



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 PM UTC

PDB ID : 3HMG / pdb_00003hmg
Title : REFINEMENT OF THE INFLUENZA VIRUS HEMAGGLUTININ BY SIMULATED ANNEALING
Authors : Weis, W.I.; Bruenger, A.T.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1989-09-11
Resolution : 2.90 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)
Validation Pipeline (wwPDB-VP)	:	2.49

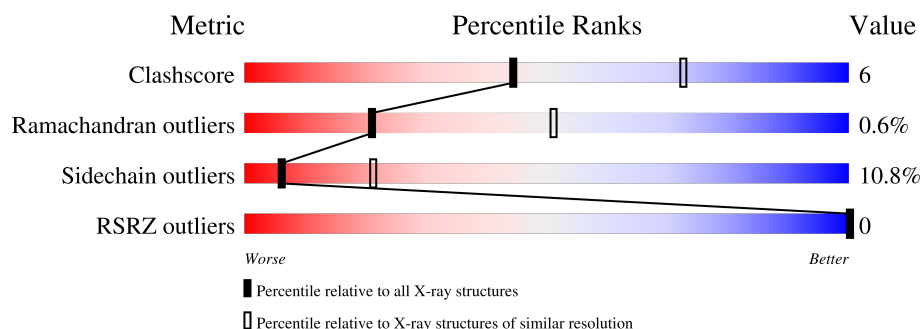
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	
3	G	3	

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Mol	Chain	Length	Quality of chain
3	H	3	 100%
3	I	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HEMAGGLUTININ.

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

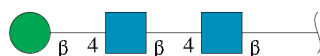
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called HEMAGGLUTININ.

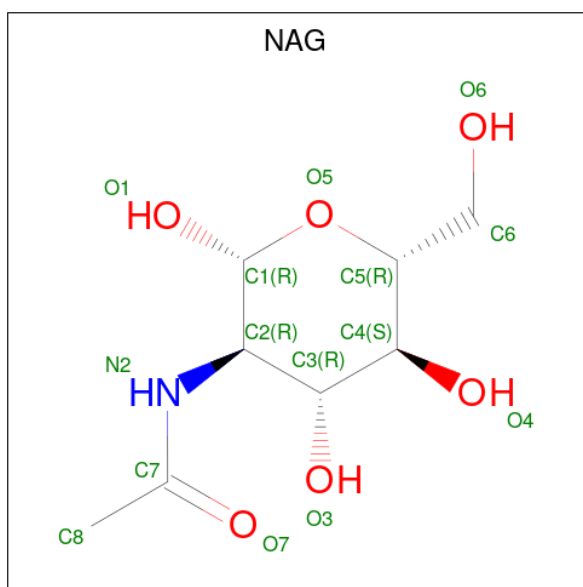
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	D	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	F	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

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

- Molecule 4 is 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	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is water.

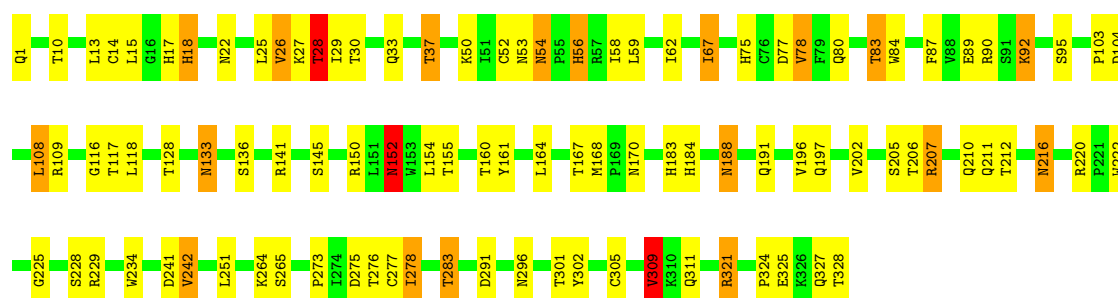
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	5	Total	O	0	0
			5	5		
5	C	6	Total	O	0	0
			6	6		
5	D	5	Total	O	0	0
			5	5		
5	E	6	Total	O	0	0
			6	6		
5	F	5	Total	O	0	0
			5	5		

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.

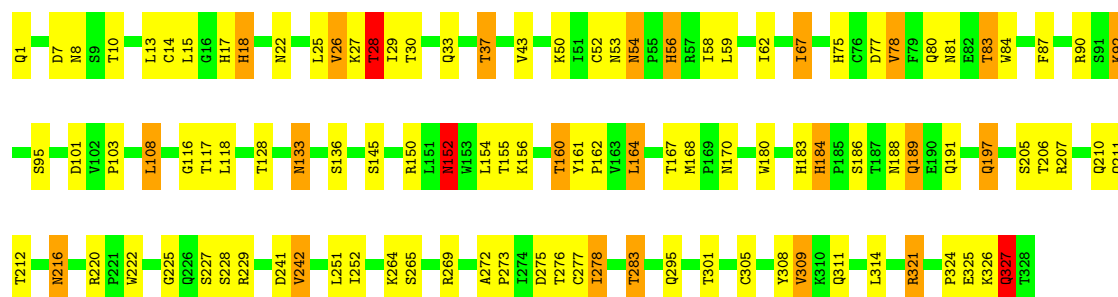
• Molecule 1: HEMAGGLUTININ

Chain A: 



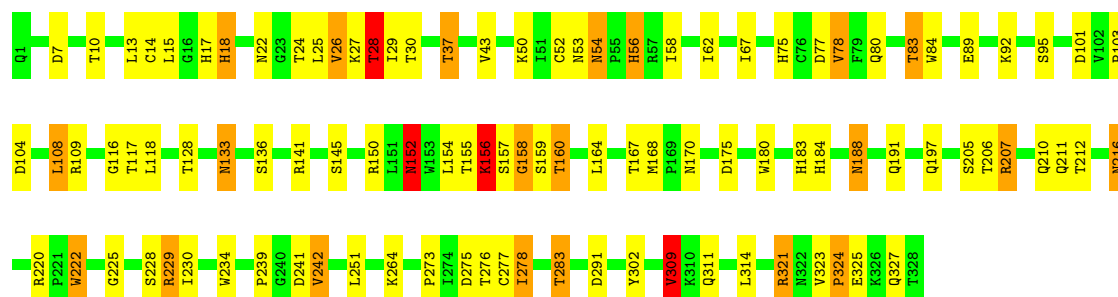
• Molecule 1: HEMAGGLUTININ

Chain C: 



• Molecule 1: HEMAGGLUTININ

Chain E: 



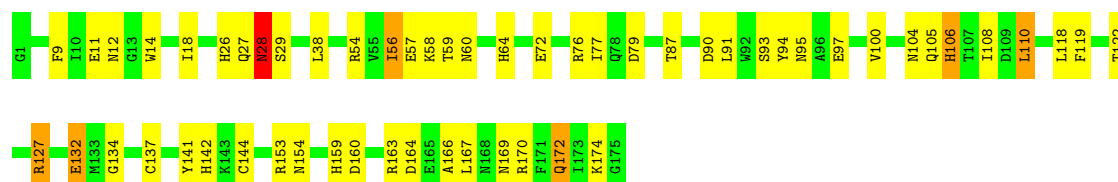
- Molecule 2: HEMAGGLUTININ

Chain B: 



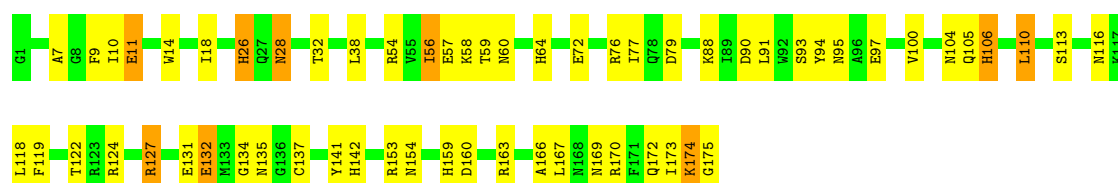
- Molecule 2: HEMAGGLUTININ

Chain D: 

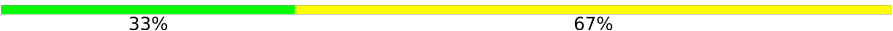


- Molecule 2: HEMAGGLUTININ

Chain F: 

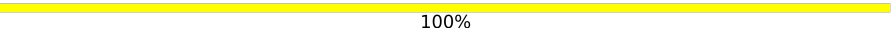


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

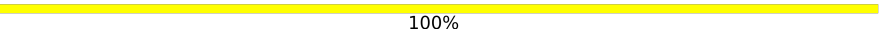


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 



- 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: 

