



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:42 AM UTC

PDB ID : 1NMA / pdb_00001nma
Title : N9 NEURAMINIDASE COMPLEXES WITH ANTIBODIES NC41 AND NC10: EMPIRICAL FREE-ENERGY CALCULATIONS CAPTURE SPECIFICITY TRENDS OBSERVED WITH MUTANT BINDING DATA
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Deposited on : 1994-05-06
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

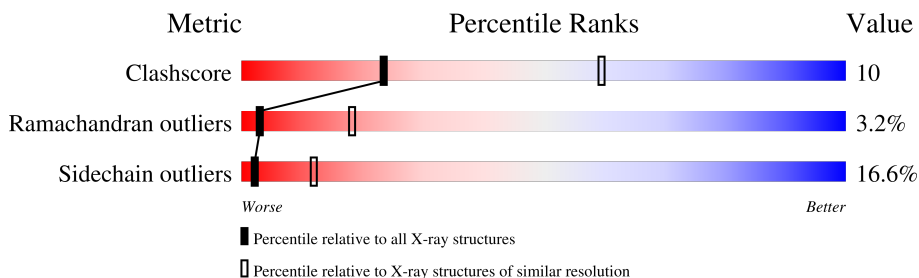
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	
2	L	109	
3	H	122	
4	A	6	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4863 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 N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	378	Total	C	N	O	S	0	0	0
			2979	1851	527	578	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	387	LYS	ARG	conflict	UNP P05803
N	389	ARG	LYS	conflict	UNP P05803

- Molecule 2 is a protein called FAB NC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	109	Total	C	N	O	S	0	0	0
			853	530	142	178	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLN	GLU	conflict	GB 501094
L	4	MET	LEU	conflict	GB 501094

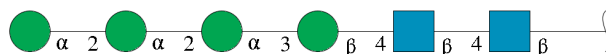
- Molecule 3 is a protein called FAB NC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	122	Total	C	N	O	S	0	0	0
			945	594	154	192	5			

There are 2 discrepancies between the modelled and reference sequences:

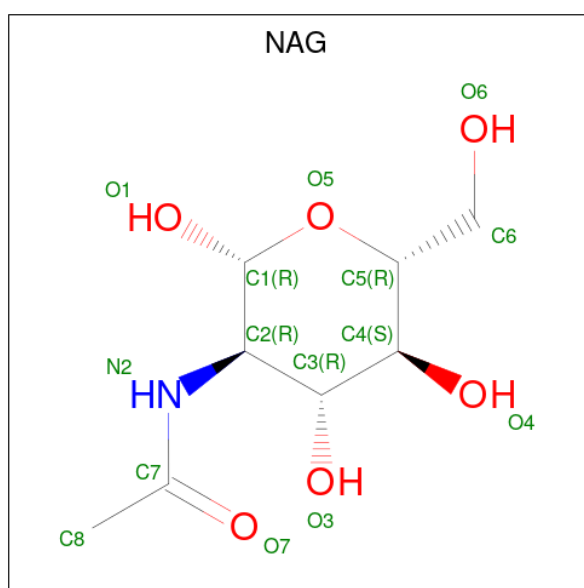
Chain	Residue	Modelled	Actual	Comment	Reference
H	7	PRO	SER	conflict	GB 501094
H	109	LEU	VAL	conflict	GB 501094

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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
4	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



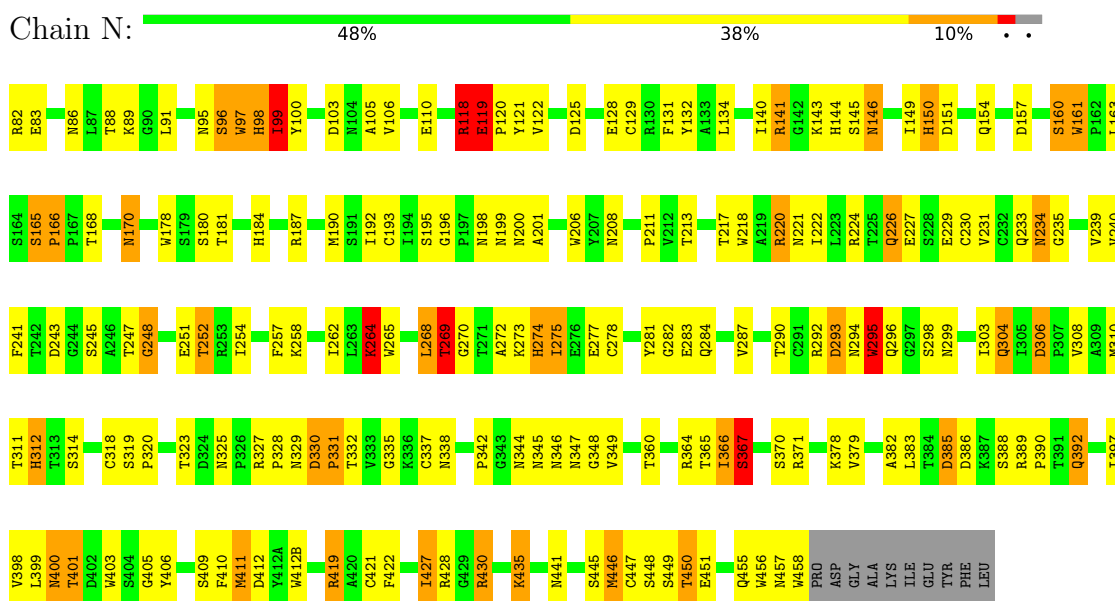
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

