



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:16 PM UTC

PDB ID : 1E05 / pdb_00001e05
Title : PLASMA ALPHA ANTITHROMBIN-III
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Deposited on : 2000-03-09
Resolution : 2.62 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

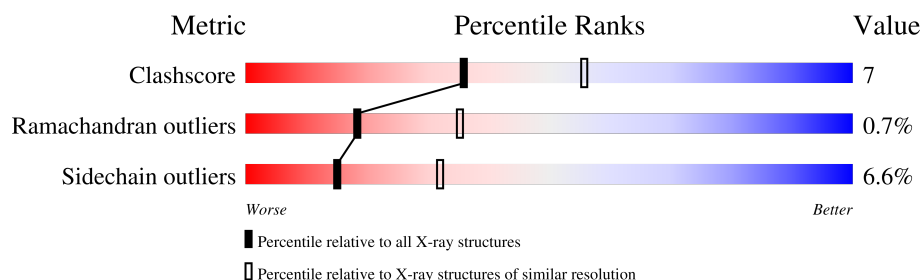
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)

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	I	432	
1	L	432	
2	A	2	
2	C	2	
3	B	3	
4	D	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GUP	D	3	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6903 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 ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	417	Total	C	N	O	S	0	0	0
			3274	2088	553	617	16			
1	L	417	Total	C	N	O	S	0	0	0
			3261	2082	542	619	18			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

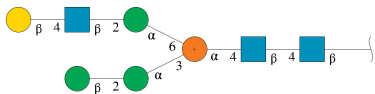
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

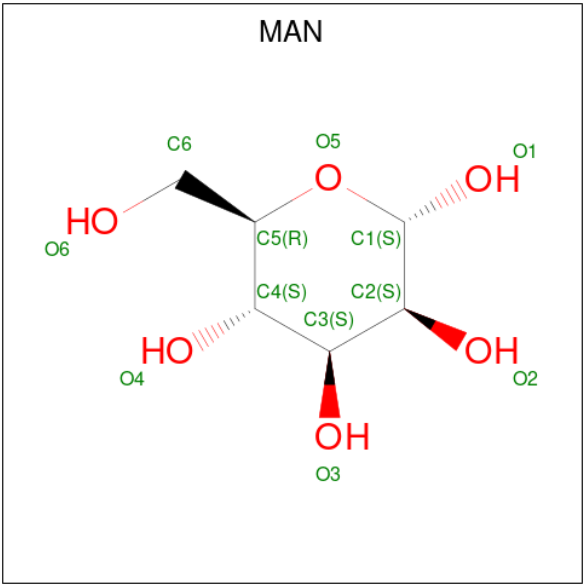
- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-L-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop

yranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



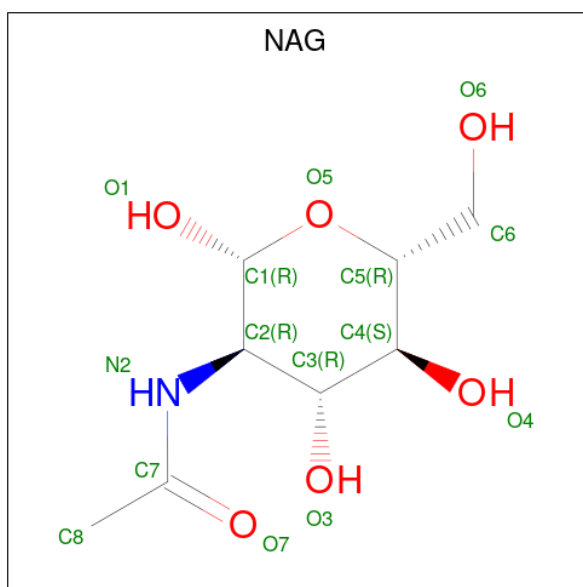
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	0	0	0
			97	54	3	40			

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



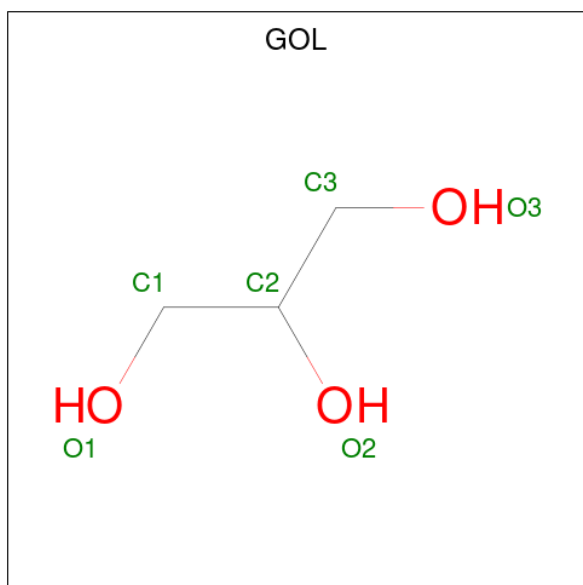
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			11	6	5		
5	L	1	Total	C	O	0	0
			11	6	5		
5	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



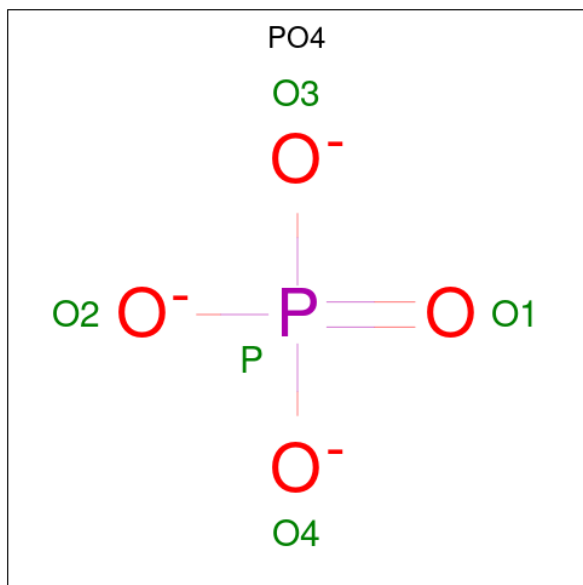
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O P 5 4 1	0	0

- Molecule 9 is water.

