



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:31 PM UTC

PDB ID : 2AAI / pdb_00002aai
Title : Crystallographic refinement of ricin to 2.5 Angstroms
Authors : Rutenber, E.; Katzin, B.J.; Montfort, W.; Villafranca, J.E.; Ernst, S.R.;
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Deposited on : 1993-09-07
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

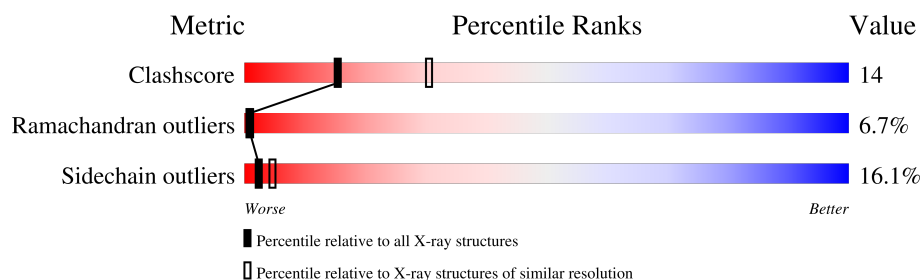
1 Overall quality at a glance

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	267	42% 35% 19% .
2	B	262	42% 38% 16% .
3	C	2	100%
3	D	2	100%
4	E	5	80% 20%
4	F	5	100%

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	NAG	E	1	X	-	-	-
4	NAG	F	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4440 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 RICIN (A CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2114	1342	372	395	5			

- Molecule 2 is a protein called RICIN (B CHAIN).

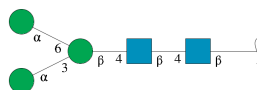
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2035	1273	357	393	12			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			
3	D	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is water.

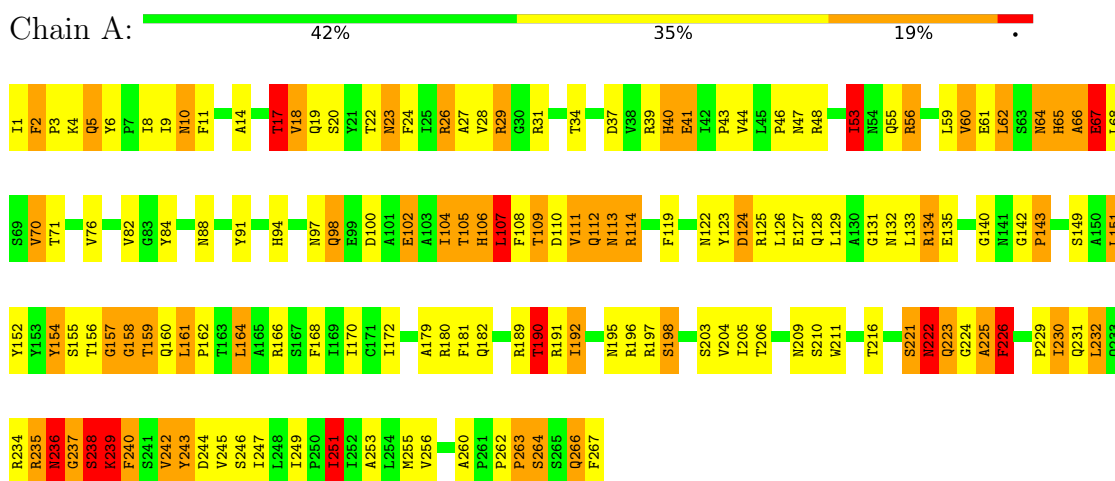
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

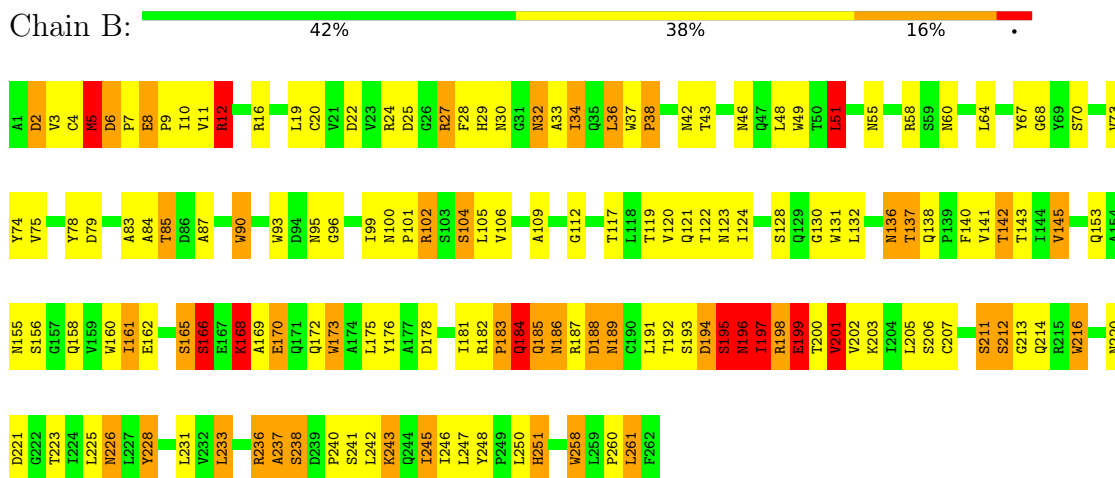
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: RICIN (B CHAIN)



• Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



BGC1
GAL2

- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:  100%BGC1
GAL2

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

Chain E:  80%  20%MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain F:  100%MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 78.49Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: BGC, GAL, NAG, BMA, 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	1.35	8/2162 (0.4%)	2.40	118/2941 (4.0%)
2	B	1.30	5/2080 (0.2%)	2.41	142/2842 (5.0%)
All	All	1.33	13/4242 (0.3%)	2.40	260/5783 (4.5%)

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	3
2	B	0	3
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	HIS	CD2-NE2	-8.63	1.28	1.37
2	B	251	HIS	CD2-NE2	-7.50	1.29	1.37
1	A	235	ARG	NE-CZ	5.90	1.39	1.33
2	B	251	HIS	CG-ND1	-5.83	1.31	1.38
1	A	143	PRO	CA-CB	-5.71	1.45	1.53
2	B	10	ILE	CA-CB	5.71	1.60	1.53
1	A	106	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	205	ILE	CA-CB	5.52	1.60	1.54
1	A	249	ILE	CA-C	5.41	1.57	1.52
2	B	184	GLN	CA-CB	-5.22	1.44	1.53
1	A	94	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	159	THR	CA-CB	5.05	1.62	1.53
2	B	29	HIS	CD2-NE2	-5.01	1.32	1.37

