



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:07 PM UTC

PDB ID : 7API / pdb\_00007api  
Title : THE S VARIANT OF HUMAN ALPHA1-ANTITRYPSIN, STRUCTURE AND IMPLICATIONS FOR FUNCTION AND METABOLISM  
Authors : Loebermann, H.; Tokuoka, R.; Deisenhofer, J.; Huber, R.  
Deposited on : 1988-09-08  
Resolution : 3.00 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>.

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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

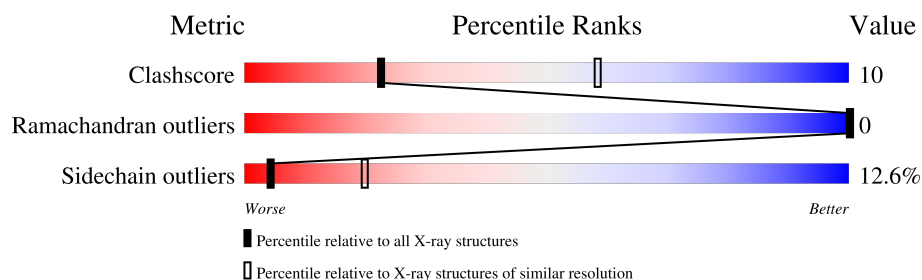
# 1 Overall quality at a glance

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  $\geq 3$ , 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	A	347	
2	B	36	
3	C	6	
4	D	2	
4	E	2	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	3	X	-	-	-
4	NAG	E	1	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3260 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.

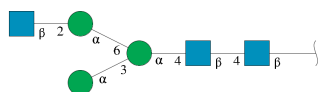
- Molecule 1 is a protein called ALPHA 1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	6	0	0
			2690	1726	441	515	8			

- Molecule 2 is a protein called ALPHA 1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	4	0	0
			291	193	46	50	2			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-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	C	6	Total	C	N	O	25	0	0
			75	42	3	30			

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



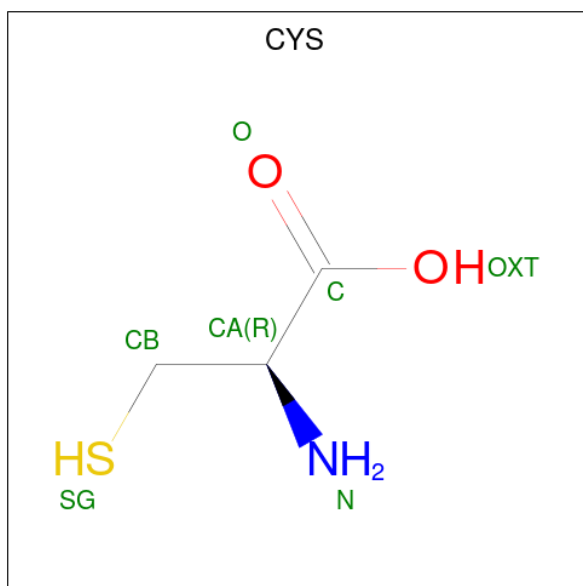
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	18	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	5	0	0
			28	16	2	10			

- Molecule 5 is CYSTEINE (CCD ID: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 6 is water.

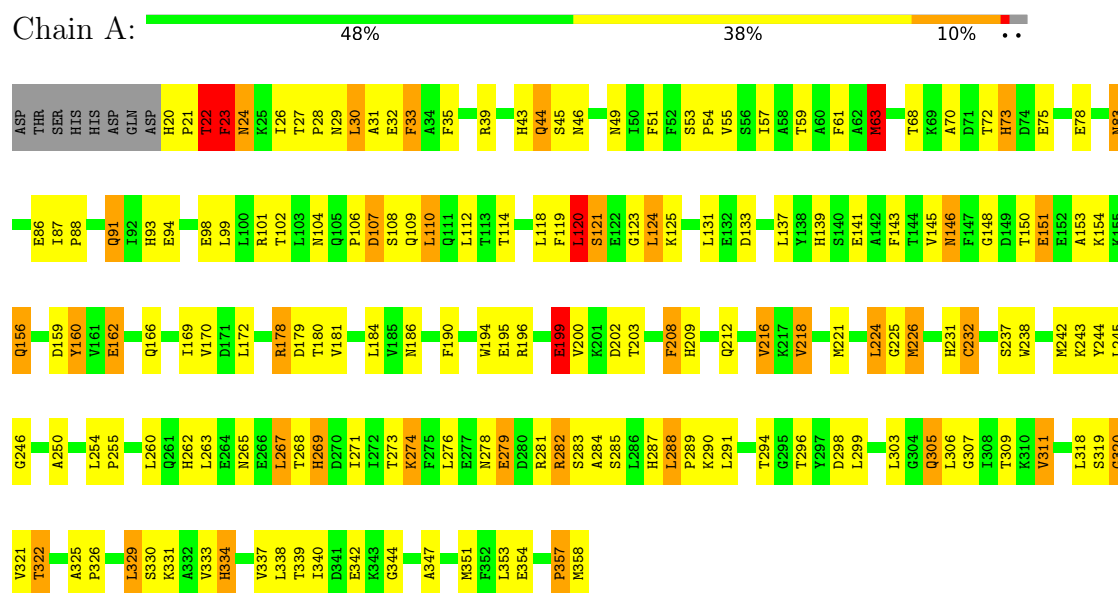
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	13	Total	O	0	0
			13	13		

