



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 1HGF / pdb_00001hgf
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 : 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
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)

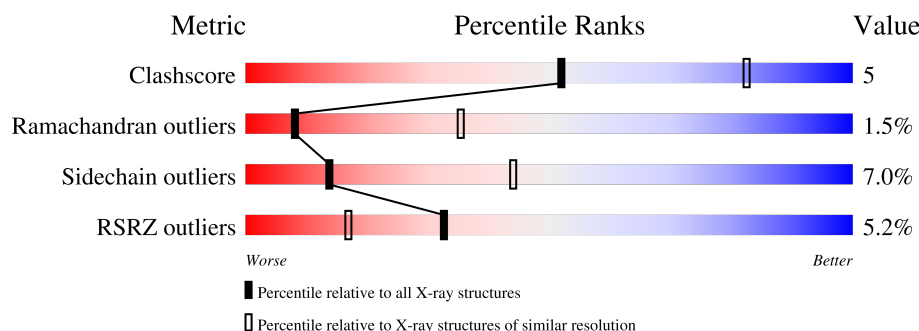
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	5% 73% 20% 6%
1	C	328	5% 73% 21%
1	E	328	6% 73% 21% 5%
2	B	175	6% 73% 22% 5%
2	D	175	4% 73% 21% 6%

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Mol	Chain	Length	Quality of chain
2	F	175	4% 76% 20% • •
3	G	3	33% 67%
3	H	3	67% 33%
3	I	3	100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15192 atoms, of which 3048 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.

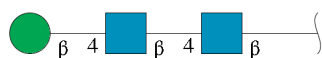
- Molecule 1 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			

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

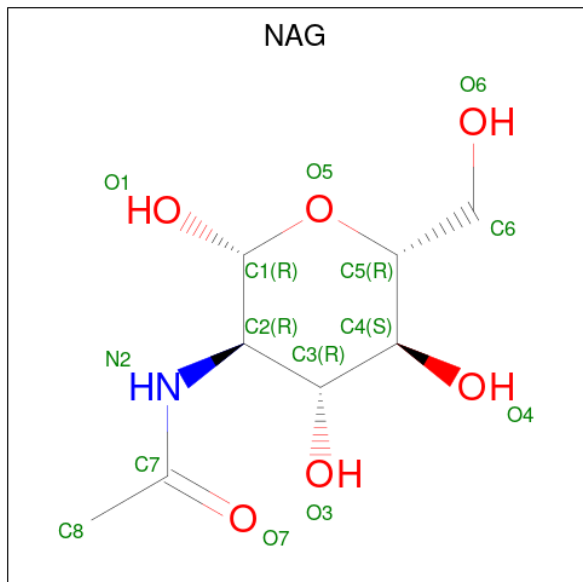
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			

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



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

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

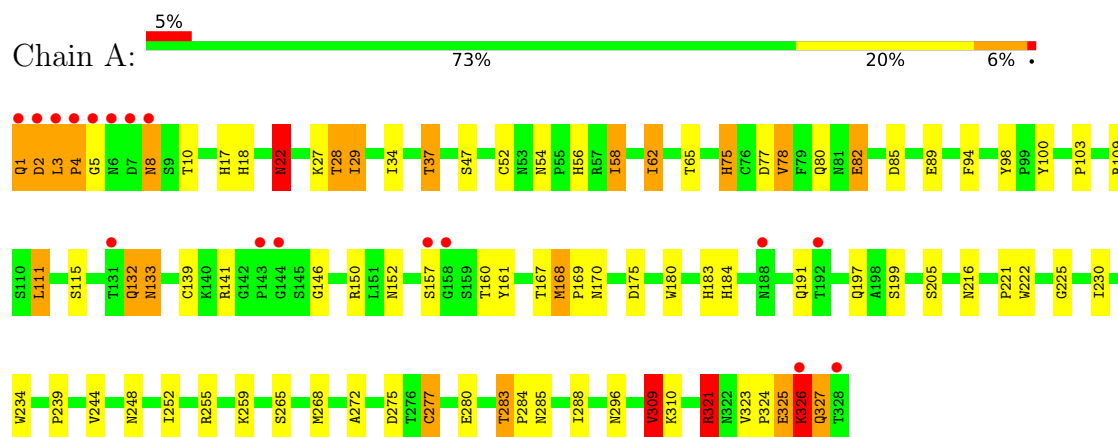


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total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

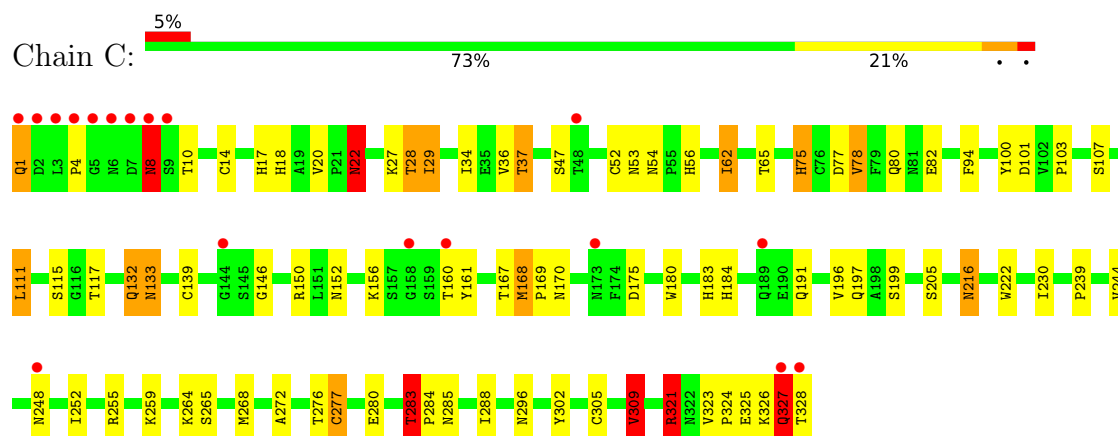
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

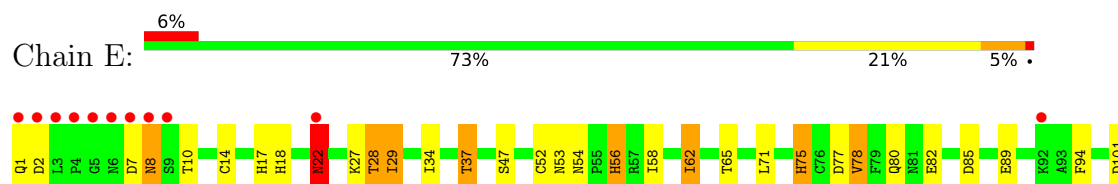
• Molecule 1: HEMAGGLUTININ, CHAIN HA1

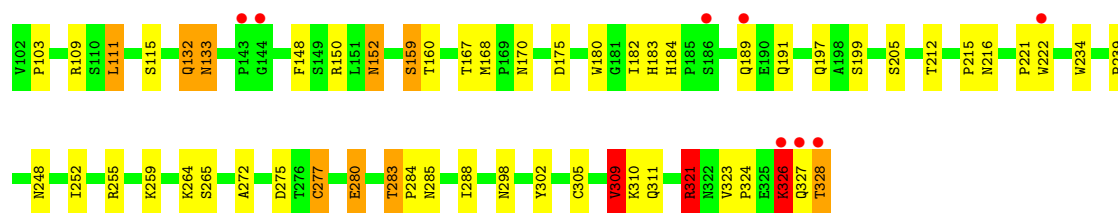


• Molecule 1: HEMAGGLUTININ, CHAIN HA1

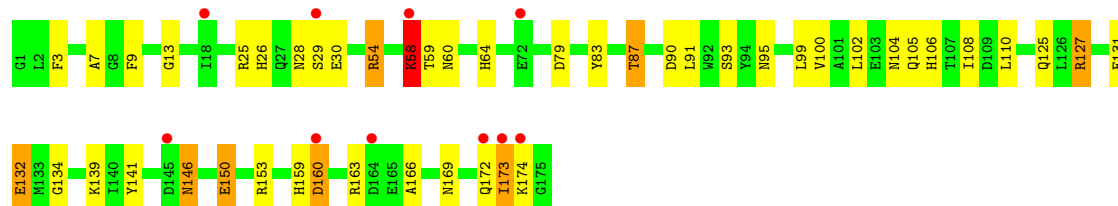
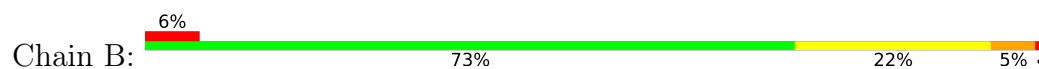


