



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 PM UTC

PDB ID : 1E04 / pdb_00001e04
Title : PLASMA BETA ANTITHROMBIN-III
Authors : Mccoy, A.J.; Skinner, R.; Abrahams, J.-P.; Pei, X.Y.; Carrell, R.W.
Deposited on : 2000-03-09
Resolution : 2.60 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

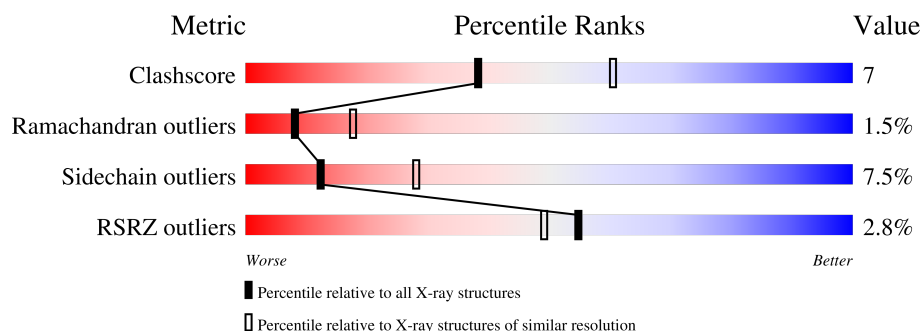
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	432	2% 69% 22% • 7%
1	L	432	3% 71% 21% • 5%
2	A	2	100%
2	B	2	100%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	C	3	 100%
4	F	5	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANTITHROMBIN-III.

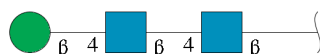
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	403	Total	C	N	O	S	0	0	0
			3179	2032	529	602	16			
1	L	412	Total	C	N	O	S	0	0	0
			3225	2057	536	614	18			

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



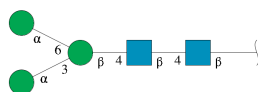
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



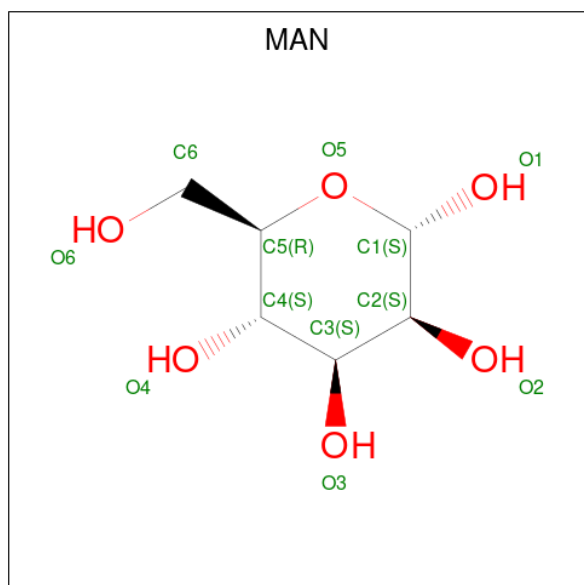
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



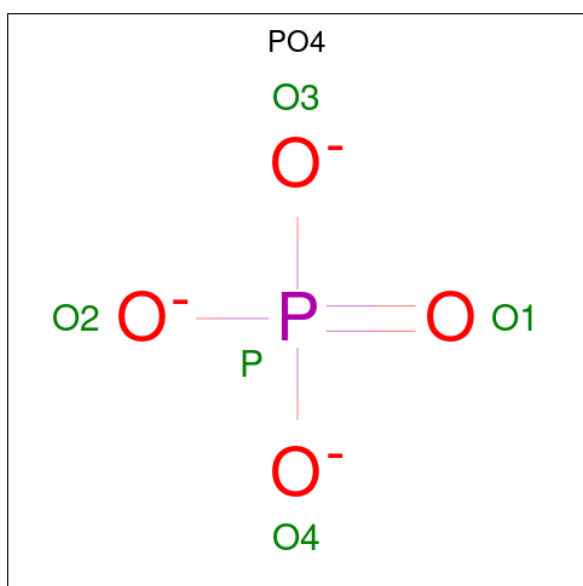
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

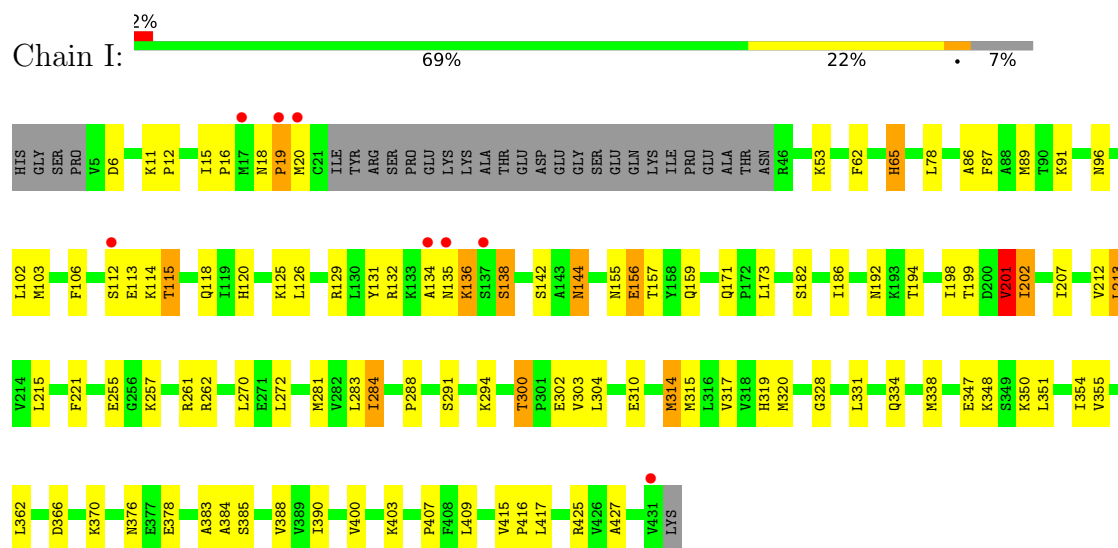
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	51	Total 51	O 51	0	0
8	L	33	Total 33	O 33	0	0

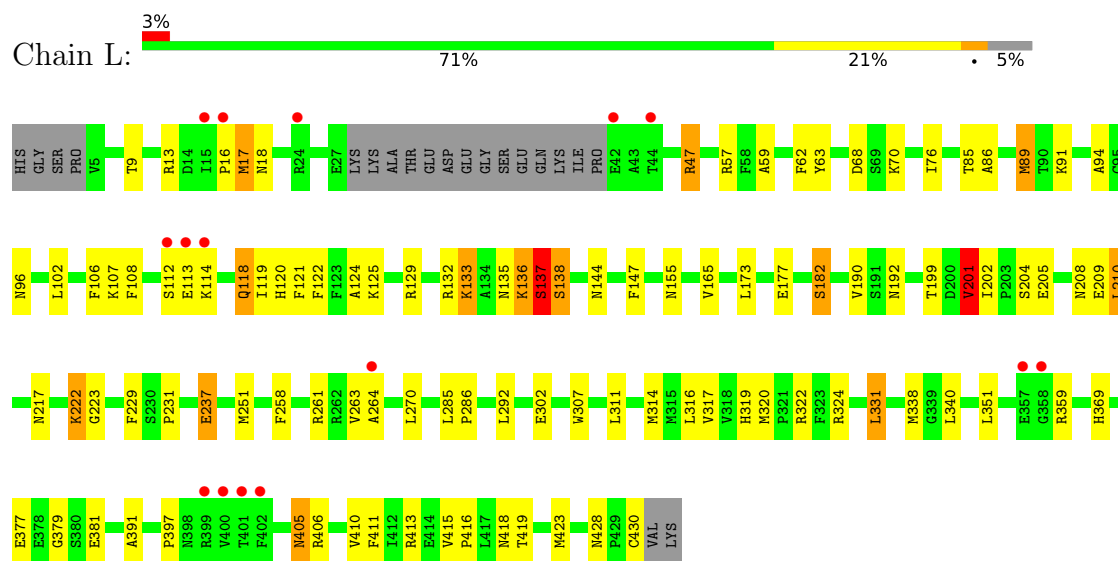
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: ANTITHROMBIN-III



