



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:39 PM UTC

PDB ID : 1BCR / pdb_00001bcr
Title : COMPLEX OF THE WHEAT SERINE CARBOXYPEPTIDASE, CPDW-II,
WITH THE MICROBIAL PEPTIDE ALDEHYDE INHIBITOR, ANTIPAIN,
AND ARGININE AT ROOM TEMPERATURE
Authors : Bullock, T.L.; Remington, S.J.
Deposited on : 1995-11-03
Resolution : 2.50 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

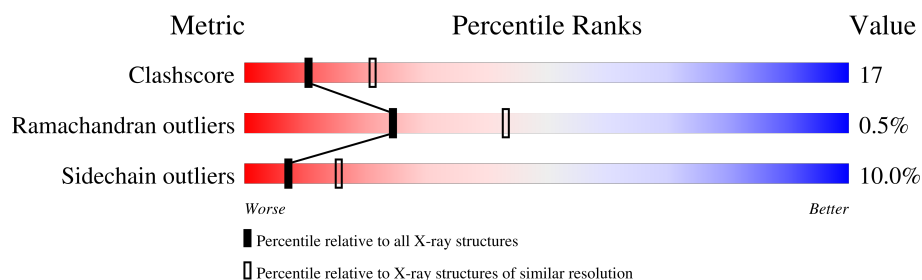
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	263	
2	B	160	
3	C	4	
4	D	3	
5	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
4	FUC	D	2	X	-	-	-
5	NAG	E	2	X	-	-	-
6	NAG	A	1131	X	-	-	-
7	ARG	A	426	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3489 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
1	A	254	Total	C	N	O	S	0	0	0
			1991	1274	333	377	7			

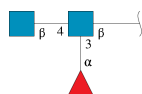
- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1196	768	205	217	6			

- Molecule 3 is a protein called ANTIPAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			18	11	5	2			

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



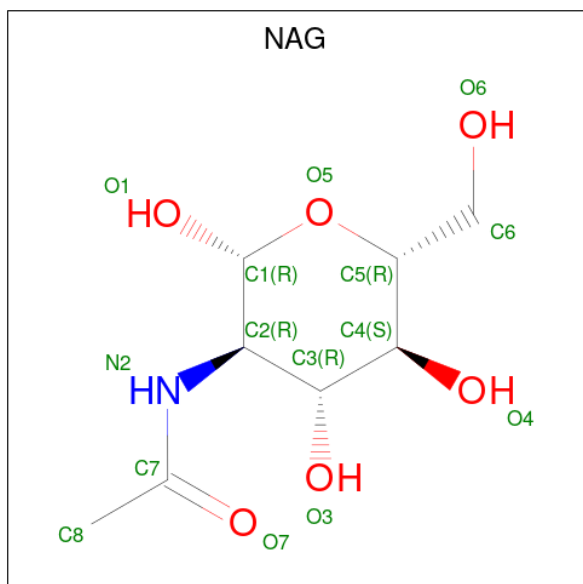
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



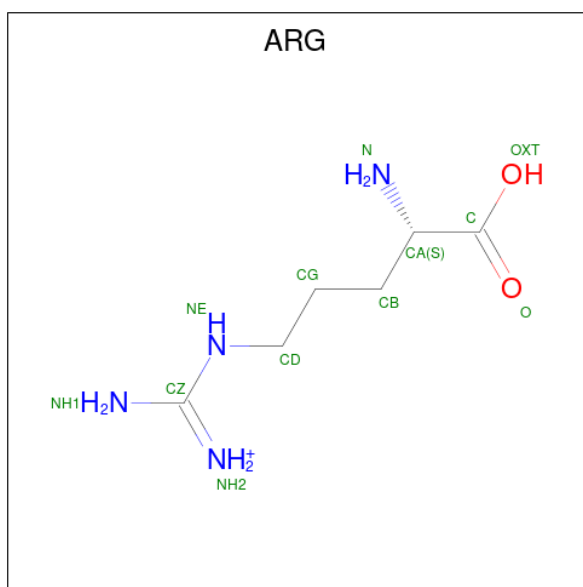
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

- Molecule 8 is water.

