



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:22 AM UTC

PDB ID : 5W1O / pdb_00005w1o
Title : Crystal Structure of HPV16 L1 Pentamer Bound to Heparin Oligosaccharides
Authors : Dasgupta, J.; Chen, X.S.
Deposited on : 2017-06-04
Resolution : 2.80 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

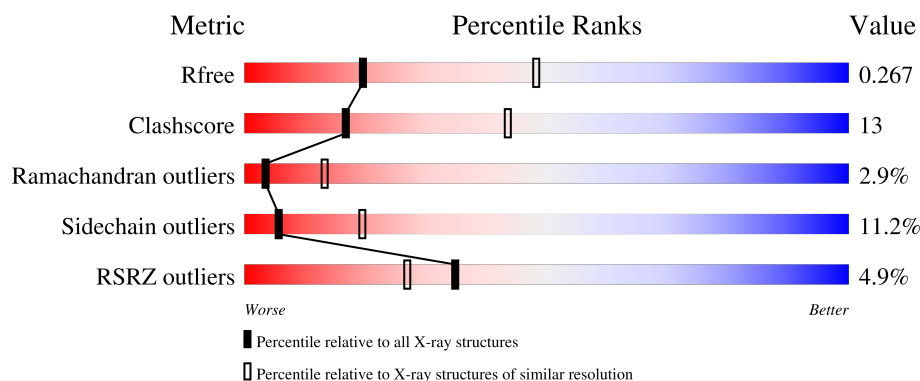
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	427	5% 68% 26% 7%
1	B	427	4% 70% 26% .
1	C	427	4% 66% 29% 5%
1	D	427	6% 68% 27% ..
1	E	427	6% 67% 28% .

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 100%
2	P	2	 100%
3	G	6	 33% 67%

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
2	JHM	F	1	-	-	X	-
2	JHM	H	1	-	-	X	-
2	JHM	I	1	-	-	X	-
2	IDS	I	2	-	-	X	-
2	JHM	J	1	-	-	X	-
2	IDS	J	2	-	-	X	-
2	JHM	M	1	-	-	X	-
2	JHM	P	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17224 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	B	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	C	427	Total	C	N	O	S	0	0	0
			3344	2125	562	637	20			
1	D	425	Total	C	N	O	S	0	0	0
			3328	2114	560	634	20			
1	E	425	Total	C	N	O	S	0	0	0
			3327	2115	559	633	20			

There are 35 discrepancies between the modelled and reference sequences:

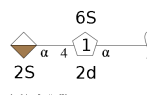
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q81007
A	432	GLY	-	linker	UNP Q81007
A	433	GLY	-	linker	UNP Q81007
A	434	GLY	-	linker	UNP Q81007
A	435	SER	-	linker	UNP Q81007
A	436	GLY	-	linker	UNP Q81007
A	437	ALA	-	linker	UNP Q81007
B	20	ALA	-	expression tag	UNP Q81007
B	432	GLY	-	linker	UNP Q81007
B	433	GLY	-	linker	UNP Q81007
B	434	GLY	-	linker	UNP Q81007
B	435	SER	-	linker	UNP Q81007
B	436	GLY	-	linker	UNP Q81007
B	437	ALA	-	linker	UNP Q81007
C	20	ALA	-	expression tag	UNP Q81007
C	432	GLY	-	linker	UNP Q81007
C	433	GLY	-	linker	UNP Q81007
C	434	GLY	-	linker	UNP Q81007
C	435	SER	-	linker	UNP Q81007

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Chain	Residue	Modelled	Actual	Comment	Reference
C	436	GLY	-	linker	UNP Q81007
C	437	ALA	-	linker	UNP Q81007
D	20	ALA	-	expression tag	UNP Q81007
D	432	GLY	-	linker	UNP Q81007
D	433	GLY	-	linker	UNP Q81007
D	434	GLY	-	linker	UNP Q81007
D	435	SER	-	linker	UNP Q81007
D	436	GLY	-	linker	UNP Q81007
D	437	ALA	-	linker	UNP Q81007
E	20	ALA	-	expression tag	UNP Q81007
E	432	GLY	-	linker	UNP Q81007
E	433	GLY	-	linker	UNP Q81007
E	434	GLY	-	linker	UNP Q81007
E	435	SER	-	linker	UNP Q81007
E	436	GLY	-	linker	UNP Q81007
E	437	ALA	-	linker	UNP Q81007

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



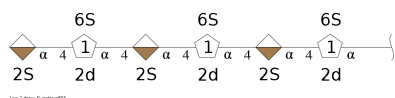
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	H	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	I	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	J	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	K	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	L	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	M	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	N	2	Total	C	O	S	0	0	0
			30	12	16	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	P	2	Total	C	O	S	0	0	0
			30	12	16	2			

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	6	Total	C	O	S	0	0	0
			90	36	48	6			

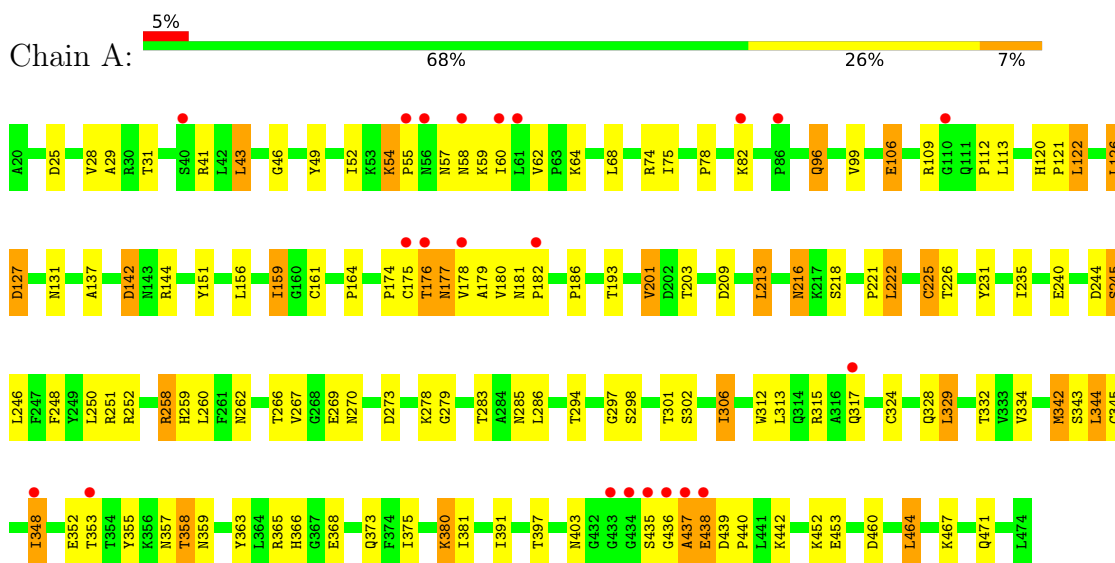
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	26	Total	O	0	0
			26	26		
4	C	34	Total	O	0	0
			34	34		
4	D	23	Total	O	0	0
			23	23		
4	E	32	Total	O	0	0
			32	32		

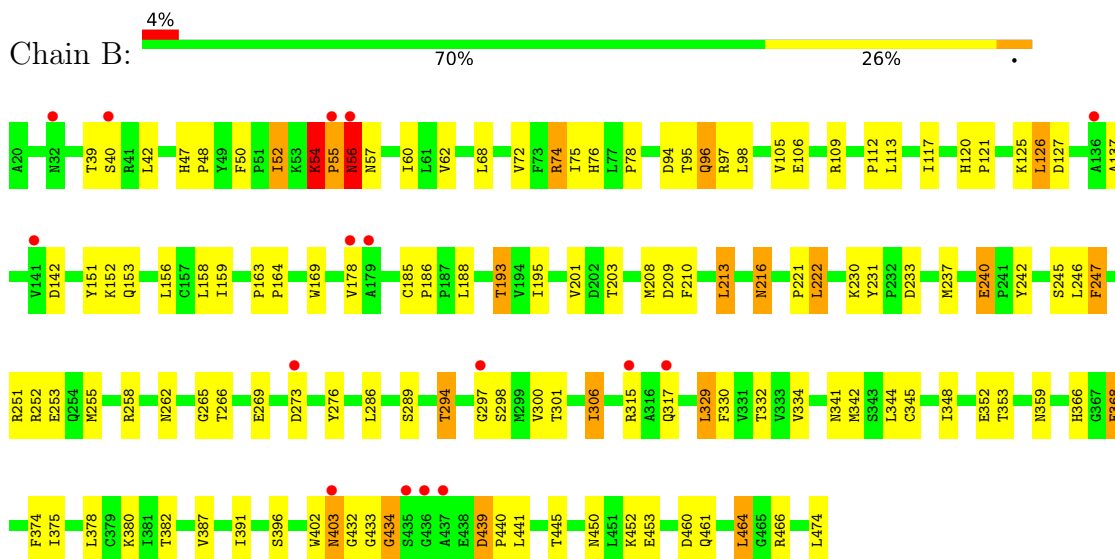
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

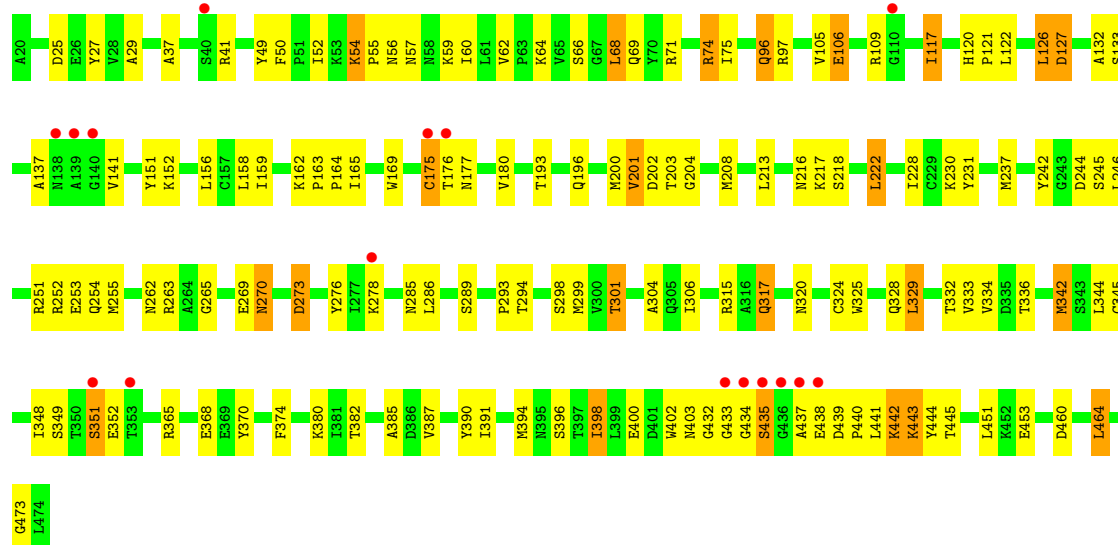
- Molecule 1: Major capsid protein L1



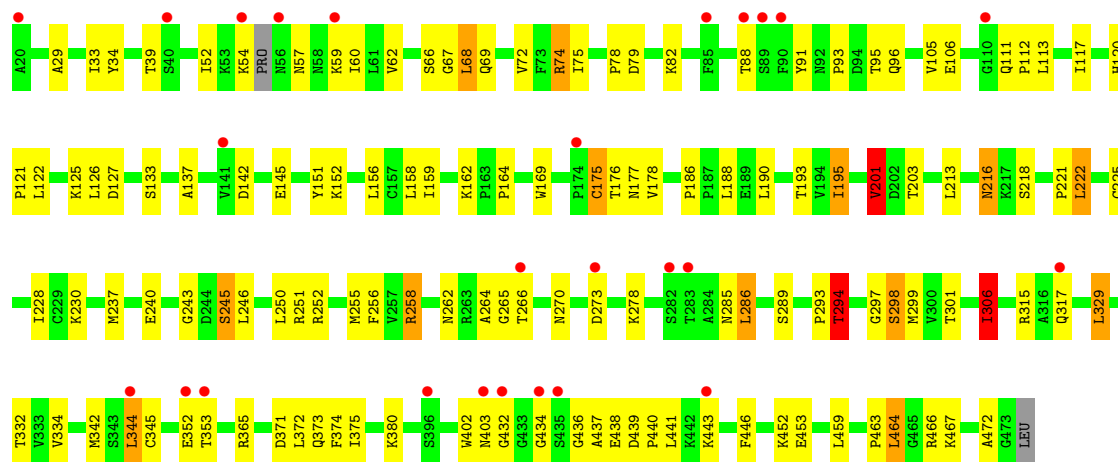
- Molecule 1: Major capsid protein L1



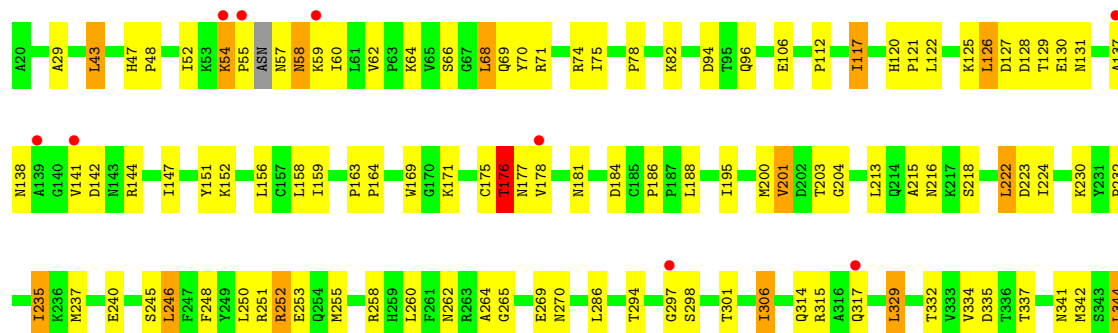
- Molecule 1: Major capsid protein L1

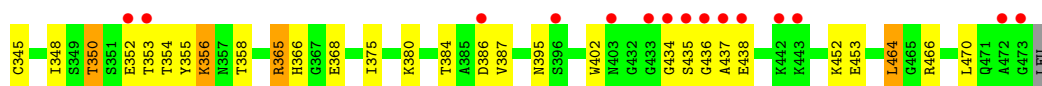


• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1





- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain F:  50%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain H:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain I:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain J:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain K:  50%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain L:  50%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain M:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain N:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain O:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain P:  100%

JHM1
IDS2

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain G:  33% 67%

JHM1
IDS2
JHM3
IDS4
JHM5
IDS6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.62Å 101.25Å 128.18Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	47.43 – 2.80 47.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.43-2.80) 93.7 (47.43-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.224 , 0.270 0.222 , 0.267	Depositor DCC
R_{free} test set	3025 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.012 for k,h,-l 0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17224	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: IDS, JHM

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	0/3430	0.93	5/4664 (0.1%)
1	B	0.58	0/3430	0.91	8/4664 (0.2%)
1	C	0.56	0/3430	0.90	6/4664 (0.1%)
1	D	0.55	0/3412	0.92	8/4638 (0.2%)
1	E	0.60	0/3412	0.93	5/4639 (0.1%)
All	All	0.57	0/17114	0.92	32/23269 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	CA-C-N	7.34	129.02	119.84
1	A	181	ASN	C-N-CA	7.34	129.02	119.84
1	E	163	PRO	O-C-N	6.35	124.23	121.31
1	B	265	GLY	N-CA-C	-6.26	105.21	111.85
1	A	306	ILE	N-CA-C	-6.19	107.22	113.47
1	A	297	GLY	N-CA-C	-6.14	100.75	111.62
1	D	265	GLY	N-CA-C	-6.08	104.64	111.63
1	C	50	PHE	CA-C-N	-6.06	113.70	119.76
1	C	50	PHE	C-N-CA	-6.06	113.70	119.76
1	C	54	LYS	CA-C-N	6.05	125.27	118.97
1	C	54	LYS	C-N-CA	6.05	125.27	118.97
1	A	96	GLN	N-CA-C	5.99	118.07	109.14
1	D	297	GLY	N-CA-C	-5.94	101.70	110.97
1	E	297	GLY	N-CA-C	-5.91	103.50	111.54
1	C	265	GLY	N-CA-C	-5.83	104.85	111.85
1	D	294	THR	CA-C-N	-5.83	114.56	120.85
1	D	294	THR	C-N-CA	-5.83	114.56	120.85
1	D	306	ILE	N-CA-C	-5.75	107.22	112.96
1	C	163	PRO	O-C-N	5.59	123.88	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	GLU	CA-C-N	5.50	124.69	118.97
1	B	240	GLU	C-N-CA	5.50	124.69	118.97
1	D	186	PRO	O-C-N	5.33	123.65	121.15
1	D	201	VAL	CB-CA-C	-5.30	105.51	111.45
1	B	96	GLN	N-CA-C	5.20	117.09	109.24
1	E	47	HIS	CA-C-N	5.19	124.81	119.05
1	E	47	HIS	C-N-CA	5.19	124.81	119.05
1	B	54	LYS	CA-C-N	5.07	126.17	119.84
1	B	54	LYS	C-N-CA	5.07	126.17	119.84
1	B	439	ASP	CA-C-N	5.06	125.13	119.87
1	B	439	ASP	C-N-CA	5.06	125.13	119.87
1	D	67	GLY	N-CA-C	-5.04	109.12	114.67
1	E	265	GLY	N-CA-C	-5.02	104.94	111.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3240	91	6
1	B	3344	0	3240	95	1
1	C	3344	0	3240	110	7
1	D	3328	0	3220	73	0
1	E	3327	0	3222	80	0
2	F	30	0	14	21	0
2	H	30	0	14	13	0
2	I	30	0	14	16	0
2	J	30	0	13	12	10
2	K	30	0	13	5	0
2	L	30	0	14	5	0
2	M	30	0	14	6	0
2	N	30	0	14	4	1
2	O	30	0	14	8	0
2	P	30	0	14	12	0
3	G	90	0	39	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	0	6	0
4	B	26	0	0	4	0
4	C	34	0	0	10	0
4	D	23	0	0	2	0
4	E	32	0	0	6	0
All	All	17224	0	16339	428	13