• Molecule 1: ANTITHROMBIN-III



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

Chain A:  100%

NAG1
NAG2

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

Chain B:  100%

NAG1
NAG2

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

Chain D:  100%

NAG1
NAG2

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

Chain E:  50% 50%

NAG1
NAG2

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

Chain C:  100%

NAG1
NAG2
BMA3

- 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%

NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.05Å 99.34Å 88.59Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 94.4 (20.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.243 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6728	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, PO4, MAN, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.51	0/3242	1.29	17/4384 (0.4%)
1	L	0.49	0/3289	1.28	23/4452 (0.5%)
All	All	0.50	0/6531	1.29	40/8836 (0.5%)

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	I	0	1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	192	ASN	OD1-CG-ND2	8.01	130.61	122.60
1	I	6	ASP	CA-CB-CG	7.94	120.54	112.60
1	I	331	LEU	N-CA-C	7.09	120.04	111.82
1	I	171	GLN	N-CA-C	6.99	118.96	109.24
1	L	208	ASN	CA-CB-CG	6.84	119.44	112.60
1	L	96	ASN	OD1-CG-ND2	6.84	129.44	122.60
1	I	96	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	I	262	ARG	CD-NE-CZ	6.66	133.73	124.40
1	L	114	LYS	N-CA-C	6.58	120.30	112.93
1	L	264	ALA	N-CA-C	6.54	120.85	112.34
1	L	108	PHE	CA-CB-CG	6.51	120.31	113.80
1	I	201	VAL	N-CA-CB	6.38	117.57	110.62
1	I	20	MET	N-CA-C	-6.30	106.56	114.56
1	L	201	VAL	N-CA-CB	6.20	117.81	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	288	PRO	CA-C-N	6.16	128.45	120.44
1	I	288	PRO	C-N-CA	6.16	128.45	120.44
1	I	106	PHE	CA-C-N	6.14	131.30	122.40
1	I	106	PHE	C-N-CA	6.14	131.30	122.40
1	I	155	ASN	OD1-CG-ND2	6.11	128.71	122.60
1	I	87	PHE	CA-CB-CG	-5.82	107.98	113.80
1	I	65	HIS	CA-CB-CG	5.63	119.43	113.80
1	L	418	ASN	CA-CB-CG	5.52	118.12	112.60
1	L	155	ASN	CA-CB-CG	5.50	118.11	112.60
1	L	155	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	L	106	PHE	CA-C-N	5.45	129.86	122.07
1	L	106	PHE	C-N-CA	5.45	129.86	122.07
1	I	348	LYS	N-CA-C	5.40	118.34	111.69
1	I	16	PRO	N-CA-C	5.40	119.50	111.41
1	L	231	PRO	CA-C-N	5.35	128.19	120.38
1	L	231	PRO	C-N-CA	5.35	128.19	120.38
1	L	147	PHE	CA-CB-CG	5.32	119.12	113.80
1	L	201	VAL	CA-C-N	-5.24	118.82	122.59
1	L	201	VAL	C-N-CA	-5.24	118.82	122.59
1	L	411	PHE	CA-CB-CG	5.24	119.04	113.80
1	L	391	ALA	N-CA-C	5.15	118.70	111.74
1	L	202	ILE	CA-C-O	5.11	122.17	119.15
1	L	89	MET	CA-C-N	5.03	127.02	120.28
1	L	89	MET	C-N-CA	5.03	127.02	120.28
1	I	192	ASN	OD1-CG-ND2	5.00	127.60	122.60
1	L	229	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	134	ALA	Mainchain

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	I	3179	0	3139	45	0
1	L	3225	0	3155	46	0
2	A	28	0	25	1	0
2	B	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
3	C	39	0	34	0	0
4	F	61	0	52	0	0
5	I	11	0	10	0	0
6	I	6	0	8	0	0
6	L	6	0	8	1	0
7	L	5	0	0	0	0
8	I	51	0	0	2	0
8	L	33	0	0	0	0
All	All	6728	0	6506	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.57	0.85
1:I:62:PHE:HA	1:I:338:MET:HE1	1.64	0.77
1:L:86:ALA:HA	1:L:89:MET:HE3	1.66	0.77
1:I:388:VAL:HG22	1:L:317:VAL:HB	1.70	0.74
1:I:86:ALA:HA	1:I:144:ASN:HD21	1.52	0.73
1:L:47:ARG:HD3	1:L:113:GLU:HG3	1.71	0.72
1:I:194:THR:HG21	1:I:198:ILE:HD12	1.73	0.70
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.76	0.68
1:L:331:LEU:HD21	1:L:369:HIS:HB2	1.76	0.66
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.80	0.64
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.63	0.63
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.80	0.63
1:I:156:GLU:HA	1:I:159:GLN:HE21	1.64	0.62
1:L:428:ASN:ND2	1:L:430:CYS:H	2.01	0.59
1:I:334:GLN:HE21	1:I:338:MET:HE3	1.67	0.58
1:L:428:ASN:HD22	1:L:430:CYS:H	1.52	0.58
1:I:11:LYS:HB3	1:I:12:PRO:HD2	1.86	0.57
1:I:198:ILE:HG23	1:I:370:LYS:HD3	1.88	0.56
1:I:314:MET:HE1	1:I:400:VAL:HB	1.87	0.56
1:I:354:ILE:HG22	1:I:362:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:LEU:HD13	1:L:182:SER:HB3	1.90	0.54
1:L:270:LEU:HD13	1:L:316:LEU:HD11	1.90	0.54
1:L:17:MET:HE1	1:L:120:HIS:HB2	1.90	0.54
1:L:144:ASN:HD22	1:L:217:ASN:HA	1.72	0.53
1:I:300:THR:HG23	1:I:303:VAL:HB	1.90	0.53
1:I:376:ASN:HD21	1:I:383:ALA:HA	1.73	0.53
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.92	0.52
1:I:135:ASN:O	1:I:136:LYS:C	2.53	0.52
1:I:173:LEU:HD13	1:I:182:SER:HB3	1.92	0.52
1:L:210:LEU:HA	1:L:359:ARG:HH22	1.75	0.52
1:I:257:LYS:HB2	1:I:315:MET:HE2	1.92	0.51
1:I:270:LEU:HD21	1:I:272:LEU:HD21	1.93	0.51
1:I:114:LYS:O	1:I:115:THR:C	2.54	0.51
1:L:204:SER:O	1:L:205:GLU:HB2	2.11	0.50
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.93	0.50
1:L:222:LYS:HD3	1:L:381:GLU:HB2	1.93	0.49
1:I:213:LEU:HD11	1:I:354:ILE:HD13	1.95	0.48
1:I:18:ASN:HB3	1:I:19:PRO:HD2	1.94	0.48
1:L:16:PRO:O	1:L:17:MET:C	2.55	0.48
1:I:291:SER:HB3	1:I:294:LYS:HG3	1.96	0.48
1:I:261:ARG:HG2	1:I:310:GLU:HB3	1.97	0.47
1:I:425:ARG:HD3	1:I:427:ALA:HB2	1.96	0.47
1:I:15:ILE:HG21	1:I:120:HIS:HB2	1.97	0.47
1:L:102:LEU:HG	1:L:340:LEU:HD11	1.97	0.47
1:I:126:LEU:HD12	1:I:417:LEU:HD13	1.95	0.47
1:L:222:LYS:HG2	1:L:381:GLU:HG3	1.97	0.47
1:L:261:ARG:HB3	1:L:311:LEU:HD23	1.98	0.46
1:L:132:ARG:O	1:L:133:LYS:HB2	2.14	0.46
1:L:136:LYS:O	1:L:137:SER:C	2.58	0.46
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.97	0.45
1:I:328:GLY:HA2	1:I:370:LYS:HG3	1.98	0.45
1:L:85:THR:HG22	1:L:89:MET:HE2	1.99	0.45
1:L:237:GLU:OE1	1:L:251:MET:HG3	2.17	0.45
1:I:390:ILE:HA	1:L:319:HIS:HB2	1.99	0.45
1:L:125:LYS:O	1:L:129:ARG:HG2	2.17	0.45
1:L:263:VAL:HG11	1:L:307:TRP:CD1	2.51	0.44
1:I:89:MET:HE2	1:I:144:ASN:HD22	1.83	0.44
1:I:125:LYS:O	1:I:129:ARG:HG2	2.18	0.43
1:I:378:GLU:HG3	1:I:384:ALA:HB3	2.00	0.43
1:I:65:HIS:HB2	8:I:2047:HOH:O	2.18	0.43
1:I:284:ILE:HB	1:I:409:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:ARG:HG2	1:L:122:PHE:CE2	2.54	0.43
1:L:18:ASN:HB2	2:E:2:NAG:H83	2.00	0.43
1:L:405:ASN:O	1:L:406:ARG:C	2.61	0.43
1:I:138:SER:HB3	1:I:221:PHE:CE1	2.54	0.42
2:A:1:NAG:H62	2:A:2:NAG:N2	2.34	0.42
1:I:86:ALA:HB1	1:I:215:LEU:HD21	2.02	0.42
1:L:286:PRO:HD3	1:L:292:LEU:HD13	2.01	0.42
1:I:131:TYR:CE1	1:I:142:SER:HB2	2.54	0.42
1:L:59:ALA:O	1:L:423:MET:HE1	2.19	0.42
1:I:202:ILE:HG21	1:I:207:ILE:HD12	2.02	0.42
1:I:415:VAL:HB	1:I:416:PRO:CD	2.48	0.42
1:L:63:TYR:HB2	1:L:423:MET:HE1	2.01	0.42
1:L:413:ARG:HD2	6:L:810:GOL:H12	2.02	0.42
1:L:18:ASN:HB2	2:E:2:NAG:C8	2.50	0.42
1:L:89:MET:CE	1:L:217:ASN:HB2	2.49	0.41
1:I:11:LYS:HB3	1:I:12:PRO:CD	2.49	0.41
1:L:121:PHE:CZ	1:L:125:LYS:HE3	2.56	0.41
1:L:190:VAL:HG21	1:L:201:VAL:HG21	2.01	0.41
1:L:124:ALA:HB2	1:L:165:VAL:HG13	2.02	0.41
1:L:70:LYS:HD2	1:L:76:ILE:HG12	2.01	0.41
2:B:1:NAG:H62	2:B:2:NAG:N2	2.35	0.41
1:I:91:LYS:HE2	1:I:103:MET:SD	2.61	0.41
1:L:223:GLY:O	1:L:379:GLY:HA3	2.21	0.41
1:L:322:ARG:HD2	1:L:377:GLU:OE1	2.20	0.41
1:L:57:ARG:HB3	1:L:107:LYS:HG3	2.03	0.41
1:I:201:VAL:HG22	8:I:2008:HOH:O	2.21	0.40
1:I:281:MET:HE1	1:I:320:MET:HE1	2.04	0.40
1:L:112:SER:O	1:L:113:GLU:C	2.65	0.40
1:L:113:GLU:HB3	1:L:118:GLN:OE1	2.21	0.40
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	399/432 (92%)	373 (94%)	21 (5%)	5 (1%)	9	21
1	L	408/432 (94%)	380 (93%)	21 (5%)	7 (2%)	7	15
All	All	807/864 (93%)	753 (93%)	42 (5%)	12 (2%)	8	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	13	ARG
1	I	112	SER
1	I	19	PRO
1	I	115	THR
1	L	138	SER
1	I	136	LYS
1	L	17	MET
1	L	133	LYS
1	L	136	LYS
1	L	137	SER
1	L	397	PRO
1	I	407	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	I	347/383 (91%)	321 (92%)	26 (8%)	12	28
1	L	349/383 (91%)	323 (93%)	26 (7%)	13	29
All	All	696/766 (91%)	644 (92%)	52 (8%)	12	28