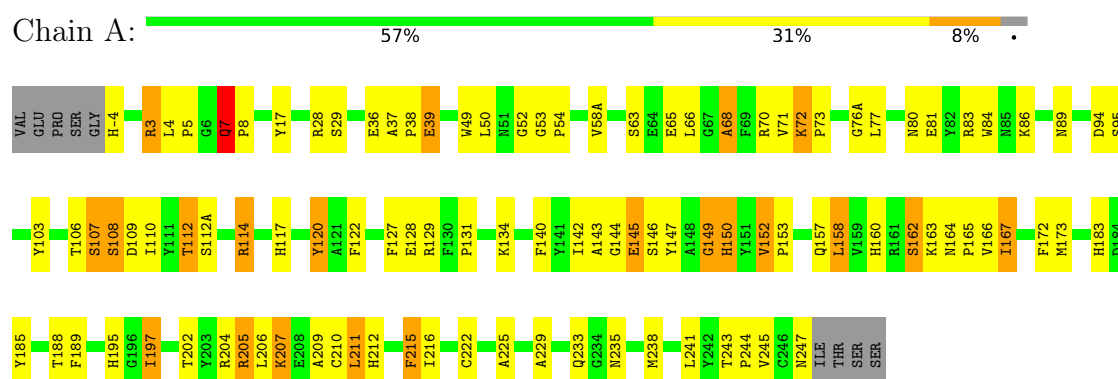
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total	O	0	0
			113	113		
8	B	76	Total	O	0	0
			76	76		
8	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

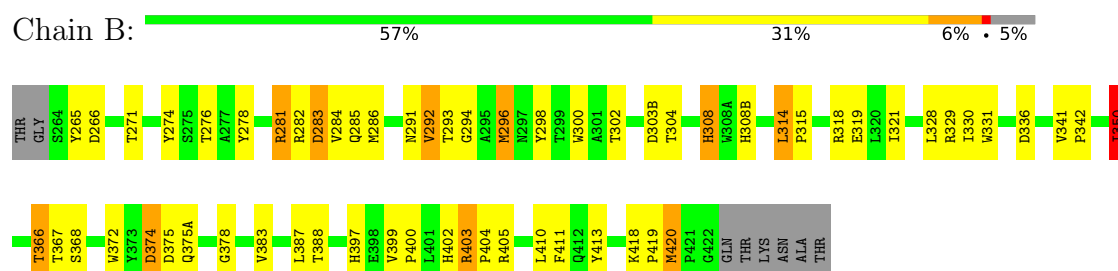
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

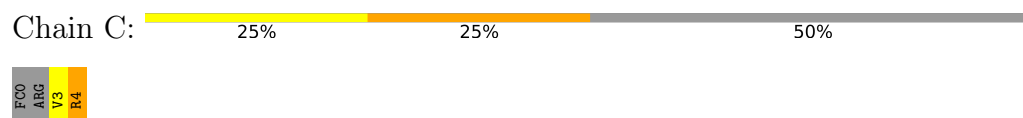
• Molecule 1: SERINE CARBOXYPEPTIDASE II



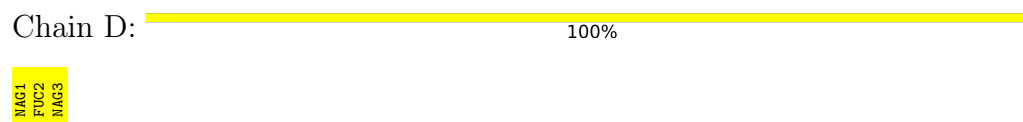
• Molecule 2: SERINE CARBOXYPEPTIDASE II



• Molecule 3: ANTIPAIN



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



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

Chain E:



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 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.40Å 98.40Å 209.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (21.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3489	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FUC, NAG, OAR