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	162.80Å 162.80Å 177.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 0.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 0.0 (0.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.238 , (Not available) 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 169.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	12180	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality

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	1.12	7/2590 (0.3%)	1.78	52/3528 (1.5%)
1	C	1.13	9/2590 (0.3%)	1.81	55/3528 (1.6%)
1	E	1.13	8/2590 (0.3%)	1.79	55/3528 (1.6%)
2	B	1.21	9/1445 (0.6%)	1.83	30/1939 (1.5%)
2	D	1.24	10/1445 (0.7%)	1.81	28/1939 (1.4%)
2	F	1.20	8/1445 (0.6%)	1.84	29/1939 (1.5%)
All	All	1.16	51/12105 (0.4%)	1.80	249/16401 (1.5%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	HIS	CD2-NE2	-7.42	1.29	1.37
2	F	159	HIS	CG-ND1	-7.37	1.30	1.38
1	E	75	HIS	CD2-NE2	-7.31	1.29	1.37
1	A	75	HIS	CD2-NE2	-7.26	1.29	1.37
1	C	184	HIS	CD2-NE2	-6.97	1.30	1.37
2	F	159	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.86	1.30	1.37
1	E	184	HIS	CD2-NE2	-6.83	1.30	1.37
1	E	56	HIS	CD2-NE2	-6.72	1.30	1.37
2	B	64	HIS	CD2-NE2	-6.61	1.30	1.37
2	B	26	HIS	CD2-NE2	-6.60	1.30	1.37
1	C	75	HIS	CD2-NE2	-6.58	1.30	1.37
2	B	64	HIS	CG-ND1	-6.55	1.31	1.38
2	D	159	HIS	CG-ND1	-6.55	1.31	1.38
1	C	17	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.43	1.30	1.37
2	D	106	HIS	CD2-NE2	-6.43	1.30	1.37
2	B	159	HIS	CG-ND1	-6.42	1.31	1.38
2	D	26	HIS	CD2-NE2	-6.37	1.30	1.37
2	B	106	HIS	CD2-NE2	-6.33	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	HIS	CD2-NE2	-6.28	1.30	1.37
2	F	142	HIS	CD2-NE2	-6.26	1.30	1.37
2	B	142	HIS	CD2-NE2	-6.12	1.31	1.37
2	D	106	HIS	CG-ND1	-6.12	1.31	1.38
2	D	159	HIS	CD2-NE2	-6.03	1.31	1.37
1	E	184	HIS	CG-ND1	-6.02	1.31	1.38
2	D	142	HIS	CG-ND1	-5.99	1.31	1.38
2	F	26	HIS	CD2-NE2	-5.96	1.31	1.37
2	D	142	HIS	CD2-NE2	-5.95	1.31	1.37
1	E	17	HIS	CD2-NE2	-5.87	1.31	1.37
2	B	26	HIS	CG-ND1	-5.86	1.31	1.38
2	B	159	HIS	CD2-NE2	-5.83	1.31	1.37
1	C	183	HIS	CD2-NE2	-5.83	1.31	1.37
1	E	183	HIS	CG-ND1	-5.78	1.31	1.38
1	E	183	HIS	CD2-NE2	-5.78	1.31	1.37
2	B	142	HIS	CG-ND1	-5.77	1.31	1.38
1	C	18	HIS	CD2-NE2	-5.76	1.31	1.37
2	F	106	HIS	CG-ND1	-5.55	1.32	1.38
1	C	67	ILE	CA-CB	5.53	1.61	1.54
1	A	184	HIS	CG-ND1	-5.53	1.32	1.38
2	F	106	HIS	CD2-NE2	-5.48	1.31	1.37
2	D	64	HIS	CG-ND1	-5.45	1.32	1.38
2	D	64	HIS	CD2-NE2	-5.41	1.31	1.37
2	F	64	HIS	CD2-NE2	-5.41	1.31	1.37
1	C	184	HIS	CG-ND1	-5.30	1.32	1.38
2	F	142	HIS	CG-ND1	-5.28	1.32	1.38
1	A	183	HIS	CD2-NE2	-5.21	1.32	1.37
2	D	26	HIS	CG-ND1	-5.19	1.32	1.38
1	A	234	TRP	CG-CD2	-5.12	1.34	1.43
1	E	234	TRP	CG-CD2	-5.11	1.34	1.43
1	C	18	HIS	CG-ND1	-5.07	1.32	1.38

