS	CG-ND1	-5.67	1.32	1.38
2	B	26	HIS	CG-ND1	-5.66	1.32	1.38
2	D	64	HIS	CD2-NE2	-5.64	1.31	1.37
1	E	17	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	183	HIS	CG-ND1	-5.59	1.32	1.38
2	F	159	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	280	GLU	CA-CB	-5.49	1.44	1.53
1	A	280	GLU	CA-CB	-5.48	1.44	1.53
1	C	17	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	135	ARG	NE-CZ	5.47	1.39	1.33
1	A	56	HIS	CG-ND1	-5.40	1.32	1.38
1	C	183	HIS	CD2-NE2	-5.40	1.31	1.37
1	E	17	HIS	CG-ND1	-5.40	1.32	1.38
1	A	135	ARG	NE-CZ	5.38	1.39	1.33
2	D	142	HIS	CD2-NE2	-5.36	1.31	1.37
1	C	17	HIS	CG-ND1	-5.36	1.32	1.38
1	A	183	HIS	CG-ND1	-5.36	1.32	1.38
2	D	26	HIS	CG-ND1	-5.34	1.32	1.38
2	B	142	HIS	CG-ND1	-5.28	1.32	1.38
1	A	326	LYS	CA-CB	5.26	1.62	1.53
1	E	56	HIS	CG-ND1	-5.26	1.32	1.38
2	D	87	THR	CA-CB	5.25	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	HIS	CG-ND1	-5.15	1.32	1.38
1	A	184	HIS	CG-ND1	-5.06	1.32	1.38
1	A	278	ILE	CA-CB	5.02	1.60	1.54
2	B	87	THR	CA-CB	5.02	1.61	1.53