### 3 Residue-property plots

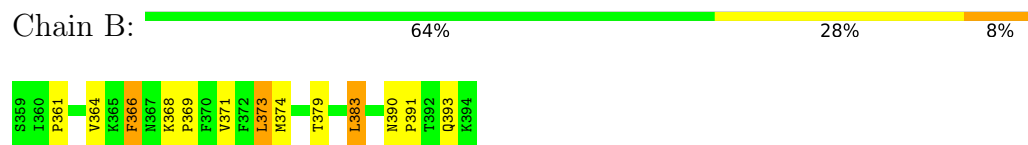
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

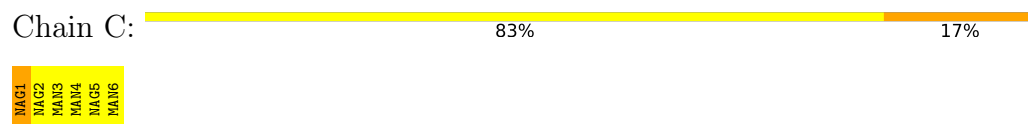
#### • Molecule 1: ALPHA 1-ANTITRYPSIN



#### • Molecule 2: ALPHA 1-ANTITRYPSIN



#### • Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:  100%

MAG1  
MAG2

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

Chain E:  50%  50%

MAG1  
MAG2

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.50Å 120.50Å 113.50Å 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	EREF	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3260	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: NAG, MAN

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	1.40	29/2744 (1.1%)	1.98	78/3707 (2.1%)
2	B	1.08	0/299	1.89	10/402 (2.5%)
All	All	1.37	29/3043 (1.0%)	1.97	88/4109 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	21

