



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:54 PM UTC

PDB ID : 1N1M / pdb_00001n1m
Title : Human Dipeptidyl Peptidase IV/CD26 in complex with an inhibitor
Authors : Rasmussen, H.B.; Branner, S.; Wiberg, F.C.; Wagtmann, N.R.
Deposited on : 2002-10-18
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)	:	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

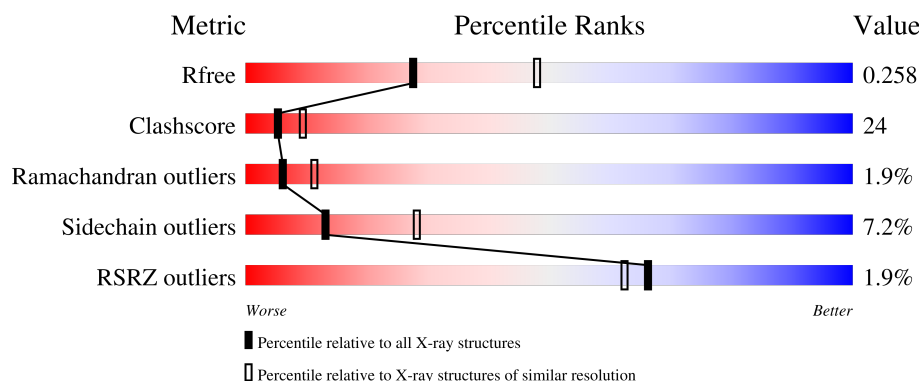
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



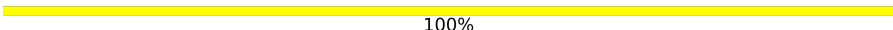
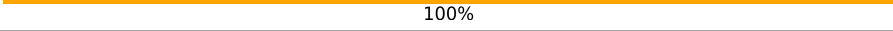
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	A	728	0.2% 60% 33% 7%
1	B	728	2% 56% 36% 7%
2	C	3	33% 67%
3	D	3	33% 67%
4	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 50% 50%
4	J	2	 50% 50%
5	F	3	 33% 67%
6	I	2	 50% 50%
7	K	3	 33% 67%
7	L	3	 67% 33%
8	M	2	 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	1	X	-	-	-
4	NAG	J	1	X	-	-	-
5	NDG	F	2	-	-	X	-
8	NAG	M	1	X	-	-	-
9	NAG	A	782	-	-	X	-

2 Entry composition [i](#)

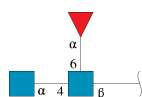
There are 12 unique types of molecules in this entry. The entry contains 13270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase IV SOLUBLE FORM.

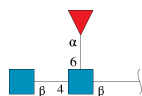
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

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



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

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



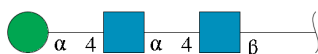
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



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

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



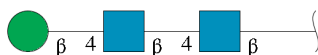
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 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.



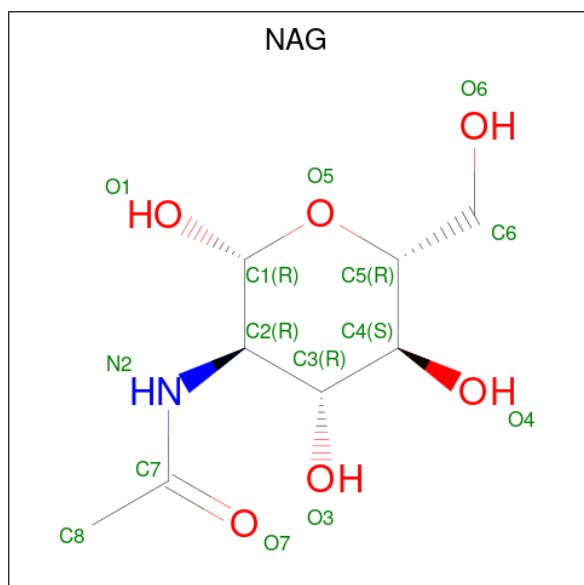
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

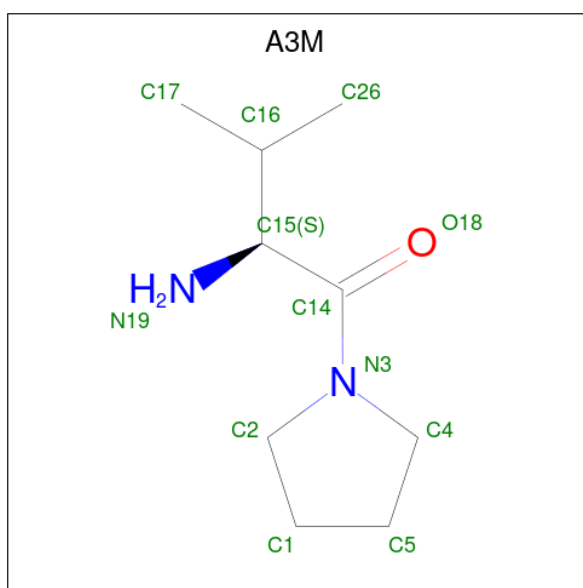


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Hg 2 2	0	0
10	B	2	Total Hg 2 2	0	0

- Molecule 11 is 2-AMINO-3-METHYL-1-PYRROLIDIN-1-YL-BUTAN-1-ONE (CCD ID: A3M) (formula: C₉H₁₈N₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 12 9 2 1	0	0
11	B	1	Total C N O 12 9 2 1	0	0

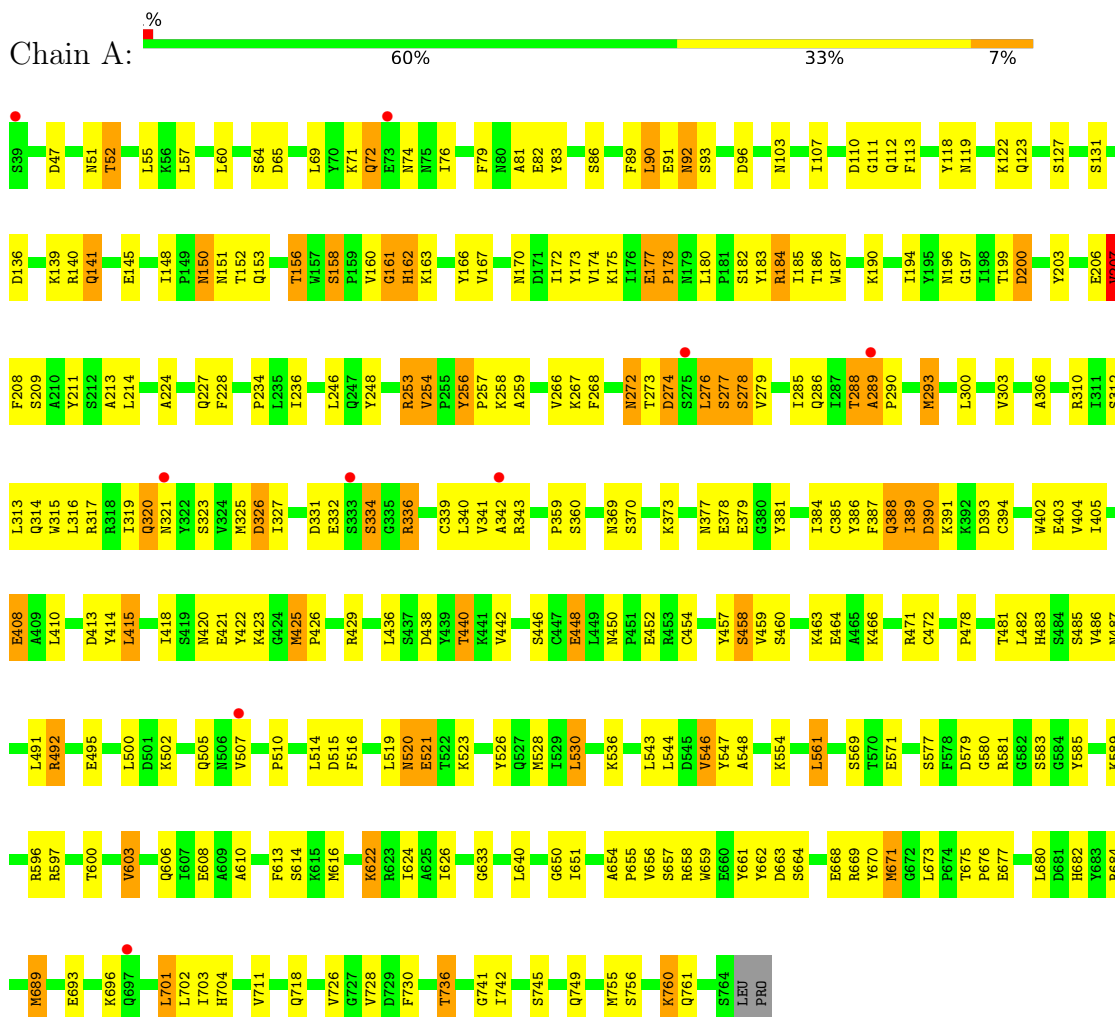
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	488	Total O 488 488	0	0
12	B	443	Total O 443 443	0	0

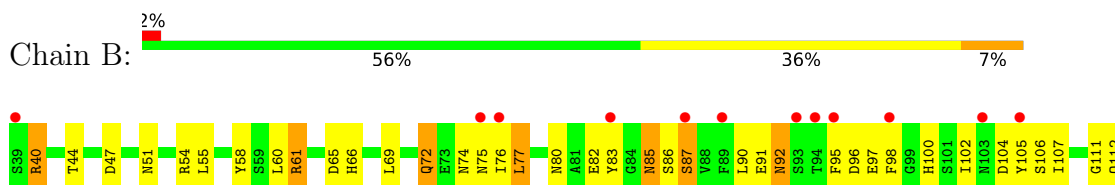
3 Residue-property plots

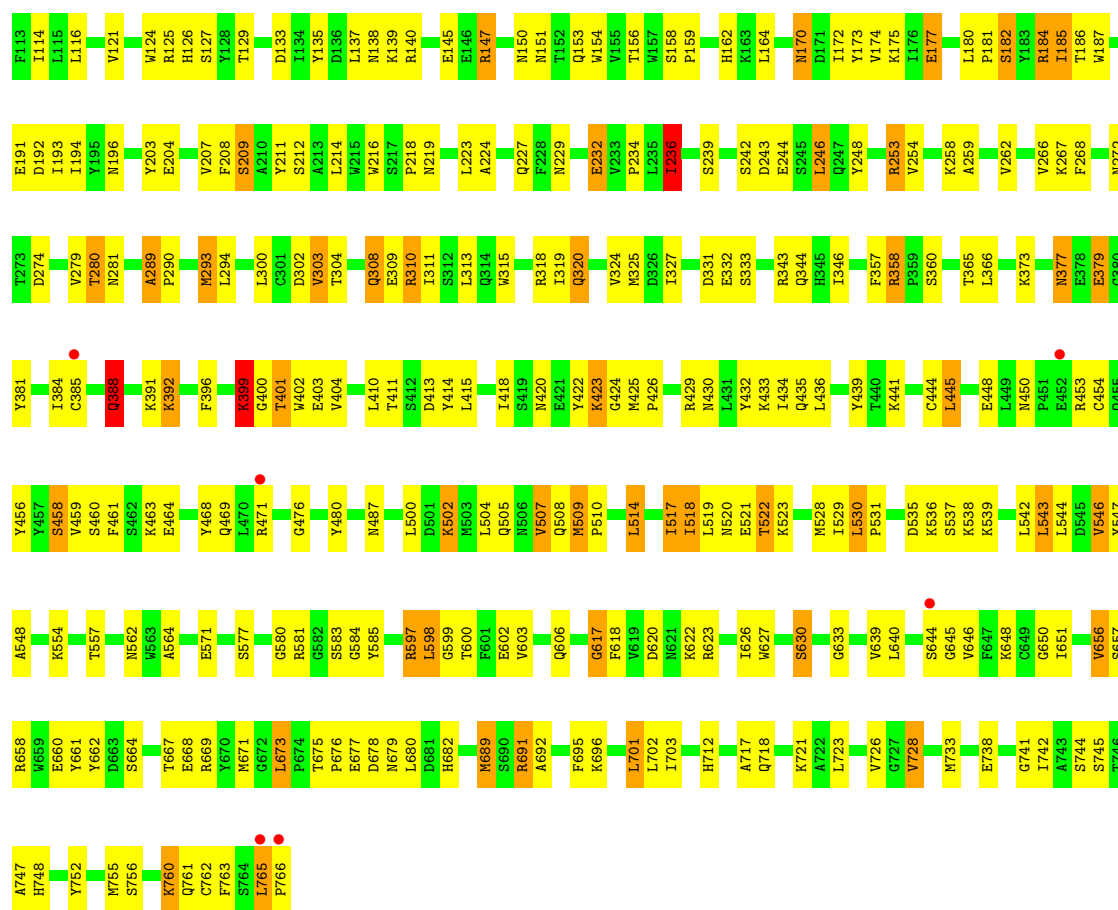
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase IV SOLUBLE FORM



• Molecule 1: Dipeptidyl peptidase IV SOLUBLE FORM





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

Chain C: 33% 67%



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

Chain D: 33% 67%



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

Chain E: 50% 50%



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

Chain G:  100%

NAG1
NAG2

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

Chain H:  50% 50%

NAG1
NAG2

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

Chain J:  50% 50%

NAG1
NAG2

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

Chain F:  33% 67%

NAG1
NDG2
MAN3

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

NAG1
FUC2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67%

NAG1
NAG2
EM13

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%



- Molecule 8: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 123.45Å 131.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.50 29.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.98-2.50) 87.3 (29.98-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.208 , 0.263 0.205 , 0.258	Depositor DCC
R_{free} test set	2987 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, MAN, NDG, HG, NAG, A3M

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	0.42	0/6119	0.98	35/8321 (0.4%)
1	B	0.41	0/6136	0.95	28/8344 (0.3%)
All	All	0.42	0/12255	0.97	63/16665 (0.4%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	LEU	CA-C-N	9.83	126.84	119.66
1	B	530	LEU	C-N-CA	9.83	126.84	119.66
1	A	160	VAL	N-CA-C	9.33	118.99	111.62
1	A	207	VAL	N-CA-C	8.53	119.38	111.45
1	B	91	GLU	N-CA-C	8.00	120.25	110.41
1	A	378	GLU	N-CA-C	-7.91	102.73	111.36
1	A	148	ILE	CA-C-N	7.89	127.95	119.90
1	A	148	ILE	C-N-CA	7.89	127.95	119.90
1	B	458	SER	N-CA-C	-7.69	97.62	109.24
1	B	401	THR	N-CA-C	7.29	120.98	109.39
1	B	425	MET	CA-C-N	7.24	126.94	119.56
1	B	425	MET	C-N-CA	7.24	126.94	119.56
1	A	425	MET	CA-C-N	7.06	126.77	119.56
1	A	425	MET	C-N-CA	7.06	126.77	119.56
1	A	206	GLU	N-CA-C	6.83	121.88	112.04
1	A	530	LEU	CA-C-N	6.81	124.63	119.66
1	A	530	LEU	C-N-CA	6.81	124.63	119.66
1	A	458	SER	N-CA-C	-6.71	99.10	109.24
1	B	399	LYS	N-CA-C	6.68	125.02	110.80
1	A	177	GLU	CA-C-N	6.62	128.12	119.84
1	A	177	GLU	C-N-CA	6.62	128.12	119.84
1	A	111	GLY	N-CA-C	-6.44	106.19	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	CYS	N-CA-C	6.37	118.79	108.41
1	A	288	THR	CB-CA-C	-6.29	106.53	114.40
1	B	236	ILE	N-CA-C	-6.29	99.31	108.87
1	A	448	GLU	N-CA-C	6.11	120.73	113.28
1	B	392	LYS	N-CA-C	6.07	119.52	111.75
1	B	617	GLY	N-CA-C	5.97	122.98	115.21
1	B	162	HIS	N-CA-C	5.91	118.00	110.61
1	B	546	VAL	N-CA-C	5.84	118.10	108.99
1	B	209	SER	N-CA-C	-5.81	105.77	112.86
1	B	656	VAL	N-CA-C	-5.78	100.10	108.71
1	A	279	VAL	N-CA-C	-5.71	106.25	111.67
1	A	633	GLY	N-CA-C	-5.68	105.50	112.77
1	B	158	SER	N-CA-C	-5.64	102.08	110.20
1	B	177	GLU	CA-C-N	5.63	126.00	119.47
1	B	177	GLU	C-N-CA	5.63	126.00	119.47
1	B	300	LEU	N-CA-C	-5.58	100.09	108.96
1	B	454	CYS	N-CA-C	5.56	117.92	108.02
1	A	450	ASN	CA-C-N	5.53	125.89	119.47
1	A	450	ASN	C-N-CA	5.53	125.89	119.47
1	A	158	SER	N-CA-C	-5.50	102.28	110.20
1	B	523	LYS	N-CA-C	5.49	118.58	109.46
1	A	274	ASP	N-CA-C	-5.48	106.60	113.72
1	A	200	ASP	N-CA-C	-5.40	102.75	110.59
1	A	360	SER	N-CA-C	5.38	117.48	110.43
1	A	656	VAL	N-CA-C	-5.32	100.78	108.87
1	A	162	HIS	N-CA-C	-5.28	104.63	111.71
1	A	492	ARG	N-CA-C	5.28	116.55	108.42
1	B	667	THR	N-CA-C	5.23	116.67	110.97
1	A	659	TRP	N-CA-C	5.22	118.43	111.75
1	B	450	ASN	CA-C-N	5.19	126.33	119.84
1	B	450	ASN	C-N-CA	5.19	126.33	119.84
1	A	671	MET	N-CA-C	5.17	119.73	113.38
1	A	546	VAL	N-CA-C	5.12	117.21	108.86
1	A	150	ASN	N-CA-C	-5.12	103.28	110.50
1	B	630	SER	CB-CA-C	-5.11	110.28	117.23
1	A	491	LEU	N-CA-C	5.10	117.24	111.02
1	A	548	ALA	N-CA-C	5.08	118.74	112.24
1	A	408	GLU	N-CA-C	5.07	119.55	112.90
1	B	319	ILE	N-CA-C	-5.07	99.39	107.15
1	B	633	GLY	N-CA-C	-5.07	106.35	112.49
1	B	388	GLN	N-CA-C	-5.00	100.36	108.52

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	5948	0	5657	260	0
1	B	5964	0	5673	302	0
2	C	38	0	33	2	0
3	D	38	0	34	7	0
4	E	28	0	25	0	0
4	G	28	0	25	1	0
4	H	28	0	25	2	0
4	J	28	0	25	4	0
5	F	39	0	33	11	0
6	I	24	0	22	2	0
7	K	39	0	34	0	0
7	L	39	0	34	1	0
8	M	28	0	24	4	0
9	A	14	0	13	8	0
9	B	28	0	26	4	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
11	A	12	0	18	2	0
11	B	12	0	18	3	0
12	A	488	0	0	15	0
12	B	443	0	0	29	0
All	All	13270	0	11719	581	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 24.