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 (428) 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:266:THR:HG21	2:F:1:JHM:C6	1.21	1.63
1:B:266:THR:CG2	2:F:1:JHM:H6A	1.19	1.62
1:A:358:THR:CB	2:F:1:JHM:H1	1.30	1.56
1:A:358:THR:CG2	2:F:1:JHM:C1	1.82	1.55
1:E:452:LYS:NZ	2:P:1:JHM:C6	1.72	1.49
1:A:358:THR:CG2	2:F:1:JHM:H1	0.95	1.41
1:A:358:THR:CB	2:F:1:JHM:C1	1.96	1.36
1:E:452:LYS:NZ	2:P:1:JHM:H6A	1.05	1.35
2:O:1:JHM:O1	2:P:2:IDS:C4	1.73	1.35
1:A:358:THR:HB	2:F:1:JHM:C1	1.56	1.34
1:A:358:THR:HG22	2:F:1:JHM:C1	1.47	1.33
1:C:196:GLN:HE22	2:I:2:IDS:C6	1.12	1.30
2:L:2:IDS:C4	2:M:1:JHM:O1	1.81	1.28
1:A:358:THR:HB	2:F:1:JHM:O5	1.39	1.22
2:H:1:JHM:H1	2:I:2:IDS:O6B	1.35	1.20
1:E:358:THR:HB	3:G:2:IDS:O6A	1.02	1.19
1:E:358:THR:CB	3:G:2:IDS:O6A	1.91	1.19
1:A:358:THR:HG22	2:F:1:JHM:O1	1.42	1.18
2:L:2:IDS:O2S	2:M:1:JHM:O8	1.62	1.18
1:C:55:PRO:HG3	2:J:1:JHM:C1	1.72	1.17
2:L:2:IDS:C4	2:M:1:JHM:C1	2.25	1.13
1:A:358:THR:HG21	2:F:1:JHM:H1	1.25	1.12
1:C:55:PRO:HG3	2:J:1:JHM:H1	1.32	1.09
1:E:452:LYS:HZ3	2:P:1:JHM:C6	1.46	1.08
1:C:55:PRO:HG3	2:J:1:JHM:O5	1.55	1.07
1:C:196:GLN:NE2	2:I:2:IDS:C6	1.85	1.05
2:H:1:JHM:H1	2:I:2:IDS:C6	1.85	1.04
2:N:1:JHM:O1	2:O:2:IDS:C4	2.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLN:NE2	2:I:2:IDS:O6B	1.92	1.01
1:E:452:LYS:HZ2	2:P:1:JHM:H6	1.26	1.01
1:E:452:LYS:HZ2	2:P:1:JHM:C6	1.67	0.98
1:D:285:ASN:ND2	2:K:1:JHM:O9	1.97	0.97
1:E:358:THR:HB	3:G:2:IDS:C6	1.92	0.97
1:E:452:LYS:NZ	2:P:1:JHM:H6	1.77	0.94
1:C:443:LYS:NZ	2:I:1:JHM:O8	2.01	0.94
1:E:71:ARG:NH2	4:E:601:HOH:O	2.02	0.93
2:H:1:JHM:C1	2:I:2:IDS:O6B	2.17	0.93
1:D:285:ASN:HA	2:K:1:JHM:O9	1.69	0.91
1:A:358:THR:CB	2:F:1:JHM:O5	2.06	0.88
1:C:55:PRO:CG	2:J:1:JHM:O5	2.22	0.87
2:N:1:JHM:H6A	2:O:2:IDS:O2S	1.76	0.85
1:E:452:LYS:HZ1	2:P:1:JHM:H6A	1.40	0.85
1:E:452:LYS:HZ1	2:P:1:JHM:C6	1.84	0.85
2:O:1:JHM:C1	2:P:2:IDS:C4	2.53	0.85
2:O:1:JHM:HO1	2:P:2:IDS:C4	1.90	0.84
1:E:270:ASN:ND2	2:M:1:JHM:O9	2.10	0.84
1:C:445:THR:HG21	2:H:1:JHM:O7	1.79	0.81
1:C:444:TYR:HE2	2:I:1:JHM:H2A	1.46	0.81
1:C:334:VAL:O	4:C:601:HOH:O	1.98	0.81
1:C:263:ARG:N	4:C:602:HOH:O	2.08	0.80
1:B:266:THR:CG2	2:F:1:JHM:C6	2.06	0.80
1:C:444:TYR:CE2	2:I:1:JHM:H2	2.18	0.78
1:E:54:LYS:HD3	1:E:55:PRO:HD2	1.65	0.78
1:C:444:TYR:CE2	2:I:1:JHM:C2	2.67	0.78
1:D:375:ILE:HG12	1:D:464:LEU:HD13	1.67	0.77
1:C:156:LEU:O	4:C:601:HOH:O	2.02	0.76
1:D:285:ASN:HA	2:K:1:JHM:S	2.27	0.74
1:A:358:THR:CA	2:F:1:JHM:O5	2.36	0.74
1:C:54:LYS:HG3	1:C:55:PRO:HD2	1.70	0.74
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.70	0.74
1:D:345:CYS:SG	4:E:602:HOH:O	2.45	0.74
1:E:358:THR:HG1	3:G:1:JHM:HO3	0.97	0.74
2:N:1:JHM:C6	2:O:2:IDS:O2S	2.36	0.73
1:C:55:PRO:CG	2:J:1:JHM:H1	2.15	0.73
1:C:55:PRO:CG	2:J:1:JHM:C1	2.62	0.72
1:D:68:LEU:HD13	1:D:151:TYR:HD1	1.54	0.72
1:A:358:THR:HA	2:F:1:JHM:O5	1.89	0.72
1:C:29:ALA:HB3	1:C:380:LYS:HG3	1.71	0.71
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:ILE:HG12	1:E:464:LEU:HD13	1.70	0.71
1:E:69:GLN:OE1	4:E:601:HOH:O	2.09	0.70
1:B:56:ASN:N	1:B:56:ASN:OD1	2.24	0.70
1:E:215:ALA:N	4:E:602:HOH:O	2.16	0.70
1:B:240:GLU:OE2	1:B:245:SER:OG	2.09	0.70
1:B:402:TRP:O	1:B:432:GLY:N	2.25	0.69
1:C:444:TYR:HE2	2:I:1:JHM:C2	2.03	0.69
1:B:266:THR:HG21	2:F:1:JHM:C5	2.19	0.69
1:D:240:GLU:OE2	1:D:245:SER:OG	2.08	0.69
1:B:345:CYS:SG	1:C:216:ASN:HB2	2.34	0.68
1:E:358:THR:OG1	3:G:1:JHM:O3	1.91	0.68
2:L:2:IDS:C4	2:M:1:JHM:O5	2.41	0.68
1:A:345:CYS:SG	1:B:216:ASN:HB2	2.34	0.68
1:A:25:ASP:OD1	4:A:601:HOH:O	2.10	0.68
1:C:270:ASN:O	4:C:603:HOH:O	2.12	0.67
1:D:175:CYS:O	1:D:177:ASN:N	2.27	0.67
1:B:440:PRO:O	4:B:601:HOH:O	2.13	0.66
1:A:375:ILE:HG12	1:A:464:LEU:HD13	1.76	0.66
1:A:436:GLY:O	1:A:438:GLU:N	2.28	0.66
1:C:59:LYS:O	4:C:604:HOH:O	2.13	0.65
1:D:54:LYS:HB3	1:D:57:ASN:HB2	1.79	0.65
1:D:298:SER:N	4:D:602:HOH:O	2.29	0.65
1:E:204:GLY:HA2	1:E:255:MET:HE2	1.80	0.64
1:C:55:PRO:HB3	2:J:1:JHM:C6	2.28	0.64
1:C:345:CYS:SG	1:D:216:ASN:HB2	2.38	0.64
1:A:373:GLN:OE1	4:A:602:HOH:O	2.15	0.63
1:B:375:ILE:HG12	1:B:464:LEU:HD13	1.80	0.63
1:E:175:CYS:O	1:E:177:ASN:N	2.30	0.62
1:B:55:PRO:HB2	1:B:56:ASN:OD1	1.99	0.62
1:B:460:ASP:HB3	1:B:461:GLN:HE21	1.63	0.62
1:B:52:ILE:HB	1:B:62:VAL:HB	1.81	0.62
1:C:55:PRO:HB3	2:J:1:JHM:O6	2.00	0.62
1:D:402:TRP:O	1:D:432:GLY:N	2.32	0.62
1:B:266:THR:CG2	2:F:1:JHM:C5	2.77	0.61
1:E:29:ALA:HB3	1:E:380:LYS:HG3	1.82	0.61
1:A:106:GLU:OE2	1:A:467:LYS:NZ	2.33	0.61
2:L:2:IDS:C4	2:M:1:JHM:H1	2.29	0.61
1:C:75:ILE:HB	1:C:329:LEU:HB3	1.82	0.61
4:A:603:HOH:O	1:B:208:MET:HE1	2.01	0.61
1:D:74:ARG:NH2	1:D:439:ASP:OD2	2.33	0.60
1:D:286:LEU:N	2:K:1:JHM:O8	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:GLU:OE2	1:E:245:SER:OG	2.14	0.59
1:A:240:GLU:OE2	1:A:245:SER:OG	2.17	0.59
1:C:55:PRO:HB3	2:J:1:JHM:O5	2.02	0.59
1:A:177:ASN:OD1	1:A:177:ASN:N	2.36	0.59
1:B:96:GLN:HB3	1:B:382:THR:HA	1.84	0.58
1:B:113:LEU:HD22	1:C:253:GLU:HG3	1.85	0.58
1:A:113:LEU:HD22	1:B:253:GLU:HG3	1.84	0.58
1:C:121:PRO:HG3	1:D:289:SER:HB3	1.85	0.58
1:D:344:LEU:HD12	1:E:186:PRO:HG2	1.85	0.58
1:A:269:GLU:OE1	1:E:365:ARG:NH2	2.36	0.58
1:C:55:PRO:CB	2:J:1:JHM:O5	2.50	0.58
1:B:341:ASN:HD22	1:B:366:HIS:HB2	1.68	0.58
1:B:258:ARG:HB3	1:B:294:THR:HG22	1.86	0.58
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.86	0.57
1:C:52:ILE:HB	1:C:62:VAL:HB	1.85	0.57
1:C:57:ASN:ND2	1:C:59:LYS:HB3	2.19	0.57
1:C:432:GLY:O	1:C:434:GLY:N	2.37	0.57
1:A:176:THR:O	1:A:176:THR:OG1	2.22	0.57
1:C:151:TYR:CG	1:C:203:THR:HB	2.39	0.57
1:C:200:MET:SD	2:H:2:IDS:O6A	2.63	0.57
1:B:348:ILE:HG22	1:B:359:ASN:OD1	2.04	0.57
1:A:343:SER:O	4:A:603:HOH:O	2.16	0.57
1:C:97:ARG:HH21	1:C:403:ASN:HB2	1.69	0.57
1:E:466:ARG:NH2	4:E:606:HOH:O	2.38	0.57
1:A:260:LEU:HD23	1:E:117:ILE:HG13	1.86	0.57
1:C:444:TYR:CE2	2:I:1:JHM:H2A	2.30	0.57
1:B:266:THR:CB	2:F:1:JHM:H6A	2.20	0.56
1:C:109:ARG:HH12	1:C:368:GLU:HG3	1.70	0.56
1:E:126:LEU:HD13	1:E:264:ALA:HB2	1.85	0.56
1:A:344:LEU:HD12	1:B:186:PRO:HG2	1.86	0.56
1:D:158:LEU:HB2	1:D:332:THR:HB	1.86	0.56
1:C:117:ILE:HG21	1:D:293:PRO:HD3	1.86	0.56
1:E:78:PRO:HD3	1:E:452:LYS:HA	1.88	0.56
1:C:244:ASP:OD1	1:C:320:ASN:ND2	2.39	0.56
1:C:175:CYS:HB3	1:C:177:ASN:HB2	1.86	0.56
1:A:175:CYS:O	1:A:177:ASN:N	2.38	0.55
1:C:285:ASN:HA	4:C:612:HOH:O	2.05	0.55
1:C:217:LYS:NZ	4:C:608:HOH:O	2.38	0.55
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.41	0.55
1:D:68:LEU:O	1:D:201:VAL:HG23	2.06	0.55
2:H:1:JHM:C2	2:I:2:IDS:O6B	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ILE:HB	1:E:329:LEU:HB3	1.87	0.55
1:D:68:LEU:HD13	1:D:151:TYR:CD1	2.39	0.55
1:B:74:ARG:NH2	1:B:439:ASP:OD2	2.39	0.55
1:C:175:CYS:O	1:C:177:ASN:N	2.40	0.55
1:C:273:ASP:OD2	1:C:273:ASP:N	2.40	0.55
1:E:57:ASN:O	1:E:59:LYS:N	2.40	0.55
1:A:29:ALA:HB3	1:A:380:LYS:HG3	1.89	0.54
1:E:358:THR:CB	3:G:1:JHM:HO3	2.17	0.54
1:D:52:ILE:HB	1:D:62:VAL:HB	1.90	0.54
1:D:345:CYS:O	4:E:602:HOH:O	2.18	0.54
1:C:68:LEU:O	1:C:201:VAL:HG23	2.07	0.54
1:C:204:GLY:HA2	1:C:255:MET:HE2	1.89	0.54
1:C:342:MET:HE1	1:D:169:TRP:CD1	2.42	0.54
1:E:64:LYS:NZ	1:E:223:ASP:O	2.40	0.54
1:C:273:ASP:HA	1:C:276:TYR:CE2	2.43	0.54
1:A:78:PRO:HD3	1:A:452:LYS:HA	1.90	0.54
1:B:273:ASP:HA	1:B:276:TYR:CE2	2.43	0.54
1:C:27:TYR:OH	1:C:394:MET:HE1	2.08	0.54
1:E:358:THR:CB	3:G:1:JHM:O3	2.56	0.54
1:E:358:THR:CA	3:G:2:IDS:O6A	2.54	0.53
1:B:120:HIS:CD2	1:B:222:LEU:HD13	2.43	0.53
1:D:151:TYR:CD2	1:D:203:THR:HB	2.44	0.53
1:C:349:SER:OG	1:C:351:SER:OG	2.27	0.53
1:D:66:SER:HB3	1:D:69:GLN:HG3	1.91	0.53
1:D:285:ASN:CA	2:K:1:JHM:O9	2.51	0.53
1:B:75:ILE:HB	1:B:329:LEU:HB3	1.90	0.53
1:A:358:THR:HG21	2:F:1:JHM:C1	2.04	0.53
1:B:266:THR:HG22	2:F:1:JHM:C6	2.26	0.52
1:D:345:CYS:SG	1:E:216:ASN:HB2	2.49	0.52
1:B:193:THR:HG21	1:B:230:LYS:HD2	1.91	0.52
2:O:1:JHM:H1	2:P:2:IDS:C4	2.36	0.52
1:E:158:LEU:HB2	1:E:332:THR:HB	1.92	0.52
1:C:54:LYS:HB3	1:C:57:ASN:HB3	1.91	0.52
1:D:122:LEU:O	1:D:218:SER:HB3	2.10	0.52
1:B:39:THR:HB	1:B:42:LEU:HD21	1.91	0.52
1:C:25:ASP:OD1	4:C:606:HOH:O	2.18	0.52
1:B:72:VAL:HG22	1:B:332:THR:HG23	1.90	0.51
1:B:209:ASP:O	1:B:213:LEU:HB2	2.10	0.51
1:B:342:MET:HE1	1:C:169:TRP:CD1	2.45	0.51
1:B:164:PRO:HG2	1:B:195:ILE:HB	1.92	0.51
1:A:52:ILE:HA	4:A:607:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PRO:HG2	1:E:344:LEU:HD12	1.93	0.51
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.46	0.51
1:A:266:THR:HB	3:G:3:JHM:O7	2.11	0.51
1:A:365:ARG:NH2	1:B:269:GLU:OE1	2.43	0.51
1:E:252:ARG:HD2	1:E:306:ILE:HD11	1.91	0.51
1:E:164:PRO:HG2	1:E:195:ILE:HB	1.93	0.51
1:A:52:ILE:HB	1:A:62:VAL:HB	1.93	0.51
1:A:75:ILE:HB	1:A:329:LEU:HB3	1.92	0.51
1:A:342:MET:HE1	1:B:169:TRP:CD1	2.46	0.51
1:C:158:LEU:HB2	1:C:332:THR:HB	1.93	0.51
2:H:1:JHM:H1	2:I:2:IDS:C4	2.41	0.51
1:C:216:ASN:OD1	1:C:218:SER:HB2	2.11	0.50
1:C:69:GLN:OE1	1:C:71:ARG:NH2	2.45	0.50
1:D:436:GLY:O	1:D:438:GLU:N	2.43	0.50
1:B:152:LYS:HB2	1:B:255:MET:HG3	1.94	0.50
1:D:466:ARG:NH2	4:D:606:HOH:O	2.45	0.50
1:B:208:MET:HE2	1:B:210:PHE:CD2	2.46	0.50
1:B:387:VAL:HG13	1:B:391:ILE:HD13	1.94	0.50
1:D:162:LYS:HB2	1:D:245:SER:HA	1.93	0.50
1:A:358:THR:CA	2:F:1:JHM:C1	2.83	0.50
1:C:325:TRP:HB3	1:C:398:ILE:CD1	2.42	0.50
1:D:240:GLU:HG2	1:D:243:GLY:H	1.76	0.50
1:A:363:TYR:CE2	1:B:185:CYS:HB2	2.46	0.50
1:B:233:ASP:OD1	4:B:602:HOH:O	2.20	0.50
1:B:159:ILE:HG22	1:B:247:PHE:HE1	1.77	0.49
1:C:64:LYS:HE3	2:H:2:IDS:C4	2.42	0.49
1:C:387:VAL:O	1:C:391:ILE:HG12	2.12	0.49
1:D:298:SER:OG	1:D:299:MET:N	2.44	0.49
1:B:97:ARG:HH21	1:B:403:ASN:HB2	1.76	0.49
1:D:120:HIS:HB2	1:D:221:PRO:HA	1.94	0.49
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.93	0.49
1:D:72:VAL:HG22	1:D:332:THR:HG23	1.94	0.49
1:D:228:ILE:HG22	1:D:230:LYS:HG2	1.94	0.49
1:E:200:MET:HE2	1:E:224:ILE:HG22	1.94	0.49
1:D:342:MET:HE1	1:E:169:TRP:CD1	2.48	0.49
1:A:122:LEU:O	1:A:218:SER:HB3	2.11	0.49
1:C:385:ALA:N	4:C:611:HOH:O	2.45	0.49
1:D:164:PRO:HG2	1:D:195:ILE:HB	1.95	0.49
1:E:201:VAL:HG21	1:E:334:VAL:HG11	1.93	0.49
1:B:237:MET:SD	1:B:246:LEU:HD23	2.53	0.49
1:B:246:LEU:HD12	1:B:246:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LYS:HD2	2:H:2:IDS:C4	2.43	0.48
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.95	0.48
1:D:270:ASN:OD1	2:J:2:IDS:C3	2.58	0.48
1:A:175:CYS:C	1:A:177:ASN:H	2.21	0.48
1:E:171:LYS:HG3	1:E:186:PRO:HB2	1.94	0.48
2:H:1:JHM:O1	2:I:2:IDS:C4	2.61	0.48
1:B:121:PRO:HG3	1:C:289:SER:HB3	1.96	0.48
1:B:353:THR:N	4:B:603:HOH:O	2.28	0.48
1:B:153:GLN:OE1	1:B:300:VAL:HG12	2.14	0.48
1:E:151:TYR:CD2	1:E:203:THR:HB	2.48	0.48
1:E:434:GLY:O	1:E:436:GLY:N	2.46	0.48
1:B:117:ILE:HG21	1:C:293:PRO:HD3	1.94	0.48
1:E:130:GLU:HB2	1:E:260:LEU:HB2	1.95	0.48
1:A:68:LEU:O	1:A:201:VAL:HG23	2.14	0.48
1:A:109:ARG:HH12	1:A:368:GLU:HG3	1.79	0.48
1:B:68:LEU:HD13	1:B:151:TYR:HD1	1.79	0.48
1:B:121:PRO:HD3	1:B:222:LEU:HD21	1.96	0.48
1:B:164:PRO:HG3	1:B:332:THR:OG1	2.14	0.48
1:B:341:ASN:ND2	1:B:366:HIS:HB2	2.29	0.48
1:D:68:LEU:CD1	1:D:151:TYR:HD1	2.24	0.48
1:D:79:ASP:HB3	1:D:82:LYS:HB2	1.96	0.48
1:B:152:LYS:HE3	1:B:253:GLU:HB2	1.96	0.47
1:A:142:ASP:OD1	1:A:144:ARG:NH2	2.43	0.47
1:B:68:LEU:O	1:B:201:VAL:HG23	2.14	0.47
1:A:28:VAL:HG13	1:A:381:ILE:HD11	1.97	0.47
1:B:109:ARG:HH12	1:B:368:GLU:HG3	1.80	0.47
1:C:162:LYS:HB2	1:C:245:SER:HA	1.95	0.47
1:C:246:LEU:O	1:C:246:LEU:HD12	2.14	0.47
1:E:366:HIS:HE1	1:E:368:GLU:OE1	1.98	0.47
1:A:267:VAL:HG11	1:A:270:ASN:HA	1.97	0.47
1:C:156:LEU:N	4:C:601:HOH:O	2.21	0.47
1:D:371:ASP:OD2	1:D:373:GLN:NE2	2.47	0.47
2:N:1:JHM:H6	2:O:2:IDS:O2S	2.14	0.47
1:E:436:GLY:O	1:E:438:GLU:N	2.48	0.47
1:C:442:LYS:HB3	1:C:442:LYS:HE3	1.72	0.47
1:D:156:LEU:HA	1:D:250:LEU:O	2.15	0.47
1:A:57:ASN:OD1	1:A:59:LYS:HB3	2.15	0.46
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.29	0.46
1:A:225:CYS:SG	1:A:226:THR:HG23	2.55	0.46
1:A:258:ARG:HG3	1:A:259:HIS:CD2	2.50	0.46
1:B:94:ASP:OD1	1:B:94:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LYS:HE2	1:D:443:LYS:HA	1.96	0.46
1:C:156:LEU:HG	1:C:334:VAL:HB	1.97	0.46
1:C:390:TYR:CE2	1:C:394:MET:HE3	2.51	0.46
1:D:121:PRO:HD3	1:D:222:LEU:HD21	1.97	0.46
1:A:52:ILE:HG12	1:B:269:GLU:CD	2.41	0.46
1:C:57:ASN:HD21	1:C:59:LYS:HB3	1.79	0.46
1:E:181:ASN:HB2	1:E:184:ASP:OD1	2.15	0.46
1:B:125:LYS:O	1:B:125:LYS:HD3	2.16	0.46
1:E:384:THR:OG1	1:E:387:VAL:HG23	2.16	0.46
1:A:126:LEU:HG	1:A:127:ASP:OD2	2.16	0.46
1:B:105:VAL:HG22	1:B:374:PHE:CD2	2.50	0.46
1:A:267:VAL:O	3:G:3:JHM:O8	2.33	0.46
1:A:246:LEU:O	1:A:246:LEU:HD12	2.16	0.46
1:C:365:ARG:HG3	1:D:188:LEU:HD21	1.97	0.46
1:C:96:GLN:HB3	1:C:382:THR:HA	1.98	0.45
1:D:29:ALA:HB3	1:D:380:LYS:HG3	1.97	0.45
1:E:122:LEU:HD13	1:E:144:ARG:NH2	2.30	0.45
1:A:54:LYS:HB3	1:A:57:ASN:HB3	1.97	0.45
1:A:260:LEU:HB3	1:E:117:ILE:HD11	1.99	0.45
1:A:278:LYS:HB2	1:D:353:THR:O	2.16	0.45
1:C:105:VAL:HG22	1:C:374:PHE:CD2	2.51	0.45
1:A:46:GLY:O	1:A:365:ARG:HD3	2.17	0.45
1:A:201:VAL:HG21	1:A:334:VAL:HG11	1.99	0.45
1:C:333:VAL:HG11	1:C:370:TYR:HE2	1.80	0.45
1:E:125:LYS:HD2	1:E:147:ILE:HD11	1.98	0.45
1:E:175:CYS:C	1:E:177:ASN:H	2.21	0.45
1:A:49:TYR:O	1:A:64:LYS:HE2	2.17	0.45
1:A:366:HIS:HE2	1:A:368:GLU:CD	2.25	0.45
1:A:164:PRO:HG3	1:A:332:THR:OG1	2.16	0.45
1:B:300:VAL:O	1:C:254:GLN:HA	2.16	0.45
1:A:156:LEU:HA	1:A:250:LEU:O	2.17	0.45
1:B:68:LEU:HD22	1:B:203:THR:HG22	1.98	0.45
1:D:201:VAL:HG21	1:D:334:VAL:HG11	1.98	0.45
1:E:120:HIS:CD2	1:E:222:LEU:HD13	2.52	0.45
1:B:156:LEU:HG	1:B:334:VAL:HB	1.98	0.45
1:C:228:ILE:HG22	1:C:230:LYS:HG2	1.98	0.45
1:C:242:TYR:CD2	1:C:394:MET:HG3	2.52	0.45
1:D:152:LYS:HB2	1:D:255:MET:HG3	1.99	0.45
1:A:266:THR:HG23	1:E:358:THR:HA	1.98	0.45
1:B:98:LEU:HD13	1:B:378:LEU:HD11	1.99	0.45
1:E:48:PRO:HB3	1:E:341:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LEU:HA	1:E:250:LEU:O	2.17	0.45
1:C:120:HIS:ND1	1:C:121:PRO:HD2	2.31	0.45
1:E:122:LEU:O	1:E:218:SER:HB3	2.16	0.45
1:B:97:ARG:HD2	1:B:402:TRP:HB3	1.99	0.44
1:B:306:ILE:HD13	1:B:306:ILE:HA	1.70	0.44
2:H:1:JHM:C1	2:I:2:IDS:C4	2.95	0.44
1:A:58:ASN:OD1	1:A:58:ASN:N	2.50	0.44
1:C:106:GLU:HB2	1:C:464:LEU:HG	2.00	0.44
1:C:396:SER:O	1:C:400:GLU:HG3	2.18	0.44
1:A:312:TRP:NE1	1:A:471:GLN:HG3	2.31	0.44
1:C:152:LYS:HB2	1:C:255:MET:HG3	1.99	0.44
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.87	0.44
1:B:466:ARG:HD2	1:C:317:GLN:O	2.18	0.44
1:C:121:PRO:HD3	1:C:222:LEU:HD21	1.99	0.44
1:C:164:PRO:HG3	1:C:332:THR:OG1	2.17	0.44
1:E:129:THR:HG21	1:E:262:ASN:OD1	2.17	0.44
1:D:365:ARG:NH2	1:E:269:GLU:OE2	2.50	0.44
1:C:237:MET:SD	1:C:246:LEU:HD23	2.58	0.44
1:C:49:TYR:O	1:C:64:LYS:HE2	2.18	0.44
1:C:97:ARG:NH2	1:C:403:ASN:HB2	2.31	0.44
1:D:39:THR:HG23	1:D:372:LEU:HB2	2.00	0.44
1:E:151:TYR:CG	1:E:203:THR:HB	2.53	0.44
1:B:151:TYR:CD2	1:B:203:THR:HB	2.53	0.44
1:C:242:TYR:CE2	1:C:394:MET:HG3	2.53	0.44
1:D:125:LYS:HD3	1:D:145:GLU:HG3	1.99	0.44
1:A:209:ASP:O	1:A:213:LEU:HB2	2.18	0.44
1:B:125:LYS:NZ	1:C:132:ALA:O	2.50	0.44
1:C:440:PRO:HG2	1:C:441:LEU:HD12	1.99	0.44
1:C:445:THR:CG2	2:H:1:JHM:O7	2.59	0.44
1:B:163:PRO:HD3	1:B:330:PHE:CE1	2.53	0.43
1:D:75:ILE:HB	1:D:329:LEU:HB3	2.00	0.43
1:D:270:ASN:OD1	2:J:2:IDS:H3	2.17	0.43
1:E:152:LYS:HE3	1:E:253:GLU:HB2	2.00	0.43
1:A:28:VAL:HG13	1:A:381:ILE:CD1	2.48	0.43
1:E:52:ILE:HB	1:E:62:VAL:HB	1.99	0.43
1:B:52:ILE:HG12	1:C:269:GLU:CD	2.44	0.43
1:D:105:VAL:HG22	1:D:374:PHE:CD2	2.54	0.43
1:A:285:ASN:HB2	4:A:609:HOH:O	2.18	0.43
1:E:176:THR:HG23	1:E:176:THR:O	2.19	0.43
1:D:463:PRO:O	1:D:467:LYS:HG3	2.18	0.43
1:C:301:THR:HG23	1:C:304:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:HB3	1:D:294:THR:HG22	2.00	0.43
1:B:242:TYR:HB2	4:B:610:HOH:O	2.19	0.43
1:C:152:LYS:NZ	1:C:202:ASP:OD1	2.50	0.43
1:C:324:CYS:HB3	1:C:328:GLN:O	2.19	0.42
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.91	0.42
1:E:355:TYR:C	1:E:356:LYS:HD3	2.44	0.42
1:E:358:THR:O	3:G:2:IDS:O6A	2.37	0.42
1:C:64:LYS:HB3	2:H:2:IDS:H3	2.00	0.42
1:A:355:TYR:HE2	1:A:357:ASN:ND2	2.16	0.42
1:B:158:LEU:HB2	1:B:332:THR:HB	2.01	0.42
1:B:159:ILE:HG22	1:B:247:PHE:CE1	2.54	0.42
1:C:68:LEU:HG	1:C:336:THR:HG22	2.02	0.42
1:A:279:GLY:HA3	1:A:283:THR:O	2.19	0.42
1:B:402:TRP:O	1:B:403:ASN:C	2.62	0.42
1:D:237:MET:SD	1:D:246:LEU:HD23	2.58	0.42
1:E:335:ASP:OD1	1:E:337:THR:OG1	2.18	0.42
1:A:439:ASP:HA	1:A:440:PRO:HD2	1.93	0.42
1:A:131:ASN:ND2	1:E:128:ASP:OD2	2.43	0.42
1:B:163:PRO:HG3	1:B:441:LEU:CD2	2.50	0.42
1:B:237:MET:O	1:B:240:GLU:HB3	2.20	0.42
1:C:325:TRP:HB3	1:C:398:ILE:HD11	2.01	0.42
1:D:306:ILE:HD13	1:D:306:ILE:HA	1.59	0.42
1:A:161:CYS:SG	1:A:244:ASP:HB3	2.60	0.42
1:B:342:MET:HB2	1:C:208:MET:SD	2.60	0.42
1:A:54:LYS:HE2	1:A:55:PRO:HD2	2.01	0.42
1:B:120:HIS:HB2	1:B:221:PRO:HA	2.01	0.42
1:D:344:LEU:N	1:D:344:LEU:HD23	2.35	0.42
1:A:159:ILE:HG13	1:A:248:PHE:HD2	1.85	0.41
1:A:363:TYR:CD2	1:B:185:CYS:HB2	2.55	0.41
1:D:78:PRO:HD3	1:D:452:LYS:HA	2.02	0.41
1:B:54:LYS:H	1:B:54:LYS:HG3	1.59	0.41
1:C:37:ALA:HB1	1:C:451:LEU:HD13	2.02	0.41
1:A:121:PRO:HG3	1:B:289:SER:HB3	2.03	0.41
1:A:151:TYR:CG	1:A:203:THR:HB	2.55	0.41
1:A:216:ASN:OD1	1:A:218:SER:HB2	2.20	0.41
1:D:126:LEU:HD13	1:D:264:ALA:HB2	2.02	0.41
1:B:74:ARG:HD3	1:B:76:HIS:CE1	2.56	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.86	0.41
1:A:269:GLU:CD	1:E:52:ILE:HG12	2.45	0.41
1:A:348:ILE:HG22	1:A:359:ASN:OD1	2.21	0.41
1:C:299:MET:HA	1:D:256:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:LEU:HD13	1:E:151:TYR:HD1	1.84	0.41
1:A:120:HIS:HB2	1:A:221:PRO:HA	2.02	0.41
1:A:178:VAL:HG23	1:A:179:ALA:O	2.20	0.41
1:C:105:VAL:HG21	1:C:159:ILE:HD13	2.03	0.41
1:C:126:LEU:HG	1:C:127:ASP:OD2	2.20	0.41
1:B:353:THR:O	1:D:278:LYS:HB2	2.20	0.41
1:A:109:ARG:HA	1:A:109:ARG:HD2	1.93	0.41
1:B:105:VAL:HG21	1:B:159:ILE:HD13	2.03	0.41
1:B:153:GLN:H	1:B:297:GLY:HA3	1.85	0.41
1:D:105:VAL:HG21	1:D:159:ILE:HD13	2.03	0.41
1:D:151:TYR:CG	1:D:203:THR:HB	2.56	0.41
1:E:57:ASN:C	1:E:59:LYS:N	2.79	0.41
1:A:324:CYS:HB3	1:A:328:GLN:O	2.20	0.41
1:B:78:PRO:HD3	1:B:452:LYS:HA	2.03	0.41
1:B:432:GLY:O	1:B:434:GLY:N	2.54	0.41
1:D:440:PRO:HG2	1:D:441:LEU:HD12	2.03	0.41
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.21	0.41
1:E:235:ILE:H	1:E:235:ILE:HG12	1.63	0.41
1:B:201:VAL:O	1:B:203:THR:HG23	2.21	0.40
1:D:74:ARG:HB2	1:D:446:PHE:HB2	2.03	0.40
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.91	0.40
1:E:237:MET:SD	1:E:246:LEU:HD23	2.61	0.40
1:B:47:HIS:HB3	1:B:50:PHE:O	2.21	0.40
1:C:122:LEU:O	1:C:218:SER:HB3	2.20	0.40
1:D:34:TYR:HB2	1:D:459:LEU:HD11	2.03	0.40
1:B:48:PRO:HB3	1:B:341:ASN:ND2	2.35	0.40
1:D:111:GLN:HB3	1:D:112:PRO:HD2	2.04	0.40
1:E:57:ASN:C	1:E:59:LYS:H	2.29	0.40
1:B:112:PRO:HB3	1:C:231:TYR:CD1	2.56	0.40
1:C:74:ARG:NH2	1:C:439:ASP:OD2	2.54	0.40
1:E:121:PRO:HD3	1:E:222:LEU:HD21	2.02	0.40