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	HIS	ND1-CE1	10.31	1.42	1.32
1	A	73	HIS	CE1-NE2	9.80	1.42	1.32
1	A	287	HIS	ND1-CE1	9.76	1.42	1.32
1	A	139	HIS	ND1-CE1	9.70	1.42	1.32
1	A	231	HIS	ND1-CE1	9.48	1.42	1.32
1	A	238	TRP	NE1-CE2	-9.46	1.27	1.37
1	A	43	HIS	ND1-CE1	9.25	1.41	1.32
1	A	194	TRP	NE1-CE2	-9.17	1.27	1.37
1	A	139	HIS	CE1-NE2	8.96	1.41	1.32
1	A	73	HIS	ND1-CE1	8.89	1.41	1.32
1	A	262	HIS	CE1-NE2	8.86	1.41	1.32
1	A	269	HIS	CE1-NE2	8.77	1.41	1.32
1	A	20	HIS	CE1-NE2	8.77	1.41	1.32
1	A	20	HIS	ND1-CE1	8.71	1.41	1.32
1	A	93	HIS	CE1-NE2	8.68	1.41	1.32
1	A	123	GLY	CA-C	8.58	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	HIS	CE1-NE2	8.56	1.41	1.32
1	A	334	HIS	CE1-NE2	8.48	1.41	1.32
1	A	43	HIS	CE1-NE2	8.32	1.40	1.32
1	A	287	HIS	CE1-NE2	8.32	1.40	1.32
1	A	269	HIS	ND1-CE1	8.24	1.40	1.32
1	A	93	HIS	ND1-CE1	8.15	1.40	1.32
1	A	262	HIS	ND1-CE1	8.09	1.40	1.32
1	A	179	ASP	N-CA	7.93	1.54	1.46
1	A	231	HIS	CE1-NE2	7.17	1.39	1.32
1	A	209	HIS	ND1-CE1	6.86	1.39	1.32
1	A	123	GLY	N-CA	6.04	1.53	1.45
1	A	124	LEU	N-CA	5.96	1.53	1.46
1	A	178	ARG	CA-C	5.88	1.60	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	CYS	CB-CA-C	-10.23	93.41	110.19
1	A	232	CYS	CA-C-O	-8.64	110.81	120.32
1	A	225	GLY	CA-C-N	-8.51	111.78	122.84
1	A	225	GLY	C-N-CA	-8.51	111.78	122.84
1	A	45	SER	CA-C-N	-8.16	109.10	122.65
1	A	45	SER	C-N-CA	-8.16	109.10	122.65
1	A	265	ASN	CA-CB-CG	-7.87	104.73	112.60
1	A	278	ASN	CA-CB-CG	-7.45	105.15	112.60
1	A	298	ASP	CA-CB-CG	-7.44	105.16	112.60
1	A	61	PHE	CA-CB-CG	-7.13	106.67	113.80
1	A	32	GLU	O-C-N	7.07	130.21	122.15
1	A	30	LEU	O-C-N	7.04	129.35	122.03
1	A	94	GLU	O-C-N	7.03	130.44	122.22
1	A	244	TYR	O-C-N	7.00	130.94	123.03
1	A	311	VAL	CB-CA-C	-6.96	101.88	112.05
1	A	23	PHE	CB-CA-C	-6.93	100.00	110.88
1	A	133	ASP	CA-CB-CG	-6.92	105.69	112.60
1	A	49	ASN	CA-CB-CG	-6.82	105.78	112.60
1	A	320	GLY	CA-C-N	-6.82	114.31	122.35
1	A	320	GLY	C-N-CA	-6.82	114.31	122.35
2	B	371	VAL	CA-C-O	-6.63	114.50	121.93
1	A	33	PHE	O-C-N	6.47	128.73	122.07
1	A	57	ILE	CB-CA-C	-6.45	103.44	112.14
1	A	53	SER	O-C-N	6.43	128.93	121.47
1	A	101	ARG	O-C-N	6.39	128.65	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	THR	O-C-N	6.37	130.61	123.48
1	A	288	LEU	O-C-N	6.17	128.42	121.94
1	A	78	GLU	CB-CG-CD	-6.14	102.16	112.60
1	A	94	GLU	N-CA-C	-6.03	104.78	111.71
1	A	156	GLN	OE1-CD-NE2	6.00	128.60	122.60
1	A	44	GLN	CB-CG-CD	-5.99	102.42	112.60
1	A	169	ILE	CA-C-N	-5.96	115.45	122.36
1	A	169	ILE	C-N-CA	-5.96	115.45	122.36
1	A	274	LYS	N-CA-C	-5.86	104.53	111.03
2	B	373	LEU	N-CA-C	5.80	116.96	108.14
1	A	159	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	22	THR	N-CA-CB	-5.73	101.66	110.20
1	A	347	ALA	CA-C-O	-5.65	114.51	121.06
1	A	216	VAL	CA-CB-CG1	5.63	119.98	110.40
1	A	75	GLU	CB-CG-CD	-5.61	103.06	112.60
1	A	21	PRO	CA-C-N	5.60	130.16	120.58
1	A	21	PRO	C-N-CA	5.60	130.16	120.58
1	A	153	ALA	O-C-N	5.60	128.14	122.09
2	B	364	VAL	CA-C-N	-5.59	115.28	123.00
2	B	364	VAL	C-N-CA	-5.59	115.28	123.00
2	B	366	PHE	CA-C-N	-5.57	114.25	122.83
2	B	366	PHE	C-N-CA	-5.57	114.25	122.83
1	A	209	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	102	THR	O-C-N	5.53	127.98	122.12
1	A	35	PHE	N-CA-C	-5.53	105.33	111.36
2	B	379	THR	N-CA-CB	-5.53	102.99	110.67
1	A	208	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	121	SER	O-C-N	5.47	129.54	122.81
1	A	44	GLN	N-CA-C	5.46	116.92	110.97
1	A	244	TYR	N-CA-C	-5.43	102.01	110.42
1	A	119	PHE	CA-CB-CG	-5.42	108.38	113.80
1	A	218	VAL	CB-CA-C	-5.36	101.60	111.36
1	A	110	LEU	CA-C-N	-5.35	115.46	123.00
1	A	110	LEU	C-N-CA	-5.35	115.46	123.00
1	A	33	PHE	N-CA-C	-5.31	105.39	111.07
1	A	340	ILE	CB-CA-C	-5.29	102.80	110.63
1	A	303	LEU	N-CA-C	-5.28	106.68	113.01
1	A	24	ASN	CA-CB-CG	-5.23	107.37	112.60
2	B	393	GLN	CB-CG-CD	-5.22	103.72	112.60
1	A	325	ALA	O-C-N	5.18	125.43	121.65
2	B	371	VAL	N-CA-CB	-5.18	102.18	112.24
1	A	172	LEU	CA-C-N	-5.17	116.53	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	LEU	C-N-CA	-5.17	116.53	122.95
1	A	274	LYS	O-C-N	5.17	127.61	122.03
1	A	24	ASN	N-CA-C	-5.15	106.83	113.01
1	A	125	LYS	CA-C-N	-5.14	113.77	122.67
1	A	125	LYS	C-N-CA	-5.14	113.77	122.67
1	A	344	GLY	CA-C-N	-5.14	113.52	122.37
1	A	344	GLY	C-N-CA	-5.14	113.52	122.37
1	A	279	GLU	CB-CG-CD	-5.12	103.90	112.60
1	A	121	SER	CA-C-N	5.10	127.37	120.38
1	A	121	SER	C-N-CA	5.10	127.37	120.38
1	A	288	LEU	CA-C-N	5.10	125.03	119.78
1	A	288	LEU	C-N-CA	5.10	125.03	119.78
1	A	202	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	357	PRO	O-C-N	5.07	129.52	123.13
1	A	262	HIS	O-C-N	5.05	127.28	122.07
1	A	141	GLU	CA-C-N	-5.04	114.97	122.74
1	A	141	GLU	C-N-CA	-5.04	114.97	122.74
2	B	371	VAL	CB-CA-C	-5.04	104.32	111.38
1	A	160	TYR	O-C-N	5.04	127.26	122.07
1	A	112	LEU	CA-C-N	5.00	130.55	122.29
1	A	112	LEU	C-N-CA	5.00	130.55	122.29