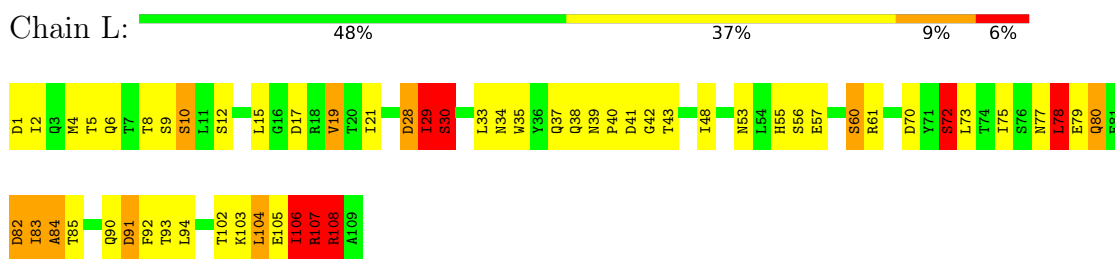
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

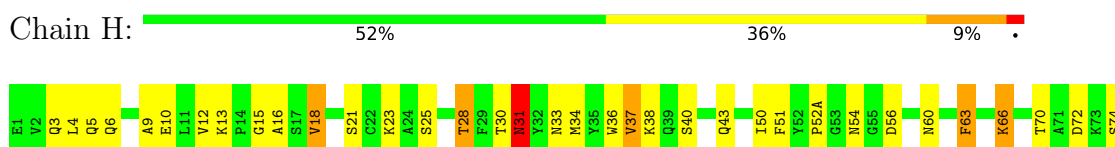
• Molecule 1: N9 NEURAMINIDASE

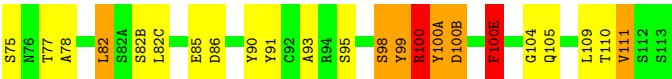


• Molecule 2: FAB NC10



• Molecule 3: FAB NC10





● Molecule 4: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	171.50Å 171.50Å 160.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	N	1.04	9/3058 (0.3%)	2.07	136/4167 (3.3%)
2	L	0.96	1/869 (0.1%)	1.99	29/1178 (2.5%)
3	H	0.91	0/969	2.05	35/1311 (2.7%)
All	All	1.00	10/4896 (0.2%)	2.05	200/6656 (3.0%)

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	N	0	2
2	L	0	2
3	H	0	2
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	98	HIS	CD2-NE2	-7.42	1.29	1.37
1	N	184	HIS	CD2-NE2	-6.87	1.30	1.37
1	N	312	HIS	CD2-NE2	-6.63	1.30	1.37
1	N	274	HIS	CD2-NE2	-6.54	1.30	1.37
1	N	144	HIS	CD2-NE2	-6.16	1.31	1.37
1	N	150	HIS	CD2-NE2	-5.82	1.31	1.37
2	L	55	HIS	CD2-NE2	-5.53	1.31	1.37
1	N	184	HIS	CG-ND1	-5.32	1.32	1.38
1	N	252	THR	CA-CB	5.22	1.61	1.53
1	N	166	PRO	CA-CB	-5.04	1.49	1.54