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	53	LYS

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Mol	Chain	Res	Type
1	I	78	LEU
1	I	102	LEU
1	I	113	GLU
1	I	118	GLN
1	I	132	ARG
1	I	138	SER
1	I	144	ASN
1	I	156	GLU
1	I	157	THR
1	I	199	THR
1	I	201	VAL
1	I	202	ILE
1	I	212	VAL
1	I	213	LEU
1	I	284	ILE
1	I	300	THR
1	I	302	GLU
1	I	304	LEU
1	I	314	MET
1	I	347	GLU
1	I	350	LYS
1	I	351	LEU
1	I	355	VAL
1	I	366	ASP
1	I	385	SER
1	L	9	THR
1	L	47	ARG
1	L	68	ASP
1	L	91	LYS
1	L	118	GLN
1	L	119	ILE
1	L	135	ASN
1	L	137	SER
1	L	138	SER
1	L	177	GLU
1	L	182	SER
1	L	199	THR
1	L	201	VAL
1	L	209	GLU
1	L	210	LEU
1	L	222	LYS
1	L	237	GLU

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Mol	Chain	Res	Type
1	L	285	LEU
1	L	302	GLU
1	L	314	MET
1	L	320	MET
1	L	324	ARG
1	L	331	LEU
1	L	405	ASN
1	L	410	VAL
1	L	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	144	ASN
1	I	159	GLN
1	I	254	GLN
1	I	334	GLN
1	L	55	ASN
1	L	71	ASN
1	L	144	ASN
1	L	217	ASN
1	L	254	GLN
1	L	336	GLN
1	L	405	ASN
1	L	428	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1	1,2	14,14,15	1.29	1 (7%)	17,19,21	1.33	2 (11%)
2	NAG	A	2	2	14,14,15	1.29	1 (7%)	17,19,21	1.75	2 (11%)
2	NAG	B	1	1,2	14,14,15	1.30	1 (7%)	17,19,21	1.26	2 (11%)
2	NAG	B	2	2	14,14,15	1.29	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	C	1	1,3	14,14,15	1.40	1 (7%)	17,19,21	1.44	2 (11%)
3	NAG	C	2	3	14,14,15	1.31	1 (7%)	17,19,21	1.23	1 (5%)
3	BMA	C	3	3	11,11,12	1.00	1 (9%)	15,15,17	1.03	1 (6%)
2	NAG	D	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	1.31	2 (11%)
2	NAG	D	2	2	14,14,15	1.29	1 (7%)	17,19,21	1.27	2 (11%)
2	NAG	E	1	1,2	14,14,15	1.44	2 (14%)	17,19,21	1.76	3 (17%)
2	NAG	E	2	2	14,14,15	1.30	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	F	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	2.38	4 (23%)
4	NAG	F	2	4	14,14,15	1.33	1 (7%)	17,19,21	1.90	5 (29%)
4	BMA	F	3	4	11,11,12	1.66	4 (36%)	15,15,17	3.19	6 (40%)
4	MAN	F	4	4	11,11,12	0.97	1 (9%)	15,15,17	1.11	0
4	MAN	F	5	4	11,11,12	0.96	0	15,15,17	1.43	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	1/1/1/1
4	MAN	F	5	4	-	2/2/19/22	1/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O7-C7	-3.89	1.14	1.23
2	A	2	NAG	O7-C7	-3.87	1.14	1.23
2	A	1	NAG	O7-C7	-3.87	1.14	1.23
3	C	2	NAG	O7-C7	-3.86	1.14	1.23
2	E	1	NAG	O7-C7	-3.84	1.14	1.23
4	F	2	NAG	O7-C7	-3.82	1.14	1.23
2	D	1	NAG	O7-C7	-3.82	1.14	1.23
2	B	2	NAG	O7-C7	-3.81	1.14	1.23
3	C	1	NAG	O7-C7	-3.80	1.14	1.23
2	B	1	NAG	O7-C7	-3.79	1.14	1.23
4	F	1	NAG	O7-C7	-3.79	1.14	1.23
2	E	2	NAG	O7-C7	-3.71	1.14	1.23
2	E	1	NAG	O5-C1	2.87	1.48	1.43
4	F	3	BMA	C1-C2	2.73	1.58	1.52
4	F	3	BMA	C4-C5	2.72	1.58	1.53
3	C	3	BMA	C1-C2	2.51	1.58	1.52
4	F	4	MAN	C1-C2	2.41	1.58	1.52
4	F	1	NAG	O5-C1	2.33	1.47	1.43
4	F	3	BMA	O2-C2	-2.32	1.38	1.43
4	F	3	BMA	C2-C3	2.12	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	C1-C2-C3	-7.71	98.41	109.64
4	F	1	NAG	C1-O5-C5	-7.21	102.52	112.19
4	F	3	BMA	O3-C3-C4	6.37	125.39	110.38
2	A	2	NAG	C2-N2-C7	5.59	130.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	-4.67	104.06	111.29
3	C	1	NAG	O5-C1-C2	-4.60	104.17	111.29
4	F	1	NAG	O5-C1-C2	-4.57	104.22	111.29
4	F	3	BMA	C3-C4-C5	-4.51	102.05	110.23
4	F	2	NAG	C2-N2-C7	4.47	128.88	122.90
2	B	1	NAG	O5-C1-C2	-4.24	104.73	111.29
2	A	1	NAG	O5-C1-C2	-4.15	104.88	111.29
2	E	1	NAG	C1-O5-C5	-4.06	106.74	112.19
2	D	1	NAG	O5-C1-C2	-4.00	105.11	111.29
3	C	2	NAG	O5-C1-C2	-3.70	105.57	111.29
2	D	2	NAG	O5-C1-C2	-3.62	105.69	111.29
4	F	5	MAN	C1-O5-C5	3.56	116.95	112.19
2	E	2	NAG	O5-C1-C2	-3.38	106.06	111.29
2	B	2	NAG	C6-C5-C4	-3.34	104.82	113.02
4	F	2	NAG	O5-C1-C2	-3.33	106.14	111.29
4	F	3	BMA	O5-C1-C2	-3.18	103.21	110.79
4	F	2	NAG	C3-C4-C5	3.13	115.91	110.23
2	B	2	NAG	C1-O5-C5	3.08	116.31	112.19
2	A	2	NAG	O5-C1-C2	-3.06	106.55	111.29
4	F	2	NAG	C4-C3-C2	2.74	115.04	111.02
4	F	1	NAG	C1-C2-N2	2.68	114.66	110.43
2	B	2	NAG	O5-C1-C2	-2.68	107.15	111.29
4	F	3	BMA	O4-C4-C3	2.62	116.55	110.38
4	F	1	NAG	C3-C4-C5	2.59	114.93	110.23
2	E	1	NAG	C1-C2-N2	2.45	114.29	110.43
4	F	2	NAG	O4-C4-C3	-2.39	104.75	110.38
2	D	2	NAG	C2-N2-C7	2.25	125.92	122.90
4	F	5	MAN	O5-C5-C6	2.25	112.04	107.66
3	C	1	NAG	C4-C3-C2	-2.22	107.77	111.02
2	A	1	NAG	C2-N2-C7	2.17	125.80	122.90
2	D	1	NAG	C1-O5-C5	-2.15	109.30	112.19
3	C	3	BMA	C1-C2-C3	-2.12	106.56	109.64
2	B	1	NAG	C4-C3-C2	-2.11	107.92	111.02
2	E	2	NAG	C1-O5-C5	2.10	115.00	112.19
4	F	3	BMA	O5-C5-C6	2.09	111.72	107.66