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	1.38	4/2054 (0.2%)	1.68	32/2803 (1.1%)
2	B	1.35	0/1236	1.72	25/1693 (1.5%)
3	C	1.77	0/6	2.40	1/7 (14.3%)
All	All	1.37	4/3296 (0.1%)	1.70	58/4503 (1.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	SER	N-CA	-6.01	1.39	1.46
1	A	94	ASP	C-N	-5.88	1.26	1.33
1	A	152	VAL	C-N	-5.35	1.27	1.34
1	A	80	ASN	C-N	-5.19	1.26	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ILE	N-CA-C	8.63	123.84	113.22
2	B	341	VAL	CA-C-N	8.24	128.30	119.89
2	B	341	VAL	C-N-CA	8.24	128.30	119.89
1	A	81	GLU	CB-CG-CD	-8.16	98.72	112.60
2	B	420	MET	CA-C-N	8.15	128.08	119.85
2	B	420	MET	C-N-CA	8.15	128.08	119.85
2	B	283	ASP	N-CA-CB	-7.94	97.07	110.49
1	A	211	LEU	N-CA-C	7.85	121.96	112.38
2	B	308	HIS	CA-CB-CG	-7.83	105.97	113.80
2	B	294	GLY	CA-C-N	7.79	136.49	122.38
2	B	294	GLY	C-N-CA	7.79	136.49	122.38
1	A	210	CYS	N-CA-C	7.58	122.53	113.28
1	A	145	GLU	CB-CA-C	-7.52	96.11	110.24
1	A	140	PHE	N-CA-CB	-7.14	98.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	GLY	O-C-N	7.10	130.61	122.38
1	A	86	LYS	N-CA-C	-7.05	104.14	112.89
2	B	418	LYS	CA-C-N	6.98	126.97	119.78
2	B	418	LYS	C-N-CA	6.98	126.97	119.78
2	B	303(B)	ASP	CA-CB-CG	-6.66	105.94	112.60
1	A	114	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	A	149	GLY	N-CA-C	-6.32	106.51	114.16
2	B	294	GLY	N-CA-C	-6.31	106.22	115.63
1	A	117	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	127	PHE	CA-CB-CG	-6.27	107.53	113.80
2	B	336	ASP	N-CA-C	6.26	120.78	113.20
1	A	189	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	112	THR	N-CA-CB	-6.19	101.22	111.49
2	B	293	THR	N-CA-C	5.91	117.80	111.36
1	A	39	GLU	N-CA-C	5.85	118.41	111.33
1	A	183	HIS	CA-CB-CG	-5.82	107.98	113.80
2	B	330	ILE	N-CA-C	5.70	116.07	107.75
1	A	167	ILE	N-CA-C	5.64	115.46	106.88
2	B	403	ARG	CA-C-N	5.61	126.85	119.84
2	B	403	ARG	C-N-CA	5.61	126.85	119.84
2	B	303(B)	ASP	N-CA-CB	-5.56	101.65	109.94
1	A	114	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	A	150	HIS	CA-CB-CG	-5.54	108.25	113.80
1	A	235	ASN	N-CA-C	5.54	118.19	109.39
2	B	419	PRO	CB-CA-C	-5.52	104.16	111.23
2	B	413	TYR	CA-CB-CG	-5.40	104.17	113.90
2	B	350	ILE	CB-CA-C	-5.37	105.01	112.04
1	A	128	GLU	N-CA-C	-5.36	105.60	111.82
1	A	68	ALA	N-CA-C	5.35	118.03	111.82
1	A	225	ALA	N-CA-C	-5.35	105.45	111.28
1	A	17	TYR	CB-CA-C	-5.34	98.57	109.94
1	A	114	ARG	CD-NE-CZ	5.29	131.81	124.40
1	A	241	LEU	N-CA-C	5.28	118.50	111.75
1	A	167	ILE	N-CA-CB	-5.27	105.28	111.60
3	C	3	VAL	N-CA-CB	-5.23	102.61	111.50
2	B	314	LEU	CA-C-O	5.19	123.11	118.33
1	A	247	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	140	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	120	TYR	CA-CB-CG	-5.11	104.71	113.90
1	A	7	GLN	N-CA-C	5.08	116.28	109.83
2	B	308(B)	HIS	CA-CB-CG	-5.07	108.73	113.80
2	B	366	THR	N-CA-CB	-5.05	103.07	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	CA-C-O	5.04	125.89	120.55
1	A	215	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

There are no planarity outliers.

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	1991	0	1839	70	0
2	B	1196	0	1130	41	0
3	C	18	0	19	4	0
4	D	38	0	34	0	0
5	E	28	0	24	4	0
6	A	14	0	13	2	0
7	A	12	0	12	6	0
8	A	113	0	0	7	0
8	B	76	0	0	4	0
8	C	3	0	0	0	0
All	All	3489	0	3071	107	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 17.