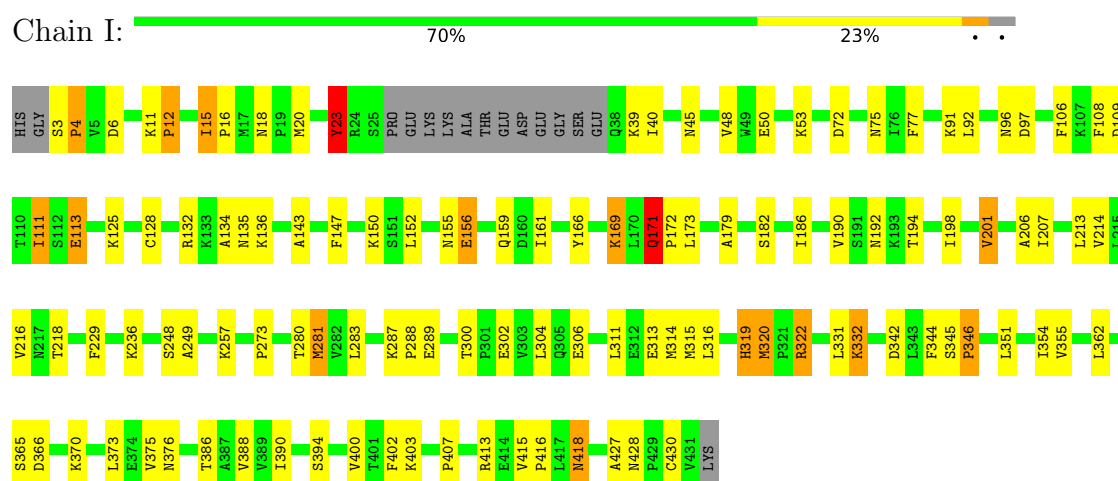
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	46	Total O 46 46	0	0
9	L	24	Total O 24 24	0	0

3 Residue-property plots [i](#)

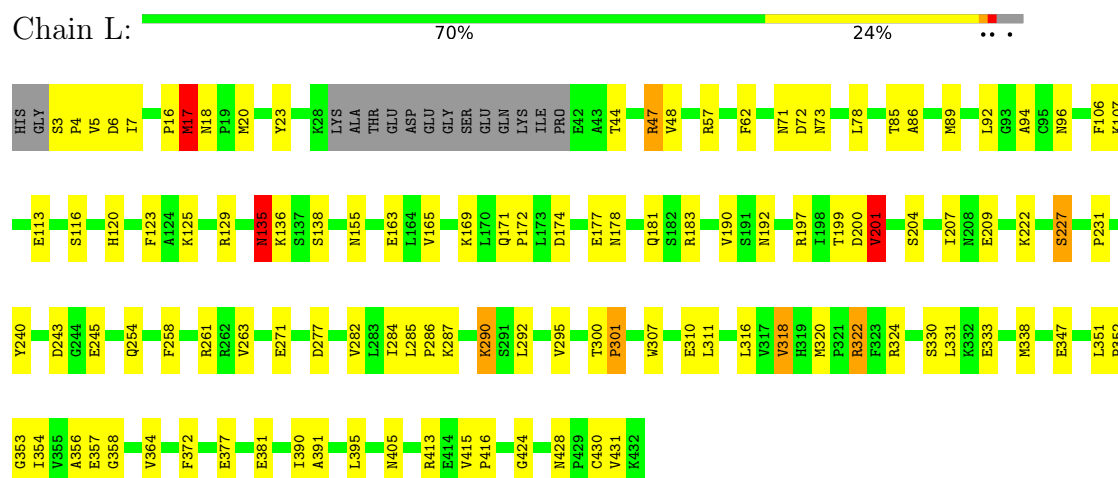
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ANTITHROMBIN-III



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





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

Chain C: 100%



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

Chain B: 100%



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-L-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 12% 62% 25%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.41 Å 98.31 Å 90.41 Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62	Depositor
% Data completeness (in resolution range)	72.0 (20.00-2.62)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6903	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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: GOL, MAN, GAL, PO4, BMA, GUP, 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	I	0.51	0/3340	1.53	43/4519 (1.0%)
1	L	0.50	0/3326	1.49	40/4500 (0.9%)
All	All	0.51	0/6666	1.51	83/9019 (0.9%)