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PHE	CA-CB-CG	15.23	129.03	113.80
1	A	222	ASN	OD1-CG-ND2	-15.09	107.51	122.60
1	A	56	ARG	N-CA-C	12.70	126.56	111.82
2	B	2	ASP	CA-CB-CG	10.96	123.56	112.60
1	A	223	GLN	N-CA-C	-10.88	93.16	109.81
1	A	64	ASN	OD1-CG-ND2	-10.82	111.78	122.60
2	B	212	SER	O-C-N	-10.69	109.72	122.87
1	A	113	ASN	CA-CB-CG	-10.39	102.21	112.60
2	B	200	THR	O-C-N	10.30	136.21	122.82
1	A	124	ASP	CA-CB-CG	10.29	122.89	112.60
1	A	132	ASN	CA-CB-CG	10.17	122.77	112.60
1	A	240	PHE	N-CA-C	10.09	132.30	110.80
1	A	65	HIS	N-CA-CB	10.07	125.29	110.49
2	B	185	GLN	N-CA-C	-10.03	100.58	113.12
1	A	64	ASN	CB-CG-ND2	10.01	131.42	116.40
2	B	200	THR	CA-C-O	9.98	131.87	120.60
1	A	17	THR	N-CA-CB	-9.93	95.54	111.62
2	B	32	ASN	OD1-CG-ND2	-9.78	112.82	122.60
2	B	198	ARG	CA-CB-CG	9.69	133.48	114.10
2	B	186	ASN	OD1-CG-ND2	-9.56	113.04	122.60
1	A	65	HIS	O-C-N	9.55	133.34	122.55
1	A	236	ASN	CA-C-O	-9.45	110.61	121.47
1	A	226	PHE	N-CA-C	9.39	130.80	110.80
2	B	79	ASP	CA-CB-CG	9.38	121.98	112.60
2	B	169	ALA	N-CA-C	-9.34	96.05	109.96
2	B	258	TRP	CG-CD2-CE3	9.11	143.01	133.90
2	B	43	THR	CA-CB-OG1	-8.88	96.29	109.60
1	A	236	ASN	O-C-N	-8.85	112.96	122.96
1	A	266	GLN	N-CA-C	8.77	129.48	110.80
1	A	37	ASP	CA-CB-CG	8.54	121.14	112.60
2	B	55	ASN	CA-CB-CG	8.42	121.02	112.60
2	B	22	ASP	O-C-N	-8.34	113.10	123.27
1	A	65	HIS	CB-CA-C	-8.28	99.46	112.05
2	B	189	ASN	OD1-CG-ND2	-8.25	114.35	122.60
2	B	68	GLY	O-C-N	-8.15	114.65	123.29
2	B	258	TRP	CB-CG-CD1	-8.13	114.70	126.90
1	A	164	LEU	N-CA-C	-8.11	102.03	111.03
1	A	71	THR	CA-CB-OG1	-8.05	97.52	109.60
2	B	251	HIS	CB-CG-CD2	-8.01	120.78	131.20
1	A	197	ARG	N-CA-C	-7.91	96.01	108.90
1	A	222	ASN	CB-CG-ND2	7.90	128.25	116.40
2	B	220	ASN	OD1-CG-ND2	-7.89	114.70	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	HIS	CA-CB-CG	7.88	121.68	113.80
1	A	238	SER	CA-C-N	7.86	136.55	121.54
1	A	238	SER	C-N-CA	7.86	136.55	121.54
2	B	183	PRO	N-CA-CB	7.85	107.32	102.92
2	B	90	TRP	CG-CD2-CE3	7.85	141.75	133.90
2	B	170	GLU	N-CA-C	7.83	121.00	110.35
2	B	176	TYR	N-CA-C	7.73	120.99	110.55
2	B	30	ASN	OD1-CG-ND2	-7.73	114.87	122.60
1	A	64	ASN	CA-CB-CG	7.71	120.31	112.60
1	A	67	GLU	N-CA-C	7.59	126.97	110.80
2	B	87	ALA	N-CA-C	-7.56	103.42	114.39
2	B	43	THR	CA-CB-CG2	7.45	123.17	110.50
1	A	159	THR	CA-CB-CG2	7.45	123.17	110.50
1	A	230	ILE	N-CA-C	-7.43	97.76	108.17
1	A	2	PHE	N-CA-C	7.37	122.47	109.58
1	A	64	ASN	O-C-N	-7.33	113.92	123.16
2	B	188	ASP	CA-CB-CG	7.27	119.87	112.60
2	B	201	VAL	CA-C-N	-7.23	113.44	122.48
2	B	201	VAL	C-N-CA	-7.23	113.44	122.48
1	A	249	ILE	N-CA-CB	-7.20	105.97	110.50
1	A	239	LYS	N-CA-C	7.12	125.95	110.80
1	A	190	THR	CA-CB-OG1	-7.09	98.97	109.60
1	A	113	ASN	O-C-N	7.07	131.54	123.48
1	A	221	SER	CA-CB-OG	7.04	125.18	111.10
2	B	211	SER	N-CA-C	7.00	120.01	110.55
1	A	236	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	245	VAL	O-C-N	-6.98	112.91	122.05
1	A	195	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	204	VAL	CA-C-O	-6.91	113.52	120.85
2	B	137	THR	N-CA-CB	-6.89	98.83	110.41
2	B	165	SER	N-CA-C	-6.87	95.91	107.99
2	B	226	ASN	OD1-CG-ND2	-6.86	115.74	122.60
2	B	196	ASN	CA-CB-CG	-6.86	105.74	112.60
1	A	98	GLN	OE1-CD-NE2	-6.85	115.75	122.60
2	B	60	ASN	OD1-CG-ND2	-6.84	115.76	122.60
2	B	3	VAL	N-CA-C	-6.81	100.15	109.55
1	A	238	SER	O-C-N	6.80	131.64	122.59
1	A	109	THR	CA-CB-OG1	-6.77	99.44	109.60
1	A	246	SER	N-CA-C	6.76	120.79	112.54
2	B	143	THR	N-CA-C	-6.74	98.74	109.59
1	A	6	TYR	CA-C-N	6.74	126.50	119.76
1	A	6	TYR	C-N-CA	6.74	126.50	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	VAL	N-CA-CB	-6.71	102.94	110.99
2	B	121	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	104	ILE	N-CA-CB	-6.69	99.21	110.65
2	B	24	ARG	N-CA-C	6.67	119.69	110.35
2	B	43	THR	N-CA-CB	-6.66	96.71	111.69
2	B	178	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	100	ASP	N-CA-C	6.64	118.17	111.07
2	B	60	ASN	CA-CB-CG	6.63	119.23	112.60
1	A	181	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	226	PHE	CB-CA-C	-6.59	97.31	110.42
2	B	106	VAL	N-CA-CB	-6.58	99.05	111.21
2	B	138	GLN	OE1-CD-NE2	-6.58	116.03	122.60
2	B	75	VAL	N-CA-C	-6.57	99.02	108.48
2	B	184	GLN	N-CA-C	6.55	124.75	110.80
2	B	104	SER	O-C-N	6.52	134.31	122.44
2	B	58	ARG	N-CA-C	6.51	119.42	108.02
1	A	238	SER	N-CA-C	6.50	124.65	110.80
2	B	238	SER	N-CA-C	-6.48	104.68	112.58
2	B	30	ASN	CB-CG-ND2	6.39	125.99	116.40
1	A	76	VAL	N-CA-CB	-6.36	99.78	110.65
2	B	112	GLY	CA-C-N	6.36	129.74	120.71
2	B	112	GLY	C-N-CA	6.36	129.74	120.71
1	A	168	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	64	ASN	CA-C-O	-6.33	114.00	121.16
1	A	97	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	71	THR	CA-CB-CG2	6.31	121.23	110.50
1	A	152	TYR	CA-C-O	-6.30	114.16	120.90
1	A	154	TYR	N-CA-C	-6.27	104.50	111.71
2	B	184	GLN	CA-CB-CG	-6.25	101.59	114.10
1	A	22	THR	CA-C-O	-6.25	114.26	120.82
1	A	222	ASN	N-CA-C	-6.23	97.53	110.80
1	A	40	HIS	CB-CG-CD2	-6.23	123.11	131.20
1	A	128	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	192	ILE	CA-CB-CG1	6.20	120.94	110.40
1	A	113	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	53	ILE	CB-CA-C	-6.18	99.99	111.79
2	B	214	GLN	N-CA-C	-6.16	105.04	113.30
2	B	156	SER	CB-CA-C	-6.15	109.46	116.54
2	B	28	PHE	CA-CB-CG	-6.14	107.66	113.80
2	B	166	SER	CA-C-N	6.12	131.22	121.18
2	B	166	SER	C-N-CA	6.12	131.22	121.18
2	B	197	ILE	CB-CG1-CD1	-6.10	100.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	VAL	CA-C-O	-6.09	113.17	120.78
2	B	155	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	210	SER	CA-CB-OG	-6.09	98.93	111.10
2	B	120	VAL	N-CA-C	-6.08	99.72	108.53