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASN	Mainchain
1	A	106	PRO	Mainchain
1	A	107	ASP	Mainchain
1	A	120	LEU	Mainchain
1	A	156	GLN	Mainchain
1	A	160	TYR	Sidechain
1	A	162	GLU	Mainchain
1	A	178	ARG	Sidechain
1	A	180	THR	Mainchain
1	A	199	GLU	Mainchain
1	A	203	THR	Mainchain
1	A	23	PHE	Mainchain
1	A	232	CYS	Mainchain
1	A	237	SER	Mainchain
1	A	289	PRO	Mainchain
1	A	290	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	296	THR	Mainchain
1	A	309	THR	Mainchain
1	A	63	MET	Mainchain
1	A	70	ALA	Mainchain
1	A	83	ASN	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2690	0	2685	62	1
2	B	291	0	306	6	0
3	C	75	0	64	1	0
4	D	28	0	25	0	0
4	E	28	0	25	2	0
5	A	7	0	3	0	0
6	A	128	0	0	0	3
6	B	13	0	0	0	0
All	All	3260	0	3108	64	3

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 (64) 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:A:27:THR:HA	1:A:30:LEU:HD12	1.61	0.80
1:A:83:ASN:HD22	1:A:86:GLU:HG3	1.53	0.74
1:A:299:LEU:HD12	1:A:351:MET:HE1	1.72	0.72
1:A:331:LYS:HB2	1:A:354:GLU:HG2	1.70	0.72
1:A:26:ILE:HA	1:A:29:ASN:HD22	1.56	0.70
1:A:110:LEU:HD11	1:A:190:PHE:HE1	1.58	0.69
1:A:88:PRO:HG2	1:A:91:GLN:HB2	1.79	0.64
1:A:146:ASN:HD22	1:A:148:GLY:H	1.45	0.63
1:A:334:HIS:HB2	1:A:351:MET:SD	2.41	0.61
1:A:329:LEU:HD21	1:A:353:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:O	1:A:33:PHE:HB3	2.01	0.60
1:A:195:GLU:HG2	1:A:245:LEU:HD23	1.84	0.59
1:A:208:PHE:HB2	1:A:218:VAL:HG21	1.83	0.59
1:A:54:PRO:HD2	2:B:383:LEU:O	2.02	0.58
1:A:121:SER:HA	1:A:145:VAL:O	2.05	0.57
1:A:31:ALA:HB1	1:A:269:HIS:HB2	1.87	0.56
1:A:195:GLU:HG3	1:A:243:LYS:HB3	1.89	0.55
1:A:255:PRO:HG3	1:A:260:LEU:HD13	1.90	0.54
1:A:55:VAL:O	1:A:59:THR:HG23	2.08	0.53
1:A:226:MET:HG2	1:A:281:ARG:HB3	1.91	0.53
1:A:330:SER:OG	1:A:354:GLU:HG3	2.09	0.53
1:A:63:MET:HE2	1:A:184:LEU:HD21	1.91	0.52
1:A:151:GLU:HA	1:A:154:LYS:HE2	1.91	0.52
1:A:26:ILE:HA	1:A:29:ASN:ND2	2.26	0.51
1:A:27:THR:HB	1:A:28:PRO:HD2	1.94	0.50
1:A:294:THR:HG22	1:A:337:VAL:HG22	1.94	0.49
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.54	0.48
1:A:27:THR:O	1:A:30:LEU:HB2	2.14	0.48
1:A:107:ASP:CG	4:E:1:NAG:HN2	2.22	0.48
1:A:291:LEU:O	1:A:339:THR:HA	2.14	0.47
1:A:110:LEU:HD11	1:A:190:PHE:CE1	2.45	0.47
1:A:162:GLU:HG3	1:A:170:VAL:HG12	1.95	0.47
1:A:246:GLY:HA2	4:E:1:NAG:H83	1.96	0.46
1:A:181:VAL:HG23	1:A:357:PRO:HD3	1.97	0.46
1:A:68:THR:HB	1:A:73:HIS:HB2	1.96	0.46
1:A:326:PRO:O	1:A:358:MET:HG2	2.17	0.45
1:A:196:ARG:HA	1:A:196:ARG:HD2	1.76	0.45
1:A:27:THR:HB	1:A:28:PRO:CD	2.47	0.44
1:A:242:MET:HB2	1:A:250:ALA:HB3	2.00	0.44
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.72	0.44
1:A:254:LEU:HB2	2:B:366:PHE:CE2	2.51	0.44
1:A:87:ILE:HA	1:A:88:PRO:HD2	1.74	0.43
1:A:282:ARG:HG3	1:A:283:SER:N	2.34	0.43
2:B:368:LYS:HB2	2:B:369:PRO:HD2	2.00	0.43
1:A:46:ASN:HD22	3:C:1:NAG:H83	1.83	0.43
2:B:390:ASN:HA	2:B:391:PRO:HD2	1.86	0.43
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.79	0.42
1:A:120:LEU:HD12	1:A:143:PHE:O	2.18	0.42
1:A:22:THR:OG1	1:A:98:GLU:HG3	2.20	0.42
1:A:199:GLU:H	1:A:199:GLU:HG2	1.37	0.42
1:A:195:GLU:HA	1:A:245:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HB	1:A:271:ILE:HD12	2.01	0.41
1:A:284:ALA:HA	2:B:361:PRO:HB2	2.02	0.41
1:A:291:LEU:HD21	2:B:391:PRO:HB3	2.01	0.41
1:A:224:LEU:HD12	1:A:285:SER:HA	2.02	0.41
1:A:226:MET:CG	1:A:281:ARG:HB3	2.49	0.41
1:A:146:ASN:HD22	1:A:146:ASN:C	2.28	0.41
1:A:271:ILE:O	1:A:274:LYS:HB2	2.21	0.40
1:A:305:GLN:C	1:A:307:GLY:H	2.29	0.40
1:A:51:PHE:CZ	1:A:338:LEU:HB2	2.57	0.40
1:A:318:LEU:C	1:A:320:GLY:N	2.77	0.40
1:A:39:ARG:HH11	1:A:39:ARG:HD2	1.72	0.40
1:A:263:LEU:O	1:A:267:LEU:HD12	2.21	0.40
1:A:124:LEU:HD11	1:A:322:THR:HG21	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:750:HOH:O	6:A:750:HOH:O[7_556]	1.50	0.70
6:A:698:HOH:O	6:A:698:HOH:O[7_556]	1.78	0.42
1:A:319:SER:OG	6:A:608:HOH:O[4_555]	2.11	0.09