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	I	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	201	VAL	N-CA-CB	8.85	119.92	110.62
1	I	155	ASN	OD1-CG-ND2	8.67	131.27	122.60
1	L	135	ASN	CB-CG-ND2	8.65	129.38	116.40
1	I	192	ASN	CB-CG-ND2	8.53	129.20	116.40
1	I	331	LEU	N-CA-C	8.26	122.46	112.38
1	I	171	GLN	N-CA-C	8.01	120.37	109.24
1	L	6	ASP	CA-CB-CG	7.89	120.49	112.60
1	L	192	ASN	OD1-CG-ND2	7.58	130.18	122.60
1	I	96	ASN	OD1-CG-ND2	7.45	130.05	122.60
1	I	135	ASN	CB-CG-ND2	7.45	127.57	116.40
1	I	12	PRO	CA-C-N	7.35	131.11	120.38
1	I	12	PRO	C-N-CA	7.35	131.11	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	229	PHE	CA-CB-CG	7.30	121.10	113.80
1	L	7	ILE	CA-C-N	7.29	131.75	120.82
1	L	7	ILE	C-N-CA	7.29	131.75	120.82
1	L	372	PHE	CA-CB-CG	7.18	120.98	113.80
1	L	354	ILE	N-CA-C	7.17	117.27	110.74
1	L	106	PHE	CA-CB-CG	-7.13	106.67	113.80
1	L	174	ASP	CA-CB-CG	7.02	119.62	112.60
1	I	206	ALA	N-CA-C	-6.91	105.40	114.31
1	L	135	ASN	N-CA-CB	6.81	120.19	109.71
1	L	135	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	I	135	ASN	CA-CB-CG	6.55	119.15	112.60
1	I	150	LYS	CA-C-N	6.42	129.53	120.28
1	I	150	LYS	C-N-CA	6.42	129.53	120.28
1	I	91	LYS	CA-C-N	6.30	128.72	120.28
1	I	91	LYS	C-N-CA	6.30	128.72	120.28
1	L	322	ARG	CD-NE-CZ	6.29	133.21	124.40
1	I	72	ASP	N-CA-C	6.22	118.87	111.71
1	L	16	PRO	CA-C-N	6.15	133.28	121.54
1	L	16	PRO	C-N-CA	6.15	133.28	121.54
1	I	108	PHE	CA-C-N	6.08	129.04	120.28
1	I	108	PHE	C-N-CA	6.08	129.04	120.28
1	I	316	LEU	N-CA-CB	-6.07	102.15	111.56
1	I	113	GLU	CA-C-N	6.05	132.15	122.83
1	I	113	GLU	C-N-CA	6.05	132.15	122.83
1	L	155	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	I	106	PHE	CA-CB-CG	-5.98	107.82	113.80
1	L	277	ASP	CA-C-N	5.95	130.80	120.68
1	L	277	ASP	C-N-CA	5.95	130.80	120.68
1	L	18	ASN	CA-CB-CG	5.90	118.50	112.60
1	L	16	PRO	CA-C-O	5.86	125.89	121.38
1	L	135	ASN	N-CA-C	5.86	118.20	109.59
1	I	135	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	I	413	ARG	CD-NE-CZ	5.82	132.54	124.40
1	L	201	VAL	CB-CA-C	-5.81	104.26	111.70
1	L	6	ASP	CB-CA-C	5.80	120.09	110.74
1	I	346	PRO	CA-C-N	5.77	128.28	120.44
1	I	346	PRO	C-N-CA	5.77	128.28	120.44
1	I	332	LYS	N-CA-C	5.72	117.19	111.07
1	L	231	PRO	CA-C-N	5.71	128.20	120.38
1	L	231	PRO	C-N-CA	5.71	128.20	120.38
1	L	135	ASN	CA-C-O	5.71	127.20	120.58
1	L	391	ALA	N-CA-C	5.70	119.29	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	243	ASP	N-CA-C	-5.61	107.44	114.56
1	I	6	ASP	CA-CB-CG	5.59	118.19	112.60
1	L	209	GLU	N-CA-C	5.57	118.11	111.71
1	I	402	PHE	CA-CB-CG	5.56	119.36	113.80
1	I	125	LYS	N-CA-C	5.56	117.34	111.28
1	L	17	MET	CA-CB-CG	5.55	125.20	114.10
1	I	430	CYS	N-CA-C	5.55	117.90	110.35
1	I	342	ASP	N-CA-C	5.51	118.00	111.33
1	L	96	ASN	CA-CB-CG	5.50	118.11	112.60
1	L	301	PRO	CA-C-N	5.50	127.65	120.28
1	L	301	PRO	C-N-CA	5.50	127.65	120.28
1	L	290	LYS	N-CA-C	5.48	117.61	110.43
1	I	40	ILE	CA-C-O	5.45	122.89	119.51
1	I	39	LYS	N-CA-C	5.43	117.24	109.14
1	I	418	ASN	CB-CG-ND2	5.41	124.52	116.40
1	I	15	ILE	N-CA-C	5.32	113.42	108.15
1	I	386	THR	N-CA-CB	5.32	120.68	110.90
1	I	23	TYR	CB-CA-C	5.30	119.90	109.72
1	L	106	PHE	CA-C-N	5.22	129.97	122.40
1	L	106	PHE	C-N-CA	5.22	129.97	122.40
1	L	318	VAL	CB-CA-C	-5.21	103.36	110.96
1	I	300	THR	N-CA-C	-5.20	102.22	108.25
1	L	92	LEU	N-CA-C	5.20	117.62	111.33
1	L	424	GLY	N-CA-C	5.19	117.59	110.69
1	I	97	ASP	N-CA-C	5.17	117.82	111.82
1	I	192	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	I	319	HIS	CA-CB-CG	5.06	118.86	113.80
1	L	73	ASN	N-CA-CB	-5.05	103.14	110.47
1	I	108	PHE	CA-C-O	5.02	125.53	119.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	113	GLU	Mainchain
1	I	166	TYR	Mainchain
1	L	107	LYS	Mainchain

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	I	3274	0	3213	51	0
1	L	3261	0	3207	46	0
2	A	28	0	25	2	0
2	C	28	0	25	0	0
3	B	39	0	34	0	0
4	D	97	0	79	1	0
5	I	11	0	10	1	0
5	L	22	0	20	1	0
6	I	28	0	26	0	0
6	L	28	0	26	1	0
7	I	6	0	8	0	0
7	L	6	0	8	1	0
8	L	5	0	0	0	0
9	I	46	0	0	0	0
9	L	24	0	0	0	0
All	All	6903	0	6681	99	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 7.