• Molecule 1: HEMAGGLUTININ, CHAIN HA1





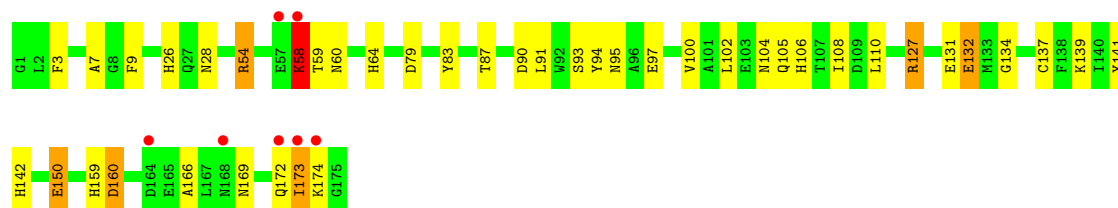
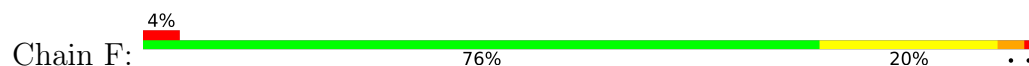
• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



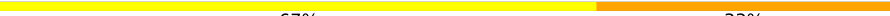
• Molecule 2: HEMAGGLUTININ, CHAIN HA1



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

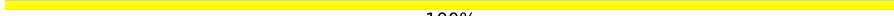


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

MAG1
MAG2
BMA3

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

Chain I:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	163.20Å 163.20Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00 7.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-3.00) 70.9 (7.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.99Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available) 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	1.18	12/2589 (0.5%)	1.82	59/3527 (1.7%)
1	C	1.15	12/2589 (0.5%)	1.79	56/3527 (1.6%)
1	E	1.22	13/2589 (0.5%)	1.80	57/3527 (1.6%)
2	B	1.19	7/1445 (0.5%)	1.76	23/1939 (1.2%)
2	D	1.23	7/1445 (0.5%)	1.77	25/1939 (1.3%)
2	F	1.21	9/1445 (0.6%)	1.76	22/1939 (1.1%)
All	All	1.19	60/12102 (0.5%)	1.79	242/16398 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	150	GLU	CA-CB	-7.68	1.40	1.53
1	E	56	HIS	CD2-NE2	-7.63	1.29	1.37
1	E	184	HIS	CD2-NE2	-7.46	1.29	1.37
1	E	305	CYS	CA-CB	-7.15	1.45	1.54
1	E	18	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	56	HIS	CD2-NE2	-7.01	1.30	1.37
2	F	159	HIS	CD2-NE2	-6.95	1.30	1.37
2	B	26	HIS	CD2-NE2	-6.79	1.30	1.37
2	B	159	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	75	HIS	CD2-NE2	-6.68	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	64	HIS	CG-ND1	-6.61	1.30	1.38
2	B	64	HIS	CD2-NE2	-6.52	1.30	1.37
2	F	64	HIS	CD2-NE2	-6.52	1.30	1.37
1	E	18	HIS	CG-ND1	-6.51	1.31	1.38
2	D	26	HIS	CD2-NE2	-6.50	1.30	1.37
2	D	159	HIS	CD2-NE2	-6.48	1.30	1.37
1	C	184	HIS	CD2-NE2	-6.48	1.30	1.37
1	E	184	HIS	CG-ND1	-6.41	1.31	1.38
2	D	64	HIS	CG-ND1	-6.31	1.31	1.38
1	A	56	HIS	CG-ND1	-6.31	1.31	1.38
2	D	106	HIS	CG-ND1	-6.30	1.31	1.38
1	C	18	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.21	1.31	1.37
1	C	56	HIS	CD2-NE2	-6.21	1.31	1.37
1	E	183	HIS	CD2-NE2	-6.17	1.31	1.37
1	C	17	HIS	CD2-NE2	-6.14	1.31	1.37
2	F	159	HIS	CG-ND1	-6.12	1.31	1.38
1	A	18	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	17	HIS	CD2-NE2	-6.07	1.31	1.37
2	D	106	HIS	CD2-NE2	-6.07	1.31	1.37
1	E	183	HIS	CG-ND1	-6.04	1.31	1.38
1	E	75	HIS	CD2-NE2	-5.99	1.31	1.37
2	D	64	HIS	CD2-NE2	-5.92	1.31	1.37
2	F	142	HIS	CD2-NE2	-5.89	1.31	1.37
1	C	75	HIS	CD2-NE2	-5.72	1.31	1.37
1	E	56	HIS	CG-ND1	-5.71	1.31	1.38
1	C	18	HIS	CG-ND1	-5.67	1.32	1.38
2	D	142	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	183	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	326	LYS	CA-CB	5.58	1.62	1.53
2	F	26	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	183	HIS	CG-ND1	-5.55	1.32	1.38
1	A	18	HIS	CG-ND1	-5.53	1.32	1.38
2	B	159	HIS	CG-ND1	-5.48	1.32	1.38
2	B	87	THR	CA-CB	5.43	1.62	1.53
1	C	305	CYS	CA-CB	-5.40	1.47	1.54
2	F	106	HIS	CD2-NE2	-5.38	1.31	1.37
1	E	280	GLU	CA-CB	-5.38	1.45	1.53
2	F	64	HIS	CG-ND1	-5.38	1.32	1.38
2	B	106	HIS	CD2-NE2	-5.33	1.31	1.37
1	E	234	TRP	CG-CD2	-5.33	1.34	1.43
1	C	184	HIS	CG-ND1	-5.22	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	HIS	CG-ND1	-5.19	1.32	1.38
2	F	26	HIS	CG-ND1	-5.18	1.32	1.38
1	C	17	HIS	CG-ND1	-5.14	1.32	1.38
1	C	20	VAL	CA-CB	-5.09	1.50	1.55
1	C	183	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	234	TRP	CG-CD2	-5.08	1.34	1.43
1	C	183	HIS	CG-ND1	-5.07	1.32	1.38
1	E	17	HIS	CD2-NE2	-5.04	1.32	1.37

