



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:13 AM UTC

PDB ID : 1BCS / pdb\_00001bcs  
Title : COMPLEX OF THE WHEAT SERINE CARBOXYPEPTIDASE, CPDW-II,  
WITH THE MICROBIAL PEPTIDE ALDEHYDE INHIBITOR, CHYMO-  
STATIN, AND ARGININE AT 100 DEGREES KELVIN  
Authors : Bullock, T.L.; Remington, S.J.  
Deposited on : 1995-11-03  
Resolution : 2.08 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](mailto: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>.

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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)  
Xtrriage (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

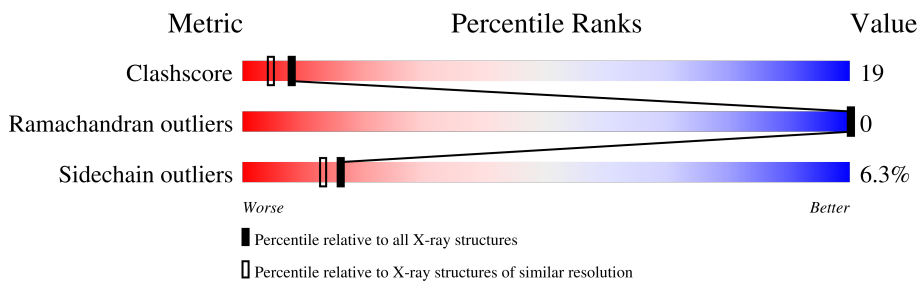
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)

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	263	62% 25% 8% . .
2	B	160	60% 26% 9% . .
3	C	4	50% 25% 25%
4	D	3	100%
5	E	2	50% 50%

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
4	NAG	D	1	-	-	X	-
4	NDG	D	3	X	-	-	-
5	NAG	E	1	-	-	X	-
5	NAG	E	2	X	-	-	-
7	NAG	A	1131	X	-	X	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 3731 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 SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	1999	1280	334	378	7	0	0	0

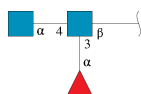
- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	1202	771	207	218	6	0	0	0

- Molecule 3 is a protein called CHYMOSTATIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	44	31	7	6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



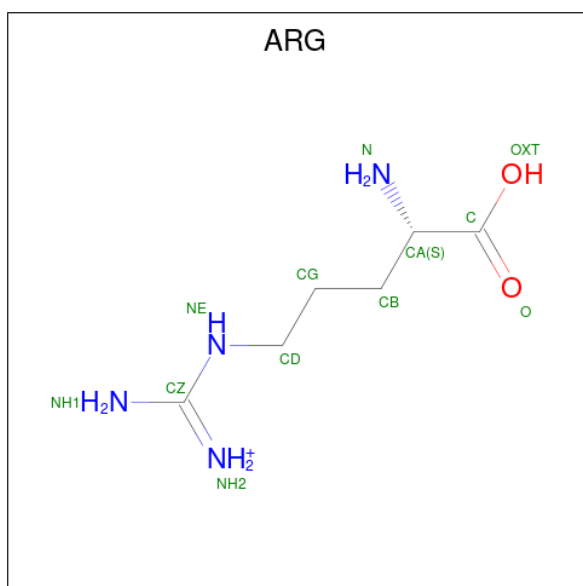
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0

- Molecule 6 is ARGinine (CCD ID: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



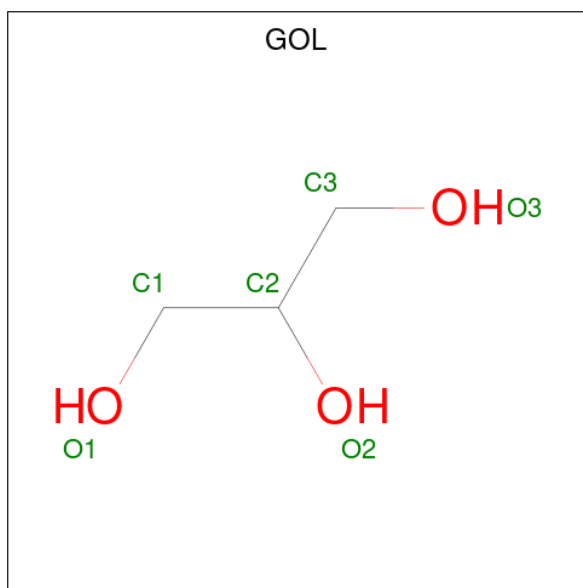
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	12	6	4	2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	226	Total O 226 226	0	0
10	B	157	Total O 157 157	0	0
10	C	1	Total O 1 1	0	0

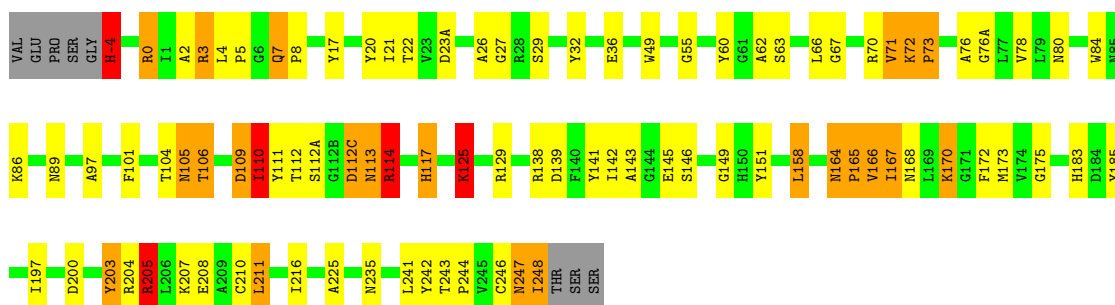
### 3 Residue-property plots [i](#)

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.