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	HIS	CA-CB-CG	8.96	122.76	113.80
2	D	169	ASN	CA-CB-CG	8.81	121.41	112.60
1	E	56	HIS	ND1-CG-CD2	8.81	114.91	106.10
1	A	75	HIS	CA-CB-CG	8.71	122.51	113.80
2	B	169	ASN	CA-CB-CG	8.53	121.13	112.60
1	C	56	HIS	ND1-CG-CD2	8.50	114.60	106.10
2	F	169	ASN	CA-CB-CG	8.36	120.96	112.60
2	D	64	HIS	ND1-CG-CD2	8.36	114.46	106.10
2	B	57	GLU	CA-CB-CG	8.23	130.57	114.10
2	B	79	ASP	CA-CB-CG	8.20	120.80	112.60
2	D	57	GLU	CA-CB-CG	8.12	130.35	114.10
1	E	326	LYS	CA-CB-CG	8.06	130.21	114.10
2	F	79	ASP	CA-CB-CG	8.02	120.62	112.60
2	F	57	GLU	CA-CB-CG	7.96	130.03	114.10
1	C	191	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	A	184	HIS	ND1-CG-CD2	7.85	113.95	106.10
1	C	75	HIS	CA-CB-CG	7.85	121.65	113.80
2	D	9	PHE	CA-CB-CG	7.79	121.59	113.80
1	A	56	HIS	ND1-CG-CD2	7.78	113.88	106.10
1	C	184	HIS	ND1-CG-CD2	7.78	113.88	106.10
2	D	106	HIS	ND1-CG-CD2	7.75	113.85	106.10
2	F	9	PHE	CA-CB-CG	7.74	121.54	113.80
2	B	64	HIS	ND1-CG-CD2	7.71	113.81	106.10
2	F	106	HIS	ND1-CG-CD2	7.68	113.78	106.10
2	D	79	ASP	CA-CB-CG	7.64	120.25	112.60
2	B	150	GLU	CB-CG-CD	7.61	125.54	112.60
2	B	159	HIS	ND1-CG-CD2	7.61	113.71	106.10
1	E	184	HIS	ND1-CG-CD2	7.56	113.66	106.10
2	D	26	HIS	ND1-CG-CD2	7.53	113.63	106.10
2	B	106	HIS	ND1-CG-CD2	7.49	113.59	106.10
2	F	26	HIS	ND1-CG-CD2	7.33	113.42	106.10
1	A	325	GLU	CA-CB-CG	7.25	128.60	114.10
2	B	9	PHE	CA-CB-CG	7.16	120.95	113.80
2	F	64	HIS	ND1-CG-CD2	7.14	113.24	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	159	HIS	ND1-CG-CD2	6.94	113.04	106.10
1	E	191	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	C	18	HIS	ND1-CG-CD2	6.88	112.98	106.10
1	E	183	HIS	ND1-CG-CD2	6.83	112.92	106.10
1	A	1	GLN	N-CA-C	-6.82	91.92	111.00
2	B	26	HIS	ND1-CG-CD2	6.81	112.91	106.10
2	B	172	GLN	OE1-CD-NE2	-6.81	115.79	122.60
2	F	172	GLN	OE1-CD-NE2	-6.80	115.80	122.60
2	D	172	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	C	37	THR	CA-CB-OG1	-6.71	99.54	109.60
1	A	18	HIS	ND1-CG-CD2	6.67	112.78	106.10
1	A	183	HIS	ND1-CG-CD2	6.67	112.77	106.10
1	C	248	ASN	N-CA-CB	-6.65	98.93	111.43
1	E	18	HIS	ND1-CG-CD2	6.65	112.75	106.10
2	D	11	GLU	CA-CB-CG	-6.60	100.91	114.10
1	E	37	THR	CA-CB-OG1	-6.58	99.72	109.60
1	C	183	HIS	ND1-CG-CD2	6.49	112.59	106.10
2	B	146	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	E	272	ALA	CA-C-N	6.44	126.20	119.76
1	E	272	ALA	C-N-CA	6.44	126.20	119.76
1	A	324	PRO	O-C-N	6.40	130.94	123.01
1	E	56	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	272	ALA	CA-C-N	6.36	126.12	119.76
1	C	272	ALA	C-N-CA	6.36	126.12	119.76
2	B	90	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	248	ASN	N-CA-CB	-6.34	99.50	111.43
1	A	115	SER	N-CA-C	-6.33	104.47	111.36
2	D	159	HIS	ND1-CG-CD2	6.31	112.41	106.10
1	A	111	LEU	N-CA-CB	-6.30	100.85	110.12
1	A	2	ASP	CA-CB-CG	6.27	118.87	112.60
1	C	111	LEU	N-CA-CB	-6.26	100.92	110.12
1	C	56	HIS	CB-CG-CD2	-6.26	123.06	131.20
2	F	90	ASP	CA-CB-CG	6.17	118.77	112.60
2	D	132	GLU	CA-CB-CG	-6.15	101.79	114.10
1	A	37	THR	CA-CB-OG1	-6.15	100.38	109.60
1	E	248	ASN	N-CA-CB	-6.14	99.88	111.43
1	A	56	HIS	CB-CG-CD2	-6.11	123.26	131.20
2	F	132	GLU	CA-CB-CG	-6.09	101.91	114.10
2	B	132	GLU	CA-CB-CG	-6.07	101.95	114.10
2	D	11	GLU	N-CA-C	6.06	118.67	111.33
1	A	325	GLU	N-CA-CB	-6.02	103.42	110.35
1	E	103	PRO	CA-C-N	-6.01	114.91	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	PRO	C-N-CA	-6.01	114.91	123.20
1	E	321	ARG	NE-CZ-NH2	-6.01	113.79	119.20
2	D	26	HIS	CG-CD2-NE2	-5.97	101.22	107.20
2	D	125	GLN	CG-CD-NE2	5.95	125.33	116.40
1	A	272	ALA	CA-C-N	5.95	125.70	119.76
1	A	272	ALA	C-N-CA	5.95	125.70	119.76
2	F	51	LYS	N-CA-CB	-5.94	101.40	110.01
1	E	28	THR	N-CA-CB	-5.94	102.18	111.56
1	C	321	ARG	NE-CZ-NH2	-5.91	113.89	119.20
2	B	125	GLN	CG-CD-NE2	5.90	125.25	116.40
1	A	28	THR	N-CA-CB	-5.88	102.28	111.56
1	E	56	HIS	CG-CD2-NE2	-5.86	101.34	107.20
1	A	191	GLN	OE1-CD-NE2	-5.85	116.75	122.60
2	D	64	HIS	CG-CD2-NE2	-5.84	101.36	107.20
1	E	1	GLN	N-CA-C	-5.83	94.67	111.00
1	C	1	GLN	N-CA-C	-5.81	94.73	111.00
2	D	135	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	E	111	LEU	N-CA-CB	-5.80	101.60	110.12
1	E	180	TRP	CG-CD2-CE3	5.80	139.70	133.90
1	A	8	ASN	CA-C-N	-5.79	112.56	123.27
1	A	8	ASN	C-N-CA	-5.79	112.56	123.27
2	B	168	ASN	CA-CB-CG	-5.79	106.81	112.60
1	E	248	ASN	CA-CB-CG	5.78	118.38	112.60
2	B	26	HIS	CG-CD2-NE2	-5.78	101.42	107.20
1	C	28	THR	N-CA-CB	-5.78	102.44	111.56
1	E	168	MET	CA-C-N	5.75	125.50	119.76
1	E	168	MET	C-N-CA	5.75	125.50	119.76
1	C	168	MET	CA-C-N	5.74	125.50	119.76
1	C	168	MET	C-N-CA	5.74	125.50	119.76
2	D	160	ASP	CA-CB-CG	-5.70	106.90	112.60
1	C	325	GLU	CB-CG-CD	5.68	122.25	112.60
1	C	115	SER	N-CA-C	-5.67	105.18	111.36
2	F	160	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	325	GLU	N-CA-C	-5.65	103.53	110.65
1	E	309	VAL	N-CA-CB	-5.65	101.36	111.92
1	C	324	PRO	O-C-N	-5.64	116.08	122.91
1	A	168	MET	CA-C-N	5.63	125.39	119.76
1	A	168	MET	C-N-CA	5.63	125.39	119.76
2	F	58	LYS	N-CA-C	5.58	122.69	110.80
1	A	321	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	E	115	SER	N-CA-C	-5.56	105.30	111.36
2	F	124	ARG	CG-CD-NE	-5.56	99.77	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASN	N-CA-CB	-5.55	103.03	111.19
1	A	54	ASN	O-C-N	-5.54	117.52	121.84
2	D	90	ASP	CA-CB-CG	5.53	118.13	112.60
2	D	124	ARG	CG-CD-NE	-5.53	99.83	112.00
2	F	11	GLU	N-CA-C	5.51	117.72	111.11
2	D	58	LYS	N-CA-C	5.50	122.52	110.80
1	A	103	PRO	CA-C-N	-5.50	115.61	123.20
1	A	103	PRO	C-N-CA	-5.50	115.61	123.20
2	F	26	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	F	168	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	262	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	103	PRO	CA-C-N	-5.48	115.64	123.20
1	C	103	PRO	C-N-CA	-5.48	115.64	123.20
2	D	168	ASN	CA-CB-CG	-5.43	107.17	112.60
1	C	54	ASN	O-C-N	-5.42	117.61	121.84
1	E	54	ASN	CA-CB-CG	-5.42	107.18	112.60
2	B	160	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	54	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	248	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	326	LYS	CA-CB-CG	5.39	124.88	114.10
1	A	180	TRP	CG-CD2-CE3	5.39	139.29	133.90
2	B	11	GLU	N-CA-C	5.39	117.58	111.11
2	B	58	LYS	N-CA-C	5.38	122.26	110.80
1	C	309	VAL	N-CA-CB	-5.37	101.88	111.92
2	F	3	PHE	CA-CB-CG	-5.36	108.44	113.80
1	E	262	THR	CA-CB-OG1	-5.35	101.57	109.60
1	C	262	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	184	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	E	28	THR	CA-CB-CG2	5.34	119.58	110.50
1	E	214	ILE	CA-C-N	5.33	125.32	120.21
1	E	214	ILE	C-N-CA	5.33	125.32	120.21
2	D	127	ARG	N-CA-C	5.32	116.39	108.31
1	C	216	ASN	CA-CB-CG	5.31	117.91	112.60
1	E	216	ASN	CA-CB-CG	5.31	117.91	112.60
1	C	56	HIS	CG-CD2-NE2	-5.31	101.89	107.20
1	C	37	THR	CA-CB-CG2	5.30	119.52	110.50
2	D	125	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	C	8	ASN	CA-C-O	5.28	126.82	120.27
1	C	82	GLU	N-CA-CB	-5.28	102.42	110.45
1	A	309	VAL	N-CA-CB	-5.27	102.06	111.92
2	D	104	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	C	277	CYS	CA-C-N	-5.25	115.40	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	CYS	C-N-CA	-5.25	115.40	122.91
1	A	321	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	C	180	TRP	CG-CD2-CE3	5.21	139.12	133.90
1	C	214	ILE	CA-C-N	5.21	125.22	120.21
1	C	214	ILE	C-N-CA	5.21	125.22	120.21
2	B	51	LYS	N-CA-CB	-5.21	102.46	110.01
1	A	180	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	214	ILE	CA-C-N	5.20	125.20	120.21
1	A	214	ILE	C-N-CA	5.20	125.20	120.21
1	C	252	ILE	N-CA-C	-5.20	99.47	106.85
1	C	184	HIS	CG-CD2-NE2	-5.19	102.01	107.20
1	E	37	THR	CA-CB-CG2	5.19	119.32	110.50
1	E	180	TRP	CE2-CD2-CG	-5.19	100.98	107.20
1	E	252	ILE	N-CA-C	-5.19	99.49	106.85
1	E	159	SER	CA-CB-OG	-5.18	100.74	111.10
2	B	124	ARG	CG-CD-NE	-5.17	100.63	112.00
2	F	63	PHE	CA-CB-CG	-5.16	108.64	113.80
1	C	36	VAL	CA-C-N	5.14	127.43	120.38
1	C	36	VAL	C-N-CA	5.14	127.43	120.38
1	A	310	LYS	CB-CG-CD	5.14	123.13	111.30
2	B	127	ARG	CG-CD-NE	-5.13	100.70	112.00
1	A	184	HIS	CG-CD2-NE2	-5.12	102.08	107.20
1	C	310	LYS	CB-CG-CD	5.12	123.08	111.30
2	B	76	ARG	N-CA-C	5.12	117.25	111.11
2	F	127	ARG	CG-CD-NE	-5.11	100.75	112.00
2	B	159	HIS	CG-CD2-NE2	-5.11	102.09	107.20
1	A	28	THR	CA-CB-CG2	5.11	119.18	110.50
1	C	54	ASN	CA-CB-CG	-5.10	107.50	112.60
2	B	54	ARG	CA-CB-CG	5.10	124.31	114.10
1	C	80	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	E	75	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	56	HIS	CG-CD2-NE2	-5.10	102.10	107.20
1	A	132	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	E	7	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	73	ASP	CA-C-N	5.06	124.50	119.24
1	A	73	ASP	C-N-CA	5.06	124.50	119.24
1	E	184	HIS	CG-CD2-NE2	-5.06	102.14	107.20
2	B	107	THR	CA-CB-OG1	-5.05	102.03	109.60
1	E	310	LYS	CB-CG-CD	5.04	122.89	111.30
2	F	159	HIS	CG-CD2-NE2	-5.03	102.17	107.20
1	E	183	HIS	CG-CD2-NE2	-5.02	102.18	107.20
1	E	291	ASP	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	HIS	CA-CB-CG	5.01	118.81	113.80
1	C	22	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	127	TRP	CE2-CD2-CG	-5.01	101.19	107.20

