



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:50 PM EDT

PDB ID : 4J0M / pdb_00004j0m
Title : Crystal structure of BRL1 (LRR) in complex with brassinolide
Authors : Chai, J.; She, J.; Han, Z.; Zhou, B.
Deposited on : 2013-01-31
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:

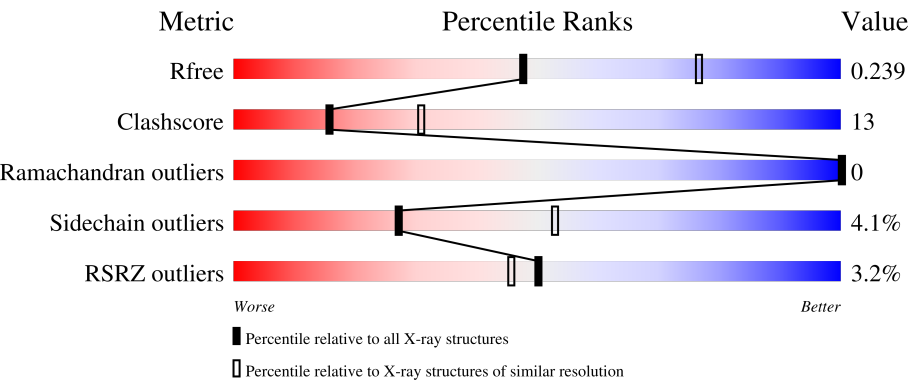
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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.



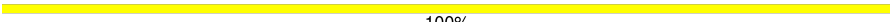
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	740	3% 76% 19% ..
1	B	740	3% 76% 20% ..
2	C	2	50% 50%
2	E	2	100%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 50%50%
2	J	2	 100%
2	K	2	 50%50%
3	D	6	 67%33%
3	I	6	 83%17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11785 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Serine/threonine-protein kinase BRI1-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			
1	B	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	HIS	-	expression tag	UNP Q9ZWC8
A	760	HIS	-	expression tag	UNP Q9ZWC8
A	761	HIS	-	expression tag	UNP Q9ZWC8
A	762	HIS	-	expression tag	UNP Q9ZWC8
A	763	HIS	-	expression tag	UNP Q9ZWC8
A	764	HIS	-	expression tag	UNP Q9ZWC8
B	759	HIS	-	expression tag	UNP Q9ZWC8
B	760	HIS	-	expression tag	UNP Q9ZWC8
B	761	HIS	-	expression tag	UNP Q9ZWC8
B	762	HIS	-	expression tag	UNP Q9ZWC8
B	763	HIS	-	expression tag	UNP Q9ZWC8
B	764	HIS	-	expression tag	UNP Q9ZWC8

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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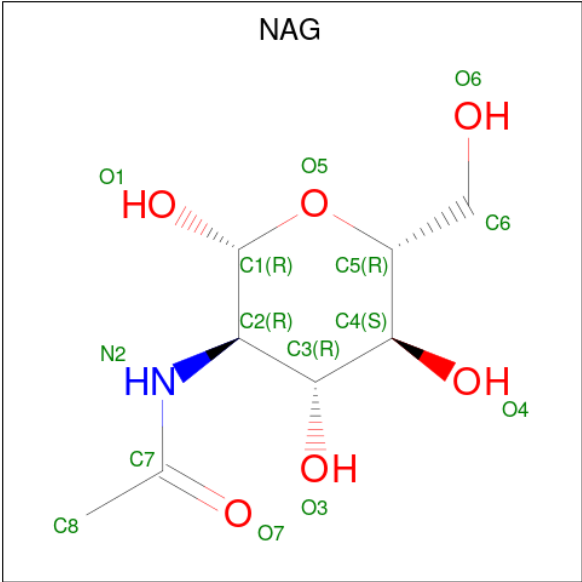
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



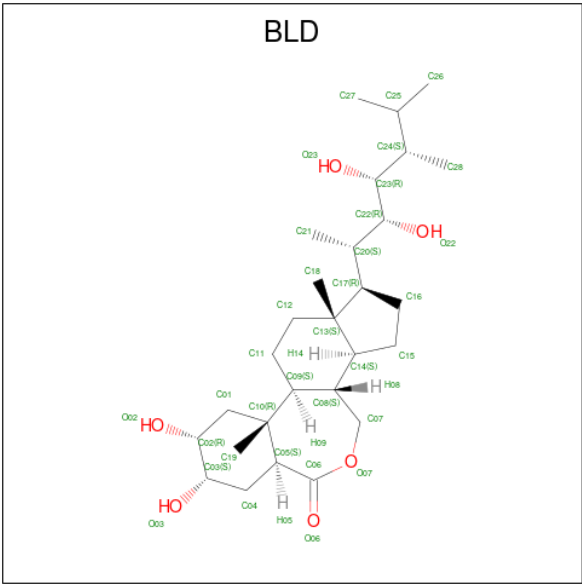
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is Brassinolide (CCD ID: BLD) (formula: $C_{28}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			34	28	6		
5	B	1	Total	C	O	0	0
			34	28	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	201	Total	O	0	0
			201	201		

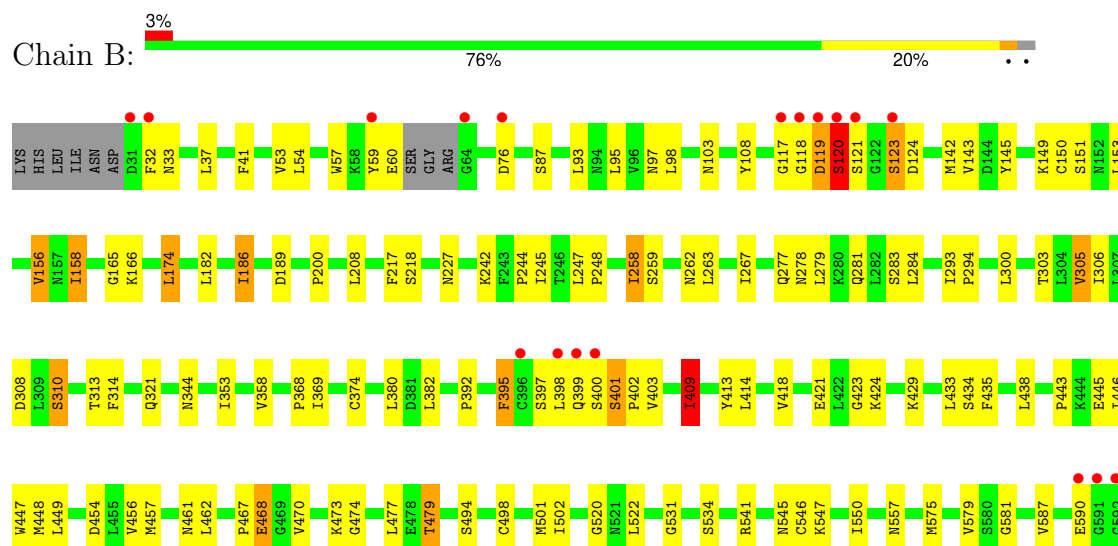
3 Residue-property plots

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: Serine/threonine-protein kinase BRI1-like 1



• Molecule 1: Serine/threonine-protein kinase BRI1-like 1





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

Chain C: 50%



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

Chain E: 100%



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

Chain F: 50%



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

Chain G: 100%



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

Chain H: 50%



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

Chain J: 100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-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 D:  67% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 3: alpha-D-mannopyranose-(1-2)-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 I:  83% 17%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.86Å 83.40Å 264.06Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	29.83 – 2.50 29.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.83-2.50) 94.3 (29.83-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.187 , 0.239 0.188 , 0.239	Depositor DCC
R_{free} test set	3786 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.6	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	11785	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: BMA, BLD, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/5561	0.97	20/7559 (0.3%)
1	B	0.55	1/5561 (0.0%)	0.99	24/7559 (0.3%)
All	All	0.55	1/11122 (0.0%)	0.98	44/15118 (0.3%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	557	ASN	C-O	-5.07	1.18	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	SER	N-CA-C	7.33	119.48	110.91
1	B	121	SER	N-CA-C	-7.29	98.24	109.24
1	A	121	SER	N-CA-C	-7.26	97.64	107.88
1	B	119	ASP	N-CA-C	-7.14	103.23	112.23
1	A	237	ASN	N-CA-C	6.88	121.38	112.92
1	A	117	GLY	N-CA-C	6.75	118.90	112.08
1	B	156	VAL	CB-CA-C	-6.46	101.69	110.42
1	A	262	ASN	N-CA-C	6.25	119.84	112.72
1	B	262	ASN	N-CA-C	6.17	120.52	112.92
1	B	395	PHE	N-CA-C	6.12	118.75	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	VAL	N-CA-C	5.95	117.83	112.17
1	B	278	ASN	N-CA-C	5.93	120.53	112.88
1	A	278	ASN	N-CA-C	5.70	120.23	112.88
1	B	461	ASN	N-CA-C	5.67	119.19	112.72
1	B	186	ILE	N-CA-C	5.66	116.95	111.91
1	A	186	ILE	N-CA-C	5.66	116.95	111.91
1	A	409	ILE	N-CA-C	5.59	117.59	111.77
1	A	413	TYR	N-CA-C	5.59	119.09	112.72
1	A	399	GLN	CB-CA-C	-5.58	109.64	117.23
1	B	313	THR	N-CA-C	5.58	119.08	112.72
1	B	189	ASP	CB-CA-C	-5.55	108.57	115.89
1	B	227	ASN	N-CA-C	5.53	120.14	113.17
1	A	534	SER	N-CA-C	5.53	119.03	112.72
1	B	33	ASN	CB-CA-C	-5.53	109.72	117.23
1	B	258	ILE	N-CA-C	5.50	117.49	111.77
1	B	103	ASN	N-CA-C	5.49	120.09	113.17
1	A	227	ASN	N-CA-C	5.47	120.06	113.17
1	A	675	ILE	N-CA-C	5.45	116.44	109.30
1	B	449	LEU	CA-C-N	5.45	124.79	118.85
1	B	449	LEU	C-N-CA	5.45	124.79	118.85
1	B	401	SER	CA-C-N	-5.44	113.67	119.98
1	B	401	SER	C-N-CA	-5.44	113.67	119.98
1	B	534	SER	N-CA-C	5.40	119.56	112.92
1	A	395	PHE	N-CA-C	5.40	117.92	111.71
1	B	438	LEU	N-CA-C	5.32	117.58	110.35
1	B	409	ILE	N-CA-C	5.32	117.22	112.17
1	B	502	ILE	N-CA-C	-5.27	107.03	111.56
1	A	457	MET	N-CA-C	5.13	120.18	112.94
1	A	362	ASN	N-CA-C	5.13	119.23	112.92
1	A	718	VAL	CB-CA-C	5.12	117.55	111.20
1	A	101	LEU	CA-C-N	5.12	124.29	118.97
1	A	101	LEU	C-N-CA	5.12	124.29	118.97
1	B	531	GLY	N-CA-C	5.08	117.77	111.93
1	A	461	ASN	N-CA-C	5.02	118.44	112.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	SER	Peptide

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	5455	0	5391	149	0
1	B	5455	0	5390	137	1
2	C	28	0	25	2	0
2	E	28	0	24	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	D	72	0	55	7	0
3	I	72	0	54	1	0
4	A	28	0	26	2	0
4	B	28	0	26	0	0
5	A	34	0	48	5	0
5	B	34	0	48	5	0
6	A	210	0	0	8	0
6	B	201	0	0	12	0
All	All	11785	0	11212	300	1

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 13.