All (107) 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:112:THR:HG23	1:A:114:ARG:HH22	1.08	1.08
1:A:5:PRO:HG2	2:B:284:VAL:HG22	1.47	0.94
1:A:3:ARG:HH11	1:A:3:ARG:HB3	1.40	0.85
1:A:112:THR:CG2	1:A:114:ARG:HH22	1.90	0.82
1:A:112:THR:HG23	1:A:114:ARG:NH2	1.92	0.82
2:B:296:MET:HE2	5:E:1:NAG:O7	1.81	0.80
1:A:5:PRO:HG2	2:B:284:VAL:CG2	2.13	0.78
1:A:134:LYS:HD3	1:A:166:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:OD1	1:A:166:VAL:HG22	1.92	0.69
1:A:36:GLU:HB3	1:A:89:ASN:OD1	1.92	0.68
1:A:134:LYS:HD3	1:A:166:VAL:CG1	2.23	0.68
1:A:108:SER:O	1:A:112:THR:HG22	1.95	0.67
1:A:3:ARG:HH11	1:A:3:ARG:CB	2.09	0.64
1:A:229:ALA:O	1:A:233:GLN:HG3	1.97	0.64
2:B:281:ARG:O	2:B:285:GLN:HG3	1.97	0.64
1:A:7:GLN:HG2	1:A:8:PRO:O	1.98	0.62
2:B:291:ASN:OD1	2:B:296:MET:HG3	1.99	0.62
1:A:152:VAL:HB	1:A:153:PRO:HD3	1.82	0.62
1:A:205:ARG:NH1	8:A:1216:HOH:O	2.31	0.62
1:A:71:VAL:HG12	1:A:72:LYS:O	2.01	0.61
1:A:173:MET:HA	2:B:331:TRP:O	2.00	0.61
1:A:84:TRP:HB3	2:B:411:PHE:CE2	2.36	0.60
1:A:53:GLY:H	3:C:4:OAR:HO	1.49	0.60
2:B:329:ARG:HD3	8:B:129:HOH:O	2.03	0.59
2:B:374:ASP:HB3	8:B:178:HOH:O	2.02	0.59
2:B:282:ARG:O	2:B:286:MET:HB2	2.03	0.59
1:A:4:LEU:H	1:A:7:GLN:NE2	2.01	0.58
2:B:300:TRP:HB2	5:E:1:NAG:H81	1.84	0.58
2:B:387:LEU:HD23	2:B:387:LEU:C	2.28	0.58
1:A:209:ALA:HB1	1:A:222:CYS:HA	1.84	0.57
1:A:52:GLY:N	7:A:426:ARG:O	2.35	0.57
1:A:243:THR:HB	1:A:244:PRO:HD2	1.85	0.57
1:A:150:HIS:O	1:A:153:PRO:HD2	2.06	0.56
1:A:70:ARG:HH11	1:A:70:ARG:HG3	1.69	0.56
1:A:195:HIS:NE2	8:A:1148:HOH:O	2.32	0.56
6:A:1131:NAG:H82	6:A:1131:NAG:C3	2.36	0.56
6:A:1131:NAG:H82	6:A:1131:NAG:O3	2.05	0.56
1:A:72:LYS:HD3	1:A:76(A):GLY:C	2.31	0.55
1:A:114:ARG:HD2	8:A:1170:HOH:O	2.08	0.54
1:A:109:ASP:HA	1:A:112:THR:CG2	2.40	0.52
1:A:188:THR:HA	2:B:342:PRO:HG2	1.92	0.52
7:A:426:ARG:N	3:C:4:OAR:HC1	2.25	0.52
1:A:146:SER:OG	1:A:147:TYR:N	2.43	0.51
1:A:58(A):VAL:HB	8:A:1178:HOH:O	2.11	0.50
1:A:65:GLU:OE1	1:A:145:GLU:OE2	2.28	0.50
2:B:278:TYR:O	2:B:281:ARG:HG3	2.12	0.49
2:B:399:VAL:HB	2:B:400:PRO:HD3	1.95	0.49
2:B:300:TRP:HB2	5:E:1:NAG:C8	2.42	0.49
2:B:265:TYR:CE1	2:B:402:HIS:CE1	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-4:HIS:N	8:A:1242:HOH:O	2.45	0.49
1:A:72:LYS:HB3	1:A:73:PRO:HD2	1.94	0.49
2:B:274:TYR:N	2:B:274:TYR:CD1	2.75	0.49
1:A:202:THR:HG22	1:A:206:LEU:HD11	1.95	0.49
1:A:112(A):SER:HB3	8:A:1230:HOH:O	2.12	0.48
2:B:342:PRO:HA	8:B:2:HOH:O	2.13	0.48