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	2539	593	2483	32	0
1	C	2539	593	2483	36	0
1	E	2539	593	2483	32	0
2	B	1421	331	1345	20	0
2	D	1421	331	1345	25	0
2	F	1421	331	1345	24	0
3	G	39	37	34	1	0
3	H	39	37	34	1	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	12	24	0	0	0
5	B	12	24	0	1	0
5	C	11	22	0	1	0
5	D	13	26	0	1	0
5	E	12	24	0	0	0
5	F	12	24	0	1	0
All	All	12237	3195	11742	137	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 (137) 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:321:ARG:HH11	1:C:321:ARG:HG2	1.47	0.79
2:D:28:ASN:HB2	2:D:144:CYS:O	1.83	0.78
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.50	0.77
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.48	0.76
2:D:83:TYR:O	2:D:87:THR:HG23	1.87	0.75
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.70	0.74
2:B:83:TYR:O	2:B:87:THR:HG23	1.88	0.73
2:F:83:TYR:O	2:F:87:THR:HG23	1.87	0.73
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.72	0.71
2:B:58:LYS:HE2	2:B:59:THR:O	1.91	0.69
2:D:58:LYS:HE2	2:D:59:THR:O	1.93	0.68
2:F:58:LYS:HE2	2:F:59:THR:O	1.92	0.68
2:B:132:GLU:HG2	2:B:134:GLY:H	1.58	0.68
2:D:132:GLU:HG2	2:D:134:GLY:H	1.59	0.67
2:F:132:GLU:HG2	2:F:134:GLY:H	1.58	0.67
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.76	0.66
5:B:413:HOH:O	2:F:87:THR:HG22	1.98	0.64
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.82	0.61
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.82	0.61
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.82	0.60
2:B:87:THR:HG22	5:D:402:HOH:O	2.02	0.60
1:A:52:CYS:HB3	1:A:277:CYS:O	2.02	0.59
2:D:87:THR:HG22	5:F:403:HOH:O	2.00	0.59
1:E:52:CYS:HB3	1:E:277:CYS:O	2.02	0.59
1:C:52:CYS:HB3	1:C:277:CYS:O	2.03	0.58
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.86	0.58
2:B:141:TYR:O	2:B:166:ALA:HA	2.05	0.57
2:D:141:TYR:O	2:D:166:ALA:HA	2.04	0.56
1:C:53:ASN:OD1	1:C:276:THR:HA	2.05	0.56
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.87	0.56
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.88	0.56
1:E:283:THR:HG22	1:E:285:ASN:H	1.71	0.56
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.06	0.55
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.06	0.55
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.89	0.55
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.89	0.55
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.87	0.55
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.89	0.55
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.89	0.54
2:F:141:TYR:O	2:F:166:ALA:HA	2.08	0.54
1:A:283:THR:HG22	1:A:285:ASN:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.08	0.53
1:C:283:THR:HG22	1:C:285:ASN:H	1.73	0.53
1:A:325:GLU:HB2	2:B:13:GLY:O	2.09	0.52
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.25	0.52
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.92	0.51
1:A:10:THR:HG22	2:B:141:TYR:HA	1.93	0.51
1:C:77:ASP:O	1:C:80:GLN:HG3	2.11	0.50
1:E:77:ASP:O	1:E:80:GLN:HG3	2.11	0.50
1:E:47:SER:HA	1:E:288:ILE:HG22	1.93	0.50
1:A:167:THR:HB	3:G:1:NAG:H62	1.94	0.50
1:E:10:THR:HG22	2:F:141:TYR:HA	1.92	0.49
1:E:326:LYS:HD2	1:E:327:GLN:H	1.77	0.49
1:A:75:HIS:HE1	1:A:94:PHE:O	1.94	0.49
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.28	0.49
1:E:167:THR:HB	3:I:1:NAG:H62	1.95	0.49
1:C:28:THR:HG22	1:C:30:THR:H	1.78	0.49
1:C:75:HIS:HE1	1:C:94:PHE:O	1.95	0.48
1:A:47:SER:HA	1:A:288:ILE:HG22	1.94	0.48
1:C:10:THR:HG22	2:D:141:TYR:HA	1.94	0.48
1:C:47:SER:HA	1:C:288:ILE:HG22	1.94	0.48
1:E:28:THR:HG22	1:E:30:THR:H	1.79	0.48
1:A:28:THR:HG22	1:A:30:THR:H	1.78	0.48
1:E:75:HIS:HE1	1:E:94:PHE:O	1.97	0.48
1:C:135:ARG:HG3	1:C:145:SER:HB2	1.96	0.48
1:A:77:ASP:O	1:A:80:GLN:HG3	2.13	0.48
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.62	0.47
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.63	0.47
1:C:167:THR:HB	3:H:1:NAG:H62	1.95	0.47
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.97	0.47
1:A:135:ARG:HG3	1:A:145:SER:HB2	1.97	0.46
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.63	0.46
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.31	0.46
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.45
2:F:127:ARG:HB3	2:F:128:GLU:H	1.67	0.45
2:B:54:ARG:NH2	1:E:27:LYS:HD3	2.30	0.45
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.81	0.45
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.98	0.45
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.82	0.45
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.82	0.44
2:B:127:ARG:HB3	2:B:128:GLU:H	1.66	0.44
2:D:91:LEU:HD13	2:F:91:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ASN:O	1:E:278:ILE:HA	2.18	0.44
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.17	0.44
1:C:27:LYS:HD3	2:F:54:ARG:NH2	2.33	0.44
2:B:132:GLU:CD	2:D:124:ARG:HE	2.26	0.44
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.18	0.43
1:A:66:LEU:HD22	1:A:267:ILE:HD12	2.01	0.43
2:D:135:ASN:OD1	2:D:135:ASN:N	2.52	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.01	0.43
1:C:135:ARG:NH1	1:C:145:SER:O	2.52	0.43
1:C:325:GLU:O	1:C:325:GLU:HG2	2.19	0.43
2:F:20:GLY:HA3	2:F:36:ALA:HB1	2.00	0.43
2:B:114:GLU:OE2	2:B:117:LYS:NZ	2.52	0.43
1:A:54:ASN:O	1:A:278:ILE:HA	2.19	0.42
1:C:66:LEU:HD22	1:C:267:ILE:HD12	2.01	0.42
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.69	0.42
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.19	0.42
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.17	0.42
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.52	0.42
2:D:26:HIS:ND1	2:D:149:ILE:HG21	2.35	0.42
1:C:115:SER:O	1:C:261:ARG:HG3	2.19	0.42
1:A:136:SER:C	1:A:145:SER:HB3	2.45	0.42
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.19	0.42
1:A:27:LYS:HD3	2:D:54:ARG:NH2	2.34	0.42
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.53	0.42
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.52	0.42
1:A:14:CYS:HA	2:B:137:CYS:HA	2.02	0.41
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.20	0.41
1:C:54:ASN:O	1:C:278:ILE:HA	2.20	0.41
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.35	0.41
1:C:15:LEU:HD23	2:D:118:LEU:HG	2.03	0.41
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.52	0.41
2:D:20:GLY:HA3	2:D:36:ALA:HB1	2.02	0.41
1:E:115:SER:O	1:E:261:ARG:HG3	2.20	0.41
1:C:37:THR:HG21	5:C:352:HOH:O	2.21	0.41
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.41
1:A:164:LEU:O	1:A:246:ASN:HA	2.20	0.41
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.52	0.41
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.54	0.41
1:C:136:SER:C	1:C:145:SER:HB3	2.45	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:ARG:HB3	2:D:128:GLU:H	1.65	0.41
2:D:174:LYS:HZ3	2:F:164:ASP:CG	2.28	0.41
1:C:29:ILE:HB	2:D:105:GLN:OE1	2.21	0.41
1:C:284:PRO:HG2	1:C:298:ASN:ND2	2.36	0.41
1:E:135:ARG:HG3	1:E:145:SER:HB2	2.02	0.41
1:E:326:LYS:HD2	1:E:327:GLN:N	2.36	0.41
1:C:201:ARG:HH11	1:C:201:ARG:HD3	1.79	0.40
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.56	0.40
2:F:26:HIS:O	2:F:32:THR:HA	2.20	0.40
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.56	0.40
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.54	0.40
1:A:115:SER:O	1:A:261:ARG:HG3	2.22	0.40
1:A:284:PRO:HG2	1:A:298:ASN:ND2	2.36	0.40
2:B:20:GLY:HA3	2:B:36:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/290 (82%)	216 (91%)	22 (9%)	8	22
1	C	290/290 (100%)	265 (91%)	25 (9%)	10	25
1	E	290/290 (100%)	261 (90%)	29 (10%)	7	19
2	B	149/149 (100%)	143 (96%)	6 (4%)	28	56
2	D	149/149 (100%)	143 (96%)	6 (4%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	149/149 (100%)	142 (95%)	7 (5%)	23	51
All	All	1265/1317 (96%)	1170 (92%)	95 (8%)	12	31