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	56	ASP	CA-CB-CG	13.40	126.00	112.60
2	L	2	ILE	N-CA-C	-12.74	89.33	107.80
1	N	386	ASP	CA-CB-CG	12.54	125.14	112.60
1	N	226	GLN	N-CA-C	12.43	127.89	112.23
1	N	157	ASP	CA-CB-CG	11.03	123.63	112.60
3	H	33	ASN	CA-CB-CG	10.77	123.36	112.60
1	N	412	ASP	CA-CB-CG	10.04	122.64	112.60
1	N	274	HIS	CA-CB-CG	9.31	123.11	113.80
1	N	198	ASN	OD1-CG-ND2	-9.23	113.37	122.60
1	N	146	ASN	OD1-CG-ND2	-9.19	113.41	122.60
1	N	243	ASP	CA-CB-CG	8.86	121.45	112.60
1	N	401	THR	N-CA-CB	-8.85	95.98	110.40
3	H	100	ARG	NE-CZ-NH2	-8.70	111.37	119.20
1	N	306	ASP	CA-CB-CG	8.43	121.03	112.60
1	N	88	THR	N-CA-CB	-8.36	98.11	110.49
3	H	100	ARG	NE-CZ-NH1	8.28	129.78	121.50
1	N	226	GLN	OE1-CD-NE2	-8.12	114.48	122.60
2	L	29	ILE	N-CA-CB	-8.03	97.98	111.23
1	N	390	PRO	N-CA-C	7.98	122.85	110.80
1	N	344	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	N	335	GLY	O-C-N	-7.85	117.90	123.95
1	N	103	ASP	CA-CB-CG	7.78	120.38	112.60
1	N	146	ASN	CB-CG-ND2	7.38	127.47	116.40
3	H	98	SER	N-CA-C	7.34	121.59	111.90
2	L	92	PHE	N-CA-C	-7.34	102.45	111.40
2	L	1	ASP	CA-CB-CG	7.31	119.91	112.60
1	N	100	TYR	N-CA-C	-7.28	102.37	112.12
3	H	86	ASP	CA-CB-CG	7.23	119.83	112.60
3	H	100(B)	ASP	CA-CB-CG	7.21	119.81	112.60
1	N	385	ASP	CA-C-N	7.21	131.26	120.31
1	N	385	ASP	C-N-CA	7.21	131.26	120.31
3	H	100	ARG	CB-CG-CD	-7.03	95.14	111.30
3	H	100	ARG	NH1-CZ-NH2	-6.99	110.22	119.30
1	N	226	GLN	CG-CD-NE2	6.87	126.71	116.40
1	N	220	ARG	N-CA-C	6.83	125.35	110.80
1	N	400	ASN	CA-CB-CG	6.82	119.42	112.60
1	N	99	ILE	CB-CA-C	-6.82	101.06	111.08
1	N	234	ASN	N-CA-C	6.80	120.79	111.54
1	N	344	ASN	CB-CG-ND2	6.77	126.55	116.40
2	L	77	ASN	CA-CB-CG	-6.76	105.84	112.60
3	H	63	PHE	CA-CB-CG	-6.74	107.06	113.80
2	L	28	ASP	CA-C-O	6.73	128.25	120.98
2	L	56	SER	N-CA-C	6.71	118.25	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	406	TYR	N-CA-C	6.70	119.95	110.23
2	L	37	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	N	403	TRP	CG-CD2-CE3	6.67	140.57	133.90
1	N	304	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	N	199	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	N	392	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	N	405	GLY	CA-C-O	-6.62	116.34	120.91
1	N	83	GLU	N-CA-C	-6.61	96.73	110.80
2	L	39	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	N	319	SER	N-CA-C	6.52	124.22	109.81
3	H	100(A)	TYR	N-CA-C	-6.46	100.61	109.71
1	N	265	TRP	CG-CD2-CE3	6.40	140.30	133.90
1	N	125	ASP	O-C-N	-6.35	116.60	121.55
3	H	33	ASN	OD1-CG-ND2	-6.33	116.27	122.60
3	H	72	ASP	CA-CB-CG	6.29	118.89	112.60
1	N	448	SER	CA-CB-OG	6.27	123.64	111.10
1	N	151	ASP	N-CA-C	6.27	120.71	111.87
1	N	119	GLU	CA-CB-CG	6.25	126.60	114.10
1	N	409	SER	N-CA-C	6.23	119.85	109.95
1	N	360	THR	CA-C-O	6.22	126.96	120.30
2	L	108	ARG	CD-NE-CZ	-6.21	115.70	124.40
2	L	6	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	N	345	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	N	347	ASN	O-C-N	-6.21	117.08	123.29
2	L	107	ARG	CG-CD-NE	-6.16	98.44	112.00
1	N	319	SER	CA-C-N	6.14	126.67	120.04
1	N	319	SER	C-N-CA	6.14	126.67	120.04
1	N	89	LYS	N-CA-C	6.11	117.86	109.18
3	H	82	LEU	N-CA-C	-6.10	99.24	109.07
1	N	338	ASN	N-CA-C	6.09	121.46	113.30
1	N	118	ARG	CD-NE-CZ	-6.06	115.92	124.40
1	N	422	PHE	CA-CB-CG	6.06	119.86	113.80
2	L	39	ASN	CA-C-N	6.06	127.41	119.84
2	L	39	ASN	C-N-CA	6.06	127.41	119.84
1	N	86	ASN	CA-CB-CG	6.05	118.65	112.60
1	N	456	TRP	CG-CD2-CE3	6.04	139.94	133.90
2	L	34	ASN	OD1-CG-ND2	-6.04	116.56	122.60
3	H	78	ALA	N-CA-C	-6.04	101.58	110.52
1	N	337	CYS	N-CA-C	6.02	117.92	111.36
1	N	131	PHE	CA-CB-CG	6.02	119.82	113.80
1	N	265	TRP	CB-CG-CD1	-6.02	117.87	126.90
2	L	19	VAL	N-CA-CB	-6.01	99.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	29	ILE	CB-CG1-CD1	-6.00	101.21	113.80
1	N	342	PRO	N-CA-C	5.99	120.05	111.13
1	N	274	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	N	269	THR	CA-CB-OG1	-5.96	100.66	109.60
2	L	61	ARG	N-CA-C	5.94	120.53	113.28
1	N	401	THR	CB-CA-C	5.93	122.38	109.99
1	N	299	ASN	N-CA-C	-5.91	101.25	110.42
1	N	448	SER	N-CA-C	5.91	118.17	110.43
2	L	35	TRP	CG-CD2-CE3	5.90	139.80	133.90
1	N	331	PRO	N-CA-C	5.90	120.26	111.41
1	N	296	GLN	N-CA-C	5.89	120.59	113.41
1	N	180	SER	N-CA-C	5.89	116.33	108.38
2	L	30	SER	CA-C-O	-5.88	112.10	120.51
3	H	100(E)	PHE	CA-CB-CG	5.88	119.68	113.80
1	N	345	ASN	CA-C-O	-5.88	114.76	121.40