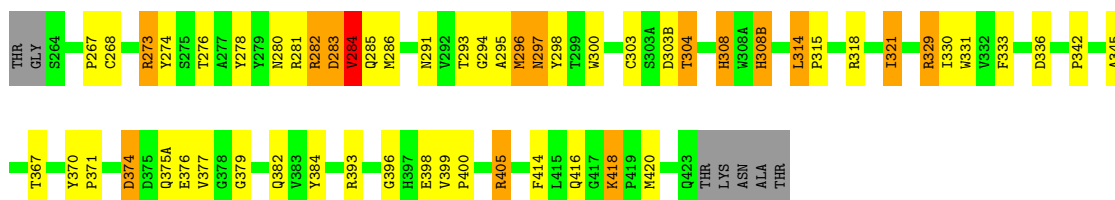
- Molecule 1: SERINE CARBOXYPEPTIDASE II

Chain A: 



- Molecule 2: SERINE CARBOXYPEPTIDASE II

Chain B: 



- Molecule 3: CHYMOSTATIN A

Chain C: 



- Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

MAGE1  
MAGE2

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.40Å 95.40Å 208.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.08	Depositor
% Data completeness (in resolution range)	(Not available) (33.00-2.08)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, FUC, CSI, NDG, GOL, NAG, PHA

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	1.42	11/2062 (0.5%)	1.78	37/2814 (1.3%)
2	B	1.45	3/1242 (0.2%)	1.87	34/1702 (2.0%)
3	C	0.91	0/19	1.48	0/21
All	All	1.43	14/3323 (0.4%)	1.81	71/4537 (1.6%)