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C1-C2-N2-C7
2	A	2	NAG	C3-C2-N2-C7

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

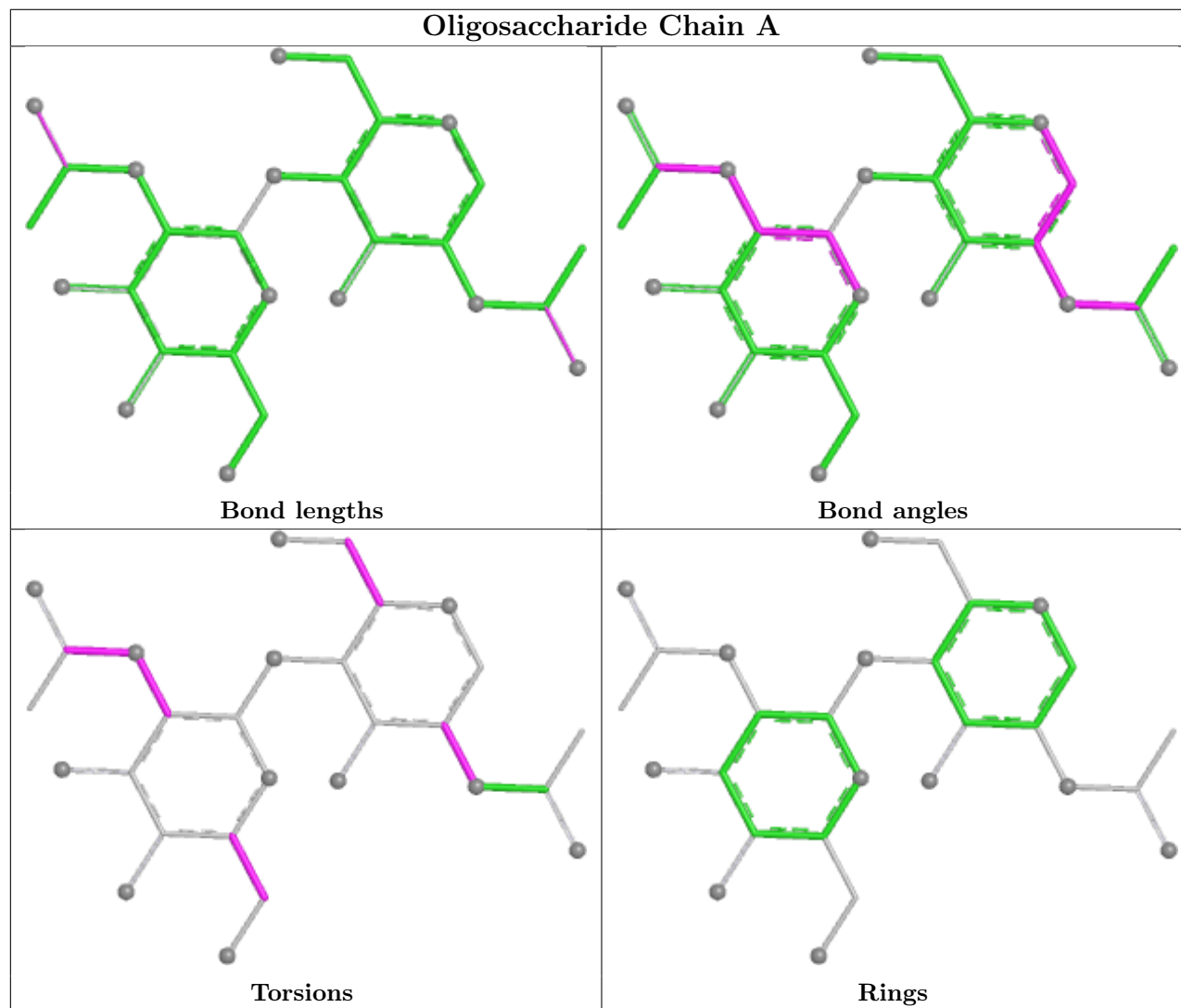
All (2) ring outliers are listed below:

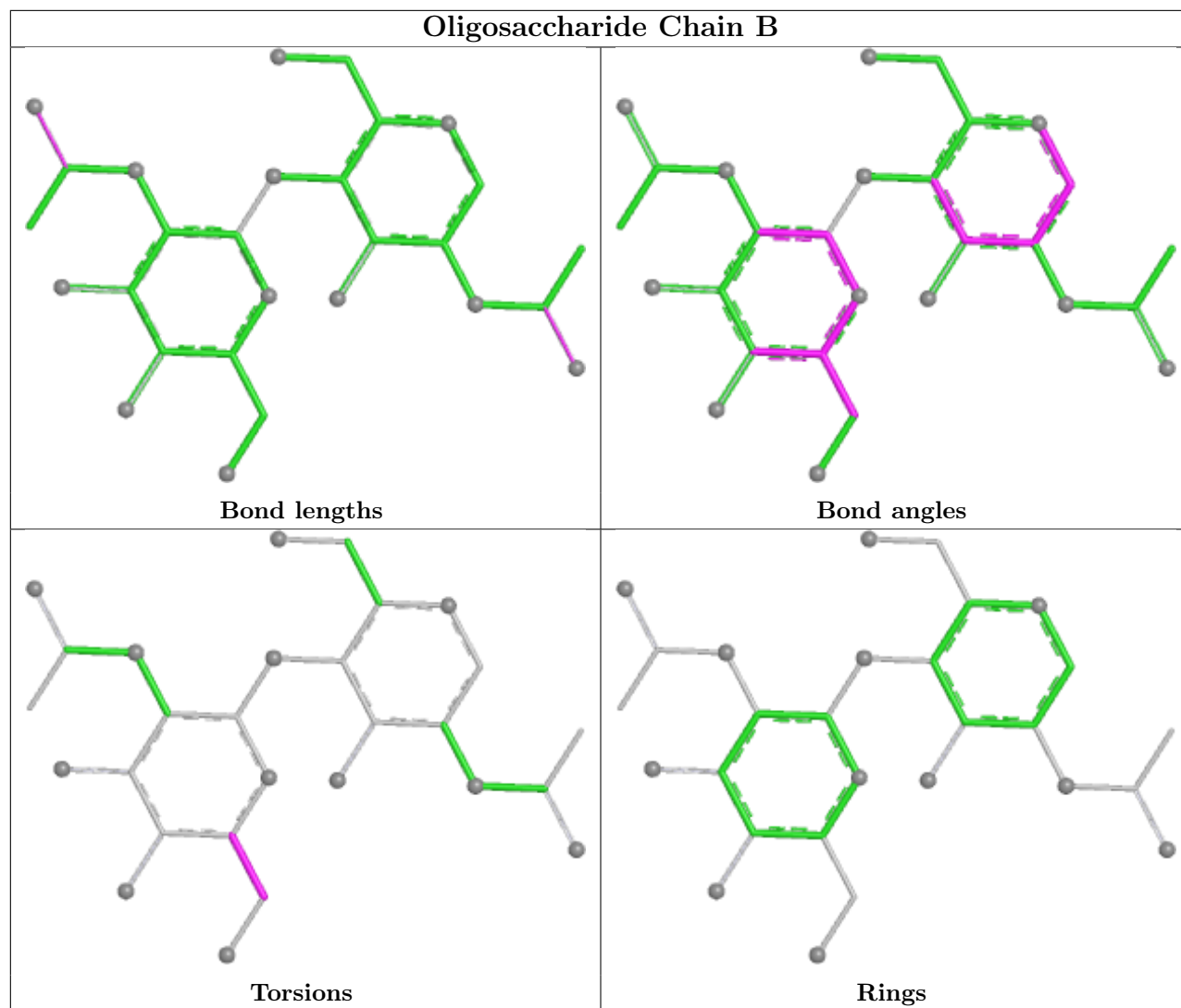
Mol	Chain	Res	Type	Atoms
4	F	5	MAN	C1-C2-C3-C4-C5-O5
4	F	4	MAN	C1-C2-C3-C4-C5-O5

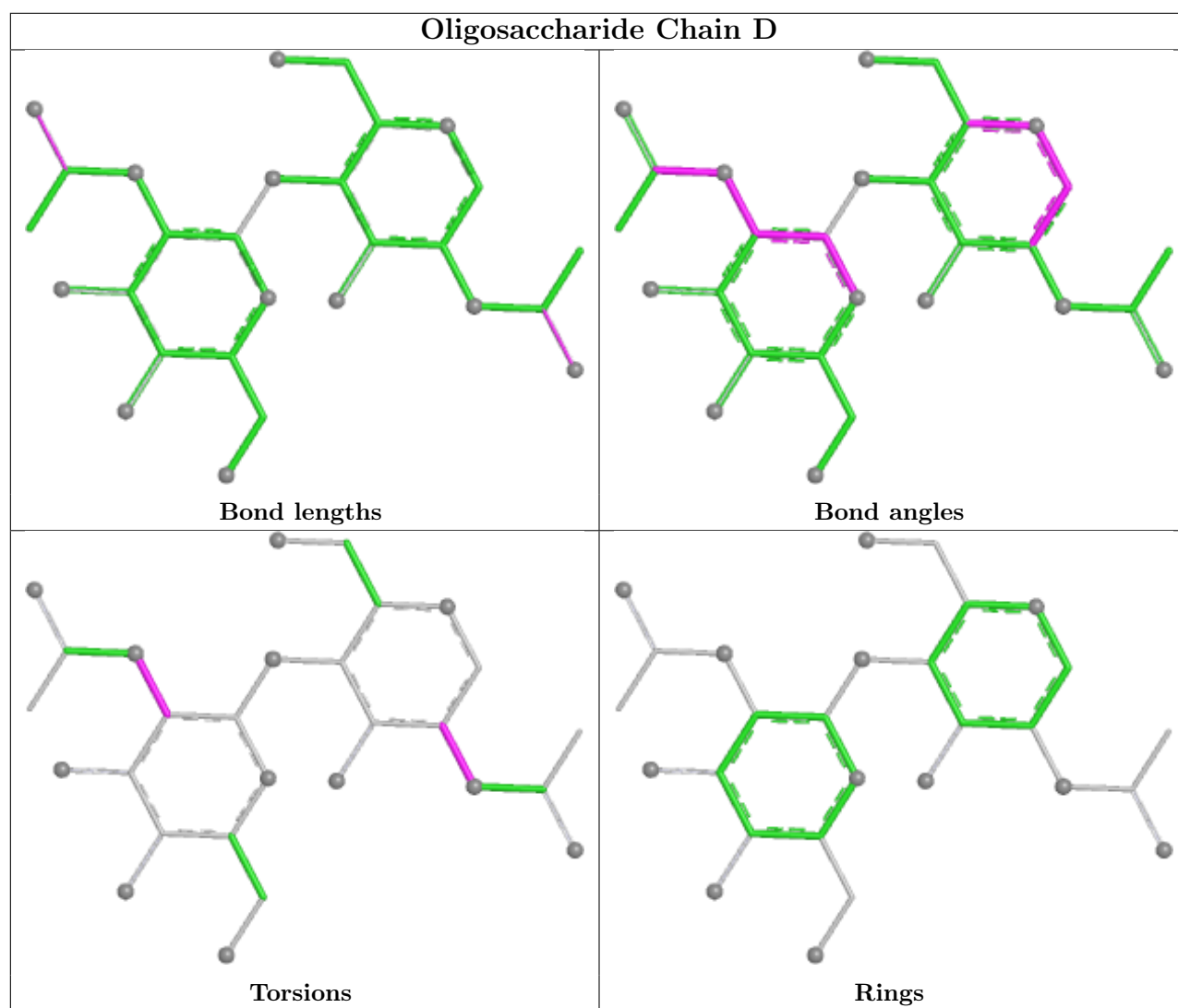
5 monomers are involved in 4 short contacts:

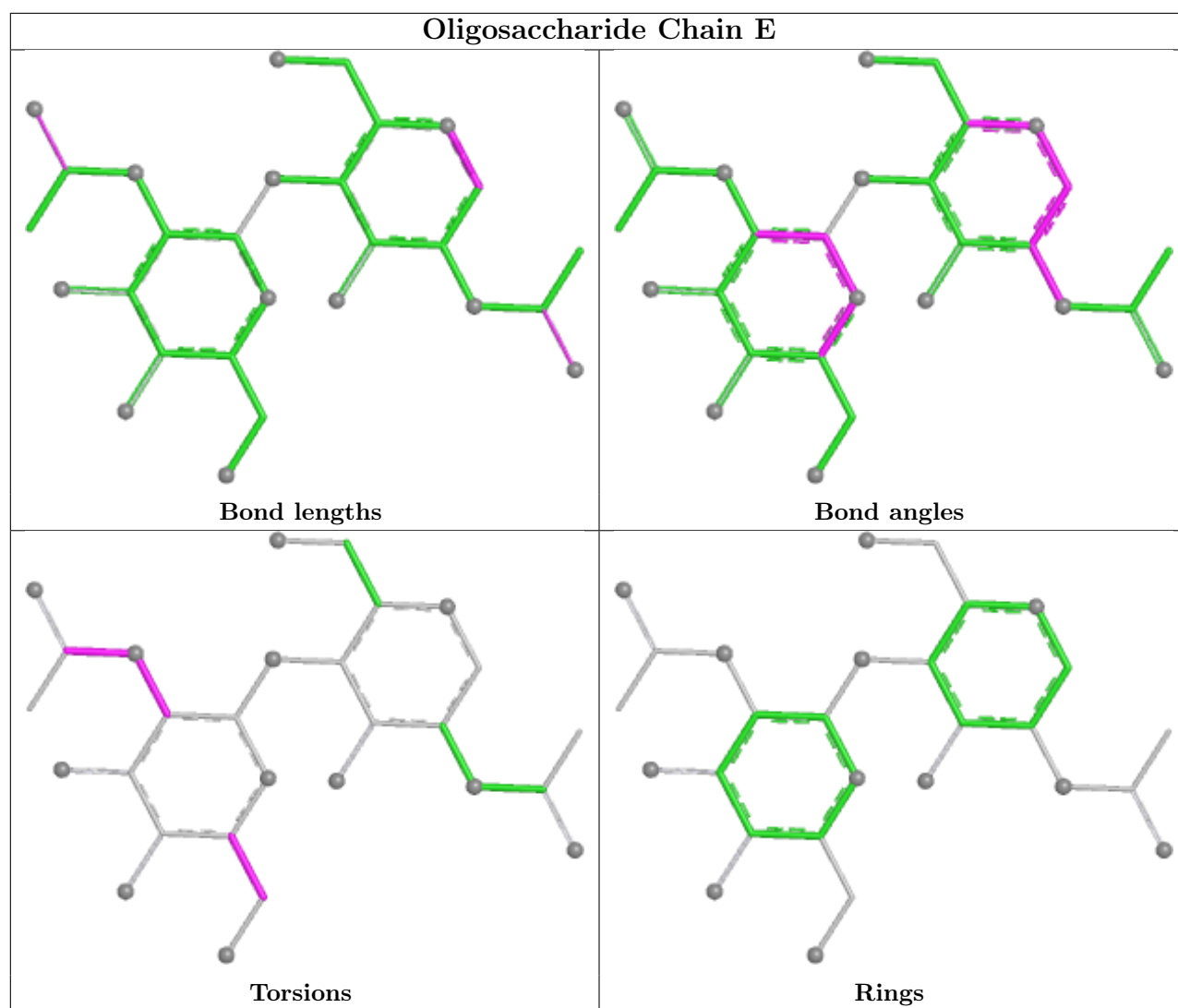
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	E	2	NAG	2	0
2	A	2	NAG	1	0
2	B	1	NAG	1	0
2	A	1	NAG	1	0