## 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	337/347 (97%)	315 (94%)	22 (6%)	0	100	100
2	B	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
All	All	371/383 (97%)	347 (94%)	24 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	297/305 (97%)	259 (87%)	38 (13%)	4	19
2	B	35/35 (100%)	32 (91%)	3 (9%)	10	36
All	All	332/340 (98%)	291 (88%)	41 (12%)	4	21

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	PHE
1	A	24	ASN
1	A	44	GLN
1	A	63	MET
1	A	72	THR
1	A	91	GLN
1	A	99	LEU
1	A	108	SER
1	A	109	GLN
1	A	114	THR
1	A	120	LEU
1	A	137	LEU
1	A	146	ASN
1	A	150	THR
1	A	151	GLU
1	A	166	GLN
1	A	186	ASN
1	A	199	GLU
1	A	200	VAL
1	A	212	GLN
1	A	216	VAL
1	A	221	MET
1	A	224	LEU
1	A	226	MET
1	A	267	LEU
1	A	273	THR

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	279	GLU
1	A	282	ARG
1	A	288	LEU
1	A	305	GLN
1	A	306	LEU
1	A	311	VAL
1	A	321	VAL
1	A	329	LEU
1	A	333	VAL
1	A	342	GLU
2	B	373	LEU
2	B	374	MET
2	B	383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	43	HIS
1	A	97	GLN
1	A	146	ASN
1	A	212	GLN
1	A	305	GLN
2	B	377	GLN
2	B	378	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

10 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	C	1	3,1	14,14,15	0.87	0	17,19,21	1.67	4 (23%)
3	NAG	C	2	3	14,14,15	1.22	2 (14%)	17,19,21	2.87	2 (11%)
3	MAN	C	3	3	11,11,12	0.90	0	15,15,17	1.19	1 (6%)
3	MAN	C	4	3	11,11,12	0.93	0	15,15,17	2.10	1 (6%)
3	NAG	C	5	3	14,14,15	1.03	1 (7%)	17,19,21	1.90	3 (17%)
3	MAN	C	6	3	11,11,12	1.09	1 (9%)	15,15,17	2.01	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	1.71	2 (11%)
4	NAG	D	2	4	14,14,15	0.68	0	17,19,21	1.51	1 (5%)
4	NAG	E	1	4,1	14,14,15	1.41	2 (14%)	17,19,21	2.01	6 (35%)
4	NAG	E	2	4	14,14,15	0.92	1 (7%)	17,19,21	2.04	4 (23%)