1	A	234	ARG	NE-CZ-NH2	-6.06	113.74	119.20
1	A	225	ALA	N-CA-C	6.06	123.70	110.80
2	B	105	LEU	CA-C-O	6.05	126.98	120.32
2	B	109	ALA	O-C-N	-6.05	115.13	123.12
2	B	247	LEU	N-CA-C	-6.05	99.54	109.40
1	A	182	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	142	GLY	O-C-N	-5.97	118.92	121.07
1	A	249	ILE	O-C-N	-5.97	115.83	120.07
2	B	136	ASN	CB-CG-ND2	5.96	125.34	116.40
1	A	182	GLN	CG-CD-NE2	5.95	125.32	116.40
2	B	212	SER	CA-C-O	-5.92	114.67	121.19
2	B	251	HIS	N-CA-C	-5.91	105.73	113.12
1	A	26	ARG	CD-NE-CZ	-5.90	116.14	124.40
2	B	131	TRP	CE2-CD2-CG	-5.89	100.13	107.20
1	A	159	THR	OG1-CB-CG2	-5.88	97.54	109.30
1	A	243	TYR	N-CA-C	-5.87	106.09	113.72
2	B	202	VAL	N-CA-C	-5.86	98.19	107.15
1	A	231	GLN	OE1-CD-NE2	-5.85	116.75	122.60
2	B	237	ALA	N-CA-C	5.85	123.26	110.80
2	B	29	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	B	198	ARG	O-C-N	5.78	130.28	122.59
1	A	67	GLU	CB-CG-CD	-5.77	102.79	112.60
2	B	251	HIS	CB-CG-ND1	5.77	131.35	122.70
2	B	60	ASN	N-CA-C	5.75	119.36	111.54
2	B	216	TRP	CG-CD1-NE1	-5.75	102.72	110.20
1	A	123	TYR	CA-C-O	-5.74	114.76	120.90
2	B	201	VAL	N-CA-C	-5.73	97.41	109.34
1	A	216	THR	CA-CB-OG1	-5.73	101.00	109.60
1	A	60	VAL	N-CA-CB	-5.73	104.24	111.46
1	A	41	GLU	N-CA-C	5.73	123.00	110.80
2	B	119	THR	O-C-N	-5.71	114.70	122.81
2	B	34	ILE	N-CA-C	-5.68	100.24	108.87
2	B	170	GLU	O-C-N	5.68	129.80	122.81
2	B	258	TRP	CG-CD1-NE1	-5.67	102.83	110.20
1	A	251	ILE	CA-C-O	-5.67	113.69	120.78
1	A	182	GLN	N-CA-C	-5.67	105.63	112.54
2	B	172	GLN	N-CA-C	-5.64	100.50	109.76
1	A	82	VAL	CB-CA-C	-5.64	103.70	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLU	CA-CB-CG	5.64	125.38	114.10
2	B	194	ASP	CA-C-N	5.64	132.31	121.54
2	B	194	ASP	C-N-CA	5.64	132.31	121.54
2	B	22	ASP	N-CA-CB	-5.63	100.80	111.00
2	B	245	ILE	N-CA-C	-5.63	99.04	107.37
2	B	12	ARG	O-C-N	-5.62	116.44	122.85
2	B	258	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	47	ASN	CA-CB-CG	5.60	118.20	112.60
2	B	168	LYS	N-CA-C	5.59	118.51	109.79
2	B	11	VAL	N-CA-CB	-5.57	102.05	112.36
2	B	138	GLN	CA-C-N	5.55	125.53	120.21
2	B	138	GLN	C-N-CA	5.55	125.53	120.21
1	A	154	TYR	O-C-N	-5.54	115.74	122.22
2	B	28	PHE	N-CA-C	5.53	119.72	112.92
2	B	195	SER	CA-CB-OG	5.49	122.07	111.10
2	B	186	ASN	CB-CG-ND2	5.47	124.61	116.40
2	B	27	ARG	CA-CB-CG	-5.46	103.17	114.10
1	A	40	HIS	CB-CG-ND1	5.46	130.90	122.70
2	B	187	ARG	N-CA-C	5.46	119.68	113.19
2	B	46	ASN	CA-CB-CG	5.45	118.05	112.60
2	B	243	LYS	CG-CD-CE	5.44	123.82	111.30
1	A	190	THR	CA-CB-CG2	5.44	119.75	110.50
2	B	221	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	132	LEU	CA-C-N	5.43	126.63	119.84
2	B	132	LEU	C-N-CA	5.43	126.63	119.84
1	A	106	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	159	THR	CA-CB-OG1	-5.43	101.45	109.60
2	B	90	TRP	CB-CG-CD1	-5.43	118.76	126.90
2	B	142	THR	CB-CA-C	-5.42	99.56	110.30
2	B	131	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	A	17	THR	CB-CA-C	5.42	122.75	110.67
2	B	37	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	A	236	ASN	N-CA-C	-5.41	102.47	110.48
2	B	161	ILE	CA-CB-CG1	-5.41	101.20	110.40
2	B	192	THR	CA-C-O	-5.41	114.52	120.36
2	B	37	TRP	CD1-CG-CD2	5.39	114.92	106.30
2	B	120	VAL	O-C-N	-5.39	117.64	123.14
1	A	180	ARG	CB-CG-CD	-5.38	98.92	111.30
2	B	37	TRP	CG-CD1-NE1	-5.38	103.20	110.20
2	B	199	GLU	CB-CG-CD	5.35	121.70	112.60
1	A	27	ALA	CA-C-N	5.34	127.29	120.56
1	A	27	ALA	C-N-CA	5.34	127.29	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	VAL	CG1-CB-CG2	-5.33	99.07	110.80
1	A	18	VAL	N-CA-C	-5.32	105.35	110.72
2	B	70	SER	CA-C-O	-5.30	113.81	120.23
2	B	6	ASP	N-CA-C	5.29	117.97	110.24
2	B	60	ASN	N-CA-CB	-5.29	103.95	111.84
1	A	159	THR	CB-CA-C	5.29	120.94	110.42
1	A	107	LEU	N-CA-C	5.29	122.06	110.80
1	A	225	ALA	CA-C-N	5.28	131.63	121.54
1	A	225	ALA	C-N-CA	5.28	131.63	121.54
2	B	258	TRP	CD1-CG-CD2	5.27	114.72	106.30
1	A	109	THR	CA-CB-CG2	5.26	119.45	110.50
1	A	104	ILE	CB-CA-C	5.23	120.27	112.16
2	B	32	ASN	CB-CG-ND2	5.23	124.24	116.40
2	B	243	LYS	N-CA-C	5.22	118.64	111.54
2	B	173	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	A	172	ILE	O-C-N	-5.20	116.47	121.83
2	B	137	THR	N-CA-C	5.17	119.43	113.18
1	A	240	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	216	TRP	CD1-CG-CD2	5.16	114.56	106.30
2	B	165	SER	CA-CB-OG	5.16	121.41	111.10
2	B	162	GLU	O-C-N	-5.14	115.94	122.78
1	A	131	GLY	N-CA-C	-5.14	107.90	115.30
2	B	166	SER	N-CA-C	5.14	121.75	110.80
2	B	9	PRO	N-CA-CB	-5.14	98.56	103.34
2	B	248	TYR	O-C-N	-5.13	117.83	121.83
1	A	237	GLY	N-CA-C	5.12	125.32	113.18
1	A	161	LEU	N-CA-C	5.12	119.90	113.25
1	A	111	VAL	O-C-N	5.10	128.03	122.57
2	B	10	ILE	N-CA-C	-5.10	99.78	107.73
1	A	84	TYR	N-CA-C	5.10	116.59	108.79
1	A	242	VAL	CG1-CB-CG2	-5.10	99.58	110.80
2	B	216	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	A	65	HIS	CB-CG-CD2	-5.09	124.59	131.20
2	B	37	TRP	CA-C-N	5.08	126.19	119.84
2	B	37	TRP	C-N-CA	5.08	126.19	119.84
1	A	2	PHE	CA-C-N	5.08	126.19	119.84
1	A	2	PHE	C-N-CA	5.08	126.19	119.84
2	B	161	ILE	N-CA-CB	-5.08	104.89	110.99
2	B	85	THR	N-CA-CB	-5.07	101.92	110.49
1	A	23	ASN	OD1-CG-ND2	-5.07	117.53	122.60
2	B	95	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	226	PHE	O-C-N	5.05	129.31	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	ARG	CA-CB-CG	-5.04	104.02	114.10
2	B	123	ASN	CA-CB-CG	5.04	117.64	112.60
2	B	137	THR	OG1-CB-CG2	5.04	119.38	109.30
1	A	28	VAL	CG1-CB-CG2	-5.04	99.72	110.80
2	B	220	ASN	CB-CG-ND2	5.03	123.94	116.40
2	B	121	GLN	CG-CD-NE2	5.01	123.92	116.40
1	A	114	ARG	CA-CB-CG	5.01	124.12	114.10
2	B	51	LEU	N-CA-C	-5.01	100.34	108.41