All (300) 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:B:120:SER:HB3	1:B:145:TYR:HB2	1.26	1.17
1:B:590:GLU:HG2	1:B:624:THR:HG21	1.25	1.12
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.06	1.11
1:A:95:LEU:H	1:A:118:GLY:HA2	1.07	1.11
1:A:399:GLN:HG3	1:A:402:PRO:HD3	1.28	1.11
1:A:95:LEU:HD22	1:A:142:MET:HE2	1.32	1.09
1:B:398:LEU:HD23	1:B:399:GLN:H	1.01	1.09
1:A:590:GLU:HG2	1:A:624:THR:HG21	1.12	1.08
1:A:95:LEU:HB2	1:A:142:MET:HE3	1.33	1.08
1:A:418:VAL:HG21	1:A:457:MET:HE1	1.29	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLY:H	1:B:142:MET:HE3	1.15	1.03
1:A:153:LEU:HD21	1:A:156:VAL:HG22	1.41	1.02
1:B:399:GLN:HG2	1:B:400:SER:H	1.20	1.02
1:B:418:VAL:HG21	1:B:457:MET:HE1	1.41	1.01
1:A:399:GLN:HG2	1:A:401:SER:HA	1.41	1.01
1:A:95:LEU:H	1:A:118:GLY:CA	1.75	0.98
1:A:480:LEU:N	1:A:501:MET:HE1	1.81	0.96
1:B:457:MET:HE2	1:B:462:LEU:HD11	1.48	0.95
1:B:95:LEU:HB2	1:B:142:MET:HE2	1.49	0.94
1:B:118:GLY:N	1:B:142:MET:HE3	1.83	0.94
1:B:448:MET:CE	1:B:473:LYS:HD2	1.98	0.94
1:A:590:GLU:HG2	1:A:624:THR:CG2	1.97	0.93
1:B:398:LEU:HD23	1:B:399:GLN:N	1.83	0.93
1:A:95:LEU:N	1:A:118:GLY:HA2	1.82	0.93
1:A:510:ARG:HG2	1:A:510:ARG:NH1	1.85	0.90
1:A:400:SER:N	1:A:401:SER:HA	1.88	0.89
1:B:590:GLU:CG	1:B:624:THR:HG21	2.01	0.89
1:A:590:GLU:CG	1:A:624:THR:HG21	2.02	0.89
1:B:498:CYS:O	1:B:522:LEU:HD22	1.73	0.88
1:B:400:SER:N	1:B:401:SER:HA	1.89	0.88
1:B:448:MET:HE2	1:B:473:LYS:HD2	1.57	0.87
1:A:281:GLN:HB3	3:D:1:NAG:H81	1.55	0.87
4:A:815:NAG:H82	4:A:815:NAG:O3	1.75	0.87
1:B:477:LEU:HB2	1:B:501:MET:HE1	1.55	0.87
1:A:119:ASP:CG	1:A:120:SER:H	1.83	0.86
1:B:305:VAL:HG23	1:B:306:ILE:HG13	1.56	0.86
1:A:399:GLN:CG	1:A:402:PRO:HD3	2.04	0.85
1:B:398:LEU:CD2	1:B:399:GLN:H	1.90	0.85
1:A:399:GLN:OE1	6:A:1080:HOH:O	1.94	0.84
1:A:153:LEU:HD21	1:A:156:VAL:CG2	2.06	0.84
1:B:120:SER:HB3	1:B:145:TYR:CB	2.08	0.83
1:B:590:GLU:HG2	1:B:624:THR:CG2	2.08	0.83
1:A:399:GLN:HG2	1:A:400:SER:H	1.44	0.82
1:B:118:GLY:H	1:B:142:MET:CE	1.94	0.81
1:B:153:LEU:HD21	1:B:156:VAL:HG22	1.62	0.81
1:A:399:GLN:HG2	1:A:400:SER:N	1.95	0.80
1:A:281:GLN:HB3	3:D:1:NAG:C8	2.12	0.79
1:B:477:LEU:CB	1:B:501:MET:HE1	2.12	0.78
1:A:258:ILE:HD12	1:A:263:LEU:CD1	2.12	0.78
1:B:477:LEU:O	1:B:501:MET:HE2	1.83	0.78
1:A:497:ARG:HD2	6:A:1104:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:HE2	1:A:462:LEU:HD11	1.65	0.76
1:A:399:GLN:CG	1:A:400:SER:H	1.96	0.76
1:A:119:ASP:HA	1:A:141:SER:OG	1.85	0.75
1:B:468:GLU:OE1	6:B:1007:HOH:O	2.03	0.75
1:B:603:GLU:OE2	1:B:605:GLU:HB2	1.87	0.74
1:B:399:GLN:HG2	1:B:400:SER:N	2.00	0.74
1:B:258:ILE:HD11	1:B:284:LEU:HD22	1.69	0.74
1:B:418:VAL:HG21	1:B:457:MET:CE	2.16	0.74
1:A:418:VAL:CG2	1:A:457:MET:HE1	2.14	0.73
1:B:501:MET:SD	6:B:1000:HOH:O	2.46	0.72
1:A:480:LEU:H	1:A:501:MET:HE1	1.53	0.72
1:A:558:ASN:OD1	2:C:1:NAG:H2	1.88	0.72
1:B:467:PRO:O	1:B:470:VAL:HG23	1.89	0.72
1:B:400:SER:N	1:B:401:SER:CA	2.53	0.71
1:A:603:GLU:OE2	1:A:605:GLU:HB2	1.91	0.71
1:A:479:THR:HA	1:A:501:MET:HE3	1.73	0.70
1:B:457:MET:HE2	1:B:462:LEU:CD1	2.20	0.70
1:B:258:ILE:HD12	1:B:263:LEU:CD1	2.22	0.70
1:B:443:PRO:HD2	1:B:446:ILE:HD12	1.73	0.69
1:A:95:LEU:HB2	1:A:142:MET:CE	2.17	0.69
1:B:165:GLY:HA3	6:B:1018:HOH:O	1.92	0.69
1:A:258:ILE:HD12	1:A:263:LEU:HD11	1.72	0.69
1:A:443:PRO:HD2	1:A:446:ILE:HD12	1.73	0.69
1:B:151:SER:HA	1:B:174:LEU:HD22	1.75	0.69
1:A:310:SER:OG	1:A:332:ASN:OD1	2.11	0.69
5:A:804:BLD:H221	5:A:804:BLD:H112	1.73	0.68
1:B:501:MET:HE3	6:B:1000:HOH:O	1.93	0.68
1:A:479:THR:C	1:A:501:MET:HE1	2.20	0.67
1:A:105:GLN:HB3	1:A:128:GLN:HG3	1.75	0.66
1:B:399:GLN:C	1:B:401:SER:HA	2.20	0.66
1:A:41:PHE:CD1	1:A:98:LEU:HD21	2.30	0.66
1:A:95:LEU:HD22	1:A:142:MET:CE	2.18	0.66
1:A:558:ASN:OD1	2:C:1:NAG:C2	2.40	0.66
1:B:374:CYS:HB3	6:B:1054:HOH:O	1.94	0.65
1:B:117:GLY:CA	1:B:142:MET:HE3	2.26	0.65
1:A:479:THR:HA	1:A:501:MET:CE	2.26	0.65
1:B:501:MET:CE	6:B:1000:HOH:O	2.44	0.65
1:A:281:GLN:CB	3:D:1:NAG:H81	2.28	0.64
1:A:399:GLN:HG2	1:A:401:SER:CA	2.24	0.64
1:A:119:ASP:CG	1:A:120:SER:N	2.54	0.64
1:A:418:VAL:HG12	1:A:446:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLN:O	1:B:303:THR:HG21	1.98	0.64
1:A:174:LEU:O	1:A:200:PRO:HG3	1.99	0.63
1:A:95:LEU:HB3	1:A:118:GLY:HA3	1.81	0.63
5:A:804:BLD:H221	5:A:804:BLD:C12	2.29	0.62
1:A:372:THR:HG22	1:A:395:PHE:CD1	2.35	0.62
1:B:392:PRO:HB2	1:B:395:PHE:CD2	2.34	0.62
1:A:399:GLN:C	1:A:401:SER:HA	2.24	0.62
1:A:631:THR:HG22	5:A:804:BLD:H228	1.81	0.61
1:A:153:LEU:CD2	1:A:156:VAL:CG2	2.78	0.61
1:A:258:ILE:HD11	1:A:284:LEU:HD22	1.80	0.61
1:B:575:MET:HE1	1:B:637:ALA:CB	2.31	0.61
1:B:123:SER:OG	1:B:124:ASP:N	2.33	0.60
1:A:642:ILE:N	1:A:642:ILE:HD13	2.16	0.60
3:D:2:NAG:H3	3:D:2:NAG:H83	1.82	0.60
1:A:399:GLN:CG	1:A:400:SER:N	2.60	0.60
1:B:392:PRO:HG2	1:B:395:PHE:HE2	1.66	0.60
5:B:801:BLD:H112	5:B:801:BLD:H221	1.82	0.60
1:B:41:PHE:CD1	1:B:98:LEU:HD21	2.36	0.60
1:A:119:ASP:OD2	1:A:120:SER:N	2.33	0.59
1:A:132:LEU:HD13	1:A:142:MET:HE1	1.85	0.59
1:A:684:GLY:HA3	1:A:706:SER:OG	2.02	0.59
1:A:510:ARG:HH11	1:A:510:ARG:CG	1.95	0.59
4:A:815:NAG:H82	4:A:815:NAG:HO3	1.68	0.59
1:A:358:VAL:CG2	1:A:382:LEU:HD23	2.33	0.58
1:A:59:TYR:CE1	1:A:60:GLU:HG3	2.39	0.58
1:A:255:THR:HB	1:A:281:GLN:HB2	1.85	0.58
1:A:596:ARG:HD3	1:A:648:TYR:CE2	2.38	0.58
1:A:753:ARG:NH1	1:A:754:PRO:HD2	2.18	0.57
1:B:631:THR:HG22	5:B:801:BLD:H228	1.85	0.57
1:B:118:GLY:HA3	1:B:120:SER:OG	2.04	0.57
1:B:59:TYR:CE1	1:B:60:GLU:HG3	2.39	0.57
1:B:279:LEU:HD23	1:B:300:LEU:HD22	1.87	0.57
1:A:510:ARG:NH1	1:A:510:ARG:CG	2.61	0.56
1:B:41:PHE:CE1	1:B:98:LEU:HD11	2.40	0.56
1:B:418:VAL:HG12	1:B:446:ILE:HD11	1.87	0.56
1:B:477:LEU:HB2	1:B:501:MET:CE	2.31	0.56
1:A:716:LEU:HD22	1:A:733:LEU:CD1	2.36	0.56
1:B:676:THR:HG22	1:B:698:ASN:HB2	1.86	0.56
1:A:400:SER:N	1:A:401:SER:CA	2.67	0.56
1:A:501:MET:CE	1:A:503:TRP:O	2.53	0.56
1:B:718:VAL:HG13	1:B:723:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HE2	1:A:59:TYR:HH	1.52	0.55
1:A:317:GLU:HG2	1:A:339:SER:O	2.07	0.55
1:B:166:LYS:N	6:B:1018:HOH:O	2.38	0.55
1:B:358:VAL:CG2	1:B:382:LEU:HD23	2.36	0.55
1:A:37:LEU:HD21	1:A:97:ASN:O	2.06	0.55
1:B:433:LEU:HB2	1:B:457:MET:HG2	1.87	0.55
1:B:308:ASP:OD1	1:B:310:SER:HB2	2.07	0.55
1:B:418:VAL:HG12	1:B:446:ILE:CD1	2.37	0.55
1:B:281:GLN:HB3	3:I:1:NAG:H81	1.90	0.54
1:B:358:VAL:HG23	1:B:382:LEU:HD23	1.89	0.54
1:B:59:TYR:CZ	1:B:60:GLU:HG3	2.43	0.54
1:B:590:GLU:CB	1:B:624:THR:HG21	2.38	0.54
1:B:32:PHE:HZ	1:B:59:TYR:HH	1.50	0.54
3:D:2:NAG:H83	3:D:2:NAG:C3	2.37	0.54
1:B:614:ARG:HB2	1:B:614:ARG:NH1	2.23	0.53
1:B:54:LEU:HD22	1:B:57:TRP:CE2	2.44	0.53
1:B:468:GLU:OE2	1:B:494:SER:HB2	2.07	0.53
1:A:80:VAL:HG23	1:A:105:GLN:HG3	1.90	0.53
1:A:241:ASP:C	1:A:242:LYS:HG3	2.34	0.53
1:B:421:GLU:O	1:B:424:LYS:HB2	2.09	0.53
1:A:581:GLY:O	1:A:630:MET:HE3	2.09	0.53
1:B:418:VAL:HG11	1:B:446:ILE:HD13	1.91	0.52
1:A:716:LEU:CD2	1:A:733:LEU:CD1	2.88	0.52
1:A:480:LEU:H	1:A:501:MET:CE	2.19	0.52
1:A:706:SER:HB2	6:A:916:HOH:O	2.10	0.52
1:B:150:CYS:O	1:B:174:LEU:HD22	2.10	0.52
5:B:801:BLD:H221	5:B:801:BLD:C12	2.40	0.51
1:A:322:PHE:O	1:A:325:CYS:HB2	2.10	0.51
1:B:108:TYR:OH	6:B:964:HOH:O	2.11	0.51
1:B:409:ILE:HG21	1:B:414:LEU:HD11	1.91	0.51
1:A:716:LEU:HD22	1:A:733:LEU:HD11	1.93	0.51
1:B:738:VAL:CG1	6:B:1044:HOH:O	2.59	0.51
1:A:395:PHE:HB2	6:A:1015:HOH:O	2.10	0.50
1:A:247:LEU:N	1:A:248:PRO:CD	2.74	0.50
1:A:409:ILE:HG21	1:A:414:LEU:HD11	1.93	0.50
1:B:217:PHE:O	1:B:244:PRO:HG3	2.12	0.50
1:B:117:GLY:HA2	1:B:142:MET:CE	2.41	0.50
1:A:502:ILE:HD11	1:A:578:SER:HB3	1.94	0.49
1:B:267:ILE:HD11	1:B:314:PHE:CZ	2.48	0.49
1:A:93:LEU:HD21	1:A:142:MET:HE1	1.94	0.49
1:A:392:PRO:HG2	1:A:395:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ASN:HB2	1:B:368:PRO:HB3	1.95	0.49
1:B:454:ASP:HA	1:B:479:THR:HG22	1.94	0.49
1:B:575:MET:HE1	1:B:637:ALA:HB2	1.95	0.49
1:B:37:LEU:HD23	1:B:37:LEU:C	2.38	0.48
3:D:2:NAG:H3	3:D:2:NAG:C8	2.43	0.48
1:A:79:ILE:HD12	1:A:101:LEU:HD22	1.95	0.48
1:B:398:LEU:HD22	1:B:399:GLN:O	2.13	0.48
1:A:308:ASP:OD1	1:A:310:SER:HB2	2.13	0.48
1:B:575:MET:HE1	1:B:637:ALA:HB1	1.94	0.48
1:A:467:PRO:O	1:A:470:VAL:HG23	2.14	0.48
1:B:247:LEU:N	1:B:248:PRO:CD	2.76	0.48
1:A:691:VAL:HG22	1:A:715:ASP:HB3	1.96	0.48
1:A:76:ASP:OD2	1:A:76:ASP:N	2.47	0.47
1:A:418:VAL:CG1	1:A:446:ILE:CD1	2.92	0.47
1:B:654:PHE:C	1:B:654:PHE:CD2	2.92	0.47
1:A:267:ILE:HD11	1:A:314:PHE:CZ	2.50	0.47
1:A:461:ASN:HB2	6:A:1053:HOH:O	2.15	0.47
1:B:418:VAL:CG1	1:B:446:ILE:CD1	2.93	0.47
1:B:429:LYS:HB3	1:B:429:LYS:HE3	1.66	0.47
1:B:447:TRP:O	1:B:474:GLY:HA3	2.14	0.47
1:B:738:VAL:HG12	6:B:1044:HOH:O	2.14	0.47
1:A:132:LEU:CD1	1:A:142:MET:HE1	2.45	0.47
1:A:153:LEU:CD2	1:A:156:VAL:HG22	2.27	0.47
1:A:635:PHE:HE2	1:A:642:ILE:HD11	1.78	0.47
1:A:470:VAL:C	1:A:472:VAL:H	2.23	0.47
1:A:575:MET:HE1	1:A:637:ALA:CB	2.45	0.46
1:B:579:VAL:HG12	1:B:633:TYR:OH	2.15	0.46
1:B:581:GLY:HA2	1:B:630:MET:HG3	1.97	0.46
3:D:2:NAG:C3	3:D:2:NAG:C8	2.92	0.46
1:A:41:PHE:CE1	1:A:98:LEU:HD11	2.50	0.46
1:B:380:LEU:CD2	1:B:395:PHE:CZ	2.98	0.46
1:B:37:LEU:HD21	1:B:97:ASN:O	2.15	0.46
1:A:501:MET:HE3	1:A:503:TRP:O	2.15	0.46
1:B:686:LEU:O	1:B:710:LEU:HD22	2.16	0.46
1:A:31:ASP:C	1:A:32:PHE:CD2	2.93	0.46
1:B:610:GLU:OE1	2:H:2:NAG:H82	2.16	0.46
1:A:358:VAL:HG23	1:A:382:LEU:HD23	1.98	0.46
1:B:117:GLY:C	1:B:142:MET:HE3	2.37	0.46
1:A:434:SER:OG	1:A:456:VAL:HG12	2.16	0.46
1:B:117:GLY:HA2	1:B:142:MET:HE3	1.98	0.46
1:A:418:VAL:HG12	1:A:446:ILE:CD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:CD2	1:B:156:VAL:HG22	2.38	0.45
1:B:545:ASN:O	1:B:547:LYS:HD2	2.16	0.45
1:A:45:SER:O	1:A:91:GLY:HA3	2.16	0.45
1:A:734:THR:HB	1:A:750:VAL:HG12	1.97	0.45
1:A:398:LEU:O	1:A:398:LEU:HG	2.16	0.45
1:B:392:PRO:HB2	1:B:395:PHE:CE2	2.52	0.45
1:B:398:LEU:CD2	1:B:399:GLN:N	2.64	0.45
1:B:691:VAL:HG23	5:B:801:BLD:H02	1.98	0.44
1:A:564:PRO:HG2	1:A:567:LEU:HG	2.00	0.44
5:A:804:BLD:H20	5:A:804:BLD:H24	1.79	0.44
2:E:1:NAG:H62	2:E:2:NAG:C1	2.47	0.44
1:A:405:GLU:OE2	6:A:999:HOH:O	2.21	0.44
1:A:470:VAL:HG12	1:A:471:CYS:SG	2.58	0.44
1:A:479:THR:CA	1:A:501:MET:HE1	2.47	0.44
1:B:418:VAL:CG1	1:B:446:ILE:HD13	2.47	0.44
1:A:241:ASP:HB3	1:A:242:LYS:HG3	2.00	0.44
1:A:576:PRO:HA	1:A:633:TYR:CE1	2.53	0.44
1:B:153:LEU:HD21	1:B:156:VAL:CG2	2.41	0.44
1:B:218:SER:HB3	1:B:242:LYS:O	2.17	0.44
1:B:258:ILE:HD12	1:B:263:LEU:HD11	1.98	0.44
1:A:83:ASP:OD1	1:A:85:ARG:NH2	2.47	0.43
1:B:635:PHE:HB3	1:B:664:TYR:CE1	2.53	0.43
1:A:32:PHE:HE2	1:A:59:TYR:OH	2.01	0.43
1:B:174:LEU:O	1:B:200:PRO:HG3	2.18	0.43
1:B:434:SER:OG	1:B:456:VAL:HG12	2.18	0.43
1:B:321:GLN:CD	1:B:321:GLN:H	2.26	0.43
1:A:392:PRO:HB2	1:A:395:PHE:CE2	2.52	0.43
1:A:503:TRP:CD1	1:A:503:TRP:C	2.96	0.43
1:A:392:PRO:HB2	1:A:395:PHE:CD2	2.54	0.43
1:B:718:VAL:HG13	1:B:718:VAL:O	2.18	0.43
1:A:473:LYS:HD2	1:A:473:LYS:HA	1.81	0.43
1:B:413:TYR:CD2	1:B:413:TYR:N	2.87	0.43
1:A:40:ALA:O	1:A:44:ASN:HB2	2.19	0.43
1:A:143:VAL:HG22	1:A:158:ILE:HD12	1.99	0.43
1:B:158:ILE:O	1:B:158:ILE:HG22	2.18	0.42
1:B:259:SER:HB3	1:B:283:SER:OG	2.19	0.42
1:B:32:PHE:CE2	1:B:59:TYR:CE1	3.07	0.42
1:A:689:ILE:HG23	1:A:689:ILE:O	2.18	0.42
1:A:417:THR:HB	6:A:971:HOH:O	2.19	0.42
1:A:679:ILE:HD12	1:A:703:LEU:HD23	2.01	0.42
1:B:93:LEU:HG	1:B:142:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG22	1:B:158:ILE:HD12	2.00	0.42
1:B:596:ARG:HD3	1:B:648:TYR:CD2	2.54	0.42
1:A:95:LEU:CB	1:A:118:GLY:HA3	2.49	0.42
1:A:501:MET:HE2	1:A:504:ILE:CG1	2.50	0.42
5:B:801:BLD:O06	5:B:801:BLD:C19	2.67	0.42
1:B:587:VAL:HB	1:B:599:GLY:CA	2.49	0.42
1:A:418:VAL:HG11	1:A:446:ILE:HD13	2.01	0.42
1:B:401:SER:O	1:B:402:PRO:C	2.62	0.42
1:A:59:TYR:HD1	1:A:60:GLU:N	2.18	0.42
1:B:245:ILE:O	1:B:248:PRO:HD2	2.20	0.42
1:B:380:LEU:HD22	1:B:395:PHE:CZ	2.55	0.42
1:B:53:VAL:HG21	1:B:87:SER:HB3	2.02	0.41
1:A:80:VAL:HG22	1:A:80:VAL:O	2.21	0.41
1:A:372:THR:HG22	1:A:395:PHE:CE1	2.55	0.41
1:B:546:CYS:HB3	6:B:901:HOH:O	2.19	0.41
1:B:590:GLU:HG2	1:B:624:THR:CB	2.50	0.41
1:A:281:GLN:N	1:A:281:GLN:OE1	2.54	0.41
1:A:596:ARG:CD	1:A:648:TYR:CD2	3.04	0.41
5:A:804:BLD:H119	5:A:804:BLD:H08	1.85	0.41
1:B:321:GLN:CD	1:B:321:GLN:N	2.78	0.41
1:A:247:LEU:HB3	1:A:248:PRO:HD3	2.03	0.41
1:A:260:ARG:HG2	1:A:286:HIS:HB2	2.02	0.41
1:A:479:THR:HA	1:A:501:MET:HE1	2.03	0.41
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.86	0.41
1:B:423:GLY:HA3	1:B:445:GLU:HB3	2.02	0.41
1:A:642:ILE:C	1:A:665:LEU:HD12	2.46	0.41
1:A:457:MET:HB2	1:A:482:LEU:CD2	2.51	0.41
1:A:93:LEU:O	1:A:117:GLY:CA	2.69	0.41
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.19	0.41
1:A:641:MET:HE3	1:A:641:MET:HB2	1.82	0.41
1:B:550:ILE:HB	1:B:642:ILE:HG12	2.03	0.41
1:B:550:ILE:HA	1:B:641:MET:HA	2.02	0.41
1:B:610:GLU:CD	1:B:610:GLU:H	2.29	0.41
1:A:32:PHE:CD2	1:A:32:PHE:N	2.89	0.41
1:B:293:ILE:HA	1:B:294:PRO:HD3	1.94	0.41
1:B:305:VAL:HG21	6:B:983:HOH:O	2.21	0.41
1:A:591:GLY:HA3	1:A:595:CYS:SG	2.60	0.40
1:A:733:LEU:HD13	1:A:733:LEU:HA	1.89	0.40
1:B:182:LEU:HB2	1:B:208:LEU:HD23	2.02	0.40
1:A:132:LEU:CD1	1:A:142:MET:CE	2.99	0.40
1:A:588:ARG:NH1	1:A:627:TYR:OH	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:GLY:O	1:B:545:ASN:ND2	2.49	0.40
1:A:546:CYS:HB3	6:A:901:HOH:O	2.22	0.40
1:B:477:LEU:O	1:B:501:MET:CE	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:OD1	1:B:541:ARG:NH1[1_545]	1.99	0.21