All (249) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	28	ASN	OD1-CG-ND2	-14.99	107.61	122.60
2	D	79	ASP	CA-CB-CG	12.92	125.52	112.60
2	F	79	ASP	CA-CB-CG	12.58	125.18	112.60
2	B	79	ASP	CA-CB-CG	12.54	125.14	112.60
2	B	172	GLN	OE1-CD-NE2	-10.90	111.70	122.60
2	F	9	PHE	CA-CB-CG	10.48	124.28	113.80
2	F	28	ASN	CB-CG-ND2	9.99	131.39	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASN	CA-CB-CG	9.55	122.15	112.60
1	E	152	ASN	OD1-CG-ND2	-9.35	113.25	122.60
2	D	9	PHE	CA-CB-CG	9.26	123.06	113.80
1	E	216	ASN	CA-CB-CG	9.26	121.86	112.60
2	B	9	PHE	CA-CB-CG	9.21	123.01	113.80
1	C	216	ASN	CA-CB-CG	9.19	121.79	112.60
2	B	95	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	E	28	THR	CA-CB-OG1	-8.69	96.56	109.60
1	C	56	HIS	ND1-CG-CD2	8.65	114.75	106.10
2	B	172	GLN	CB-CG-CD	8.49	127.04	112.60
1	A	28	THR	CA-CB-OG1	-8.31	97.14	109.60
2	F	95	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	E	56	HIS	ND1-CG-CD2	8.19	114.29	106.10
1	C	152	ASN	OD1-CG-ND2	-8.10	114.50	122.60
2	B	95	ASN	CB-CG-ND2	8.10	128.55	116.40
2	B	159	HIS	ND1-CG-CD2	7.96	114.06	106.10
2	F	95	ASN	CB-CG-ND2	7.95	128.32	116.40
1	C	184	HIS	ND1-CG-CD2	7.88	113.98	106.10
2	B	172	GLN	CG-CD-NE2	7.85	128.17	116.40
1	E	28	THR	CA-CB-CG2	7.85	123.84	110.50
1	C	189	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	A	152	ASN	OD1-CG-ND2	-7.78	114.82	122.60
2	F	159	HIS	ND1-CG-CD2	7.60	113.70	106.10
2	D	95	ASN	CB-CG-ND2	7.60	127.80	116.40
1	C	327	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	E	7	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	26	VAL	N-CA-CB	-7.53	99.79	112.44
1	C	28	THR	CA-CB-OG1	-7.53	98.31	109.60
2	D	95	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	A	28	THR	CA-CB-CG2	7.45	123.16	110.50
1	A	184	HIS	ND1-CG-CD2	7.45	113.55	106.10
2	B	106	HIS	ND1-CG-CD2	7.35	113.45	106.10
2	D	172	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	56	HIS	ND1-CG-CD2	7.25	113.34	106.10
1	C	28	THR	CA-CB-CG2	7.21	122.76	110.50
2	D	159	HIS	ND1-CG-CD2	7.20	113.30	106.10
1	E	184	HIS	ND1-CG-CD2	7.11	113.21	106.10
2	F	106	HIS	ND1-CG-CD2	7.00	113.11	106.10
2	D	153	ARG	NE-CZ-NH1	-6.98	114.52	121.50
2	D	104	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	C	26	VAL	N-CA-CB	-6.91	100.84	112.44
2	B	90	ASP	CA-CB-CG	6.83	119.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ASN	N-CA-C	6.82	120.90	111.90
1	C	197	GLN	CA-CB-CG	-6.78	100.53	114.10
2	B	154	ASN	CA-CB-CG	6.78	119.38	112.60
2	D	90	ASP	CA-CB-CG	6.74	119.34	112.60
2	B	132	GLU	CA-CB-CG	-6.73	100.64	114.10
2	D	132	GLU	CA-CB-CG	-6.73	100.65	114.10
1	A	75	HIS	CA-CB-CG	6.68	120.48	113.80
2	F	132	GLU	CA-CB-CG	-6.67	100.76	114.10
2	F	154	ASN	CA-CB-CG	6.62	119.22	112.60
1	C	191	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	C	283	THR	O-C-N	-6.60	117.19	121.88
1	E	26	VAL	N-CA-CB	-6.60	100.16	112.36
1	A	197	GLN	CA-CB-CG	-6.59	100.92	114.10
2	D	106	HIS	ND1-CG-CD2	6.57	112.67	106.10
2	F	90	ASP	CA-CB-CG	6.55	119.15	112.60
1	E	152	ASN	CB-CG-ND2	6.54	126.21	116.40
1	E	56	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	A	133	ASN	N-CA-C	6.46	120.42	111.90
1	C	56	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	E	191	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	E	197	GLN	CA-CB-CG	-6.42	101.26	114.10
1	A	170	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	E	75	HIS	CA-CB-CG	6.38	120.18	113.80
2	D	28	ASN	CB-CG-ND2	6.26	125.79	116.40
1	E	133	ASN	N-CA-C	6.26	120.16	111.90
1	C	183	HIS	ND1-CG-CD2	6.22	112.32	106.10
2	F	104	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	B	104	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	283	THR	CA-CB-OG1	-6.17	100.35	109.60
1	C	26	VAL	CA-CB-CG2	-6.16	99.92	110.40
1	E	156	LYS	N-CA-C	6.15	118.65	110.53
1	A	56	HIS	CB-CG-CD2	-6.14	123.22	131.20
2	D	154	ASN	CA-CB-CG	6.14	118.74	112.60
1	C	75	HIS	CA-CB-CG	6.14	119.94	113.80
1	C	188	ASN	CA-CB-CG	-6.11	106.50	112.60
1	E	101	ASP	CA-CB-CG	6.09	118.69	112.60
2	D	170	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	E	37	THR	CA-CB-OG1	-6.00	100.59	109.60
1	C	152	ASN	CB-CG-ND2	6.00	125.40	116.40
1	C	103	PRO	N-CA-C	-6.00	101.79	111.03
1	C	327	GLN	CG-CD-NE2	5.99	125.39	116.40
1	A	161	TYR	CA-C-N	5.99	126.45	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	TYR	C-N-CA	5.99	126.45	120.52
1	A	188	ASN	CA-CB-CG	-5.93	106.67	112.60
1	A	283	THR	O-C-N	-5.93	117.67	121.88
2	F	56	ILE	N-CA-CB	-5.91	101.47	111.23
1	A	37	THR	N-CA-CB	-5.91	101.12	110.22
1	E	183	HIS	ND1-CG-CD2	5.91	112.01	106.10
2	D	27	GLN	N-CA-C	-5.87	99.33	108.90
1	E	207	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	E	103	PRO	N-CA-C	-5.85	102.02	111.03
1	A	26	VAL	CA-CB-CG2	-5.85	100.46	110.40
1	C	37	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	78	VAL	CB-CA-C	-5.81	103.15	112.16
2	D	170	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	C	168	MET	CA-C-N	5.77	125.53	119.76
1	C	168	MET	C-N-CA	5.77	125.53	119.76
1	E	18	HIS	CB-CG-CD2	-5.77	123.69	131.20
2	B	60	ASN	CA-CB-CG	5.77	118.37	112.60
1	E	180	TRP	CG-CD2-CE3	5.77	139.67	133.90
2	D	56	ILE	N-CA-CB	-5.74	101.77	111.23
1	E	54	ASN	O-C-N	-5.73	117.37	121.84
1	E	184	HIS	CB-CG-CD2	-5.71	123.77	131.20
2	F	11	GLU	CB-CG-CD	5.71	122.31	112.60
2	F	170	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	183	HIS	ND1-CG-CD2	5.71	111.81	106.10
1	A	321	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	C	28	THR	N-CA-CB	-5.70	101.80	111.31
2	D	60	ASN	CA-CB-CG	5.69	118.29	112.60
1	C	78	VAL	CB-CA-C	-5.68	103.35	112.16
2	D	28	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	C	170	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	152	ASN	CB-CG-ND2	5.65	124.88	116.40
1	C	37	THR	N-CA-CB	-5.65	101.52	110.22
2	F	60	ASN	OD1-CG-ND2	-5.64	116.96	122.60
2	B	153	ARG	NE-CZ-NH1	-5.63	115.87	121.50
2	D	172	GLN	CG-CD-NE2	5.63	124.84	116.40
1	E	283	THR	O-C-N	-5.62	117.89	121.88
1	E	160	THR	N-CA-C	5.60	118.20	109.52
2	F	60	ASN	CA-CB-CG	5.60	118.20	112.60
2	B	159	HIS	CG-CD2-NE2	-5.58	101.62	107.20
1	A	191	GLN	OE1-CD-NE2	-5.58	117.03	122.60
2	B	76	ARG	N-CA-C	5.57	117.03	111.07
1	A	28	THR	N-CA-CB	-5.56	102.02	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	HIS	CG-CD2-NE2	-5.56	101.64	107.20
1	A	275	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	160	THR	N-CA-C	5.55	117.84	109.23
1	A	117	THR	CA-CB-OG1	-5.54	101.28	109.60
2	F	170	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	E	291	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	33	GLN	CB-CG-CD	-5.53	103.20	112.60
2	B	170	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	E	117	THR	CA-CB-OG1	-5.52	101.32	109.60
1	E	104	ASP	CA-C-O	5.52	128.10	121.65
2	B	60	ASN	OD1-CG-ND2	-5.50	117.10	122.60
2	B	27	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	168	MET	CA-C-N	5.45	125.36	119.85
1	A	168	MET	C-N-CA	5.45	125.36	119.85
1	E	283	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	37	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	324	PRO	O-C-N	5.43	129.74	123.06
2	B	150	GLU	CB-CG-CD	5.43	121.84	112.60
1	C	8	ASN	CA-CB-CG	5.43	118.03	112.60
2	F	153	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	E	188	ASN	CA-CB-CG	-5.42	107.18	112.60
1	E	222	TRP	CE2-CD2-CE3	5.42	124.22	118.80
1	E	83	THR	N-CA-CB	-5.42	101.45	111.52
1	E	17	HIS	CB-CG-CD2	-5.41	124.16	131.20
2	B	95	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	207	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	E	24	THR	CA-C-O	-5.41	114.86	120.70
1	E	309	VAL	N-CA-CB	-5.41	102.36	112.36
1	C	81	ASN	CA-CB-CG	5.40	118.00	112.60
2	D	95	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	54	ASN	O-C-N	-5.38	117.65	121.84
1	A	103	PRO	N-CA-C	-5.37	102.77	111.03
1	C	54	ASN	O-C-N	-5.36	117.66	121.84
1	C	180	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	E	170	ASN	OD1-CG-ND2	-5.36	117.25	122.60
1	C	184	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	A	321	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	C	269	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	C	128	THR	N-CA-C	5.34	117.45	108.96
1	C	117	THR	CA-CB-OG1	-5.33	101.60	109.60
2	F	76	ARG	N-CA-C	5.33	116.77	111.07
1	E	141	ARG	N-CA-C	-5.33	98.69	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	26	VAL	CA-CB-CG2	-5.33	101.34	110.40
1	E	28	THR	N-CA-CB	-5.33	102.41	111.31
1	C	83	THR	N-CA-CB	-5.32	101.62	111.52
1	A	104	ASP	CA-C-O	5.32	127.88	121.65
1	E	75	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	C	272	ALA	CA-C-N	5.31	125.07	119.76
1	C	272	ALA	C-N-CA	5.31	125.07	119.76
2	F	124	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	C	7	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	160	ASP	CA-CB-CG	-5.29	107.31	112.60
1	E	275	ASP	CA-CB-CG	5.28	117.88	112.60
1	E	37	THR	N-CA-CB	-5.28	102.10	110.22
2	D	60	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	E	128	THR	N-CA-C	5.25	117.32	108.96
2	F	160	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	18	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	A	325	GLU	CA-CB-CG	5.24	124.58	114.10
1	C	321	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	E	168	MET	CA-C-N	5.22	125.12	119.85
1	E	168	MET	C-N-CA	5.22	125.12	119.85
1	C	33	GLN	CB-CG-CD	-5.21	103.74	112.60
1	C	321	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	216	ASN	CB-CG-ND2	5.20	124.21	116.40
1	A	184	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	D	94	TYR	N-CA-C	-5.20	105.51	111.07
2	D	14	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	D	164	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	27	LYS	CB-CA-C	-5.17	100.78	109.83
1	A	291	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	153	ARG	CB-CG-CD	-5.17	99.41	111.30
1	C	326	LYS	O-C-N	5.17	127.67	122.09
2	F	135	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	83	THR	N-CA-CB	-5.15	101.93	111.52
1	A	309	VAL	N-CA-CB	-5.15	102.83	112.36
1	E	167	THR	CA-CB-OG1	-5.15	101.87	109.60
1	E	321	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	296	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	67	ILE	CA-C-O	-5.13	115.61	120.95
1	E	78	VAL	CB-CA-C	-5.12	104.22	112.16
2	F	14	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	E	27	LYS	CA-CB-CG	5.12	124.33	114.10
2	D	76	ARG	N-CA-C	5.11	116.54	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	ASP	CA-CB-CG	5.11	117.71	112.60
1	E	229	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	141	ARG	N-CA-C	-5.10	99.09	108.02
1	E	56	HIS	CG-CD2-NE2	-5.10	102.10	107.20
1	A	167	THR	CA-CB-OG1	-5.10	101.95	109.60
1	C	27	LYS	CB-CA-C	-5.09	100.91	109.83
2	D	160	ASP	CA-CB-CG	-5.09	107.51	112.60
2	F	124	ARG	CA-CB-CG	-5.08	103.93	114.10
1	E	180	TRP	CB-CG-CD1	-5.08	119.28	126.90
2	B	170	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	F	94	TYR	N-CA-C	-5.08	105.64	111.07
1	C	167	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	27	LYS	CA-CB-CG	5.07	124.24	114.10
1	C	17	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	C	183	HIS	CG-CD2-NE2	-5.06	102.14	107.20
2	B	135	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	C	275	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	17	HIS	CB-CG-CD2	-5.05	124.63	131.20
2	F	116	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	141	ARG	CA-CB-CG	-5.05	104.00	114.10
1	C	67	ILE	CA-C-O	-5.04	115.70	120.95
1	A	128	THR	N-CA-C	5.04	116.97	108.96
2	D	108	ILE	CA-C-O	-5.04	115.71	120.95
1	E	141	ARG	CA-CB-CG	-5.03	104.04	114.10
2	B	95	ASN	CA-C-O	-5.03	115.52	120.90
2	B	106	HIS	CG-CD2-NE2	-5.02	102.18	107.20
1	C	252	ILE	N-CA-C	-5.02	99.72	106.85
1	E	184	HIS	CG-CD2-NE2	-5.01	102.19	107.20
2	F	127	ARG	CG-CD-NE	-5.01	100.98	112.00
2	B	14	TRP	CE2-CD2-CG	-5.01	101.19	107.20
2	F	10	ILE	N-CA-CB	-5.00	105.36	111.67
2	B	124	ARG	CA-CB-CG	-5.00	104.10	114.10