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	ASN	CA-CB-CG	12.82	125.42	112.60
2	D	169	ASN	CA-CB-CG	12.41	125.01	112.60
2	F	169	ASN	CA-CB-CG	12.16	124.76	112.60
2	F	9	PHE	CA-CB-CG	11.46	125.26	113.80
2	D	9	PHE	CA-CB-CG	11.16	124.96	113.80
2	B	9	PHE	CA-CB-CG	10.78	124.58	113.80
1	A	75	HIS	CA-CB-CG	9.77	123.57	113.80
1	E	75	HIS	CA-CB-CG	9.65	123.45	113.80
1	A	8	ASN	CA-CB-CG	9.43	122.03	112.60
1	C	75	HIS	CA-CB-CG	8.96	122.76	113.80
2	B	159	HIS	ND1-CG-CD2	8.94	115.04	106.10
2	F	79	ASP	CA-CB-CG	8.90	121.50	112.60
1	E	8	ASN	OD1-CG-ND2	-8.72	113.88	122.60
2	D	159	HIS	ND1-CG-CD2	8.57	114.67	106.10
2	B	79	ASP	CA-CB-CG	8.56	121.16	112.60
1	E	56	HIS	ND1-CG-CD2	8.55	114.66	106.10
1	A	324	PRO	O-C-N	8.50	133.52	123.06
2	F	150	GLU	CA-CB-CG	-8.12	97.86	114.10
1	C	56	HIS	ND1-CG-CD2	8.11	114.21	106.10
1	A	56	HIS	ND1-CG-CD2	7.92	114.02	106.10
1	E	37	THR	CA-CB-OG1	-7.89	97.77	109.60
1	C	37	THR	CA-CB-OG1	-7.88	97.77	109.60
2	F	169	ASN	OD1-CG-ND2	-7.82	114.78	122.60
2	D	79	ASP	CA-CB-CG	7.81	120.41	112.60
2	B	169	ASN	OD1-CG-ND2	-7.75	114.85	122.60
2	F	159	HIS	ND1-CG-CD2	7.66	113.76	106.10
1	C	115	SER	N-CA-C	-7.57	102.97	111.07
2	F	106	HIS	ND1-CG-CD2	7.55	113.65	106.10
1	A	115	SER	N-CA-C	-7.52	103.02	111.14
1	E	216	ASN	CA-CB-CG	7.51	120.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	216	ASN	CA-CB-CG	7.46	120.06	112.60
2	D	169	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	C	216	ASN	CA-CB-CG	7.42	120.03	112.60
2	B	106	HIS	ND1-CG-CD2	7.42	113.52	106.10
1	C	111	LEU	N-CA-CB	-7.37	99.28	110.12
1	E	326	LYS	CA-CB-CG	7.35	128.81	114.10
2	D	106	HIS	ND1-CG-CD2	7.26	113.36	106.10
1	E	309	VAL	N-CA-CB	-7.23	100.30	112.44
1	C	132	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	C	184	HIS	ND1-CG-CD2	7.17	113.27	106.10
1	E	321	ARG	NE-CZ-NH2	-7.17	112.75	119.20
1	A	326	LYS	CA-CB-CG	7.14	128.38	114.10
1	C	248	ASN	N-CA-CB	-7.13	100.18	110.80
1	A	277	CYS	CA-C-N	-7.13	114.35	123.19
1	A	277	CYS	C-N-CA	-7.13	114.35	123.19
2	B	28	ASN	CA-CB-CG	7.10	119.70	112.60
1	A	324	PRO	CA-C-N	7.04	132.48	122.05
1	A	324	PRO	C-N-CA	7.04	132.48	122.05
1	C	277	CYS	CA-C-N	-7.04	114.46	123.19
1	C	277	CYS	C-N-CA	-7.04	114.46	123.19
1	E	180	TRP	CG-CD2-CE3	7.03	140.93	133.90
1	E	8	ASN	CB-CG-ND2	7.03	126.94	116.40
2	D	104	ASN	OD1-CG-ND2	-6.97	115.62	122.60
1	E	277	CYS	CA-C-N	-6.97	114.55	123.19
1	E	277	CYS	C-N-CA	-6.97	114.55	123.19
1	E	132	GLN	OE1-CD-NE2	-6.96	115.64	122.60
1	A	184	HIS	ND1-CG-CD2	6.87	112.97	106.10
2	D	27	GLN	CA-CB-CG	-6.83	100.45	114.10
2	B	150	GLU	CB-CG-CD	6.81	124.18	112.60
1	E	111	LEU	N-CA-CB	-6.80	100.12	110.12
2	F	104	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	A	37	THR	CA-CB-OG1	-6.78	99.42	109.60
1	A	248	ASN	N-CA-CB	-6.77	100.72	110.80
1	A	111	LEU	N-CA-CB	-6.76	100.18	110.12
1	E	248	ASN	N-CA-CB	-6.76	100.73	110.80
2	F	132	GLU	CA-CB-CG	-6.76	100.59	114.10
2	D	132	GLU	CA-CB-CG	-6.74	100.61	114.10
2	D	135	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	E	184	HIS	ND1-CG-CD2	6.71	112.81	106.10
2	D	11	GLU	N-CA-C	6.70	119.44	111.33
1	C	309	VAL	N-CA-CB	-6.70	101.19	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	169	ASN	CB-CG-ND2	6.70	126.44	116.40
2	B	132	GLU	CA-CB-CG	-6.69	100.72	114.10
1	E	82	GLU	N-CA-CB	-6.67	100.31	110.45
1	C	28	THR	CA-CB-CG2	6.67	121.84	110.50
1	C	29	ILE	N-CA-C	-6.65	104.28	110.53
1	A	321	ARG	NE-CZ-NH2	-6.60	113.26	119.20
2	B	169	ASN	CB-CG-ND2	6.58	126.26	116.40
1	C	321	ARG	NE-CZ-NH2	-6.55	113.30	119.20
1	A	321	ARG	CB-CG-CD	-6.55	96.23	111.30
1	E	272	ALA	CA-C-N	6.54	126.30	119.76
1	E	272	ALA	C-N-CA	6.54	126.30	119.76
1	A	132	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	E	191	GLN	OE1-CD-NE2	-6.53	116.08	122.60
1	A	28	THR	CA-CB-CG2	6.52	121.59	110.50
1	E	132	GLN	CG-CD-NE2	6.52	126.18	116.40
2	D	169	ASN	CB-CG-ND2	6.51	126.16	116.40
1	C	28	THR	CA-CB-OG1	-6.49	99.86	109.60
1	C	191	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	28	THR	CA-CB-OG1	-6.48	99.88	109.60
1	C	272	ALA	CA-C-N	6.48	126.24	119.76
1	C	272	ALA	C-N-CA	6.48	126.24	119.76
1	C	170	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	E	28	THR	CA-CB-CG2	6.38	121.34	110.50
1	E	115	SER	N-CA-C	-6.36	104.26	111.07
1	E	321	ARG	CB-CG-CD	-6.36	96.66	111.30
2	D	3	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	325	GLU	CA-CB-CG	6.34	126.78	114.10
1	A	184	HIS	CA-C-N	6.33	126.29	120.03
1	A	184	HIS	C-N-CA	6.33	126.29	120.03
1	A	133	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	54	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	132	GLN	CG-CD-NE2	6.29	125.83	116.40
1	E	8	ASN	CA-CB-CG	6.28	118.88	112.60
1	C	321	ARG	CB-CG-CD	-6.27	96.87	111.30
1	C	54	ASN	CA-CB-CG	-6.27	106.33	112.60
1	E	28	THR	CA-CB-OG1	-6.24	100.24	109.60
1	E	28	THR	N-CA-CB	-6.24	100.89	111.31
2	F	108	ILE	CA-C-O	-6.23	114.25	120.85
1	E	101	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	29	ILE	N-CA-C	-6.19	104.71	110.53
1	C	132	GLN	CG-CD-NE2	6.19	125.69	116.40
1	E	56	HIS	CB-CG-CD2	-6.17	123.18	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	ASN	CA-CB-CG	6.17	118.77	112.60
1	E	22	ASN	CA-CB-CG	6.15	118.75	112.60
1	C	180	TRP	CG-CD2-CE3	6.15	140.05	133.90
1	C	183	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	A	85	ASP	N-CA-C	-6.12	104.88	112.90
1	A	180	TRP	CG-CD2-CE3	6.11	140.01	133.90
1	C	22	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	272	ALA	CA-C-N	6.10	125.86	119.76
1	A	272	ALA	C-N-CA	6.10	125.86	119.76
1	C	184	HIS	CA-C-N	6.10	126.07	120.03
1	C	184	HIS	C-N-CA	6.10	126.07	120.03
2	D	108	ILE	CA-C-O	-6.08	114.41	120.85
1	E	183	HIS	ND1-CG-CD2	6.08	112.18	106.10
1	E	159	SER	CA-CB-OG	-6.07	98.97	111.10
1	A	78	VAL	CB-CA-C	-6.04	102.80	112.16
1	E	54	ASN	CA-CB-CG	-6.04	106.56	112.60
1	C	56	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	E	1	GLN	N-CA-C	-6.01	94.16	111.00
2	D	25	ARG	O-C-N	-5.98	115.62	123.16
1	E	37	THR	CA-CB-CG2	5.94	120.59	110.50
2	F	3	PHE	CA-CB-CG	-5.93	107.87	113.80
2	D	32	THR	CA-C-O	-5.93	114.50	121.44
1	C	28	THR	N-CA-CB	-5.93	101.41	111.31
1	C	252	ILE	N-CA-C	-5.91	97.33	106.72
1	C	37	THR	CA-CB-CG2	5.90	120.53	110.50
2	F	60	ASN	CA-CB-CG	5.89	118.49	112.60
2	D	160	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	22	ASN	CA-CB-CG	5.87	118.47	112.60
2	F	28	ASN	OD1-CG-ND2	-5.87	116.73	122.60
2	F	150	GLU	CB-CG-CD	-5.85	102.65	112.60
1	A	8	ASN	N-CA-CB	-5.84	101.26	110.49
1	E	326	LYS	N-CA-CB	-5.83	100.63	110.49
2	F	95	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	82	GLU	CB-CG-CD	5.81	122.47	112.60
1	A	170	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	C	78	VAL	CB-CA-C	-5.80	103.58	112.05
2	D	95	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	56	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	28	THR	N-CA-CB	-5.78	101.66	111.31
1	E	85	ASP	N-CA-C	-5.77	105.34	112.90
2	B	160	ASP	CA-CB-CG	-5.77	106.83	112.60
1	C	133	ASN	OD1-CG-ND2	-5.75	116.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	HIS	CG-CD2-NE2	-5.72	101.48	107.20
1	A	309	VAL	N-CA-CB	-5.71	101.80	112.36
1	A	183	HIS	ND1-CG-CD2	5.70	111.80	106.10
1	C	101	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	37	THR	CA-C-O	-5.64	114.57	120.55
1	E	252	ILE	N-CA-C	-5.62	97.78	106.72
2	B	104	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	C	1	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	F	90	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	108	ILE	CA-C-O	-5.51	115.01	120.85
1	E	168	MET	CA-C-N	5.51	125.94	119.99
1	E	168	MET	C-N-CA	5.51	125.94	119.99
1	E	170	ASN	OD1-CG-ND2	-5.47	117.12	122.60
2	F	160	ASP	CA-CB-CG	-5.47	107.13	112.60
1	E	180	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	C	107	SER	CA-CB-OG	-5.46	100.19	111.10
1	E	133	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	E	309	VAL	CB-CA-C	5.45	118.83	110.55
1	C	8	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	E	184	HIS	CA-C-N	5.43	125.41	120.03
1	E	184	HIS	C-N-CA	5.43	125.41	120.03
1	A	310	LYS	CB-CG-CD	5.42	123.76	111.30
2	B	25	ARG	O-C-N	-5.41	116.87	123.10
1	C	168	MET	CA-C-N	5.40	125.82	119.99
1	C	168	MET	C-N-CA	5.40	125.82	119.99
1	E	180	TRP	CB-CG-CD1	-5.38	118.83	126.90
1	E	56	HIS	CG-CD2-NE2	-5.37	101.83	107.20
1	C	82	GLU	N-CA-CB	-5.36	102.77	110.44
1	E	275	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	60	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	275	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	296	ASN	N-CA-CB	-5.32	102.67	111.49
1	C	325	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	2	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	283	THR	O-C-N	-5.30	117.24	121.80
2	D	60	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	180	TRP	CB-CG-CD1	-5.27	119.00	126.90
1	E	222	TRP	CE2-CD2-CE3	5.26	124.06	118.80
1	A	252	ILE	N-CA-C	-5.26	98.36	106.72
1	A	8	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	C	36	VAL	CA-C-N	5.26	127.32	120.28