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

Mol	Chain	Res	Type
1	A	82	GLU
1	A	103	PRO
1	A	140	LYS
1	A	141	ARG
1	A	145	SER
1	A	150	ARG
1	A	155	THR
1	A	157	SER
1	A	160	THR
1	A	189	GLN
1	A	199	SER
1	A	228	SER
1	A	248	ASN
1	A	259	LYS
1	A	265	SER
1	A	277	CYS
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	30	GLU
2	B	52	LEU
2	B	87	THR
2	B	110	LEU
2	B	127	ARG
2	B	160	ASP
1	C	8	ASN
1	C	28	THR
1	C	34	ILE
1	C	37	THR
1	C	54	ASN
1	C	58	ILE
1	C	78	VAL
1	C	103	PRO

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Mol	Chain	Res	Type
1	C	140	LYS
1	C	141	ARG
1	C	150	ARG
1	C	155	THR
1	C	159	SER
1	C	160	THR
1	C	199	SER
1	C	228	SER
1	C	248	ASN
1	C	259	LYS
1	C	265	SER
1	C	277	CYS
1	C	278	ILE
1	C	280	GLU
1	C	283	THR
1	C	309	VAL
1	C	321	ARG
2	D	52	LEU
2	D	87	THR
2	D	110	LEU
2	D	127	ARG
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	54	ASN
1	E	78	VAL
1	E	82	GLU
1	E	103	PRO
1	E	140	LYS
1	E	141	ARG
1	E	149	SER
1	E	150	ARG
1	E	155	THR
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	199	SER
1	E	228	SER

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Mol	Chain	Res	Type
1	E	248	ASN
1	E	259	LYS
1	E	265	SER
1	E	277	CYS
1	E	278	ILE
1	E	280	GLU
1	E	283	THR
1	E	309	VAL
1	E	321	ARG
1	E	326	LYS
2	F	11	GLU
2	F	52	LEU
2	F	87	THR
2	F	110	LEU
2	F	127	ARG
2	F	150	GLU
2	F	160	ASP