1	N	241	PHE	CA-CB-CG	5.86	119.66	113.80
2	L	91	ASP	CA-CB-CG	5.84	118.44	112.60
1	N	98	HIS	CB-CG-CD2	-5.84	123.61	131.20
3	H	60	ASN	OD1-CG-ND2	-5.83	116.77	122.60
3	H	100	ARG	CB-CA-C	-5.83	99.68	109.53
1	N	278	CYS	N-CA-C	5.82	118.01	108.52
2	L	72	SER	N-CA-C	5.79	118.92	109.59
1	N	88	THR	CA-CB-OG1	-5.78	100.94	109.60
1	N	430	ARG	CA-CB-CG	-5.77	102.55	114.10
1	N	441	ASN	N-CA-C	5.76	116.16	108.38
1	N	344	ASN	O-C-N	-5.76	116.30	123.04
1	N	82	ARG	N-CA-C	-5.75	94.90	111.00
2	L	41	ASP	CA-C-O	5.75	126.53	120.33
1	N	410	PHE	CA-CB-CG	5.73	119.53	113.80
3	H	105	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	N	233	GLN	OE1-CD-NE2	-5.71	116.89	122.60
3	H	31	ASN	CA-CB-CG	5.70	118.30	112.60
1	N	345	ASN	CB-CG-ND2	5.70	124.95	116.40
1	N	293	ASP	CA-CB-CG	5.70	118.30	112.60
1	N	403	TRP	CB-CG-CD1	-5.70	118.36	126.90
3	H	6	GLN	CA-C-N	5.70	126.01	119.92
3	H	6	GLN	C-N-CA	5.70	126.01	119.92
3	H	85	GLU	CA-CB-CG	5.68	125.46	114.10
1	N	145	SER	N-CA-C	-5.67	105.09	112.23
1	N	208	ASN	N-CA-CB	-5.66	102.14	111.53
2	L	107	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	N	161	TRP	CG-CD2-CE3	5.64	139.54	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	106	ILE	CA-CB-CG1	-5.62	100.84	110.40
1	N	144	HIS	CB-CG-CD2	-5.62	123.89	131.20
2	L	82	ASP	CA-CB-CG	5.60	118.20	112.60
2	L	34	ASN	CA-CB-CG	5.59	118.19	112.60
1	N	106	VAL	N-CA-CB	-5.59	103.42	110.57
3	H	43	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	N	419	ARG	CB-CG-CD	-5.57	98.49	111.30
1	N	347	ASN	CA-C-O	-5.56	115.33	121.28
1	N	200	ASN	CA-CB-CG	5.54	118.14	112.60
1	N	105	ALA	N-CA-C	5.51	122.53	110.80
1	N	88	THR	CB-CA-C	5.51	119.29	110.09
1	N	367	SER	N-CA-C	5.50	117.49	108.52
1	N	240	VAL	N-CA-C	5.49	115.80	108.11
3	H	40	SER	CA-C-O	-5.49	114.98	120.64
1	N	323	THR	CA-CB-OG1	-5.45	101.43	109.60
1	N	178	TRP	N-CA-C	5.43	119.22	112.59
1	N	399	LEU	O-C-N	-5.43	116.65	122.85
1	N	299	ASN	CA-CB-CG	5.43	118.03	112.60
1	N	329	ASN	OD1-CG-ND2	-5.42	117.19	122.60
1	N	103	ASP	O-C-N	-5.41	116.86	123.30
1	N	198	ASN	CB-CG-ND2	5.41	124.51	116.40
1	N	184	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	N	160	SER	CA-CB-OG	5.38	121.86	111.10
1	N	308	VAL	N-CA-C	5.38	115.58	110.53
3	H	99	TYR	CA-CB-CG	5.36	123.54	113.90
2	L	19	VAL	CB-CA-C	5.35	119.06	110.82
1	N	221	ASN	O-C-N	5.33	128.40	123.50
1	N	411	MET	O-C-N	-5.32	117.18	123.41
3	H	63	PHE	N-CA-C	5.31	117.82	111.71
1	N	392	GLN	O-C-N	-5.26	117.79	123.42
3	H	70	THR	N-CA-CB	-5.26	103.09	111.62
1	N	330	ASP	N-CA-C	5.26	121.43	109.81
1	N	264	LYS	CA-CB-CG	5.26	124.62	114.10
3	H	36	TRP	CG-CD2-CE3	5.26	139.16	133.90
3	H	9	ALA	N-CA-C	5.24	116.25	108.60
3	H	36	TRP	CB-CG-CD1	-5.23	119.05	126.90
1	N	455	GLN	N-CA-CB	-5.23	102.34	110.29
1	N	318	CYS	N-CA-C	5.23	118.92	112.54
1	N	125	ASP	CA-CB-CG	5.23	117.83	112.60
2	L	75	ILE	N-CA-C	-5.22	100.23	107.80
3	H	99	TYR	N-CA-CB	5.22	119.31	110.49
1	N	412(B)	TRP	CG-CD2-CE3	5.22	139.12	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	312	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	N	412(B)	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	N	298	SER	N-CA-C	-5.20	106.97	113.72
1	N	455	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	N	365	THR	O-C-N	-5.19	117.09	122.96
1	N	265	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	N	264	LYS	CB-CG-CD	-5.17	99.42	111.30
3	H	36	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	N	269	THR	CA-CB-CG2	5.14	119.25	110.50
1	N	273	LYS	N-CA-C	5.14	117.55	111.33
1	N	165	SER	CA-C-N	5.13	123.36	119.66
1	N	165	SER	C-N-CA	5.13	123.36	119.66
1	N	143	LYS	N-CA-C	5.13	117.61	111.71
1	N	97	TRP	CE2-CD2-CG	-5.12	101.06	107.20
3	H	18	VAL	N-CA-CB	-5.12	106.51	112.34
1	N	125	ASP	CA-C-O	-5.11	115.58	120.64
1	N	121	TYR	CA-CB-CG	5.10	123.08	113.90
1	N	150	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	N	218	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	N	272	ALA	CA-C-N	5.05	127.30	120.38
1	N	272	ALA	C-N-CA	5.05	127.30	120.38
1	N	220	ARG	CB-CG-CD	5.05	122.92	111.30
1	N	265	TRP	CG-CD1-NE1	-5.05	103.64	110.20
1	N	401	THR	CA-CB-OG1	-5.04	102.05	109.60
1	N	445	SER	CA-CB-OG	5.03	121.17	111.10
1	N	295	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	N	345	ASN	CA-CB-CG	5.02	117.62	112.60
1	N	348	GLY	O-C-N	-5.02	118.91	123.78
1	N	88	THR	CA-CB-CG2	5.01	119.02	110.50
1	N	247	THR	N-CA-C	-5.01	104.59	111.81
3	H	37	VAL	N-CA-CB	-5.00	103.24	111.45