All (13) 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:C:278:LYS:CE	2:J:2:IDS:O6B[2_545]	1.60	0.60
1:C:278:LYS:CE	2:J:2:IDS:O6A[2_545]	1.65	0.55
1:A:353:THR:CG2	2:J:2:IDS:O2S[2_545]	1.81	0.39
1:A:353:THR:OG1	2:J:2:IDS:O2[2_545]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:CE	2:J:2:IDS:C6[2_545]	1.86	0.34
1:A:353:THR:OG1	2:J:2:IDS:O1S[2_545]	1.91	0.29
1:C:278:LYS:CG	2:J:2:IDS:O6A[2_545]	1.95	0.25
1:A:59:LYS:NZ	2:N:1:JHM:O1[2_546]	1.96	0.24
1:C:278:LYS:CB	2:J:2:IDS:O6A[2_545]	2.01	0.19
1:A:353:THR:OG1	2:J:2:IDS:S[2_545]	2.09	0.11
1:C:278:LYS:CD	2:J:2:IDS:O6A[2_545]	2.12	0.08
1:A:437:ALA:CB	3:G:6:IDS:O1S[2_546]	2.13	0.07
1:B:450:ASN:ND2	1:C:435:SER:O[2_645]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/427 (100%)	391 (92%)	22 (5%)	12 (3%)	4	14
1	B	425/427 (100%)	384 (90%)	27 (6%)	14 (3%)	3	11
1	C	425/427 (100%)	390 (92%)	24 (6%)	11 (3%)	4	15
1	D	421/427 (99%)	388 (92%)	23 (6%)	10 (2%)	4	17
1	E	421/427 (99%)	386 (92%)	20 (5%)	15 (4%)	2	10
All	All	2117/2135 (99%)	1939 (92%)	116 (6%)	62 (3%)	3	13

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	182	PRO
1	A	435	SER
1	A	437	ALA
1	A	460	ASP
1	B	55	PRO
1	B	56	ASN