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

Mol	Chain	Res	Type
1	A	132	GLN
1	A	171	ASN
1	A	216	ASN
2	B	27	GLN
1	C	132	GLN
1	C	171	ASN
2	D	28	ASN
2	D	49	ASN
1	E	96	ASN
1	E	132	GLN
1	E	171	ASN
1	E	189	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	3,1	14,14,15	0.60	0	17,19,21	0.77	0
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	1.19	1 (5%)
3	BMA	G	3	3	11,11,12	0.55	0	15,15,17	1.16	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.89	1 (7%)	17,19,21	0.87	0
3	NAG	H	2	3	14,14,15	0.50	0	17,19,21	1.17	1 (5%)
3	BMA	H	3	3	11,11,12	0.51	0	15,15,17	1.25	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.62	0	17,19,21	0.87	0
3	NAG	I	2	3	14,14,15	0.44	0	17,19,21	1.09	1 (5%)
3	BMA	I	3	3	11,11,12	0.76	0	15,15,17	0.86	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	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	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	3,1	-	1/6/23/26	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	H	1	NAG	O5-C1	-2.15	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C4-C3-C2	-2.94	106.70	111.02
3	H	3	BMA	C1-O5-C5	2.94	116.13	112.19
3	G	3	BMA	C1-O5-C5	2.67	115.77	112.19
3	H	2	NAG	C4-C3-C2	-2.66	107.12	111.02
3	I	2	NAG	C4-C3-C2	-2.61	107.20	111.02
3	H	3	BMA	C6-C5-C4	-2.56	106.74	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

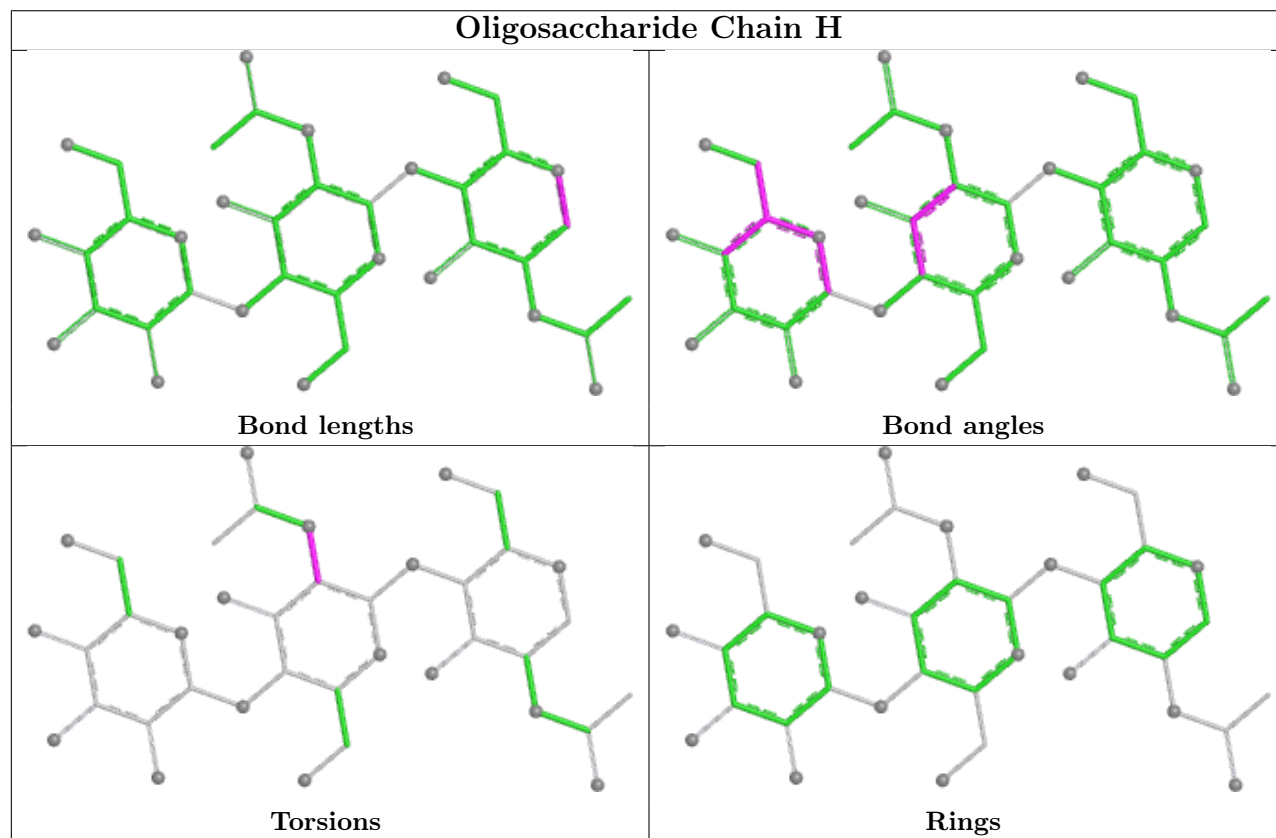
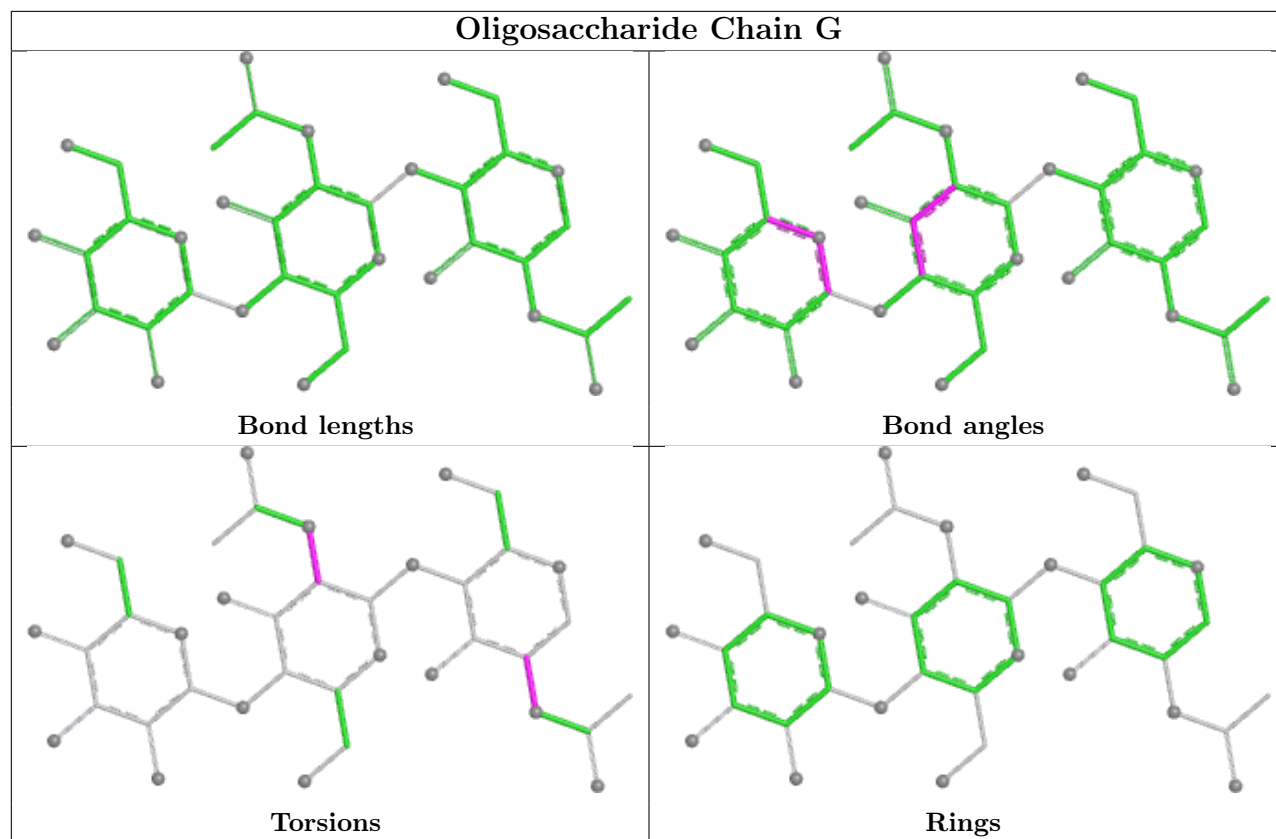
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7