All (99) 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:I:75:ASN:HD21	1:I:428:ASN:H	1.21	0.88
1:I:16:PRO:HD2	1:I:161:ILE:HD11	1.57	0.84
1:I:75:ASN:ND2	1:I:427:ALA:H	1.77	0.83
1:I:75:ASN:HD22	1:I:427:ALA:H	1.30	0.80
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.66	0.77
1:L:86:ALA:HA	1:L:89:MET:HE3	1.67	0.76
1:L:47:ARG:HD3	1:L:113:GLU:HG3	1.68	0.74
1:I:194:THR:HG21	1:I:198:ILE:HD12	1.73	0.71
1:I:169:LYS:HD3	1:I:171:GLN:HG2	1.75	0.69
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.76	0.68
1:L:71:ASN:HD22	1:L:72:ASP:H	1.44	0.66
1:L:287:LYS:HD3	1:L:290:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.79	0.64
1:I:15:ILE:HG23	1:I:161:ILE:HD12	1.82	0.60
1:L:71:ASN:HD22	1:L:72:ASP:N	2.00	0.59
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.84	0.59
1:L:20:MET:HG3	1:L:353:GLY:HA2	1.85	0.58
1:I:156:GLU:HA	1:I:159:GLN:HE21	1.69	0.58
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.86	0.57
1:I:50:GLU:HB3	1:I:111:ILE:HG23	1.87	0.56
1:L:3:SER:HB2	1:L:4:PRO:HD2	1.88	0.56
1:L:222:LYS:HD2	1:L:381:GLU:HB2	1.87	0.55
1:L:356:ALA:O	1:L:357:GLU:HB2	2.07	0.55
1:I:190:VAL:HG13	1:I:218:THR:HG21	1.89	0.54
1:I:213:LEU:HD11	1:I:354:ILE:HD13	1.90	0.54
1:I:190:VAL:HG11	1:I:201:VAL:HG21	1.88	0.54
1:I:257:LYS:HE2	1:I:313:GLU:HB3	1.89	0.54
1:L:57:ARG:HG2	1:L:301:PRO:HG2	1.90	0.53
1:I:75:ASN:ND2	1:I:428:ASN:H	1.99	0.53
1:L:428:ASN:ND2	1:L:430:CYS:H	2.08	0.52
1:I:320:MET:HE1	1:I:375:VAL:HG11	1.92	0.51
1:L:183:ARG:HG3	1:L:207:ILE:HD12	1.93	0.51
1:L:85:THR:HG22	1:L:89:MET:HE2	1.93	0.50
1:I:314:MET:HE1	1:I:400:VAL:HG23	1.92	0.50
1:L:23:TYR:H	1:L:116:SER:HB2	1.76	0.50
1:L:352:PRO:O	1:L:358:GLY:HA2	2.13	0.49
1:I:18:ASN:HD21	1:I:92:LEU:HA	1.77	0.49
1:L:428:ASN:HD21	1:L:430:CYS:HB2	1.78	0.48
1:I:134:ALA:HB3	1:I:136:LYS:HG2	1.94	0.48
1:I:147:PHE:HB2	1:I:214:VAL:HG12	1.94	0.48
4:D:1:NAG:H62	4:D:2:NAG:N2	2.29	0.48
1:L:322:ARG:HD2	1:L:377:GLU:OE1	2.13	0.48
1:L:286:PRO:HG3	1:L:292:LEU:HD13	1.95	0.48
1:I:287:LYS:HB2	1:I:288:PRO:HD2	1.95	0.47
1:I:143:ALA:HB3	1:I:218:THR:HG22	1.96	0.47
1:L:227:SER:HB2	1:L:254:GLN:HE22	1.78	0.47
1:I:173:LEU:HD13	1:I:182:SER:HB3	1.97	0.47
1:I:186:ILE:HG21	1:I:216:VAL:HG21	1.97	0.47
1:I:20:MET:HB2	2:A:2:NAG:H83	1.96	0.47
1:L:295:VAL:HG13	1:L:307:TRP:HH2	1.79	0.47
1:I:273:PRO:HB3	1:I:280:THR:HG22	1.97	0.46
1:I:132:ARG:HG3	1:I:136:LYS:HE2	1.98	0.46
1:I:3:SER:N	1:I:4:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:PHE:HB2	1:I:214:VAL:CG1	2.46	0.45
1:L:261:ARG:NE	1:L:310:GLU:HG2	2.31	0.45
1:I:415:VAL:HB	1:I:416:PRO:CD	2.46	0.45
1:L:261:ARG:HG2	1:L:310:GLU:HB3	1.98	0.45
1:I:171:GLN:HA	1:I:172:PRO:HD3	1.85	0.45
1:I:179:ALA:HB1	1:I:207:ILE:HG22	1.99	0.45
1:I:394:SER:HB3	1:L:240:TYR:H	1.82	0.45
1:I:45:ASN:HB3	1:I:48:VAL:HG22	1.99	0.44
1:L:413:ARG:HE	7:L:901:GOL:H2	1.80	0.44
1:L:364:VAL:HG22	1:L:390:ILE:HD13	1.99	0.44
1:I:3:SER:N	1:I:4:PRO:CD	2.79	0.44
1:L:17:MET:SD	1:L:120:HIS:HB2	2.58	0.44
1:I:23:TYR:OH	1:I:109:ASP:HA	2.18	0.44
1:L:415:VAL:HB	1:L:416:PRO:HD3	2.00	0.44
1:I:388:VAL:HG12	1:I:390:ILE:HG13	2.00	0.43
1:I:198:ILE:HG23	1:I:370:LYS:HD3	2.00	0.43
1:I:11:LYS:HB3	1:I:12:PRO:HD2	2.01	0.43
1:L:271:GLU:HG3	1:L:282:VAL:HG22	2.00	0.43
1:L:428:ASN:HD22	1:L:430:CYS:H	1.65	0.43
1:L:135:ASN:HA	6:L:821:NAG:C1	2.49	0.42
5:L:843:MAN:H2	5:L:844:MAN:H2	2.01	0.42
1:I:257:LYS:HB2	1:I:315:MET:HE2	2.01	0.42
1:I:92:LEU:HD21	1:I:161:ILE:HG21	2.01	0.42
1:L:171:GLN:HA	1:L:172:PRO:HD3	1.89	0.42
1:I:3:SER:HB2	1:I:4:PRO:HD3	2.01	0.42
1:L:200:ASP:O	1:L:201:VAL:C	2.61	0.42
1:L:357:GLU:O	1:L:358:GLY:C	2.63	0.42
1:I:322:ARG:HH11	1:I:322:ARG:HD2	1.70	0.42
1:L:163:GLU:OE2	1:L:169:LYS:HG2	2.20	0.41
1:L:261:ARG:HB3	1:L:311:LEU:HD23	2.01	0.41
5:I:803:MAN:C1	2:A:2:NAG:H61	2.50	0.41
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.55	0.41
1:I:332:LYS:HG3	1:I:344:PHE:CD1	2.56	0.41
1:L:62:PHE:HA	1:L:338:MET:HE1	2.01	0.41
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.85	0.41
1:L:125:LYS:O	1:L:129:ARG:HG2	2.21	0.41
1:L:178:ASN:HB3	1:L:181:GLN:HB3	2.02	0.41
1:L:190:VAL:HG11	1:L:201:VAL:HG22	2.03	0.41
1:I:354:ILE:HG22	1:I:362:LEU:HD13	2.02	0.41
1:L:300:THR:HB	1:L:301:PRO:HD2	2.02	0.41
1:L:44:THR:O	1:L:48:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.03	0.40
1:L:183:ARG:NH1	1:L:204:SER:HA	2.36	0.40
1:I:75:ASN:ND2	1:I:427:ALA:N	2.58	0.40
1:I:236:LYS:HA	1:I:249:ALA:O	2.22	0.40
1:I:345:SER:HA	1:I:346:PRO:HD3	1.98	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	I	413/432 (96%)	388 (94%)	22 (5%)	3 (1%)	18	35
1	L	413/432 (96%)	374 (91%)	36 (9%)	3 (1%)	18	35
All	All	826/864 (96%)	762 (92%)	58 (7%)	6 (1%)	18	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	4	PRO
1	L	245	GLU
1	L	136	LYS
1	L	263	VAL
1	I	407	PRO
1	I	111	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	354/383 (92%)	331 (94%)	23 (6%)	15	33
1	L	355/383 (93%)	331 (93%)	24 (7%)	14	30
All	All	709/766 (93%)	662 (93%)	47 (7%)	15	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	23	TYR
1	I	53	LYS
1	I	128	CYS
1	I	152	LEU
1	I	156	GLU
1	I	169	LYS
1	I	171	GLN
1	I	201	VAL
1	I	248	SER
1	I	281	MET
1	I	289	GLU
1	I	302	GLU
1	I	304	LEU
1	I	306	GLU
1	I	311	LEU
1	I	320	MET
1	I	322	ARG
1	I	351	LEU
1	I	355	VAL
1	I	365	SER
1	I	366	ASP
1	I	376	ASN
1	I	418	ASN
1	L	5	VAL
1	L	17	MET
1	L	47	ARG
1	L	78	LEU
1	L	123	PHE
1	L	135	ASN
1	L	138	SER
1	L	177	GLU
1	L	197	ARG
1	L	199	THR