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Mol	Chain	Res	Type
1	B	57	ASN
1	B	137	ALA
1	B	403	ASN
1	C	137	ALA
1	C	433	GLY
1	C	437	ALA
1	D	137	ALA
1	D	176	THR
1	D	298	SER
1	D	403	ASN
1	D	437	ALA
1	E	137	ALA
1	E	176	THR
1	E	352	GLU
1	E	353	THR
1	E	402	TRP
1	E	435	SER
1	E	437	ALA
1	A	41	ARG
1	A	403	ASN
1	B	126	LEU
1	B	142	ASP
1	B	298	SER
1	B	434	GLY
1	C	435	SER
1	C	460	ASP
1	D	434	GLY
1	E	58	ASN
1	E	395	ASN
1	A	142	ASP
1	A	176	THR
1	B	40	SER
1	B	216	ASN
1	C	41	ARG
1	C	298	SER
1	C	402	TRP
1	D	142	ASP
1	A	126	LEU
1	A	298	SER
1	B	396	SER
1	C	126	LEU
1	C	176	THR

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Mol	Chain	Res	Type
1	D	216	ASN
1	E	142	ASP
1	E	248	PHE
1	A	174	PRO
1	B	54	LYS
1	D	472	ALA
1	E	126	LEU
1	E	298	SER
1	E	350	THR
1	E	131	ASN
1	B	433	GLY
1	C	473	GLY
1	D	93	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/368 (100%)	321 (87%)	47 (13%)	4	15
1	B	368/368 (100%)	337 (92%)	31 (8%)	10	32
1	C	368/368 (100%)	328 (89%)	40 (11%)	6	21
1	D	366/368 (100%)	327 (89%)	39 (11%)	6	21
1	E	366/368 (100%)	318 (87%)	48 (13%)	4	14
All	All	1836/1840 (100%)	1631 (89%)	205 (11%)	6	19

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	43	LEU
1	A	54	LYS
1	A	60	ILE
1	A	74	ARG
1	A	82	LYS

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	99	VAL
1	A	106	GLU
1	A	122	LEU
1	A	127	ASP
1	A	159	ILE
1	A	177	ASN
1	A	180	VAL
1	A	193	THR
1	A	201	VAL
1	A	213	LEU
1	A	216	ASN
1	A	222	LEU
1	A	225	CYS
1	A	235	ILE
1	A	245	SER
1	A	251	ARG
1	A	252	ARG
1	A	258	ARG
1	A	273	ASP
1	A	286	LEU
1	A	294	THR
1	A	301	THR
1	A	302	SER
1	A	306	ILE
1	A	313	LEU
1	A	315	ARG
1	A	317	GLN
1	A	329	LEU
1	A	342	MET
1	A	344	LEU
1	A	348	ILE
1	A	352	GLU
1	A	358	THR
1	A	380	LYS
1	A	391	ILE
1	A	397	THR
1	A	438	GLU
1	A	442	LYS
1	A	453	GLU
1	A	464	LEU
1	B	52	ILE

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Mol	Chain	Res	Type
1	B	54	LYS
1	B	56	ASN
1	B	60	ILE
1	B	74	ARG
1	B	95	THR
1	B	106	GLU
1	B	127	ASP
1	B	178	VAL
1	B	188	LEU
1	B	193	THR
1	B	213	LEU
1	B	222	LEU
1	B	247	PHE
1	B	251	ARG
1	B	252	ARG
1	B	286	LEU
1	B	294	THR
1	B	301	THR
1	B	306	ILE
1	B	315	ARG
1	B	317	GLN
1	B	329	LEU
1	B	344	LEU
1	B	352	GLU
1	B	368	GLU
1	B	380	LYS
1	B	445	THR
1	B	453	GLU
1	B	464	LEU
1	B	474	LEU
1	C	56	ASN
1	C	60	ILE
1	C	66	SER
1	C	68	LEU
1	C	74	ARG
1	C	96	GLN
1	C	106	GLU
1	C	117	ILE
1	C	127	ASP
1	C	133	SER
1	C	141	VAL
1	C	165	ILE

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Mol	Chain	Res	Type
1	C	175	CYS
1	C	180	VAL
1	C	193	THR
1	C	201	VAL
1	C	213	LEU
1	C	222	LEU
1	C	251	ARG
1	C	252	ARG
1	C	270	ASN
1	C	273	ASP
1	C	286	LEU
1	C	294	THR
1	C	301	THR
1	C	306	ILE
1	C	315	ARG
1	C	317	GLN
1	C	329	LEU
1	C	342	MET
1	C	344	LEU
1	C	348	ILE
1	C	351	SER
1	C	352	GLU
1	C	398	ILE
1	C	438	GLU
1	C	442	LYS
1	C	443	LYS
1	C	453	GLU
1	C	464	LEU
1	D	33	ILE
1	D	59	LYS
1	D	60	ILE
1	D	68	LEU
1	D	74	ARG
1	D	88	THR
1	D	91	TYR
1	D	95	THR
1	D	96	GLN
1	D	106	GLU
1	D	113	LEU
1	D	117	ILE
1	D	127	ASP
1	D	133	SER

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Mol	Chain	Res	Type
1	D	175	CYS
1	D	178	VAL
1	D	193	THR
1	D	195	ILE
1	D	201	VAL
1	D	213	LEU
1	D	222	LEU
1	D	225	CYS
1	D	245	SER
1	D	251	ARG
1	D	252	ARG
1	D	258	ARG
1	D	266	THR
1	D	273	ASP
1	D	286	LEU
1	D	294	THR
1	D	301	THR
1	D	306	ILE
1	D	315	ARG
1	D	317	GLN
1	D	329	LEU
1	D	344	LEU
1	D	352	GLU
1	D	453	GLU
1	D	464	LEU
1	E	43	LEU
1	E	54	LYS
1	E	58	ASN
1	E	60	ILE
1	E	66	SER
1	E	68	LEU
1	E	74	ARG
1	E	82	LYS
1	E	94	ASP
1	E	96	GLN
1	E	106	GLU
1	E	117	ILE
1	E	127	ASP
1	E	138	ASN
1	E	141	VAL
1	E	159	ILE
1	E	176	THR

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Mol	Chain	Res	Type
1	E	178	VAL
1	E	188	LEU
1	E	201	VAL
1	E	213	LEU
1	E	222	LEU
1	E	230	LYS
1	E	235	ILE
1	E	246	LEU
1	E	251	ARG
1	E	252	ARG
1	E	258	ARG
1	E	286	LEU
1	E	294	THR
1	E	301	THR
1	E	306	ILE
1	E	314	GLN
1	E	315	ARG
1	E	317	GLN
1	E	329	LEU
1	E	342	MET
1	E	344	LEU
1	E	345	CYS
1	E	348	ILE
1	E	350	THR
1	E	354	THR
1	E	356	LYS
1	E	365	ARG
1	E	386	ASP
1	E	453	GLU
1	E	464	LEU
1	E	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	341	ASN
1	A	357	ASN
1	A	373	GLN
1	A	392	HIS
1	B	143	ASN
1	B	341	ASN

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Mol	Chain	Res	Type
1	B	357	ASN
1	C	96	GLN
1	C	143	ASN
1	C	168	HIS
1	C	196	GLN
1	C	314	GLN
1	C	319	HIS
1	C	341	ASN
1	C	366	HIS
1	D	153	GLN
1	E	216	ASN
1	E	341	ASN
1	E	357	ASN
1	E	366	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	JHM	F	1	2	15,15,15	1.03	0	19,22,22	1.21	2 (10%)
2	IDS	F	2	2	15,15,17	2.01	1 (6%)	14,22,26	1.51	3 (21%)
3	JHM	G	1	3	15,15,15	1.04	1 (6%)	19,22,22	1.20	2 (10%)
3	IDS	G	2	3	16,16,17	1.99	3 (18%)	16,24,26	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	JHM	G	3	3	14,14,15	0.96	1 (7%)	19,20,22	1.40	3 (15%)
3	IDS	G	4	3	16,16,17	1.98	3 (18%)	16,24,26	4.11	4 (25%)
3	JHM	G	5	3	14,14,15	0.96	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	G	6	3	15,15,17	2.02	2 (13%)	14,22,26	1.56	3 (21%)
2	JHM	H	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.22	2 (10%)
2	IDS	H	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.55	3 (21%)
2	JHM	I	1	2	15,15,15	1.05	1 (6%)	19,22,22	1.23	2 (10%)
2	IDS	I	2	2	15,15,17	1.99	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	J	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	J	2	2	15,15,17	2.00	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	K	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	K	2	2	15,15,17	1.99	1 (6%)	14,22,26	1.52	3 (21%)
2	JHM	L	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.22	2 (10%)
2	IDS	L	2	2	15,15,17	2.03	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	M	1	2	15,15,15	1.02	0	19,22,22	1.22	2 (10%)
2	IDS	M	2	2	15,15,17	2.01	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	N	1	2	15,15,15	1.02	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	N	2	2	15,15,17	2.00	1 (6%)	14,22,26	1.52	3 (21%)
2	JHM	O	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.19	2 (10%)
2	IDS	O	2	2	15,15,17	2.00	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	P	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	P	2	2	15,15,17	1.99	1 (6%)	14,22,26	1.49	3 (21%)

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	JHM	F	1	2	-	1/6/22/22	0/1/1/1
2	IDS	F	2	2	-	0/9/22/29	0/1/1/1
3	JHM	G	1	3	-	1/6/22/22	0/1/1/1
3	IDS	G	2	3	-	0/9/26/29	0/1/1/1
3	JHM	G	3	3	-	0/6/20/22	0/1/1/1
3	IDS	G	4	3	-	0/9/26/29	0/1/1/1
3	JHM	G	5	3	-	0/6/20/22	0/1/1/1
3	IDS	G	6	3	-	0/9/22/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JHM	H	1	2	-	0/6/22/22	0/1/1/1
2	IDS	H	2	2	-	0/9/22/29	0/1/1/1
2	JHM	I	1	2	-	0/6/22/22	0/1/1/1
2	IDS	I	2	2	-	0/9/22/29	0/1/1/1
2	JHM	J	1	2	-	1/6/22/22	0/1/1/1
2	IDS	J	2	2	-	0/9/22/29	0/1/1/1
2	JHM	K	1	2	-	1/6/22/22	0/1/1/1
2	IDS	K	2	2	-	0/9/22/29	0/1/1/1
2	JHM	L	1	2	-	0/6/22/22	0/1/1/1
2	IDS	L	2	2	-	0/9/22/29	0/1/1/1
2	JHM	M	1	2	-	0/6/22/22	0/1/1/1
2	IDS	M	2	2	-	0/9/22/29	0/1/1/1
2	JHM	N	1	2	-	1/6/22/22	0/1/1/1
2	IDS	N	2	2	-	0/9/22/29	0/1/1/1
2	JHM	O	1	2	-	1/6/22/22	0/1/1/1
2	IDS	O	2	2	-	0/9/22/29	0/1/1/1
2	JHM	P	1	2	-	0/6/22/22	0/1/1/1
2	IDS	P	2	2	-	0/9/22/29	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	IDS	O2-C2	-6.78	1.37	1.47
2	N	2	IDS	O2-C2	-6.77	1.37	1.47
2	L	2	IDS	O2-C2	-6.75	1.37	1.47
2	J	2	IDS	O2-C2	-6.74	1.37	1.47
2	O	2	IDS	O2-C2	-6.73	1.37	1.47
3	G	4	IDS	O2-C2	-6.72	1.37	1.47
2	H	2	IDS	O2-C2	-6.71	1.37	1.47
2	P	2	IDS	O2-C2	-6.70	1.37	1.47
3	G	6	IDS	O2-C2	-6.69	1.37	1.47
2	I	2	IDS	O2-C2	-6.69	1.37	1.47
2	K	2	IDS	O2-C2	-6.68	1.37	1.47
3	G	2	IDS	O2-C2	-6.66	1.37	1.47
2	M	2	IDS	O2-C2	-6.65	1.37	1.47
2	M	2	IDS	O6B-C6	-2.30	1.23	1.30
3	G	4	IDS	O6B-C6	-2.29	1.23	1.30
3	G	6	IDS	O6B-C6	-2.28	1.23	1.30
2	L	2	IDS	O6B-C6	-2.26	1.23	1.30
2	H	2	IDS	O6B-C6	-2.25	1.23	1.30
2	I	1	JHM	C3-C4	2.17	1.55	1.52
3	G	2	IDS	O4-C4	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	JHM	C3-C4	2.11	1.55	1.52
2	K	1	JHM	C3-C4	2.11	1.55	1.52
2	L	1	JHM	C3-C4	2.07	1.55	1.52
2	H	1	JHM	C3-C4	2.06	1.55	1.52
3	G	3	JHM	C3-C4	2.06	1.55	1.52
3	G	1	JHM	C3-C4	2.05	1.55	1.52
2	P	1	JHM	C3-C4	2.04	1.55	1.52
2	N	1	JHM	C3-C4	2.02	1.55	1.52
2	O	1	JHM	C3-C4	2.01	1.55	1.52
3	G	2	IDS	C4-C5	-2.00	1.49	1.53
3	G	5	JHM	C3-C4	2.00	1.55	1.52
3	G	4	IDS	C4-C5	-2.00	1.49	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4	IDS	O4-C4-C5	15.22	144.52	109.76
3	G	4	IDS	O4-C4-C3	-4.28	100.30	110.38
3	G	3	JHM	C2-C3-C4	-3.51	107.14	111.16
3	G	5	JHM	C2-C3-C4	-3.46	107.20	111.16
2	J	1	JHM	C3-C4-C5	-3.36	106.62	109.99
2	N	1	JHM	C3-C4-C5	-3.32	106.66	109.99
2	I	1	JHM	C3-C4-C5	-3.31	106.67	109.99
2	L	1	JHM	C3-C4-C5	-3.30	106.68	109.99
2	H	1	JHM	C3-C4-C5	-3.30	106.68	109.99
2	K	1	JHM	C3-C4-C5	-3.29	106.69	109.99
2	F	1	JHM	C3-C4-C5	-3.29	106.69	109.99
3	G	3	JHM	C3-C4-C5	-3.27	106.71	109.99
3	G	5	JHM	C3-C4-C5	-3.27	106.71	109.99
3	G	1	JHM	C3-C4-C5	-3.25	106.73	109.99
2	P	1	JHM	C3-C4-C5	-3.25	106.73	109.99
2	O	1	JHM	C3-C4-C5	-3.24	106.74	109.99
2	M	1	JHM	C3-C4-C5	-3.23	106.75	109.99
3	G	6	IDS	O6B-C6-C5	3.19	121.01	112.71
2	M	2	IDS	O6B-C6-C5	3.18	120.97	112.71
2	L	2	IDS	O6B-C6-C5	3.16	120.94	112.71
2	H	2	IDS	O6B-C6-C5	3.16	120.94	112.71
2	F	2	IDS	O6B-C6-C5	2.94	120.36	112.71
2	N	2	IDS	O6B-C6-C5	2.92	120.31	112.71
2	I	2	IDS	O6B-C6-C5	2.92	120.29	112.71
2	O	2	IDS	O6B-C6-C5	2.91	120.27	112.71
2	P	2	IDS	O6B-C6-C5	2.90	120.26	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	IDS	O6B-C6-C5	2.90	120.25	112.71
2	K	2	IDS	O6B-C6-C5	2.90	120.25	112.71
2	P	2	IDS	C1-C2-C3	2.83	113.82	109.84
2	O	2	IDS	C1-C2-C3	2.82	113.81	109.84
2	N	2	IDS	C1-C2-C3	2.80	113.78	109.84
2	L	2	IDS	C1-C2-C3	2.79	113.78	109.84
3	G	6	IDS	C1-C2-C3	2.77	113.75	109.84
2	M	2	IDS	C1-C2-C3	2.77	113.74	109.84
2	K	2	IDS	C1-C2-C3	2.77	113.74	109.84
2	I	2	IDS	C1-C2-C3	2.77	113.73	109.84
2	H	2	IDS	C1-C2-C3	2.73	113.69	109.84
2	J	2	IDS	C1-C2-C3	2.71	113.66	109.84
2	F	2	IDS	C1-C2-C3	2.71	113.66	109.84
2	M	1	JHM	C2-C3-C4	-2.43	107.16	110.67
2	I	1	JHM	C2-C3-C4	-2.43	107.17	110.67
2	K	1	JHM	C2-C3-C4	-2.42	107.17	110.67
3	G	1	JHM	C2-C3-C4	-2.41	107.19	110.67
2	H	1	JHM	C2-C3-C4	-2.40	107.20	110.67
2	N	1	JHM	C2-C3-C4	-2.40	107.20	110.67
2	P	1	JHM	C2-C3-C4	-2.40	107.21	110.67
2	F	1	JHM	C2-C3-C4	-2.39	107.22	110.67
2	F	2	IDS	O6B-C6-O6A	-2.39	118.66	124.08
2	O	1	JHM	C2-C3-C4	-2.39	107.22	110.67
2	L	1	JHM	C2-C3-C4	-2.39	107.22	110.67
2	J	1	JHM	C2-C3-C4	-2.38	107.23	110.67
3	G	4	IDS	O6B-C6-O6A	-2.38	118.68	124.08
2	J	2	IDS	O6B-C6-O6A	-2.38	118.69	124.08
3	G	2	IDS	O6B-C6-O6A	-2.37	118.70	124.08
2	N	2	IDS	O6B-C6-O6A	-2.36	118.73	124.08
3	G	6	IDS	O6B-C6-O6A	-2.35	118.74	124.08
2	P	2	IDS	O6B-C6-O6A	-2.35	118.75	124.08
2	K	2	IDS	O6B-C6-O6A	-2.34	118.77	124.08
2	L	2	IDS	O6B-C6-O6A	-2.34	118.77	124.08
2	I	2	IDS	O6B-C6-O6A	-2.34	118.78	124.08
2	M	2	IDS	O6B-C6-O6A	-2.33	118.79	124.08
2	O	2	IDS	O6B-C6-O6A	-2.33	118.79	124.08
2	H	2	IDS	O6B-C6-O6A	-2.32	118.81	124.08
3	G	5	JHM	C1-C2-C3	-2.22	107.00	110.61
3	G	3	JHM	C1-C2-C3	-2.22	107.01	110.61
3	G	4	IDS	O6B-C6-C5	2.05	121.04	113.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