2:B:410:LEU:HA	2:B:420:MET:HE1	1.95	0.48
1:A:7:GLN:HB2	1:A:77:LEU:HD12	1.95	0.48
2:B:283:ASP:O	2:B:286:MET:HB3	2.14	0.48
1:A:53:GLY:HA3	1:A:54:PRO:C	2.38	0.48
1:A:160:HIS:HE1	8:B:128:HOH:O	1.96	0.47
2:B:298:TYR:O	5:E:1:NAG:H3	2.14	0.47
1:A:207:LYS:O	1:A:211:LEU:HG	2.14	0.46
1:A:70:ARG:HG3	1:A:70:ARG:NH1	2.30	0.46
2:B:276:THR:HA	2:B:300:TRP:HZ3	1.79	0.46
1:A:233:GLN:HE22	1:A:238:MET:HE3	1.81	0.46
2:B:374:ASP:O	2:B:375:ASP:HB2	2.15	0.46
7:A:426:ARG:N	3:C:4:OAR:C	2.79	0.46
1:A:28:ARG:HD3	1:A:109:ASP:OD2	2.17	0.45
2:B:367:THR:HB	2:B:383:VAL:HB	1.99	0.45
2:B:266:ASP:O	2:B:271:THR:HG23	2.17	0.45
1:A:145:GLU:OE1	7:A:426:ARG:OXT	2.35	0.44
2:B:403:ARG:N	2:B:404:PRO:HD3	2.33	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.62	0.44
2:B:314:LEU:N	2:B:315:PRO:CD	2.80	0.44
2:B:276:THR:HA	2:B:300:TRP:CZ3	2.53	0.44
2:B:314:LEU:O	2:B:318:ARG:HG3	2.18	0.44
1:A:152:VAL:N	1:A:153:PRO:CD	2.81	0.43
1:A:209:ALA:CB	1:A:222:CYS:HA	2.48	0.43
1:A:146:SER:HB2	2:B:397:HIS:NE2	2.33	0.43
1:A:53:GLY:N	7:A:426:ARG:N	2.67	0.43
1:A:122:PHE:CD2	1:A:122:PHE:C	2.97	0.43
1:A:164:ASN:OD1	1:A:165:PRO:HD2	2.19	0.43
2:B:375:ASP:HB3	2:B:375(A):GLN:H	1.46	0.43
1:A:162:SER:O	1:A:163:LYS:HB2	2.19	0.42
1:A:157:GLN:NE2	2:B:319:GLU:OE1	2.39	0.42
1:A:103:TYR:CD1	1:A:103:TYR:C	2.97	0.42
1:A:72:LYS:O	2:B:274:TYR:HB3	2.20	0.42
1:A:120:TYR:CD2	1:A:120:TYR:C	2.97	0.42
1:A:142:ILE:O	1:A:172:PHE:HB2	2.20	0.41
2:B:403:ARG:N	2:B:404:PRO:CD	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ALA:HB1	1:A:38:PRO:HD2	2.03	0.41
1:A:129:ARG:C	1:A:131:PRO:HD3	2.46	0.41
1:A:147:TYR:C	1:A:149:GLY:H	2.27	0.41
2:B:350:ILE:N	2:B:350:ILE:HD13	2.35	0.41
7:A:426:ARG:N	3:C:4:OAR:O	2.53	0.41
1:A:106:THR:O	1:A:108:SER:N	2.52	0.41
2:B:271:THR:HG23	2:B:271:THR:H	1.61	0.41
2:B:304:THR:O	2:B:308:HIS:HD2	2.04	0.41
1:A:68:ALA:HA	1:A:83:ARG:HB3	2.03	0.41
1:A:50:LEU:O	1:A:144:GLY:HA3	2.21	0.40
2:B:387:LEU:HD23	2:B:388:THR:N	2.36	0.40
1:A:-4:HIS:HB3	1:A:129:ARG:HG2	2.02	0.40
1:A:49:TRP:HA	1:A:143:ALA:O	2.20	0.40
1:A:212:HIS:HB2	8:A:1214:HOH:O	2.22	0.40
1:A:209:ALA:HB1	1:A:222:CYS:CA	2.51	0.40
2:B:372:TRP:CH2	2:B:378:GLY:HA3	2.57	0.40
1:A:71:VAL:HG12	2:B:274:TYR:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/263 (96%)	238 (94%)	13 (5%)	1 (0%)	30	49
2	B	150/160 (94%)	140 (93%)	9 (6%)	1 (1%)	18	34
All	All	402/423 (95%)	378 (94%)	22 (6%)	2 (0%)	24	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	SER