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Mol	Chain	Res	Type
1	L	201	VAL
1	L	227	SER
1	L	284	ILE
1	L	285	LEU
1	L	318	VAL
1	L	320	MET
1	L	324	ARG
1	L	330	SER
1	L	331	LEU
1	L	333	GLU
1	L	347	GLU
1	L	395	LEU
1	L	405	ASN
1	L	431	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	18	ASN
1	I	64	GLN
1	I	71	ASN
1	I	75	ASN
1	I	127	ASN
1	I	159	GLN
1	I	171	GLN
1	I	178	ASN
1	I	254	GLN
1	I	428	ASN
1	L	71	ASN
1	L	118	GLN
1	L	120	HIS
1	L	181	GLN
1	L	217	ASN
1	L	254	GLN
1	L	268	GLN
1	L	319	HIS
1	L	336	GLN
1	L	405	ASN
1	L	428	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 ⓘ

15 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$
2	NAG	A	1	1,2	14,14,15	1.27	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	A	2	2	14,14,15	1.17	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	B	1	1,3	14,14,15	1.38	2 (14%)	17,19,21	2.36	5 (29%)
3	NAG	B	2	3	14,14,15	1.26	1 (7%)	17,19,21	1.10	2 (11%)
3	BMA	B	3	3	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
2	NAG	C	1	1,2	14,14,15	1.28	1 (7%)	17,19,21	0.78	0
2	NAG	C	2	2	14,14,15	1.22	1 (7%)	17,19,21	1.41	4 (23%)
4	NAG	D	1	4,1	14,14,15	1.26	1 (7%)	17,19,21	1.14	1 (5%)
4	NAG	D	2	4	14,14,15	1.27	1 (7%)	17,19,21	1.60	2 (11%)
4	GUP	D	3	4	11,11,12	0.80	0	15,15,17	2.26	4 (26%)
4	MAN	D	4	4	11,11,12	1.44	1 (9%)	15,15,17	2.97	5 (33%)
4	NAG	D	5	4	14,14,15	1.48	3 (21%)	17,19,21	2.12	6 (35%)
4	GAL	D	6	4	11,11,12	3.18	3 (27%)	15,15,17	1.70	4 (26%)
4	MAN	D	7	4	11,11,12	0.95	1 (9%)	15,15,17	2.05	2 (13%)
4	BMA	D	8	4	11,11,12	0.73	0	15,15,17	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	GUP	D	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	NAG	D	5	4	-	2/6/23/26	0/1/1/1
4	GAL	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	2/2/19/22	0/1/1/1
4	BMA	D	8	4	-	2/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	GAL	C2-C3	-9.55	1.37	1.52
4	D	4	MAN	O2-C2	-4.05	1.34	1.43
4	D	5	NAG	O7-C7	-3.90	1.14	1.23
2	C	2	NAG	O7-C7	-3.88	1.14	1.23
4	D	2	NAG	O7-C7	-3.82	1.14	1.23
3	B	2	NAG	O7-C7	-3.79	1.14	1.23
2	A	1	NAG	O7-C7	-3.78	1.14	1.23
3	B	1	NAG	O7-C7	-3.77	1.14	1.23
4	D	1	NAG	O7-C7	-3.77	1.14	1.23
2	A	2	NAG	O7-C7	-3.72	1.14	1.23
2	C	1	NAG	O7-C7	-3.71	1.14	1.23
4	D	6	GAL	O3-C3	3.33	1.51	1.43
4	D	6	GAL	C4-C3	2.94	1.60	1.52
3	B	1	NAG	O5-C5	-2.48	1.38	1.43
4	D	5	NAG	C2-N2	2.28	1.50	1.46
4	D	7	MAN	O5-C1	-2.19	1.40	1.43
4	D	5	NAG	O4-C4	-2.08	1.37	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	MAN	O2-C2-C3	7.53	125.74	110.15
4	D	7	MAN	C1-O5-C5	6.63	121.07	112.19
3	B	1	NAG	C1-O5-C5	6.48	120.87	112.19
4	D	4	MAN	O2-C2-C1	5.72	122.31	109.22
4	D	5	NAG	O4-C4-C5	5.54	122.96	109.32
3	B	1	NAG	C3-C4-C5	4.63	118.62	110.23
4	D	2	NAG	C1-O5-C5	4.62	118.37	112.19
4	D	3	GUP	O6-C6-C5	4.41	126.37	111.33
4	D	3	GUP	C1-O5-C5	-4.26	106.48	112.19
4	D	3	GUP	O5-C5-C6	4.20	115.84	107.66
4	D	4	MAN	C1-C2-C3	-4.13	103.63	109.64
4	D	5	NAG	O4-C4-C3	3.73	119.16	110.38
4	D	2	NAG	C4-C3-C2	-3.49	105.90	111.02
2	A	2	NAG	C3-C4-C5	3.37	116.34	110.23
4	D	6	GAL	O3-C3-C4	-3.15	102.96	110.38
4	D	6	GAL	C2-C3-C4	3.12	116.35	110.86
2	A	2	NAG	C1-O5-C5	-3.05	108.09	112.19
4	D	6	GAL	C3-C4-C5	-3.01	104.77	110.23
4	D	3	GUP	C6-C5-C4	3.01	120.41	113.02
2	C	2	NAG	C1-C2-N2	2.99	115.15	110.43
3	B	1	NAG	C6-C5-C4	-2.77	106.21	113.02
4	D	6	GAL	O3-C3-C2	2.77	115.71	110.05
4	D	7	MAN	C3-C4-C5	-2.60	105.51	110.23
3	B	1	NAG	O3-C3-C4	-2.59	104.27	110.38
4	D	1	NAG	O5-C1-C2	-2.58	107.29	111.29
2	A	1	NAG	O5-C1-C2	-2.57	107.31	111.29
4	D	4	MAN	C3-C4-C5	-2.56	105.59	110.23
2	C	2	NAG	O5-C1-C2	-2.54	107.36	111.29
4	D	5	NAG	O5-C5-C6	-2.54	102.72	107.66
4	D	5	NAG	O5-C5-C4	-2.46	104.85	110.83
3	B	1	NAG	O5-C5-C6	-2.42	102.94	107.66
4	D	4	MAN	O5-C1-C2	-2.34	105.22	110.79
3	B	2	NAG	O4-C4-C3	2.32	115.84	110.38
2	C	2	NAG	C3-C4-C5	2.24	114.29	110.23
4	D	5	NAG	C4-C3-C2	2.17	114.20	111.02
4	D	5	NAG	O5-C1-C2	2.09	114.52	111.29
2	C	2	NAG	C2-N2-C7	2.06	125.66	122.90
3	B	2	NAG	O4-C4-C5	-2.05	104.27	109.32
3	B	3	BMA	C1-O5-C5	2.03	114.90	112.19
3	B	3	BMA	O5-C5-C4	-2.02	105.92	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	3	GUP	C5