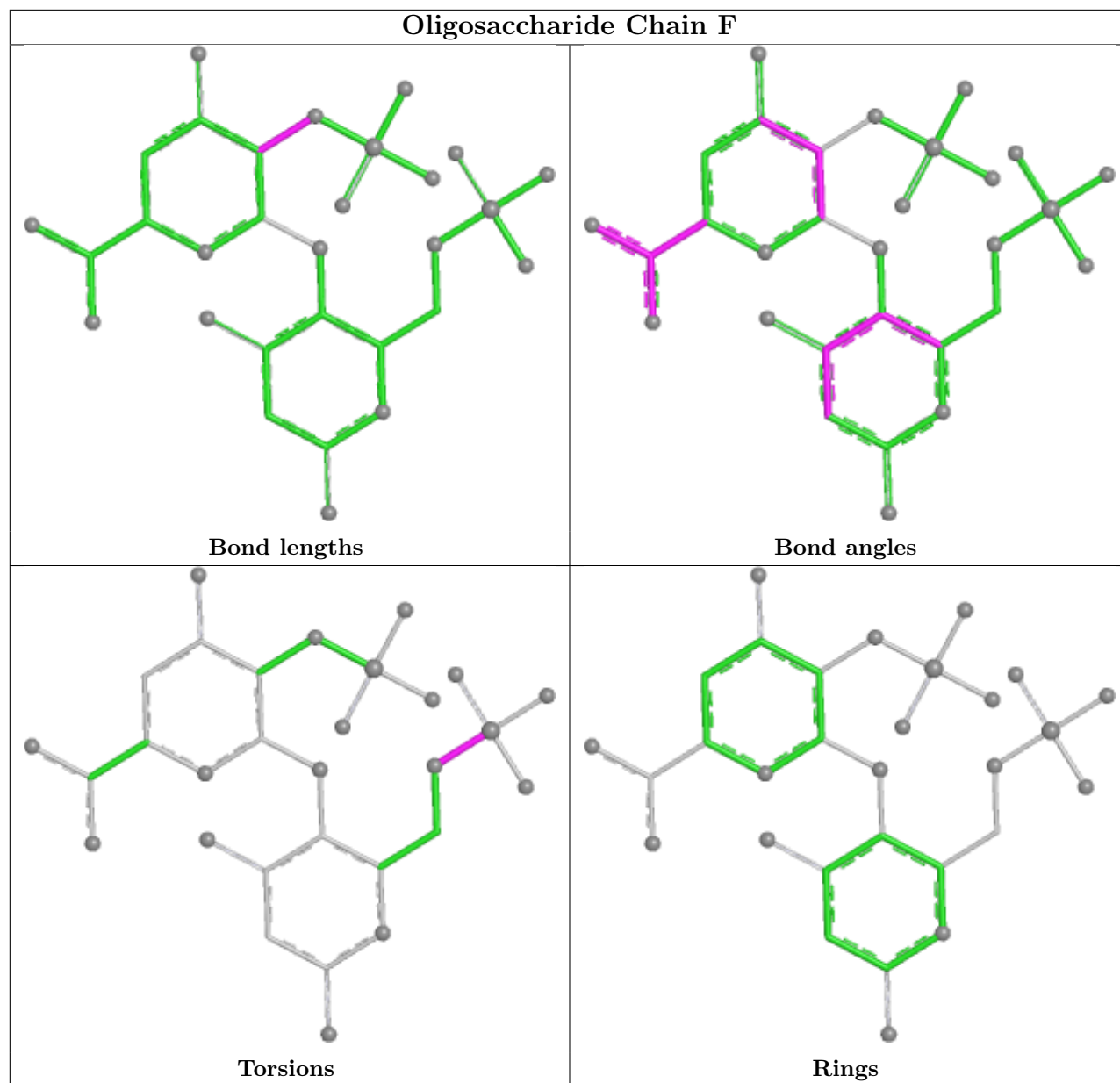
Mol	Chain	Res	Type	Atoms
2	F	1	JHM	C6-O6-S-O8
2	J	1	JHM	C6-O6-S-O8
2	K	1	JHM	C6-O6-S-O8
2	N	1	JHM	C6-O6-S-O8
2	O	1	JHM	C6-O6-S-O8
3	G	1	JHM	C6-O6-S-O8

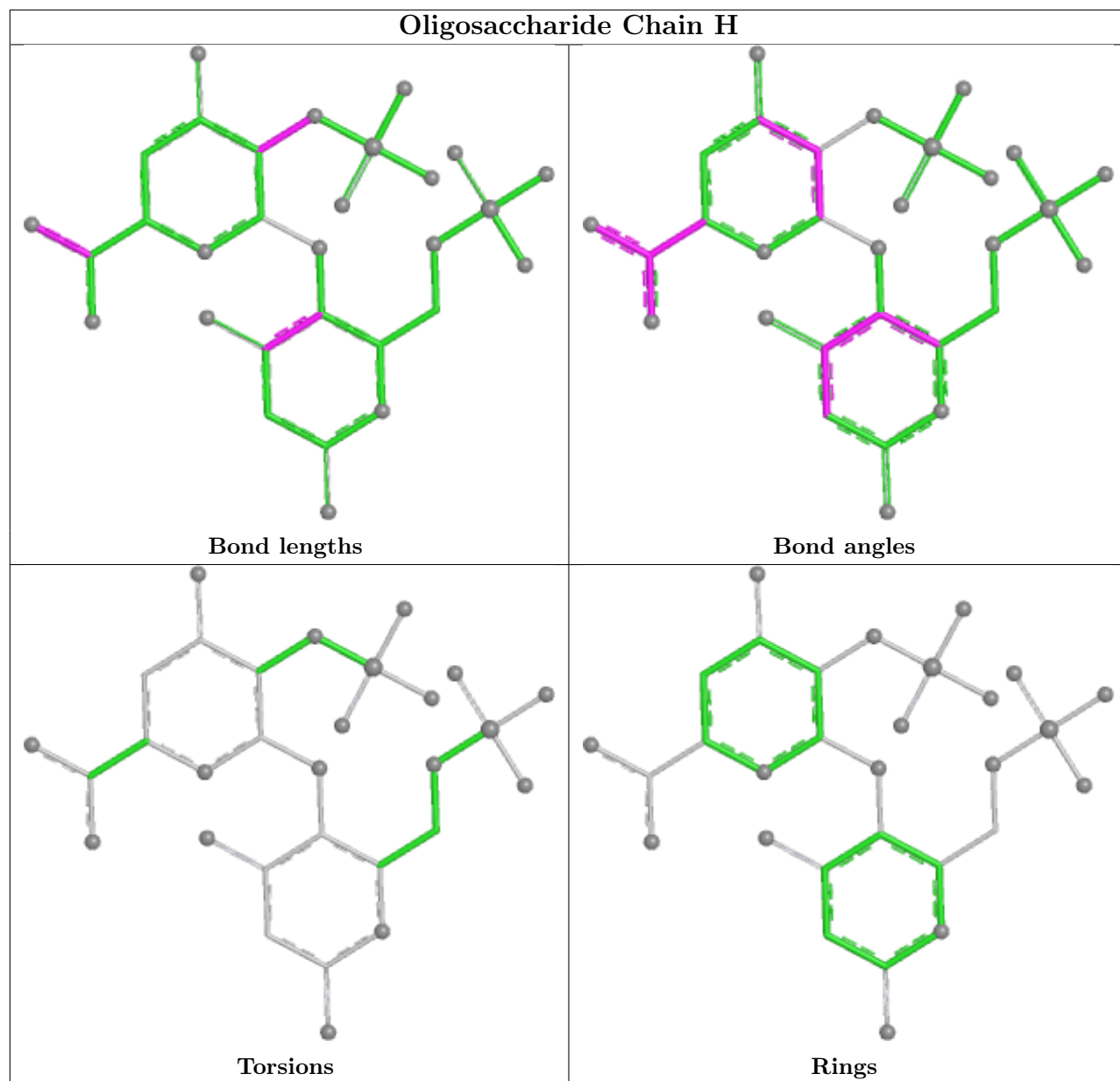
There are no ring outliers.

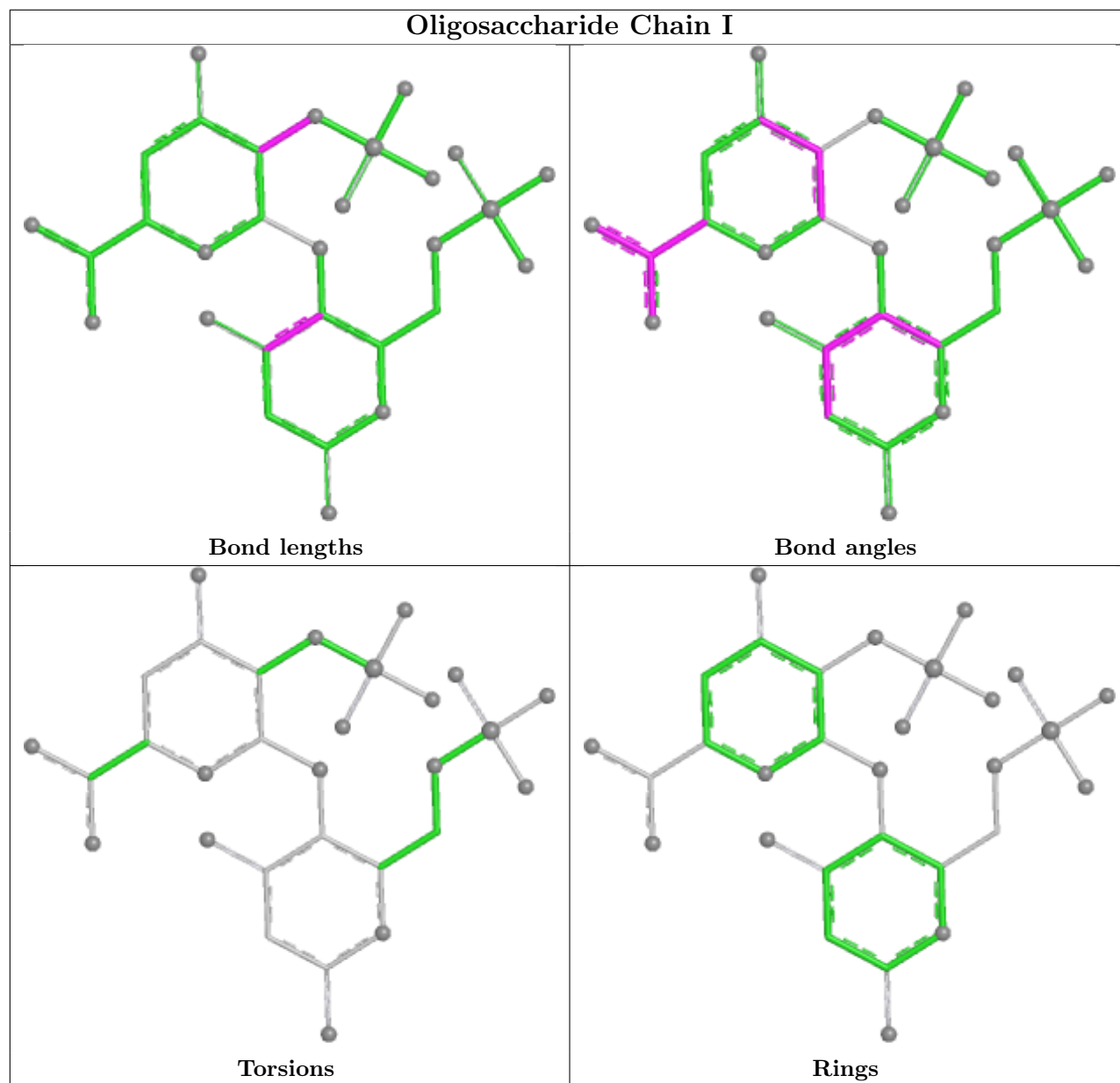
19 monomers are involved in 105 short contacts:

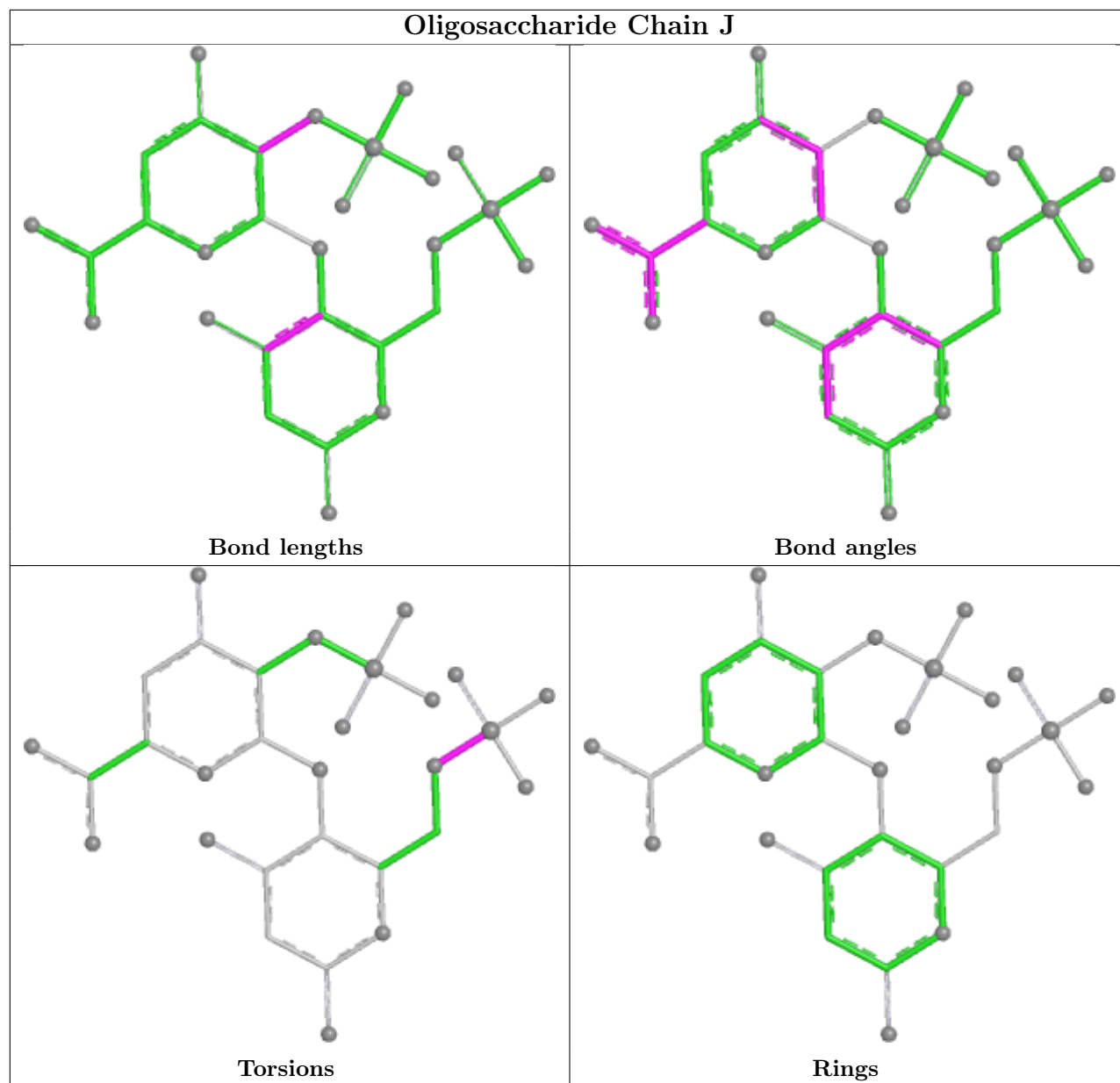
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	IDS	2	10
3	G	2	IDS	5	0
2	K	1	JHM	5	0
2	I	1	JHM	6	0
2	O	2	IDS	4	0
3	G	6	IDS	0	1
2	H	2	IDS	4	0
2	L	2	IDS	5	0
2	H	1	JHM	9	0
2	P	2	IDS	4	0
2	I	2	IDS	10	0
2	N	1	JHM	4	1
3	G	1	JHM	4	0
2	J	1	JHM	10	0
3	G	3	JHM	2	0
2	P	1	JHM	8	0
2	M	1	JHM	6	0
2	O	1	JHM	4	0
2	F	1	JHM	21	0

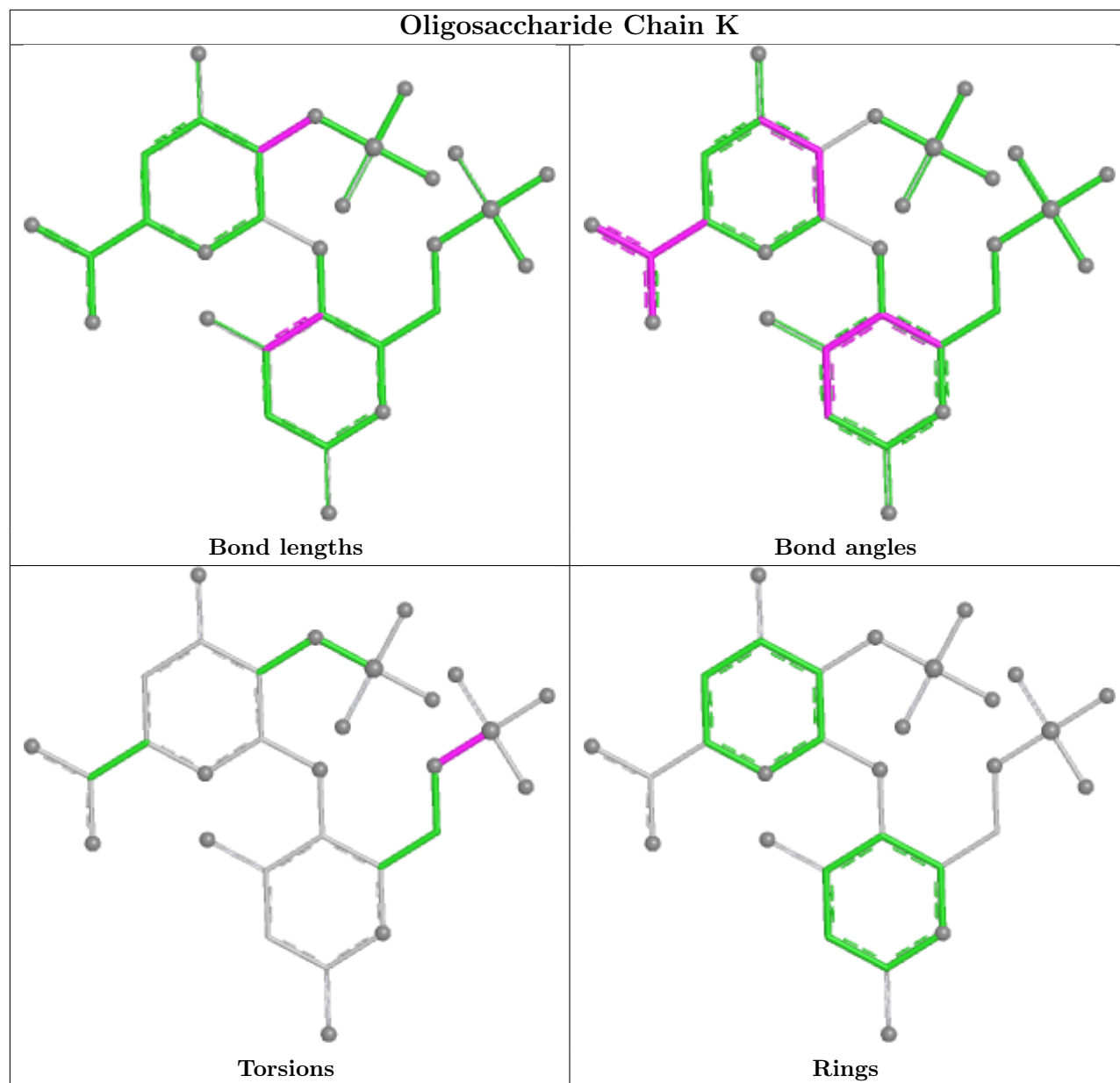
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