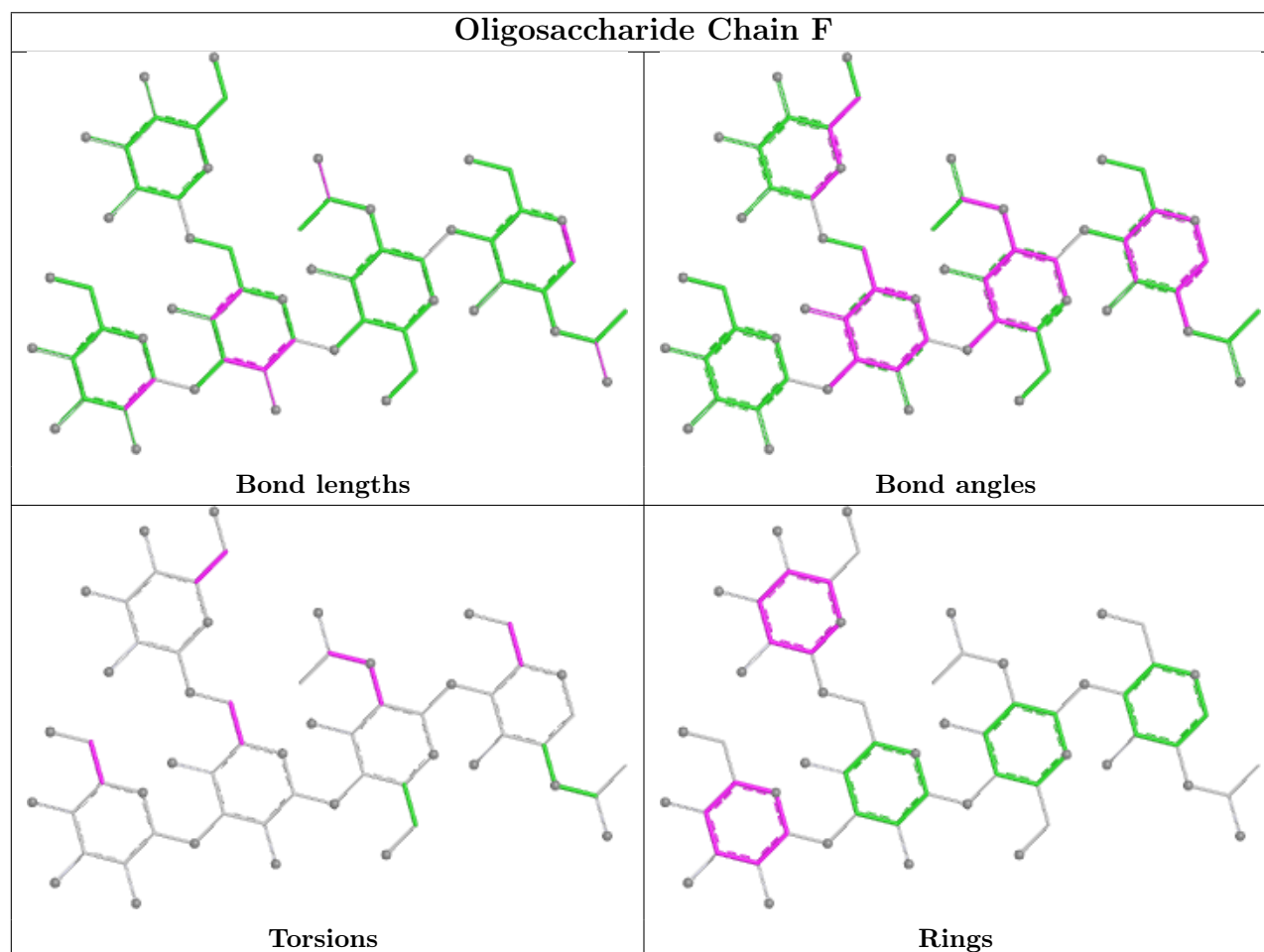
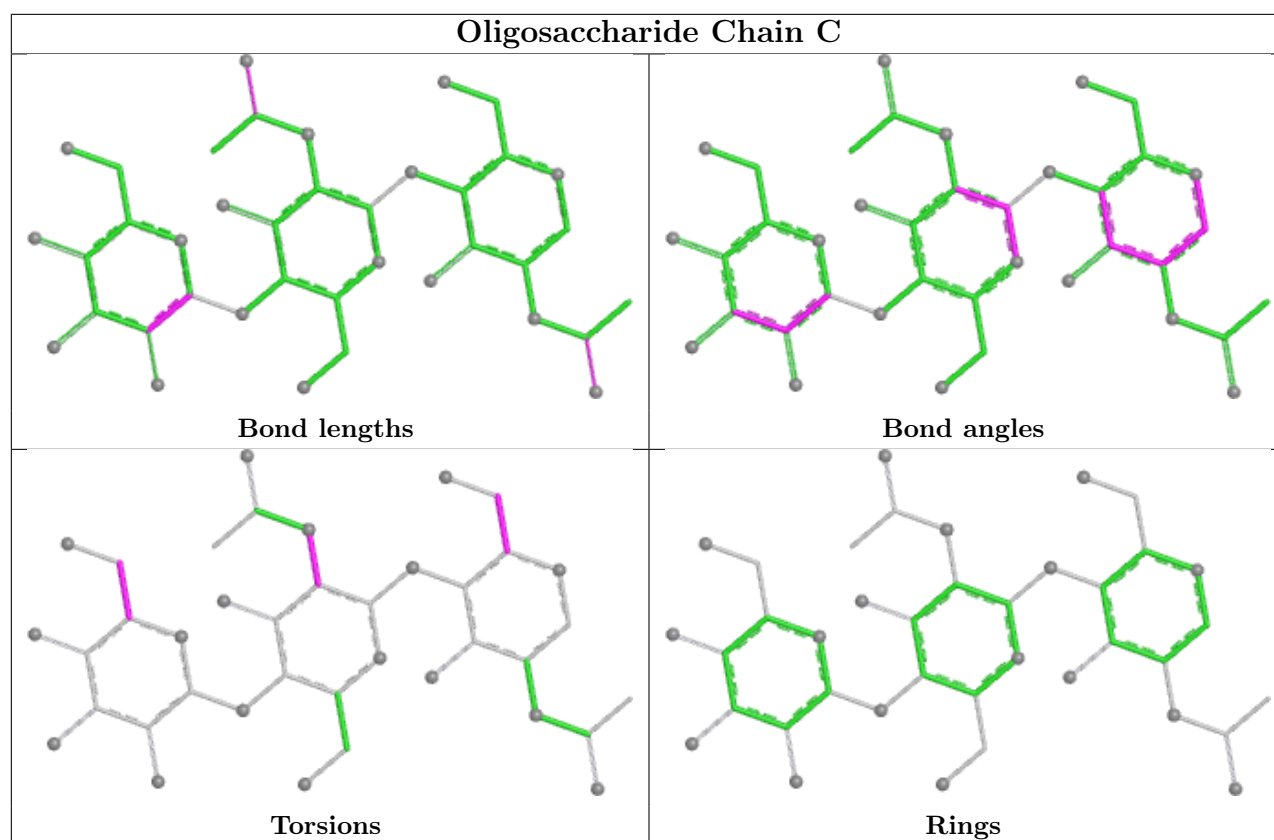
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