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	720/740 (97%)	685 (95%)	35 (5%)	0	100	100
1	B	720/740 (97%)	693 (96%)	27 (4%)	0	100	100
All	All	1440/1480 (97%)	1378 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/641 (98%)	599 (96%)	28 (4%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	627/641 (98%)	604 (96%)	23 (4%)	30	57
All	All	1254/1282 (98%)	1203 (96%)	51 (4%)	27	53

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	158	ILE
1	A	186	ILE
1	A	212	ASN
1	A	220	LEU
1	A	237	ASN
1	A	241	ASP
1	A	255	THR
1	A	305	VAL
1	A	325	CYS
1	A	353	ILE
1	A	371	LEU
1	A	403	VAL
1	A	407	ILE
1	A	435	PHE
1	A	437	GLU
1	A	453	SER
1	A	510	ARG
1	A	579	VAL
1	A	593	THR
1	A	613	GLU
1	A	618	VAL
1	A	630	MET
1	A	642	ILE
1	A	687	LYS
1	A	718	VAL
1	A	722	ASN
1	A	724	THR
1	B	76	ASP
1	B	119	ASP
1	B	123	SER
1	B	149	LYS
1	B	158	ILE
1	B	174	LEU
1	B	186	ILE
1	B	305	VAL

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Mol	Chain	Res	Type
1	B	310	SER
1	B	353	ILE
1	B	369	ILE
1	B	397	SER
1	B	403	VAL
1	B	409	ILE
1	B	435	PHE
1	B	468	GLU
1	B	479	THR
1	B	614	ARG
1	B	628	SER
1	B	630	MET
1	B	718	VAL
1	B	722	ASN
1	B	733	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	344	ASN
1	A	555	ASN
1	B	43	GLN
1	B	52	ASN
1	B	175	GLN
1	B	262	ASN
1	B	344	ASN
1	B	399	GLN
1	B	483	ASN
1	B	484	ASN
1	B	555	ASN
1	B	666	GLN
1	B	672	HIS
1	B	696	HIS

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 ⓘ

26 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	0.51	0	17,19,21	1.67	1 (5%)
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	1.33	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.58	0	17,19,21	1.84	4 (23%)
3	NAG	D	2	3	14,14,15	1.90	4 (28%)	17,19,21	2.15	5 (29%)
3	BMA	D	3	3	11,11,12	1.09	1 (9%)	15,15,17	1.41	2 (13%)
3	MAN	D	4	3	11,11,12	1.42	3 (27%)	15,15,17	1.82	3 (20%)
3	MAN	D	5	3	11,11,12	3.96	1 (9%)	15,15,17	1.33	1 (6%)
3	MAN	D	6	3	11,11,12	2.03	5 (45%)	15,15,17	1.55	3 (20%)
2	NAG	E	1	2,1	14,14,15	1.93	3 (21%)	17,19,21	2.63	6 (35%)
2	NAG	E	2	2	14,14,15	1.66	3 (21%)	17,19,21	2.41	5 (29%)
2	NAG	F	1	2,1	14,14,15	0.59	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.47	0	17,19,21	0.89	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.48	0	17,19,21	2.29	7 (41%)
2	NAG	G	2	2	14,14,15	0.47	0	17,19,21	1.07	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.51	0	17,19,21	1.77	1 (5%)
2	NAG	H	2	2	14,14,15	0.48	0	17,19,21	1.51	1 (5%)
3	NAG	I	1	3,1	14,14,15	2.06	7 (50%)	17,19,21	2.12	3 (17%)
3	NAG	I	2	3	14,14,15	2.31	6 (42%)	17,19,21	2.54	2 (11%)
3	BMA	I	3	3	11,11,12	1.06	2 (18%)	15,15,17	1.31	2 (13%)
3	MAN	I	4	3	11,11,12	1.66	3 (27%)	15,15,17	1.70	3 (20%)
3	MAN	I	5	3	11,11,12	2.16	4 (36%)	15,15,17	2.96	4 (26%)
3	MAN	I	6	3	11,11,12	2.34	5 (45%)	15,15,17	1.38	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	1	2,1	14,14,15	0.66	0	17,19,21	1.09	2 (11%)
2	NAG	J	2	2	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
2	NAG	K	2	2	14,14,15	0.51	0	17,19,21	0.78	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	MAN	I	5	3	-	2/2/19/22	0/1/1/1
3	MAN	I	6	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	MAN	O6-C6	-12.91	0.88	1.42
3	I	2	NAG	O5-C1	-4.89	1.35	1.43
3	I	6	MAN	O5-C1	-4.44	1.36	1.43
3	I	1	NAG	O5-C1	-4.39	1.36	1.43
3	I	5	MAN	O5-C1	-4.06	1.36	1.43
3	I	4	MAN	O5-C1	-3.74	1.37	1.43
3	I	2	NAG	O5-C5	-3.71	1.36	1.43
3	I	6	MAN	O5-C5	-3.71	1.36	1.43
3	D	2	NAG	O5-C1	-3.60	1.37	1.43
3	D	6	MAN	O5-C5	-3.59	1.36	1.43
2	E	1	NAG	C2-N2	-3.42	1.40	1.46
2	E	1	NAG	O5-C1	-3.36	1.38	1.43
3	D	6	MAN	O5-C1	-3.33	1.38	1.43
3	D	2	NAG	O5-C5	-3.32	1.37	1.43
3	I	1	NAG	C2-N2	-3.10	1.41	1.46
3	I	6	MAN	O2-C2	-3.09	1.36	1.43
3	I	5	MAN	O5-C5	-3.04	1.37	1.43
2	E	2	NAG	O5-C1	-3.03	1.38	1.43
3	D	6	MAN	O4-C4	-2.94	1.35	1.43
3	I	5	MAN	O3-C3	-2.88	1.35	1.43
3	I	2	NAG	C2-N2	-2.85	1.41	1.46
3	I	5	MAN	O4-C4	-2.77	1.36	1.43
3	I	6	MAN	O4-C4	-2.76	1.36	1.43
3	D	2	NAG	O3-C3	-2.76	1.36	1.43
2	E	1	NAG	O3-C3	-2.76	1.36	1.43
3	D	2	NAG	C7-N2	-2.61	1.25	1.34
3	I	2	NAG	O7-C7	-2.60	1.17	1.23
3	D	4	MAN	O2-C2	-2.57	1.37	1.43
3	I	4	MAN	O4-C4	-2.57	1.36	1.43
2	E	2	NAG	C2-N2	-2.57	1.42	1.46
3	I	1	NAG	O3-C3	-2.54	1.36	1.43
3	I	2	NAG	O3-C3	-2.53	1.36	1.43
3	I	6	MAN	O3-C3	-2.39	1.37	1.43
3	D	3	BMA	O5-C1	-2.38	1.39	1.43
3	I	4	MAN	O2-C2	-2.36	1.38	1.43
3	D	4	MAN	O4-C4	-2.34	1.37	1.43
3	I	1	NAG	O5-C5	-2.31	1.38	1.43
3	I	1	NAG	O4-C4	-2.30	1.37	1.43
3	D	4	MAN	O5-C1	-2.29	1.39	1.43
3	I	1	NAG	C1-C2	-2.27	1.49	1.52
3	D	6	MAN	O3-C3	-2.21	1.37	1.43
3	I	3	BMA	O5-C1	-2.17	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	BMA	O5-C5	-2.17	1.39	1.43
2	E	2	NAG	O5-C5	-2.16	1.39	1.43
3	I	2	NAG	C7-N2	-2.11	1.27	1.34
3	I	1	NAG	O7-C7	-2.07	1.18	1.23
3	D	6	MAN	O2-C2	-2.02	1.39	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	O5-C1-C2	-7.80	99.22	111.29
3	I	5	MAN	C1-O5-C5	7.52	122.26	112.19
3	I	5	MAN	O5-C5-C6	-7.36	93.33	107.66
2	G	1	NAG	C1-O5-C5	6.93	121.48	112.19
2	H	1	NAG	C1-O5-C5	6.59	121.02	112.19
3	D	2	NAG	O5-C1-C2	-6.59	101.10	111.29
2	E	1	NAG	O5-C1-C2	-6.46	101.30	111.29
2	E	2	NAG	C3-C4-C5	-6.39	98.65	110.23
2	C	1	NAG	C1-O5-C5	6.33	120.66	112.19
3	I	1	NAG	O5-C1-C2	-5.54	102.72	111.29
3	I	2	NAG	C3-C4-C5	-5.46	100.34	110.23
2	E	1	NAG	C6-C5-C4	-5.29	100.02	113.02
2	H	2	NAG	C1-O5-C5	5.23	119.19	112.19
3	I	1	NAG	C1-O5-C5	5.14	119.07	112.19
3	D	1	NAG	C2-N2-C7	-4.58	116.77	122.90
2	C	2	NAG	C1-O5-C5	4.47	118.17	112.19
2	E	1	NAG	C1-O5-C5	4.38	118.05	112.19
3	D	4	MAN	C2-C3-C4	-4.34	103.23	110.86
2	E	2	NAG	C2-N2-C7	-4.27	117.18	122.90
2	J	2	NAG	C2-N2-C7	-4.20	117.27	122.90
3	I	4	MAN	C2-C3-C4	-4.20	103.48	110.86
3	D	4	MAN	C1-O5-C5	4.01	117.56	112.19
2	E	2	NAG	C4-C3-C2	-3.67	105.64	111.02
2	G	1	NAG	O5-C1-C2	3.57	116.82	111.29
2	E	1	NAG	O3-C3-C4	-3.57	101.97	110.38
3	D	6	MAN	C1-O5-C5	3.45	116.81	112.19
3	D	5	MAN	C1-O5-C5	3.44	116.79	112.19
3	D	1	NAG	C1-O5-C5	3.34	116.66	112.19
3	D	2	NAG	C2-N2-C7	3.23	127.23	122.90
3	D	2	NAG	C4-C3-C2	-2.98	106.65	111.02
3	I	5	MAN	C1-C2-C3	-2.93	105.38	109.64
3	I	6	MAN	C6-C5-C4	-2.89	105.93	113.02
3	I	4	MAN	C1-O5-C5	2.88	116.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	O3-C3-C2	2.72	115.60	110.05
2	J	1	NAG	C1-O5-C5	2.70	115.80	112.19
2	G	2	NAG	C1-O5-C5	2.61	115.69	112.19
2	F	2	NAG	C1-O5-C5	2.58	115.64	112.19
2	E	2	NAG	C1-C2-N2	2.58	114.49	110.43
3	D	4	MAN	O6-C6-C5	2.56	120.06	111.33
2	G	1	NAG	O5-C5-C4	2.51	116.94	110.83
3	D	1	NAG	C3-C4-C5	2.50	114.76	110.23
3	D	6	MAN	C6-C5-C4	-2.47	106.94	113.02
2	K	1	NAG	C4-C3-C2	2.47	114.63	111.02
3	I	5	MAN	O2-C2-C3	-2.46	105.06	110.15
3	I	6	MAN	O4-C4-C3	-2.39	104.74	110.38
3	I	4	MAN	O6-C6-C5	2.39	119.48	111.33
3	I	1	NAG	C6-C5-C4	-2.39	107.15	113.02
2	J	1	NAG	O5-C1-C2	-2.37	107.62	111.29
3	I	3	BMA	C1-O5-C5	2.34	115.32	112.19
3	I	3	BMA	O5-C1-C2	-2.30	105.30	110.79
2	E	2	NAG	O5-C5-C4	-2.29	105.25	110.83
3	D	2	NAG	O3-C3-C2	2.26	114.10	109.40
2	G	2	NAG	C2-N2-C7	-2.26	119.88	122.90
2	G	1	NAG	C6-C5-C4	-2.14	107.76	113.02
2	G	1	NAG	C2-N2-C7	2.13	125.75	122.90
3	D	6	MAN	O4-C4-C5	-2.10	104.15	109.32
3	D	3	BMA	C1-O5-C5	2.09	114.98	112.19
2	F	2	NAG	C2-N2-C7	-2.08	120.11	122.90
2	G	1	NAG	C1-C2-N2	-2.07	107.17	110.43
3	D	1	NAG	C6-C5-C4	-2.07	107.94	113.02
2	G	1	NAG	C3-C4-C5	2.04	113.94	110.23
3	D	2	NAG	C3-C4-C5	-2.03	106.56	110.23
2	E	1	NAG	C1-C2-N2	-2.01	107.26	110.43
2	E	1	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	I	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	I	6	MAN	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	3	BMA	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	I	5	MAN	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
3	D	4	MAN	C4-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
3	I	4	MAN	C4-C5-C6-O6
2	F	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
3	D	3	BMA	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 12 short contacts:

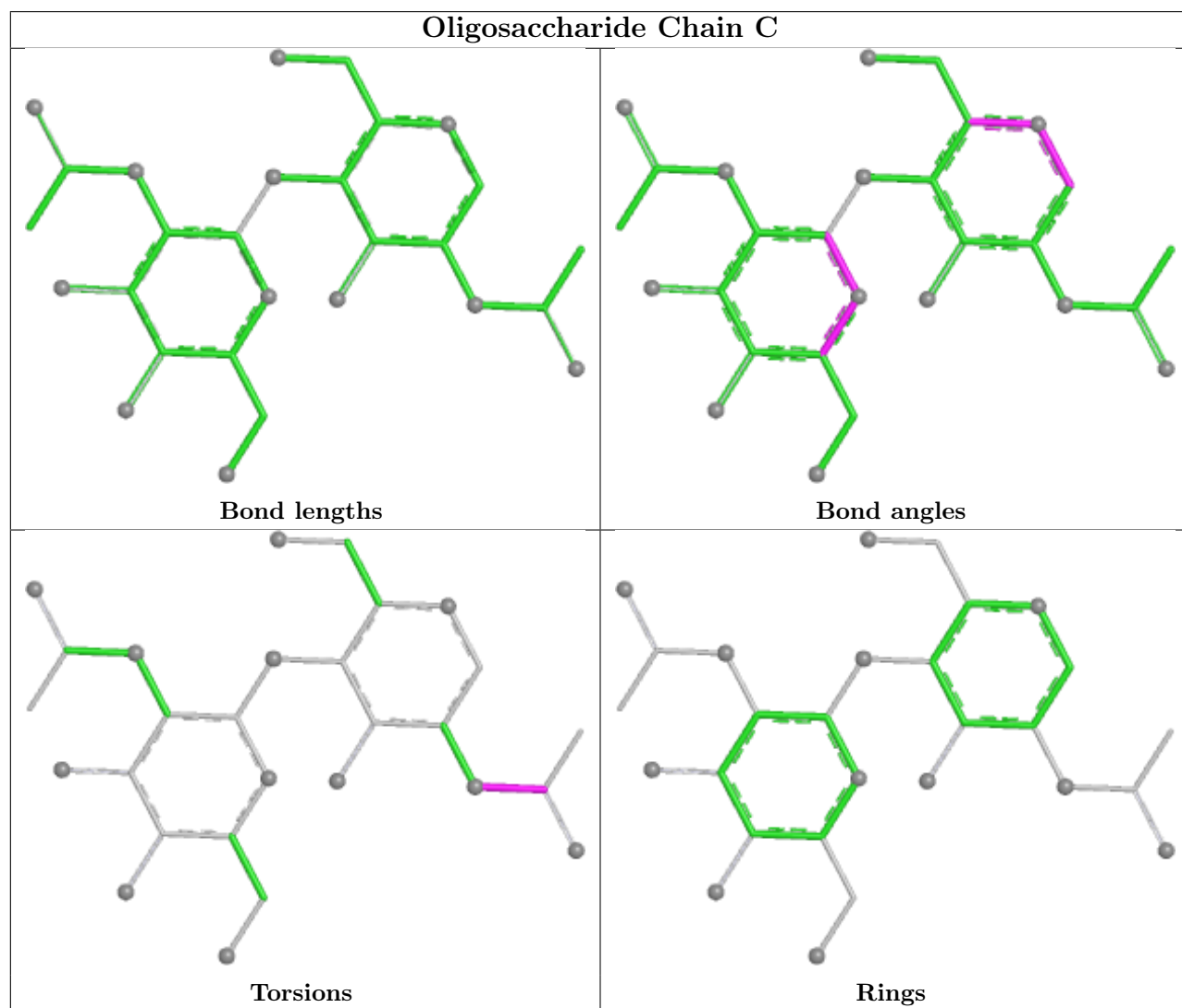
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
2	H	2	NAG	1	0
2	C	1	NAG	2	0
3	D	1	NAG	3	0

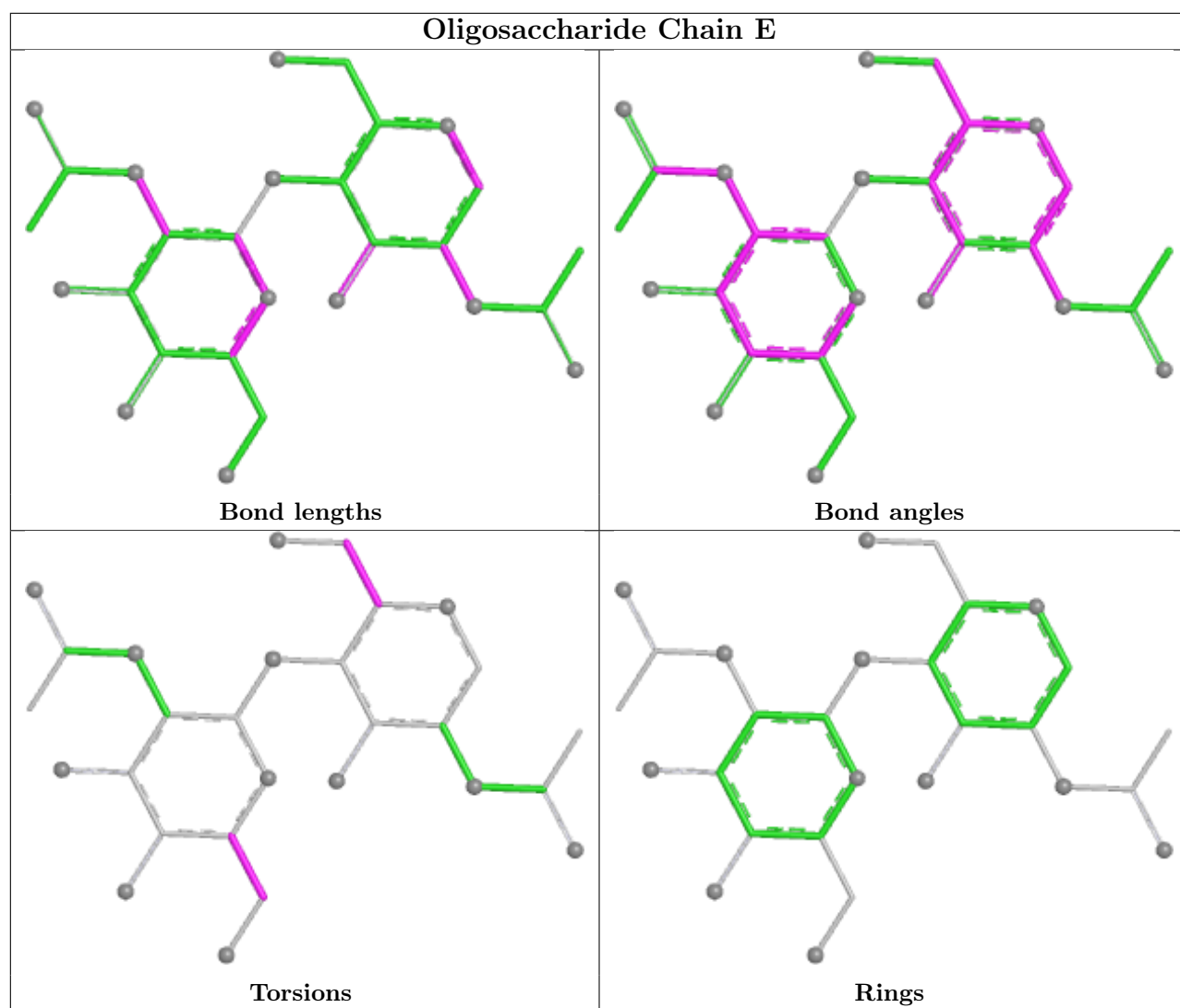
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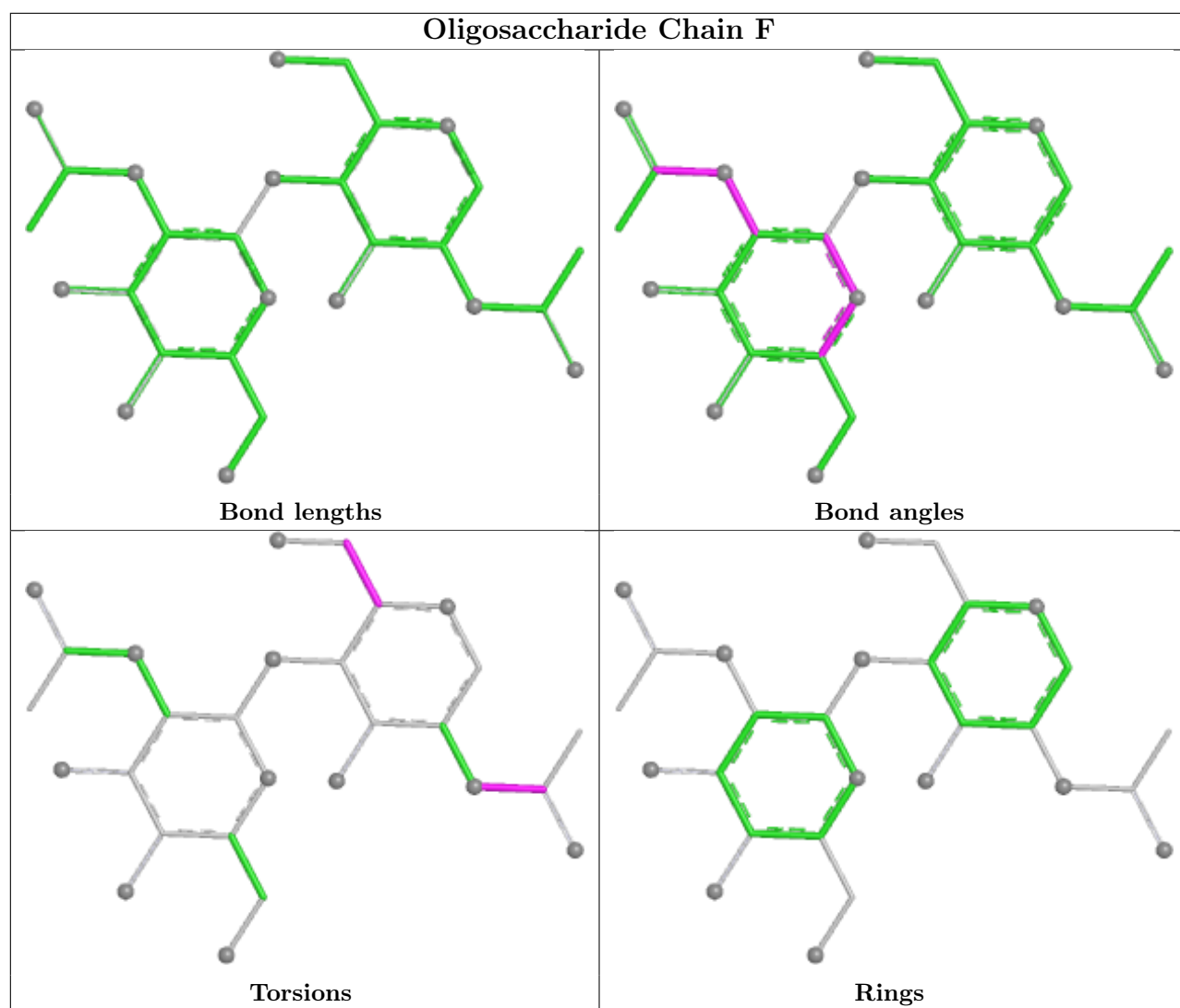
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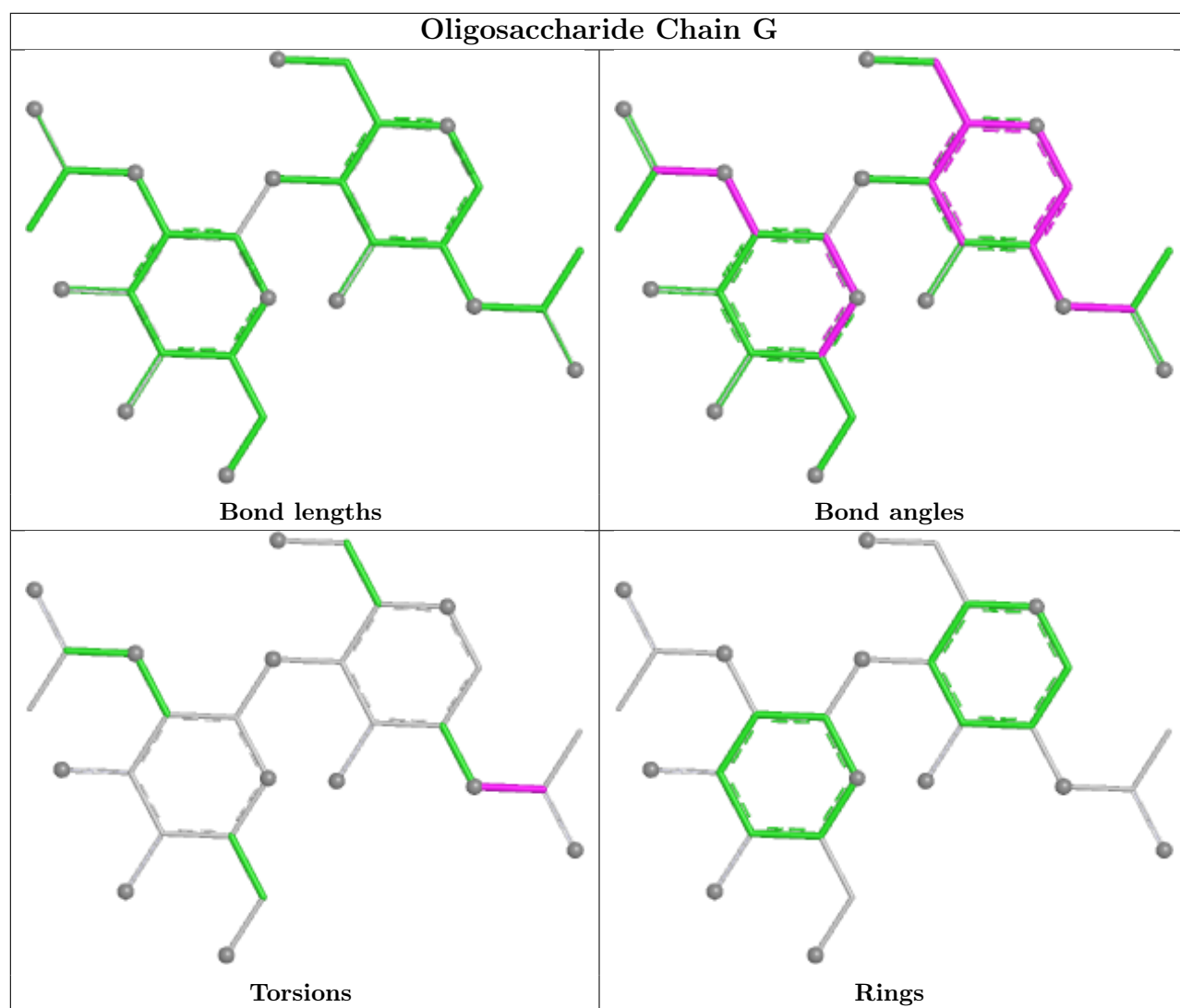
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	D	2	NAG	4	0
2	E	1	NAG	1	0