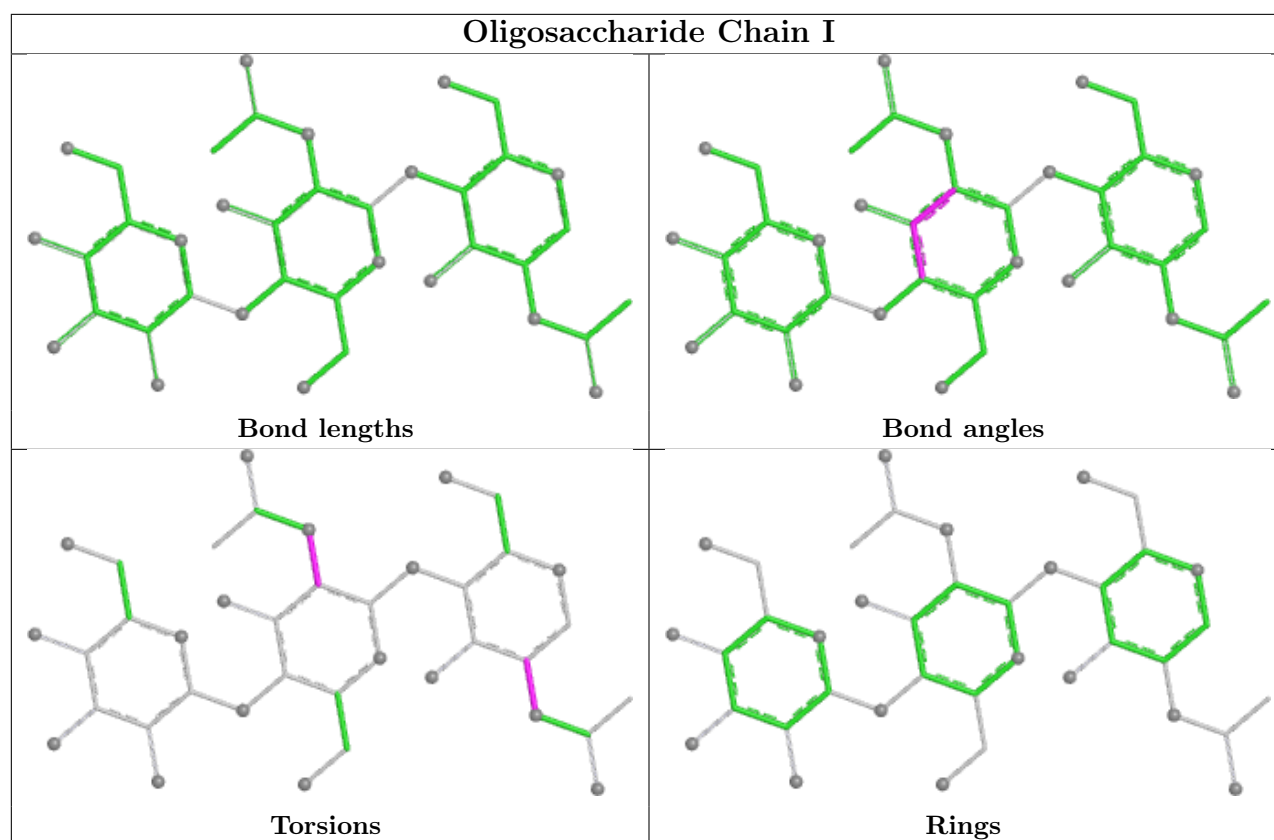
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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](#)