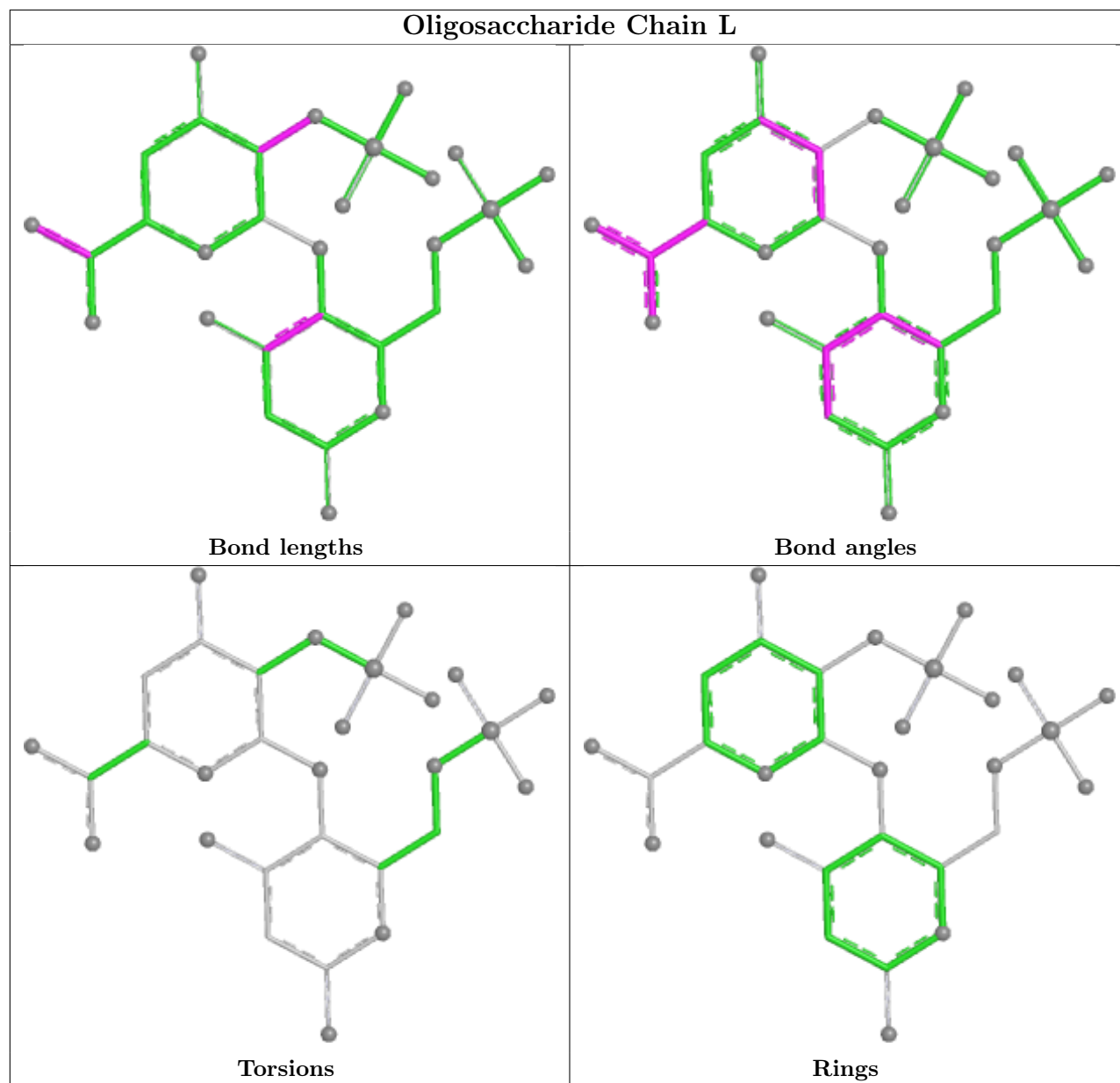




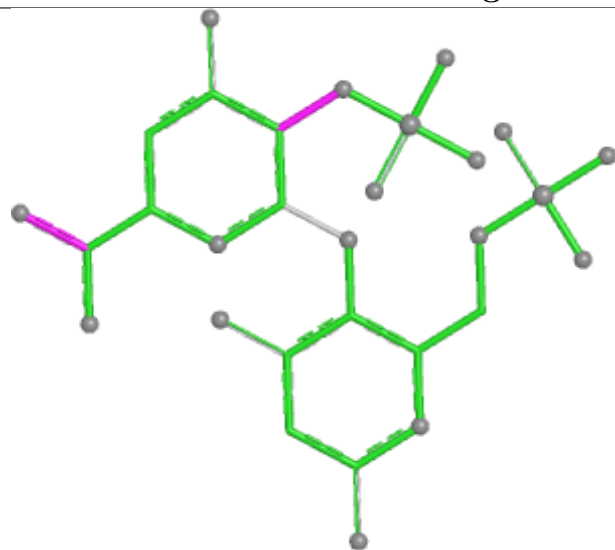




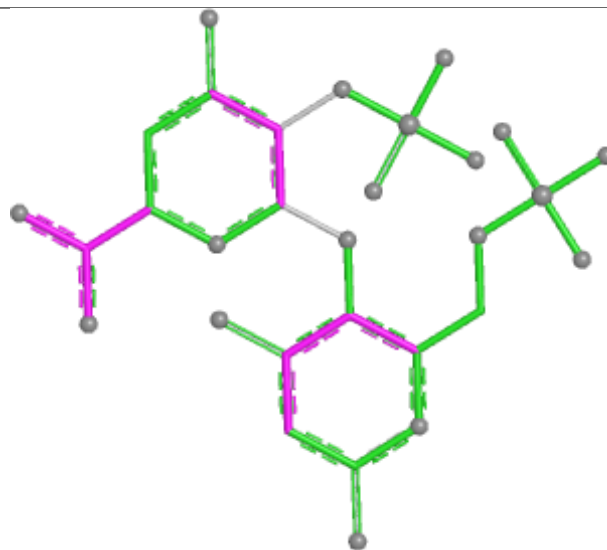




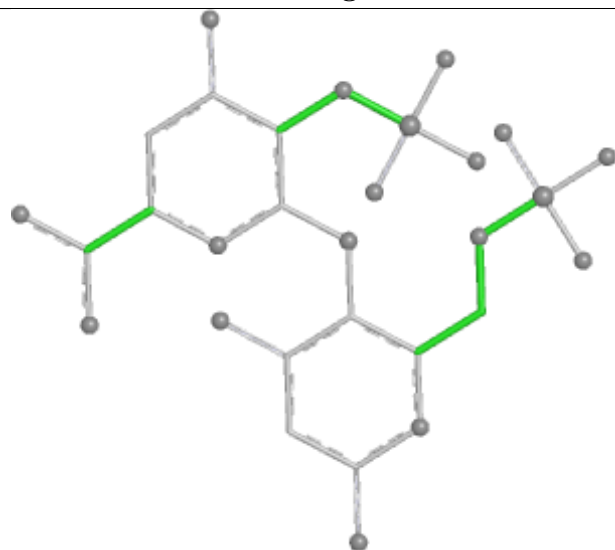
Oligosaccharide Chain M



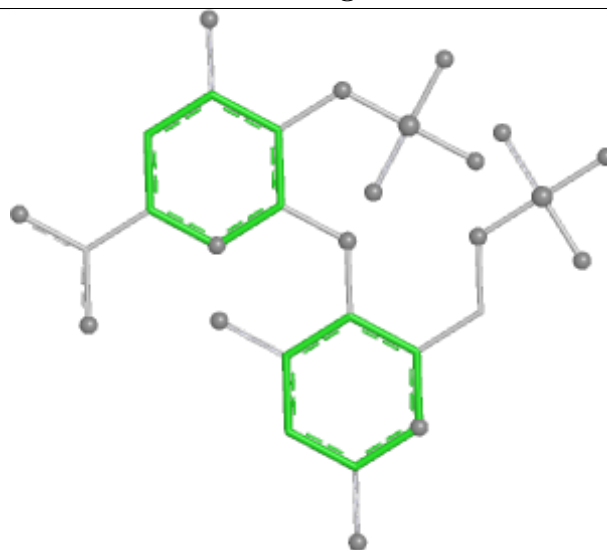
Bond lengths



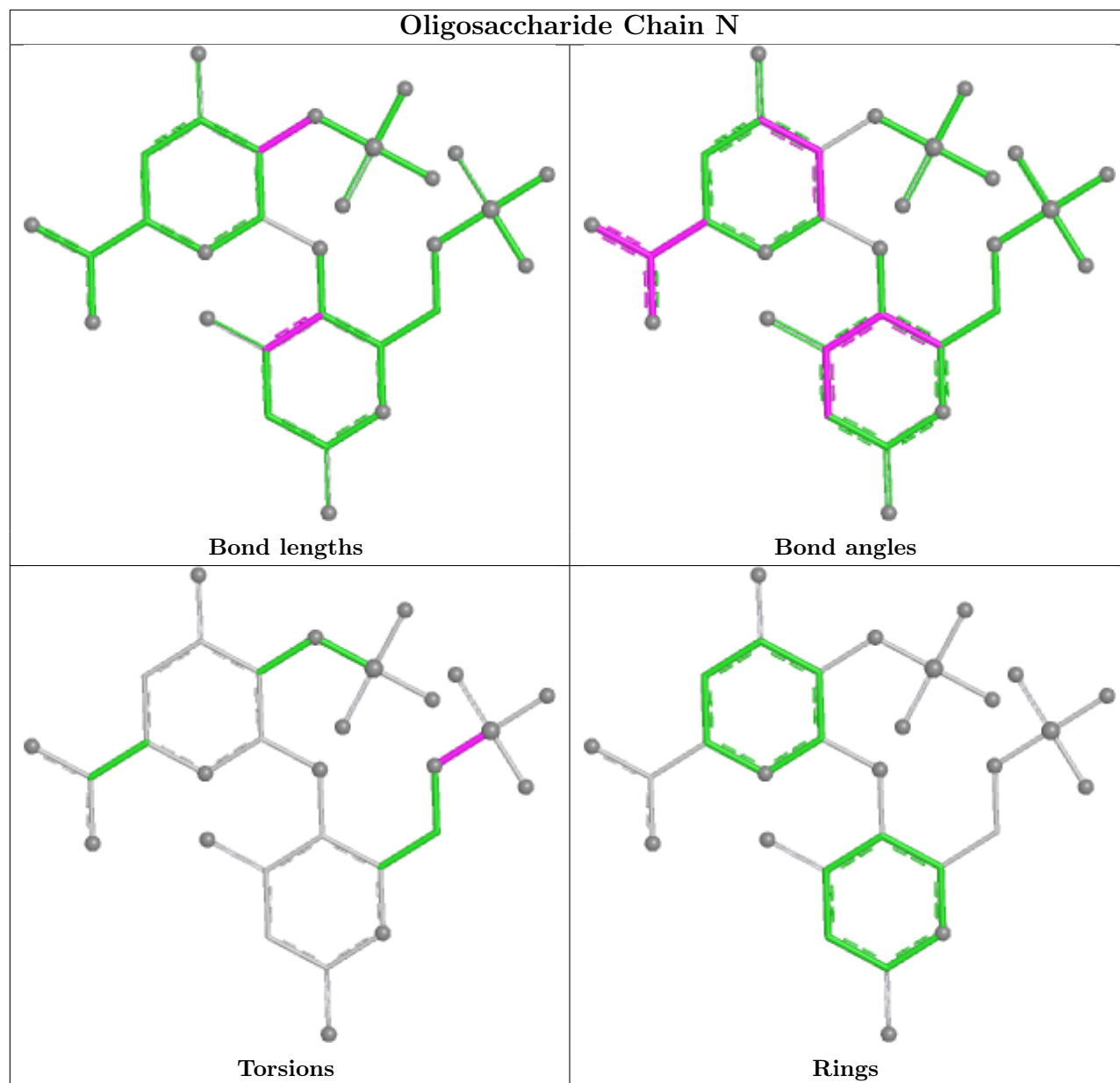
Bond angles

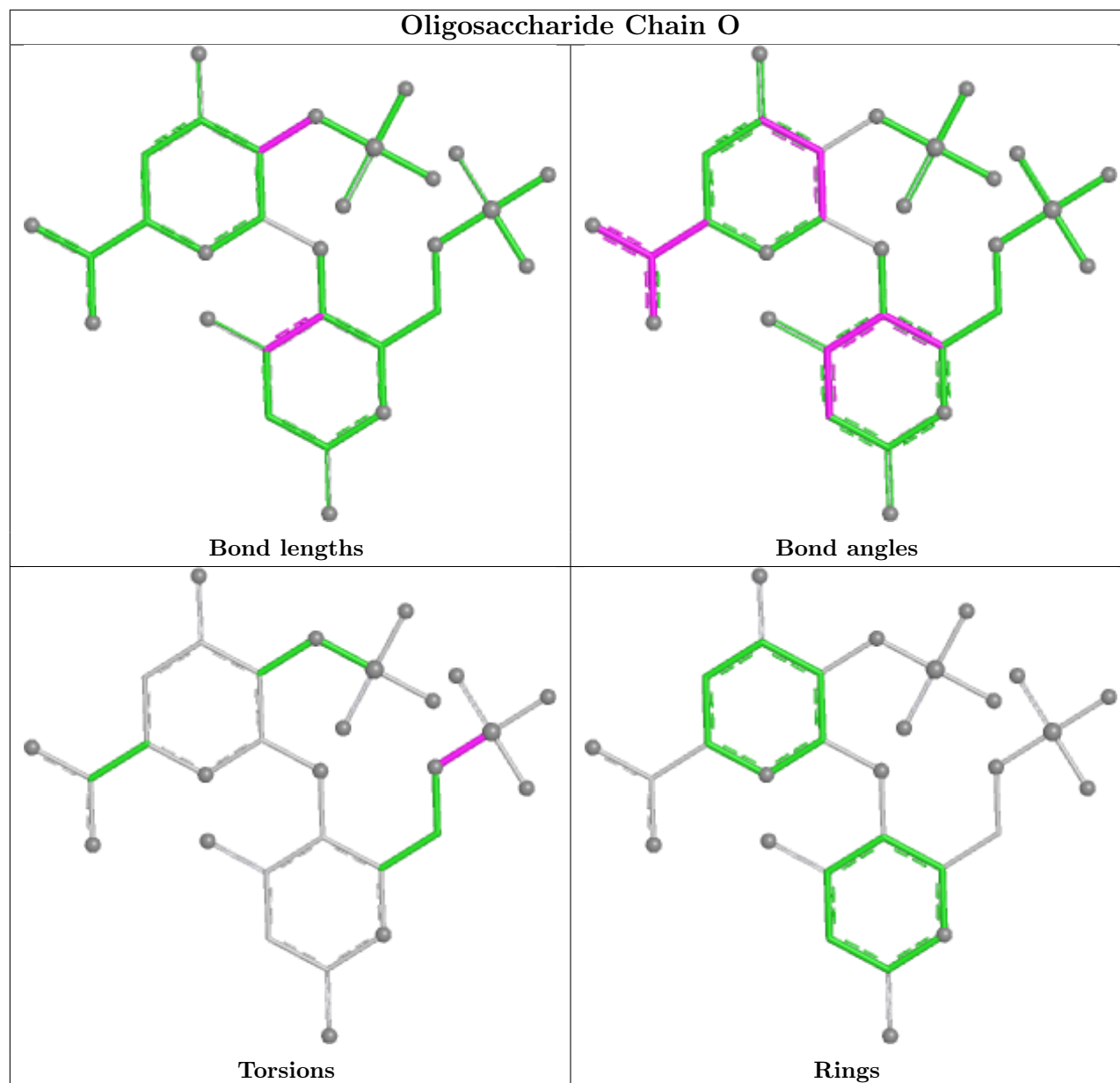


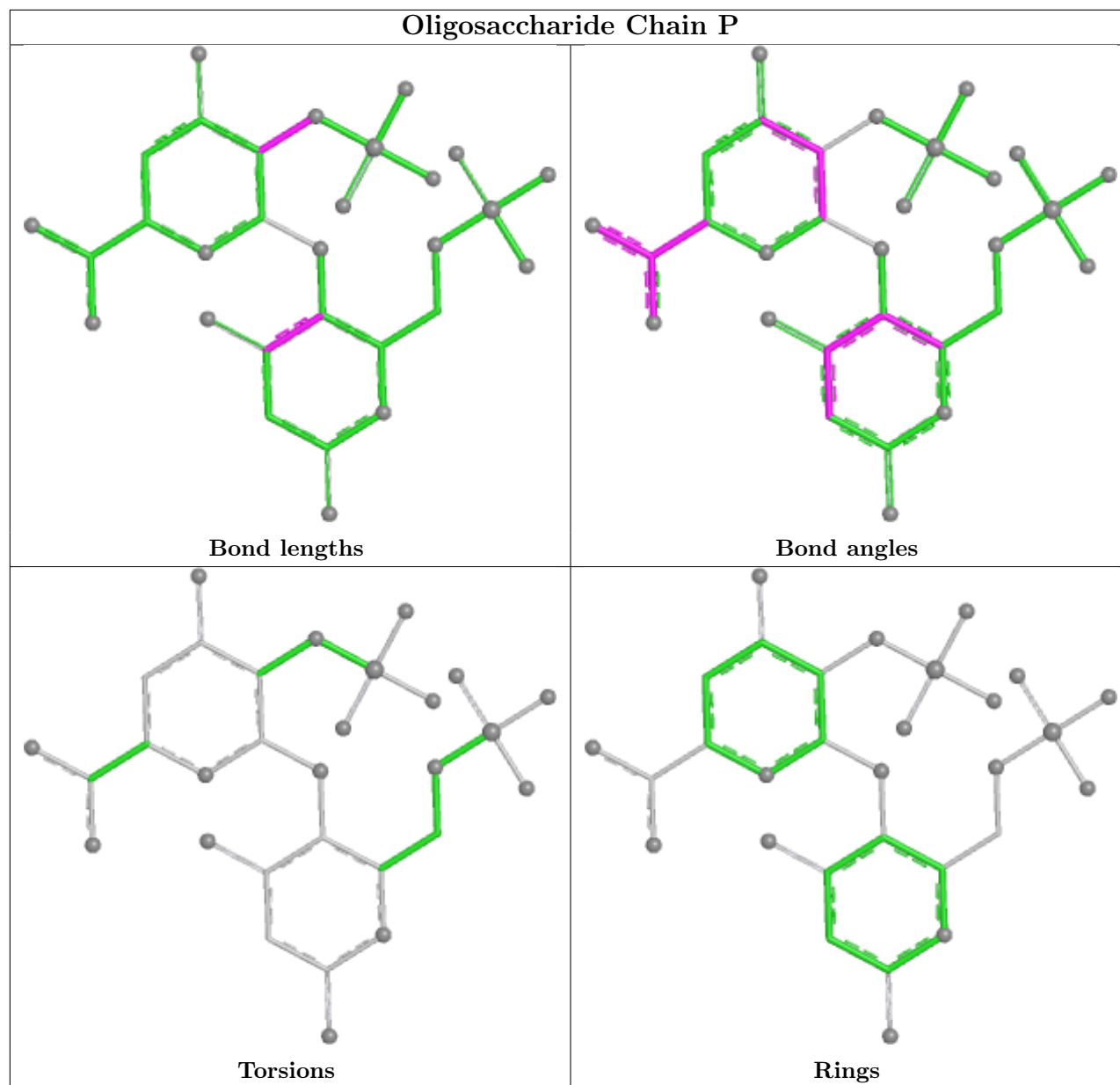
Torsions

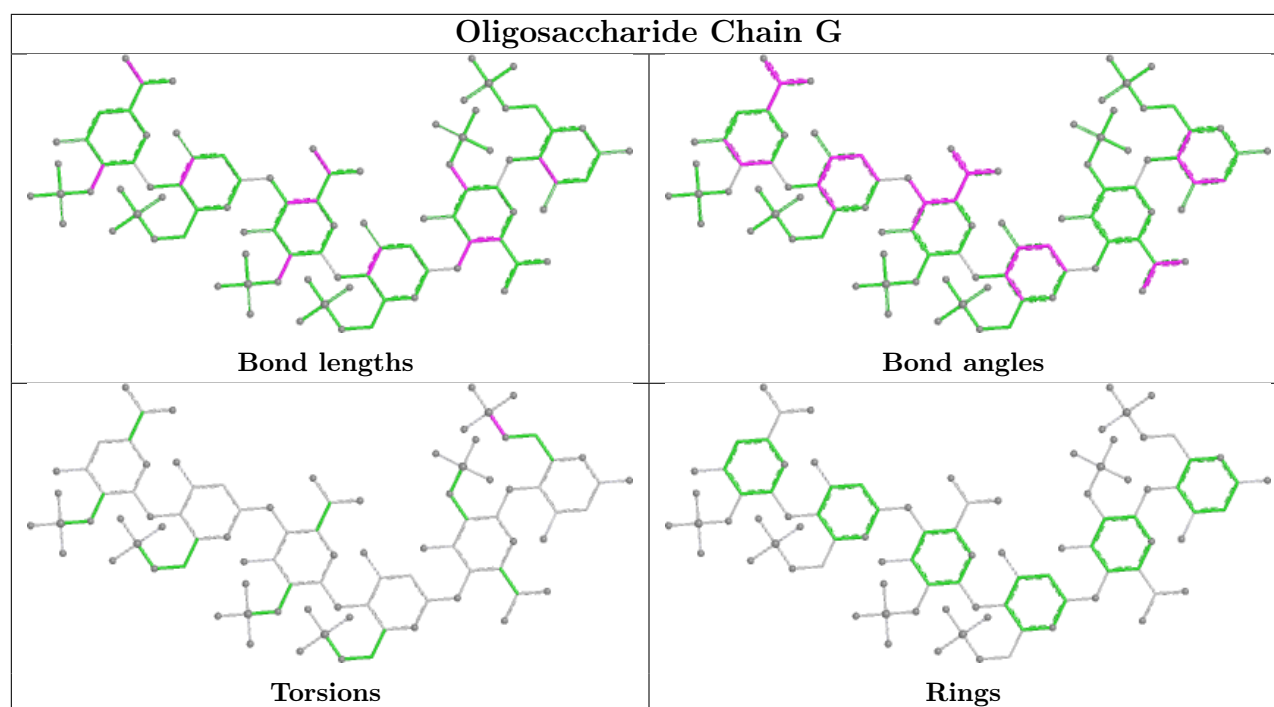


Rings









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	427/427 (100%)	0.10	22 (5%)	33	25	19, 38, 86, 131	0
1	B	427/427 (100%)	0.11	16 (3%)	45	36	20, 36, 88, 133	0
1	C	427/427 (100%)	0.16	16 (3%)	45	36	20, 39, 95, 144	0
1	D	425/427 (99%)	0.19	26 (6%)	27	20	18, 39, 94, 141	0
1	E	425/427 (99%)	0.11	24 (5%)	30	23	19, 34, 81, 115	0
All	All	2131/2135 (99%)	0.13	104 (4%)	35	27	18, 37, 91, 144	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	437	ALA	5.2
1	A	353	THR	5.1
1	E	435	SER	5.1
1	B	403	ASN	4.6
1	E	403	ASN	4.6
1	E	353	THR	4.3
1	B	56	ASN	3.9
1	B	141	VAL	3.9
1	E	434	GLY	3.8
1	A	40	SER	3.7
1	D	317	GLN	3.7
1	C	351	SER	3.7
1	D	353	THR	3.7
1	D	40	SER	3.6
1	C	139	ALA	3.5
1	A	437	ALA	3.5
1	C	433	GLY	3.5
1	A	317	GLN	3.4
1	E	55	PRO	3.4
1	C	438	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	434	GLY	3.3
1	D	435	SER	3.3
1	C	435	SER	3.2
1	E	473	GLY	3.2
1	D	352	GLU	3.2
1	D	90	PHE	3.2
1	B	297	GLY	3.2
1	A	86	PRO	3.2
1	D	141	VAL	3.1
1	D	432	GLY	3.1
1	B	136	ALA	3.1
1	B	436	GLY	3.1
1	E	386	ASP	3.0
1	D	110	GLY	3.0
1	E	472	ALA	3.0
1	A	58	ASN	2.9
1	D	56	ASN	2.9
1	A	110	GLY	2.9
1	B	437	ALA	2.9
1	B	40	SER	2.9
1	B	317	GLN	2.9
1	D	174	PRO	2.8
1	C	278	LYS	2.8
1	C	40	SER	2.8
1	C	138	ASN	2.8
1	B	273	ASP	2.8
1	E	352	GLU	2.7
1	E	437	ALA	2.7
1	E	59	LYS	2.7
1	C	110	GLY	2.7
1	B	178	VAL	2.7
1	B	435	SER	2.7
1	A	176	THR	2.6
1	D	283	THR	2.6
1	A	178	VAL	2.6
1	E	178	VAL	2.6
1	E	137	ALA	2.6
1	B	55	PRO	2.6
1	C	436	GLY	2.6
1	A	55	PRO	2.6
1	E	433	GLY	2.6
1	E	436	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	59	LYS	2.6
1	A	348	ILE	2.6
1	B	32	ASN	2.6
1	D	54	LYS	2.5
1	E	297	GLY	2.5
1	E	442	LYS	2.5
1	C	434	GLY	2.5
1	A	60	ILE	2.5
1	A	56	ASN	2.5
1	B	179	ALA	2.4
1	A	435	SER	2.4
1	D	434	GLY	2.4