There are no chirality outliers.

There are no planarity outliers.

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	2533	0	2470	37	0
1	C	2533	0	2470	43	0
1	E	2533	0	2470	36	0
2	B	1421	0	1345	21	0
2	D	1421	0	1345	18	0
2	F	1421	0	1345	24	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
4	A	42	0	39	0	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
4	D	14	0	13	0	0
4	E	42	0	39	0	0
4	F	14	0	13	0	0
5	A	6	0	0	0	0
5	B	5	0	0	0	0
5	C	6	0	0	0	0
5	D	5	0	0	0	0
5	E	6	0	0	0	0
5	F	5	0	0	0	0
All	All	12180	0	11703	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PRO:HG2	1:E:327:GLN:HA	1.63	0.81
1:A:53:ASN:OD1	1:A:276:THR:HA	1.93	0.68
1:E:53:ASN:OD1	1:E:276:THR:HA	1.95	0.67
1:C:77:ASP:O	1:C:80:GLN:HG3	1.94	0.67
1:C:53:ASN:OD1	1:C:276:THR:HA	1.94	0.66
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.78	0.65
1:E:77:ASP:O	1:E:80:GLN:HG3	1.96	0.65
1:A:160:THR:HA	1:A:196:VAL:HG21	1.80	0.63
1:E:67:ILE:HD12	1:E:108:LEU:HD13	1.80	0.63
1:A:1:GLN:N	2:F:175:GLY:HA3	2.13	0.63
1:A:1:GLN:H2	2:F:175:GLY:HA3	1.63	0.62
2:B:132:GLU:HG2	2:B:134:GLY:H	1.64	0.62
1:A:77:ASP:O	1:A:80:GLN:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:GLY:HA3	1:C:1:GLN:H2	1.66	0.61
2:F:132:GLU:HG2	2:F:134:GLY:H	1.65	0.61
1:C:161:TYR:HB3	1:C:197:GLN:NE2	2.16	0.60
1:C:67:ILE:HD12	1:C:108:LEU:HD13	1.84	0.60
2:D:28:ASN:HB2	2:D:144:CYS:O	2.02	0.60
2:B:175:GLY:HA3	1:C:1:GLN:N	2.17	0.59
2:D:132:GLU:HG2	2:D:134:GLY:H	1.67	0.59
1:A:67:ILE:HD12	1:A:108:LEU:HD13	1.85	0.59
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.38	0.58
1:C:50:LYS:HD2	1:C:273:PRO:HG2	1.85	0.58
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.86	0.58
1:E:50:LYS:HD2	1:E:273:PRO:HG2	1.86	0.57
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.39	0.57
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.40	0.57
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.40	0.56
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.41	0.56
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.41	0.55
1:A:50:LYS:HD2	1:A:273:PRO:HG2	1.87	0.55
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.89	0.55
2:B:141:TYR:O	2:B:166:ALA:HA	2.06	0.55
1:E:10:THR:HG22	2:F:141:TYR:HA	1.89	0.55
1:A:10:THR:HG22	2:B:141:TYR:HA	1.88	0.54
2:B:127:ARG:NH2	2:F:131:GLU:OE1	2.40	0.54
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.89	0.54
1:C:161:TYR:HB3	1:C:197:GLN:HE22	1.72	0.53
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.08	0.53
2:D:141:TYR:O	2:D:166:ALA:HA	2.09	0.53
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.90	0.53
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.90	0.52
1:C:136:SER:C	1:C:145:SER:HB2	2.34	0.52
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.57	0.52
1:A:136:SER:C	1:A:145:SER:HB2	2.34	0.52
1:E:136:SER:C	1:E:145:SER:HB2	2.35	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.10	0.51
1:C:54:ASN:O	1:C:278:ILE:HA	2.11	0.51
1:C:10:THR:HG22	2:D:141:TYR:HA	1.93	0.51
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.59	0.50
1:C:28:THR:HG23	2:D:105:GLN:OE1	2.12	0.50
1:C:207:ARG:HG2	1:C:241:ASP:OD1	2.11	0.50
1:E:207:ARG:HG2	1:E:241:ASP:OD1	2.10	0.50
1:C:220:ARG:HD3	1:C:229:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HG2	1:A:241:ASP:OD1	2.11	0.50
1:A:54:ASN:O	1:A:278:ILE:HA	2.12	0.50
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.59	0.50
1:E:220:ARG:HD3	1:E:229:ARG:HG2	1.94	0.49
2:B:131:GLU:OE1	2:D:127:ARG:NH2	2.45	0.49
1:E:156:LYS:HD3	1:E:158:GLY:O	2.13	0.49
1:C:309:VAL:HG22	2:D:93:SER:HA	1.94	0.49
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.95	0.49
1:A:309:VAL:HG22	2:B:93:SER:HA	1.94	0.48
2:F:58:LYS:HE2	2:F:59:THR:O	2.12	0.48
2:B:14:TRP:CZ2	2:B:25:ARG:HD3	2.49	0.48
1:C:133:ASN:H	1:C:152:ASN:ND2	2.12	0.48
1:E:54:ASN:O	1:E:278:ILE:HA	2.13	0.48
2:D:58:LYS:HE2	2:D:59:THR:O	2.14	0.48
1:A:220:ARG:HD3	1:A:229:ARG:HG2	1.96	0.48
2:B:58:LYS:HE2	2:B:59:THR:O	2.13	0.47
1:A:52:CYS:HB3	1:A:277:CYS:O	2.14	0.47
1:C:325:GLU:HB2	2:D:12:ASN:ND2	2.29	0.47
1:E:206:THR:HA	1:E:242:VAL:O	2.14	0.47
1:E:52:CYS:HB3	1:E:277:CYS:O	2.15	0.47
1:C:15:LEU:HD11	2:D:122:THR:HG21	1.97	0.47
1:C:52:CYS:HB3	1:C:277:CYS:O	2.13	0.47
1:C:206:THR:HA	1:C:242:VAL:O	2.15	0.47
1:E:309:VAL:HG22	2:F:93:SER:HA	1.96	0.46
1:A:133:ASN:H	1:A:152:ASN:ND2	2.13	0.46
1:A:206:THR:HA	1:A:242:VAL:O	2.15	0.45
1:A:15:LEU:HD11	2:B:122:THR:HG21	1.98	0.45
1:C:321:ARG:HG3	1:C:321:ARG:HH21	1.82	0.45
1:A:28:THR:HG22	1:A:30:THR:H	1.82	0.45
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.32	0.45
2:F:172:GLN:OE1	2:F:174:LYS:HB3	2.17	0.45
1:A:321:ARG:HH21	1:A:321:ARG:HG3	1.82	0.45
1:E:15:LEU:HD11	2:F:122:THR:HG21	1.98	0.45
1:E:133:ASN:H	1:E:152:ASN:HD21	1.65	0.45
1:A:133:ASN:H	1:A:152:ASN:HD21	1.64	0.45
1:A:28:THR:HG23	2:B:105:GLN:OE1	2.17	0.44
2:B:54:ARG:O	2:B:57:GLU:HB2	2.18	0.44
1:C:43:VAL:HG23	1:C:314:LEU:HB2	1.99	0.44
1:E:89:GLU:OE2	1:E:109:ARG:NH2	2.49	0.44
1:E:321:ARG:HH21	1:E:321:ARG:HG3	1.82	0.44
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASN:H	1:C:152:ASN:HD21	1.63	0.44
1:E:133:ASN:H	1:E:152:ASN:ND2	2.14	0.44
1:A:301:THR:HB	1:A:305:CYS:SG	2.57	0.44
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.53	0.43
1:A:90:ARG:HG3	1:A:92:LYS:HE2	1.99	0.43
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.34	0.43
2:F:54:ARG:O	2:F:57:GLU:HB2	2.18	0.43
2:D:54:ARG:O	2:D:57:GLU:HB2	2.17	0.43
1:C:59:LEU:HD23	1:C:87:PHE:CD1	2.53	0.43
1:C:161:TYR:CE1	1:C:164:LEU:HD22	2.53	0.43
1:C:186:SER:OG	1:C:227:SER:HB2	2.17	0.43
1:E:43:VAL:HG23	1:E:314:LEU:HB2	2.00	0.43
1:A:89:GLU:OE2	1:A:109:ARG:NH2	2.51	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.01	0.43
1:E:14:CYS:HA	2:F:137:CYS:HA	2.01	0.43
1:A:59:LEU:HD23	1:A:87:PHE:CD1	2.54	0.43
1:A:264:LYS:HD2	1:A:302:TYR:OH	2.18	0.43
1:C:216:ASN:HB2	1:C:220:ARG:HH12	1.84	0.42
1:C:90:ARG:HG3	1:C:92:LYS:HE2	2.00	0.42
2:D:106:HIS:CE1	2:D:110:LEU:HD12	2.53	0.42
2:D:163:ARG:O	2:D:167:LEU:HB2	2.19	0.42
2:B:164:ASP:OD1	2:F:173:ILE:HA	2.19	0.42
1:E:230:ILE:HD13	1:E:230:ILE:HG21	1.84	0.42
1:E:216:ASN:HB2	1:E:220:ARG:HH12	1.84	0.42
1:C:28:THR:HG22	1:C:30:THR:H	1.84	0.42
2:F:26:HIS:O	2:F:32:THR:HA	2.20	0.42
2:B:106:HIS:CE1	2:B:110:LEU:HD12	2.55	0.42
1:E:264:LYS:HD2	1:E:302:TYR:OH	2.20	0.42
1:A:14:CYS:HA	2:B:137:CYS:HA	2.02	0.42
1:E:175:ASP:OD2	1:E:239:PRO:HD3	2.20	0.42
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.55	0.42
1:C:161:TYR:HD1	1:C:162:PRO:O	2.02	0.41
2:F:163:ARG:O	2:F:167:LEU:HB2	2.20	0.41
1:C:184:HIS:ND1	1:C:216:ASN:N	2.67	0.41
2:F:106:HIS:CE1	2:F:110:LEU:HD12	2.55	0.41
2:B:14:TRP:CH2	2:B:25:ARG:HD3	2.56	0.41
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.56	0.41
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.36	0.41
1:A:202:VAL:O	1:A:212:THR:HA	2.21	0.41
2:B:110:LEU:O	2:B:113:SER:HB3	2.21	0.41
1:C:301:THR:HB	1:C:305:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HH21	1:A:109:ARG:HD2	1.64	0.40
1:C:161:TYR:HE1	1:C:164:LEU:HD22	1.87	0.40
2:D:91:LEU:HD13	2:F:91:LEU:HD13	2.02	0.40
1:C:295:GLN:O	1:C:308:TYR:HA	2.22	0.40
1:E:323:VAL:HG21	2:F:7:ALA:HB2	2.03	0.40
1:E:28:THR:HG22	1:E:30:THR:H	1.85	0.40
2:F:110:LEU:O	2:F:113:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/328 (99%)	312 (96%)	11 (3%)	3 (1%)	14	41
1	C	326/328 (99%)	315 (97%)	8 (2%)	3 (1%)	14	41
1	E	326/328 (99%)	313 (96%)	10 (3%)	3 (1%)	14	41
2	B	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
2	D	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
2	F	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
All	All	1497/1509 (99%)	1429 (96%)	59 (4%)	9 (1%)	21	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	GLN
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	E	158	GLY