1	C	36	VAL	C-N-CA	5.26	127.32	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	127	ARG	CA-CB-CG	-5.25	103.59	114.10
1	E	29	ILE	N-CA-C	-5.24	105.60	110.53
1	E	152	ASN	CA-CB-CG	5.24	117.83	112.60
1	C	180	TRP	CE2-CD2-CG	-5.23	100.92	107.20
1	A	1	GLN	N-CA-C	-5.23	96.36	111.00
1	A	62	ILE	CA-CB-CG2	-5.23	101.61	110.50
1	E	62	ILE	CA-CB-CG2	-5.22	101.62	110.50
1	C	62	ILE	CA-CB-CG2	-5.22	101.62	110.50
1	E	180	TRP	CG-CD1-NE1	-5.22	103.41	110.20
1	A	325	GLU	CA-C-O	-5.21	115.91	122.63
1	C	296	ASN	N-CA-CB	-5.20	102.85	111.49
1	C	22	ASN	OD1-CG-ND2	-5.20	117.41	122.60
1	A	141	ARG	CA-CB-CG	-5.19	103.71	114.10
1	A	37	THR	CA-CB-CG2	5.18	119.31	110.50
1	E	310	LYS	CB-CG-CD	5.17	123.20	111.30
2	B	90	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	159	HIS	CG-CD2-NE2	-5.16	102.04	107.20
2	B	99	LEU	CA-C-O	-5.16	115.59	121.00
1	A	191	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	D	163	ARG	N-CA-C	5.15	116.58	111.07
2	B	3	PHE	CA-CB-CG	-5.13	108.67	113.80
2	D	159	HIS	CG-CD2-NE2	-5.12	102.08	107.20
2	B	146	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	C	327	GLN	CA-CB-CG	5.09	124.28	114.10
1	C	184	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	180	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	C	222	TRP	CE2-CD2-CE3	5.08	123.88	118.80
1	A	58	ILE	N-CA-CB	-5.08	105.18	110.72
2	F	94	TYR	N-CA-C	-5.08	105.64	111.07
1	E	180	TRP	CD1-CG-CD2	5.07	114.41	106.30
1	A	180	TRP	CB-CG-CD1	-5.06	119.31	126.90
2	D	28	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	168	MET	CA-C-N	5.05	125.44	119.99
1	A	168	MET	C-N-CA	5.05	125.44	119.99
1	A	37	THR	N-CA-CB	-5.04	102.70	110.12
1	E	78	VAL	CB-CA-C	-5.04	104.34	112.16
2	D	125	GLN	CG-CD-NE2	5.04	123.97	116.40
2	B	58	LYS	N-CA-C	5.04	121.53	110.80
2	D	94	TYR	N-CA-C	-5.04	105.68	111.07
2	B	125	GLN	CG-CD-NE2	5.03	123.95	116.40
2	F	58	LYS	N-CA-C	5.01	121.48	110.80
1	C	117	THR	CA-CB-OG1	-5.01	102.08	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	TYR	CA-C-O	-5.01	115.50	119.71
2	D	58	LYS	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain
1	C	161	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	590	2473	31	0
1	C	2532	590	2473	33	0
1	E	2532	590	2473	34	0
2	B	1421	333	1345	20	0
2	D	1421	333	1345	19	0
2	F	1421	333	1345	18	0
3	G	39	37	34	1	0
3	H	39	37	34	2	0
3	I	39	37	34	1	0
4	A	42	42	39	0	0
4	B	14	14	13	0	0
4	C	42	42	39	0	0
4	D	14	14	13	0	0
4	E	42	42	39	0	0
4	F	14	14	13	0	0
All	All	12144	3048	11712	121	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 5.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:O	2:B:87:THR:HG23	1.85	0.77
2:F:83:TYR:O	2:F:87:THR:HG23	1.86	0.75
2:D:83:TYR:O	2:D:87:THR:HG23	1.87	0.74
2:D:27:GLN:HG3	2:D:32:THR:HG22	1.69	0.71
2:F:132:GLU:HG2	2:F:134:GLY:H	1.55	0.71
2:B:132:GLU:HG2	2:B:134:GLY:H	1.56	0.70
2:D:132:GLU:HG2	2:D:134:GLY:H	1.56	0.70
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.61	0.65
1:A:10:THR:HG22	2:B:141:TYR:HA	1.79	0.64
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.62	0.64
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.79	0.63
1:C:283:THR:HG22	1:C:285:ASN:H	1.62	0.63
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.63	0.63
2:D:28:ASN:HB2	2:D:144:CYS:O	1.99	0.63
1:E:10:THR:HG22	2:F:141:TYR:HA	1.80	0.62
1:C:77:ASP:O	1:C:80:GLN:HG3	1.98	0.62
1:E:283:THR:HG22	1:E:285:ASN:H	1.65	0.62
1:C:10:THR:HG22	2:D:141:TYR:HA	1.82	0.62
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.80	0.62
1:A:77:ASP:O	1:A:80:GLN:HG3	2.00	0.62
1:E:77:ASP:O	1:E:80:GLN:HG3	1.99	0.62
1:C:132:GLN:HE21	1:C:152:ASN:HD21	1.47	0.61
1:A:132:GLN:HE21	1:A:152:ASN:HD21	1.46	0.61
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.83	0.61
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.83	0.61
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.84	0.60
1:E:132:GLN:HE21	1:E:152:ASN:HD21	1.47	0.60
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.82	0.60
1:A:325:GLU:HB2	2:B:13:GLY:O	2.02	0.60
1:A:283:THR:HG22	1:A:285:ASN:H	1.65	0.59
1:C:53:ASN:OD1	1:C:276:THR:HA	2.04	0.57
2:F:58:LYS:HE2	2:F:59:THR:O	2.07	0.55
2:B:58:LYS:HE2	2:B:59:THR:O	2.07	0.55
1:E:52:CYS:HB3	1:E:277:CYS:O	2.09	0.53
2:B:141:TYR:O	2:B:166:ALA:HA	2.09	0.52
1:C:27:LYS:HD3	2:F:54:ARG:NH2	2.25	0.52
2:D:58:LYS:HE2	2:D:59:THR:O	2.09	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.10	0.52
2:B:54:ARG:NH2	1:E:27:LYS:HD3	2.25	0.51
1:C:52:CYS:HB3	1:C:277:CYS:O	2.10	0.51
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.10	0.51
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG23	1:E:221:PRO:HG3	1.93	0.50
1:A:27:LYS:HD3	2:D:54:ARG:NH2	2.26	0.50
1:A:3:LEU:HB2	1:A:4:PRO:HD2	1.95	0.49
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.13	0.49
1:A:52:CYS:HB3	1:A:277:CYS:O	2.12	0.49
2:D:141:TYR:O	2:D:166:ALA:HA	2.12	0.49
1:E:326:LYS:HD2	1:E:327:GLN:H	1.76	0.49
1:A:167:THR:HB	3:G:1:NAG:H62	1.95	0.48
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.96	0.48
1:A:268:MET:SD	1:A:284:PRO:HD3	2.53	0.48
1:C:132:GLN:HE21	1:C:152:ASN:ND2	2.10	0.48
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.48
1:C:167:THR:HB	3:H:1:NAG:H62	1.96	0.48
1:A:283:THR:HG22	1:A:285:ASN:N	2.29	0.47
1:E:132:GLN:HE21	1:E:152:ASN:ND2	2.12	0.47
1:A:326:LYS:HG2	1:A:327:GLN:N	2.29	0.47
1:C:283:THR:HG22	1:C:285:ASN:N	2.28	0.47
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.47	0.47
1:E:167:THR:HB	3:I:1:NAG:H62	1.96	0.47
1:E:283:THR:HG22	1:E:285:ASN:N	2.30	0.47
1:C:327:GLN:HG2	1:C:328:THR:N	2.30	0.47
1:A:309:VAL:HG22	2:B:93:SER:HA	1.96	0.46
1:C:1:GLN:HA	1:C:1:GLN:OE1	2.15	0.46
1:A:47:SER:HA	1:A:288:ILE:HG22	1.96	0.46
1:A:132:GLN:HE21	1:A:152:ASN:ND2	2.11	0.46
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.45
1:E:29:ILE:HB	2:F:105:GLN:OE1	2.17	0.45
1:A:29:ILE:HB	2:B:105:GLN:OE1	2.17	0.45
1:C:29:ILE:HB	2:D:105:GLN:OE1	2.17	0.45
2:B:30:GLU:HB2	2:B:146:ASN:ND2	2.32	0.45
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.49	0.44
1:E:47:SER:HA	1:E:288:ILE:HG22	1.99	0.44
1:C:47:SER:HA	1:C:288:ILE:HG22	2.00	0.44
1:A:221:PRO:HG3	1:C:244:VAL:HG23	1.98	0.44
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.99	0.44
1:C:139:CYS:HB3	1:C:146:GLY:O	2.18	0.43
1:C:309:VAL:HG22	2:D:93:SER:HA	1.99	0.43
1:A:75:HIS:HE1	1:A:94:PHE:O	2.01	0.43
1:A:221:PRO:HA	3:H:2:NAG:O7	2.18	0.43
1:E:75:HIS:HE1	1:E:94:PHE:O	2.01	0.43
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PRO:HG3	1:E:328:THR:HG23	2.01	0.43
1:C:327:GLN:HE21	1:C:328:THR:C	2.27	0.43
1:E:53:ASN:HA	1:E:58:ILE:HD13	1.99	0.43
1:C:100:TYR:HA	1:C:230:ILE:O	2.18	0.43
1:E:323:VAL:HG21	2:F:7:ALA:HB2	2.01	0.43
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.01	0.42
1:C:156:LYS:HD3	1:C:196:VAL:CG2	2.49	0.42
2:D:173:ILE:HD13	2:D:173:ILE:HA	1.93	0.42
1:C:323:VAL:HG21	2:D:7:ALA:HB2	2.02	0.42
1:C:10:THR:HG21	2:D:139:LYS:HE2	2.02	0.42
1:E:109:ARG:HH11	1:E:109:ARG:HD2	1.68	0.42
2:B:150:GLU:OE1	2:B:153:ARG:NH1	2.53	0.42
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.47	0.42
1:C:264:LYS:HE3	1:C:302:TYR:OH	2.20	0.42
1:C:168:MET:HA	1:C:169:PRO:HD3	1.86	0.42
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.35	0.42
2:B:131:GLU:OE1	2:D:127:ARG:NH1	2.52	0.42
1:E:309:VAL:HG22	2:F:93:SER:HA	2.01	0.42
1:E:321:ARG:HH11	1:E:321:ARG:CG	2.31	0.42
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.52	0.41
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.35	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
1:A:323:VAL:HG21	2:B:7:ALA:HB2	2.01	0.41
2:B:163:ARG:NH2	2:F:131:GLU:OE2	2.53	0.41
1:A:168:MET:HA	1:A:169:PRO:HD3	1.87	0.41
1:C:14:CYS:HA	2:D:137:CYS:HA	2.03	0.41
1:A:100:TYR:HA	1:A:230:ILE:O	2.21	0.41
1:C:268:MET:SD	1:C:284:PRO:HD3	2.61	0.41
1:A:139:CYS:HB3	1:A:146:GLY:O	2.21	0.41
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.56	0.41
1:C:75:HIS:HE1	1:C:94:PHE:O	2.04	0.41
1:E:71:LEU:O	1:E:148:PHE:HB3	2.20	0.41
1:E:264:LYS:HE3	1:E:302:TYR:OH	2.20	0.41
1:A:10:THR:HG21	2:B:139:LYS:HE2	2.03	0.40
1:E:10:THR:HG21	2:F:139:LYS:HE2	2.02	0.40
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.54	0.40
2:B:173:ILE:HD13	2:B:173:ILE:HA	1.94	0.40
1:C:8:ASN:HB2	2:D:169:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	303 (93%)	15 (5%)	8 (2%)	4	23
1	C	326/328 (99%)	303 (93%)	19 (6%)	4 (1%)	10	40
1	E	326/328 (99%)	306 (94%)	18 (6%)	2 (1%)	21	56
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	32
2	D	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	7	32
2	F	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	32
All	All	1497/1509 (99%)	1393 (93%)	81 (5%)	23 (2%)	8	35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LEU
2	B	58	LYS
2	B	173	ILE
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	326	LYS
1	C	4	PRO
1	A	327	GLN
1	C	326	LYS
2	F	172	GLN
1	A	62	ILE
2	B	172	GLN
1	C	62	ILE
2	D	172	GLN
1	E	62	ILE
1	A	22	ASN
1	A	4	PRO