All (581) 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)
5:F:2:NDG:H6C2	5:F:3:MAN:H2	1.26	1.13
1:A:581:ARG:CZ	9:A:782:NAG:H61	1.81	1.08
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.40	1.02
1:B:172:ILE:HG22	1:B:185:ILE:HD11	1.42	1.00
8:M:1:NAG:H62	8:M:2:NDG:HA	1.25	0.98
1:B:203:TYR:CD2	1:B:207:VAL:HG21	2.01	0.95
1:B:61:ARG:HH22	1:B:107:ILE:H	1.17	0.93
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.31	0.93
1:B:72:GLN:HE21	1:B:77:LEU:HD21	1.30	0.92
1:B:308:GLN:HG3	4:J:1:NAG:H62	1.49	0.92
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.00	0.91
8:M:1:NAG:H62	8:M:2:NDG:N2	1.83	0.91
1:A:172:ILE:H	1:A:186:THR:HG22	1.35	0.91
1:A:110:ASP:HB3	1:A:112:GLN:HG3	1.53	0.90
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.53	0.90
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.69	0.90
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.69	0.89
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.04	0.88
1:A:172:ILE:H	1:A:186:THR:CG2	1.86	0.88
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.73	0.88
3:D:1:NAG:H4	3:D:2:NAG:HN2	1.36	0.88
1:A:276:LEU:H	1:A:276:LEU:HD23	1.39	0.87
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.39	0.86
1:B:756:SER:O	1:B:760:LYS:HG2	1.75	0.86
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.58	0.85
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.59	0.84
1:B:318:ARG:HD3	1:B:668:GLU:OE1	1.77	0.84
1:B:40:ARG:NH1	1:B:508:GLN:HG2	1.92	0.83
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.76	0.83
1:B:72:GLN:NE2	1:B:77:LEU:HD21	1.92	0.83
1:B:399:LYS:HB2	1:B:402:TRP:HZ2	1.45	0.81
1:B:399:LYS:HB2	1:B:402:TRP:CZ2	2.15	0.81
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.15	0.81
1:B:676:PRO:HG2	1:B:677:GLU:OE2	1.81	0.80
1:B:377:ASN:C	1:B:377:ASN:HD22	1.88	0.80
1:A:194:ILE:HD13	5:F:1:NAG:H82	1.62	0.80
9:A:782:NAG:H4	12:A:1109:HOH:O	1.82	0.80
5:F:2:NDG:H6C2	5:F:3:MAN:C2	2.11	0.78
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.82	0.78
1:A:736:THR:HG21	1:B:717:ALA:O	1.83	0.78
3:D:1:NAG:H4	3:D:2:NAG:N2	1.96	0.78
1:A:600:THR:O	1:A:603:VAL:HG13	1.85	0.77
1:A:289:ALA:HB2	12:A:1181:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.67	0.76
1:B:77:LEU:HD23	1:B:77:LEU:H	1.48	0.76
1:B:219:ASN:HB2	1:B:308:GLN:CD	2.12	0.75
1:A:293:MET:HE2	1:A:317:ARG:HG3	1.69	0.75
1:B:184:ARG:HD3	1:B:186:THR:O	1.87	0.75
1:A:253:ARG:HH22	1:B:253:ARG:HH22	0.85	0.74
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.68	0.74
1:B:60:LEU:HD13	1:B:469:GLN:OE1	1.87	0.73
1:B:121:VAL:HB	1:B:129:THR:CG2	2.19	0.73
1:B:644:SER:O	1:B:646:VAL:N	2.22	0.73
1:B:691:ARG:HD2	12:B:1156:HOH:O	1.88	0.73
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.70	0.72
1:A:613:PHE:O	1:A:616:MET:HB2	1.89	0.72
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.89	0.72
1:B:90:LEU:HD21	1:B:95:PHE:CE2	2.21	0.72
1:A:452:GLU:HG3	12:A:1410:HOH:O	1.88	0.72
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.55	0.72
1:A:203:TYR:HA	1:A:207:VAL:CG1	2.20	0.72
1:B:207:VAL:HG23	1:B:208:PHE:N	2.05	0.71
1:A:438:ASP:OD1	1:A:440:THR:HB	1.90	0.71
1:B:377:ASN:ND2	1:B:379:GLU:H	1.89	0.71
1:A:579:ASP:HB3	1:A:583:SER:OG	1.90	0.71
1:A:203:TYR:HA	1:A:207:VAL:HG12	1.72	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.71	0.71
1:B:308:GLN:HA	1:B:308:GLN:OE1	1.91	0.71
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.06	0.70
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.72	0.70
1:B:504:LEU:HD22	1:B:509:MET:CE	2.20	0.70
1:B:308:GLN:CG	4:J:1:NAG:H62	2.22	0.70
1:B:509:MET:HG3	1:B:510:PRO:HD2	1.74	0.69
1:B:327:ILE:HB	1:B:343:ARG:HG2	1.74	0.69
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.28	0.69
1:B:232:GLU:HB3	1:B:262:VAL:HG11	1.75	0.69
1:A:319:ILE:HG22	1:A:321:ASN:HB2	1.75	0.69
1:B:517:ILE:HG12	1:B:518:ILE:N	2.08	0.69
1:B:520:ASN:O	1:B:522:THR:HG22	1.94	0.68
1:B:77:LEU:HD23	1:B:77:LEU:N	2.09	0.68
1:B:170:ASN:N	1:B:170:ASN:HD22	1.91	0.68
1:A:82:GLU:HG2	12:A:1241:HOH:O	1.93	0.68
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:2:NDG:C6	5:F:3:MAN:H2	2.14	0.68
1:A:272:ASN:ND2	1:A:274:ASP:H	1.92	0.67
1:B:76:ILE:CG2	1:B:90:LEU:HB3	2.25	0.67
1:B:279:VAL:O	1:B:280:THR:HB	1.92	0.67
1:B:51:ASN:HD21	1:B:54:ARG:HD3	1.57	0.67
1:A:290:PRO:HG3	1:A:326:ASP:OD2	1.94	0.67
1:B:546:VAL:HG22	1:B:547:TYR:N	2.10	0.67
1:A:276:LEU:HD23	1:A:276:LEU:N	2.11	0.66
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.31	0.66
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.77	0.66
1:A:340:LEU:O	1:A:343:ARG:HB3	1.97	0.65
1:B:74:ASN:O	1:B:92:ASN:HA	1.95	0.65
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.31	0.65
1:A:289:ALA:CB	1:A:290:PRO:CA	2.75	0.65
1:B:74:ASN:HB3	1:B:92:ASN:OD1	1.97	0.65
1:B:522:THR:HG21	12:B:1153:HOH:O	1.94	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:B:121:VAL:HA	12:B:1250:HOH:O	1.96	0.65
1:A:194:ILE:CD1	5:F:1:NAG:H82	2.27	0.65
1:A:341:VAL:C	1:A:343:ARG:H	2.04	0.65
1:B:765:LEU:HB3	1:B:766:PRO:OXT	1.98	0.64
1:A:289:ALA:CB	1:A:290:PRO:HA	2.18	0.64
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.79	0.64
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.79	0.64
1:B:54:ARG:HD3	12:B:1321:HOH:O	1.98	0.64
1:B:528:MET:HE2	1:B:530:LEU:HD21	1.80	0.64
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.64
3:D:2:NAG:O7	3:D:2:NAG:C3	2.45	0.64
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.97	0.63
1:B:302:ASP:OD1	1:B:304:THR:HG23	1.98	0.63
1:B:402:TRP:HA	12:B:1148:HOH:O	1.98	0.63
1:B:86:SER:O	1:B:87:SER:HB2	1.98	0.63
1:B:502:LYS:O	1:B:505:GLN:HG2	1.98	0.63
3:D:2:NAG:O7	3:D:2:NAG:H3	1.97	0.63
5:F:2:NDG:O7	5:F:2:NDG:H3	1.97	0.63
1:A:520:ASN:O	1:A:521:GLU:HB2	1.97	0.63
1:B:112:GLN:HB3	1:B:138:ASN:ND2	2.13	0.63
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.79	0.63
1:A:47:ASP:HA	1:A:52:THR:HG23	1.80	0.62
1:A:203:TYR:CD2	1:A:207:VAL:HG11	2.34	0.62
1:B:279:VAL:HG23	1:B:280:THR:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.35	0.62
1:B:289:ALA:CB	1:B:290:PRO:HA	2.22	0.62
1:B:61:ARG:NH2	1:B:107:ILE:H	1.95	0.62
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.29	0.62
1:A:377:ASN:HB2	1:A:381:TYR:H	1.65	0.62
1:A:756:SER:O	1:A:760:LYS:HG2	2.00	0.61
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.35	0.61
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.63	0.61
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.97	0.61
1:B:280:THR:HG23	1:B:281:ASN:N	2.13	0.61
1:A:662:TYR:CE2	11:A:954:A3M:HC21	2.36	0.61
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.00	0.61
9:A:782:NAG:H62	12:A:1179:HOH:O	2.01	0.61
1:B:75:ASN:ND2	1:B:92:ASN:HB2	2.14	0.60
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.35	0.60
1:A:341:VAL:O	1:A:342:ALA:HB3	2.01	0.60
1:B:504:LEU:HD22	1:B:509:MET:HE2	1.81	0.60
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.46	0.60
9:A:782:NAG:O7	9:A:782:NAG:H3	2.00	0.60
1:B:765:LEU:CB	1:B:766:PRO:HA	2.32	0.60
1:B:147:ARG:HG3	12:B:1255:HOH:O	2.01	0.60
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.83	0.60
1:B:272:ASN:C	1:B:272:ASN:HD22	2.09	0.59
1:B:358:ARG:HD2	12:B:1229:HOH:O	2.01	0.59
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.38	0.59
1:A:334:SER:HB3	1:A:336:ARG:HD2	1.84	0.59
1:B:203:TYR:HA	1:B:207:VAL:HG22	1.84	0.59
1:B:571:GLU:OE1	1:B:765:LEU:HD22	2.02	0.59
1:B:744:SER:HB3	1:B:747:ALA:HB3	1.84	0.59
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.68	0.58
1:B:279:VAL:O	1:B:280:THR:CB	2.50	0.58
1:A:172:ILE:N	1:A:186:THR:HG22	2.14	0.58
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.85	0.58
1:B:332:GLU:OE2	4:J:2:NAG:H4	2.03	0.58
1:A:502:LYS:O	1:A:505:GLN:HG2	2.02	0.58
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.34	0.58
1:B:83:TYR:CE2	6:I:2:FUC:H4	2.38	0.58
1:B:207:VAL:CG2	1:B:208:PHE:N	2.66	0.58
1:B:344:GLN:HE21	1:B:346:ILE:HD11	1.68	0.58
1:A:170:ASN:N	1:A:170:ASN:HD22	2.01	0.58
1:A:662:TYR:CZ	11:A:954:A3M:HC21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:LEU:HD22	1:B:703:ILE:HG13	1.86	0.58
1:B:542:LEU:C	1:B:542:LEU:HD23	2.29	0.57
12:B:1359:HOH:O	7:L:3:BMA:H4	2.04	0.57
1:A:519:LEU:O	1:A:520:ASN:C	2.47	0.57
1:A:684:ARG:HG3	12:A:1149:HOH:O	2.04	0.57
1:B:504:LEU:HD22	1:B:509:MET:HE1	1.85	0.57
1:B:648:LYS:HD3	1:B:762:CYS:SG	2.43	0.57
1:B:172:ILE:HG22	1:B:185:ILE:CD1	2.25	0.57
1:A:92:ASN:HD22	1:A:93:SER:H	1.51	0.57
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.39	0.57
1:B:150:ASN:O	1:B:151:ASN:HB2	2.04	0.57
8:M:1:NAG:H4	8:M:2:NDG:H3	1.85	0.57
1:A:187:TRP:HE3	4:G:2:NAG:H83	1.69	0.57
3:D:1:NAG:H62	3:D:3:FUC:O2	2.04	0.57
1:B:154:TRP:NE1	1:B:156:THR:HG23	2.19	0.57
1:B:203:TYR:O	1:B:207:VAL:HG22	2.05	0.57
1:B:415:LEU:C	1:B:415:LEU:HD23	2.29	0.57
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.69	0.57
1:B:373:LYS:HE2	12:B:1374:HOH:O	2.05	0.57
1:B:546:VAL:CG2	1:B:547:TYR:N	2.68	0.57
1:B:280:THR:CG2	1:B:281:ASN:N	2.68	0.56
1:A:581:ARG:NH2	9:A:782:NAG:H61	2.20	0.56
1:B:121:VAL:HB	1:B:129:THR:HG23	1.87	0.56
1:B:293:MET:HE3	1:B:315:TRP:C	2.31	0.56
1:B:504:LEU:HD13	1:B:509:MET:HE2	1.87	0.56
1:B:358:ARG:NH1	12:B:956:HOH:O	2.36	0.56
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.88	0.56
1:A:580:GLY:O	1:A:583:SER:HB2	2.06	0.56
1:B:194:ILE:HD13	1:B:229:ASN:HA	1.87	0.56
1:A:528:MET:CE	1:A:530:LEU:HD21	2.35	0.56
1:A:236:ILE:HG22	1:A:254:VAL:O	2.06	0.56
1:A:293:MET:HE2	1:A:317:ARG:CG	2.34	0.56
1:A:272:ASN:HD22	1:A:274:ASP:H	1.54	0.56
1:B:121:VAL:HB	1:B:129:THR:HG22	1.87	0.56
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.88	0.56
1:A:150:ASN:O	1:A:151:ASN:HB2	2.06	0.56
1:B:58:TYR:HD1	1:B:60:LEU:HD11	1.71	0.56
1:B:154:TRP:HE1	1:B:156:THR:CG2	2.18	0.56
1:B:377:ASN:ND2	1:B:379:GLU:N	2.54	0.56
1:B:529:ILE:HD13	12:B:1174:HOH:O	2.06	0.56
1:A:312:SER:HB2	1:A:325:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LYS:HB2	1:A:622:LYS:NZ	2.20	0.55
1:B:69:LEU:HD11	1:B:107:ILE:HD12	1.87	0.55
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.54	0.55
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.55
5:F:2:NDG:O7	5:F:2:NDG:C3	2.54	0.55
1:A:175:LYS:NZ	1:A:182:SER:HB2	2.20	0.55
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.88	0.55
1:B:606:GLN:NE2	12:B:964:HOH:O	2.39	0.55
1:A:341:VAL:HG22	1:A:342:ALA:H	1.72	0.55
1:A:369:ASN:O	1:A:389:ILE:HG23	2.05	0.55
1:B:518:ILE:HD11	1:B:521:GLU:HA	1.88	0.55
1:B:75:ASN:HD21	1:B:92:ASN:HB2	1.71	0.55
1:B:765:LEU:HB3	1:B:766:PRO:CA	2.36	0.55
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.31	0.55
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.42	0.55
1:A:90:LEU:O	1:A:90:LEU:HD13	2.07	0.55
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.89	0.55
1:B:86:SER:O	1:B:87:SER:CB	2.56	0.54
1:B:718:GLN:HE22	1:B:721:LYS:HZ1	1.55	0.54
1:A:103:ASN:HB3	12:A:1436:HOH:O	2.07	0.54
1:B:518:ILE:HD13	1:B:518:ILE:C	2.32	0.54
1:A:174:VAL:HG23	1:A:185:ILE:HG13	1.89	0.54
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.43	0.54
1:B:765:LEU:CB	1:B:766:PRO:CA	2.85	0.54
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.89	0.54
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.06	0.54
1:B:358:ARG:HH11	1:B:358:ARG:CB	2.15	0.54
1:B:539:LYS:HE3	1:B:617:GLY:O	2.07	0.54
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.89	0.54
1:A:626:ILE:O	1:A:650:GLY:HA2	2.08	0.54
1:A:651:ILE:HG21	1:A:755:MET:CE	2.38	0.54
1:B:677:GLU:CD	1:B:677:GLU:H	2.16	0.54
1:B:413:ASP:HB3	1:B:414:TYR:HD1	1.72	0.53
1:B:487:ASN:HB2	12:B:1324:HOH:O	2.08	0.53
1:A:315:TRP:O	1:A:323:SER:HB2	2.08	0.53
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.90	0.53
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.43	0.53
1:B:147:ARG:HH11	1:B:147:ARG:HB3	1.74	0.53
1:A:65:ASP:HB2	1:A:464:GLU:HG2	1.90	0.53
1:A:658:ARG:HB3	1:A:689:MET:HE2	1.90	0.53
1:B:765:LEU:HB2	1:B:766:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.53
1:A:122:LYS:HG2	1:A:123:GLN:N	2.23	0.53
1:A:207:VAL:HG22	1:A:208:PHE:CD1	2.44	0.53
1:A:272:ASN:HD22	1:A:273:THR:N	2.06	0.53
1:A:597:ARG:HG3	1:A:600:THR:HG21	1.89	0.53
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.43	0.52
1:B:60:LEU:HD13	1:B:469:GLN:CD	2.34	0.52
1:B:154:TRP:NE1	1:B:156:THR:CG2	2.72	0.52
1:A:93:SER:HA	1:A:96:ASP:OD1	2.10	0.52
1:A:730:PHE:CZ	1:B:733:MET:HE1	2.44	0.52
1:B:528:MET:HE1	1:B:618:PHE:CE1	2.44	0.52
1:B:627:TRP:CZ3	1:B:755:MET:HE1	2.44	0.52
1:B:598:LEU:HB2	1:B:671:MET:SD	2.49	0.52
1:A:60:LEU:HD12	1:A:60:LEU:C	2.35	0.52
1:A:377:ASN:HB2	1:A:381:TYR:N	2.23	0.52
1:A:388:GLN:O	1:A:390:ASP:N	2.42	0.52
1:B:76:ILE:HG23	1:B:76:ILE:O	2.08	0.52
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.45	0.52
1:B:318:ARG:HG2	12:B:988:HOH:O	2.10	0.52
1:B:519:LEU:O	1:B:522:THR:HG23	2.10	0.52
1:B:692:ALA:O	1:B:695:PHE:HB2	2.09	0.52
1:A:314:GLN:NE2	1:A:373:LYS:NZ	2.58	0.52
1:B:344:GLN:NE2	12:B:1038:HOH:O	2.42	0.52
1:B:418:ILE:HA	1:B:430:ASN:O	2.10	0.52
1:A:286:GLN:HE21	1:A:288:THR:HG22	1.75	0.52
1:A:589:LYS:HB3	12:A:964:HOH:O	2.09	0.52
1:A:405:ILE:HG13	1:A:429:ARG:CD	2.40	0.51
1:B:311:ILE:HG12	1:B:313:LEU:CD1	2.40	0.51
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.46	0.51
1:B:662:TYR:CE2	11:B:955:A3M:HC21	2.45	0.51
1:A:276:LEU:HD23	12:A:1345:HOH:O	2.09	0.51
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.46	0.51
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.92	0.51
1:A:158:SER:CB	1:A:163:LYS:HB2	2.40	0.51
1:A:334:SER:HB3	1:A:336:ARG:CD	2.40	0.51
1:B:98:PHE:CD1	1:B:100:HIS:HB2	2.45	0.51
1:B:236:ILE:HG22	1:B:254:VAL:O	2.09	0.51
1:A:546:VAL:CG2	1:A:547:TYR:N	2.74	0.51
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.93	0.51
1:B:536:LYS:HG2	1:B:618:PHE:CD2	2.46	0.51