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	100	ARG	Sidechain
3	H	90	TYR	Sidechain
2	L	107	ARG	Sidechain
2	L	108	ARG	Sidechain
1	N	248	GLY	Peptide
1	N	327	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2979	0	2800	56	0
2	L	853	0	810	20	0
3	H	945	0	882	18	0
4	A	72	0	61	0	0
5	N	14	0	13	0	0
All	All	4863	0	4566	93	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 10.

All (93) 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:L:12:SER:HB2	2:L:107:ARG:HD3	1.48	0.95
3:H:3:GLN:HB2	3:H:25:SER:HB3	1.56	0.87
3:H:12:VAL:HG21	3:H:82(C):LEU:HD22	1.64	0.79
1:N:366:ILE:HD11	1:N:400:ASN:HB3	1.69	0.72
2:L:12:SER:CB	2:L:107:ARG:HD3	2.22	0.70
1:N:190:MET:HE3	1:N:192:ILE:HD11	1.77	0.66
3:H:66:LYS:O	3:H:82:LEU:HA	1.98	0.64
1:N:235:GLY:HA3	1:N:258:LYS:HE3	1.78	0.64
2:L:38:GLN:O	2:L:84:ALA:HB1	1.99	0.63
1:N:349:VAL:HG22	1:N:371:ARG:HE	1.67	0.59
2:L:38:GLN:HG3	2:L:42:GLY:O	2.02	0.59
2:L:83:ILE:HD12	2:L:106:ILE:HD12	1.85	0.58
3:H:12:VAL:HG23	3:H:111:VAL:HG13	1.85	0.58
3:H:28:THR:HB	3:H:31:ASN:CG	2.28	0.58
1:N:149:ILE:HD12	1:N:430:ARG:HB3	1.84	0.58
3:H:82(C):LEU:HD23	3:H:109:LEU:HD21	1.85	0.58
1:N:264:LYS:HD3	1:N:310:MET:HE2	1.86	0.58
2:L:15:LEU:HD11	2:L:80:GLN:HB2	1.86	0.58
1:N:427:ILE:HD13	1:N:428:ARG:H	1.68	0.57
1:N:435:LYS:HD3	1:N:435:LYS:H	1.70	0.57
1:N:168:THR:OG1	1:N:170:ASN:HB2	2.05	0.56
1:N:245:SER:HB3	1:N:248:GLY:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:269:THR:H	1:N:312:HIS:HE1	1.53	0.55
1:N:99:ILE:HD12	1:N:458:TRP:CZ2	2.41	0.55
1:N:248:GLY:HA2	1:N:295:TRP:CD2	2.42	0.55
1:N:99:ILE:H	1:N:99:ILE:HD13	1.71	0.55
2:L:85:THR:HA	2:L:102:THR:O	2.07	0.55
1:N:397:ILE:HG22	1:N:398:VAL:HG23	1.89	0.55
1:N:95:ASN:HD22	1:N:450:THR:HA	1.71	0.54
2:L:29:ILE:HD11	2:L:90:GLN:CB	2.37	0.54
1:N:110:GLU:HG2	1:N:141:ARG:NH1	2.22	0.54
2:L:17:ASP:O	2:L:78:LEU:HB2	2.08	0.53
1:N:235:GLY:O	1:N:258:LYS:HG2	2.09	0.53
1:N:330:ASP:HB3	1:N:389:ARG:HH21	1.74	0.52
1:N:320:PRO:HB3	1:N:331:PRO:O	2.10	0.51
2:L:48:ILE:HA	2:L:53:ASN:O	2.11	0.51
3:H:28:THR:HB	3:H:31:ASN:OD1	2.10	0.50
1:N:118:ARG:HE	1:N:119:GLU:H	1.59	0.50
1:N:283:GLU:HG3	1:N:284:GLN:H	1.77	0.50
2:L:10:SER:HA	2:L:103:LYS:O	2.11	0.50
1:N:149:ILE:HG23	1:N:150:HIS:ND1	2.28	0.49
2:L:9:SER:HA	2:L:102:THR:HA	1.95	0.49
1:N:257:PHE:CE1	1:N:262:ILE:HG12	2.48	0.48
1:N:196:GLY:HA3	1:N:201:ALA:HA	1.95	0.48
3:H:15:GLY:O	3:H:82(B):SER:HA	2.13	0.48
3:H:38:LYS:HD3	3:H:63:PHE:HZ	1.78	0.48
1:N:235:GLY:C	1:N:258:LYS:HG2	2.39	0.47
3:H:37:VAL:HG13	3:H:91:TYR:HB2	1.96	0.47
1:N:231:VAL:HG11	1:N:282:GLY:HA3	1.96	0.47
1:N:96:SER:HB2	1:N:451:GLU:O	2.15	0.47
1:N:269:THR:H	1:N:312:HIS:CE1	2.32	0.47