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
3	C	1	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ASN	C-N	-7.99	1.24	1.34
1	A	110	ILE	CA-CB	-7.61	1.45	1.54
2	B	420	MET	C-N	-6.74	1.25	1.33
1	A	73	PRO	CA-C	-6.16	1.44	1.52
1	A	165	PRO	N-CA	-6.07	1.39	1.47
1	A	166	VAL	CA-C	-5.63	1.44	1.52
1	A	112(C)	ASP	CG-OD1	5.53	1.35	1.25
2	B	304	THR	C-N	-5.47	1.27	1.33
1	A	60	TYR	CA-C	-5.34	1.48	1.53
2	B	374	ASP	CA-C	-5.25	1.46	1.52
1	A	183	HIS	CA-C	-5.19	1.46	1.52
1	A	22	THR	CA-C	-5.07	1.46	1.52
1	A	208	GLU	CD-OE1	5.04	1.34	1.25
1	A	72	LYS	CA-CB	-5.02	1.46	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASN	CA-CB-CG	-10.14	102.45	112.60
1	A	164	ASN	CA-C-O	9.63	128.59	119.24
1	A	117	HIS	CA-CB-CG	-9.18	104.62	113.80
1	A	110	ILE	CB-CG1-CD1	-9.13	94.64	113.80
1	A	-4	HIS	N-CA-CB	8.50	124.96	110.50
1	A	211	LEU	N-CA-C	8.41	122.64	112.38
1	A	114	ARG	NE-CZ-NH1	8.39	129.89	121.50
2	B	308(B)	HIS	CA-CB-CG	-8.21	105.59	113.80
2	B	393	ARG	NE-CZ-NH2	-8.20	111.82	119.20
2	B	329	ARG	NE-CZ-NH2	-7.75	112.22	119.20
1	A	114	ARG	NE-CZ-NH2	-7.65	112.31	119.20
2	B	398	GLU	CA-CB-CG	-7.61	98.88	114.10
2	B	282	ARG	CB-CA-C	7.59	122.80	110.88
2	B	393	ARG	CD-NE-CZ	7.35	134.69	124.40
1	A	97	ALA	CA-C-N	-7.34	113.17	123.08
1	A	97	ALA	C-N-CA	-7.34	113.17	123.08
2	B	329	ARG	CD-NE-CZ	7.31	134.64	124.40
1	A	110	ILE	N-CA-CB	-7.31	93.98	111.23
2	B	329	ARG	NE-CZ-NH1	7.04	128.54	121.50
2	B	375(A)	GLN	CB-CA-C	7.02	121.34	109.55
2	B	393	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	A	114	ARG	CD-NE-CZ	6.68	133.75	124.40
1	A	158	LEU	CB-CA-C	-6.67	100.42	110.88
2	B	314	LEU	CA-C-O	6.58	124.38	118.33
2	B	297	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	71	VAL	CB-CA-C	-6.35	102.90	111.15
1	A	76	ALA	N-CA-C	6.33	119.16	111.82
1	A	200	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	106	THR	N-CA-CB	-6.23	100.11	110.39
1	A	149	GLY	N-CA-C	-6.20	106.06	113.99
1	A	7	GLN	N-CA-C	6.12	117.36	109.65
1	A	63	SER	N-CA-C	6.06	120.80	113.41
1	A	125	LYS	CG-CD-CE	6.06	125.23	111.30
1	A	146	SER	CB-CA-C	-6.03	109.03	117.23
1	A	105	ASN	OD1-CG-ND2	6.02	128.62	122.60
2	B	416	GLN	OE1-CD-NE2	-5.70	116.90	122.60
2	B	405	ARG	CA-C-O	5.68	126.57	120.55
2	B	296	MET	N-CA-C	-5.68	98.47	108.23
1	A	210	CYS	N-CA-C	5.67	120.35	113.38
1	A	203	TYR	CA-C-O	5.62	126.51	120.55
2	B	345	ALA	N-CA-C	-5.62	105.06	111.07
2	B	374	ASP	N-CA-CB	5.62	119.53	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	295	ALA	N-CA-C	5.60	119.73	113.01
2	B	416	GLN	CA-CB-CG	5.51	125.12	114.10
1	A	80	ASN	CA-C-O	5.51	126.47	120.58
1	A	139	ASP	CA-CB-CG	-5.51	107.09	112.60
1	A	89	ASN	CA-CB-CG	-5.50	107.10	112.60
2	B	405	ARG	CD-NE-CZ	5.47	132.06	124.40
2	B	405	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	73	PRO	N-CA-CB	5.44	108.09	103.35
1	A	205	ARG	CD-NE-CZ	5.44	132.01	124.40
2	B	308	HIS	CA-CB-CG	-5.37	108.43	113.80
2	B	336	ASP	N-CA-C	5.32	119.52	113.19
2	B	379	GLY	N-CA-C	-5.28	103.58	110.45
1	A	151	TYR	N-CA-C	5.27	117.43	111.11
2	B	284	VAL	N-CA-CB	5.26	118.47	110.58
2	B	342	PRO	N-CA-C	5.26	119.30	111.41
1	A	235	ASN	N-CA-C	5.25	118.84	110.70
2	B	283	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	284	VAL	CA-CB-CG1	5.24	119.31	110.40
2	B	284	VAL	CA-CB-CG2	5.18	119.21	110.40
1	A	241	LEU	N-CA-C	5.12	117.59	111.71
1	A	242	TYR	CA-CB-CG	-5.10	104.71	113.90
1	A	113	ASN	N-CA-C	5.10	116.53	111.07
2	B	278	TYR	N-CA-C	5.09	116.52	111.07
2	B	396	GLY	CA-C-N	5.09	127.10	120.28
2	B	396	GLY	C-N-CA	5.09	127.10	120.28
1	A	109	ASP	CA-CB-CG	-5.08	107.52	112.60
2	B	321	ILE	N-CA-C	-5.06	105.61	110.72
1	A	247	ASN	N-CA-C	5.03	119.42	113.28
2	B	384	TYR	CB-CA-C	-5.01	101.45	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	CSI	CB

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1999	0	1853	76	0
2	B	1202	0	1135	57	0
3	C	44	0	36	3	0
4	D	38	0	33	9	0
5	E	28	0	24	11	0
6	A	12	0	12	1	0
7	A	14	0	13	7	0
8	A	6	0	8	1	0
9	B	4	0	3	1	0
10	A	226	0	0	5	0
10	B	157	0	0	7	0
10	C	1	0	0	0	0
All	All	3731	0	3117	126	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 19.