2:C:1:NAG:O3	2:C:2:NDG:C5	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:98:PHE:HB2	2.11	0.50
1:B:344:GLN:O	1:B:392:LYS:HE2	2.11	0.50
1:A:610:ALA:HA	1:A:613:PHE:HD2	1.77	0.50
1:B:207:VAL:HG23	1:B:208:PHE:CD1	2.46	0.50
1:B:360:SER:HB3	1:B:373:LYS:HZ2	1.76	0.50
1:B:528:MET:CE	1:B:530:LEU:HD21	2.40	0.50
1:A:745:SER:O	1:A:749:GLN:HG3	2.11	0.50
1:B:104:ASP:OD1	1:B:105:TYR:N	2.45	0.50
1:B:696:LYS:HD2	12:B:1382:HOH:O	2.11	0.50
1:B:181:PRO:HA	12:B:1378:HOH:O	2.12	0.50
1:B:207:VAL:CG2	1:B:208:PHE:H	2.25	0.50
1:B:289:ALA:HA	1:B:294:LEU:HG	1.94	0.50
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.94	0.50
1:B:520:ASN:HB2	9:B:780:NAG:H61	1.94	0.50
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.36	0.50
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.12	0.50
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.12	0.49
1:A:273:THR:O	1:A:276:LEU:HD21	2.11	0.49
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.47	0.49
1:B:528:MET:HE1	1:B:618:PHE:CZ	2.48	0.49
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.10	0.49
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.27	0.49
1:B:280:THR:HB	12:B:1091:HOH:O	2.13	0.49
1:B:630:SER:OG	11:B:955:A3M:HC42	2.12	0.49
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.43	0.49
1:B:599:GLY:H	1:B:602:GLU:CD	2.18	0.49
1:B:657:SER:HB2	1:B:689:MET:CE	2.43	0.49
1:A:664:SER:HB2	1:A:668:GLU:OE2	2.12	0.49
1:B:80:ASN:HB3	1:B:85:ASN:HB2	1.95	0.49
1:B:191:GLU:O	1:B:193:ILE:HG12	2.12	0.49
3:D:1:NAG:O6	3:D:2:NAG:H2	2.13	0.49
1:A:369:ASN:C	1:A:389:ILE:HG23	2.37	0.49
1:B:154:TRP:HE1	1:B:156:THR:HG23	1.77	0.49
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.47	0.49
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.94	0.49
1:B:696:LYS:HE3	12:B:1327:HOH:O	2.11	0.49
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.93	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.45	0.49
1:B:738:GLU:OE2	1:B:744:SER:HB2	2.13	0.49
1:B:538:LYS:HD3	1:B:539:LYS:N	2.28	0.49
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.46	0.48
1:B:597:ARG:HG3	1:B:600:THR:HG21	1.94	0.48
1:B:86:SER:O	6:I:1:NAG:H81	2.13	0.48
1:B:581:ARG:CZ	9:B:780:NAG:H5	2.43	0.48
1:B:671:MET:HE1	1:B:682:HIS:CD2	2.48	0.48
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.79	0.48
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.49	0.48
1:B:58:TYR:CD1	1:B:60:LEU:HD11	2.48	0.48
1:B:325:MET:CE	1:B:373:LYS:HD2	2.44	0.48
1:B:325:MET:HE1	1:B:373:LYS:HD2	1.95	0.48
1:A:314:GLN:HE22	1:A:373:LYS:HZ1	1.61	0.48
1:B:174:VAL:HG23	1:B:185:ILE:HD12	1.94	0.48
1:B:599:GLY:N	1:B:602:GLU:OE2	2.31	0.48
1:A:736:THR:HG23	12:B:957:HOH:O	2.14	0.48
1:B:203:TYR:CA	1:B:207:VAL:HG22	2.44	0.48
1:B:422:TYR:C	1:B:424:GLY:H	2.22	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.96	0.48
1:B:597:ARG:NH2	1:B:682:HIS:HB2	2.28	0.48
1:B:763:PHE:HB2	1:B:765:LEU:CD1	2.44	0.48
1:A:92:ASN:H	1:A:92:ASN:ND2	2.02	0.48
1:A:60:LEU:HD12	1:A:60:LEU:O	2.14	0.47
1:A:408:GLU:HG3	1:A:459:VAL:HG12	1.95	0.47
1:B:279:VAL:HG23	1:B:280:THR:N	2.28	0.47
1:B:453:ARG:HG3	1:B:476:GLY:HA3	1.95	0.47
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.49	0.47
1:A:197:GLY:C	1:A:213:ALA:HB3	2.39	0.47
1:A:341:VAL:HG22	1:A:342:ALA:N	2.28	0.47
1:A:581:ARG:NE	9:A:782:NAG:H61	2.25	0.47
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.48	0.47
1:A:458:SER:OG	1:A:471:ARG:HB2	2.15	0.47
1:B:420:ASN:ND2	1:B:426:PRO:HA	2.29	0.47
1:B:662:TYR:CZ	11:B:955:A3M:HC21	2.49	0.47
1:B:399:LYS:HB3	1:B:400:GLY:H	1.32	0.47
1:A:334:SER:CB	1:A:336:ARG:HD2	2.44	0.47
1:A:377:ASN:HB2	1:A:381:TYR:O	2.14	0.47
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.47
1:A:266:VAL:HG22	1:A:267:LYS:N	2.30	0.47
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.49	0.47
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.50	0.47
1:B:536:LYS:HG2	1:B:618:PHE:HD2	1.80	0.47
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.30	0.47
1:A:289:ALA:HB1	1:A:290:PRO:C	2.39	0.47
1:B:433:LYS:HB3	1:B:445:LEU:HD21	1.96	0.47
1:B:463:LYS:HE3	12:B:1305:HOH:O	2.14	0.47
1:A:675:THR:C	1:A:680:LEU:HB2	2.40	0.46
1:B:272:ASN:HD22	1:B:274:ASP:H	1.63	0.46
1:A:273:THR:HA	1:A:276:LEU:HD22	1.97	0.46
1:B:76:ILE:HG22	1:B:90:LEU:HB3	1.98	0.46
1:B:520:ASN:ND2	9:B:780:NAG:H4	2.31	0.46
1:B:562:ASN:HB2	12:B:994:HOH:O	2.15	0.46
1:B:192:ASP:O	1:B:193:ILE:HD13	2.15	0.46
1:B:544:LEU:HD21	1:B:606:GLN:HE21	1.79	0.46
1:A:671:MET:HE1	1:A:682:HIS:HD2	1.80	0.46
1:A:420:ASN:HB2	1:A:426:PRO:HA	1.98	0.46
1:B:429:ARG:HB3	1:B:456:TYR:HA	1.98	0.46
1:A:83:TYR:OH	2:C:3:FUC:H62	2.15	0.46
1:A:581:ARG:NH1	9:A:782:NAG:H61	2.28	0.46
1:A:657:SER:OG	1:A:689:MET:HE1	2.16	0.46
1:B:137:LEU:C	1:B:139:LYS:H	2.24	0.46
1:B:518:ILE:HD13	1:B:518:ILE:O	2.15	0.46
1:A:173:TYR:HB3	1:A:182:SER:OG	2.16	0.46
1:A:256:TYR:CD1	1:A:256:TYR:C	2.93	0.46
1:B:411:THR:HG22	12:B:1292:HOH:O	2.16	0.46
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.41	0.46
1:A:152:THR:HG23	1:A:167:VAL:O	2.16	0.46
1:A:689:MET:HG3	1:B:244:GLU:OE1	2.15	0.46
1:B:675:THR:C	1:B:680:LEU:HB2	2.41	0.46
1:B:293:MET:HG2	1:B:315:TRP:HB3	1.97	0.45
8:M:1:NAG:H62	8:M:2:NDG:C7	2.42	0.45
1:A:74:ASN:C	1:A:92:ASN:HB3	2.42	0.45
1:B:236:ILE:O	1:B:253:ARG:HA	2.16	0.45
1:B:266:VAL:HG22	1:B:267:LYS:N	2.30	0.45
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.97	0.45
1:A:207:VAL:HG22	1:A:208:PHE:HD1	1.80	0.45
1:B:671:MET:HE1	1:B:682:HIS:HD2	1.82	0.45
1:A:119:ASN:HD22	1:A:131:SER:CB	2.30	0.45
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.16	0.45
1:A:293:MET:CE	1:A:317:ARG:HG3	2.42	0.45
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.97	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.74	0.45
1:A:314:GLN:NE2	1:A:373:LYS:HZ1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:O	1:A:379:GLU:HG2	2.16	0.45
1:A:415:LEU:C	1:A:415:LEU:HD13	2.41	0.45
1:A:74:ASN:O	1:A:92:ASN:HB3	2.17	0.45
1:A:81:ALA:O	1:A:492:ARG:NH2	2.46	0.45
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.42	0.45
4:H:1:NAG:H4	4:H:2:NAG:H2	1.77	0.45
1:B:289:ALA:HB1	1:B:290:PRO:C	2.40	0.45
1:A:57:LEU:HD23	12:A:1127:HOH:O	2.17	0.45
1:A:614:SER:HB3	1:A:624:ILE:HD11	1.98	0.45
1:A:658:ARG:HD2	1:A:661:TYR:CE1	2.52	0.44
1:B:77:LEU:N	1:B:77:LEU:CD2	2.80	0.44
1:B:365:THR:O	1:B:366:LEU:C	2.60	0.44
1:B:657:SER:HB2	1:B:689:MET:HE1	1.99	0.44
1:A:93:SER:CB	1:A:96:ASP:OD2	2.65	0.44
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.53	0.44
1:A:341:VAL:C	1:A:343:ARG:N	2.71	0.44
1:A:614:SER:C	1:A:616:MET:H	2.24	0.44
1:A:277:SER:O	1:A:278:SER:HB3	2.17	0.44
1:B:102:ILE:HD12	1:B:116:LEU:HB3	2.00	0.44
1:B:246:LEU:HD13	1:B:248:TYR:O	2.18	0.44
1:A:571:GLU:CD	1:A:760:LYS:HE3	2.43	0.44
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.17	0.44
1:B:96:ASP:O	1:B:97:GLU:HB2	2.17	0.44
1:B:562:ASN:OD1	1:B:564:ALA:HB3	2.17	0.44
3:D:1:NAG:C4	3:D:2:NAG:N2	2.76	0.44
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.33	0.44
1:B:154:TRP:CZ2	1:B:212:SER:HB2	2.53	0.44
1:B:280:THR:CB	12:B:1091:HOH:O	2.64	0.44
1:A:76:ILE:HB	1:A:90:LEU:HD11	1.98	0.44
1:B:214:LEU:HD12	1:B:214:LEU:O	2.18	0.44
1:A:64:SER:C	1:A:463:LYS:HG2	2.43	0.44
1:A:161:GLY:HA3	12:A:1369:HOH:O	2.16	0.44
1:A:319:ILE:O	1:A:321:ASN:N	2.44	0.44
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.01	0.44
1:A:610:ALA:HA	1:A:613:PHE:CD2	2.53	0.44
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.33	0.44
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.43	0.44
1:B:366:LEU:HB2	12:B:1371:HOH:O	2.16	0.44
1:A:651:ILE:HG23	1:A:701:LEU:HB3	1.99	0.43
1:B:744:SER:HB3	1:B:747:ALA:CB	2.48	0.43
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:O	1:B:137:LEU:HD12	2.17	0.43
1:B:580:GLY:O	1:B:583:SER:OG	2.31	0.43
1:A:90:LEU:CD1	1:A:90:LEU:N	2.81	0.43
1:A:386:TYR:O	1:A:394:CYS:HB2	2.19	0.43
1:A:408:GLU:HG3	1:A:459:VAL:CG1	2.49	0.43
1:A:425:MET:HA	1:A:426:PRO:HD2	1.78	0.43
1:A:546:VAL:HG22	1:A:547:TYR:N	2.32	0.43
1:B:309:GLU:OE1	4:J:1:NAG:O6	2.35	0.43
1:B:648:LYS:HE2	1:B:762:CYS:O	2.19	0.43
1:B:742:ILE:O	1:B:742:ILE:HG22	2.17	0.43
1:A:495:GLU:HA	12:A:1210:HOH:O	2.17	0.43
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.00	0.43
1:B:218:PRO:HG2	1:B:308:GLN:OE1	2.18	0.43
1:B:765:LEU:HB3	1:B:766:PRO:C	2.44	0.43
1:A:704:HIS:CE1	1:A:711:VAL:O	2.71	0.43
1:B:471:ARG:HD2	12:B:1001:HOH:O	2.17	0.43
1:A:276:LEU:N	1:A:276:LEU:CD2	2.78	0.43
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.49	0.43
1:B:346:ILE:HD12	1:B:346:ILE:N	2.33	0.43
1:B:357:PHE:O	1:B:358:ARG:HB3	2.18	0.43
1:A:139:LYS:O	1:A:141:GLN:NE2	2.52	0.43
1:A:459:VAL:HG22	1:A:460:SER:N	2.33	0.43
1:A:673:LEU:N	1:A:673:LEU:HD12	2.33	0.43
1:B:58:TYR:HD1	1:B:60:LEU:CD1	2.31	0.43
1:B:75:ASN:ND2	12:B:1360:HOH:O	2.51	0.43
1:B:420:ASN:HD22	1:B:426:PRO:HA	1.83	0.43
5:F:1:NAG:H62	5:F:2:NDG:O5	2.19	0.43
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.43
1:A:651:ILE:HG23	1:A:701:LEU:HD13	2.00	0.43
1:A:388:GLN:CB	1:A:391:LYS:HD3	2.49	0.43
9:B:780:NAG:O7	9:B:780:NAG:C3	2.67	0.43
1:A:402:TRP:HA	12:A:987:HOH:O	2.18	0.43
1:A:689:MET:HG3	1:B:244:GLU:CD	2.44	0.43
1:B:124:TRP:CZ2	1:B:254:VAL:HG21	2.54	0.43
1:A:203:TYR:CD2	1:A:207:VAL:CG1	3.02	0.42
1:A:285:ILE:N	1:A:285:ILE:HD12	2.33	0.42
1:B:258:LYS:O	1:B:259:ALA:C	2.62	0.42
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.54	0.42
1:B:673:LEU:HD12	1:B:673:LEU:HA	1.77	0.42
1:B:748:HIS:CE1	1:B:752:TYR:CE2	3.07	0.42
1:A:199:THR:HA	1:A:228:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.20	0.42
1:B:434:ILE:HD11	1:B:439:TYR:HA	2.01	0.42
1:B:458:SER:OG	1:B:471:ARG:HB2	2.19	0.42
1:B:744:SER:O	1:B:745:SER:C	2.62	0.42
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.54	0.42
1:A:93:SER:HB2	1:A:96:ASP:OD2	2.19	0.42
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.34	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.19	0.42
5:F:1:NAG:C6	5:F:2:NDG:C1	2.97	0.42
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.55	0.42
1:B:331:ASP:C	1:B:333:SER:H	2.27	0.42
1:A:258:LYS:O	1:A:259:ALA:C	2.61	0.42
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.85	0.42
1:B:657:SER:CB	1:B:689:MET:HE1	2.50	0.42
1:A:200:ASP:OD1	1:A:200:ASP:C	2.63	0.42
1:A:402:TRP:CE3	1:A:421:GLU:HB2	2.54	0.42
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.54	0.42
1:B:303:VAL:O	1:B:303:VAL:HG22	2.19	0.42
1:A:520:ASN:OD1	9:A:782:NAG:O5	2.37	0.42
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.50	0.42
1:B:177:GLU:HB2	1:B:180:LEU:CG	2.49	0.42
1:B:381:TYR:CZ	1:B:401:THR:HG23	2.55	0.42
4:H:2:NAG:O7	4:H:2:NAG:H3	2.20	0.42
1:A:370:SER:HB2	1:A:387:PHE:O	2.20	0.42
1:A:174:VAL:HG23	1:A:185:ILE:CG1	2.50	0.42
1:A:314:GLN:HG3	1:A:325:MET:HG3	2.01	0.42
1:A:405:ILE:N	1:A:418:ILE:O	2.50	0.41
1:B:44:THR:HG1	1:B:47:ASP:CG	2.27	0.41
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.02	0.41
1:A:183:TYR:HE1	1:A:277:SER:O	2.02	0.41
1:B:622:LYS:O	1:B:623:ARG:HG3	2.20	0.41
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.19	0.41
1:B:471:ARG:HH11	1:B:480:TYR:HE2	1.68	0.41
1:B:504:LEU:HA	1:B:507:VAL:HG13	2.01	0.41
1:B:548:ALA:HA	12:B:1182:HOH:O	2.21	0.41
5:F:1:NAG:C6	5:F:2:NDG:O5	2.68	0.41
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.90	0.41
1:B:331:ASP:OD1	1:B:333:SER:HB3	2.20	0.41
1:A:89:PHE:O	1:A:90:LEU:HB3	2.20	0.41
1:A:190:LYS:HA	12:A:1046:HOH:O	2.20	0.41
1:A:316:LEU:HD11	1:A:320:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:N	1:A:670:TYR:O	2.49	0.41
1:B:139:LYS:HE2	1:B:139:LYS:HB3	1.92	0.41
1:B:459:VAL:HG22	1:B:460:SER:N	2.36	0.41
1:B:535:ASP:OD1	1:B:537:SER:HB2	2.20	0.41
1:B:542:LEU:HD23	1:B:543:LEU:N	2.34	0.41
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.51	0.41
1:B:147:ARG:HB3	1:B:147:ARG:NH1	2.33	0.41
1:B:388:GLN:CB	1:B:391:LYS:HB2	2.50	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.19	0.41
1:B:741:GLY:O	1:B:742:ILE:C	2.62	0.41
1:A:486:VAL:HG13	1:A:487:ASN:N	2.36	0.41
1:A:515:ASP:OD2	1:A:516:PHE:N	2.49	0.41
1:A:156:THR:HG21	1:A:214:LEU:CD1	2.36	0.41
1:A:326:ASP:OD1	1:A:339:CYS:HB3	2.21	0.41
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.50	0.41
1:A:388:GLN:HB2	1:A:391:LYS:HB2	2.03	0.41
1:B:691:ARG:NH1	12:B:1156:HOH:O	2.48	0.41
1:A:208:PHE:O	1:A:209:SER:HB3	2.21	0.41
1:A:257:PRO:O	1:A:663:ASP:HA	2.20	0.41
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.86	0.41
1:A:658:ARG:NH1	12:A:1074:HOH:O	2.53	0.41
1:B:324:VAL:HG22	1:B:346:ILE:HG13	2.02	0.41
1:B:518:ILE:HG12	1:B:522:THR:H	1.86	0.41
1:B:584:GLY:O	1:B:585:TYR:HB2	2.21	0.41
1:A:64:SER:O	1:A:463:LYS:HG2	2.21	0.41
1:A:701:LEU:HD22	1:A:703:ILE:HG13	2.03	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB2	2.03	0.41
1:A:526:TYR:CD1	1:A:526:TYR:C	2.99	0.40
1:A:554:LYS:HB3	1:A:554:LYS:HE3	1.80	0.40
1:A:654:ALA:N	1:A:655:PRO:CD	2.84	0.40
1:A:696:LYS:CG	1:A:728:VAL:HG22	2.52	0.40
1:B:242:SER:OG	1:B:243:ASP:N	2.54	0.40
1:A:413:ASP:HB3	1:A:414:TYR:HD1	1.87	0.40
1:B:658:ARG:HD3	1:B:660:GLU:HB2	2.03	0.40
1:A:118:TYR:O	1:A:119:ASN:HB2	2.21	0.40
1:B:435:GLN:HB3	1:B:441:LYS:HB2	2.03	0.40
5:F:1:NAG:H61	5:F:2:NDG:C1	2.51	0.40
1:A:227:GLN:O	1:A:266:VAL:HA	2.22	0.40
1:A:272:ASN:ND2	1:A:272:ASN:C	2.75	0.40
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.44	0.40
1:B:519:LEU:O	1:B:520:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CE1	1:A:173:TYR:HB2	2.56	0.40
1:A:208:PHE:HE1	1:A:300:LEU:O	2.05	0.40
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.02	0.40
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	661 (91%)	50 (7%)	13 (2%)	6	12
1	B	726/728 (100%)	654 (90%)	58 (8%)	14 (2%)	6	11
All	All	1450/1456 (100%)	1315 (91%)	108 (7%)	27 (2%)	6	11