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Mol	Chain	Res	Type
2	B	292	VAL

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	204/215 (95%)	183 (90%)	21 (10%)	7	14
2	B	123/133 (92%)	112 (91%)	11 (9%)	9	20
3	C	1/2 (50%)	1 (100%)	0	100	100
All	All	328/350 (94%)	296 (90%)	32 (10%)	7	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	GLN
1	A	29	SER
1	A	39	GLU
1	A	63	SER
1	A	66	LEU
1	A	72	LYS
1	A	107	SER
1	A	108	SER
1	A	110	ILE
1	A	158	LEU
1	A	162	SER
1	A	167	ILE
1	A	185	TYR
1	A	197	ILE
1	A	204	ARG
1	A	205	ARG
1	A	207	LYS
1	A	215	PHE
1	A	216	ILE
1	A	245	VAL

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Mol	Chain	Res	Type
2	B	281	ARG
2	B	292	VAL
2	B	296	MET
2	B	302	THR
2	B	321	ILE
2	B	328	LEU
2	B	350	ILE
2	B	366	THR
2	B	368	SER
2	B	374	ASP
2	B	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-4	HIS
1	A	7	GLN
1	A	117	HIS
1	A	217	HIS
1	A	233	GLN
1	A	235	ASN
2	B	289	HIS
2	B	308	HIS
2	B	402	HIS
2	B	412	GLN
2	B	416	GLN

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	OAR	C	4	1,3	10,10,10	1.06	1 (10%)	9,11,11	1.39	1 (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
3	OAR	C	4	1,3	-	3/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	OAR	CB-CA	-2.09	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	OAR	CB-CA-C	-3.27	107.78	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	OAR	NE-CD-CG-CB
3	C	4	OAR	O-C-CA-CB
3	C	4	OAR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	OAR	4	0

5.5 Carbohydrates

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	1,4	14,14,15	0.78	0	17,19,21	2.33	5 (29%)
4	FUC	D	2	4	10,10,11	3.49	3 (30%)	14,14,16	3.69	8 (57%)
4	NAG	D	3	4	14,14,15	2.08	6 (42%)	17,19,21	3.54	7 (41%)
5	NAG	E	1	2,5	14,14,15	1.00	1 (7%)	17,19,21	2.76	6 (35%)
5	NAG	E	2	5	14,14,15	1.48	3 (21%)	17,19,21	3.55	8 (47%)

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	FUC	O5-C1	8.71	1.58	1.43
4	D	2	FUC	O5-C5	5.78	1.55	1.43
4	D	3	NAG	O4-C4	4.69	1.54	1.43
4	D	2	FUC	C4-C3	3.11	1.60	1.52
4	D	3	NAG	C1-C2	2.94	1.56	1.52
4	D	3	NAG	O5-C5	2.74	1.48	1.43
5	E	2	NAG	C4-C5	2.73	1.58	1.53
5	E	1	NAG	C1-C2	2.59	1.55	1.52
4	D	3	NAG	C3-C2	2.58	1.57	1.52
4	D	3	NAG	C4-C5	2.41	1.58	1.53
5	E	2	NAG	C2-N2	2.36	1.50	1.46
4	D	3	NAG	C4-C3	2.29	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	C1-C2	2.10	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	NAG	O6-C6-C5	11.60	150.83	111.33
5	E	2	NAG	C1-C2-N2	9.53	125.45	110.43
4	D	2	FUC	O3-C3-C2	8.77	127.94	110.05
4	D	2	FUC	C2-C3-C4	-7.91	96.95	110.86
5	E	1	NAG	O6-C6-C5	7.56	137.09	111.33
4	D	1	NAG	C1-O5-C5	6.18	120.47	112.19
5	E	2	NAG	O6-C6-C5	5.79	131.06	111.33
5	E	1	NAG	C1-O5-C5	4.68	118.46	112.19
4	D	1	NAG	O6-C6-C5	-4.44	96.22	111.33
5	E	2	NAG	O7-C7-C8	-4.44	114.15	122.05
4	D	3	NAG	C1-C2-N2	4.33	117.26	110.43
5	E	2	NAG	C1-O5-C5	4.18	117.79	112.19
5	E	2	NAG	C3-C4-C5	3.97	117.43	110.23
5	E	1	NAG	C3-C4-C5	3.92	117.34	110.23
4	D	3	NAG	O4-C4-C5	3.92	118.97	109.32
4	D	2	FUC	O2-C2-C3	3.83	118.08	110.15
4	D	1	NAG	O5-C1-C2	3.49	116.69	111.29
5	E	2	NAG	C2-N2-C7	3.39	127.45	122.90
4	D	3	NAG	O4-C4-C3	3.35	118.26	110.38
5	E	1	NAG	C4-C3-C2	3.32	115.89	111.02
4	D	3	NAG	C4-C3-C2	2.95	115.34	111.02
5	E	2	NAG	O5-C5-C4	2.94	117.97	110.83
4	D	1	NAG	O5-C5-C6	-2.61	102.58	107.66
4	D	2	FUC	C1-C2-C3	2.59	113.42	109.64
4	D	2	FUC	O3-C3-C4	-2.48	104.53	110.38
4	D	2	FUC	C6-C5-C4	2.40	117.47	113.08
5	E	2	NAG	O7-C7-N2	2.36	126.16	121.98
5	E	1	NAG	O4-C4-C5	-2.35	103.54	109.32
4	D	1	NAG	O3-C3-C2	-2.30	104.63	109.40
4	D	3	NAG	C1-O5-C5	2.29	115.26	112.19
4	D	2	FUC	O5-C5-C4	2.29	113.68	109.55
5	E	1	NAG	O5-C5-C4	2.27	116.34	110.83
4	D	3	NAG	C3-C4-C5	2.21	114.25	110.23
4	D	2	FUC	C3-C4-C5	-2.20	106.47	109.81