All (126) 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:0:ARG:HG3	1:A:17:TYR:CE2	2.08	0.88
1:A:173:MET:HE1	2:B:414:PHE:HB2	1.57	0.85
1:A:113:ASN:ND2	7:A:1131:NAG:N2	2.26	0.83
1:A:5:PRO:HG2	2:B:284:VAL:HG12	1.64	0.78
1:A:173:MET:HE3	2:B:414:PHE:CD1	2.19	0.76
2:B:374:ASP:HB3	10:B:3066:HOH:O	1.85	0.76
1:A:105:ASN:HD21	4:D:1:NAG:C1	2.02	0.73
2:B:296:MET:O	5:E:1:NAG:H3	1.89	0.72
1:A:4:LEU:H	1:A:7:GLN:NE2	1.87	0.72
2:B:303(B):ASP:HA	3:C:1:PHE:CD2	2.25	0.71
2:B:285:GLN:HE22	5:E:1:NAG:H83	1.54	0.70
1:A:105:ASN:HD21	4:D:1:NAG:C2	2.04	0.70
5:E:1:NAG:O3	5:E:2:NAG:H61	1.90	0.70
1:A:110:ILE:HG22	1:A:111:TYR:CD1	2.27	0.69
1:A:3:ARG:NH1	1:A:7:GLN:O	2.26	0.68
1:A:-4:HIS:HB3	1:A:129:ARG:O	1.93	0.68
2:B:318:ARG:HD3	10:B:3007:HOH:O	1.92	0.68
2:B:418:LYS:NZ	10:B:2972:HOH:O	2.27	0.68
2:B:291:ASN:HD21	2:B:294:GLY:HA2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:426:ARG:N	3:C:4:PHA:O	2.27	0.67
2:B:293:THR:HG21	4:D:3:NDG:H8C3	1.78	0.65
2:B:304:THR:O	2:B:308:HIS:HD2	1.77	0.65
1:A:164:ASN:OD1	1:A:166:VAL:HG22	1.97	0.65
1:A:71:VAL:HG12	1:A:72:LYS:O	1.98	0.64
1:A:173:MET:HE2	2:B:331:TRP:HB3	1.80	0.63
2:B:291:ASN:OD1	2:B:296:MET:HB2	1.97	0.63
4:D:2:FUC:H5	4:D:3:NDG:C1	2.28	0.63
1:A:0:ARG:HG3	1:A:17:TYR:CZ	2.32	0.63
1:A:72:LYS:HD3	1:A:76(A):GLY:C	2.24	0.63
1:A:125:LYS:N	1:A:125:LYS:HD2	2.13	0.63
1:A:3:ARG:HD2	10:A:1156:HOH:O	2.00	0.61
1:A:205:ARG:HD2	1:A:225:ALA:HB2	1.81	0.61
2:B:297:ASN:HB3	10:B:3033:HOH:O	2.01	0.60
1:A:4:LEU:H	1:A:7:GLN:HE21	1.51	0.59
1:A:248:ILE:HD11	2:B:273:ARG:HG2	1.84	0.59
1:A:207:LYS:O	1:A:211:LEU:HG	2.02	0.59
2:B:300:TRP:HB2	5:E:1:NAG:H81	1.83	0.58
1:A:104:THR:HG21	1:A:109:ASP:HB2	1.84	0.58
1:A:105:ASN:HD21	4:D:1:NAG:H2	1.67	0.58
1:A:106:THR:O	1:A:109:ASP:HB2	2.03	0.58
2:B:282:ARG:O	2:B:286:MET:HG3	2.04	0.58
2:B:297:ASN:OD1	2:B:297:ASN:N	2.31	0.57
1:A:173:MET:HE2	2:B:331:TRP:CB	2.35	0.56
2:B:291:ASN:ND2	2:B:294:GLY:HA2	2.19	0.56
2:B:298:TYR:O	5:E:1:NAG:N2	2.39	0.56
2:B:321:ILE:HG13	2:B:330:ILE:HD12	1.87	0.56
1:A:205:ARG:HD2	1:A:225:ALA:CB	2.35	0.56
2:B:329:ARG:HD3	10:B:3012:HOH:O	2.06	0.55
1:A:173:MET:CE	2:B:414:PHE:HB2	2.33	0.55
2:B:374:ASP:CG	2:B:405:ARG:HH11	2.11	0.55
1:A:36:GLU:OE1	8:A:450:GOL:H32	2.07	0.55
1:A:105:ASN:ND2	4:D:1:NAG:H83	2.21	0.55
1:A:101:PHE:HD1	2:B:296:MET:HE1	1.72	0.54
1:A:105:ASN:ND2	4:D:1:NAG:C1	2.70	0.54
2:B:281:ARG:HB2	2:B:284:VAL:HG13	1.90	0.54
4:D:1:NAG:H61	4:D:3:NDG:H2	1.90	0.53
1:A:70:ARG:HB2	1:A:78:VAL:HG23	1.91	0.53
1:A:246:CYS:HA	2:B:267:PRO:HG2	1.89	0.53
1:A:20:TYR:HB3	1:A:29:SER:OG	2.10	0.52
1:A:167:ILE:HA	10:A:1197:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA3	1:A:105:ASN:HB2	1.91	0.52
1:A:173:MET:HE3	2:B:414:PHE:CG	2.45	0.52
1:A:203:TYR:O	1:A:207:LYS:HG3	2.11	0.51
2:B:376:GLU:HG3	10:B:3066:HOH:O	2.11	0.51
5:E:1:NAG:C3	5:E:2:NAG:H61	2.42	0.50
2:B:374:ASP:OD2	2:B:405:ARG:NH1	2.27	0.50
2:B:303(B):ASP:HA	3:C:1:PHE:CE2	2.46	0.50
1:A:113:ASN:ND2	7:A:1131:NAG:C2	2.76	0.49
1:A:142:ILE:O	1:A:172:PHE:HA	2.13	0.49
1:A:216:ILE:HG22	10:A:1236:HOH:O	2.11	0.49