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	B	289	ALA
1	B	399	LYS
1	B	645	GLY
1	B	765	LEU
1	A	289	ALA
1	A	332	GLU
1	A	389	ILE
1	A	520	ASN
1	B	85	ASN
1	B	140	ARG
1	B	280	THR
1	B	678	ASP
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	277	SER
1	A	320	GLN
1	A	521	GLU
1	B	40	ARG
1	B	87	SER
1	B	92	ASN
1	B	106	SER
1	B	423	LYS
1	A	334	SER
1	B	320	GLN
1	A	71	LYS
1	A	178	PRO
1	A	161	GLY

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	651/653 (100%)	606 (93%)	45 (7%)	14	30
1	B	653/653 (100%)	604 (92%)	49 (8%)	12	26
All	All	1304/1306 (100%)	1210 (93%)	94 (7%)	13	28

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	52	THR
1	A	72	GLN
1	A	90	LEU
1	A	91	GLU
1	A	92	ASN
1	A	141	GLN
1	A	145	GLU
1	A	156	THR
1	A	184	ARG

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Mol	Chain	Res	Type
1	A	207	VAL
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	256	TYR
1	A	272	ASN
1	A	276	LEU
1	A	293	MET
1	A	303	VAL
1	A	326	ASP
1	A	336	ARG
1	A	385	CYS
1	A	388	GLN
1	A	390	ASP
1	A	393	ASP
1	A	415	LEU
1	A	440	THR
1	A	442	VAL
1	A	448	GLU
1	A	482	LEU
1	A	485	SER
1	A	507	VAL
1	A	514	LEU
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	603	VAL
1	A	608	GLU
1	A	622	LYS
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	736	THR
1	A	760	LYS
1	A	761	GLN
1	B	61	ARG
1	B	66	HIS
1	B	72	GLN
1	B	77	LEU
1	B	145	GLU
1	B	147	ARG
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	182	SER
1	B	184	ARG
1	B	185	ILE
1	B	209	SER
1	B	223	LEU
1	B	232	GLU
1	B	236	ILE
1	B	239	SER
1	B	246	LEU
1	B	253	ARG
1	B	293	MET
1	B	303	VAL
1	B	308	GLN
1	B	310	ARG
1	B	358	ARG
1	B	377	ASN
1	B	379	GLU
1	B	388	GLN
1	B	410	LEU
1	B	436	LEU
1	B	445	LEU
1	B	448	GLU
1	B	502	LYS
1	B	507	VAL
1	B	509	MET
1	B	514	LEU
1	B	517	ILE
1	B	518	ILE
1	B	522	THR
1	B	543	LEU
1	B	597	ARG
1	B	598	LEU
1	B	656	VAL
1	B	673	LEU
1	B	679	ASN
1	B	689	MET
1	B	691	ARG
1	B	701	LEU
1	B	702	LEU
1	B	728	VAL
1	B	760	LYS
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	100	HIS
1	A	119	ASN
1	A	123	GLN
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	286	GLN
1	A	314	GLN
1	A	338	ASN
1	A	388	GLN
1	A	435	GLN
1	A	483	HIS
1	A	487	ASN
1	A	505	GLN
1	A	508	GLN
1	A	533	HIS
1	A	572	ASN
1	A	586	GLN
1	A	606	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	112	GLN
1	B	123	GLN
1	B	126	HIS
1	B	138	ASN
1	B	141	GLN
1	B	169	ASN
1	B	170	ASN
1	B	227	GLN
1	B	272	ASN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	338	ASN
1	B	344	GLN
1	B	377	ASN
1	B	430	ASN
1	B	435	GLN
1	B	455	GLN
1	B	572	ASN
1	B	595	ASN
1	B	606	GLN
1	B	679	ASN
1	B	685	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN

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 ⓘ

27 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	C	1	2,1	14,14,15	0.77	0	17,19,21	1.15	1 (5%)
2	NDG	C	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.46	3 (17%)
2	FUC	C	3	2	10,10,11	0.50	0	14,14,16	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1	3,1	14,14,15	0.79	0	17,19,21	0.74	1 (5%)
3	NAG	D	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.62	0
3	FUC	D	3	3	10,10,11	0.62	0	14,14,16	0.38	0
4	NAG	E	1	4,1	14,14,15	0.50	0	17,19,21	0.88	1 (5%)
4	NAG	E	2	4	14,14,15	0.57	0	17,19,21	0.61	0
5	NAG	F	1	5,1	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
5	NDG	F	2	5	14,14,15	0.85	1 (7%)	17,19,21	1.24	3 (17%)
5	MAN	F	3	5	11,11,12	0.72	0	15,15,17	0.43	0
4	NAG	G	1	4,1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
4	NAG	G	2	4	14,14,15	0.64	0	17,19,21	0.66	0
4	NAG	H	1	4,1	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
4	NAG	H	2	4	14,14,15	0.68	0	17,19,21	0.62	0
6	NAG	I	1	6,1	14,14,15	0.64	0	17,19,21	0.77	1 (5%)
6	FUC	I	2	6	10,10,11	0.58	0	14,14,16	0.37	0
4	NAG	J	1	4,1	14,14,15	0.77	0	17,19,21	1.00	2 (11%)
4	NAG	J	2	4	14,14,15	0.57	0	17,19,21	0.58	0
7	NAG	K	1	7,1	14,14,15	0.46	0	17,19,21	0.81	1 (5%)
7	NAG	K	2	7	14,14,15	0.56	0	17,19,21	0.81	1 (5%)
7	BMA	K	3	7	11,11,12	0.65	0	15,15,17	0.32	0
7	NAG	L	1	7,1	14,14,15	0.65	0	17,19,21	0.80	1 (5%)
7	NAG	L	2	7	14,14,15	0.89	1 (7%)	17,19,21	1.35	3 (17%)
7	BMA	L	3	7	11,11,12	0.73	0	15,15,17	0.94	1 (6%)
8	NAG	M	1	8,1	14,14,15	0.78	0	17,19,21	1.11	2 (11%)
8	NDG	M	2	8	14,14,15	0.79	1 (7%)	17,19,21	0.92	1 (5%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NDG	C	2	2	-	2/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	NDG	F	2	5	-	3/6/23/26	0/1/1/1
5	MAN	F	3	5	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
6	NAG	I	1	6,1	-	1/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1
4	NAG	J	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	NAG	L	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	3/6/23/26	0/1/1/1
7	BMA	L	3	7	-	2/2/19/22	0/1/1/1
8	NAG	M	1	8,1	1/1/5/7	2/6/23/26	0/1/1/1
8	NDG	M	2	8	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.76	1.56	1.52
2	C	2	NDG	C1-C2	2.46	1.55	1.52
5	F	2	NDG	C1-C2	2.34	1.55	1.52
8	M	2	NDG	C1-C2	2.24	1.55	1.52
7	L	2	NAG	C1-C2	2.05	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NDG	O5-C1-C2	3.94	117.39	111.29
7	L	2	NAG	C4-C3-C2	-3.58	105.78	111.02
2	C	2	NDG	C1-O5-C5	2.93	116.11	112.19
2	C	1	NAG	C4-C3-C2	2.84	115.18	111.02
8	M	1	NAG	C2-N2-C7	-2.60	119.42	122.90
7	L	3	BMA	C1-C2-C3	2.57	113.39	109.64
5	F	1	NAG	C2-N2-C7	-2.55	119.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C4-C3-C2	-2.45	107.43	111.02
8	M	1	NAG	C4-C3-C2	2.42	114.57	111.02
7	L	1	NAG	C2-N2-C7	-2.42	119.65	122.90
7	K	2	NAG	C2-N2-C7	-2.41	119.68	122.90
5	F	2	NDG	C4-C3-C2	-2.39	107.51	111.02
2	C	2	NDG	C2-N2-C7	-2.38	119.71	122.90
8	M	2	NDG	C2-N2-C7	-2.34	119.76	122.90
4	J	1	NAG	C2-N2-C7	-2.25	119.88	122.90
7	K	1	NAG	C2-N2-C7	-2.18	119.98	122.90
3	D	1	NAG	C2-N2-C7	-2.17	119.99	122.90
4	H	1	NAG	C2-N2-C7	-2.12	120.06	122.90
6	I	1	NAG	C2-N2-C7	-2.12	120.06	122.90
4	E	1	NAG	C2-N2-C7	-2.10	120.08	122.90
5	F	2	NDG	O4-C4-C5	2.09	114.47	109.32
7	L	2	NAG	O4-C4-C5	2.09	114.46	109.32
5	F	2	NDG	C1-O5-C5	2.04	114.92	112.19
7	L	2	NAG	C2-N2-C7	-2.04	120.17	122.90
4	G	1	NAG	C2-N2-C7	-2.01	120.21	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1
4	J	1	NAG	C1
8	M	1	NAG	C1

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
5	F	2	NDG	C3-C2-N2-C7
7	L	3	BMA	C4-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
5	F	3	MAN	C4-C5-C6-O6
7	L	3	BMA	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	3	MAN	O5-C5-C6-O6
8	M	1	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
8	M	2	NDG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	K	2	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
8	M	2	NDG	O5-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C3-C2-N2-C7
5	F	2	NDG	O5-C5-C6-O6
2	C	2	NDG	C8-C7-N2-C2
4	J	2	NAG	C4-C5-C6-O6
2	C	2	NDG	O7-C7-N2-C2
6	I	1	NAG	O5-C5-C6-O6
7	L	2	NAG	C1-C2-N2-C7
4	E	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	F	2	NDG	C4-C5-C6-O6

There are no ring outliers.