1:N:270:GLY:HA3	1:N:314:SER:OG	2.16	0.46
1:N:129:CYS:HB2	1:N:163:LEU:HD22	1.98	0.45
2:L:29:ILE:HD11	2:L:90:GLN:HB3	1.97	0.45
1:N:275:ILE:HD13	1:N:303:ILE:HD11	1.97	0.45
1:N:166:PRO:HB2	1:N:168:THR:HG23	1.99	0.45
1:N:98:HIS:CE1	1:N:419:ARG:HH21	2.34	0.45
1:N:274:HIS:CE1	1:N:294:ASN:HB3	2.51	0.45
2:L:15:LEU:HD11	2:L:80:GLN:CB	2.46	0.45
1:N:325:ASN:ND2	1:N:367:SER:O	2.50	0.45
1:N:427:ILE:HD13	1:N:428:ARG:N	2.31	0.45
2:L:103:LYS:HD3	2:L:104:LEU:N	2.32	0.44
1:N:269:THR:N	1:N:312:HIS:HE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:TRP:HA	1:N:211:PRO:HA	2.00	0.44
1:N:379:VAL:HG12	1:N:382:ALA:HB2	2.00	0.44
2:L:29:ILE:HD13	2:L:29:ILE:HG21	1.73	0.43
3:H:75:SER:O	3:H:77:THR:HG23	2.18	0.43
3:H:5:GLN:NE2	3:H:25:SER:HB2	2.33	0.43
2:L:12:SER:HA	2:L:105:GLU:O	2.18	0.43
3:H:100:ARG:NH1	3:H:100:ARG:HG3	2.33	0.43
1:N:385:ASP:HB3	1:N:388:SER:OG	2.17	0.43
3:H:4:LEU:HB2	3:H:104:GLY:HA2	2.01	0.43
1:N:332:THR:HA	1:N:389:ARG:HH12	1.82	0.43
3:H:38:LYS:HD3	3:H:63:PHE:CZ	2.53	0.43
3:H:93:ALA:HB1	3:H:100(E):PHE:HB3	2.01	0.42
1:N:161:TRP:NE1	1:N:165:SER:O	2.51	0.42
1:N:446:MET:HE2	1:N:446:MET:HB2	1.81	0.42
2:L:12:SER:HB2	2:L:107:ARG:CD	2.34	0.42
1:N:95:ASN:ND2	1:N:450:THR:HA	2.33	0.41
1:N:274:HIS:HB3	1:N:293:ASP:OD1	2.20	0.41
1:N:132:TYR:CE2	1:N:160:SER:HB3	2.55	0.41
3:H:51:PHE:O	3:H:52(A):PRO:HD3	2.20	0.41
1:N:328:PRO:HB3	2:L:93:THR:HB	2.03	0.41
1:N:283:GLU:HG3	1:N:284:GLN:N	2.36	0.41
1:N:226:GLN:O	1:N:227:GLU:HB2	2.21	0.40
1:N:421:CYS:HA	1:N:447:CYS:HA	2.02	0.40
2:L:21:ILE:O	2:L:72:SER:HA	2.22	0.40
3:H:100(E):PHE:CD1	3:H:100(E):PHE:N	2.89	0.40
1:N:91:LEU:HD21	1:N:281:TYR:HE1	1.87	0.40
1:N:181:THR:HG21	1:N:239:VAL:HG21	2.03	0.40
1:N:268:LEU:HD22	1:N:269:THR:H	1.85	0.40
1:N:98:HIS:CE1	1:N:447:CYS:HB2	2.57	0.40
1:N:378:LYS:HB2	1:N:392:GLN:HB3	2.02	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	N	376/388 (97%)	326 (87%)	43 (11%)	7 (2%)	6	30
2	L	107/109 (98%)	85 (79%)	12 (11%)	10 (9%)	0	2
3	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	32
All	All	603/619 (97%)	521 (86%)	63 (10%)	19 (3%)	3	18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	220	ARG
1	N	222	ILE
2	L	78	LEU
2	L	80	GLN
1	N	170	ASN
2	L	43	THR
2	L	60	SER
3	H	16	ALA
3	H	99	TYR
1	N	264	LYS
1	N	277	GLU
2	L	82	ASP
1	N	217	THR
1	N	295	TRP
2	L	8	THR
2	L	30	SER
2	L	84	ALA
2	L	29	ILE
2	L	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	332/340 (98%)	285 (86%)	47 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	97/97 (100%)	77 (79%)	20 (21%)	1	7
3	H	100/100 (100%)	79 (79%)	21 (21%)	1	6
All	All	529/537 (98%)	441 (83%)	88 (17%)	2	12