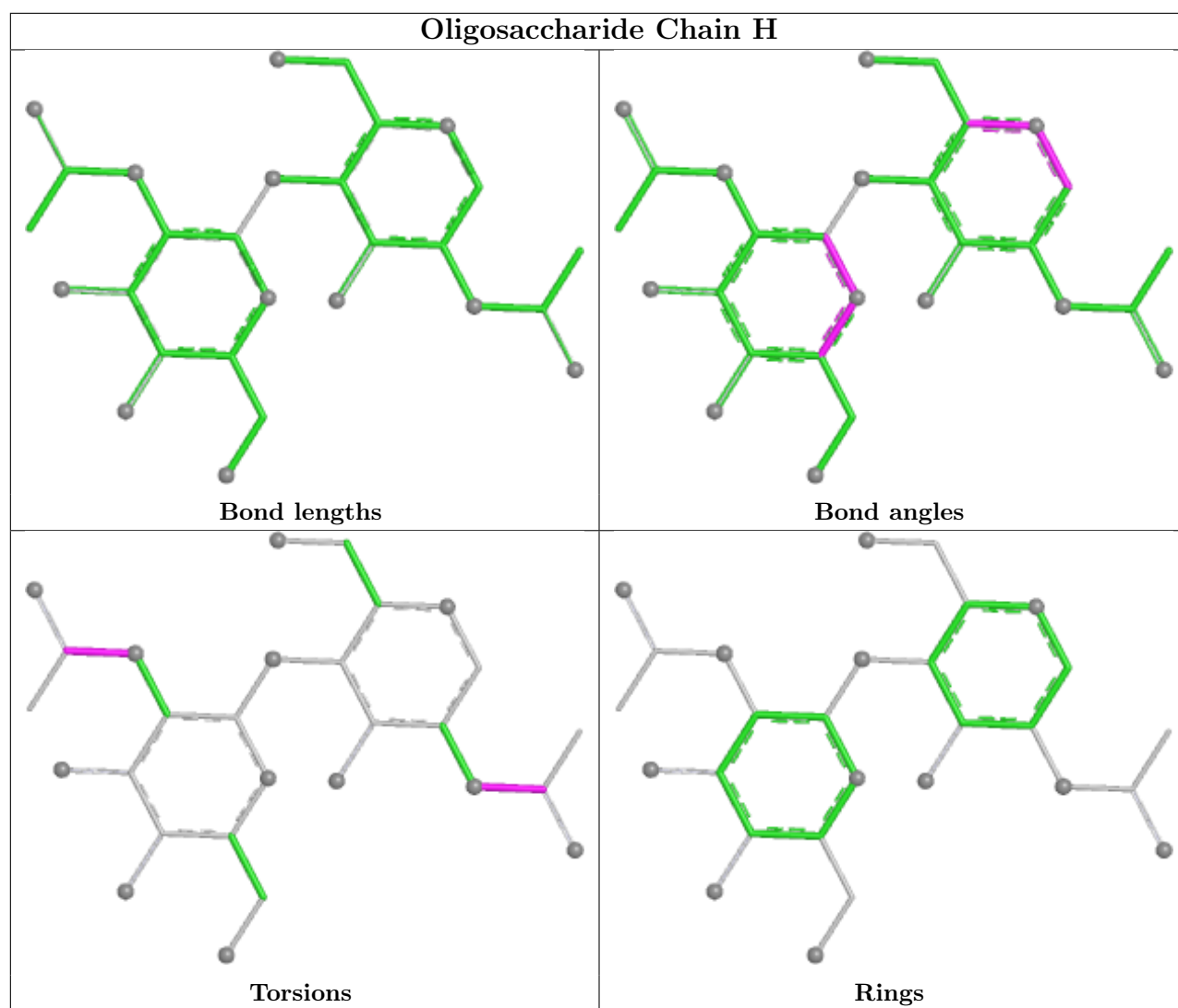
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