All (2) chirality outliers are listed below:

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

All (12) torsion outliers are listed below:

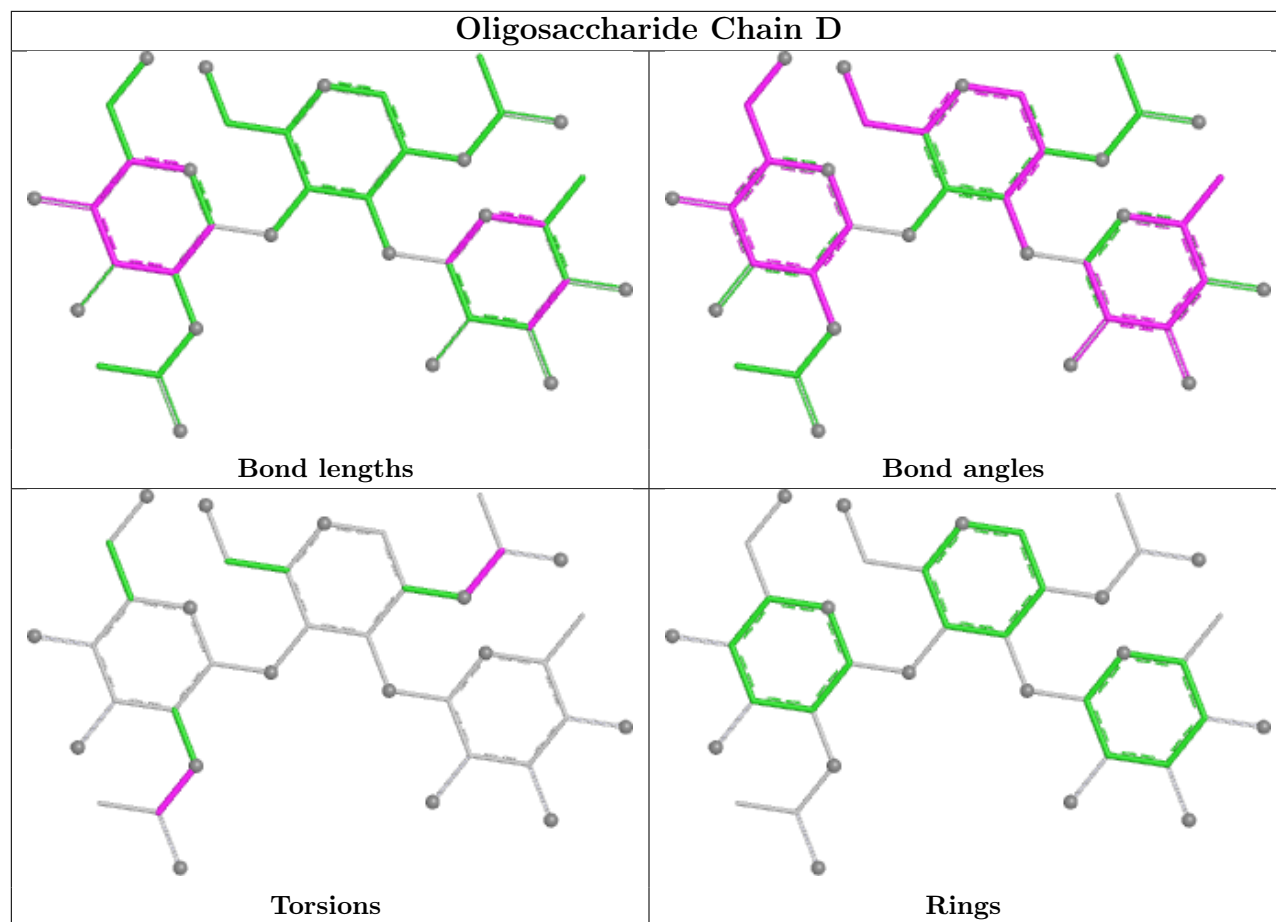
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
4	D	3	NAG	C8-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	3	NAG	O7-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7