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Mol	Chain	Res	Type
1	A	327	GLN
1	A	22	ASN
1	C	22	ASN
1	E	22	ASN

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%)	258 (89%)	31 (11%)	6	22
1	C	289/289 (100%)	255 (88%)	34 (12%)	5	17
1	E	289/289 (100%)	254 (88%)	35 (12%)	5	16
2	B	149/149 (100%)	135 (91%)	14 (9%)	8	26
2	D	149/149 (100%)	134 (90%)	15 (10%)	7	24
2	F	149/149 (100%)	136 (91%)	13 (9%)	9	30
All	All	1314/1314 (100%)	1172 (89%)	142 (11%)	6	21

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	18	HIS
1	A	25	LEU
1	A	26	VAL
1	A	28	THR
1	A	29	ILE
1	A	37	THR
1	A	58	ILE
1	A	78	VAL
1	A	83	THR
1	A	92	LYS
1	A	95	SER
1	A	108	LEU
1	A	118	LEU

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Mol	Chain	Res	Type
1	A	150	ARG
1	A	152	ASN
1	A	154	LEU
1	A	155	THR
1	A	164	LEU
1	A	188	ASN
1	A	205	SER
1	A	210	GLN
1	A	211	GLN
1	A	228	SER
1	A	242	VAL
1	A	251	LEU
1	A	265	SER
1	A	278	ILE
1	A	283	THR
1	A	309	VAL
1	A	328	THR
2	B	18	ILE
2	B	25	ARG
2	B	38	LEU
2	B	56	ILE
2	B	72	GLU
2	B	77	ILE
2	B	100	VAL
2	B	110	LEU
2	B	118	LEU
2	B	127	ARG
2	B	150	GLU
2	B	169	ASN
2	B	172	GLN
2	B	174	LYS
1	C	13	LEU
1	C	18	HIS
1	C	25	LEU
1	C	26	VAL
1	C	28	THR
1	C	29	ILE
1	C	37	THR
1	C	58	ILE
1	C	78	VAL
1	C	83	THR
1	C	92	LYS

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Mol	Chain	Res	Type
1	C	95	SER
1	C	108	LEU
1	C	118	LEU
1	C	150	ARG
1	C	152	ASN
1	C	154	LEU
1	C	155	THR
1	C	156	LYS
1	C	160	THR
1	C	164	LEU
1	C	189	GLN
1	C	205	SER
1	C	210	GLN
1	C	211	GLN
1	C	228	SER
1	C	242	VAL
1	C	251	LEU
1	C	265	SER
1	C	278	ILE
1	C	283	THR
1	C	309	VAL
1	C	324	PRO
1	C	327	GLN
2	D	11	GLU
2	D	18	ILE
2	D	28	ASN
2	D	29	SER
2	D	38	LEU
2	D	56	ILE
2	D	72	GLU
2	D	77	ILE
2	D	100	VAL
2	D	110	LEU
2	D	118	LEU
2	D	127	ARG
2	D	169	ASN
2	D	172	GLN
2	D	174	LYS
1	E	13	LEU
1	E	18	HIS
1	E	25	LEU
1	E	26	VAL