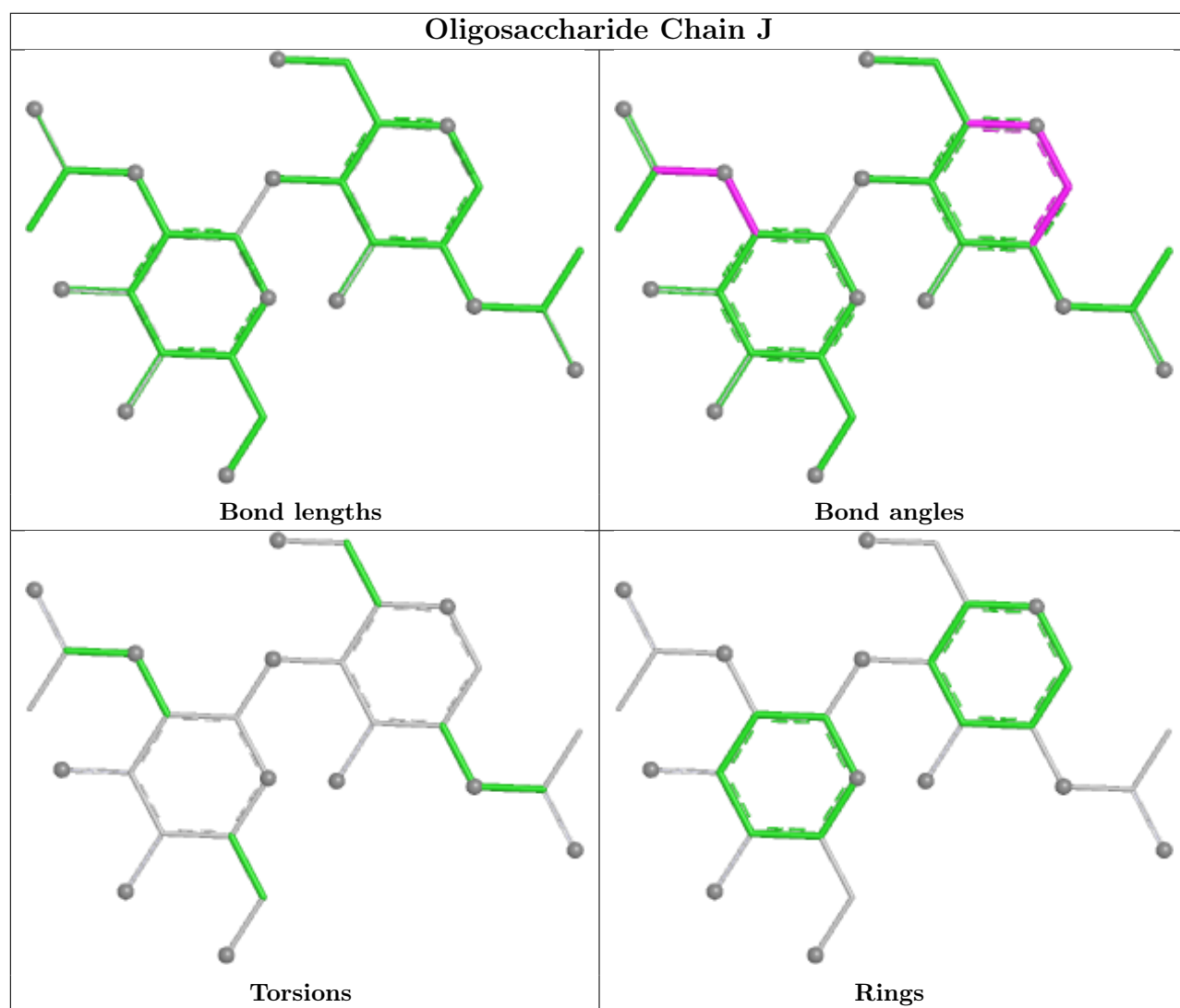




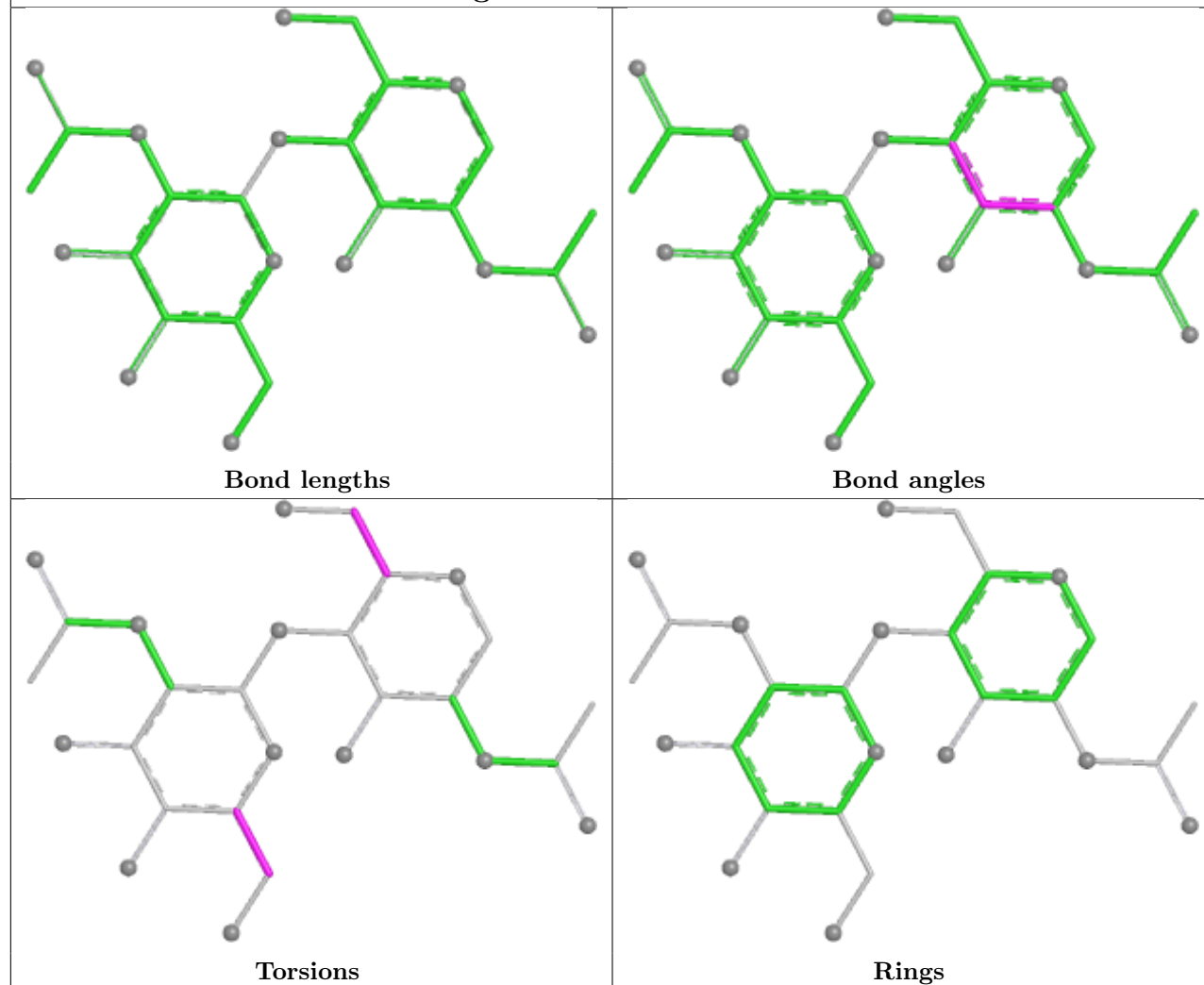




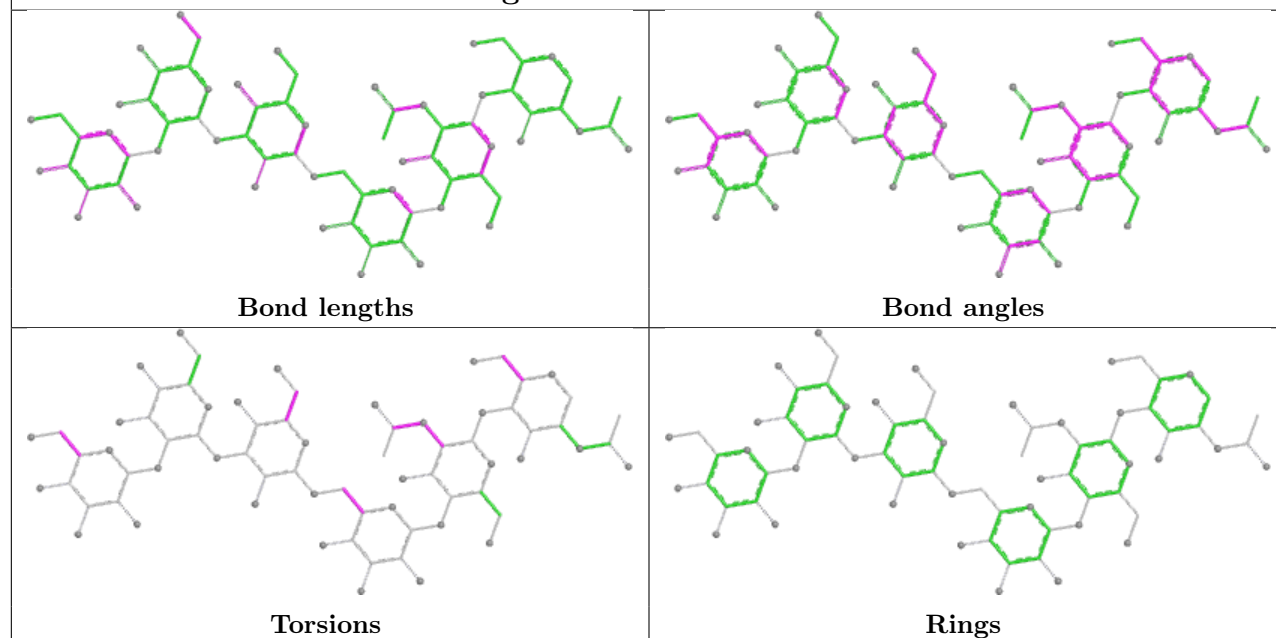


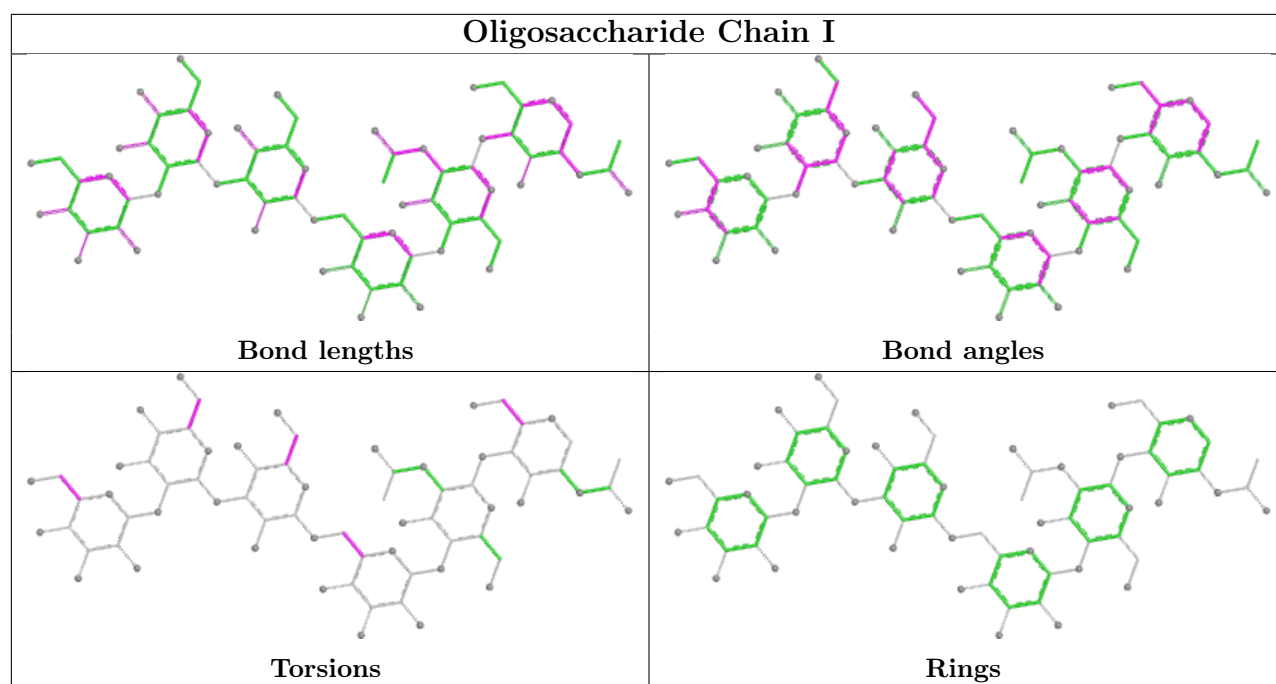


Oligosaccharide Chain K



Oligosaccharide Chain D





5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NAG	A	803	1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
4	NAG	A	815	1	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
4	NAG	B	805	1	14,14,15	0.61	0	17,19,21	1.10	0
4	NAG	B	802	1	14,14,15	0.46	0	17,19,21	0.94	0
5	BLD	B	801	-	36,37,37	2.03	8 (22%)	49,59,59	2.67	19 (38%)
5	BLD	A	804	-	36,37,37	1.98	7 (19%)	49,59,59	2.80	20 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	NAG	A	815	1	-	5/6/23/26	0/1/1/1
4	NAG	B	805	1	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
5	BLD	B	801	-	-	2/20/85/85	0/4/4/4
5	BLD	A	804	-	-	1/20/85/85	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	BLD	O06-C06	6.72	1.38	1.21
5	A	804	BLD	O06-C06	6.60	1.37	1.21
5	B	801	BLD	O07-C07	-5.29	1.37	1.45
5	A	804	BLD	O07-C07	-5.22	1.37	1.45
5	A	804	BLD	C19-C10	-3.11	1.49	1.54
5	B	801	BLD	C19-C10	-3.11	1.49	1.54
5	B	801	BLD	C20-C17	-2.91	1.49	1.54
5	A	804	BLD	C10-C05	-2.64	1.52	1.56
5	B	801	BLD	C08-C14	2.54	1.58	1.53
5	A	804	BLD	C20-C17	-2.52	1.50	1.54
5	A	804	BLD	C13-C14	-2.41	1.50	1.55
5	B	801	BLD	C10-C05	-2.37	1.52	1.56
5	B	801	BLD	O07-C06	2.36	1.37	1.34
5	B	801	BLD	C13-C14	-2.20	1.50	1.55
5	A	804	BLD	O22-C22	-2.13	1.37	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	BLD	O07-C06-O06	-6.73	106.74	116.97
5	A	804	BLD	C19-C10-C05	-6.27	99.36	109.89
5	B	801	BLD	C18-C13-C12	-6.26	101.37	110.61
5	B	801	BLD	C12-C13-C17	6.24	125.79	116.60
5	A	804	BLD	C18-C13-C12	-6.13	101.57	110.61
5	B	801	BLD	C19-C10-C05	-6.04	99.76	109.89
5	A	804	BLD	C01-C10-C05	5.53	115.76	107.11
5	B	801	BLD	C13-C17-C20	-5.38	111.24	118.99
5	B	801	BLD	C10-C01-C02	5.03	122.43	114.17
5	A	804	BLD	C12-C13-C17	4.89	123.80	116.60
5	A	804	BLD	C01-C10-C09	4.88	115.28	106.91
5	A	804	BLD	C01-C02-C03	4.85	116.80	111.40
5	A	804	BLD	C19-C10-C09	-4.70	105.03	110.47
5	B	801	BLD	O07-C06-O06	-4.67	109.87	116.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	BLD	C01-C02-C03	4.60	116.53	111.40
5	A	804	BLD	C10-C01-C02	4.46	121.50	114.17
5	B	801	BLD	C01-C10-C05	4.35	113.92	107.11
5	A	804	BLD	C13-C17-C20	-4.06	113.15	118.99
5	B	801	BLD	C16-C17-C13	3.85	108.37	103.84
5	A	804	BLD	C04-C03-C02	3.64	114.87	110.38
4	A	815	NAG	C1-O5-C5	3.63	117.06	112.19
5	A	804	BLD	C16-C17-C20	3.60	117.95	112.64
5	B	801	BLD	C01-C10-C09	3.54	112.98	106.91
4	A	803	NAG	C1-O5-C5	3.49	116.86	112.19
5	A	804	BLD	C16-C17-C13	3.23	107.64	103.84
5	A	804	BLD	C07-O07-C06	-3.07	116.72	120.98
5	B	801	BLD	C07-O07-C06	-3.07	116.73	120.98
5	B	801	BLD	C21-C20-C17	-2.96	107.42	112.78
5	B	801	BLD	C16-C17-C20	2.90	116.92	112.64
4	A	815	NAG	C2-N2-C7	-2.84	119.09	122.90
5	B	801	BLD	C04-C03-C02	2.70	113.72	110.38
5	B	801	BLD	C14-C08-C09	2.69	112.60	109.09
5	A	804	BLD	C12-C13-C14	2.49	110.98	107.25
4	A	803	NAG	C4-C3-C2	2.43	114.58	111.02
5	A	804	BLD	C11-C12-C13	2.35	116.70	112.74
5	B	801	BLD	C13-C14-C08	2.33	117.73	114.41
5	B	801	BLD	C27-C25-C26	2.32	116.96	110.58
5	B	801	BLD	C19-C10-C09	-2.30	107.80	110.47
5	A	804	BLD	C15-C14-C13	2.29	106.53	103.84
5	A	804	BLD	C14-C08-C09	2.14	111.89	109.09
5	A	804	BLD	C24-C23-C22	-2.14	110.21	114.86
5	B	801	BLD	C26-C25-C24	2.10	116.55	112.45
5	A	804	BLD	C27-C25-C26	2.01	116.11	110.58

There are no chirality outliers.

All (8) torsion outliers are listed below:

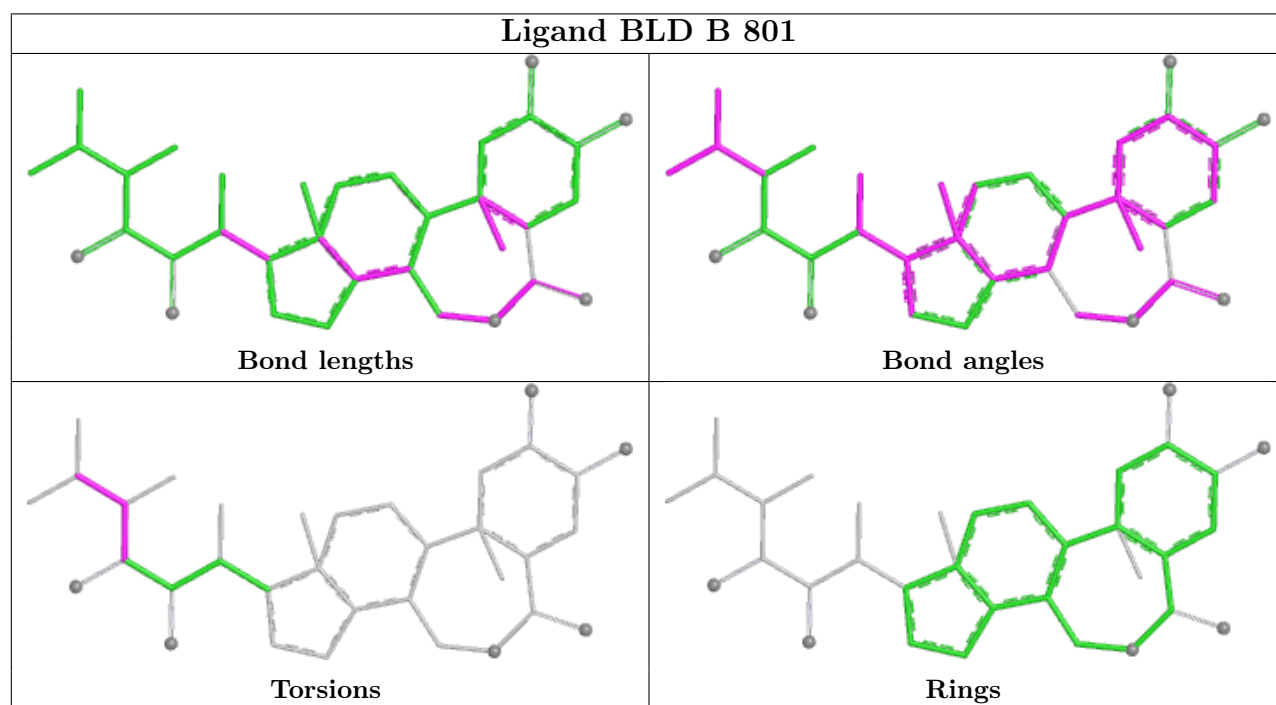
Mol	Chain	Res	Type	Atoms
4	A	815	NAG	C3-C2-N2-C7
4	A	815	NAG	C8-C7-N2-C2
4	A	815	NAG	O7-C7-N2-C2
5	A	804	BLD	C23-C24-C25-C27
5	B	801	BLD	C23-C24-C25-C27
4	A	815	NAG	C4-C5-C6-O6
4	A	815	NAG	O5-C5-C6-O6
5	B	801	BLD	O23-C23-C24-C28