12 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	0.78	0	17,19,21	1.24	3 (17%)
4	NAG	F	401	2	14,14,15	0.74	0	17,19,21	1.39	1 (5%)
4	NAG	B	401	2	14,14,15	0.67	0	17,19,21	1.35	1 (5%)
4	NAG	C	329	1	14,14,15	0.72	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	E	329	1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
4	NAG	D	401	2	14,14,15	0.72	0	17,19,21	1.38	1 (5%)
4	NAG	E	348	1	14,14,15	0.63	0	17,19,21	1.60	3 (17%)
4	NAG	A	329	1	14,14,15	0.78	1 (7%)	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	348	1	14,14,15	0.68	0	17,19,21	1.63	4 (23%)
4	NAG	A	334	1	14,14,15	0.86	0	17,19,21	1.22	1 (5%)
4	NAG	A	348	1	14,14,15	0.60	0	17,19,21	1.60	4 (23%)
4	NAG	E	334	1	14,14,15	0.80	0	17,19,21	1.17	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
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	F	401	2	-	0/6/23/26	0/1/1/1
4	NAG	B	401	2	-	0/6/23/26	0/1/1/1
4	NAG	C	329	1	-	0/6/23/26	0/1/1/1
4	NAG	E	329	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	NAG	E	348	1	-	2/6/23/26	0/1/1/1
4	NAG	A	329	1	-	0/6/23/26	0/1/1/1
4	NAG	C	348	1	-	2/6/23/26	0/1/1/1
4	NAG	A	334	1	-	0/6/23/26	0/1/1/1
4	NAG	A	348	1	-	2/6/23/26	0/1/1/1
4	NAG	E	334	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	329	NAG	C4-C5	2.29	1.57	1.53
4	C	329	NAG	C4-C5	2.21	1.57	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	NAG	C1-O5-C5	4.41	118.10	112.19
4	D	401	NAG	C1-O5-C5	4.29	117.94	112.19
4	B	401	NAG	C1-O5-C5	4.04	117.60	112.19
4	A	348	NAG	C1-O5-C5	4.02	117.57	112.19
4	E	348	NAG	C1-O5-C5	3.86	117.36	112.19
4	C	348	NAG	C1-O5-C5	3.61	117.02	112.19
4	C	348	NAG	C8-C7-N2	3.12	121.28	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	334	NAG	C1-O5-C5	2.87	116.03	112.19
4	E	348	NAG	C8-C7-N2	2.86	120.87	116.12
4	A	348	NAG	C8-C7-N2	2.80	120.75	116.12
4	E	329	NAG	C1-O5-C5	2.45	115.47	112.19
4	E	334	NAG	C1-O5-C5	2.41	115.41	112.19
4	C	348	NAG	C3-C4-C5	-2.35	105.96	110.23
4	C	334	NAG	C1-O5-C5	2.34	115.32	112.19
4	E	348	NAG	C3-C4-C5	-2.33	106.01	110.23
4	A	348	NAG	O4-C4-C5	2.29	114.96	109.32
4	C	348	NAG	O4-C4-C5	2.19	114.72	109.32
4	C	334	NAG	C1-C2-N2	2.14	113.80	110.43
4	C	334	NAG	O5-C1-C2	-2.09	108.05	111.29
4	A	348	NAG	C3-C4-C5	-2.07	106.48	110.23
4	E	334	NAG	O5-C1-C2	-2.04	108.13	111.29
4	C	329	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	348	NAG	O5-C5-C6-O6
4	E	348	NAG	O5-C5-C6-O6
4	A	348	NAG	O5-C5-C6-O6
4	A	348	NAG	C4-C5-C6-O6
4	C	348	NAG	C4-C5-C6-O6
4	E	348	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.04	19 (5%) 29 25	8, 23, 42, 139	0
1	C	328/328 (100%)	0.06	20 (6%) 27 24	8, 23, 42, 145	0
1	E	328/328 (100%)	0.04	20 (6%) 27 24	8, 23, 42, 140	0
2	B	175/175 (100%)	-0.00	10 (5%) 29 26	3, 18, 41, 89	0
2	D	175/175 (100%)	-0.04	15 (8%) 16 13	3, 18, 41, 89	0
2	F	175/175 (100%)	-0.11	9 (5%) 33 29	3, 17, 41, 89	0
All	All	1509/1509 (100%)	0.01	93 (6%) 26 23	3, 21, 42, 145	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	GLY	8.0
1	E	4	PRO	7.4
1	E	3	LEU	7.3
1	C	5	GLY	7.3
1	C	6	ASN	6.9
1	E	7	ASP	6.6
1	A	2	ASP	6.5
1	E	328	THR	6.3
2	D	175	GLY	6.1
1	E	8	ASN	5.7
1	E	6	ASN	5.6
2	F	175	GLY	5.5
1	A	7	ASP	5.5
1	C	2	ASP	5.4
2	F	172	GLN	5.2
2	B	173	ILE	5.2
1	E	2	ASP	5.1
1	C	3	LEU	4.9
2	D	58	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	4.7
2	F	173	ILE	4.6
2	F	60	ASN	4.5
1	A	328	THR	4.5
1	E	1	GLN	4.3
1	A	158	GLY	4.3
1	C	4	PRO	4.3
2	B	168	ASN	4.3
1	E	327	GLN	4.2
1	A	1	GLN	4.2
2	D	174	LYS	4.1
2	F	58	LYS	4.1
2	B	164	ASP	4.1
1	A	3	LEU	4.1
1	A	326	LYS	4.0
1	E	145	SER	4.0
1	A	5	GLY	4.0
1	C	327	GLN	3.9
2	D	173	ILE	3.8
1	C	8	ASN	3.8
1	C	328	THR	3.7
1	C	9	SER	3.6
2	B	172	GLN	3.6
1	E	92	LYS	3.5
2	B	174	LYS	3.4
1	A	327	GLN	3.4
1	C	143	PRO	3.3
2	D	57	GLU	3.3
2	D	156	THR	3.3
2	D	72	GLU	3.2
2	F	57	GLU	3.2
2	D	60	ASN	3.1
1	A	144	GLY	3.1
2	B	145	ASP	3.0
2	F	72	GLU	3.0
1	E	291	ASP	3.0
1	C	160	THR	3.0
2	B	19	ASP	2.9
1	C	144	GLY	2.8
2	D	145	ASP	2.8
2	D	172	GLN	2.7
1	E	187	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	7	ASP	2.7
2	F	174	LYS	2.7
1	E	326	LYS	2.7
1	A	9	SER	2.6
1	C	216	ASN	2.6
1	E	22	ASN	2.5
1	E	135	ARG	2.5
2	D	148	CYS	2.5
2	F	169	ASN	2.5
1	A	140	LYS	2.5
2	D	158	ASP	2.4
1	C	192	THR	2.4
1	E	48	THR	2.4
1	A	145	SER	2.4
1	A	4	PRO	2.4
1	A	8	ASN	2.3
2	D	151	SER	2.3
1	E	137	ASN	2.3
1	C	1	GLN	2.3
1	E	222	TRP	2.3
1	C	158	GLY	2.3
1	C	240	GLY	2.3
2	B	18	ILE	2.2
2	D	154	ASN	2.2
1	A	48	THR	2.2
1	A	22	ASN	2.1
2	B	171	PHE	2.1
1	C	197	GLN	2.1
1	C	10	THR	2.1
2	D	155	GLY	2.1
2	B	175	GLY	2.0
1	A	189	GLN	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.

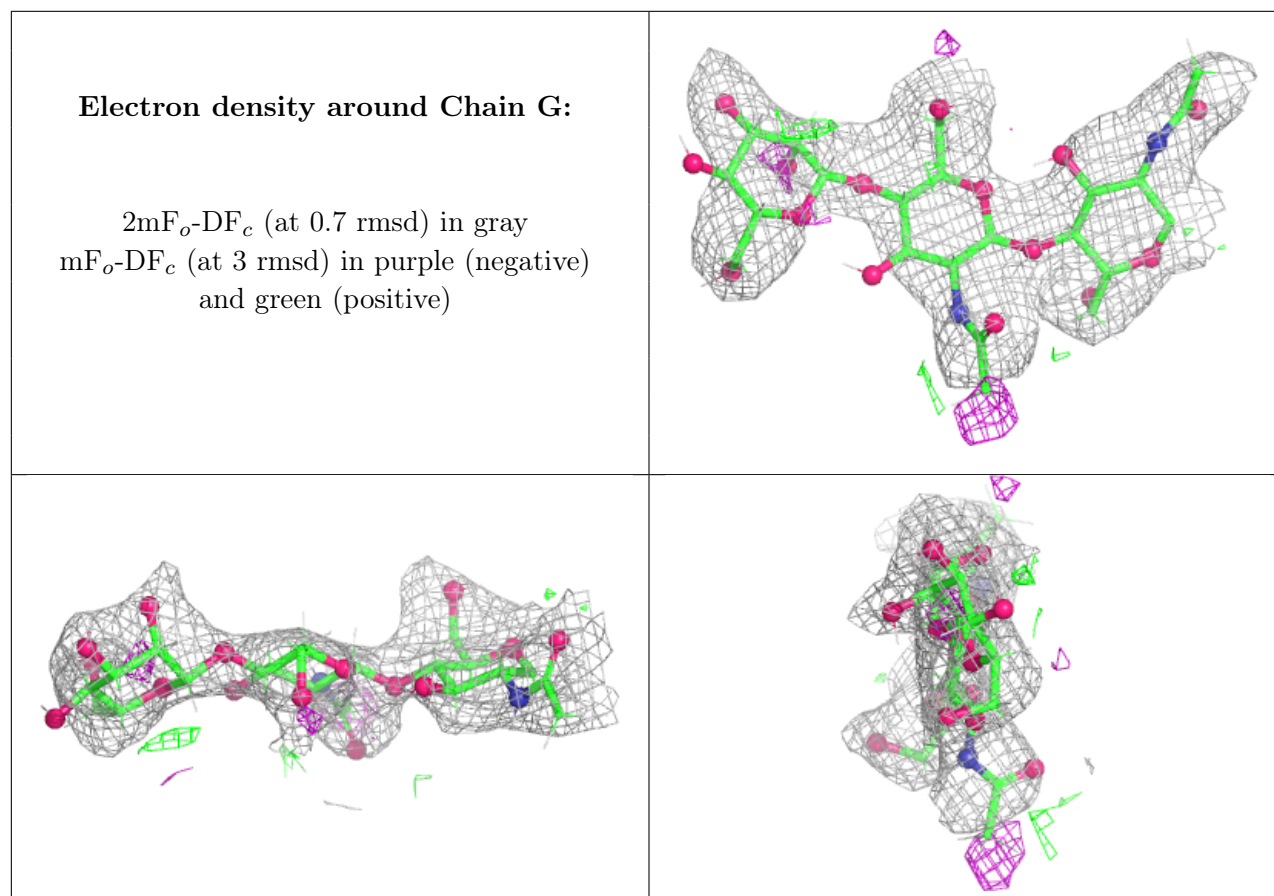
6.3 Carbohydrates [i](#)