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	96	SER
1	N	97	TRP
1	N	99	ILE
1	N	118	ARG
1	N	119	GLU
1	N	120	PRO
1	N	122	VAL
1	N	128	GLU
1	N	134	LEU
1	N	140	ILE
1	N	141	ARG
1	N	146	ASN
1	N	154	GLN
1	N	187	ARG
1	N	193	CYS
1	N	195	SER
1	N	213	THR
1	N	224	ARG
1	N	229	GLU
1	N	230	CYS
1	N	234	ASN
1	N	251	GLU
1	N	252	THR
1	N	254	ILE
1	N	268	LEU
1	N	269	THR
1	N	275	ILE
1	N	287	VAL
1	N	290	THR
1	N	292	ARG
1	N	304	GLN
1	N	306	ASP
1	N	311	THR
1	N	346	ASN

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Mol	Chain	Res	Type
1	N	364	ARG
1	N	366	ILE
1	N	367	SER
1	N	370	SER
1	N	383	LEU
1	N	401	THR
1	N	411	MET
1	N	427	ILE
1	N	435	LYS
1	N	446	MET
1	N	449	SER
1	N	450	THR
1	N	457	ASN
2	L	4	MET
2	L	5	THR
2	L	10	SER
2	L	19	VAL
2	L	28	ASP
2	L	30	SER
2	L	33	LEU
2	L	57	GLU
2	L	60	SER
2	L	70	ASP
2	L	72	SER
2	L	73	LEU
2	L	78	LEU
2	L	79	GLU
2	L	83	ILE
2	L	91	ASP
2	L	94	LEU
2	L	104	LEU
2	L	106	ILE
2	L	108	ARG
3	H	10	GLU
3	H	13	LYS
3	H	18	VAL
3	H	21	SER
3	H	23	LYS
3	H	28	THR
3	H	30	THR
3	H	31	ASN
3	H	34	MET

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Mol	Chain	Res	Type
3	H	50	ILE
3	H	54	ASN
3	H	66	LYS
3	H	74	SER
3	H	95	SER
3	H	98	SER
3	H	100	ARG
3	H	100(A)	TYR
3	H	100(B)	ASP
3	H	100(E)	PHE
3	H	110	THR
3	H	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	95	ASN
1	N	98	HIS
1	N	104	ASN
1	N	136	GLN
1	N	198	ASN
1	N	216	ASN
1	N	226	GLN
1	N	234	ASN
1	N	304	GLN
1	N	312	HIS
1	N	325	ASN
1	N	346	ASN
1	N	392	GLN
2	L	27	GLN
2	L	37	GLN
2	L	38	GLN
2	L	55	HIS
3	H	5	GLN
3	H	39	GLN
3	H	81	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 ⓘ

6 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$
4	NAG	A	1	4,1	14,14,15	1.74	5 (35%)	17,19,21	1.92	3 (17%)
4	NAG	A	2	4	14,14,15	1.34	2 (14%)	17,19,21	1.62	5 (29%)
4	BMA	A	3	4	11,11,12	0.92	0	15,15,17	0.87	1 (6%)
4	MAN	A	4	4	11,11,12	0.82	0	15,15,17	1.49	4 (26%)
4	MAN	A	5	4	11,11,12	1.12	1 (9%)	15,15,17	1.54	3 (20%)
4	MAN	A	6	4	11,11,12	0.83	0	15,15,17	1.23	2 (13%)

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	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5	4	-	2/2/19/22	0/1/1/1
4	MAN	A	6	4	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	C1-C2	3.34	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	C3-C2	3.02	1.58	1.52
4	A	2	NAG	C4-C5	2.95	1.59	1.53
4	A	2	NAG	O5-C1	-2.75	1.39	1.43
4	A	1	NAG	C8-C7	2.24	1.55	1.50
4	A	1	NAG	O4-C4	2.18	1.48	1.43
4	A	5	MAN	C2-C3	-2.09	1.49	1.52
4	A	1	NAG	O5-C5	2.03	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C2-N2-C7	4.68	129.18	122.90
4	A	1	NAG	C1-C2-N2	-4.50	103.33	110.43
4	A	2	NAG	C4-C3-C2	-3.67	105.65	111.02
4	A	5	MAN	C1-O5-C5	3.12	116.37	112.19
4	A	5	MAN	O3-C3-C2	3.00	116.18	110.05
4	A	2	NAG	C1-C2-N2	-2.97	105.75	110.43
4	A	6	MAN	C1-O5-C5	2.91	116.09	112.19
4	A	2	NAG	C8-C7-N2	2.73	120.64	116.12
4	A	4	MAN	O5-C5-C4	-2.61	104.48	110.83
4	A	4	MAN	C1-O5-C5	2.61	115.68	112.19
4	A	6	MAN	O4-C4-C3	-2.49	104.52	110.38
4	A	1	NAG	O3-C3-C4	-2.43	104.65	110.38
4	A	3	BMA	C1-C2-C3	2.35	113.07	109.64
4	A	2	NAG	O3-C3-C2	2.25	114.07	109.40
4	A	4	MAN	O5-C5-C6	2.24	112.01	107.66
4	A	5	MAN	O4-C4-C3	-2.23	105.11	110.38
4	A	2	NAG	O7-C7-N2	-2.12	118.24	121.98
4	A	4	MAN	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