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	GUP	O5-C5-C6-O6
2	A	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6
4	D	3	GUP	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	D	6	GAL	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
4	D	8	BMA	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	D	6	GAL	C4-C5-C6-O6
4	D	8	BMA	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
4	D	5	NAG	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
4	D	5	NAG	C4-C5-C6-O6
4	D	7	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	7	MAN	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
2	A	2	NAG	C8-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	A	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

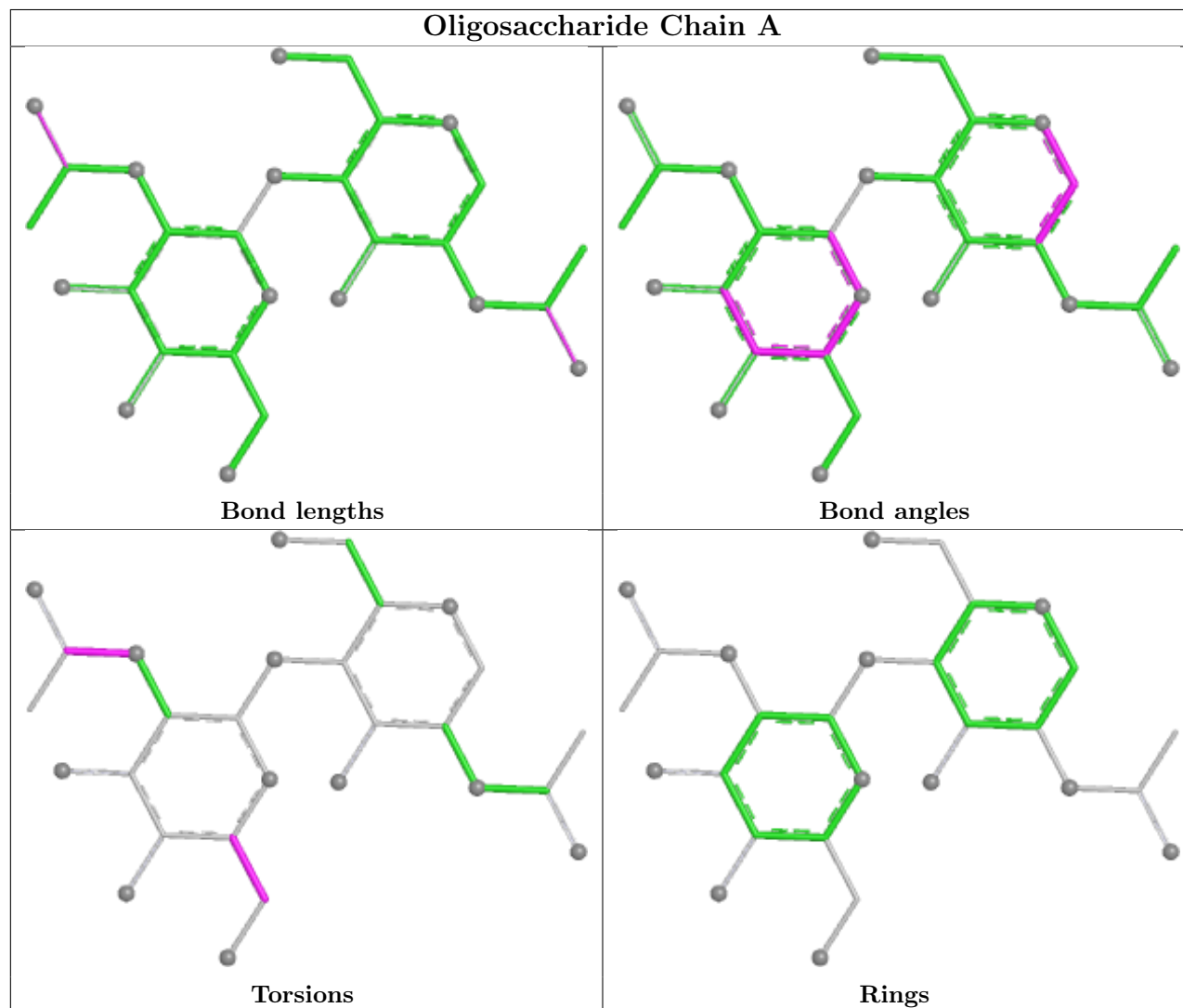
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	D	2	NAG	1	0