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLY	Mainchain
1	A	262	PRO	Peptide
1	A	56	ARG	Sidechain
2	B	170	GLU	Mainchain
2	B	199	GLU	Mainchain
2	B	74	TYR	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	2114	0	2083	66	0
2	B	2035	0	1974	51	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
4	E	61	0	52	1	0
4	F	61	0	52	0	0
5	A	61	0	0	2	0
5	B	62	0	0	4	0
All	All	4440	0	4203	115	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 14.

All (115) 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:1:ILE:HG23	1:A:2:PHE:H	1.51	0.76
1:A:236:ASN:HD21	1:A:238:SER:HB2	1.53	0.73
1:A:225:ALA:HB1	1:A:226:PHE:CD1	2.29	0.67
2:B:193:SER:HA	2:B:201:VAL:O	1.94	0.67
2:B:198:ARG:HB3	2:B:199:GLU:OE1	1.94	0.67
1:A:224:GLY:HA2	5:A:625:HOH:O	1.94	0.67
1:A:1:ILE:HG12	1:A:53:ILE:HD11	1.76	0.66
2:B:102:ARG:HB2	5:B:671:HOH:O	1.95	0.66
1:A:1:ILE:HG23	1:A:2:PHE:N	2.13	0.62
1:A:225:ALA:HB3	1:A:244:ASP:HA	1.81	0.62
2:B:165:SER:HB3	2:B:168:LYS:HB2	1.82	0.62
2:B:201:VAL:HG12	2:B:203:LYS:NZ	2.15	0.61
1:A:260:ALA:O	2:B:4:CYS:SG	2.58	0.61
1:A:266:GLN:HG3	1:A:267:PHE:N	2.15	0.61
2:B:12:ARG:HD3	2:B:20:CYS:SG	2.42	0.60
1:A:44:VAL:HG22	1:A:255:MET:HE3	1.84	0.60
1:A:229:PRO:HB3	1:A:243:TYR:CE2	2.37	0.59
1:A:53:ILE:HG21	1:A:106:HIS:CD2	2.37	0.58
2:B:16:ARG:HH11	2:B:128:SER:HB3	1.67	0.58
1:A:91:TYR:OH	1:A:155:SER:HA	2.04	0.58
1:A:154:TYR:CE1	1:A:159:THR:HG23	2.39	0.57
2:B:78:TYR:HD2	2:B:83:ALA:HB2	1.69	0.57
1:A:236:ASN:ND2	1:A:238:SER:HB2	2.18	0.56
1:A:119:PHE:HB2	1:A:125:ARG:HG2	1.86	0.56
2:B:182:ARG:NE	2:B:207:CYS:SG	2.78	0.56
2:B:236:ARG:HD3	2:B:242:LEU:HD13	1.87	0.55
1:A:40:HIS:H	1:A:267:PHE:HB3	1.72	0.55
2:B:67:TYR:HB3	2:B:73:VAL:HB	1.89	0.55
1:A:9:ILE:HD11	1:A:31:ARG:HG2	1.87	0.54
2:B:145:VAL:HG21	2:B:261:LEU:HD12	1.90	0.54
1:A:66:ALA:O	1:A:67:GLU:HB2	2.07	0.54
2:B:141:VAL:HA	2:B:173:TRP:O	2.07	0.53
2:B:153:GLN:HG2	5:B:651:HOH:O	2.08	0.53
1:A:39:ARG:HA	1:A:267:PHE:HB2	1.90	0.53
1:A:88:ASN:HB2	1:A:112:GLN:OE1	2.09	0.52
1:A:221:SER:O	1:A:222:ASN:HB2	2.08	0.52
1:A:206:THR:HG22	1:A:232:LEU:HD12	1.90	0.52
1:A:266:GLN:HG3	1:A:267:PHE:CG	2.45	0.52
1:A:102:GLU:O	1:A:105:THR:HB	2.10	0.52
1:A:53:ILE:HG21	1:A:106:HIS:HD2	1.75	0.52
2:B:99:ILE:HD11	2:B:104:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TRP:CZ3	2:B:100:ASN:HB2	2.45	0.51
1:A:60:VAL:HG12	1:A:62:LEU:HD13	1.93	0.51
2:B:27:ARG:O	2:B:32:ASN:ND2	2.43	0.51
1:A:29:ARG:HD2	1:A:179:ALA:O	2.10	0.51
1:A:39:ARG:HA	1:A:267:PHE:CB	2.42	0.49
1:A:23:ASN:HA	1:A:26:ARG:HD3	1.93	0.49
2:B:90:TRP:CE3	2:B:100:ASN:HB2	2.47	0.49
1:A:64:ASN:HB3	1:A:66:ALA:HB3	1.95	0.48
2:B:78:TYR:CD2	2:B:83:ALA:HB2	2.48	0.48
2:B:201:VAL:HG12	2:B:203:LYS:HZ2	1.77	0.48
2:B:238:SER:O	2:B:240:PRO:HD3	2.14	0.47
1:A:229:PRO:HA	1:A:242:VAL:O	2.14	0.47
2:B:34:ILE:HD12	2:B:49:TRP:HH2	1.79	0.47
2:B:161:ILE:HD12	2:B:258:TRP:CZ3	2.50	0.47
2:B:8:GLU:HA	2:B:51:LEU:O	2.15	0.47
2:B:12:ARG:CG	2:B:12:ARG:HH11	2.28	0.47
2:B:93:TRP:CZ2	4:E:2:NAG:H83	2.49	0.47
1:A:224:GLY:O	1:A:225:ALA:HB2	2.15	0.47
2:B:186:ASN:OD1	2:B:189:ASN:ND2	2.48	0.47
1:A:222:ASN:HB3	1:A:223:GLN:O	2.15	0.46
1:A:40:HIS:O	1:A:41:GLU:HB2	2.15	0.46
2:B:201:VAL:HA	2:B:203:LYS:HZ2	1.80	0.46
2:B:191:LEU:HD23	2:B:216:TRP:CE2	2.50	0.46
1:A:70:VAL:HG11	1:A:151:LEU:HD23	1.97	0.46
2:B:161:ILE:HD12	2:B:258:TRP:HZ3	1.80	0.45
2:B:124:ILE:O	2:B:212:SER:HB3	2.16	0.45
1:A:154:TYR:CD1	1:A:159:THR:HA	2.52	0.45
2:B:175:LEU:HD22	2:B:181:ILE:HG12	1.99	0.45
2:B:213:GLY:HA2	2:B:226:ASN:HD21	1.82	0.45
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.63	0.45
1:A:191:ARG:NH2	1:A:198:SER:HB3	2.31	0.45
2:B:233:LEU:HD22	2:B:245:ILE:HG21	1.99	0.45
2:B:160:TRP:CD2	2:B:243:LYS:HD3	2.52	0.45
1:A:18:VAL:HB	1:A:189:ARG:HG3	1.98	0.45
1:A:157:GLY:O	1:A:158:GLY:C	2.59	0.44
2:B:223:THR:HG21	2:B:250:LEU:HD23	1.99	0.44
1:A:11:PHE:HB2	1:A:24:PHE:CD1	2.53	0.44
1:A:251:ILE:HD13	2:B:260:PRO:HG2	2.00	0.44
1:A:43:PRO:HD2	1:A:253:ALA:O	2.18	0.43
2:B:199:GLU:HA	2:B:246:ILE:HB	2.00	0.43
2:B:228:TYR:N	5:B:675:HOH:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PRO:O	2:B:185:GLN:N	2.51	0.43
1:A:191:ARG:HH21	1:A:198:SER:HB3	1.83	0.43
1:A:4:LYS:NZ	1:A:55:GLN:HE22	2.17	0.43
1:A:211:TRP:CH2	1:A:256:VAL:HB	2.53	0.43
2:B:19:LEU:HB2	2:B:36:LEU:HG	2.01	0.43
2:B:96:GLY:O	2:B:130:GLY:HA2	2.19	0.43
1:A:190:THR:HG23	1:A:196:ARG:HH12	1.84	0.42
1:A:122:ASN:HD22	1:A:124:ASP:HB2	1.84	0.42
1:A:140:GLY:C	1:A:143:PRO:HD2	2.43	0.42
2:B:100:ASN:ND2	5:B:671:HOH:O	2.52	0.42
1:A:4:LYS:O	1:A:5:GLN:HG2	2.19	0.42
2:B:64:LEU:HD23	2:B:90:TRP:NE1	2.34	0.42
2:B:233:LEU:HD22	2:B:245:ILE:CG2	2.49	0.42
1:A:236:ASN:ND2	1:A:236:ASN:O	2.52	0.42
1:A:154:TYR:HD1	1:A:159:THR:HA	1.84	0.41
2:B:213:GLY:CA	2:B:226:ASN:HD21	2.32	0.41
1:A:10:ASN:HB3	1:A:61:GLU:HB3	2.03	0.41
1:A:39:ARG:HG2	1:A:267:PHE:HD2	1.84	0.41
1:A:161:LEU:HB3	1:A:162:PRO:HD3	2.02	0.41
1:A:8:ILE:HA	1:A:59:LEU:O	2.21	0.41
1:A:1:ILE:CG2	1:A:2:PHE:H	2.27	0.41
1:A:166:ARG:O	1:A:170:ILE:HG13	2.21	0.41
2:B:140:PHE:CD2	2:B:142:THR:HG23	2.56	0.41
1:A:238:SER:OG	1:A:239:LYS:HD3	2.20	0.41
1:A:267:PHE:HE2	5:A:310:HOH:O	2.02	0.41
1:A:17:THR:HG22	1:A:20:SER:H	1.85	0.41
1:A:68:LEU:HD12	1:A:149:SER:HA	2.02	0.41
1:A:107:LEU:HD13	1:A:107:LEU:HA	1.91	0.41
1:A:108:PHE:O	1:A:111:VAL:HG22	2.21	0.41
2:B:195:SER:O	2:B:197:ILE:N	2.53	0.41
1:A:119:PHE:HA	1:A:125:ARG:NH1	2.36	0.41
2:B:33:ALA:HB1	2:B:117:THR:HG23	2.03	0.41
2:B:2:ASP:HB3	2:B:5:MET:SD	2.62	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	265/267 (99%)	231 (87%)	17 (6%)	17 (6%)	1	1
2	B	260/262 (99%)	222 (85%)	20 (8%)	18 (7%)	1	1
All	All	525/529 (99%)	453 (86%)	37 (7%)	35 (7%)	1	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	14	ALA
1	A	66	ALA
1	A	67	GLU
1	A	222	ASN
1	A	226	PHE
1	A	239	LYS
1	A	240	PHE
1	A	263	PRO
2	B	42	ASN
2	B	166	SER
2	B	184	GLN
2	B	195	SER
2	B	199	GLU
2	B	228	TYR
1	A	105	THR
1	A	134	ARG
1	A	237	GLY
1	A	264	SER
2	B	5	MET
2	B	25	ASP
2	B	196	ASN
2	B	201	VAL
2	B	206	SER
1	A	5	GLN