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	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	3.98	1.57	1.52
3	C	2	NAG	C1-C2	2.91	1.56	1.52
3	C	5	NAG	C1-C2	2.49	1.55	1.52
3	C	2	NAG	C4-C5	2.12	1.57	1.53
4	E	2	NAG	C1-C2	2.12	1.55	1.52
4	D	1	NAG	C1-C2	2.05	1.55	1.52
3	C	6	MAN	C2-C3	2.04	1.55	1.52
4	E	1	NAG	C3-C2	2.00	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	9.58	125.02	112.19
3	C	4	MAN	C1-O5-C5	7.21	121.85	112.19
4	E	2	NAG	C1-O5-C5	6.98	121.54	112.19
3	C	6	MAN	C1-O5-C5	6.82	121.32	112.19
3	C	5	NAG	C1-O5-C5	5.81	119.98	112.19
4	D	2	NAG	C1-O5-C5	5.31	119.30	112.19
3	C	2	NAG	O5-C5-C6	-4.88	98.17	107.66
4	D	1	NAG	C1-O5-C5	4.76	118.57	112.19
4	E	1	NAG	C1-C2-N2	3.80	116.42	110.43
4	E	1	NAG	C1-O5-C5	3.73	117.18	112.19
4	E	1	NAG	O5-C1-C2	-3.64	105.65	111.29
3	C	3	MAN	C1-O5-C5	3.53	116.92	112.19
3	C	1	NAG	O5-C1-C2	-3.42	105.99	111.29
3	C	5	NAG	O5-C1-C2	-3.33	106.15	111.29
3	C	1	NAG	C1-O5-C5	3.05	116.28	112.19
3	C	6	MAN	O5-C5-C6	3.02	113.55	107.66
3	C	1	NAG	O4-C4-C3	-2.96	103.40	110.38
4	E	2	NAG	O5-C1-C2	-2.55	107.35	111.29
4	E	1	NAG	O7-C7-N2	2.34	126.11	121.98
3	C	1	NAG	O7-C7-C8	-2.28	117.99	122.05
4	E	1	NAG	C4-C3-C2	2.28	114.36	111.02
4	E	2	NAG	O7-C7-N2	2.26	125.98	121.98
4	E	2	NAG	C2-N2-C7	2.24	125.90	122.90
4	E	1	NAG	C3-C4-C5	-2.17	106.29	110.23
4	D	1	NAG	C4-C3-C2	2.17	114.20	111.02
3	C	5	NAG	O7-C7-N2	2.11	125.71	121.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	MAN	C1

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Mol	Chain	Res	Type	Atom
4	E	1	NAG	C1

All (10) torsion outliers are listed below:

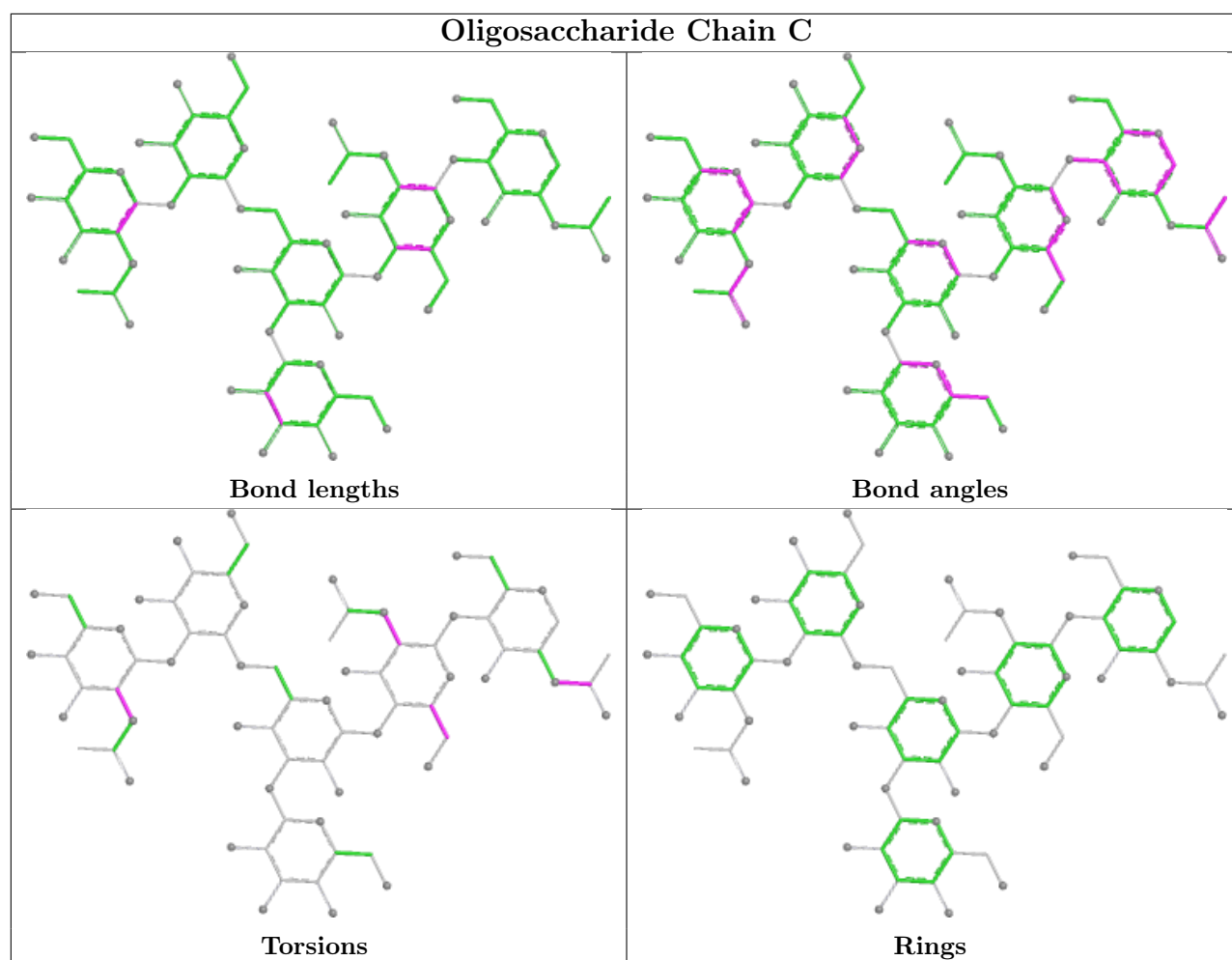
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
3	C	5	NAG	C1-C2-N2-C7
3	C	5	NAG	C3-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6