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Mol	Chain	Res	Type
1	E	28	THR
1	E	29	ILE
1	E	37	THR
1	E	58	ILE
1	E	78	VAL
1	E	83	THR
1	E	92	LYS
1	E	95	SER
1	E	108	LEU
1	E	118	LEU
1	E	150	ARG
1	E	152	ASN
1	E	154	LEU
1	E	155	THR
1	E	156	LYS
1	E	157	SER
1	E	159	SER
1	E	160	THR
1	E	164	LEU
1	E	188	ASN
1	E	205	SER
1	E	210	GLN
1	E	211	GLN
1	E	228	SER
1	E	242	VAL
1	E	251	LEU
1	E	278	ILE
1	E	283	THR
1	E	309	VAL
1	E	324	PRO
1	E	325	GLU
2	F	11	GLU
2	F	18	ILE
2	F	28	ASN
2	F	38	LEU
2	F	56	ILE
2	F	72	GLU
2	F	77	ILE
2	F	100	VAL
2	F	110	LEU
2	F	118	LEU
2	F	127	ARG

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Mol	Chain	Res	Type
2	F	169	ASN
2	F	174	LYS

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	1	GLN
1	A	96	ASN
1	A	132	GLN
1	A	152	ASN
1	A	171	ASN
1	A	248	ASN
1	A	327	GLN
2	B	27	GLN
2	B	65	GLN
1	C	96	ASN
1	C	132	GLN
1	C	152	ASN
1	C	171	ASN
1	C	248	ASN
2	D	65	GLN
1	E	1	GLN
1	E	96	ASN
1	E	132	GLN
1	E	152	ASN
1	E	171	ASN
1	E	248	ASN
2	F	12	ASN
2	F	28	ASN
2	F	65	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	1,3	14,14,15	0.55	0	17,19,21	1.12	1 (5%)
3	NAG	G	2	3	14,14,15	0.46	0	17,19,21	1.13	2 (11%)
3	BMA	G	3	3	11,11,12	0.57	0	15,15,17	0.81	0
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	1.19	1 (5%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	1.17	2 (11%)
3	BMA	H	3	3	11,11,12	0.88	0	15,15,17	1.62	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.70	0	17,19,21	1.13	3 (17%)
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	1.10	1 (5%)
3	BMA	I	3	3	11,11,12	1.21	1 (9%)	15,15,17	1.40	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	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	1,3	-	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	BMA	C4-C3	2.83	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	5.37	119.38	112.19
3	I	2	NAG	C4-C3-C2	-2.97	106.67	111.02
3	G	2	NAG	C4-C3-C2	-2.88	106.80	111.02
3	H	2	NAG	C4-C3-C2	-2.83	106.87	111.02
3	I	3	BMA	O5-C5-C4	-2.73	104.19	110.83
3	I	1	NAG	C2-N2-C7	2.62	126.41	122.90
3	G	1	NAG	C6-C5-C4	-2.45	107.01	113.02
3	H	1	NAG	C6-C5-C4	-2.43	107.05	113.02
3	I	3	BMA	C6-C5-C4	2.38	118.87	113.02
3	I	3	BMA	O2-C2-C1	2.27	114.43	109.22
3	H	2	NAG	C1-O5-C5	2.13	115.05	112.19
3	I	1	NAG	C1-O5-C5	2.09	114.99	112.19
3	I	1	NAG	C6-C5-C4	-2.07	107.93	113.02
3	G	2	NAG	C1-O5-C5	2.04	114.92	112.19
3	I	3	BMA	O5-C5-C6	2.02	111.59	107.66

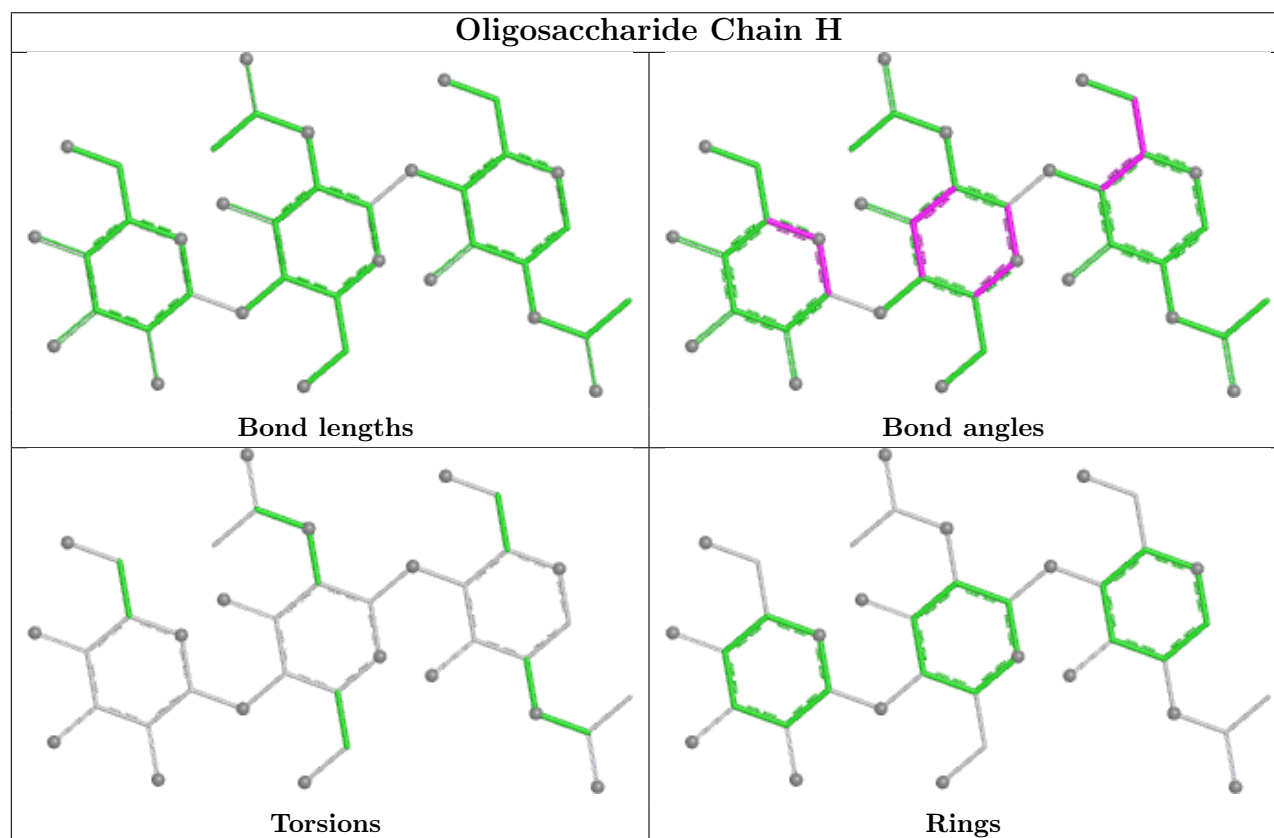
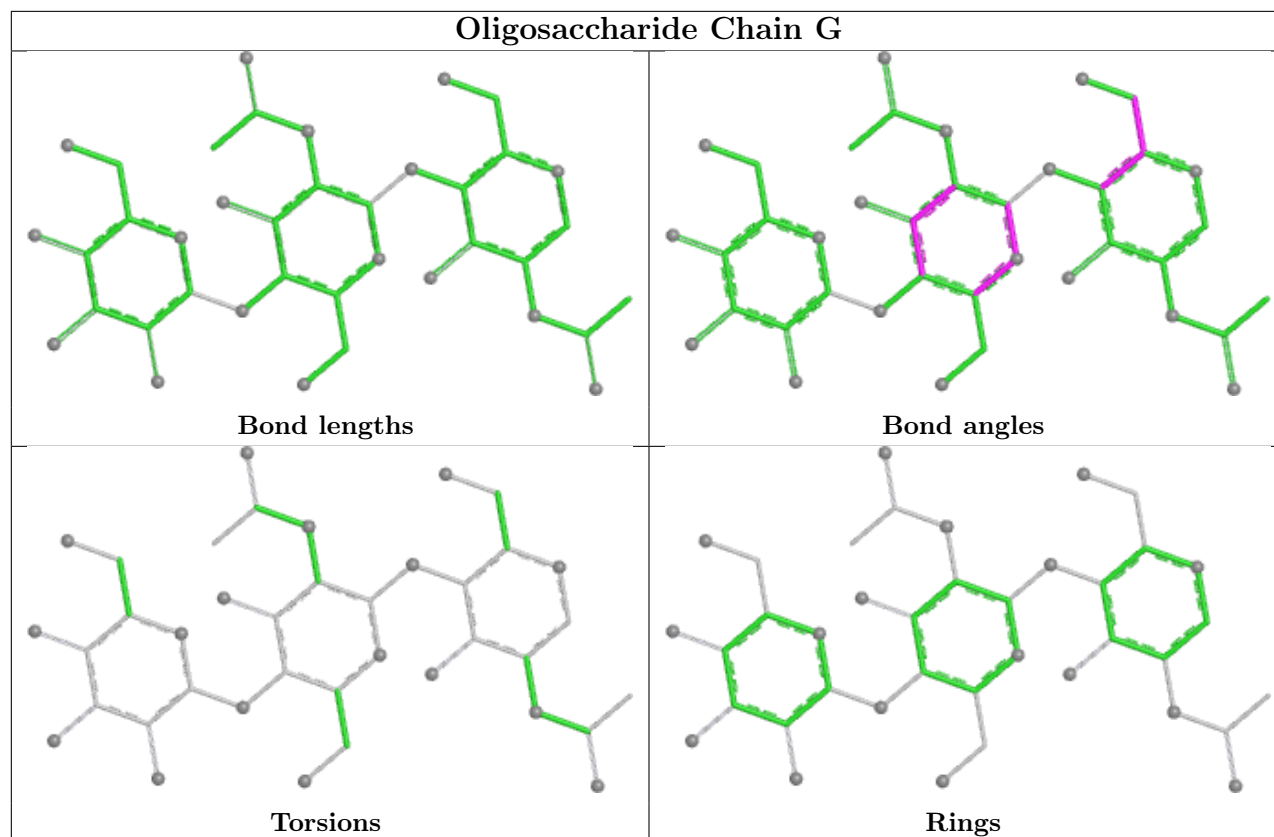
There are no chirality outliers.