1:A:7:GLN:HG2	1:A:8:PRO:O	2.13	0.49
1:A:66:LEU:HB2	1:A:84:TRP:CG	2.48	0.49
1:A:138:ARG:O	1:A:168:ASN:HB3	2.12	0.49
2:B:274:TYR:N	2:B:274:TYR:CD1	2.75	0.48
1:A:72:LYS:HB3	1:A:73:PRO:HD2	1.96	0.47
2:B:308(B):HIS:N	2:B:308(B):HIS:CD2	2.81	0.47
2:B:314:LEU:N	2:B:315:PRO:CD	2.77	0.47
5:E:1:NAG:O3	5:E:2:NAG:O5	2.28	0.47
1:A:114:ARG:HD2	10:A:1165:HOH:O	2.13	0.47
2:B:291:ASN:ND2	5:E:1:NAG:C1	2.78	0.47
1:A:145:GLU:HA	1:A:175:GLY:O	2.14	0.47
2:B:283:ASP:HA	2:B:286:MET:HE3	1.97	0.47
2:B:370:TYR:HB2	2:B:371:PRO:HD2	1.95	0.47
1:A:173:MET:HA	2:B:331:TRP:O	2.15	0.46
1:A:243:THR:HB	1:A:244:PRO:HD2	1.96	0.46
1:A:175:GLY:HA3	2:B:333:PHE:CZ	2.51	0.46
1:A:141:TYR:CE2	1:A:170:LYS:HB2	2.51	0.46
1:A:164:ASN:OD1	1:A:165:PRO:HD2	2.16	0.46
2:B:377:VAL:H	9:B:461:ACT:H2	1.79	0.46
1:A:72:LYS:HD3	1:A:76(A):GLY:CA	2.46	0.46
2:B:291:ASN:ND2	5:E:1:NAG:O5	2.49	0.46
1:A:113:ASN:HD21	7:A:1131:NAG:HN2	1.65	0.45
2:B:280:ASN:OD1	2:B:300:TRP:N	2.42	0.45
7:A:1131:NAG:C8	7:A:1131:NAG:C1	2.95	0.45
1:A:66:LEU:HD23	1:A:66:LEU:H	1.81	0.45
1:A:26:ALA:O	1:A:105:ASN:HB2	2.17	0.45
5:E:1:NAG:H2	5:E:2:NAG:O6	2.17	0.45
1:A:32:TYR:CD1	1:A:32:TYR:C	2.93	0.45
2:B:318:ARG:NH2	10:B:2984:HOH:O	2.50	0.44
2:B:367:THR:O	2:B:382:GLN:HG3	2.16	0.44
2:B:418:LYS:HB3	2:B:418:LYS:HE3	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASN:O	1:A:117:HIS:HD2	2.01	0.44
2:B:304:THR:O	2:B:308:HIS:CD2	2.65	0.44
1:A:55:GLY:O	2:B:303:CYS:HA	2.18	0.43
1:A:173:MET:CE	2:B:331:TRP:CE3	3.02	0.43
1:A:110:ILE:HD12	1:A:110:ILE:HG21	1.18	0.43
1:A:248:ILE:HD11	2:B:273:ARG:CG	2.47	0.43
1:A:49:TRP:HA	1:A:143:ALA:O	2.19	0.42
1:A:113:ASN:HD22	7:A:1131:NAG:C7	2.32	0.42
1:A:173:MET:CE	2:B:331:TRP:CB	2.97	0.42
2:B:268:CYS:O	2:B:273:ARG:HB2	2.20	0.42
2:B:303(B):ASP:OD1	2:B:304:THR:N	2.52	0.42
1:A:84:TRP:C	1:A:86:LYS:H	2.28	0.41
4:D:1:NAG:N2	4:D:2:FUC:C1	2.82	0.41
2:B:276:THR:HA	2:B:300:TRP:CZ3	2.56	0.41
1:A:142:ILE:O	1:A:172:PHE:HB2	2.19	0.41
1:A:113:ASN:ND2	7:A:1131:NAG:C1	2.84	0.41
1:A:3:ARG:NH1	1:A:8:PRO:C	2.79	0.41
2:B:399:VAL:HB	2:B:400:PRO:HD3	2.02	0.41
1:A:113:ASN:ND2	7:A:1131:NAG:C7	2.83	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.80	0.41
2:B:291:ASN:CG	5:E:1:NAG:C1	2.94	0.41
1:A:2:ALA:HB3	10:A:1326:HOH:O	2.20	0.40
1:A:62:ALA:O	1:A:67:GLY:HA3	2.20	0.40
1:A:23(A):ASP:OD1	1:A:26:ALA:N	2.40	0.40
1:A:110:ILE:HG23	1:A:110:ILE:HD13	1.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	253/263 (96%)	243 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	151/160 (94%)	142 (94%)	9 (6%)	0	100	100
3	C	1/4 (25%)	1 (100%)	0	0	100	100
All	All	405/427 (95%)	386 (95%)	19 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	205/215 (95%)	187 (91%)	18 (9%)	9	6
2	B	123/133 (92%)	120 (98%)	3 (2%)	43	47
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	330/350 (94%)	309 (94%)	21 (6%)	16	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	HIS
1	A	0	ARG
1	A	3	ARG
1	A	21	ILE
1	A	110	ILE
1	A	112	THR
1	A	112(A)	SER
1	A	112(C)	ASP
1	A	114	ARG
1	A	125	LYS
1	A	167	ILE
1	A	170	LYS
1	A	185	TYR
1	A	197	ILE
1	A	204	ARG
1	A	205	ARG