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	157	GLY
2	B	197	ILE
2	B	237	ALA
1	A	156	THR
2	B	7	PRO
2	B	84	ALA
2	B	85	THR
2	B	38	PRO
2	B	101	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/226 (100%)	183 (81%)	43 (19%)	1	3
2	B	227/227 (100%)	197 (87%)	30 (13%)	4	8
All	All	453/453 (100%)	380 (84%)	73 (16%)	2	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	THR
1	A	19	GLN
1	A	29	ARG
1	A	34	THR
1	A	46	PRO
1	A	48	ARG
1	A	53	ILE
1	A	62	LEU
1	A	65	HIS
1	A	67	GLU
1	A	70	VAL
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	102	GLU
1	A	104	ILE
1	A	107	LEU
1	A	109	THR
1	A	110	ASP
1	A	113	ASN
1	A	114	ARG
1	A	126	LEU
1	A	129	LEU
1	A	133	LEU
1	A	135	GLU
1	A	151	LEU
1	A	160	GLN
1	A	164	LEU
1	A	190	THR
1	A	192	ILE
1	A	198	SER
1	A	203	SER
1	A	222	ASN
1	A	226	PHE
1	A	230	ILE
1	A	232	LEU
1	A	235	ARG
1	A	236	ASN
1	A	238	SER
1	A	239	LYS
1	A	247	ILE
1	A	251	ILE
1	A	263	PRO
1	A	264	SER
2	B	5	MET
2	B	6	ASP
2	B	8	GLU
2	B	12	ARG
2	B	36	LEU
2	B	38	PRO
2	B	48	LEU
2	B	51	LEU
2	B	122	THR
2	B	136	ASN
2	B	137	THR
2	B	158	GLN

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Mol	Chain	Res	Type
2	B	166	SER
2	B	168	LYS
2	B	184	GLN
2	B	188	ASP
2	B	194	ASP
2	B	196	ASN
2	B	197	ILE
2	B	199	GLU
2	B	201	VAL
2	B	205	LEU
2	B	211	SER
2	B	225	LEU
2	B	231	LEU
2	B	233	LEU
2	B	236	ARG
2	B	241	SER
2	B	251	HIS
2	B	261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	47	ASN
1	A	54	ASN
1	A	55	GLN
1	A	64	ASN
1	A	98	GLN
1	A	113	ASN
1	A	128	GLN
1	A	132	ASN
1	A	209	ASN
1	A	223	GLN
1	A	236	ASN
2	B	81	ASN
2	B	100	ASN
2	B	121	GLN
2	B	136	ASN
2	B	186	ASN
2	B	189	ASN
2	B	196	ASN
2	B	214	GLN

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Mol	Chain	Res	Type
2	B	220	ASN
2	B	226	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 ⓘ