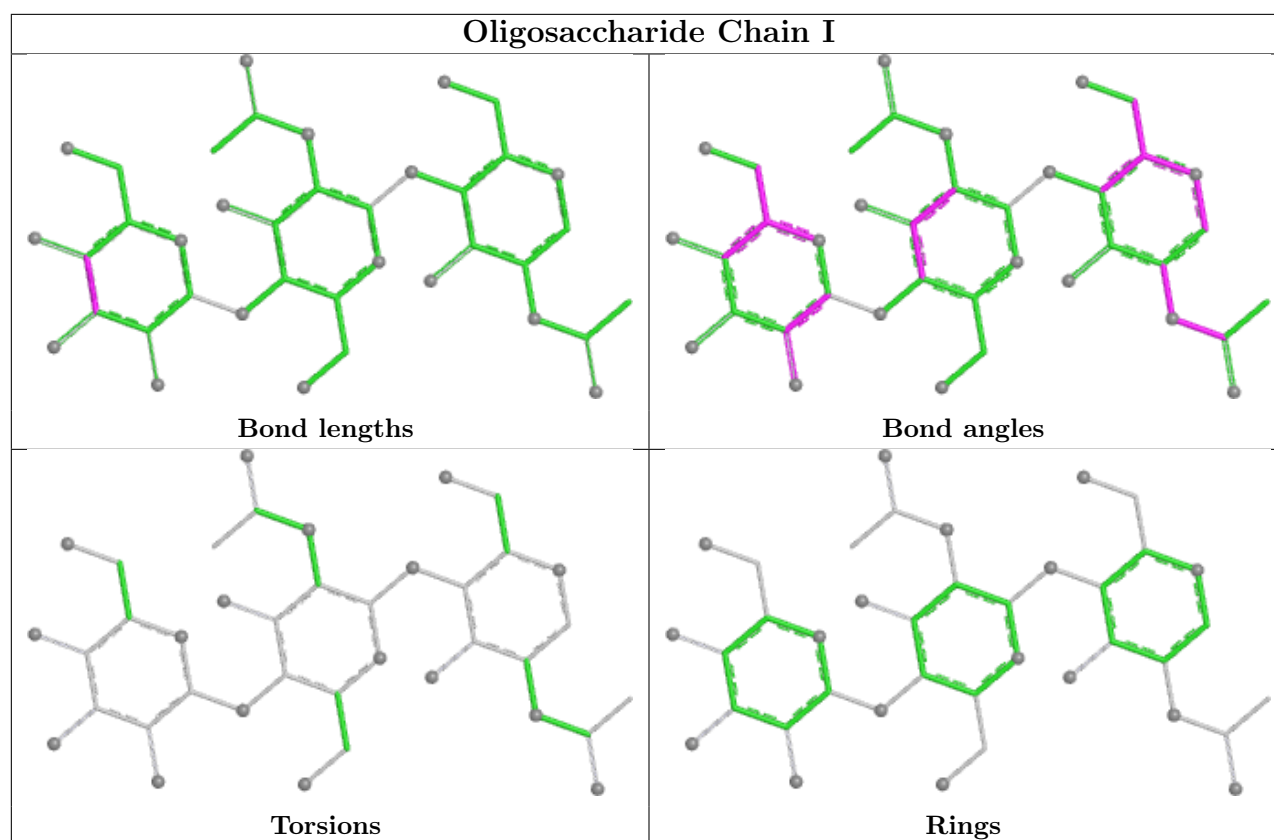
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [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	329	1	14,14,15	0.76	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	F	401	2	14,14,15	0.51	0	17,19,21	1.00	0
4	NAG	E	348	1	14,14,15	0.80	0	17,19,21	1.17	1 (5%)
4	NAG	A	329	1	14,14,15	0.91	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	E	329	1	14,14,15	0.80	0	17,19,21	0.96	1 (5%)
4	NAG	B	401	2	14,14,15	0.63	0	17,19,21	0.97	0
4	NAG	C	334	1	14,14,15	0.94	0	17,19,21	1.43	3 (17%)
4	NAG	D	401	2	14,14,15	0.44	0	17,19,21	0.92	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	0.74	0	17,19,21	1.15	1 (5%)
4	NAG	E	334	1	14,14,15	0.87	0	17,19,21	1.41	3 (17%)
4	NAG	A	334	1	14,14,15	0.94	0	17,19,21	1.45	3 (17%)
4	NAG	A	348	1	14,14,15	0.70	0	17,19,21	1.31	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	329	1	-	0/6/23/26	0/1/1/1
4	NAG	F	401	2	-	0/6/23/26	0/1/1/1
4	NAG	E	348	1	-	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	B	401	2	-	0/6/23/26	0/1/1/1
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	NAG	C	348	1	-	2/6/23/26	0/1/1/1
4	NAG	E	334	1	-	1/6/23/26	0/1/1/1
4	NAG	A	334	1	-	1/6/23/26	0/1/1/1
4	NAG	A	348	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	2.28	1.57	1.53
4	C	329	NAG	C4-C5	2.12	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	348	NAG	C1-O5-C5	3.50	116.88	112.19
4	E	329	NAG	C1-O5-C5	3.15	116.41	112.19
4	A	334	NAG	C1-O5-C5	2.95	116.14	112.19
4	A	329	NAG	C1-O5-C5	2.93	116.11	112.19
4	E	348	NAG	C1-O5-C5	2.89	116.06	112.19
4	C	329	NAG	C1-O5-C5	2.84	116.00	112.19
4	E	334	NAG	C1-C2-N2	2.68	114.66	110.43
4	E	334	NAG	C1-O5-C5	2.67	115.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	334	NAG	C1-O5-C5	2.61	115.68	112.19
4	C	348	NAG	C1-O5-C5	2.58	115.64	112.19
4	A	334	NAG	C2-N2-C7	-2.57	119.45	122.90
4	A	334	NAG	C1-C2-N2	2.48	114.34	110.43
4	C	334	NAG	C1-C2-N2	2.36	114.16	110.43
4	A	348	NAG	C8-C7-N2	2.29	119.92	116.12
4	E	334	NAG	C8-C7-N2	2.27	119.88	116.12
4	C	334	NAG	C8-C7-N2	2.24	119.83	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	334	NAG	C1-C2-N2-C7
4	E	334	NAG	C1-C2-N2-C7
4	C	348	NAG	C4-C5-C6-O6
4	C	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-2.40	0 100 100	5, 23, 53, 141	0
1	C	328/328 (100%)	-2.40	0 100 100	5, 24, 48, 145	0
1	E	328/328 (100%)	-2.40	0 100 100	4, 23, 50, 143	0
2	B	175/175 (100%)	-2.43	0 100 100	3, 18, 48, 97	0
2	D	175/175 (100%)	-2.43	0 100 100	3, 18, 47, 98	0
2	F	175/175 (100%)	-2.43	0 100 100	3, 18, 48, 98	0
All	All	1509/1509 (100%)	-2.41	0 100 100	3, 22, 51, 145	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