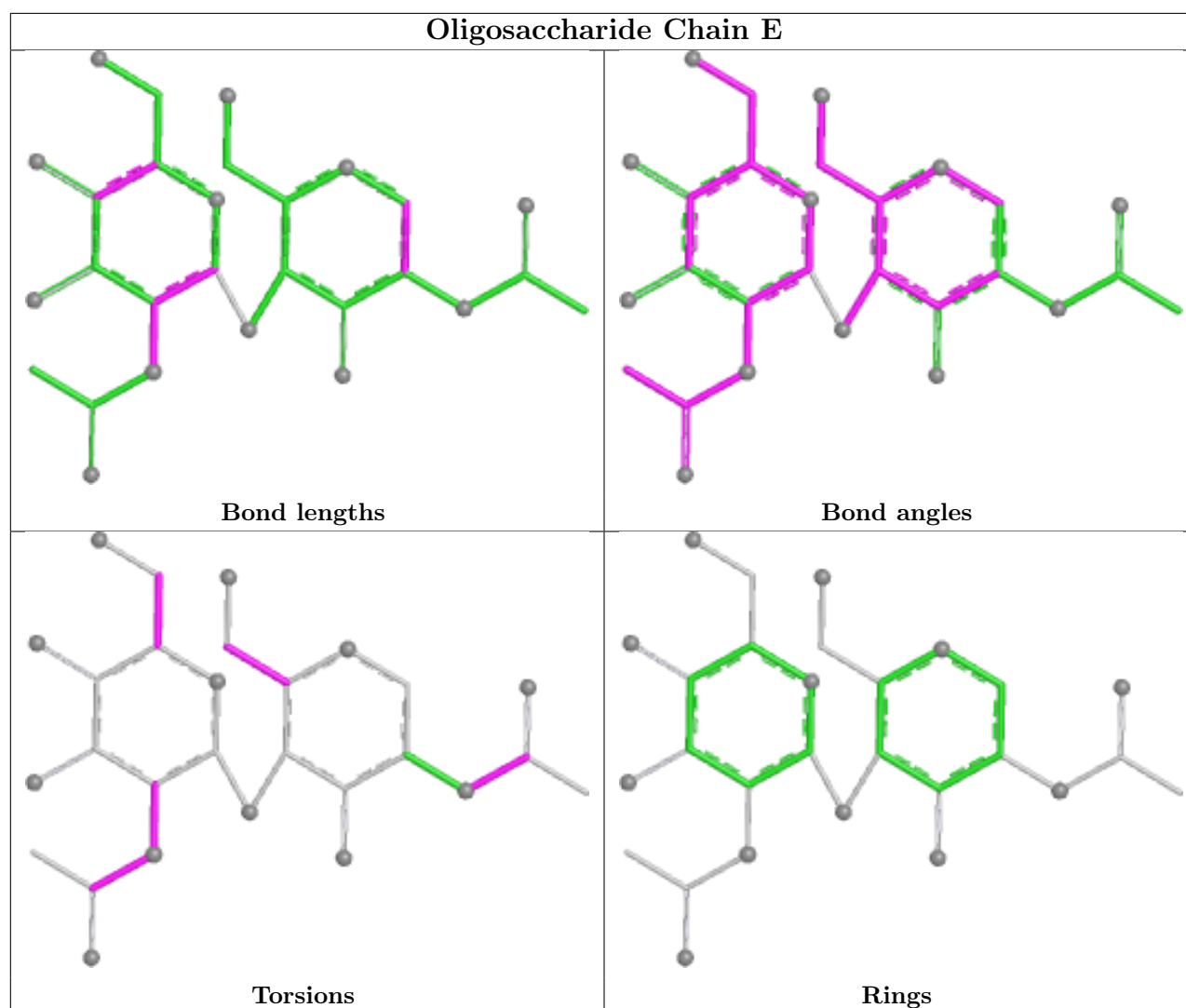
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	4	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](#)

2 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	A	1131	1	14,14,15	0.91	0	17,19,21	2.15	6 (35%)
7	ARG	A	426	-	10,11,11	0.74	0	9,13,13	1.04	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	NAG	A	1131	1	1/1/5/7	5/6/23/26	1/1/1/1
7	ARG	A	426	-	-	5/11/11/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1131	NAG	C1-O5-C5	4.90	118.75	112.19
6	A	1131	NAG	C4-C3-C2	-4.11	105.00	111.02
6	A	1131	NAG	C2-N2-C7	3.20	127.18	122.90
6	A	1131	NAG	O6-C6-C5	2.65	120.35	111.33
6	A	1131	NAG	O7-C7-C8	-2.44	117.71	122.05
6	A	1131	NAG	C8-C7-N2	2.09	119.58	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1131	NAG	C2

All (10) torsion outliers are listed below:

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

All (1) ring outliers are listed below:

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

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1131	NAG	2	0
7	A	426	ARG	6	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.