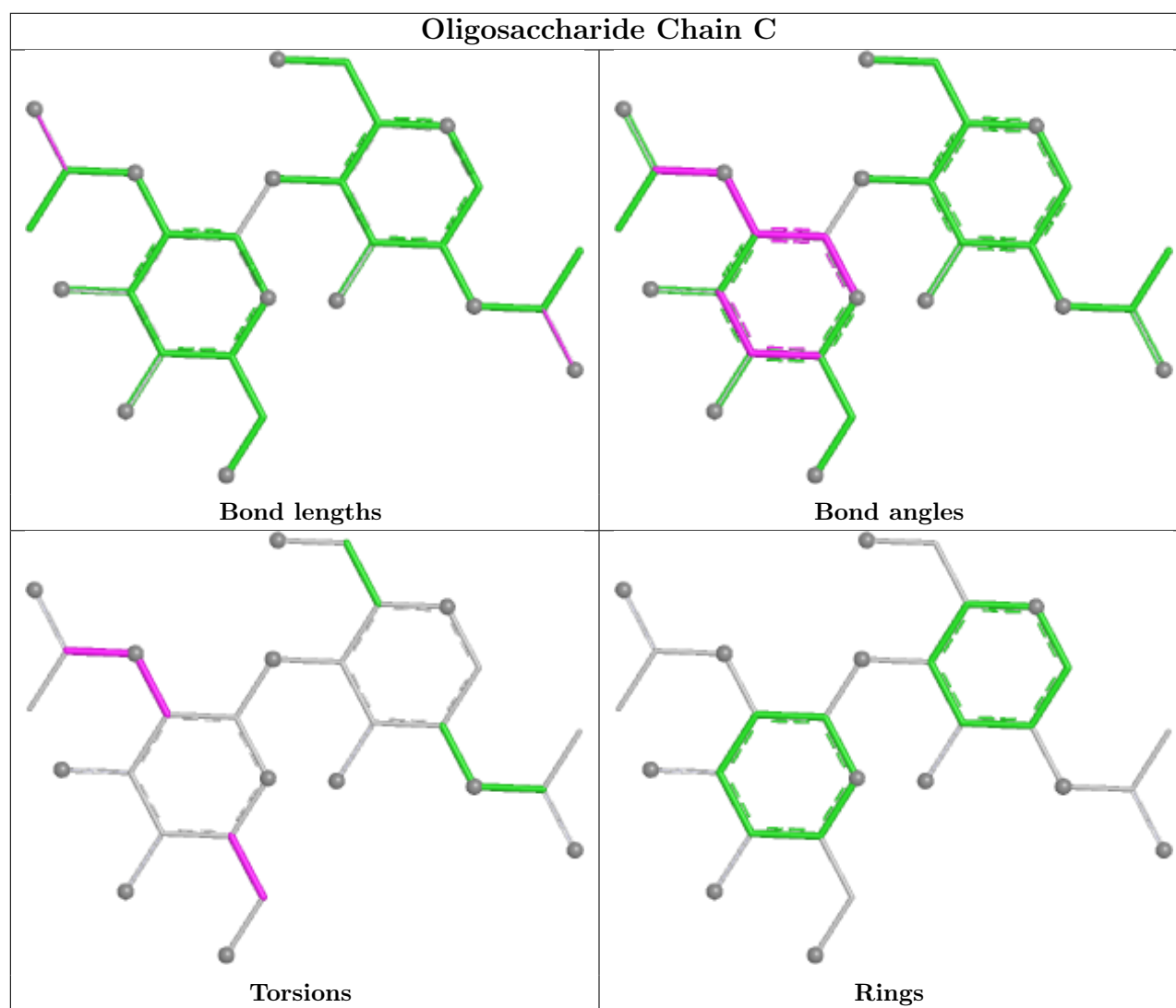
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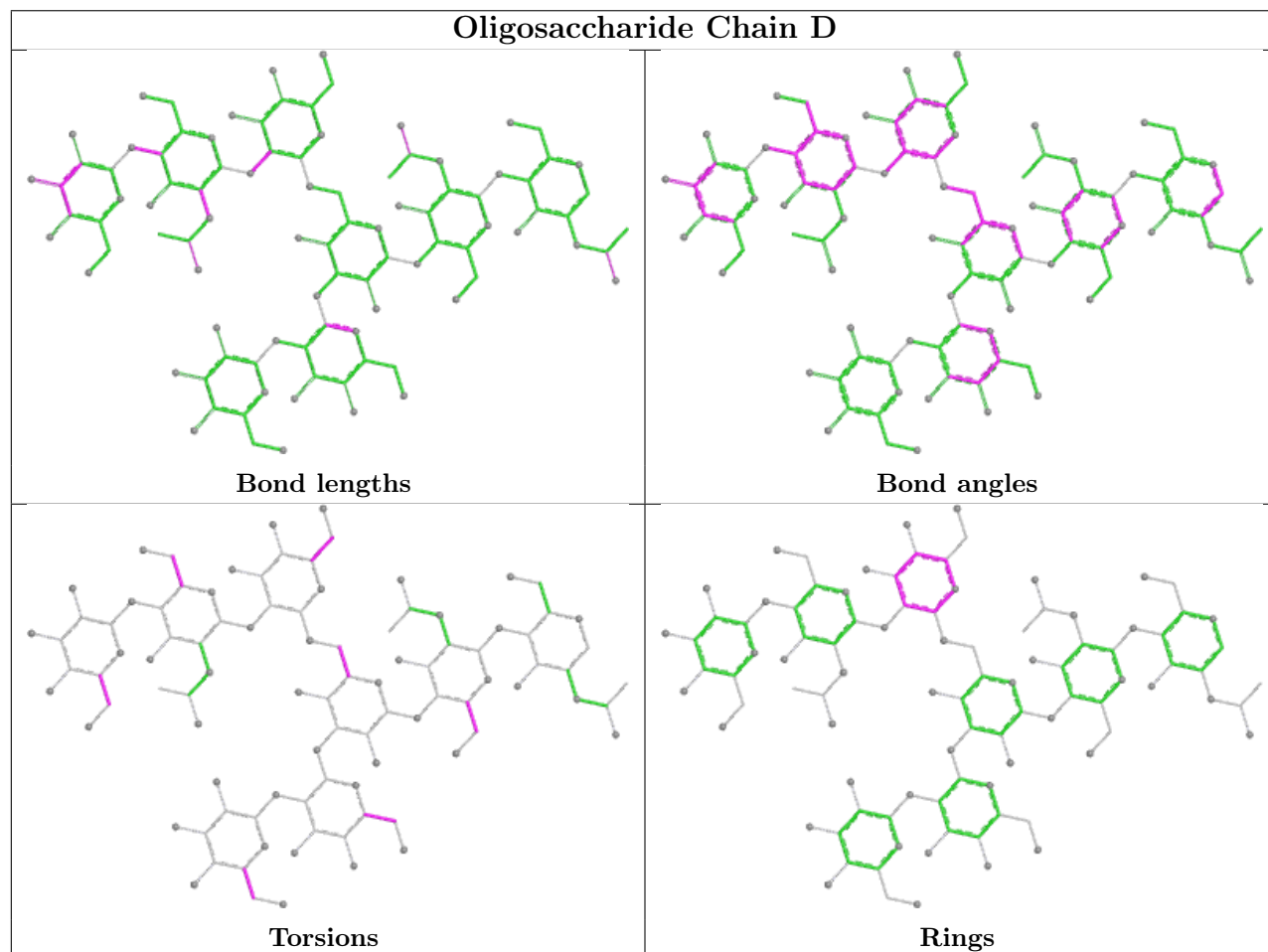
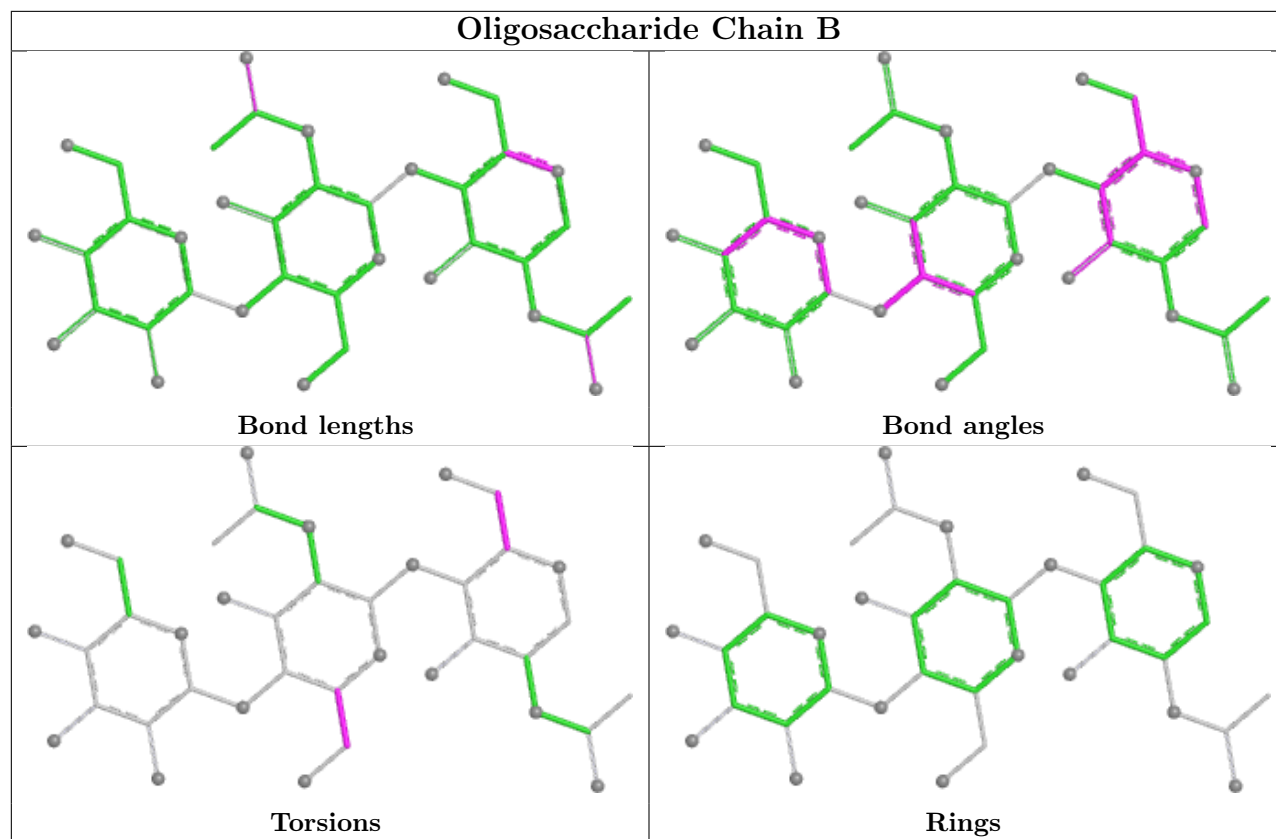
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	NAG	2	0