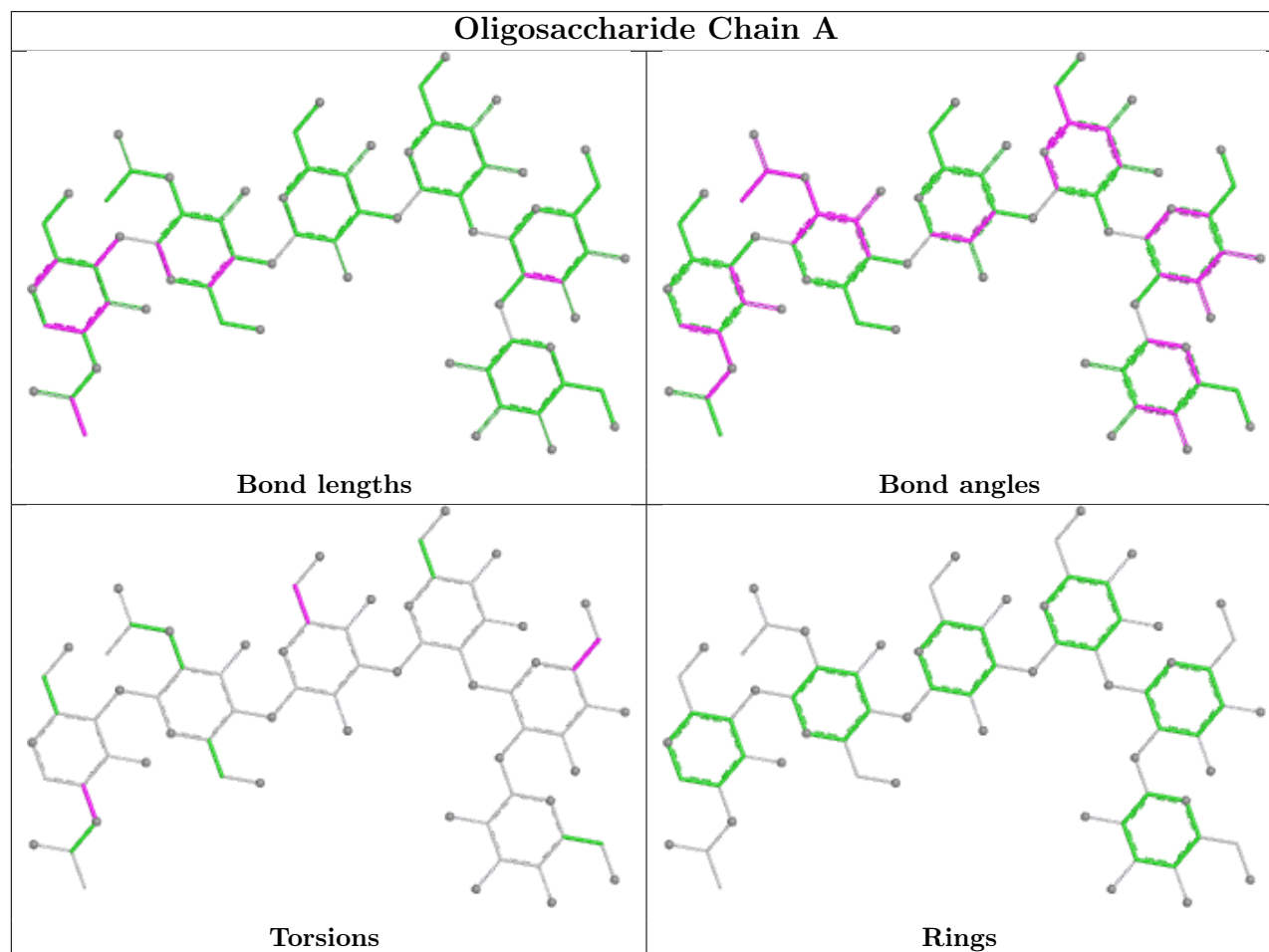
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5	MAN	O5-C5-C6-O6
4	A	5	MAN	C4-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C3-C2-N2-C7

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	N	475(A)	1	14,14,15	0.97	1 (7%)	17,19,21	1.49	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	N	475(A)	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(A)	NAG	C4-C5	-2.19	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(A)	NAG	C1-C2-N2	-3.24	105.33	110.43
5	N	475(A)	NAG	C8-C7-N2	2.61	120.45	116.12
5	N	475(A)	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	475(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.