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Mol	Chain	Res	Type
1	C	22	ASN
1	E	22	ASN
1	A	5	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%)	264 (91%)	25 (9%)	9	35
1	C	289/289 (100%)	267 (92%)	22 (8%)	12	41
1	E	289/289 (100%)	263 (91%)	26 (9%)	9	34
2	B	149/149 (100%)	143 (96%)	6 (4%)	28	62
2	D	149/149 (100%)	142 (95%)	7 (5%)	23	58
2	F	149/149 (100%)	143 (96%)	6 (4%)	28	62
All	All	1314/1314 (100%)	1222 (93%)	92 (7%)	14	44

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	8	ASN
1	A	22	ASN
1	A	28	THR
1	A	34	ILE
1	A	37	THR
1	A	58	ILE
1	A	65	THR
1	A	78	VAL
1	A	82	GLU
1	A	103	PRO
1	A	111	LEU
1	A	150	ARG
1	A	157	SER
1	A	160	THR

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	199	SER
1	A	205	SER
1	A	259	LYS
1	A	265	SER
1	A	280	GLU
1	A	283	THR
1	A	309	VAL
1	A	321	ARG
1	A	326	LYS
2	B	29	SER
2	B	54	ARG
2	B	100	VAL
2	B	110	LEU
2	B	127	ARG
2	B	160	ASP
1	C	8	ASN
1	C	22	ASN
1	C	28	THR
1	C	34	ILE
1	C	37	THR
1	C	65	THR
1	C	78	VAL
1	C	103	PRO
1	C	111	LEU
1	C	150	ARG
1	C	160	THR
1	C	197	GLN
1	C	199	SER
1	C	205	SER
1	C	259	LYS
1	C	265	SER
1	C	280	GLU
1	C	283	THR
1	C	309	VAL
1	C	321	ARG
1	C	324	PRO
1	C	327	GLN
2	D	11	GLU
2	D	54	ARG
2	D	100	VAL
2	D	110	LEU

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Mol	Chain	Res	Type
2	D	127	ARG
2	D	150	GLU
2	D	160	ASP
1	E	2	ASP
1	E	7	ASP
1	E	8	ASN
1	E	22	ASN
1	E	28	THR
1	E	34	ILE
1	E	37	THR
1	E	65	THR
1	E	78	VAL
1	E	103	PRO
1	E	111	LEU
1	E	150	ARG
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	197	GLN
1	E	199	SER
1	E	205	SER
1	E	259	LYS
1	E	265	SER
1	E	280	GLU
1	E	283	THR
1	E	309	VAL
1	E	321	ARG
1	E	326	LYS
1	E	328	THR
2	F	54	ARG
2	F	100	VAL
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	132	GLN
1	A	171	ASN

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Mol	Chain	Res	Type
2	B	49	ASN
2	B	146	ASN
1	C	6	ASN
1	C	17	HIS
1	C	132	GLN
1	C	171	ASN
1	C	211	GLN
1	C	327	GLN
2	D	12	ASN
2	D	28	ASN
2	D	49	ASN
2	D	169	ASN
1	E	8	ASN
1	E	132	GLN
1	E	171	ASN
1	E	189	GLN
2	F	12	ASN
2	F	26	HIS
2	F	42	GLN
2	F	49	ASN
2	F	168	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	3,1	14,14,15	0.56	0	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
3	BMA	G	3	3	11,11,12	0.88	0	15,15,17	1.05	0
3	NAG	H	1	3,1	14,14,15	0.72	0	17,19,21	0.85	0
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
3	BMA	H	3	3	11,11,12	0.79	0	15,15,17	1.34	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.58	0	17,19,21	0.80	0
3	NAG	I	2	3	14,14,15	0.49	0	17,19,21	1.08	1 (5%)
3	BMA	I	3	3	11,11,12	0.84	0	15,15,17	1.23	1 (6%)

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	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	BMA	C1-O5-C5	2.86	116.02	112.19
3	H	3	BMA	C1-O5-C5	2.72	115.83	112.19
3	G	2	NAG	C4-C3-C2	-2.62	107.18	111.02
3	H	2	NAG	C4-C3-C2	-2.54	107.30	111.02
3	I	2	NAG	C4-C3-C2	-2.37	107.54	111.02
3	H	3	BMA	C6-C5-C4	-2.33	107.30	113.02

There are no chirality outliers.