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	248	ILE
2	B	273	ARG
2	B	284	VAL
2	B	418	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	117	HIS
1	A	160	HIS
1	A	233	GLN
1	A	247	ASN
2	B	285	GLN
2	B	308	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
3	PHA	C	4	3,1	10,11,11	1.91	1 (10%)	8,13,13	0.67	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
3	PHA	C	4	3,1	-	0/5/6/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	PHA	O-C	5.47	1.40	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	PHA	1	0

## 5.5 Carbohydrates i

5 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	D	1	4	14,14,15	1.32	2 (14%)	17,19,21	2.45	7 (41%)
4	FUC	D	2	4	10,10,11	3.18	4 (40%)	14,14,16	3.22	7 (50%)
4	NDG	D	3	4	14,14,15	0.90	0	17,19,21	4.03	6 (35%)
5	NAG	E	1	5	14,14,15	0.56	0	17,19,21	3.00	9 (52%)
5	NAG	E	2	5	14,14,15	2.03	4 (28%)	17,19,21	3.76	9 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
4	NDG	D	3	4	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	E	1	5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	2/2/5/7	5/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	FUC	O5-C1	7.36	1.56	1.43
4	D	2	FUC	O5-C5	5.32	1.54	1.43
5	E	2	NAG	C1-C2	4.02	1.57	1.52
5	E	2	NAG	C2-N2	3.35	1.51	1.46
5	E	2	NAG	C3-C2	3.25	1.59	1.52
5	E	2	NAG	C4-C3	3.16	1.60	1.52
4	D	1	NAG	C1-C2	-2.97	1.48	1.52
4	D	1	NAG	C3-C2	-2.30	1.47	1.52
4	D	2	FUC	C2-C3	-2.23	1.49	1.52
4	D	2	FUC	C4-C3	2.20	1.58	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	O6-C6-C5	12.18	152.81	111.33
4	D	3	NDG	O6-C6-C5	11.56	150.68	111.33
4	D	3	NDG	O5-C1-C2	-8.62	97.95	111.29
4	D	2	FUC	O3-C3-C2	7.45	125.27	110.05
4	D	2	FUC	C2-C3-C4	-6.72	99.04	110.86
4	D	1	NAG	O5-C1-C2	-5.73	102.43	111.29
5	E	1	NAG	O5-C1-C2	4.99	119.02	111.29
5	E	2	NAG	C1-C2-N2	4.90	118.16	110.43
5	E	1	NAG	O3-C3-C4	4.82	121.75	110.38
5	E	1	NAG	C1-C2-N2	-4.82	102.83	110.43
5	E	2	NAG	C3-C4-C5	4.48	118.35	110.23
5	E	1	NAG	O6-C6-C5	-4.39	96.38	111.33
4	D	1	NAG	C3-C4-C5	4.23	117.90	110.23
4	D	3	NDG	C4-C3-C2	-4.22	104.83	111.02
4	D	3	NDG	C1-C2-N2	4.21	117.08	110.43
5	E	1	NAG	C8-C7-N2	-4.16	109.22	116.12
4	D	1	NAG	O7-C7-C8	4.08	129.31	122.05
4	D	3	NDG	O7-C7-C8	3.86	128.93	122.05
5	E	2	NAG	C2-N2-C7	3.62	127.76	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	O3-C3-C2	3.59	116.85	109.40
4	D	2	FUC	O5-C5-C4	3.27	115.43	109.55
4	D	2	FUC	O4-C4-C5	3.17	116.73	109.74
4	D	1	NAG	C8-C7-N2	-3.12	110.94	116.12
5	E	2	NAG	O5-C5-C6	2.96	113.42	107.66
5	E	1	NAG	C4-C3-C2	2.79	115.10	111.02
5	E	1	NAG	C1-O5-C5	2.78	115.91	112.19
4	D	2	FUC	O3-C3-C4	-2.77	103.84	110.38
5	E	2	NAG	C4-C3-C2	2.72	115.00	111.02
4	D	2	FUC	O2-C2-C3	2.65	115.64	110.15
5	E	1	NAG	O7-C7-C8	2.55	126.59	122.05
5	E	2	NAG	O4-C4-C3	2.36	115.94	110.38
4	D	1	NAG	C1-O5-C5	-2.32	109.07	112.19
4	D	3	NDG	O7-C7-N2	-2.28	117.96	121.98
5	E	2	NAG	O7-C7-C8	-2.26	118.02	122.05
4	D	2	FUC	C6-C5-C4	2.26	117.21	113.08
4	D	1	NAG	O3-C3-C4	-2.19	105.22	110.38
4	D	1	NAG	O5-C5-C6	2.11	111.78	107.66
5	E	2	NAG	O7-C7-N2	2.11	125.71	121.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	3	NDG	C2
5	E	2	NAG	C5
5	E	2	NAG	C2

All (14) torsion outliers are listed below:

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

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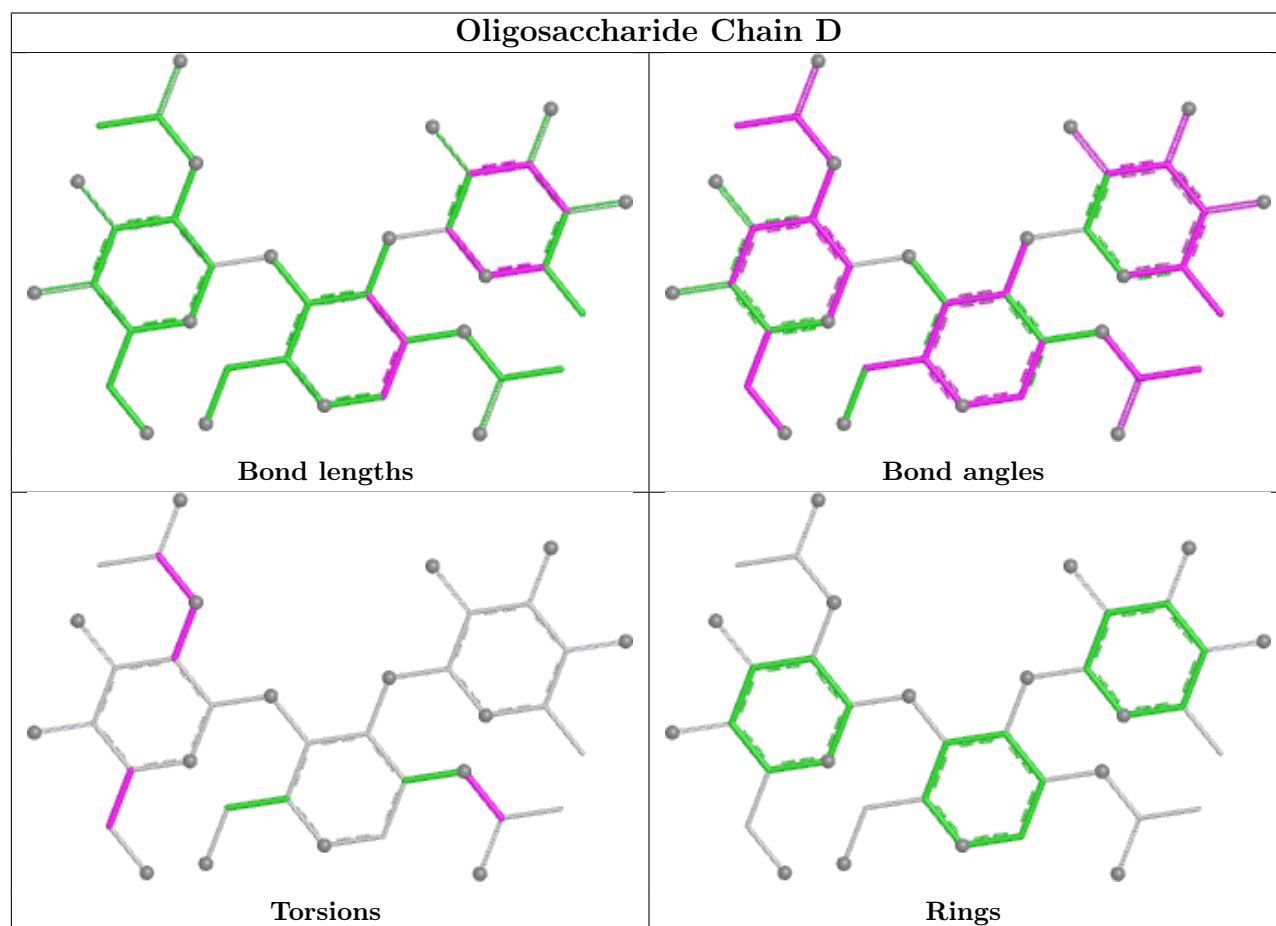
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
4	D	3	NDG	C3-C2-N2-C7