14 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	BGC	C	1	3	12,12,12	1.28	1 (8%)	17,17,17	1.68	3 (17%)
3	GAL	C	2	3	11,11,12	0.97	1 (9%)	15,15,17	1.21	1 (6%)
3	BGC	D	1	3	12,12,12	1.17	1 (8%)	17,17,17	2.04	3 (17%)
3	GAL	D	2	3	11,11,12	1.09	1 (9%)	15,15,17	1.84	6 (40%)
4	NAG	E	1	2,4	14,14,15	1.26	2 (14%)	17,19,21	1.84	5 (29%)
4	NAG	E	2	4	14,14,15	1.79	6 (42%)	17,19,21	3.67	7 (41%)
4	BMA	E	3	4	11,11,12	1.59	2 (18%)	15,15,17	3.65	8 (53%)
4	MAN	E	4	4	11,11,12	1.36	1 (9%)	15,15,17	0.99	0
4	MAN	E	5	4	11,11,12	2.15	5 (45%)	15,15,17	2.14	7 (46%)
4	NAG	F	1	2,4	14,14,15	0.86	0	17,19,21	1.49	4 (23%)
4	NAG	F	2	4	14,14,15	1.07	1 (7%)	17,19,21	2.96	8 (47%)
4	BMA	F	3	4	11,11,12	1.86	2 (18%)	15,15,17	1.91	6 (40%)
4	MAN	F	4	4	11,11,12	1.23	1 (9%)	15,15,17	2.69	11 (73%)
4	MAN	F	5	4	11,11,12	1.40	0	15,15,17	3.22	9 (60%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	O5-C5	4.06	1.51	1.43
4	E	5	MAN	C2-C3	3.80	1.58	1.52
4	E	4	MAN	C2-C3	-3.76	1.46	1.52
4	E	3	BMA	O2-C2	3.36	1.50	1.43
4	E	2	NAG	C1-C2	3.26	1.56	1.52
4	E	2	NAG	C3-C2	3.11	1.59	1.52
4	F	3	BMA	C2-C3	3.08	1.57	1.52
4	E	2	NAG	O5-C5	2.83	1.49	1.43
4	E	5	MAN	C1-C2	2.77	1.58	1.52
4	E	5	MAN	C6-C5	2.62	1.60	1.51
4	E	1	NAG	O5-C1	-2.39	1.39	1.43
3	C	1	BGC	O1-C1	2.39	1.47	1.39
3	C	2	GAL	C2-C3	-2.38	1.48	1.52
4	E	5	MAN	O3-C3	2.34	1.48	1.43
4	F	2	NAG	O5-C1	-2.28	1.39	1.43
3	D	2	GAL	O4-C4	2.20	1.48	1.43
4	E	5	MAN	O5-C5	2.16	1.47	1.43
4	E	2	NAG	C4-C3	2.16	1.57	1.52
4	E	1	NAG	C1-C2	-2.13	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	BGC	C6-C5	2.11	1.58	1.51
4	E	2	NAG	O3-C3	2.10	1.48	1.43
4	F	4	MAN	C2-C3	2.07	1.55	1.52
4	E	3	BMA	O3-C3	2.07	1.48	1.43
4	E	2	NAG	O4-C4	2.05	1.48	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C1-C2-C3	-8.71	96.96	109.64
4	E	2	NAG	O5-C1-C2	-8.02	98.88	111.29
4	E	2	NAG	C1-O5-C5	-8.01	101.44	112.19
4	F	2	NAG	C2-N2-C7	-7.45	112.92	122.90
4	F	5	MAN	O5-C1-C2	-7.35	93.25	110.79
3	D	1	BGC	C3-C4-C5	-6.50	98.45	110.23
4	E	2	NAG	C3-C4-C5	-6.27	98.86	110.23
4	E	2	NAG	C4-C3-C2	-6.21	101.92	111.02
4	E	3	BMA	O5-C5-C6	5.26	117.91	107.66
4	E	3	BMA	C6-C5-C4	-5.02	100.69	113.02
4	F	2	NAG	C1-C2-N2	-4.97	102.61	110.43
4	E	3	BMA	C3-C4-C5	4.94	119.18	110.23
4	F	2	NAG	O5-C1-C2	-4.73	103.97	111.29
4	E	3	BMA	C1-O5-C5	-4.67	105.92	112.19
4	F	5	MAN	C1-O5-C5	4.13	117.72	112.19
3	C	1	BGC	C6-C5-C4	-4.08	103.00	113.02
4	F	5	MAN	O4-C4-C5	4.06	119.32	109.32
4	F	1	NAG	O5-C1-C2	3.90	117.33	111.29
4	F	5	MAN	C3-C4-C5	-3.80	103.35	110.23
4	F	5	MAN	O4-C4-C3	-3.79	101.44	110.38
4	F	4	MAN	O5-C1-C2	-3.75	101.83	110.79
4	F	3	BMA	O6-C6-C5	3.75	124.10	111.33
4	E	1	NAG	C8-C7-N2	3.68	122.22	116.12
4	F	4	MAN	O2-C2-C3	-3.62	102.66	110.15
4	F	4	MAN	C2-C3-C4	-3.60	104.53	110.86
3	D	2	GAL	O2-C2-C3	-3.58	102.74	110.15
3	D	1	BGC	O5-C1-C2	3.51	116.47	110.30
4	F	4	MAN	O2-C2-C1	3.44	117.09	109.22
3	C	1	BGC	O5-C5-C6	3.39	114.85	106.44
4	F	5	MAN	O3-C3-C4	-3.34	102.49	110.38
4	F	4	MAN	C1-C2-C3	-3.28	104.87	109.64
4	F	2	NAG	O7-C7-N2	-3.28	116.19	121.98
4	E	5	MAN	C1-C2-C3	3.19	114.30	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	BGC	O5-C5-C4	3.12	115.33	109.70
4	E	5	MAN	C2-C3-C4	-3.09	105.43	110.86
4	E	5	MAN	O3-C3-C2	3.04	116.27	110.05
4	E	1	NAG	O5-C1-C2	2.96	115.87	111.29
4	F	2	NAG	C1-O5-C5	-2.95	108.23	112.19
4	F	2	NAG	O7-C7-C8	2.90	127.22	122.05
4	E	1	NAG	C1-C2-N2	-2.89	105.89	110.43
4	E	5	MAN	O4-C4-C3	-2.87	103.61	110.38
4	F	3	BMA	O2-C2-C1	-2.78	102.85	109.22
4	F	3	BMA	C1-O5-C5	-2.78	108.47	112.19
4	F	5	MAN	O3-C3-C2	2.73	115.63	110.05
4	F	4	MAN	C6-C5-C4	-2.73	106.32	113.02
4	F	4	MAN	O3-C3-C4	-2.69	104.03	110.38
4	E	5	MAN	C6-C5-C4	-2.66	106.49	113.02
4	E	2	NAG	O6-C6-C5	-2.62	102.42	111.33
4	F	2	NAG	O5-C5-C4	-2.57	104.58	110.83
4	E	2	NAG	C1-C2-N2	2.56	114.46	110.43
4	F	4	MAN	C3-C4-C5	-2.54	105.62	110.23
3	C	2	GAL	C1-C2-C3	2.54	113.34	109.64
4	E	3	BMA	O5-C5-C4	2.53	116.99	110.83
4	F	1	NAG	C1-O5-C5	2.53	115.58	112.19
4	F	3	BMA	C6-C5-C4	-2.48	106.94	113.02
4	F	4	MAN	O3-C3-C2	2.46	115.07	110.05
3	D	1	BGC	O4-C4-C5	2.42	115.30	109.32
3	D	2	GAL	C1-O5-C5	2.39	115.39	112.19
4	E	1	NAG	C4-C3-C2	-2.33	107.60	111.02
4	F	3	BMA	C3-C4-C5	2.33	114.46	110.23
3	D	2	GAL	C1-C2-C3	2.30	113.00	109.64
3	D	2	GAL	O2-C2-C1	2.27	114.43	109.22
4	F	1	NAG	C3-C4-C5	-2.27	106.12	110.23
3	D	2	GAL	C6-C5-C4	-2.26	107.48	113.02
4	F	1	NAG	C1-C2-N2	-2.25	106.88	110.43
4	F	4	MAN	O6-C6-C5	-2.25	103.68	111.33
3	D	2	GAL	O3-C3-C4	-2.24	105.10	110.38
4	F	4	MAN	O5-C5-C6	2.24	112.02	107.66
4	E	5	MAN	O5-C5-C6	2.21	111.96	107.66
4	E	3	BMA	O2-C2-C1	2.20	114.26	109.22
4	E	3	BMA	O4-C4-C5	-2.19	103.92	109.32
4	E	2	NAG	O4-C4-C5	2.19	114.73	109.32
4	F	5	MAN	C2-C3-C4	-2.14	107.09	110.86
4	F	5	MAN	O2-C2-C1	-2.10	104.42	109.22
4	E	5	MAN	O3-C3-C4	-2.09	105.44	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	O2-C2-C3	2.06	114.42	110.15
4	F	2	NAG	C4-C3-C2	-2.01	108.07	111.02
4	E	1	NAG	O4-C4-C5	2.01	114.27	109.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	1	NAG	C1
4	F	1	NAG	C1