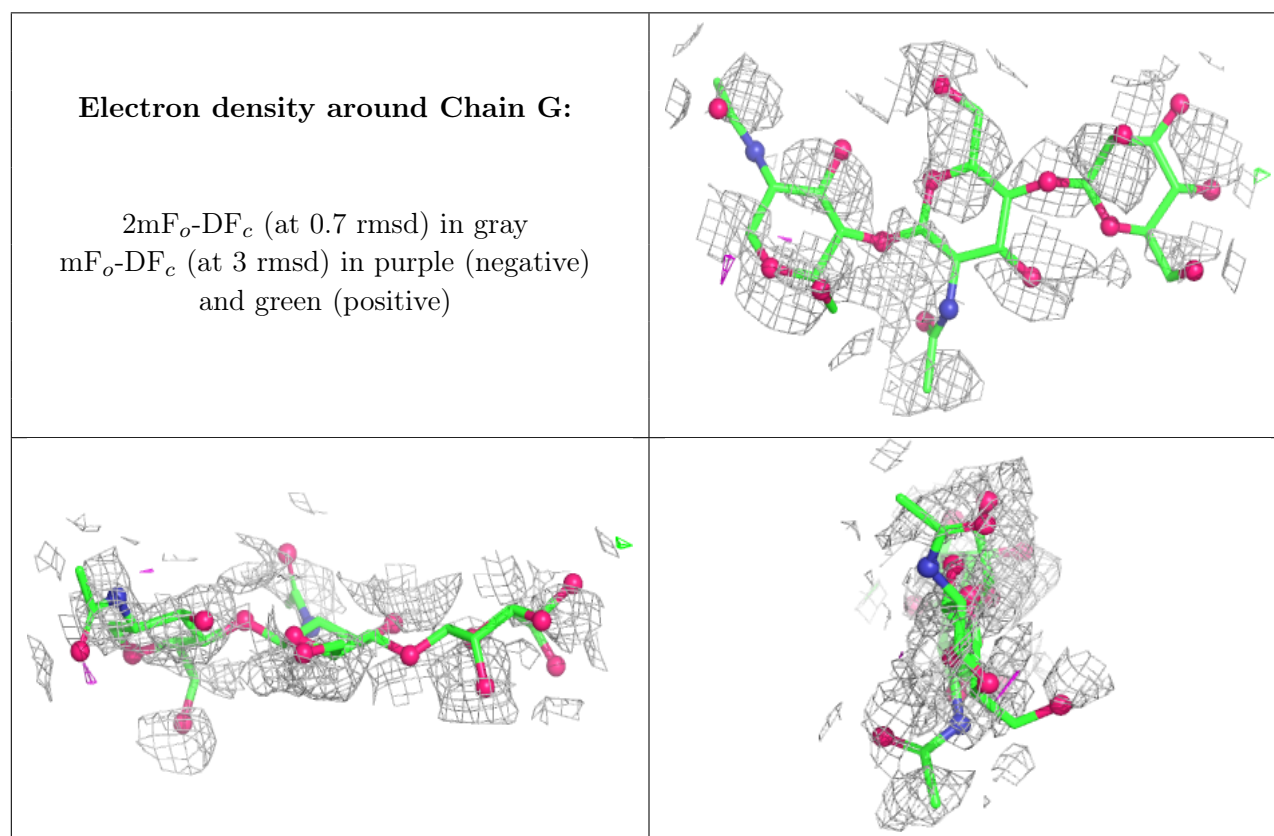
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	I	1	14/15	0.28	0.00	41,44,46,48	0
3	NAG	H	2	14/15	0.52	0.00	51,54,57,58	0
3	BMA	G	3	11/12	0.64	0.00	59,61,62,62	0
3	NAG	H	1	14/15	0.64	0.00	42,45,48,48	0
3	BMA	I	3	11/12	0.75	0.00	61,63,64,64	0
3	NAG	G	1	14/15	0.78	0.00	43,46,47,49	0

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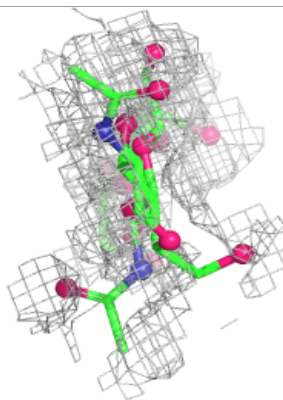
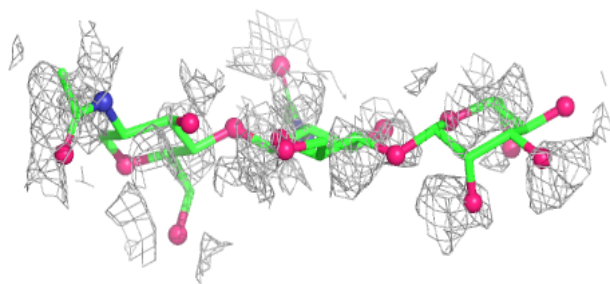
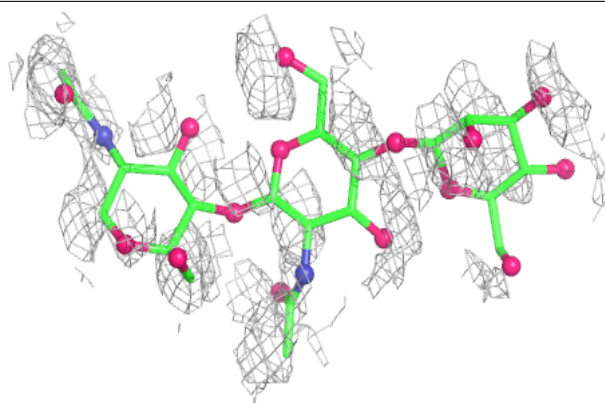
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	I	2	14/15	0.83	0.00	51,55,56,59	0
3	BMA	H	3	11/12	0.84	0.00	61,63,66,66	0
3	NAG	G	2	14/15	0.84	0.00	52,54,56,58	0

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.

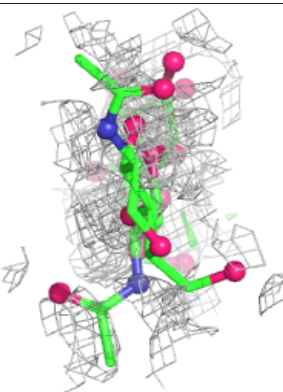
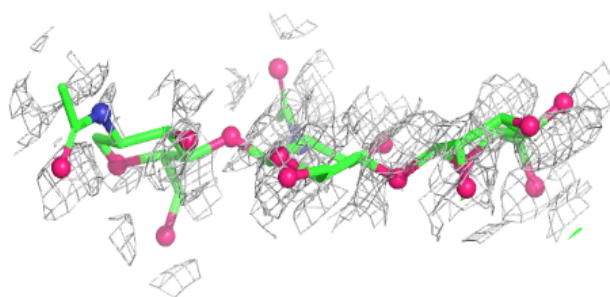
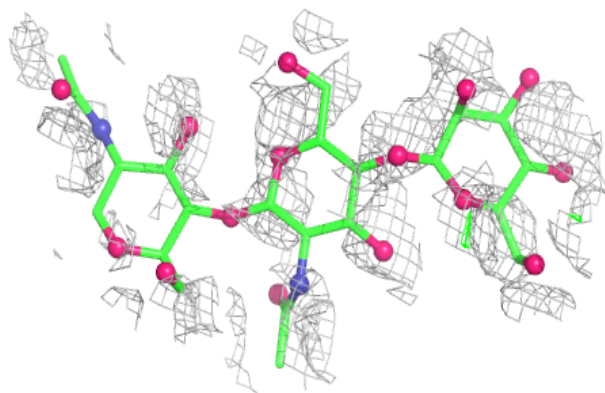


Electron density around Chain H:

$2mF_o-DF_c$ (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	0.58	0.00	36,39,42,42	0
4	NAG	B	401	14/15	0.59	0.00	50,54,55,56	0
4	NAG	F	401	14/15	0.66	0.00	49,52,54,55	0
4	NAG	E	329	14/15	0.68	0.00	38,42,43,45	0
4	NAG	E	348	14/15	0.69	0.00	34,38,40,42	0
4	NAG	C	329	14/15	0.69	0.00	38,42,43,44	0
4	NAG	D	401	14/15	0.72	0.00	50,53,55,56	0
4	NAG	E	334	14/15	0.76	0.00	36,39,41,41	0
4	NAG	A	329	14/15	0.77	0.00	38,42,43,44	0
4	NAG	C	348	14/15	0.78	0.00	35,39,41,43	0
4	NAG	A	348	14/15	0.84	0.00	34,38,40,41	0
4	NAG	A	334	14/15	0.85	0.00	35,39,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.