19 monomers are involved in 34 short contacts:

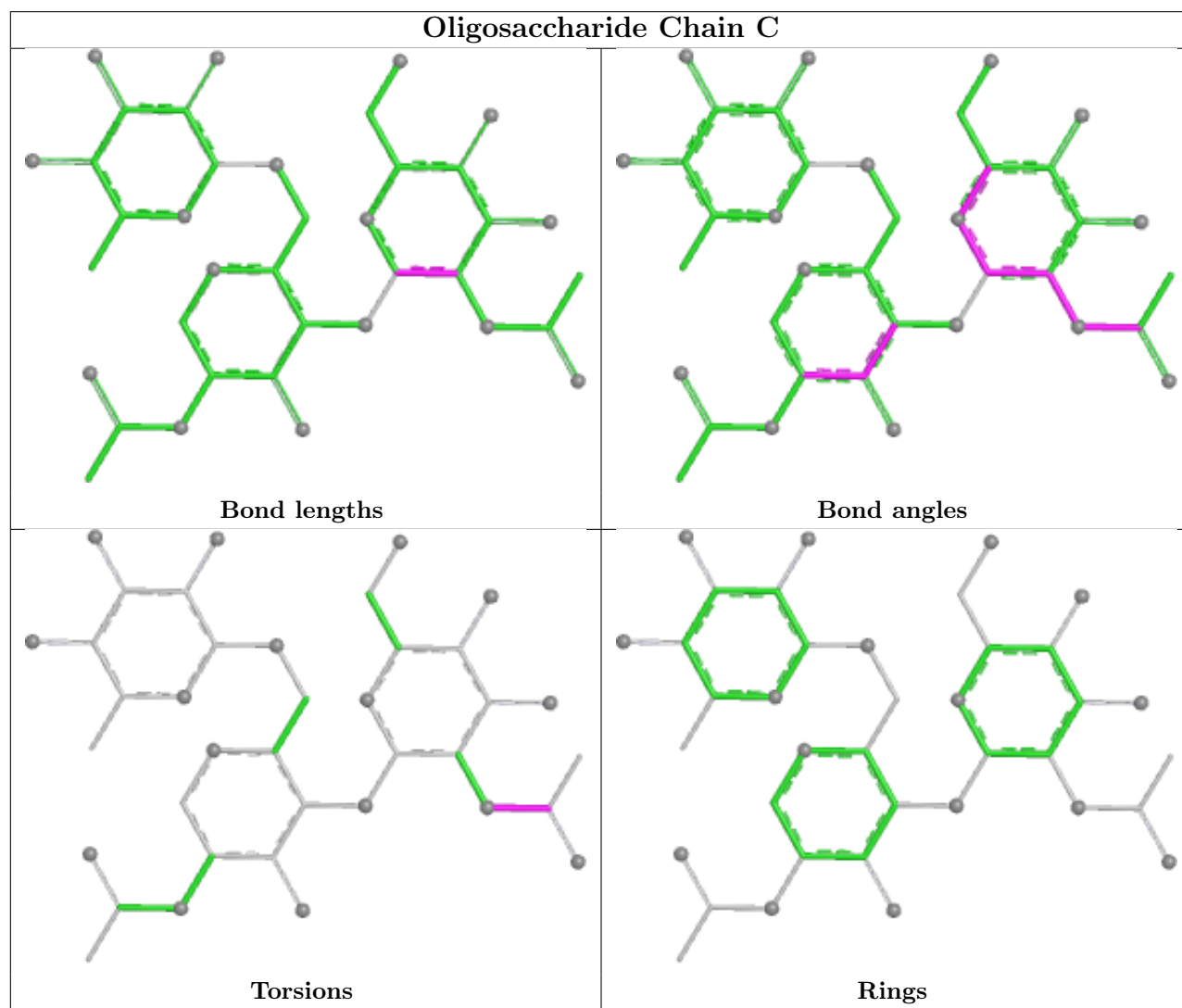
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
3	D	2	NAG	6	0
3	D	1	NAG	5	0
5	F	3	MAN	3	0
5	F	2	NDG	9	0
4	H	1	NAG	1	0
3	D	3	FUC	1	0
5	F	1	NAG	6	0
4	G	2	NAG	1	0
2	C	3	FUC	1	0
4	J	1	NAG	3	0
2	C	2	NDG	1	0
4	J	2	NAG	1	0
6	I	2	FUC	1	0
7	L	3	BMA	1	0
8	M	2	NDG	4	0

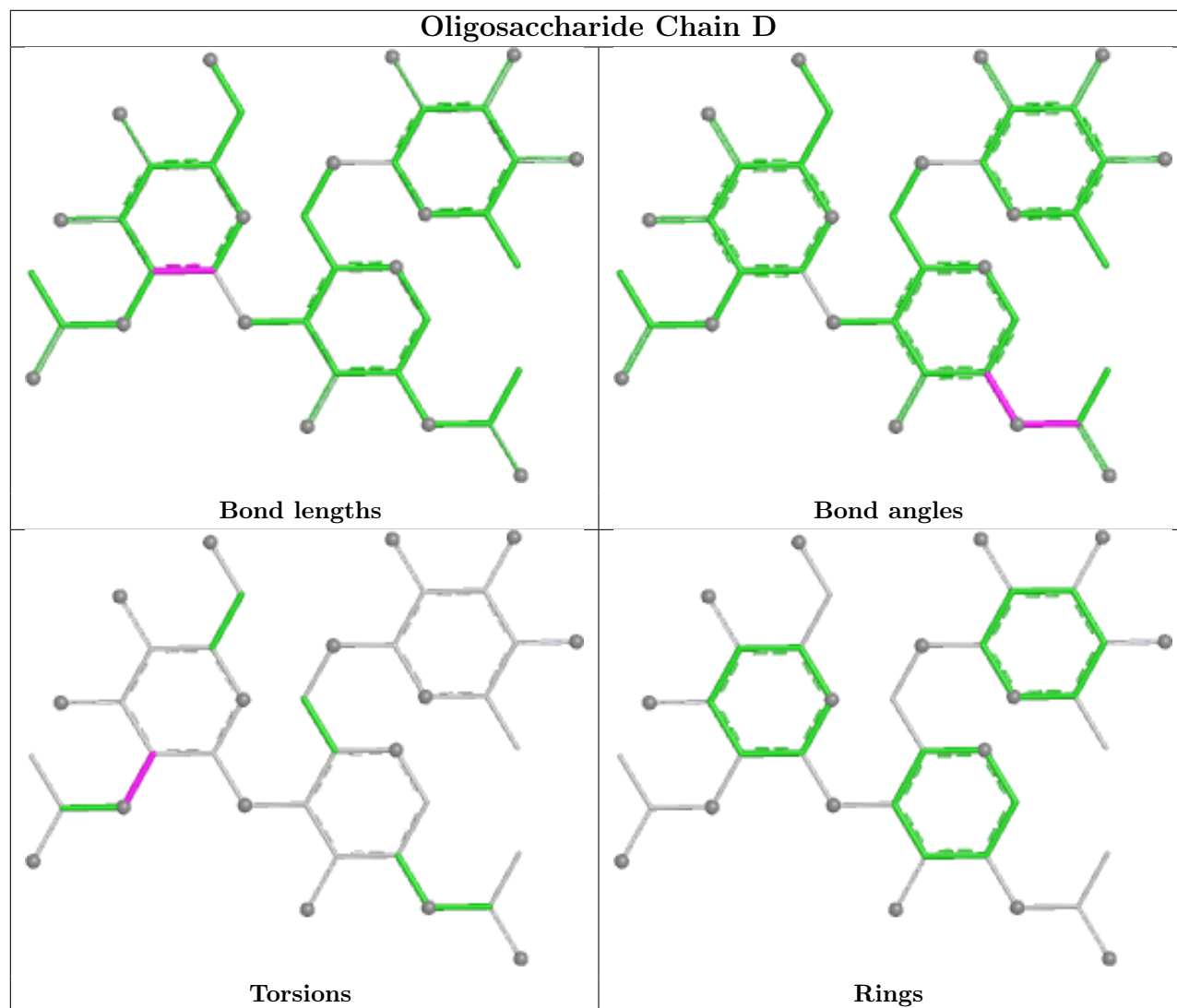
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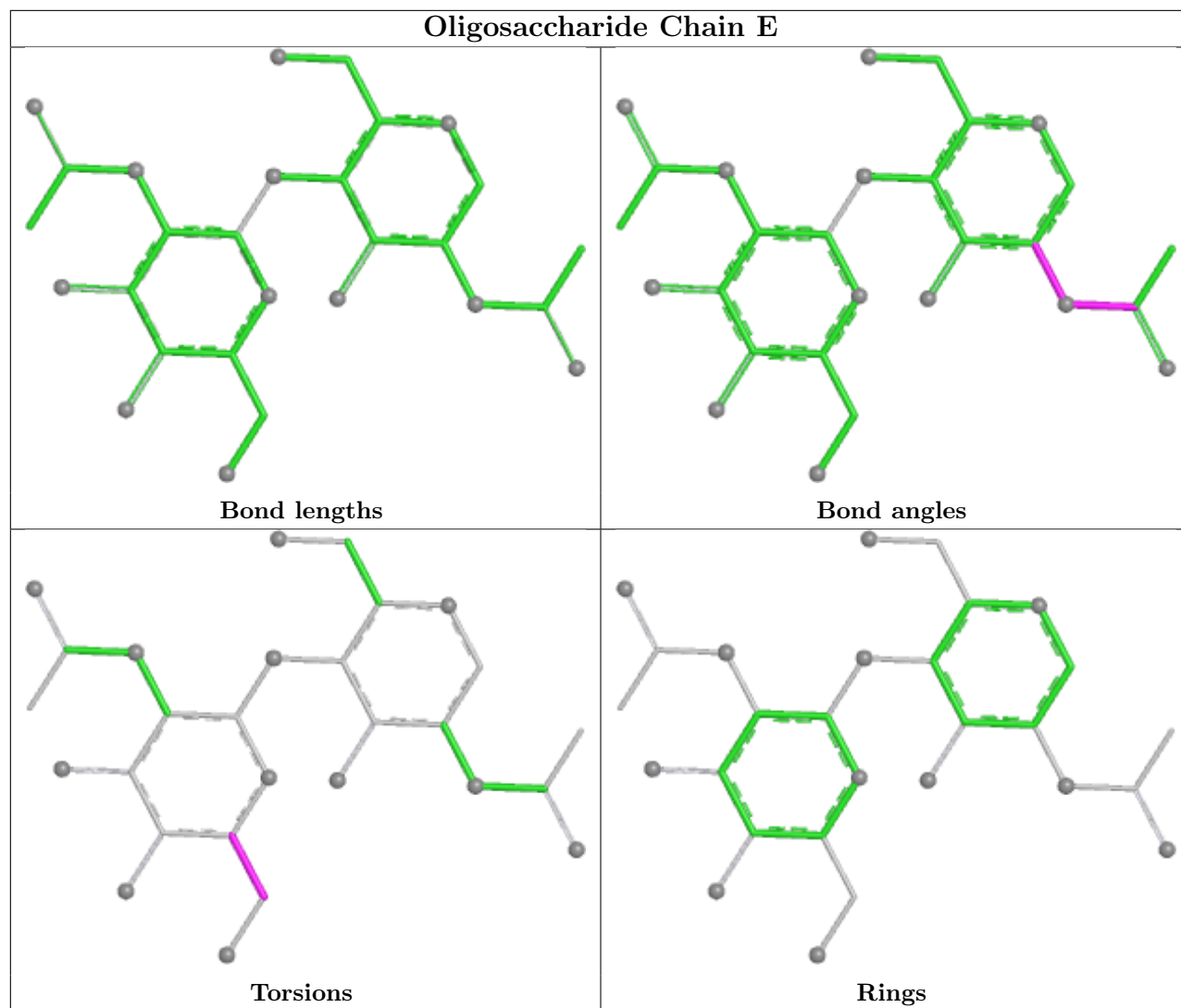
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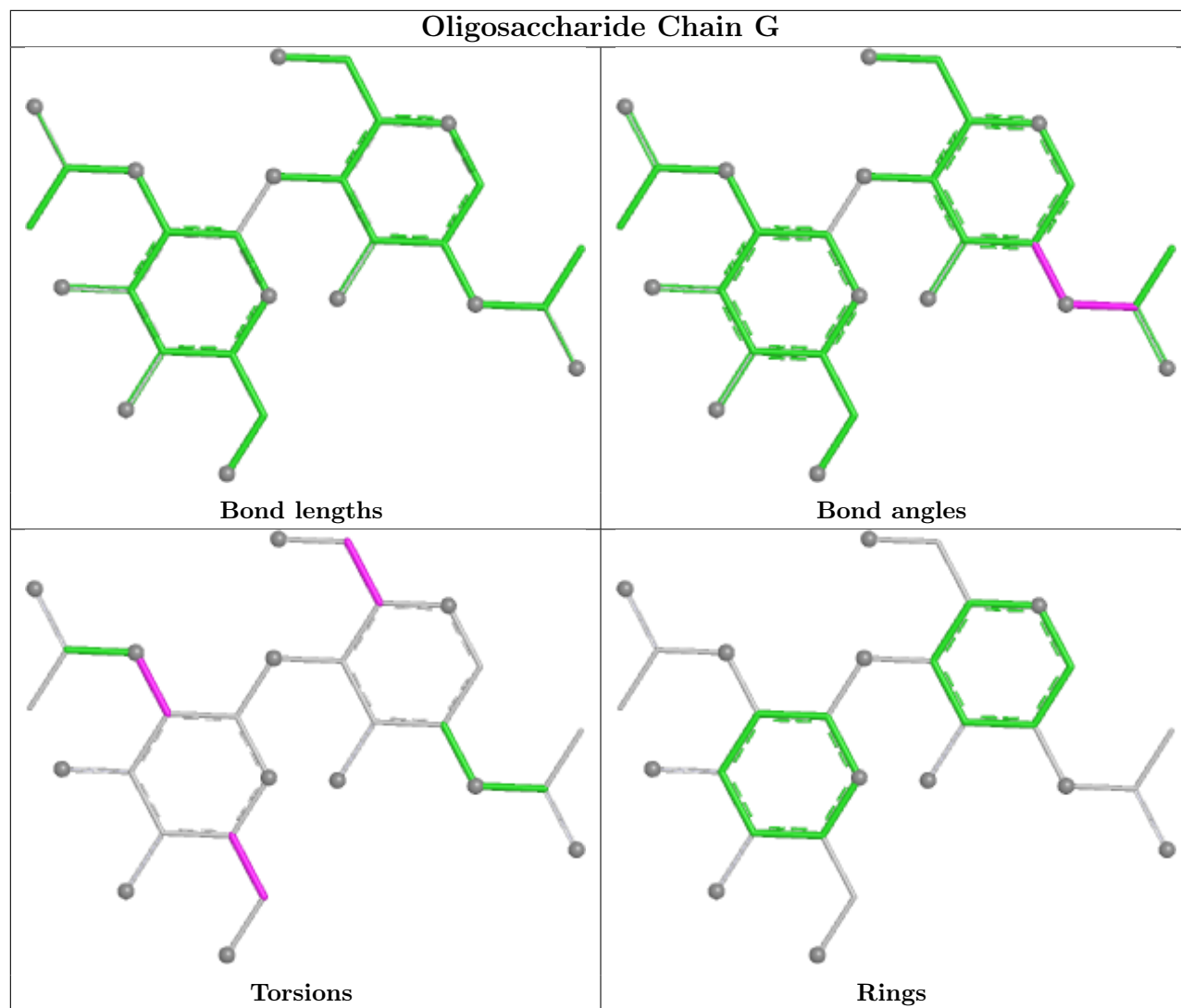
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0
4	H	2	NAG	2	0
8	M	1	NAG	4	0

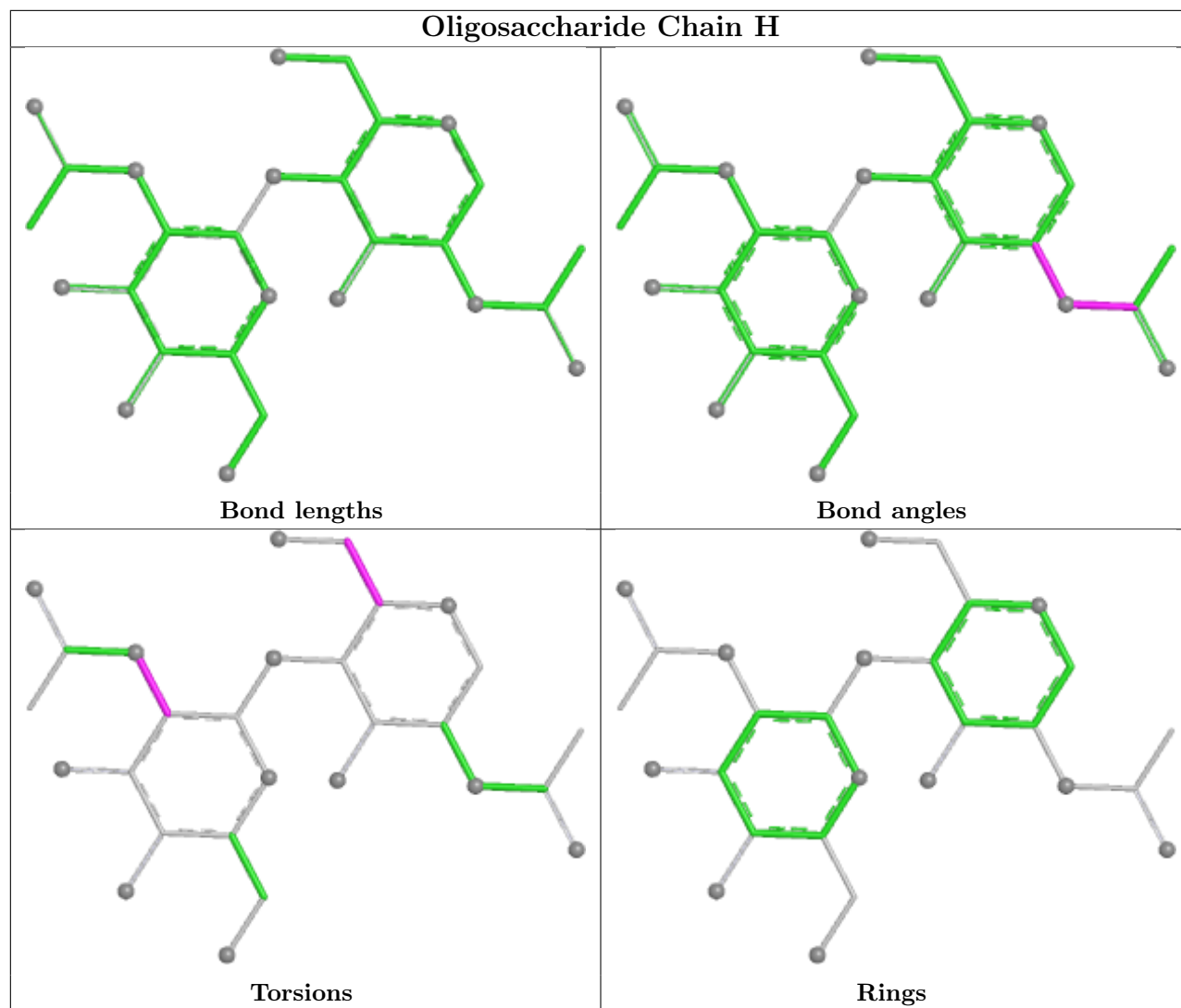
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