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

10 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
6	NAG	I	861	1	14,14,15	1.24	1 (7%)	17,19,21	1.43	3 (17%)
6	NAG	I	821	1	14,14,15	1.32	1 (7%)	17,19,21	1.48	2 (11%)
5	MAN	I	803	-	11,11,12	0.71	0	15,15,17	1.54	2 (13%)
5	MAN	L	843	-	11,11,12	0.85	0	15,15,17	1.45	2 (13%)
6	NAG	L	801	1	14,14,15	1.26	1 (7%)	17,19,21	1.25	1 (5%)
7	GOL	I	901	-	5,5,5	0.75	0	5,5,5	0.65	0
8	PO4	L	501	-	4,4,4	1.01	0	6,6,6	0.68	0
7	GOL	L	901	-	5,5,5	0.76	0	5,5,5	0.60	0
5	MAN	L	844	-	11,11,12	0.83	0	15,15,17	0.93	0
6	NAG	L	821	1	14,14,15	1.30	2 (14%)	17,19,21	1.42	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
6	NAG	I	861	1	-	0/6/23/26	0/1/1/1
6	NAG	I	821	1	-	1/6/23/26	0/1/1/1
5	MAN	I	803	-	-	2/2/19/22	0/1/1/1
5	MAN	L	843	-	-	1/2/19/22	0/1/1/1
6	NAG	L	801	1	-	3/6/23/26	0/1/1/1
7	GOL	I	901	-	-	2/4/4/4	-
7	GOL	L	901	-	-	1/4/4/4	-
5	MAN	L	844	-	-	2/2/19/22	1/1/1/1
6	NAG	L	821	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	801	NAG	O7-C7	-3.85	1.14	1.23
6	I	861	NAG	O7-C7	-3.80	1.14	1.23
6	I	821	NAG	O7-C7	-3.76	1.14	1.23
6	L	821	NAG	O7-C7	-3.75	1.14	1.23
6	L	821	NAG	C2-N2	2.08	1.49	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	821	NAG	C3-C4-C5	4.54	118.46	110.23
6	I	821	NAG	C1-O5-C5	4.34	118.01	112.19
5	I	803	MAN	C1-C2-C3	-4.16	103.59	109.64
6	I	861	NAG	O5-C1-C2	-4.13	104.90	111.29
6	L	801	NAG	C1-O5-C5	3.62	117.03	112.19
5	L	843	MAN	C1-O5-C5	3.43	116.79	112.19
6	I	821	NAG	C4-C3-C2	-2.48	107.38	111.02
5	L	843	MAN	C2-C3-C4	2.37	115.03	110.86
5	I	803	MAN	C3-C4-C5	2.13	114.09	110.23
6	L	821	NAG	C1-O5-C5	2.13	115.03	112.19
6	I	861	NAG	C1-C2-N2	2.12	113.78	110.43
6	I	861	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	901	GOL	C1-C2-C3-O3
5	I	803	MAN	O5-C5-C6-O6
5	I	803	MAN	C4-C5-C6-O6
6	L	801	NAG	O5-C5-C6-O6
6	L	801	NAG	C4-C5-C6-O6
5	L	844	MAN	C4-C5-C6-O6
7	L	901	GOL	C1-C2-C3-O3
5	L	843	MAN	O5-C5-C6-O6
6	L	821	NAG	O5-C5-C6-O6
5	L	844	MAN	O5-C5-C6-O6
7	I	901	GOL	O2-C2-C3-O3
6	L	821	NAG	C8-C7-N2-C2
6	L	801	NAG	C3-C2-N2-C7
6	L	821	NAG	O7-C7-N2-C2
6	I	821	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	844	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	803	MAN	1	0
5	L	843	MAN	1	0
7	L	901	GOL	1	0
5	L	844	MAN	1	0
6	L	821	NAG	1	0

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.