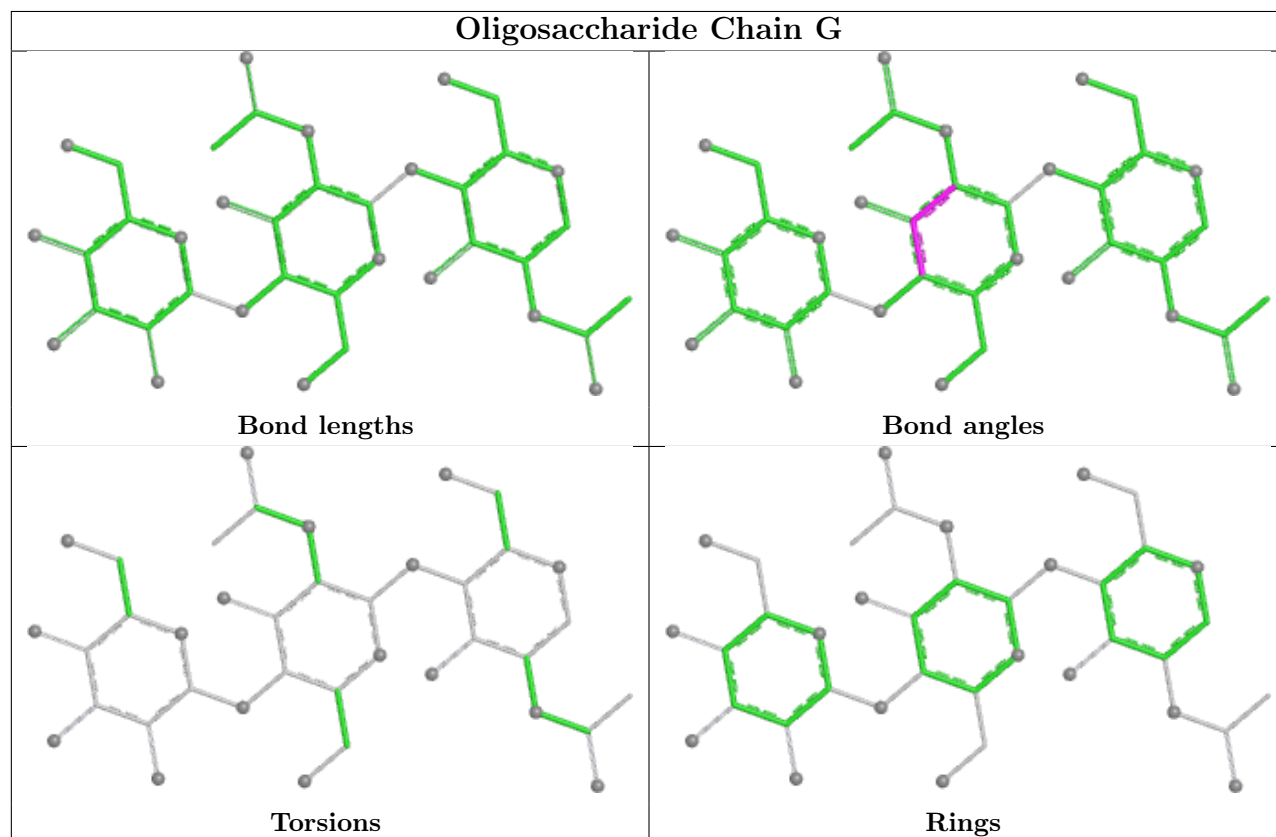
There are no torsion outliers.

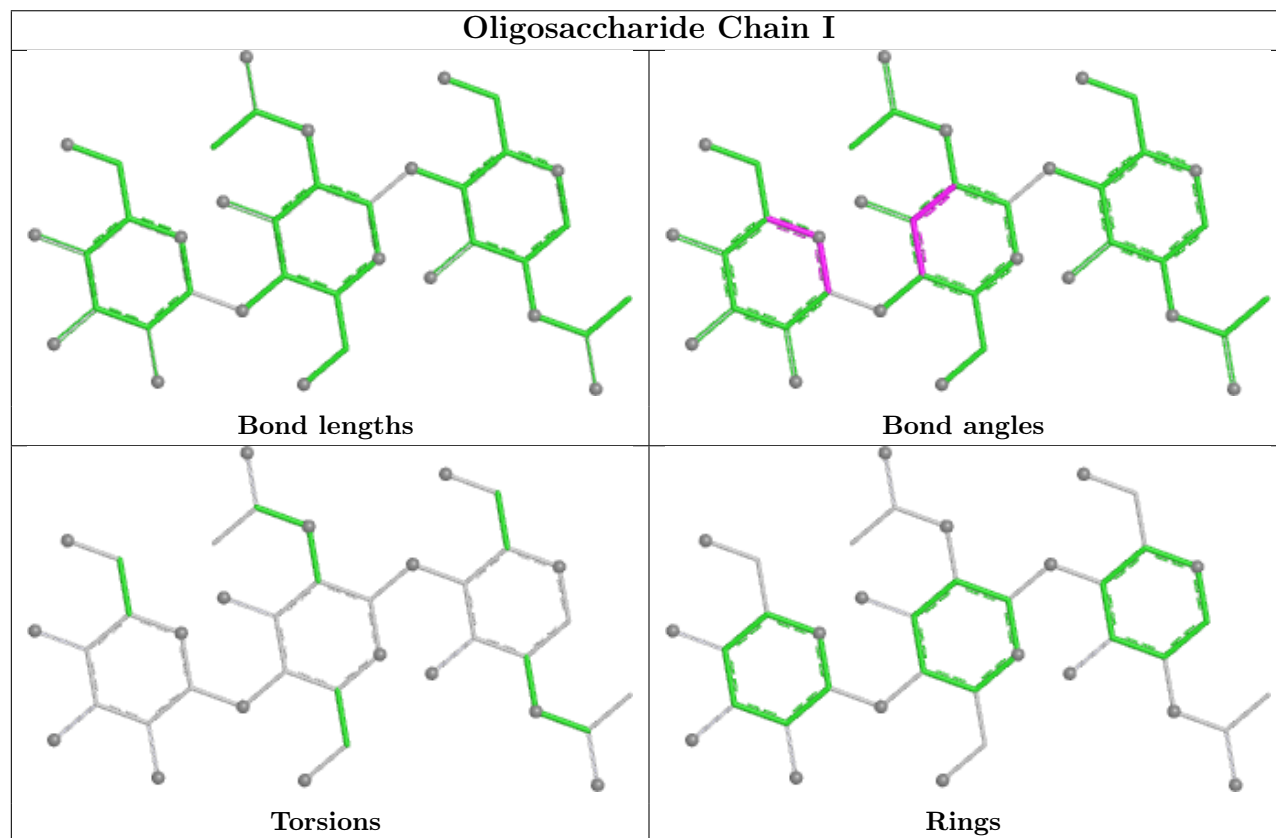
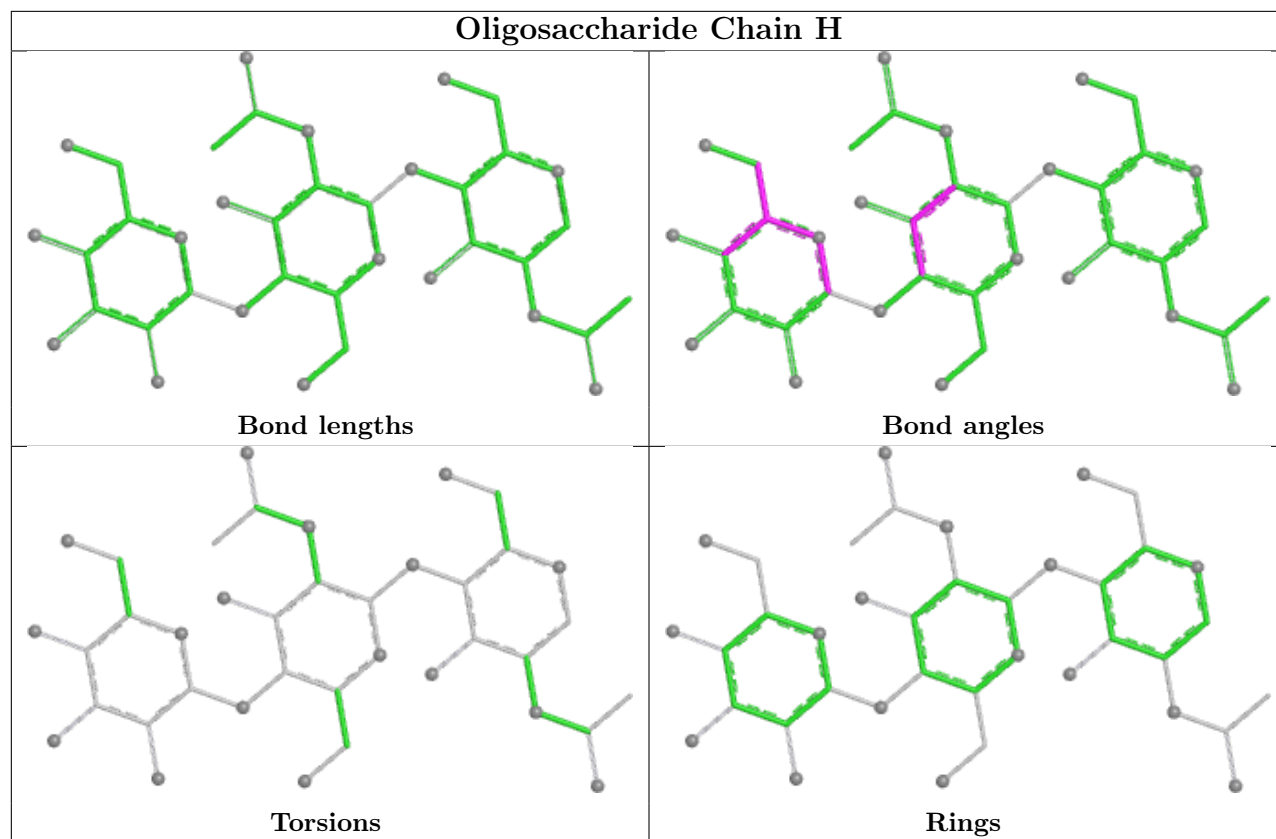
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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