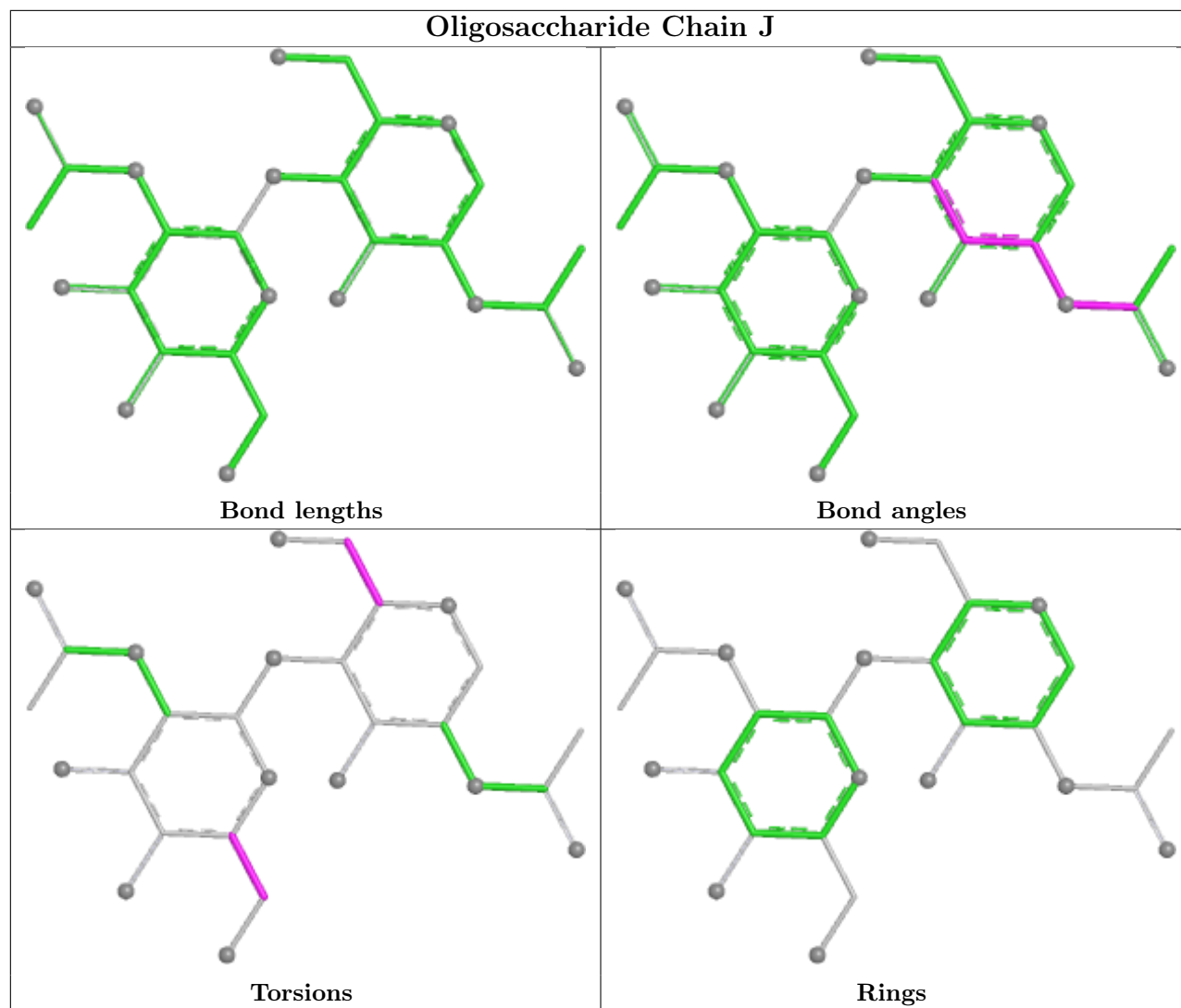


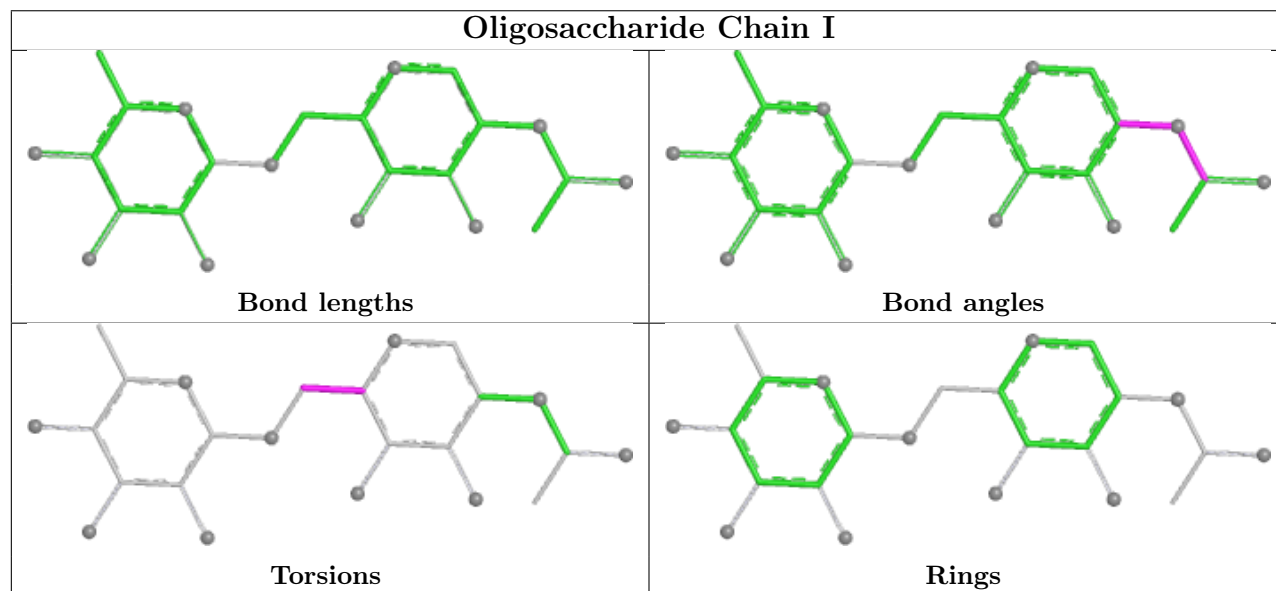
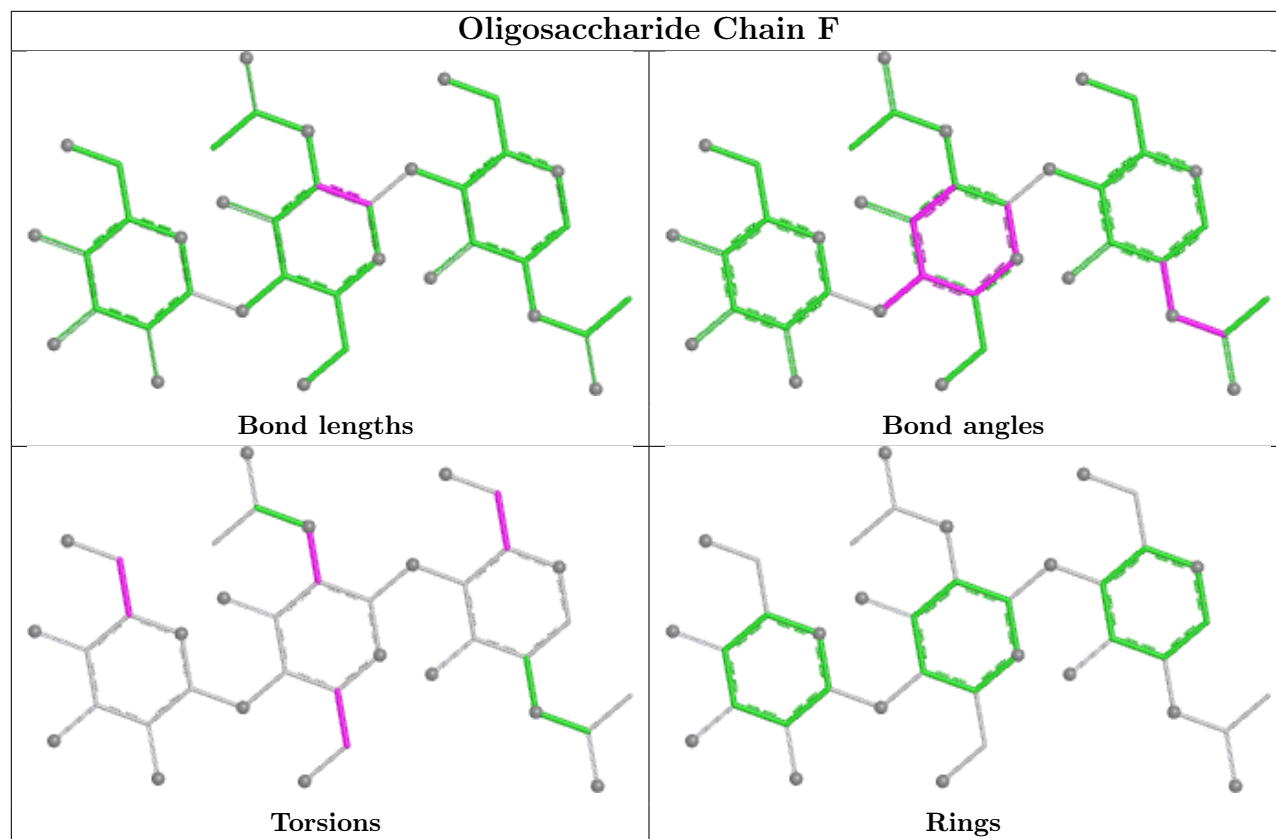


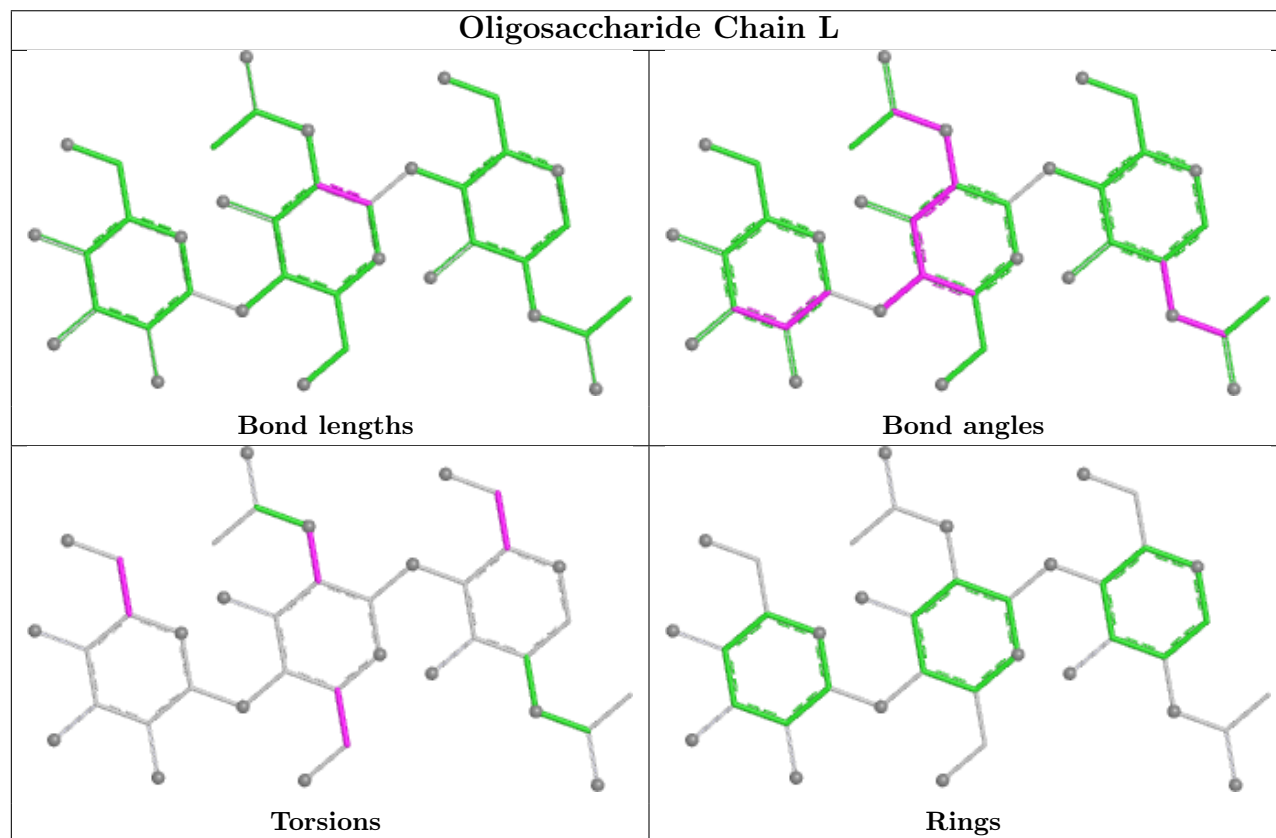
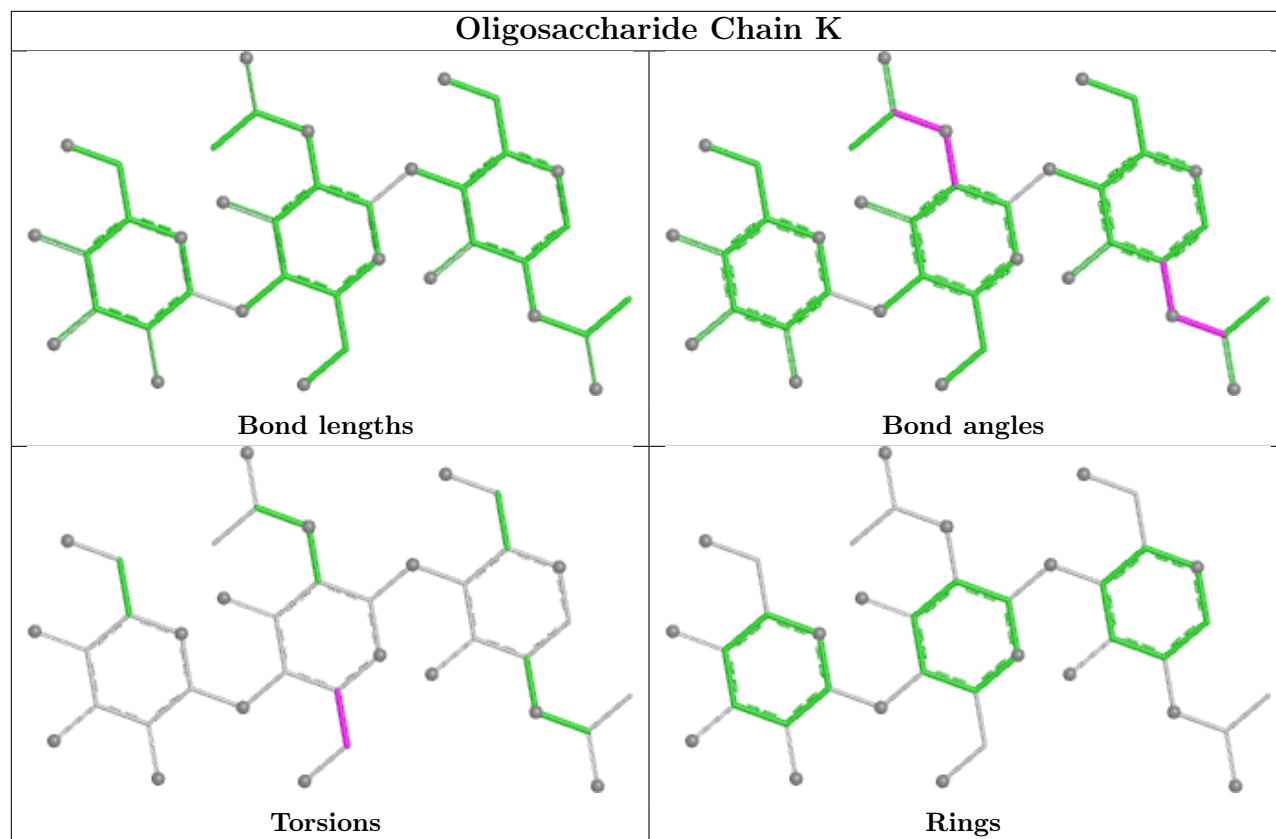