All (19) torsion outliers are listed below:

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

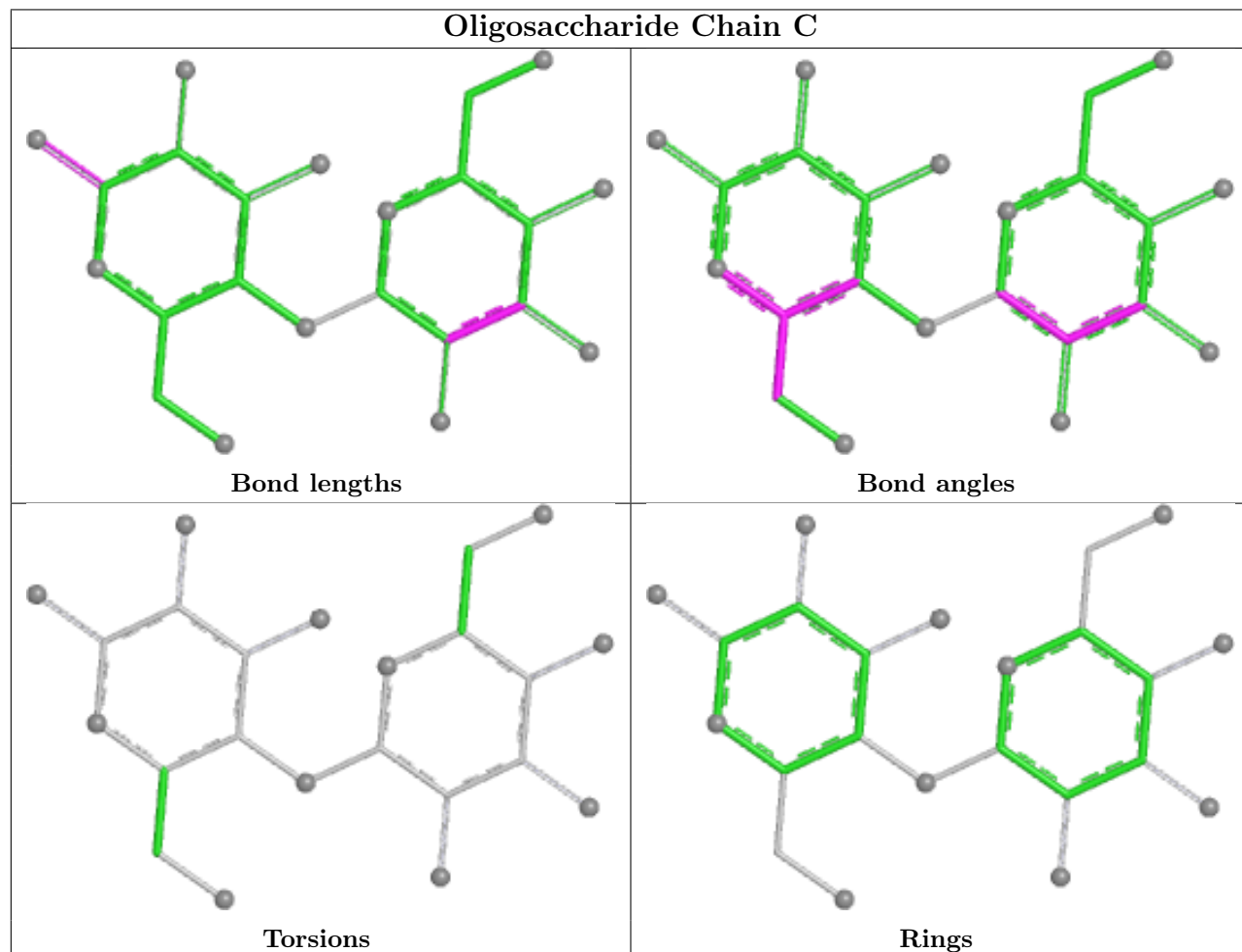
All (2) ring outliers are listed below:

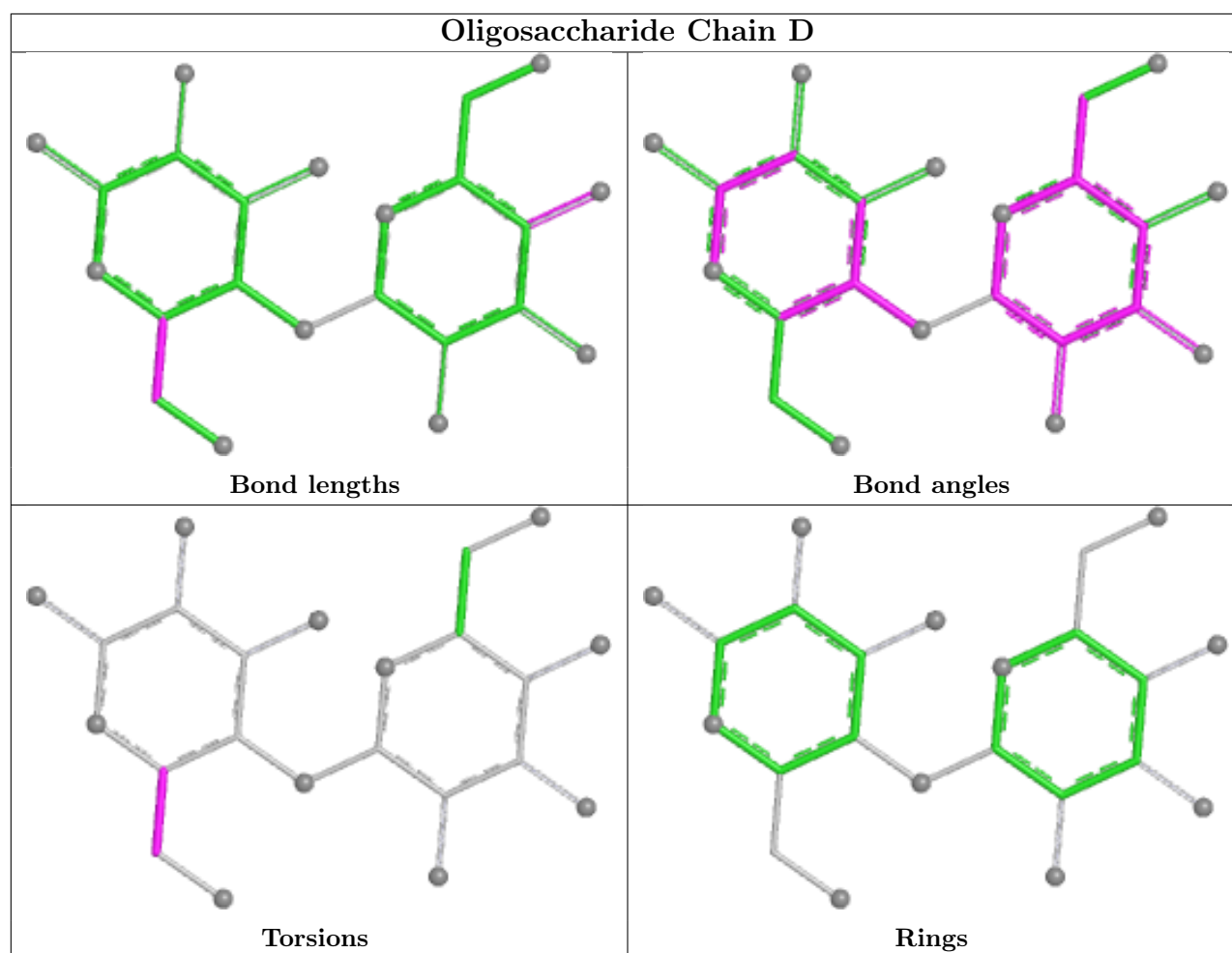
Mol	Chain	Res	Type	Atoms
4	F	5	MAN	C1-C2-C3-C4-C5-O5
4	F	4	MAN	C1-C2-C3-C4-C5-O5