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.

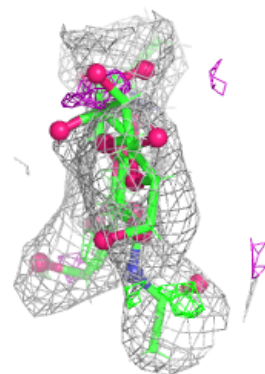
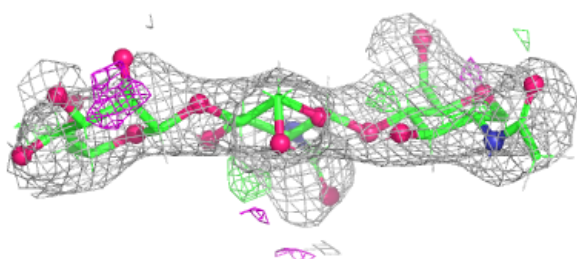
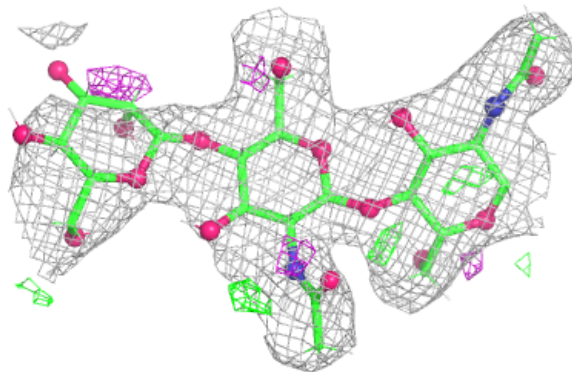
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	G	3	11/12	0.63	0.15	0,0,64,67	0
3	BMA	I	3	11/12	0.69	0.16	0,0,67,69	0
3	BMA	H	3	11/12	0.76	0.14	0,0,67,69	0
3	NAG	G	2	14/15	0.80	0.14	0,0,57,59	0
3	NAG	G	1	14/15	0.85	0.10	0,0,45,49	0
3	NAG	H	1	14/15	0.86	0.12	0,0,45,48	0
3	NAG	I	2	14/15	0.86	0.13	0,0,57,60	0
3	NAG	H	2	14/15	0.86	0.10	0,0,56,60	0
3	NAG	I	1	14/15	0.90	0.10	0,0,44,48	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.

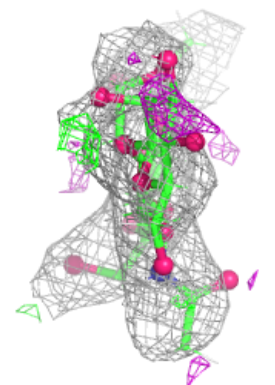
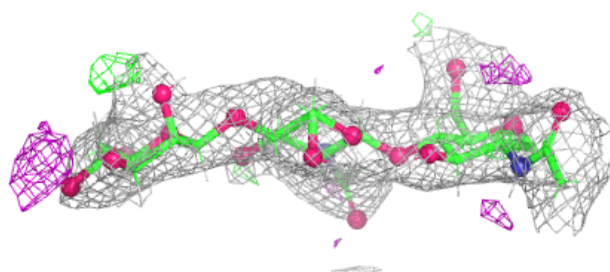
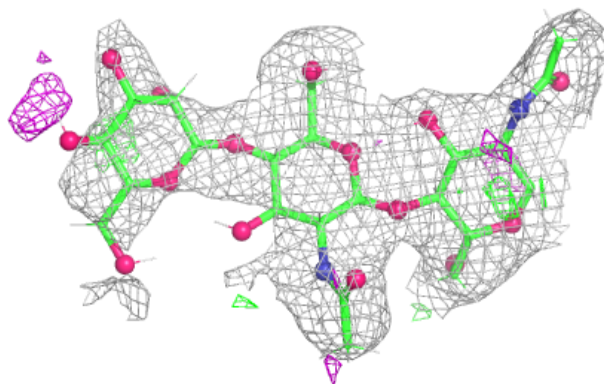


Electron density around Chain H:

$2mF_o-DF_c$ (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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	334	14/15	0.73	0.17	0,0,49,51	0
4	NAG	C	348	14/15	0.75	0.18	0,0,50,51	0
4	NAG	D	401	14/15	0.77	0.17	0,0,67,67	0
4	NAG	B	401	14/15	0.78	0.18	0,0,67,67	0
4	NAG	F	401	14/15	0.78	0.18	0,0,67,67	0
4	NAG	A	334	14/15	0.80	0.09	0,0,48,50	0
4	NAG	A	329	14/15	0.83	0.16	0,0,51,52	0
4	NAG	C	329	14/15	0.83	0.11	0,0,51,51	0
4	NAG	E	329	14/15	0.85	0.14	0,0,51,52	0
4	NAG	A	348	14/15	0.87	0.10	0,0,49,52	0
4	NAG	E	348	14/15	0.90	0.14	0,0,50,51	0
4	NAG	E	334	14/15	0.91	0.09	0,0,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.