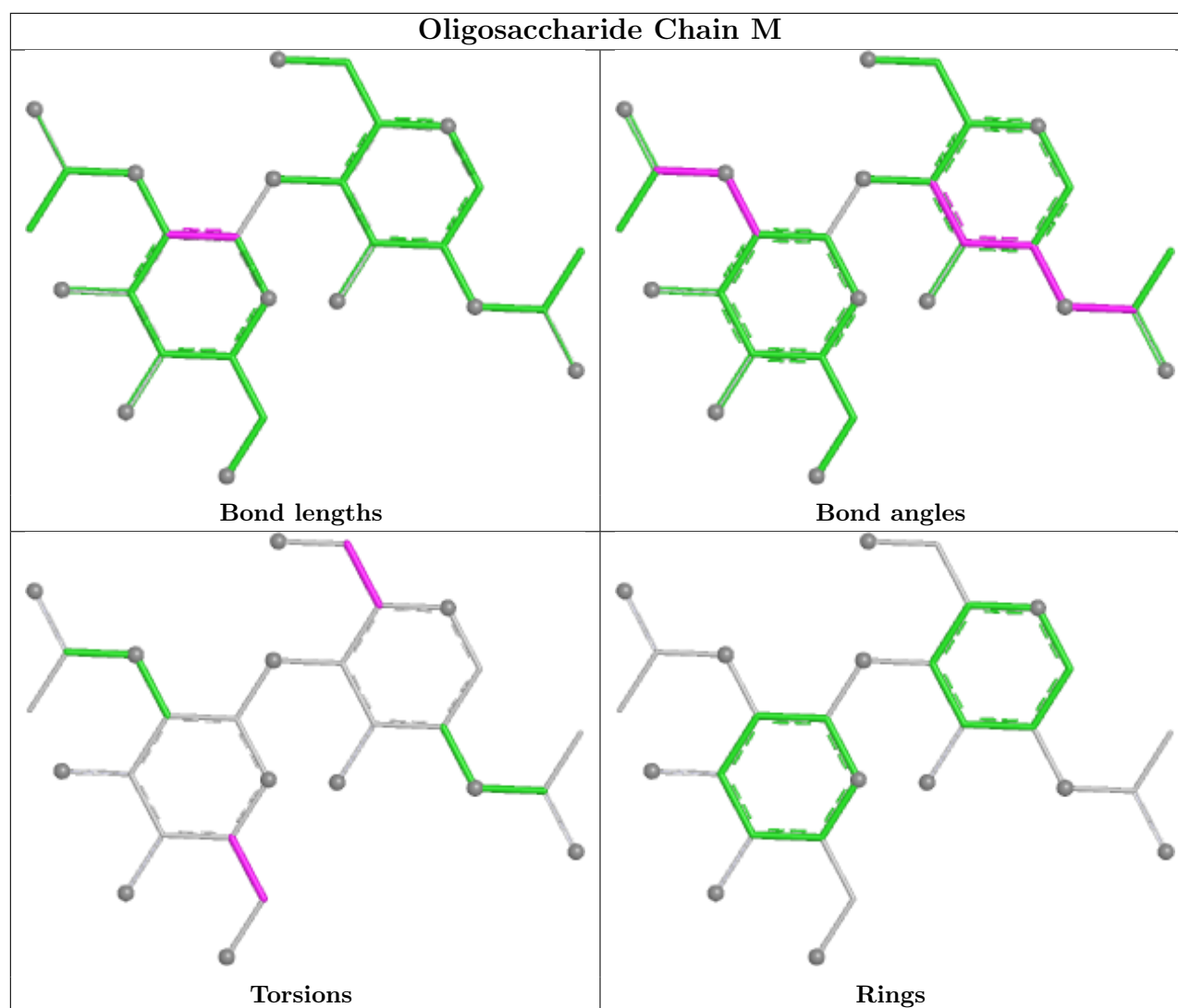












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
9	NAG	A	782	1	14,14,15	0.92	1 (7%)	17,19,21	0.78	0
11	A3M	B	955	-	11,12,12	4.66	5 (45%)	13,16,16	2.28	6 (46%)
11	A3M	A	954	-	11,12,12	4.42	5 (45%)	13,16,16	2.31	6 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	769	1	14,14,15	0.66	0	17,19,21	0.79	1 (5%)
9	NAG	B	780	1	14,14,15	0.85	1 (7%)	17,19,21	0.70	1 (5%)

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
9	NAG	A	782	1	-	1/6/23/26	0/1/1/1
11	A3M	B	955	-	-	2/12/19/19	0/1/1/1
11	A3M	A	954	-	-	2/12/19/19	0/1/1/1
9	NAG	B	769	1	-	2/6/23/26	0/1/1/1
9	NAG	B	780	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	955	A3M	O18-C14	9.41	1.39	1.22
11	A	954	A3M	O18-C14	8.76	1.38	1.22
11	B	955	A3M	C14-N3	8.41	1.47	1.35
11	A	954	A3M	C14-N3	8.05	1.46	1.35
11	B	955	A3M	C15-C14	-6.51	1.46	1.53
11	A	954	A3M	C15-C14	-5.85	1.47	1.53
11	A	954	A3M	C26-C16	4.93	1.69	1.52
11	B	955	A3M	C26-C16	4.90	1.69	1.52
11	A	954	A3M	C1-C2	2.65	1.60	1.51
9	A	782	NAG	C1-C2	2.62	1.55	1.52
11	B	955	A3M	C1-C2	2.48	1.60	1.51
9	B	780	NAG	C1-C2	2.09	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	955	A3M	C4-N3-C2	-5.37	104.27	111.37
11	A	954	A3M	C4-N3-C2	-5.14	104.57	111.37
11	A	954	A3M	O18-C14-N3	-3.53	117.40	121.61
11	A	954	A3M	C2-N3-C14	-3.01	113.58	124.03
11	B	955	A3M	C2-N3-C14	-3.01	113.58	124.03
11	B	955	A3M	O18-C14-N3	-2.93	118.11	121.61
11	A	954	A3M	O18-C14-C15	-2.31	115.59	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	769	NAG	C2-N2-C7	-2.17	120.00	122.90
11	B	955	A3M	O18-C14-C15	-2.16	115.87	119.95
11	B	955	A3M	C1-C5-C4	-2.16	99.11	105.10
11	B	955	A3M	C4-N3-C14	-2.09	116.77	124.03
11	A	954	A3M	C1-C5-C4	-2.05	99.41	105.10
9	B	780	NAG	C1-O5-C5	2.05	114.94	112.19
11	A	954	A3M	C4-N3-C14	-2.05	116.93	124.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	780	NAG	C3-C2-N2-C7
11	A	954	A3M	C15-C14-N3-C2
11	A	954	A3M	O18-C14-N3-C2
11	B	955	A3M	C15-C14-N3-C2
11	B	955	A3M	O18-C14-N3-C2
9	B	769	NAG	O5-C5-C6-O6
9	B	769	NAG	C4-C5-C6-O6
9	A	782	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	782	NAG	8	0
11	B	955	A3M	3	0
11	A	954	A3M	2	0
9	B	780	NAG	4	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	A	726/728 (99%)	-0.08	9 (1%) 76 73	14, 30, 54, 65	0
1	B	728/728 (100%)	0.03	18 (2%) 58 54	13, 31, 61, 88	0
All	All	1454/1456 (99%)	-0.02	27 (1%) 66 62	13, 30, 58, 88	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	3.6
1	B	39	SER	3.2
1	B	766	PRO	2.8
1	B	103	ASN	2.6
1	A	342	ALA	2.6
1	B	94	THR	2.6
1	B	95	PHE	2.5
1	B	765	LEU	2.5
1	A	289	ALA	2.5
1	B	76	ILE	2.4
1	B	385	CYS	2.4
1	B	105	TYR	2.4
1	B	89	PHE	2.3
1	A	73	GLU	2.3
1	A	507	VAL	2.3
1	B	75	ASN	2.3
1	B	452	GLU	2.3
1	A	275	SER	2.2
1	B	93	SER	2.2
1	A	321	ASN	2.2
1	B	471	ARG	2.2
1	B	87	SER	2.1
1	A	333	SER	2.0
1	B	644	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	697	GLN	2.0
1	B	98	PHE	2.0
1	B	83	TYR	2.0

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

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

6.3 Carbohydrates [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
3	FUC	D	3	10/11	0.19	0.18	79,80,80,80	0
3	NAG	D	2	14/15	0.25	0.17	78,80,80,80	0
4	NAG	H	2	14/15	0.45	0.16	63,65,65,66	0
5	MAN	F	3	11/12	0.48	0.17	71,72,72,73	0
2	NDG	C	2	14/15	0.55	0.14	65,66,67,67	0
8	NDG	M	2	14/15	0.57	0.16	62,64,65,65	0
6	FUC	I	2	10/11	0.58	0.18	73,73,73,73	0
7	BMA	K	3	11/12	0.59	0.15	58,59,59,59	0
3	NAG	D	1	14/15	0.60	0.15	70,73,77,78	0
5	NDG	F	2	14/15	0.63	0.15	63,65,66,69	0
4	NAG	G	2	14/15	0.66	0.16	69,70,70,70	0
7	BMA	L	3	11/12	0.70	0.13	53,54,55,55	0
4	NAG	E	2	14/15	0.71	0.13	56,58,59,59	0
4	NAG	J	2	14/15	0.71	0.13	58,60,60,61	0
8	NAG	M	1	14/15	0.72	0.14	52,54,57,60	0
7	NAG	K	2	14/15	0.77	0.12	51,53,54,56	0
6	NAG	I	1	14/15	0.78	0.12	68,69,71,72	0
4	NAG	H	1	14/15	0.79	0.12	56,59,60,63	0
4	NAG	G	1	14/15	0.82	0.12	64,65,66,67	0
7	NAG	L	2	14/15	0.84	0.12	46,47,49,51	0
2	FUC	C	3	10/11	0.86	0.10	63,63,63,64	0
4	NAG	E	1	14/15	0.87	0.10	48,49,51,54	0
5	NAG	F	1	14/15	0.87	0.12	50,52,55,59	0
2	NAG	C	1	14/15	0.87	0.09	59,60,62,64	0
4	NAG	J	1	14/15	0.88	0.09	50,52,54,56	0

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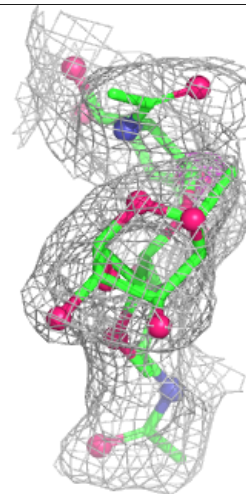
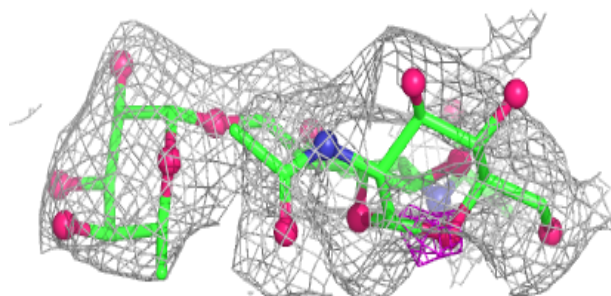
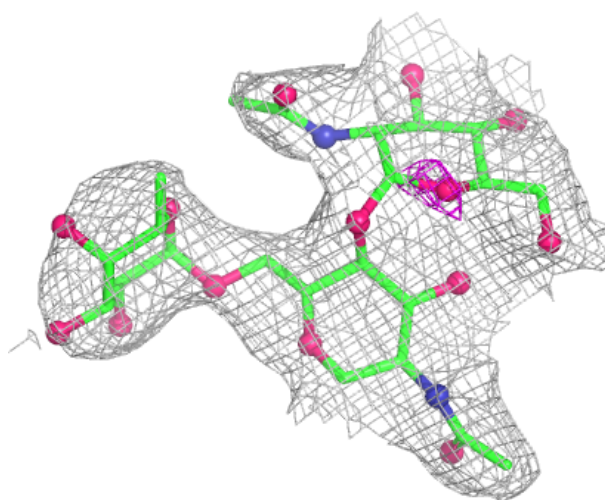
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	K	1	14/15	0.90	0.10	39,40,44,48	0
7	NAG	L	1	14/15	0.94	0.08	39,41,42,44	0

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.

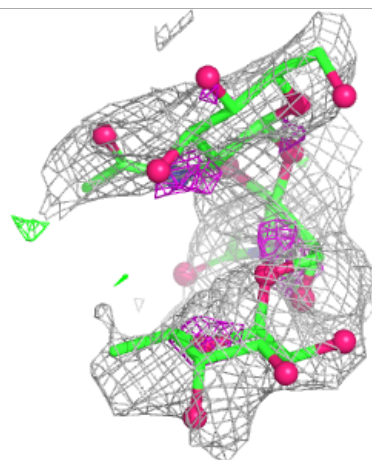
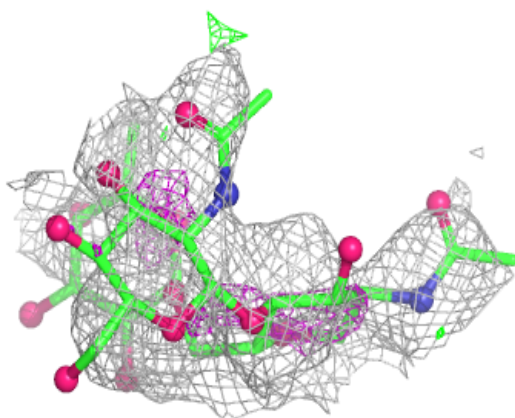
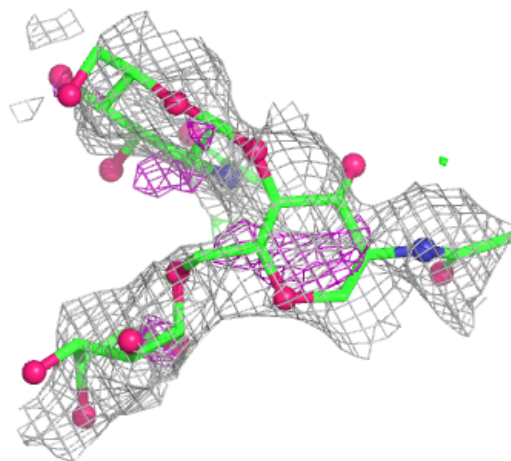
Electron density around Chain C:

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



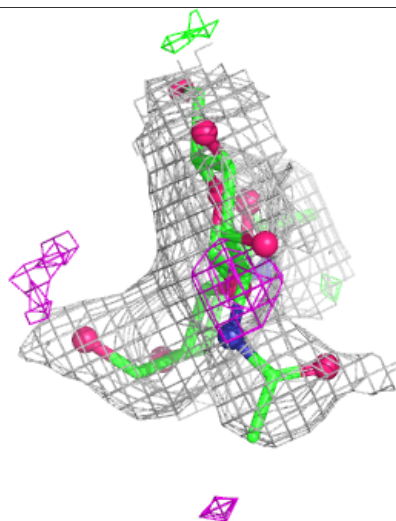
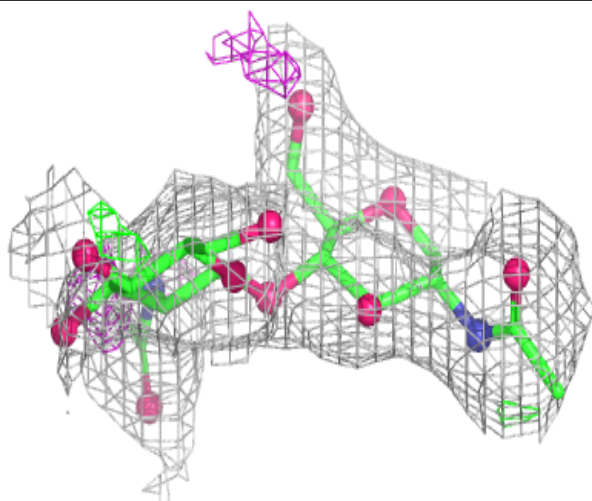
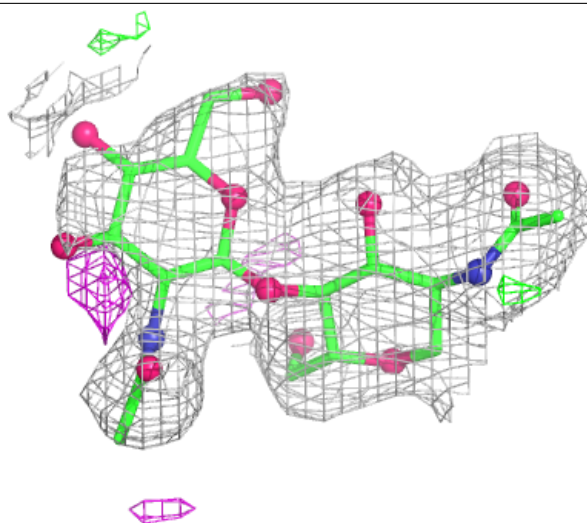
Electron density around Chain D:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