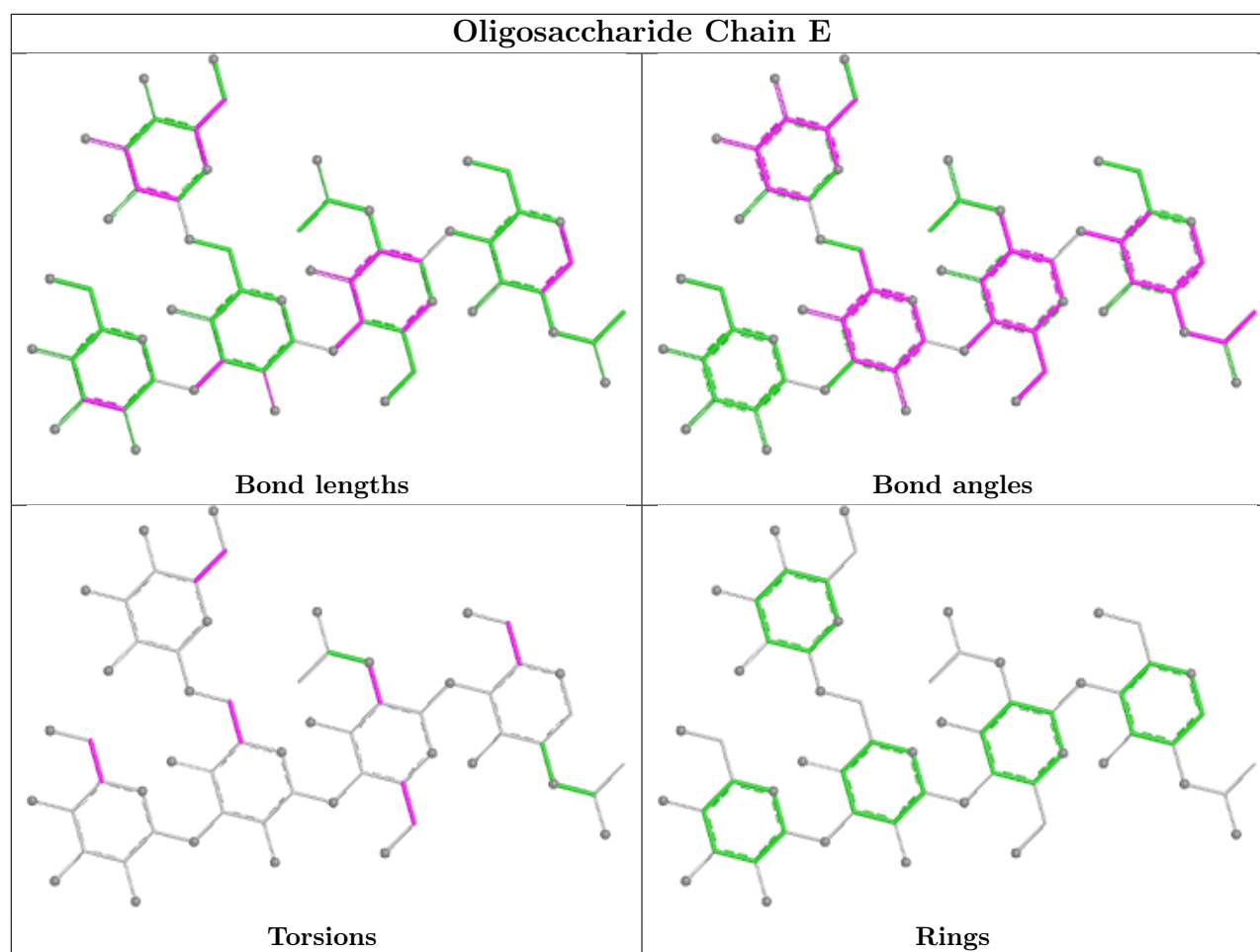
1 monomer is involved in 1 short contact:

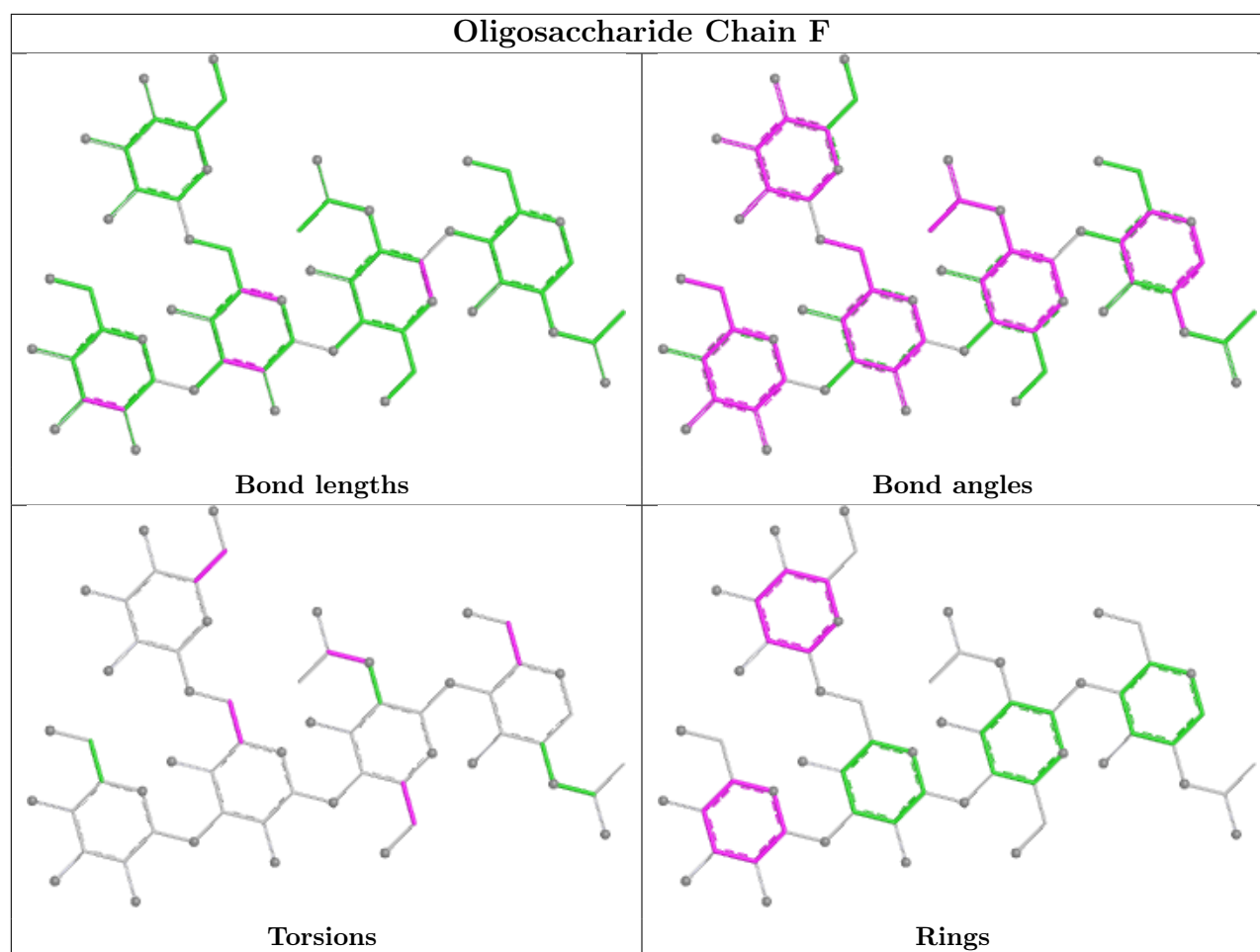
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0

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](#)

There are no ligands in this entry.

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.