5.6 Ligand geometry

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	A	334	1	14,14,15	0.80	0	17,19,21	1.35	1 (5%)
4	NAG	F	401	2	14,14,15	0.67	0	17,19,21	1.51	2 (11%)
4	NAG	A	329	1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
4	NAG	E	329	1	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
4	NAG	E	334	1	14,14,15	0.68	0	17,19,21	1.29	1 (5%)
4	NAG	B	401	2	14,14,15	0.62	0	17,19,21	1.45	2 (11%)
4	NAG	D	401	2	14,14,15	0.67	0	17,19,21	1.52	1 (5%)
4	NAG	E	348	1	14,14,15	0.78	0	17,19,21	1.44	4 (23%)
4	NAG	A	348	1	14,14,15	0.72	0	17,19,21	1.44	4 (23%)
4	NAG	C	334	1	14,14,15	0.83	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	C	348	1	14,14,15	0.79	0	17,19,21	1.50	3 (17%)
4	NAG	C	329	1	14,14,15	0.66	0	17,19,21	0.95	1 (5%)

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	A	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	A	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	E	334	1	-	0/6/23/26	0/1/1/1
4	NAG	B	401	2	-	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	348	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	C	348	1	-	2/6/23/26	0/1/1/1
4	NAG	C	329	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	334	NAG	C6-C5	2.16	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	NAG	C1-O5-C5	4.69	118.47	112.19
4	F	401	NAG	C1-O5-C5	4.51	118.22	112.19
4	B	401	NAG	C1-O5-C5	4.01	117.56	112.19
4	A	334	NAG	C1-O5-C5	3.84	117.33	112.19
4	E	334	NAG	C1-O5-C5	3.56	116.95	112.19
4	C	334	NAG	C1-O5-C5	3.34	116.67	112.19
4	C	348	NAG	C8-C7-N2	3.04	121.17	116.12
4	A	348	NAG	C1-O5-C5	3.04	116.26	112.19
4	E	348	NAG	C1-O5-C5	2.90	116.07	112.19
4	C	348	NAG	C1-O5-C5	2.64	115.73	112.19
4	C	329	NAG	C1-O5-C5	2.51	115.55	112.19
4	A	329	NAG	C1-O5-C5	2.45	115.47	112.19
4	A	348	NAG	C8-C7-N2	2.43	120.15	116.12
4	E	329	NAG	C1-O5-C5	2.40	115.41	112.19
4	E	348	NAG	C8-C7-N2	2.33	119.99	116.12
4	A	348	NAG	O4-C4-C5	2.30	114.99	109.32
4	E	348	NAG	C3-C4-C5	-2.28	106.10	110.23
4	F	401	NAG	C8-C7-N2	2.22	119.81	116.12
4	E	348	NAG	O4-C4-C5	2.21	114.76	109.32
4	A	348	NAG	C3-C4-C5	-2.14	106.36	110.23
4	C	348	NAG	O4-C4-C5	2.11	114.52	109.32
4	B	401	NAG	C8-C7-N2	2.06	119.54	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	E	348	NAG	C4-C5-C6-O6
4	C	348	NAG	C4-C5-C6-O6
4	C	348	NAG	O5-C5-C6-O6
4	E	348	NAG	O5-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%)	-0.02	17 (5%) 33 17	3, 20, 39, 140	0
1	C	328/328 (100%)	-0.00	18 (5%) 30 15	3, 20, 39, 138	0
1	E	328/328 (100%)	-0.10	19 (5%) 29 15	3, 20, 38, 137	0
2	B	175/175 (100%)	-0.15	10 (5%) 29 15	2, 14, 38, 87	0
2	D	175/175 (100%)	-0.17	7 (4%) 42 23	2, 14, 37, 88	0
2	F	175/175 (100%)	-0.25	7 (4%) 42 23	2, 14, 37, 87	0
All	All	1509/1509 (100%)	-0.09	78 (5%) 33 17	2, 18, 39, 140	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	ASN	6.2
1	C	327	GLN	6.2
1	E	327	GLN	5.5
1	A	2	ASP	5.4
1	E	7	ASP	4.9
1	E	8	ASN	4.9
1	A	328	THR	4.8
1	E	3	LEU	4.6
2	D	174	LYS	4.6
1	E	5	GLY	4.5
1	E	2	ASP	4.4
2	B	173	ILE	4.4
1	C	8	ASN	4.2
1	E	1	GLN	4.2
1	A	8	ASN	4.0
2	F	172	GLN	4.0
2	B	174	LYS	4.0
1	A	6	ASN	3.9
1	A	5	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	3.8
2	B	172	GLN	3.7
1	C	3	LEU	3.7
1	C	5	GLY	3.7
2	F	174	LYS	3.6
1	C	1	GLN	3.5
1	E	143	PRO	3.5
1	E	328	THR	3.5
1	E	4	PRO	3.3
2	D	175	GLY	3.3
1	C	160	THR	3.2
1	C	144	GLY	3.2
1	C	7	ASP	3.1
1	A	143	PRO	3.1
1	E	9	SER	3.0
1	A	3	LEU	2.9
2	B	145	ASP	2.9
2	D	173	ILE	2.9
2	F	173	ILE	2.9
1	C	4	PRO	2.8
1	E	6	ASN	2.7
1	C	328	THR	2.7
1	A	158	GLY	2.7
1	E	22	ASN	2.7
1	C	2	ASP	2.6
1	A	131	THR	2.6
2	D	58	LYS	2.6
1	A	157	SER	2.6
2	D	172	GLN	2.6
2	F	58	LYS	2.6
2	B	58	LYS	2.6
1	E	222	TRP	2.5
1	C	189	GLN	2.5
1	E	92	LYS	2.5
2	B	18	ILE	2.5
1	E	189	GLN	2.5
1	A	1	GLN	2.4
1	E	326	LYS	2.4
1	C	48	THR	2.3
1	A	192	THR	2.3
2	F	164	ASP	2.3
2	B	72	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	57	GLU	2.3
2	B	160	ASP	2.3
1	C	9	SER	2.3
1	E	186	SER	2.3
1	C	173	ASN	2.3
2	D	160	ASP	2.2
2	F	168	ASN	2.2
1	A	144	GLY	2.2
1	A	188	ASN	2.2
1	C	248	ASN	2.2
2	D	150	GLU	2.2
1	C	158	GLY	2.1
2	B	29	SER	2.1
1	A	326	LYS	2.1
1	E	144	GLY	2.0
1	A	4	PRO	2.0
2	B	164	ASP	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.