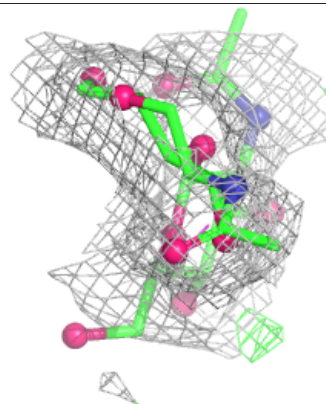
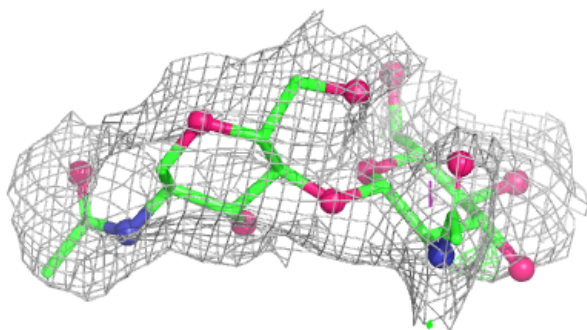
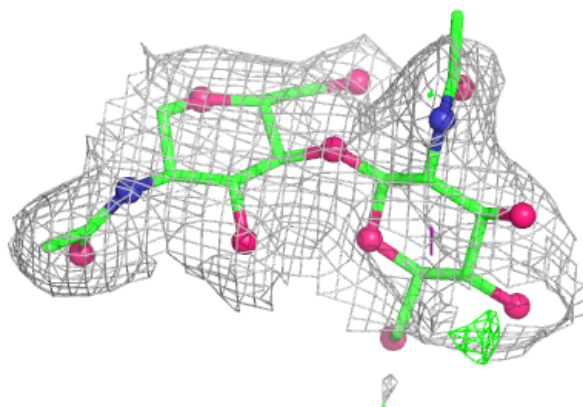
Electron density around Chain E:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



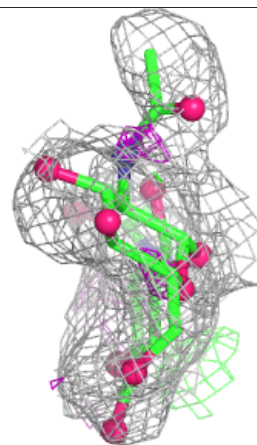
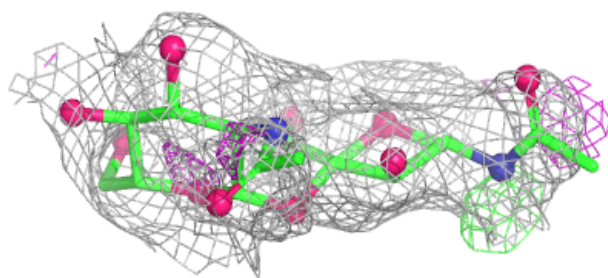
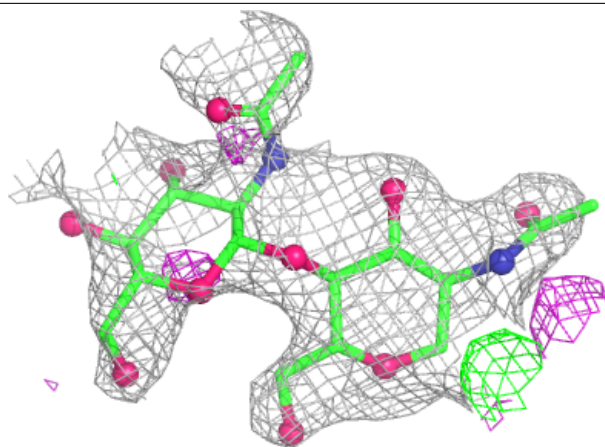
Electron density around Chain G:

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



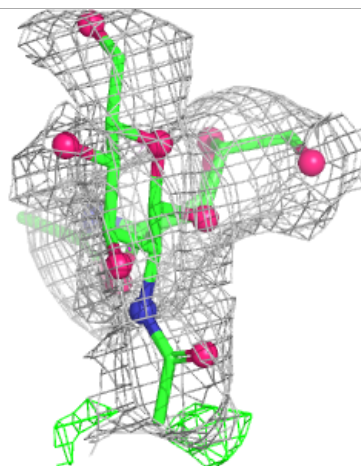
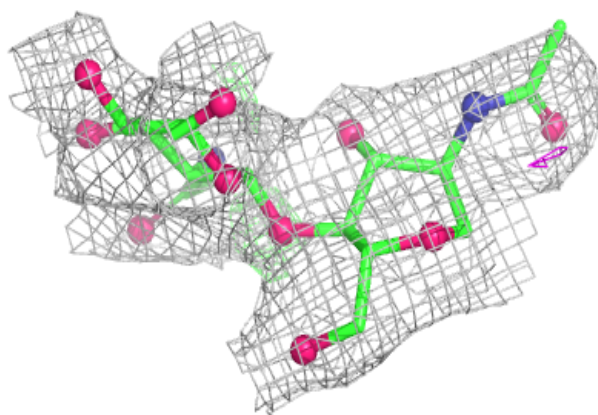
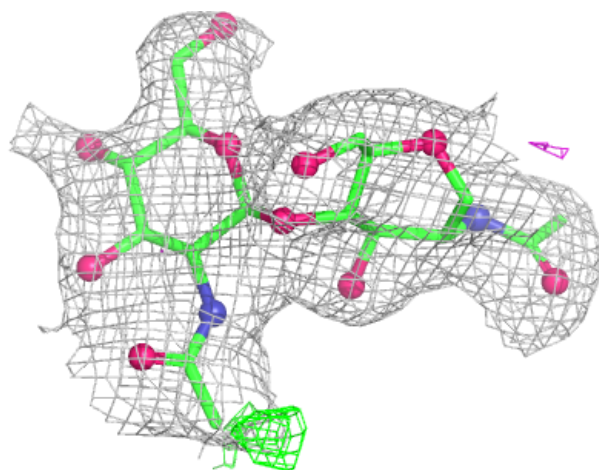
Electron density around Chain H:

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



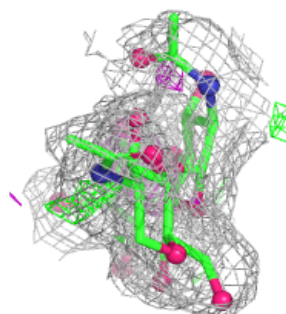
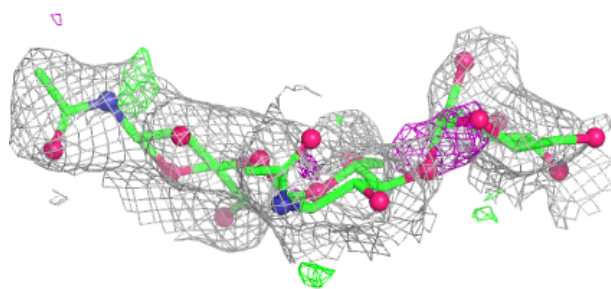
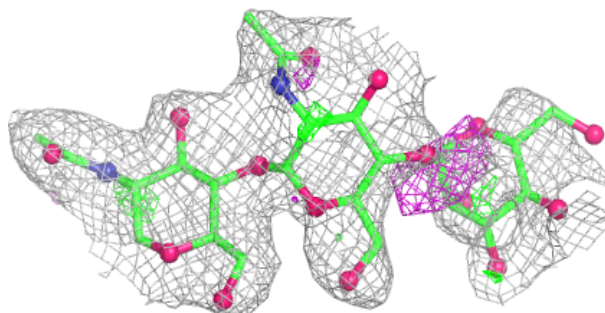
Electron density around Chain J:

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

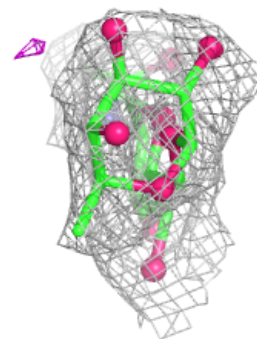
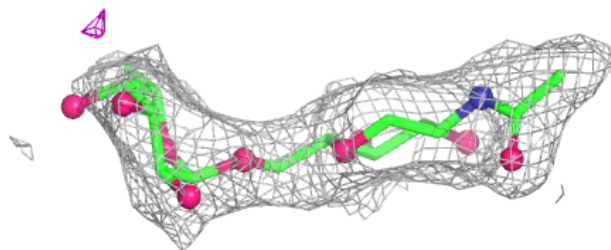
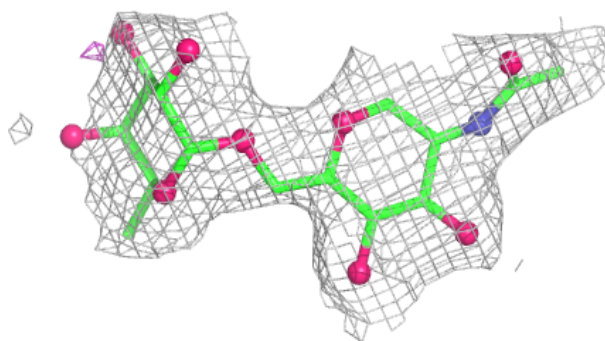


Electron density around Chain F:

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

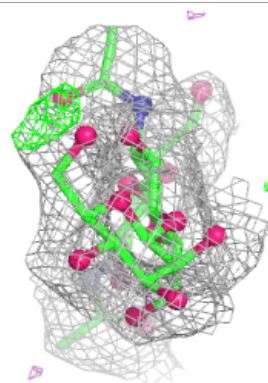
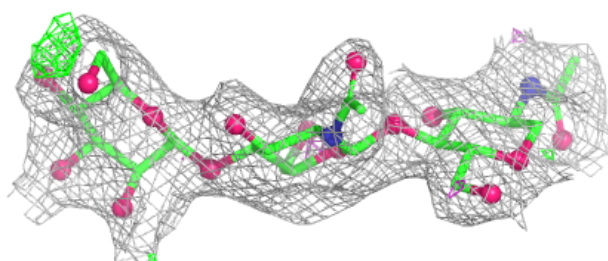
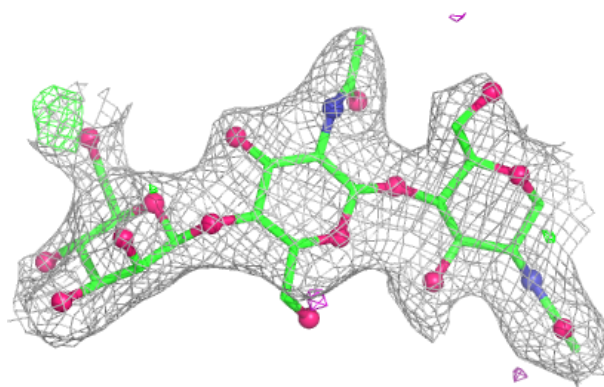
**Electron density around Chain I:**

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

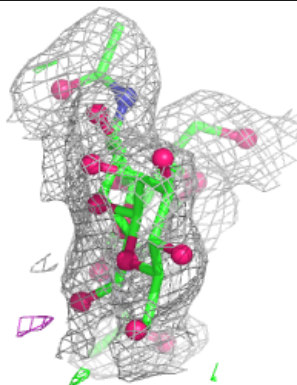
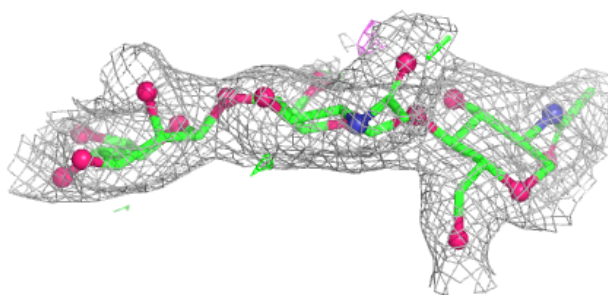
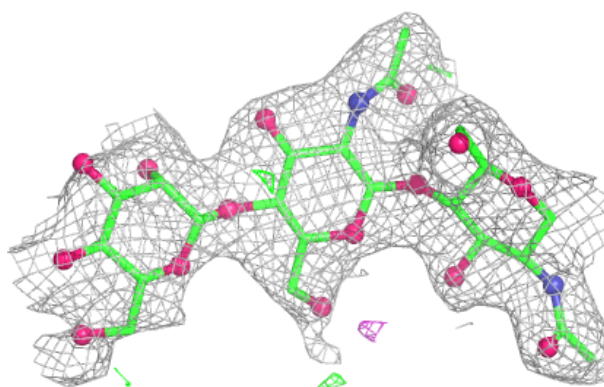


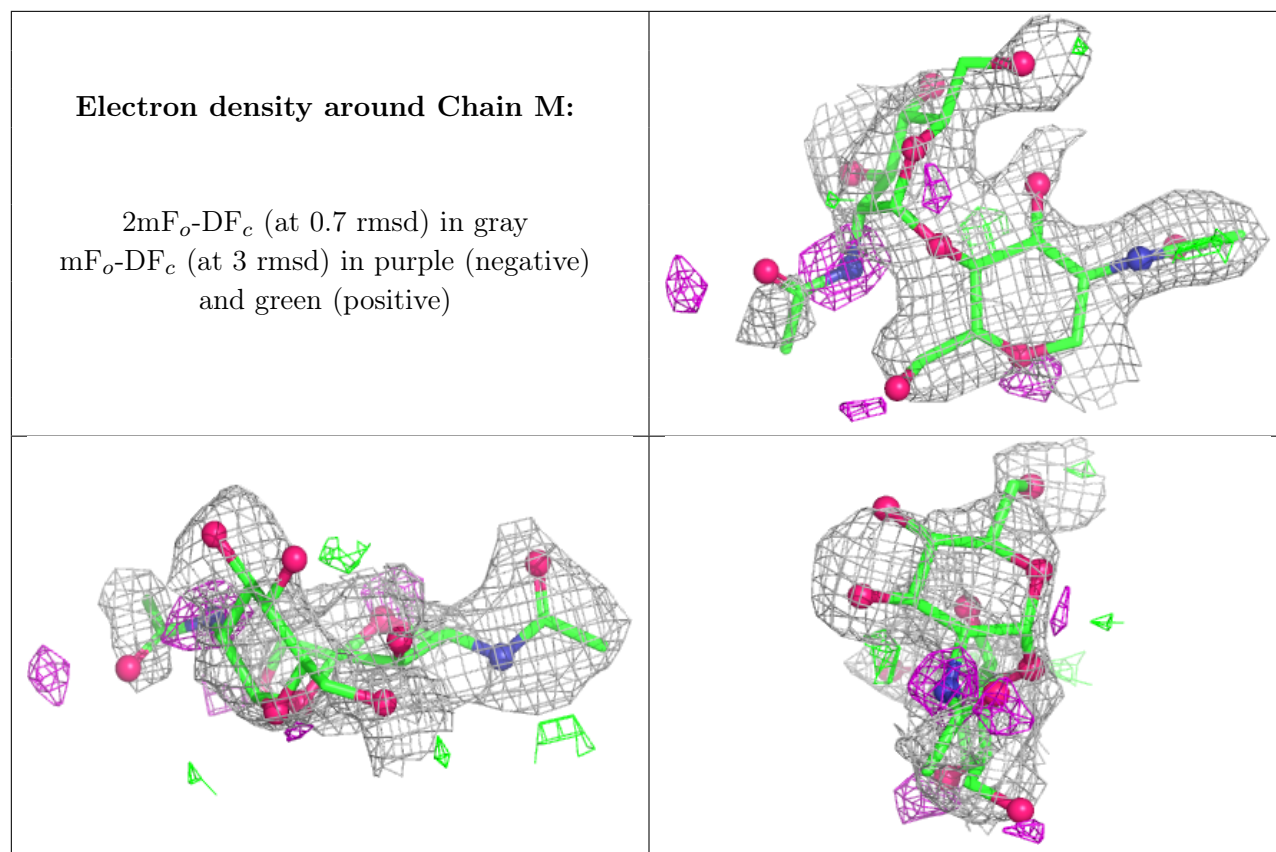
Electron density around Chain K:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
9	NAG	A	782	14/15	0.44	0.17	63,65,66,66	0
9	NAG	B	769	14/15	0.61	0.15	62,64,64,64	0
9	NAG	B	780	14/15	0.64	0.14	60,62,63,63	0
11	A3M	A	954	12/12	0.93	0.09	18,19,19,19	0
11	A3M	B	955	12/12	0.93	0.11	22,23,24,24	0
10	HG	A	950	1/1	0.98	0.05	56,56,56,56	0
10	HG	B	952	1/1	0.99	0.06	36,36,36,36	0
10	HG	B	953	1/1	0.99	0.05	60,60,60,60	0
10	HG	A	951	1/1	1.00	0.05	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.