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	$\# Z > 2$
7	PO4	L	811	-	4,4,4	0.99	0	6,6,6	0.59	0
5	MAN	I	803	-	11,11,12	0.82	0	15,15,17	0.89	0
6	GOL	I	809	-	5,5,5	0.77	0	5,5,5	0.44	0
6	GOL	L	810	-	5,5,5	0.79	0	5,5,5	0.45	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
5	MAN	I	803	-	-	2/2/19/22	1/1/1/1
6	GOL	I	809	-	-	1/4/4/4	-
6	GOL	L	810	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	803	MAN	O5-C5-C6-O6
5	I	803	MAN	C4-C5-C6-O6
6	I	809	GOL	C1-C2-C3-O3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	803	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	810	GOL	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	I	403/432 (93%)	-0.07	8 (1%) 65 60	26, 45, 82, 127	0
1	L	412/432 (95%)	-0.01	15 (3%) 46 40	26, 47, 98, 120	0
All	All	815/864 (94%)	-0.04	23 (2%) 55 49	26, 45, 95, 127	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	19	PRO	4.6
1	L	264	ALA	4.2
1	I	134	ALA	3.3
1	I	17	MET	3.1
1	I	20	MET	2.9
1	L	24	ARG	2.9
1	L	357	GLU	2.8
1	L	400	VAL	2.8
1	L	402	PHE	2.8
1	L	358	GLY	2.8
1	I	431	VAL	2.7
1	L	16	PRO	2.6
1	L	42	GLU	2.6
1	L	399	ARG	2.5
1	L	401	THR	2.5
1	L	15	ILE	2.3
1	L	114	LYS	2.3
1	I	135	ASN	2.3
1	I	137	SER	2.2
1	L	44	THR	2.2
1	L	113	GLU	2.1
1	I	112	SER	2.0
1	L	112	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

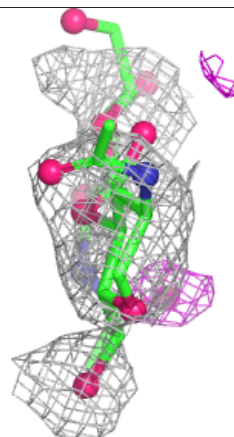
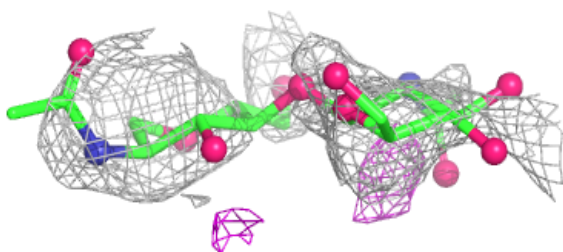
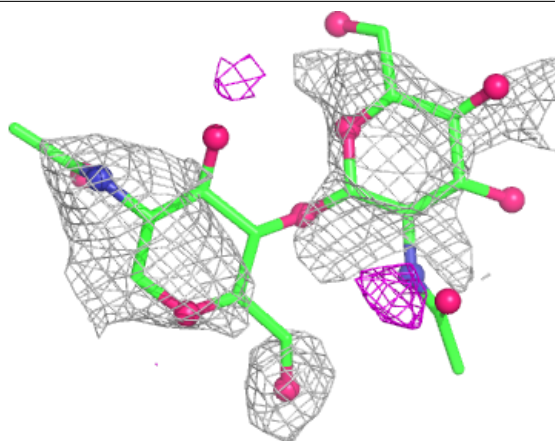
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	105,110,118,124	0
2	NAG	A	2	14/15	-	-	129,133,136,136	0
2	NAG	B	1	14/15	-	-	67,73,83,91	0
2	NAG	B	2	14/15	-	-	96,102,103,103	0
2	NAG	E	1	14/15	0.27	0.19	99,106,113,121	0
2	NAG	E	2	14/15	0.33	0.23	126,129,130,131	0
3	NAG	C	1	14/15	0.51	0.17	120,129,134,141	0
3	NAG	C	2	14/15	0.51	0.16	146,150,151,153	0
4	NAG	F	2	14/15	0.56	0.17	117,120,126,131	0
4	NAG	F	1	14/15	0.67	0.16	87,92,100,109	0
3	BMA	C	3	11/12	-	-	155,156,156,156	0
2	NAG	D	2	14/15	0.70	0.15	127,129,130,130	0
2	NAG	D	1	14/15	0.83	0.15	104,107,114,121	0
4	BMA	F	3	11/12	-	-	136,140,143,146	0
4	MAN	F	4	11/12	-	-	149,150,151,152	0
4	MAN	F	5	11/12	-	-	138,140,140,141	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

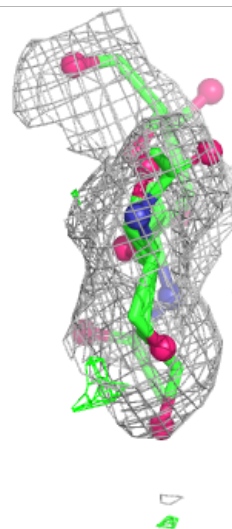
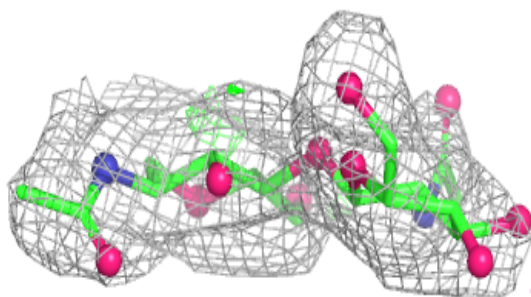
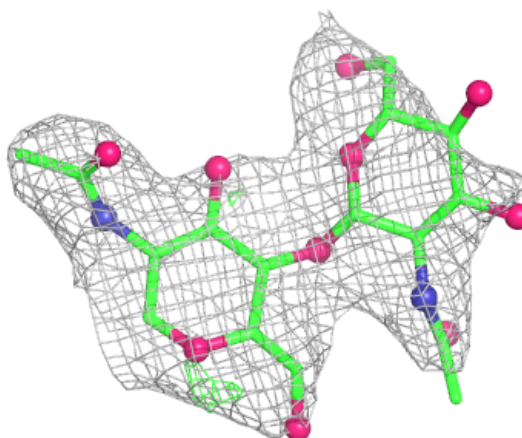
Electron density around Chain A:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



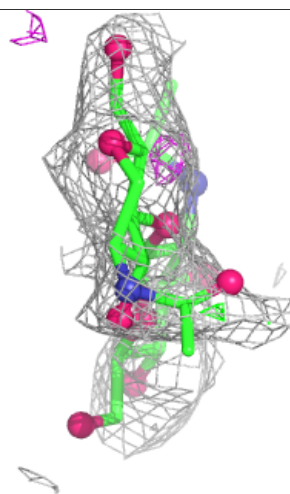
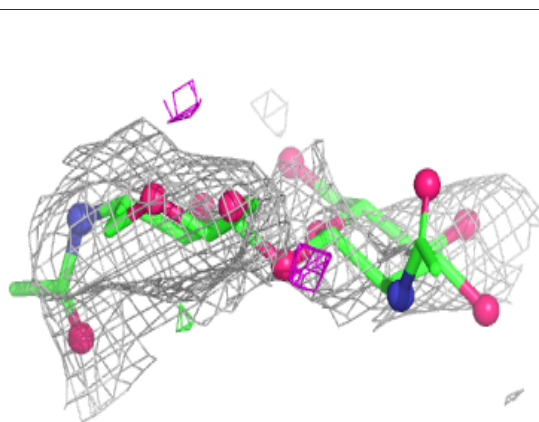
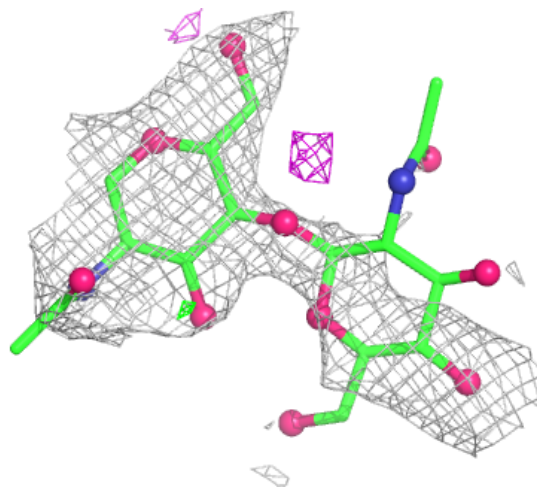
Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