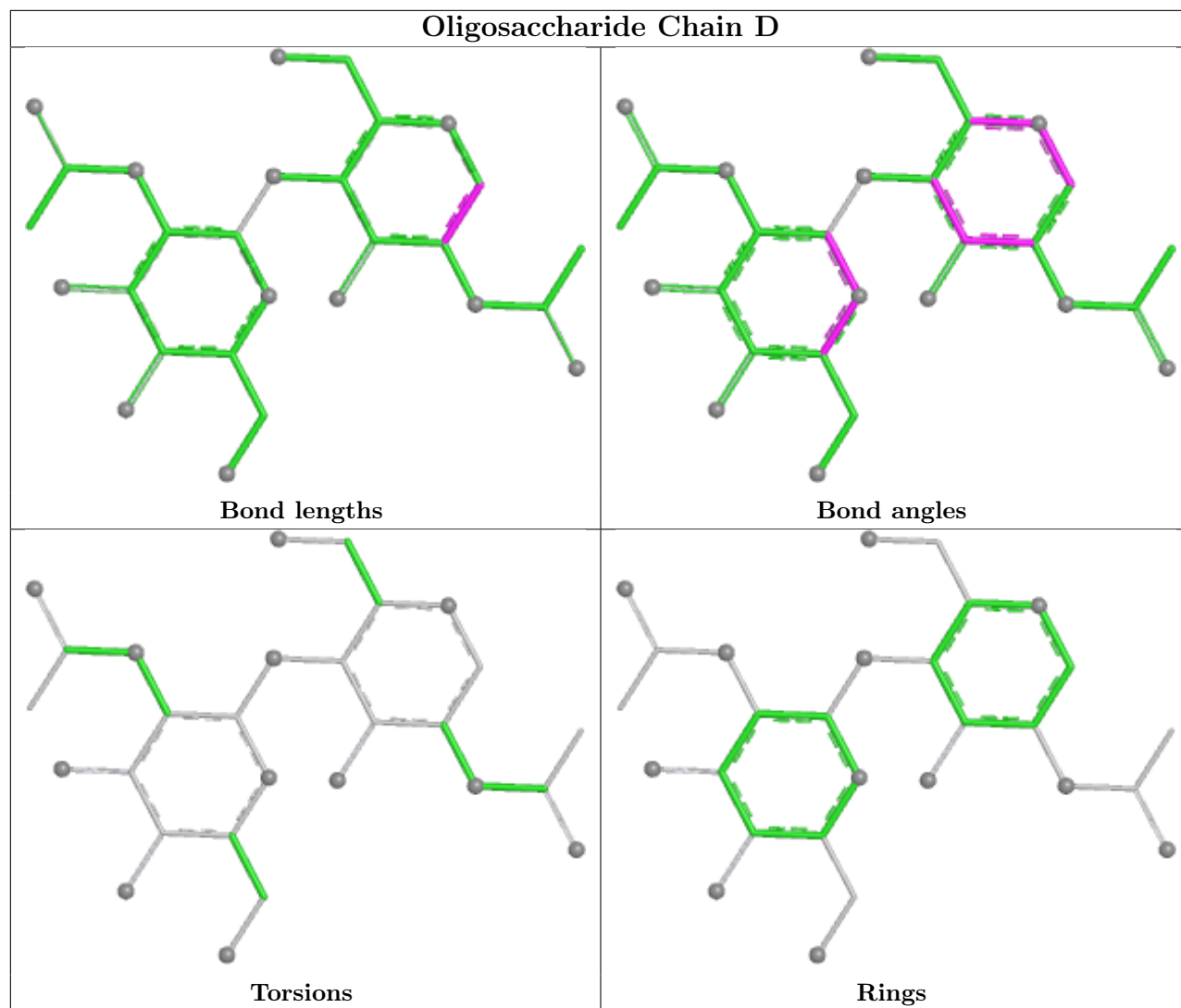
There are no ring outliers.