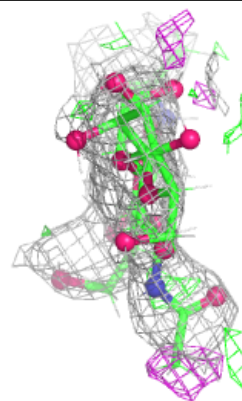
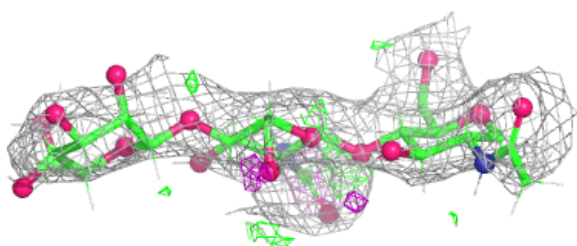
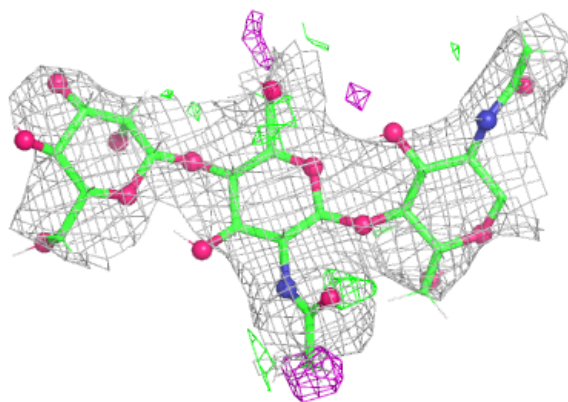
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.61	0.18	0,0,60,63	0
3	BMA	H	3	11/12	0.71	0.18	0,0,71,72	0
3	BMA	I	3	11/12	0.72	0.20	0,0,73,75	0
3	NAG	H	1	14/15	0.74	0.14	0,0,49,51	0
3	NAG	H	2	14/15	0.75	0.16	0,0,60,64	0
3	NAG	I	2	14/15	0.79	0.15	0,0,60,64	0
3	BMA	G	3	11/12	0.79	0.14	0,0,69,70	0
3	NAG	G	1	14/15	0.86	0.12	0,0,48,52	0
3	NAG	I	1	14/15	0.86	0.12	0,0,47,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

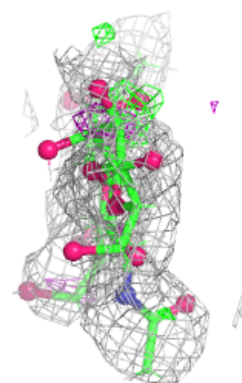
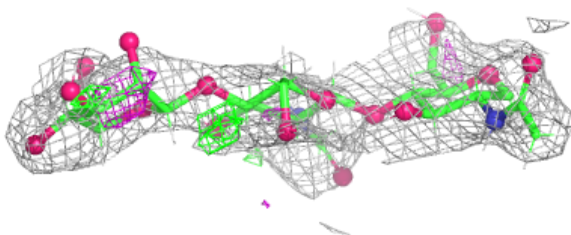
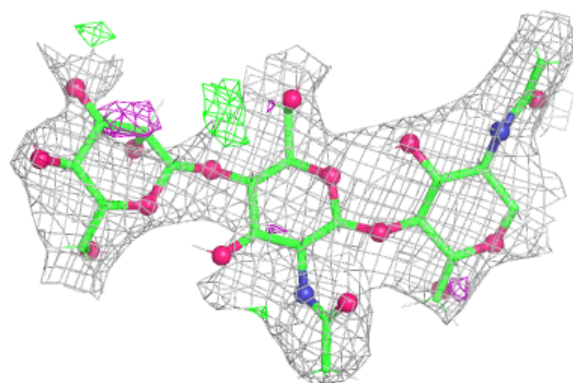
Electron density around Chain G:

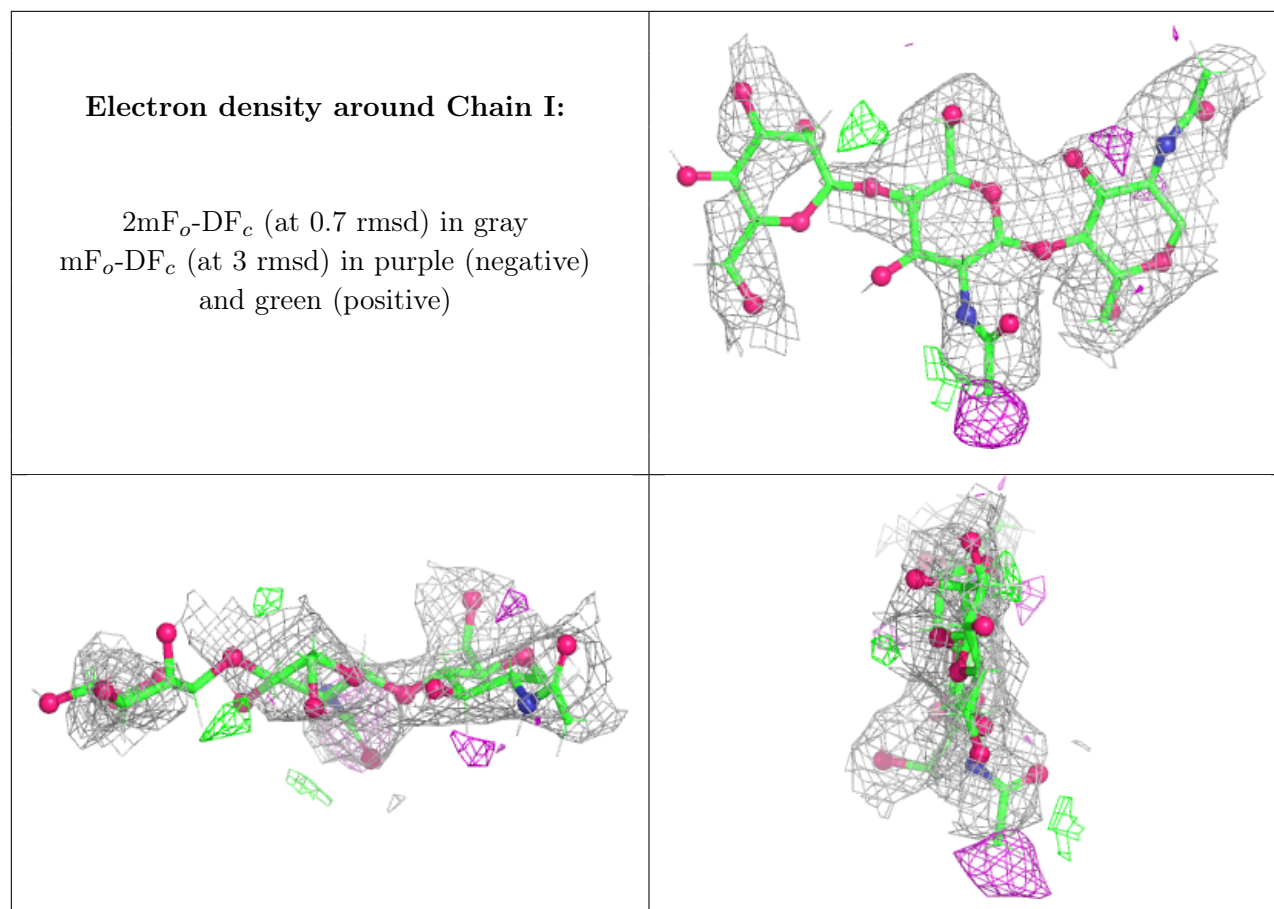
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	334	14/15	0.76	0.15	0,0,45,46	0
4	NAG	F	401	14/15	0.78	0.18	0,0,60,60	0
4	NAG	D	401	14/15	0.79	0.16	0,0,59,60	0
4	NAG	A	334	14/15	0.79	0.14	0,0,44,46	0
4	NAG	C	348	14/15	0.80	0.16	0,0,45,48	0
4	NAG	A	329	14/15	0.81	0.19	0,0,45,47	0
4	NAG	B	401	14/15	0.82	0.17	0,0,59,60	0
4	NAG	C	329	14/15	0.84	0.14	0,0,45,47	0
4	NAG	E	348	14/15	0.85	0.16	0,0,45,47	0
4	NAG	A	348	14/15	0.86	0.11	0,0,45,46	0
4	NAG	E	329	14/15	0.90	0.13	0,0,45,47	0
4	NAG	E	334	14/15	0.90	0.09	0,0,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.