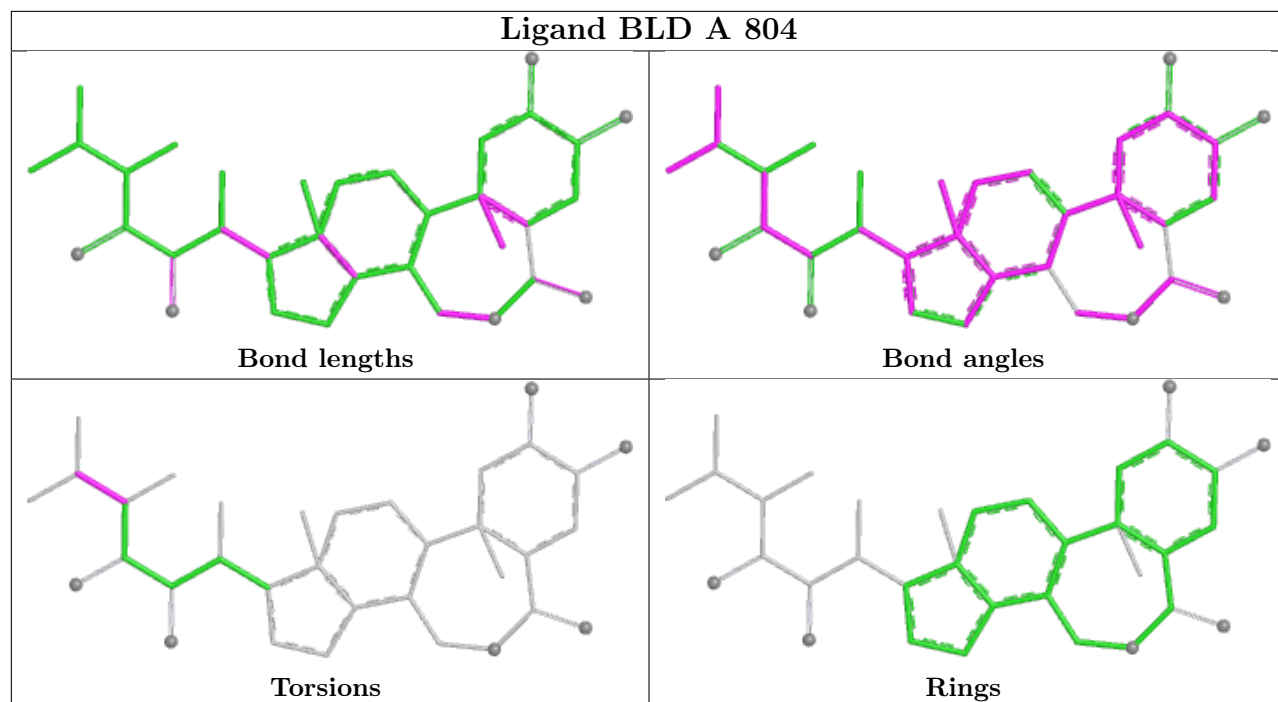
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	815	NAG	2	0
5	B	801	BLD	5	0
5	A	804	BLD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	724/740 (97%)	-0.25	23 (3%)	50	46	11, 22, 48, 88	0
1	B	724/740 (97%)	-0.25	24 (3%)	49	45	12, 23, 50, 97	0
All	All	1448/1480 (97%)	-0.25	47 (3%)	50	46	11, 22, 49, 97	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	SER	5.5
1	A	400	SER	5.1
1	A	398	LEU	4.8
1	B	64	GLY	4.6
1	B	119	ASP	4.6
1	A	118	GLY	4.5
1	B	400	SER	4.4
1	A	119	ASP	4.2
1	A	59	TYR	3.7
1	A	120	SER	3.6
1	A	32	PHE	3.6
1	A	756	GLY	3.6
1	B	398	LEU	3.6
1	A	591	GLY	3.4
1	B	592	GLY	3.4
1	B	31	ASP	3.3
1	A	64	GLY	3.3
1	B	757	SER	3.2
1	B	619	HIS	3.1
1	B	590	GLU	3.0
1	A	397	SER	2.8
1	B	118	GLY	2.8
1	B	756	GLY	2.8
1	B	59	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	121	SER	2.8
1	A	619	HIS	2.7
1	A	117	GLY	2.6
1	B	76	ASP	2.6
1	A	597	GLY	2.6
1	A	401	SER	2.5
1	A	595	CYS	2.5
1	B	123	SER	2.4
1	B	595	CYS	2.4
1	B	399	GLN	2.4
1	B	117	GLY	2.3
1	A	757	SER	2.3
1	B	396	CYS	2.3
1	B	591	GLY	2.2
1	B	593	THR	2.2
1	B	618	VAL	2.2
1	A	593	THR	2.1
1	A	396	CYS	2.1
1	A	590	GLU	2.1
1	A	33	ASN	2.1
1	B	32	PHE	2.1
1	A	399	GLN	2.1
1	A	76	ASP	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
2	NAG	H	2	14/15	0.67	0.14	49,68,74,77	0
2	NAG	H	1	14/15	0.77	0.12	40,50,57,58	0
2	NAG	C	1	14/15	0.77	0.16	25,41,51,52	0
2	NAG	K	2	14/15	0.77	0.12	44,60,63,64	0
2	NAG	G	1	14/15	0.78	0.14	28,41,47,52	0

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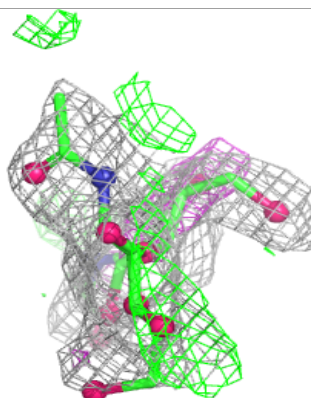
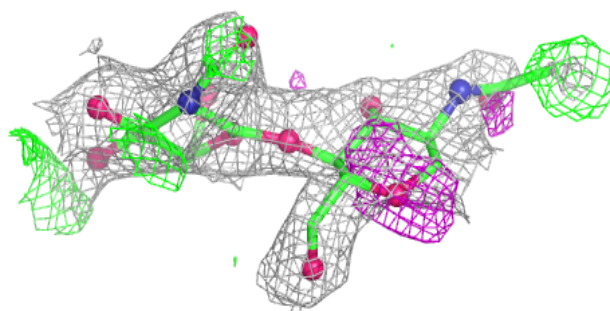
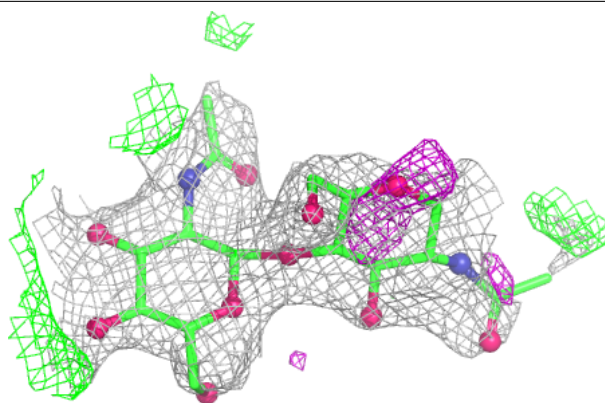
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	2	14/15	0.80	0.11	31,52,62,66	0
2	NAG	C	2	14/15	0.82	0.11	38,54,62,63	0
3	BMA	D	3	11/12	0.85	0.10	28,34,41,43	0
2	NAG	G	2	14/15	0.86	0.10	35,44,48,49	0
3	BMA	I	3	11/12	0.86	0.09	25,29,36,38	0
3	MAN	I	4	11/12	0.86	0.08	16,22,24,25	0
3	MAN	D	4	11/12	0.88	0.07	18,23,25,27	0
2	NAG	E	2	14/15	0.89	0.09	28,34,44,45	0
2	NAG	J	2	14/15	0.90	0.08	22,35,43,46	0
3	MAN	D	5	11/12	0.90	0.10	16,20,24,42	0
2	NAG	F	1	14/15	0.91	0.08	28,38,46,46	0
2	NAG	K	1	14/15	0.91	0.08	29,42,54,54	0
3	MAN	I	5	11/12	0.93	0.07	16,22,26,33	0
3	NAG	I	2	14/15	0.94	0.07	19,25,30,31	0
3	NAG	D	2	14/15	0.94	0.09	16,26,32,32	0
2	NAG	E	1	14/15	0.95	0.06	16,24,33,33	0
3	NAG	I	1	14/15	0.95	0.07	18,23,32,32	0
3	NAG	D	1	14/15	0.96	0.07	17,22,25,33	0
2	NAG	J	1	14/15	0.96	0.06	16,23,29,31	0
3	MAN	I	6	11/12	0.96	0.06	15,20,24,32	0
3	MAN	D	6	11/12	0.97	0.06	16,19,23,29	0

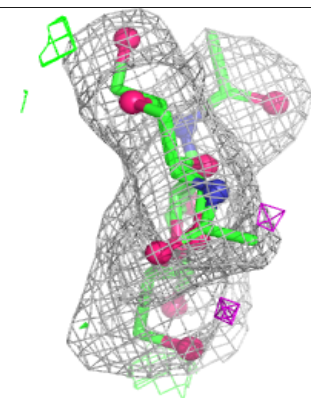
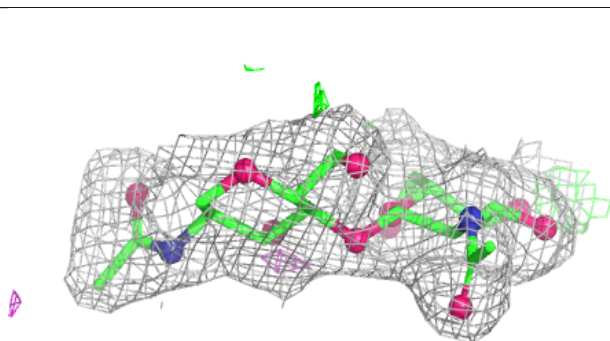
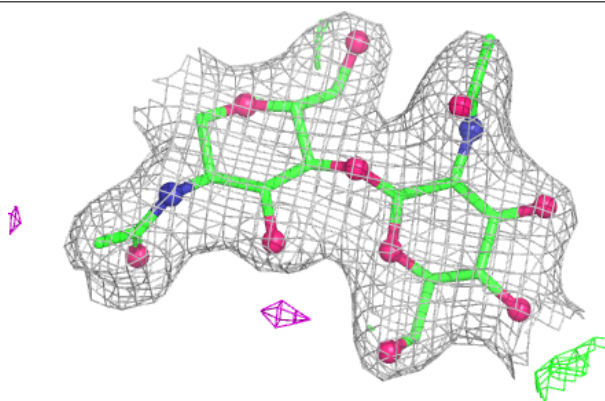
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

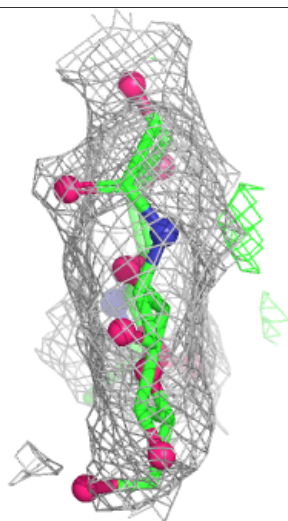
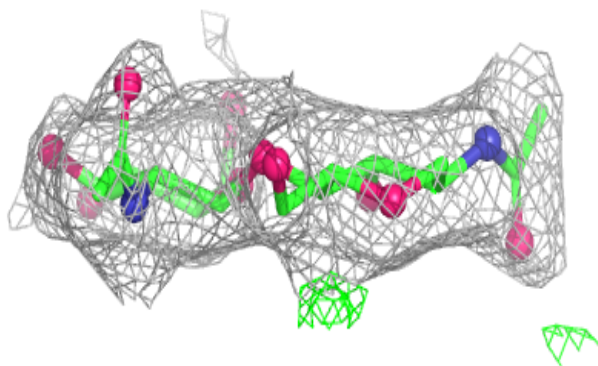
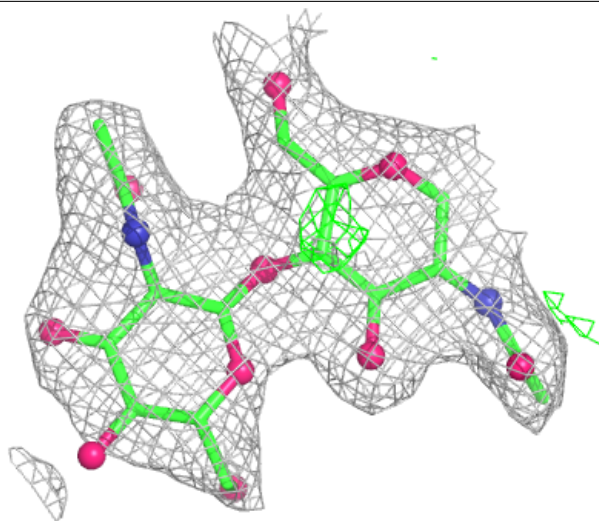
**Electron density around Chain E:**

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



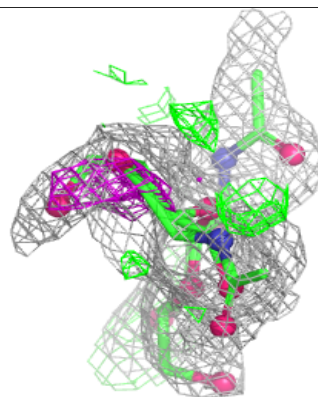
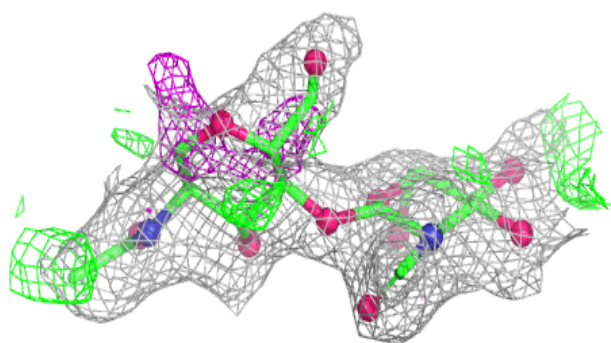
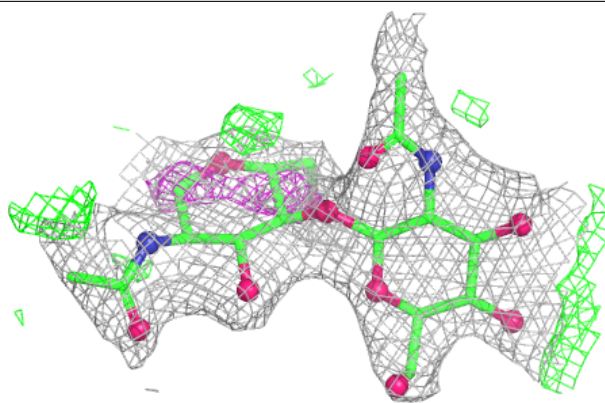
Electron density around Chain F:

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

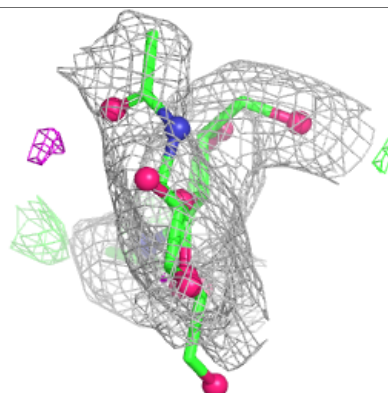
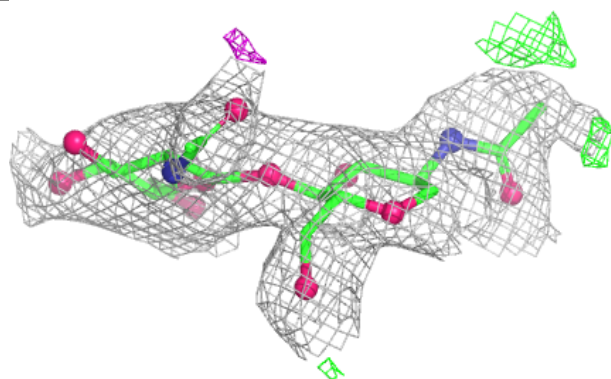
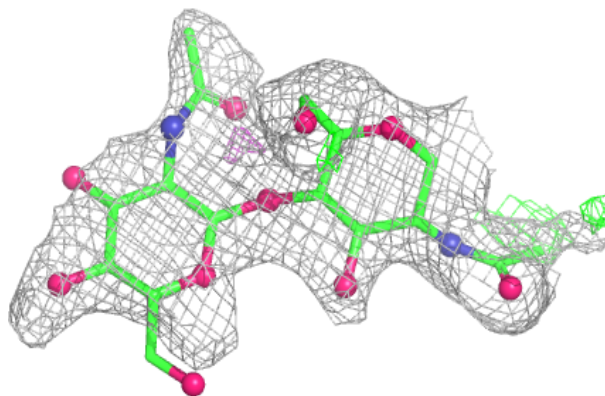


Electron density around Chain G:

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

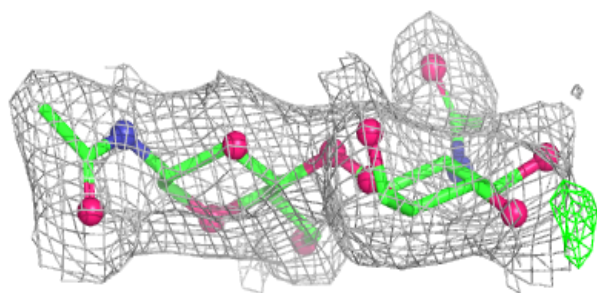
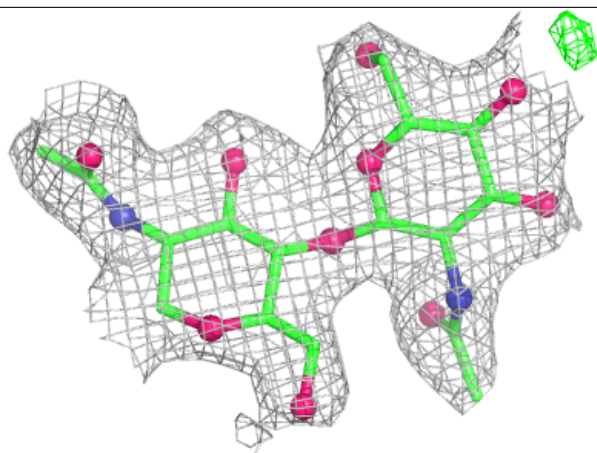
**Electron density around Chain H:**

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



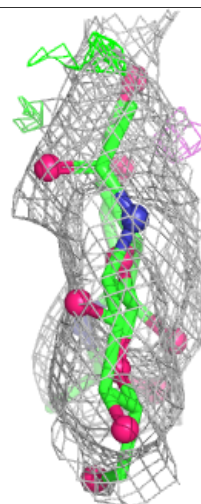
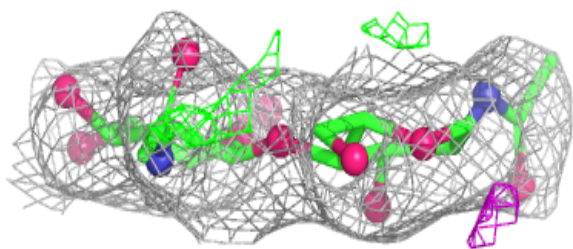
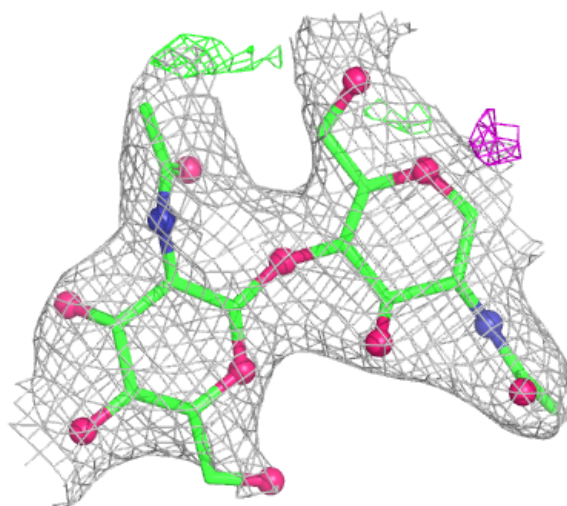
Electron density around Chain J:

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



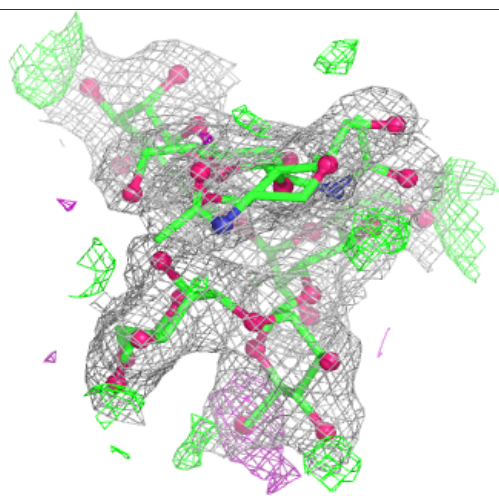
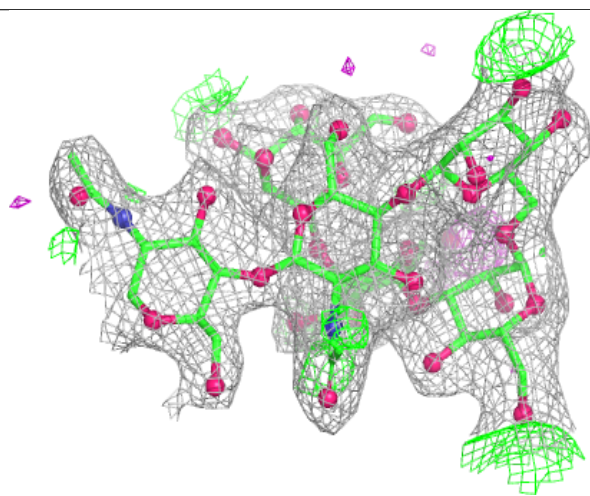
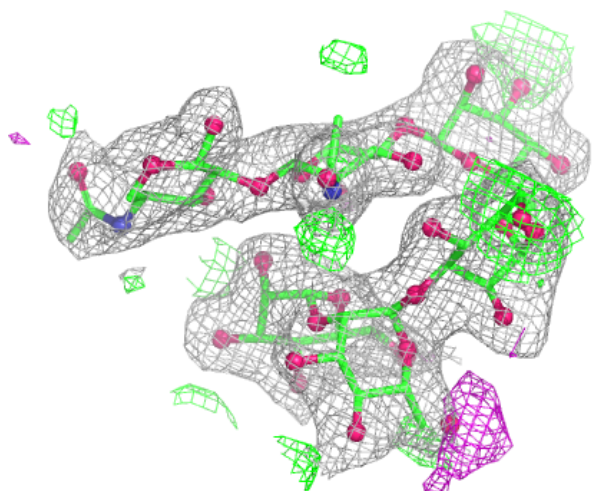
Electron density around Chain K:

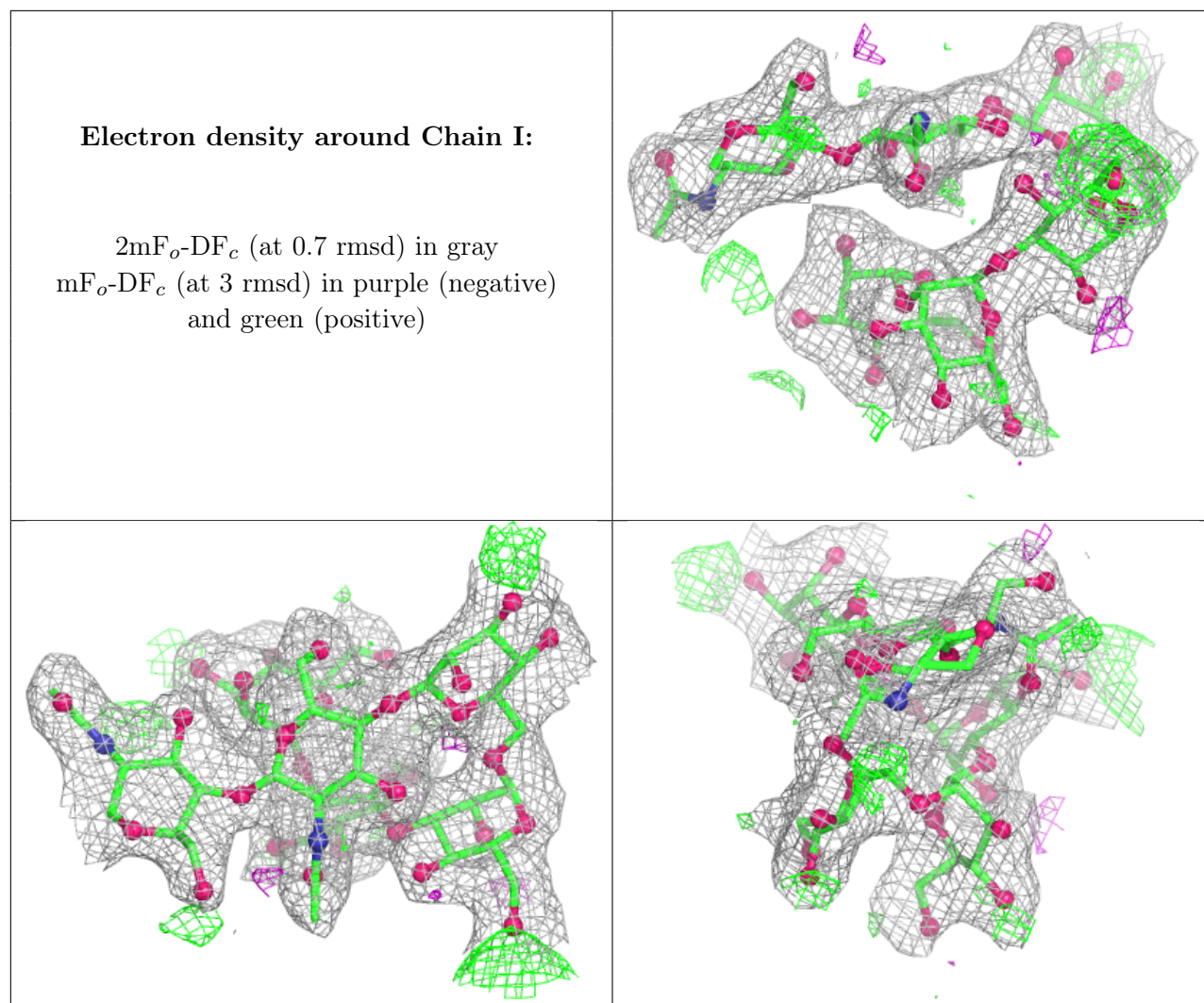
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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.

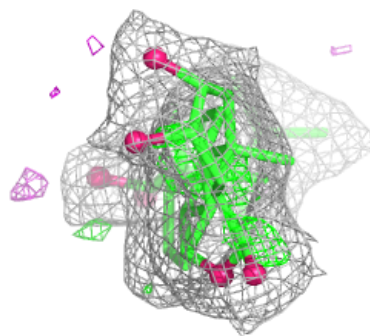
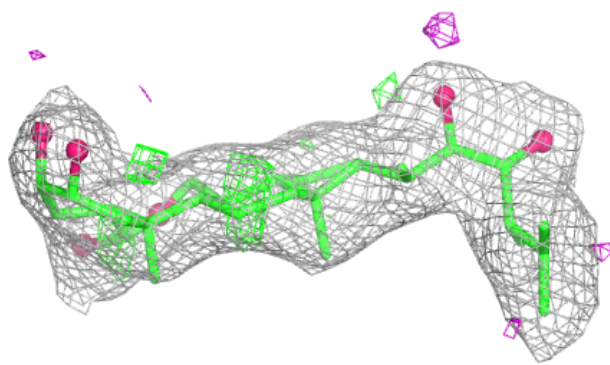
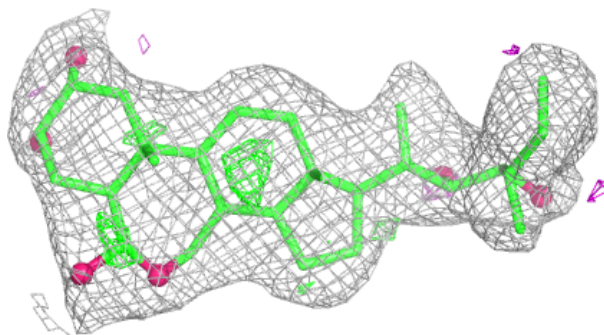
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	815	14/15	0.73	0.17	33,49,60,64	0
4	NAG	B	802	14/15	0.82	0.12	37,48,54,59	0
4	NAG	B	805	14/15	0.83	0.12	30,39,48,52	0
4	NAG	A	803	14/15	0.86	0.10	30,40,48,48	0
5	BLD	A	804	34/34	0.91	0.10	15,22,30,35	23
5	BLD	B	801	34/34	0.92	0.10	17,23,28,29	23

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

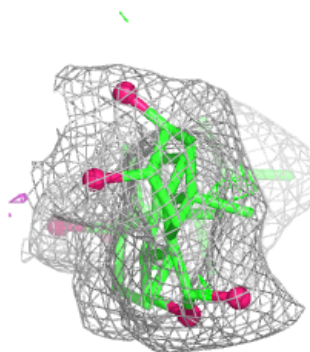
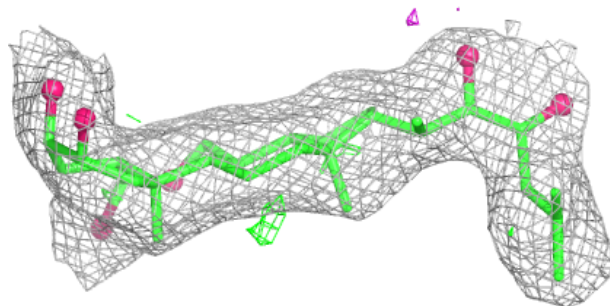
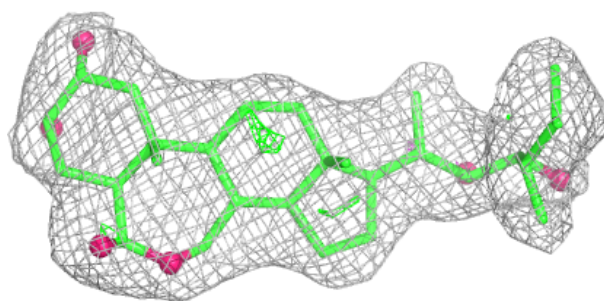
Electron density around BLD A 804:

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



Electron density around BLD B 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.