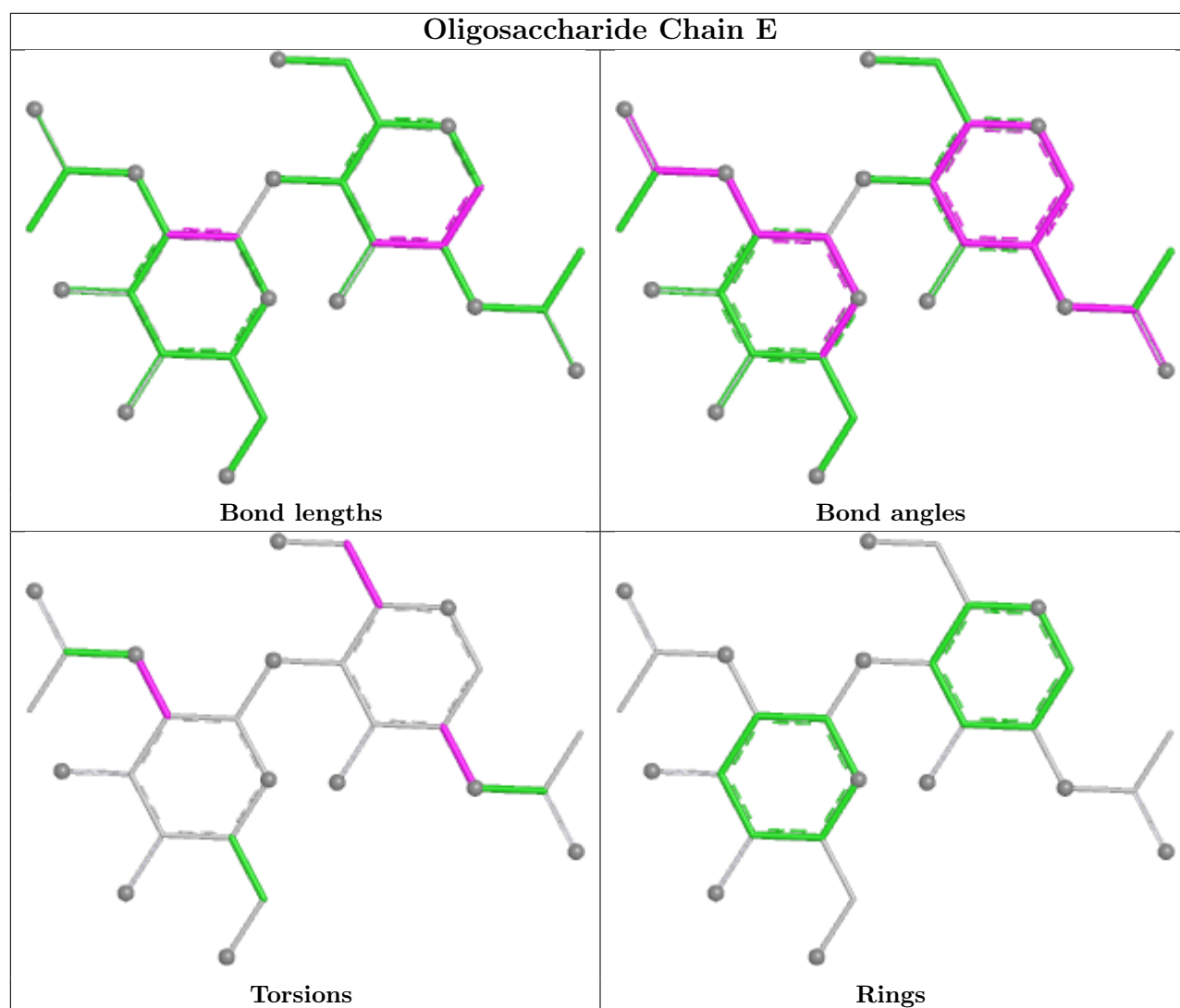
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0
3	C	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

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	CYS	A	395	1	5,6,6	1.70	1 (20%)	3,7,7	2.14	2 (66%)

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	CYS	A	395	1	-	3/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	395	CYS	CB-CA	3.58	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	395	CYS	OXT-C-O	-2.77	117.80	124.08
5	A	395	CYS	CB-CA-C	2.45	112.33	109.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	395	CYS	N-CA-CB-SG
5	A	395	CYS	C-CA-CB-SG
5	A	395	CYS	OXT-C-CA-N

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.