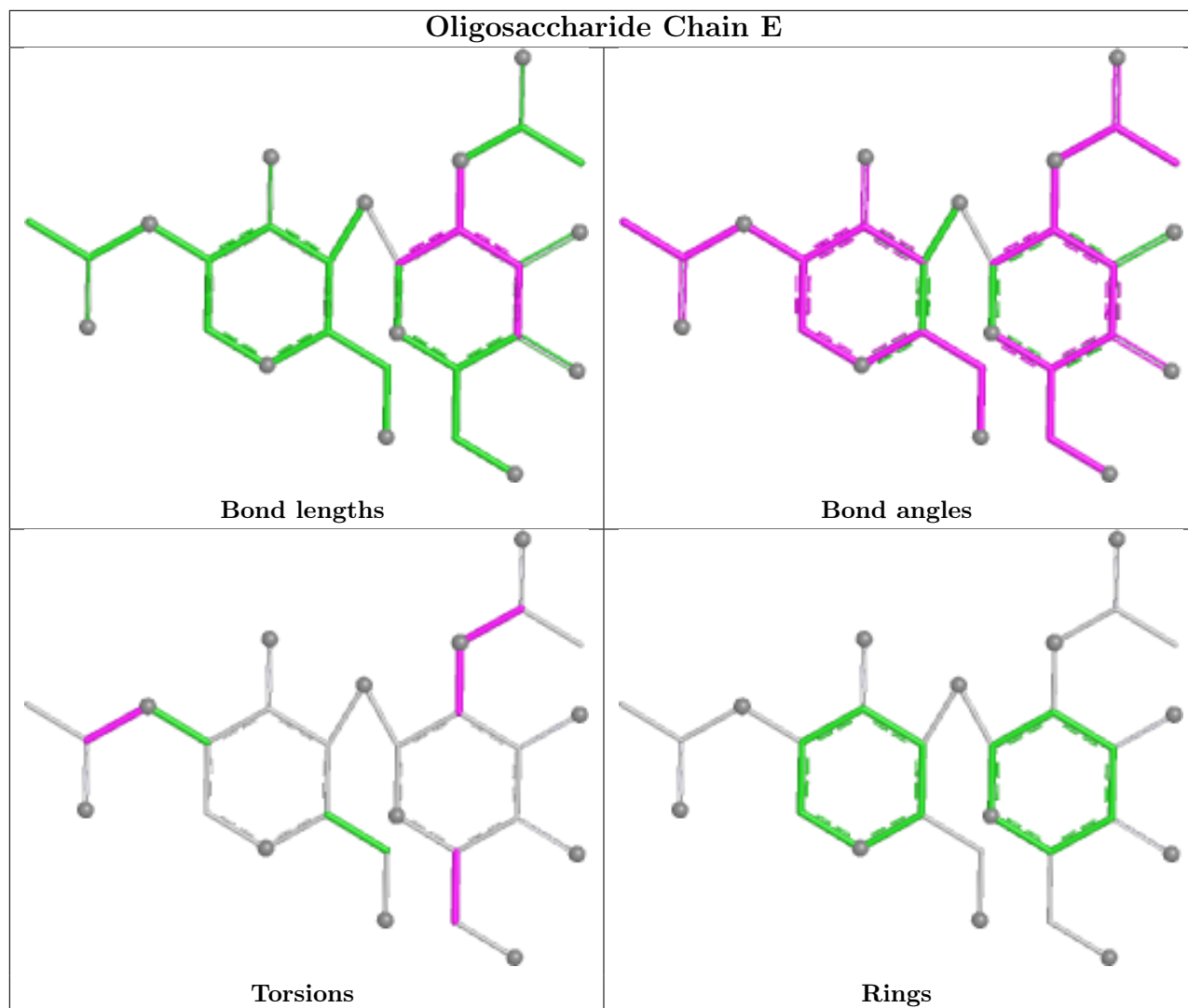
There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	4	0
4	D	2	FUC	2	0
4	D	1	NAG	7	0
5	E	1	NAG	11	0
4	D	3	NDG	3	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](#)

4 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	ARG	A	426	-	10,11,11	0.97	0	9,13,13	3.62	5 (55%)
8	GOL	A	450	-	5,5,5	0.54	0	5,5,5	0.53	0
7	NAG	A	1131	-	14,14,15	1.05	1 (7%)	17,19,21	2.41	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ACT	B	461	-	3,3,3	1.09	0	3,3,3	0.95	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
6	ARG	A	426	-	-	5/11/11/11	-
8	GOL	A	450	-	-	3/4/4/4	-
7	NAG	A	1131	-	1/1/5/7	5/6/23/26	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1131	NAG	O5-C1	-2.23	1.39	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	426	ARG	OXT-C-O	8.13	142.53	124.08
7	A	1131	NAG	O6-C6-C5	5.91	131.47	111.33
6	A	426	ARG	CB-CA-N	5.34	124.05	110.12
7	A	1131	NAG	C8-C7-N2	3.78	122.39	116.12
6	A	426	ARG	CG-CB-CA	-3.52	101.85	113.22
7	A	1131	NAG	C2-N2-C7	3.45	127.53	122.90
7	A	1131	NAG	C4-C3-C2	-2.77	106.96	111.02
7	A	1131	NAG	O5-C5-C6	-2.59	102.62	107.66
7	A	1131	NAG	O7-C7-C8	-2.55	117.51	122.05
6	A	426	ARG	CG-CD-NE	-2.10	106.32	112.20
6	A	426	ARG	NE-CZ-NH2	-2.03	117.20	120.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1131	NAG	C2

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	426	ARG	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	A	1131	NAG	C1-C2-N2-C7
7	A	1131	NAG	C8-C7-N2-C2
7	A	1131	NAG	O7-C7-N2-C2
8	A	450	GOL	O1-C1-C2-C3
7	A	1131	NAG	O5-C5-C6-O6
7	A	1131	NAG	C4-C5-C6-O6
8	A	450	GOL	O1-C1-C2-O2
8	A	450	GOL	O2-C2-C3-O3
6	A	426	ARG	O-C-CA-CB
6	A	426	ARG	OXT-C-CA-CB
6	A	426	ARG	NE-CD-CG-CB
6	A	426	ARG	C-CA-CB-CG

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1131	NAG	C1-C2-C3-C4-C5-O5

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	426	ARG	1	0
8	A	450	GOL	1	0
7	A	1131	NAG	7	0
9	B	461	ACT	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.