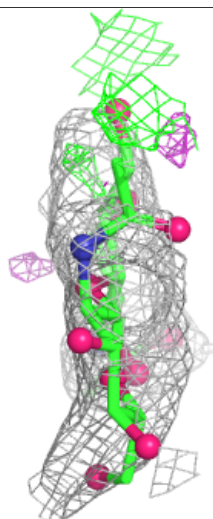
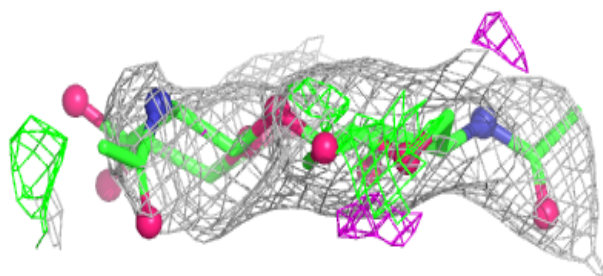
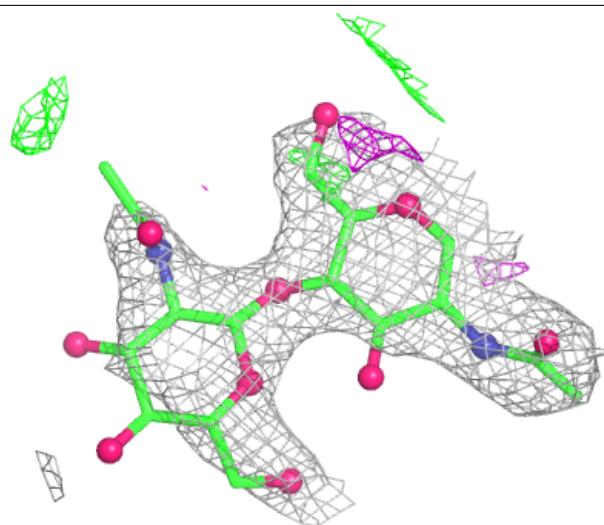
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



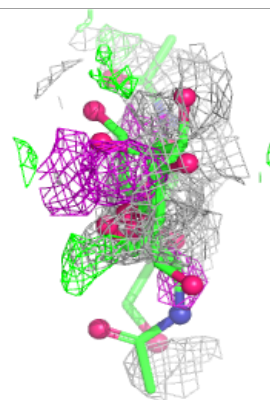
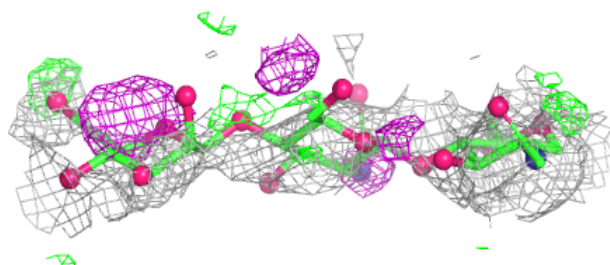
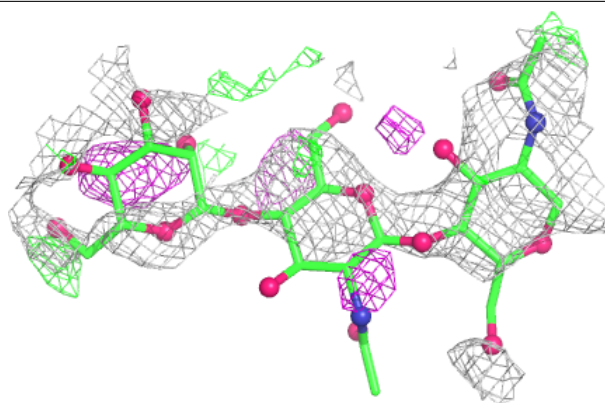
Electron density around Chain E:

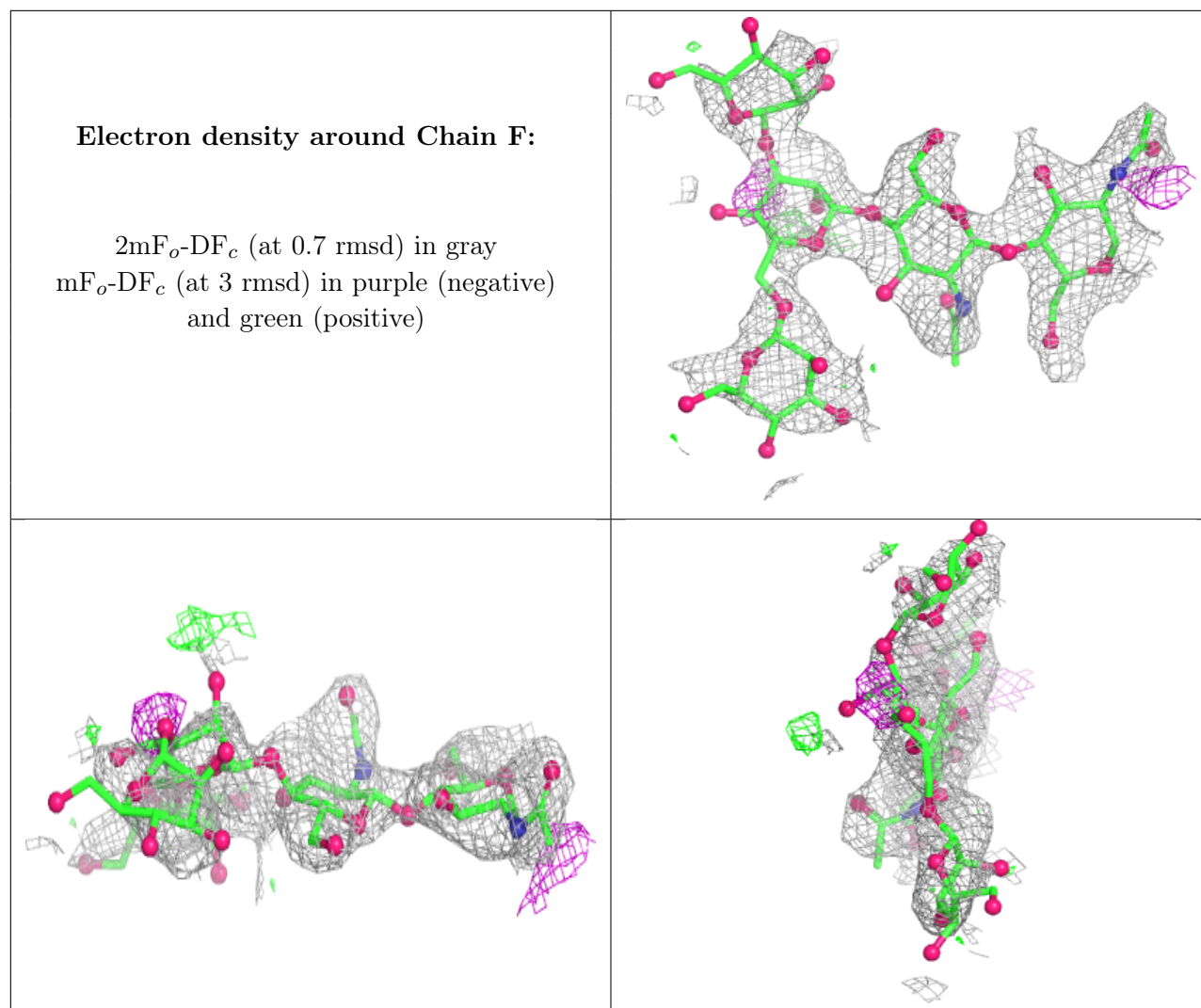
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	I	803	11/12	0.54	0.15	139,139,140,140	0
7	PO4	L	811	5/5	0.81	0.18	83,83,84,85	0
6	GOL	I	809	6/6	0.87	0.17	55,59,60,60	0
6	GOL	L	810	6/6	0.89	0.12	47,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.