1	B	315	ARG	2.4
1	E	443	LYS	2.3
1	E	54	LYS	2.3
1	C	140	GLY	2.3
1	C	175	CYS	2.3
1	D	282	SER	2.3
1	D	396	SER	2.3
1	A	182	PRO	2.3
1	A	61	LEU	2.3
1	C	176	THR	2.3
1	C	353	THR	2.3
1	E	396	SER	2.3
1	A	175	CYS	2.2
1	A	436	GLY	2.2
1	D	20	ALA	2.2
1	E	139	ALA	2.2
1	D	443	LYS	2.2
1	D	266	THR	2.1
1	D	89	SER	2.1
1	D	88	THR	2.1
1	D	85	PHE	2.1
1	D	344	LEU	2.1
1	E	317	GLN	2.1
1	A	433	GLY	2.1
1	E	438	GLU	2.1
1	E	141	VAL	2.1
1	D	403	ASN	2.1
1	D	273	ASP	2.1
1	A	82	LYS	2.0
1	A	438	GLU	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](#)

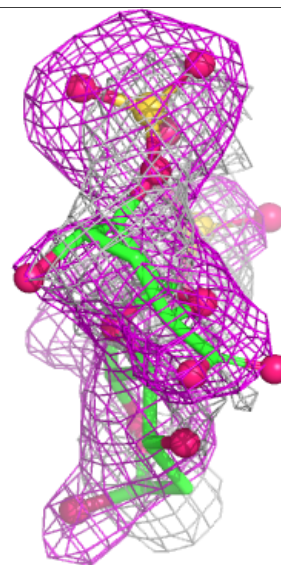
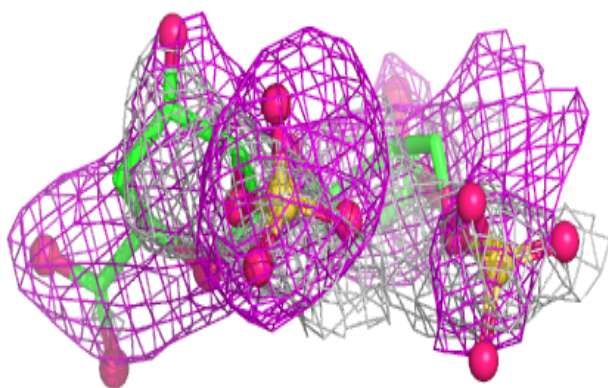
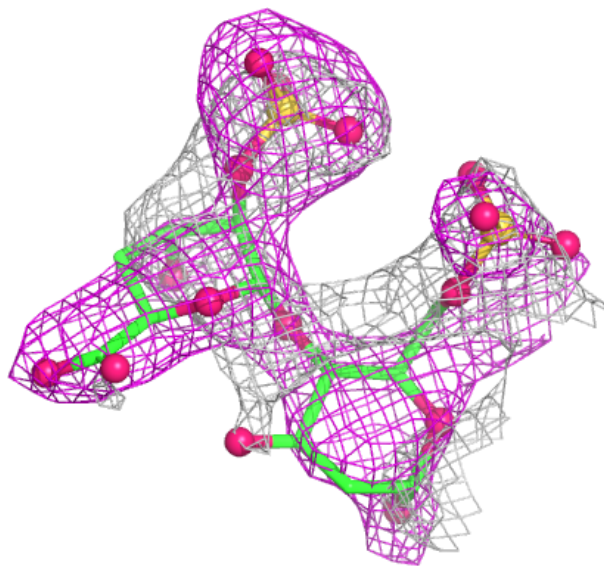
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	JHM	L	1	15/15	-0.10	0.24	46,66,88,89	0
2	JHM	O	1	15/15	0.01	0.23	46,66,88,89	0
3	JHM	G	1	15/15	0.04	0.22	46,66,88,89	0
3	JHM	G	5	14/15	0.05	0.25	46,66,88,89	0
2	JHM	J	1	15/15	0.08	0.27	46,66,88,89	0
3	JHM	G	3	14/15	0.11	0.23	46,66,88,89	0
2	JHM	I	1	15/15	0.11	0.21	46,66,88,89	0
2	JHM	K	1	15/15	0.14	0.23	46,66,88,89	0
2	JHM	N	1	15/15	0.14	0.21	46,66,88,89	0
2	JHM	P	1	15/15	0.15	0.22	46,66,88,89	0
2	JHM	M	1	15/15	0.18	0.20	46,66,88,89	0
2	JHM	F	1	15/15	0.19	0.21	46,66,88,89	0
2	JHM	H	1	15/15	0.20	0.23	46,66,88,89	0
2	IDS	K	2	15/17	0.37	0.24	30,31,38,42	0
2	IDS	P	2	15/17	0.40	0.22	30,31,38,42	0
3	IDS	G	2	16/17	0.42	0.24	30,32,42,69	0
3	IDS	G	6	15/17	0.45	0.22	30,31,38,42	0
2	IDS	O	2	15/17	0.46	0.20	30,31,38,42	0
2	IDS	F	2	15/17	0.49	0.19	30,31,38,42	0
2	IDS	J	2	15/17	0.50	0.23	30,31,38,42	0
2	IDS	M	2	15/17	0.51	0.21	30,31,38,42	0
2	IDS	H	2	15/17	0.51	0.24	30,31,38,42	0
2	IDS	N	2	15/17	0.51	0.20	30,31,38,42	0
3	IDS	G	4	16/17	0.52	0.19	30,32,42,69	0
2	IDS	I	2	15/17	0.56	0.19	30,31,38,42	0
2	IDS	L	2	15/17	0.58	0.19	30,31,38,42	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.

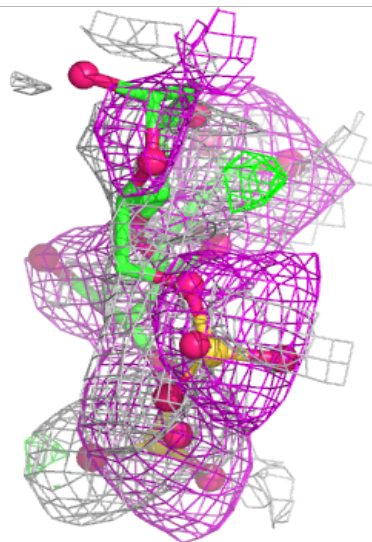
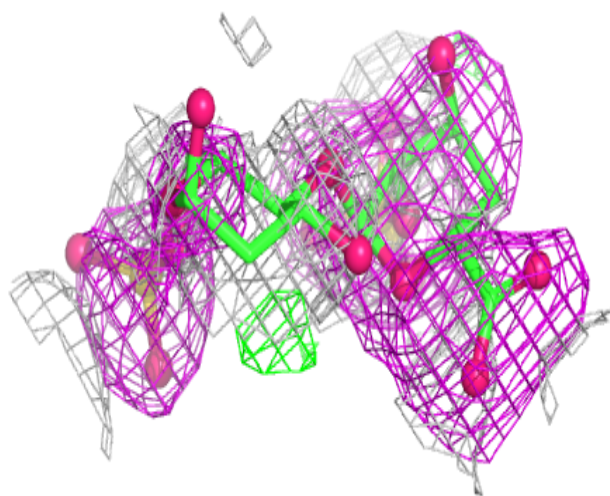
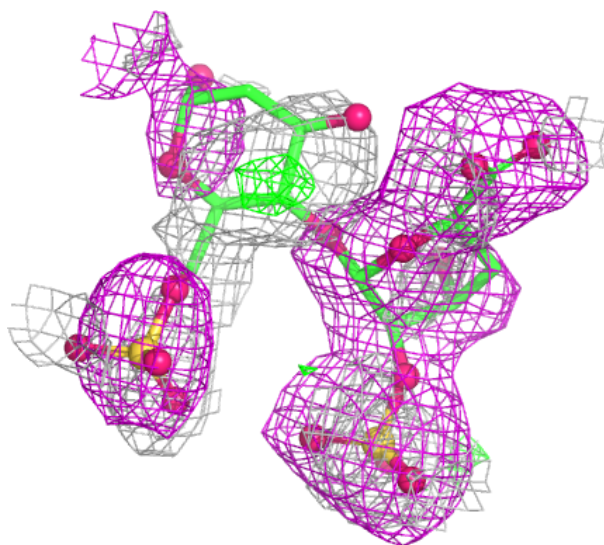
Electron density around Chain F:

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



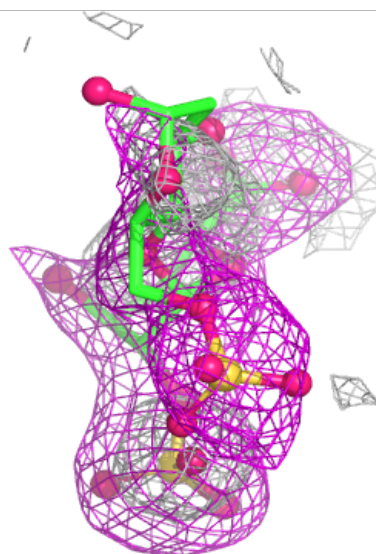
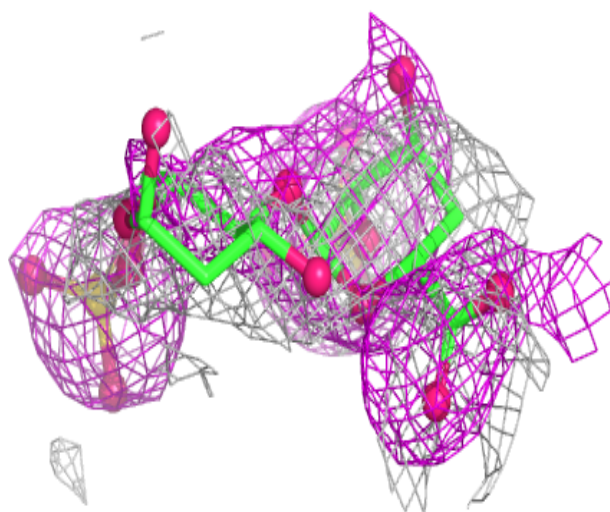
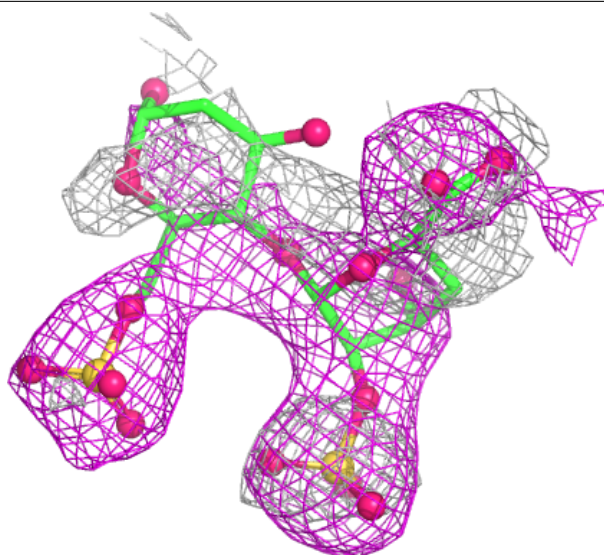
Electron density around Chain H:

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



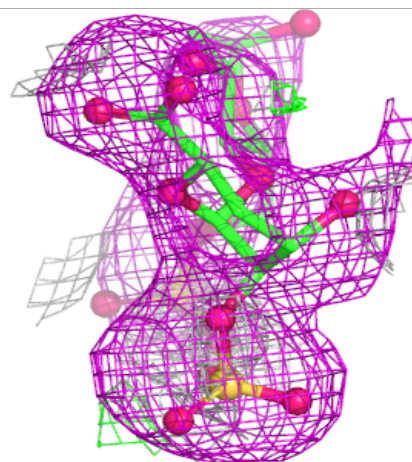
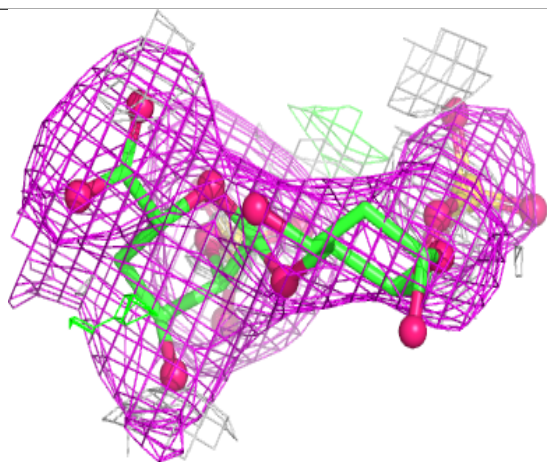
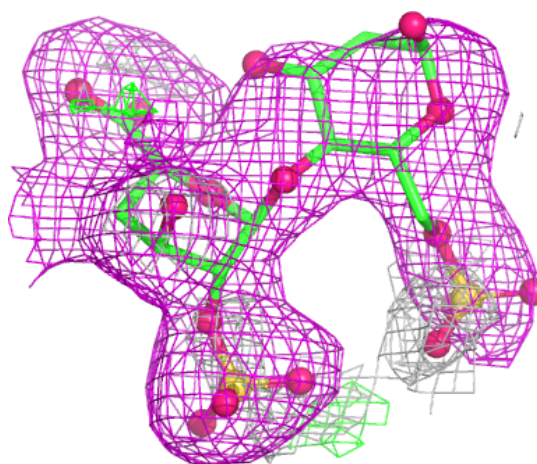
Electron density around Chain I:

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



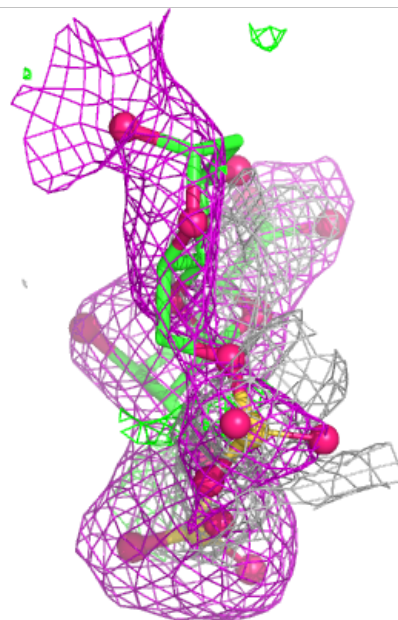
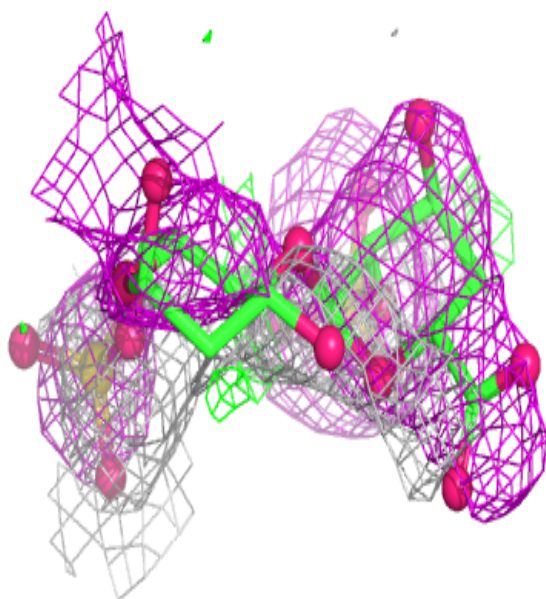
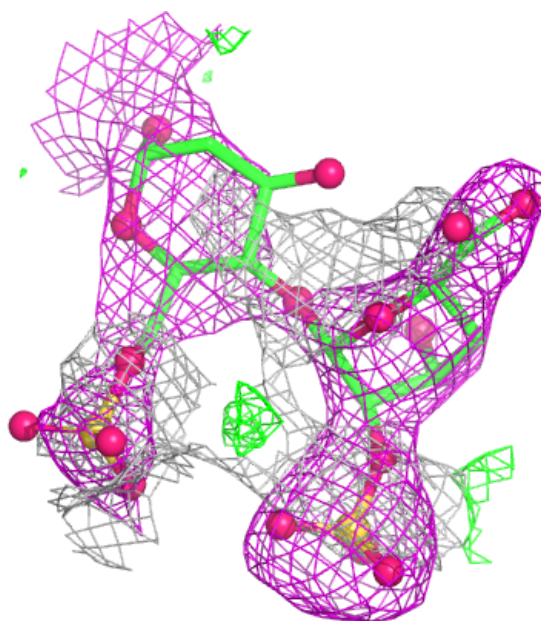
Electron density around Chain J:

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



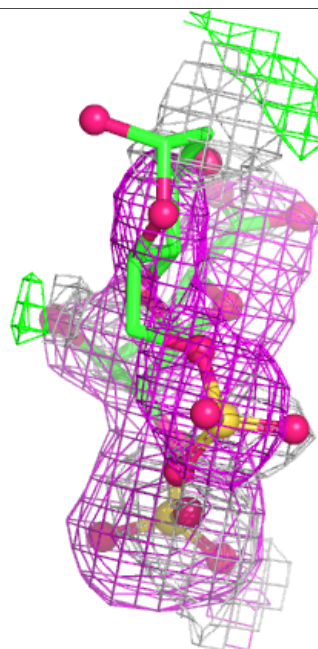
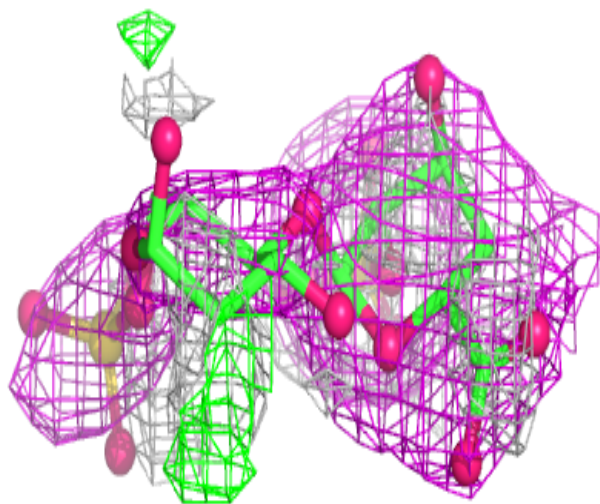
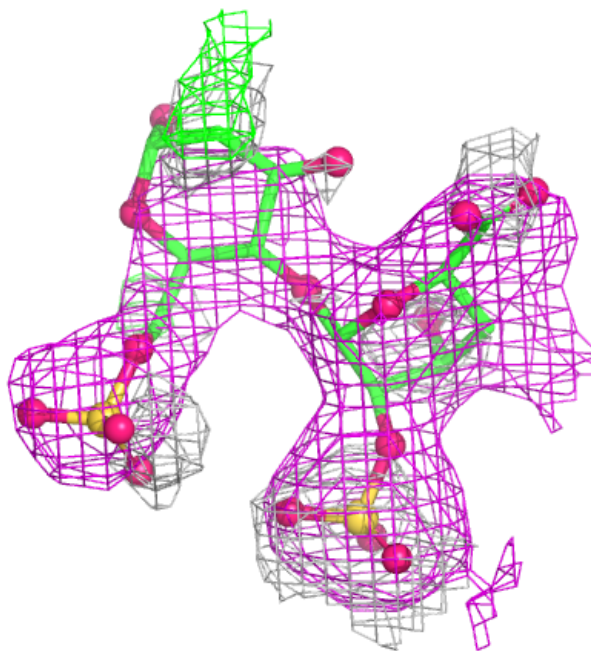
Electron density around Chain K:

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and green (positive)



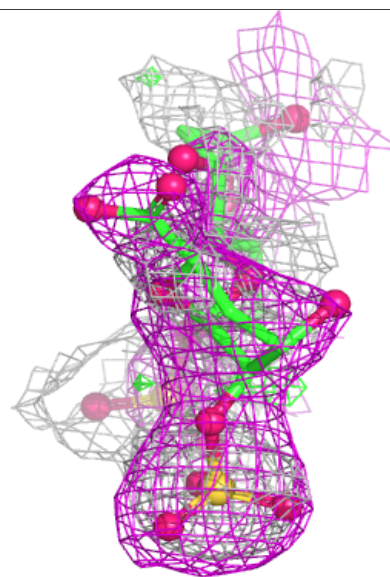
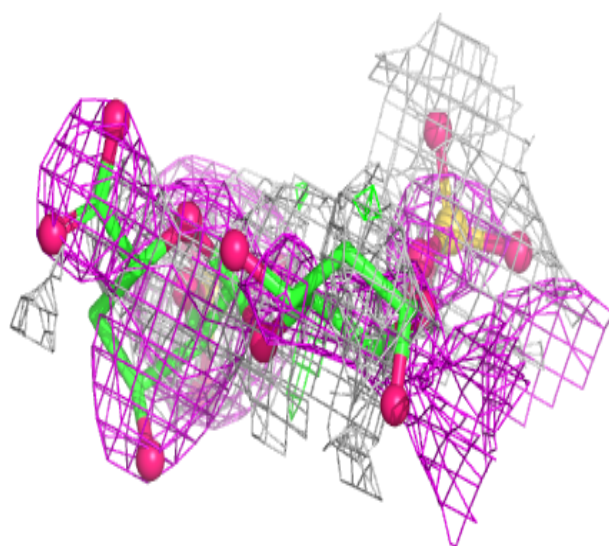
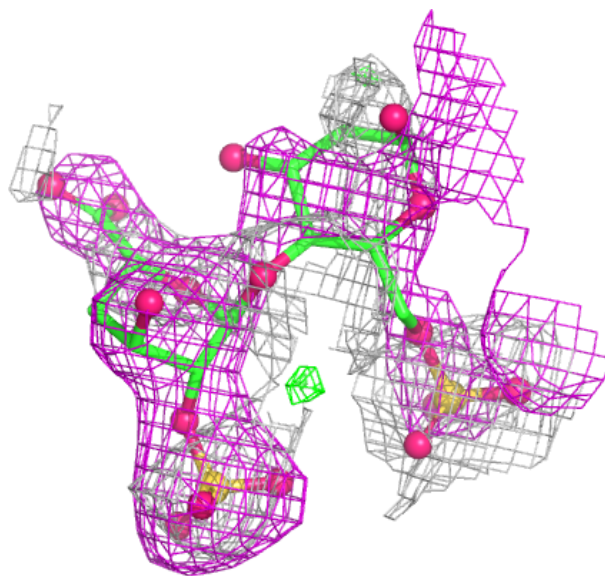
Electron density around Chain L:

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



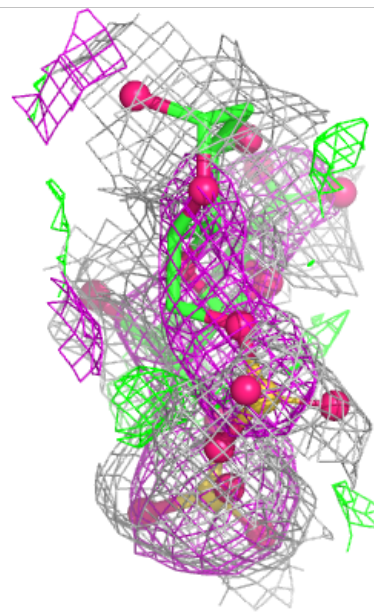
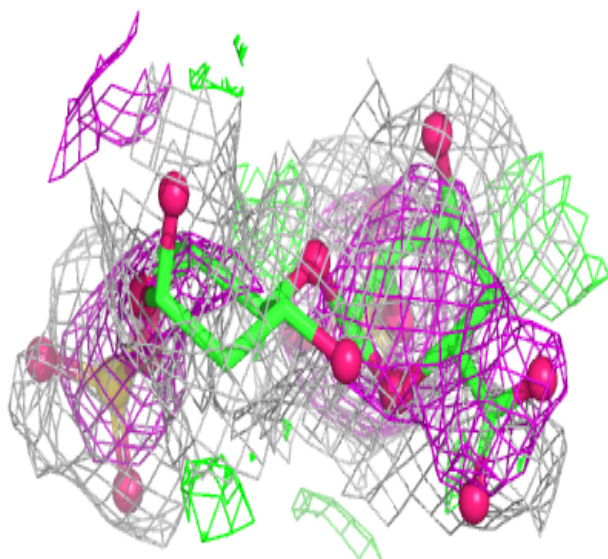
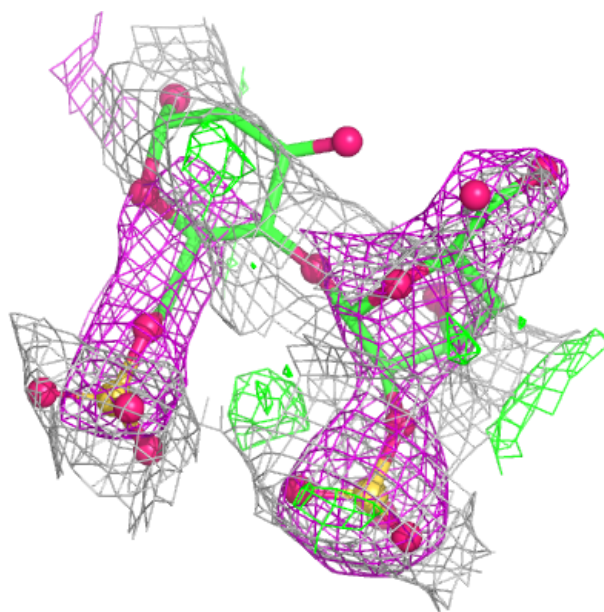
Electron density around Chain M:

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



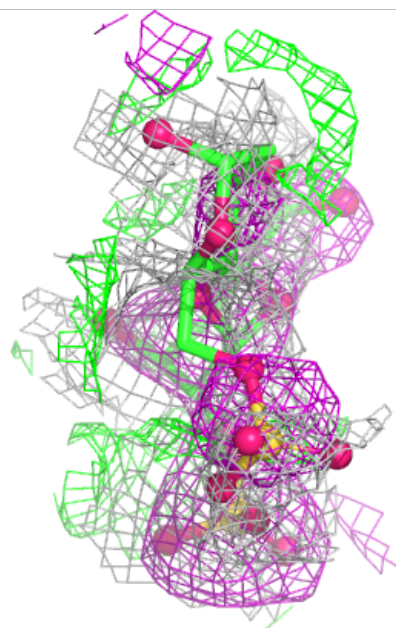
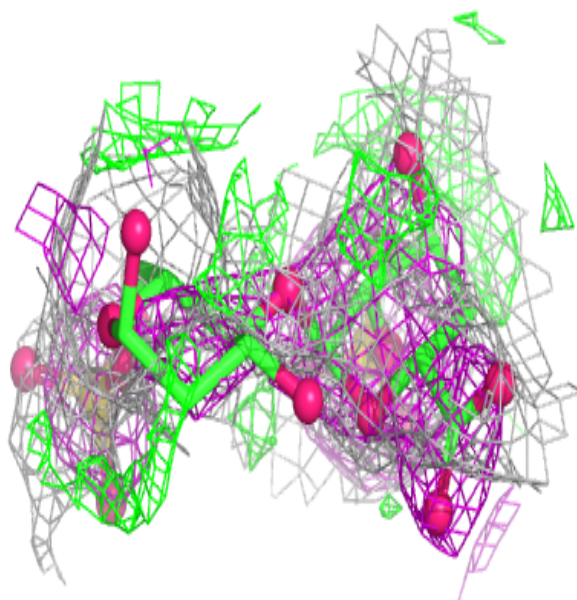
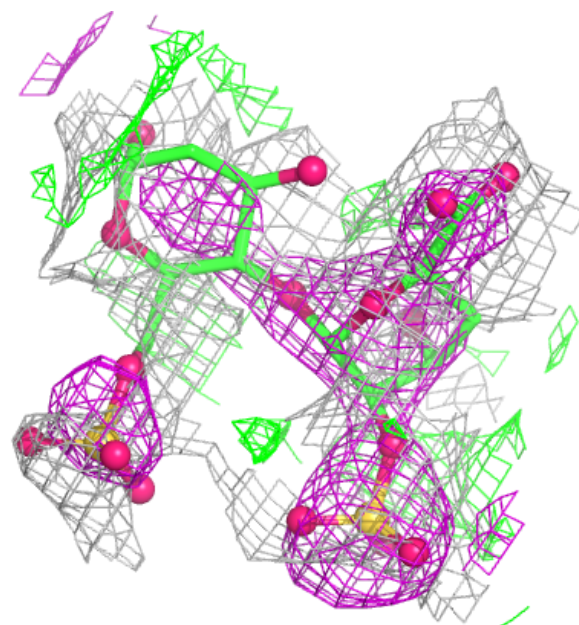
Electron density around Chain N:

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



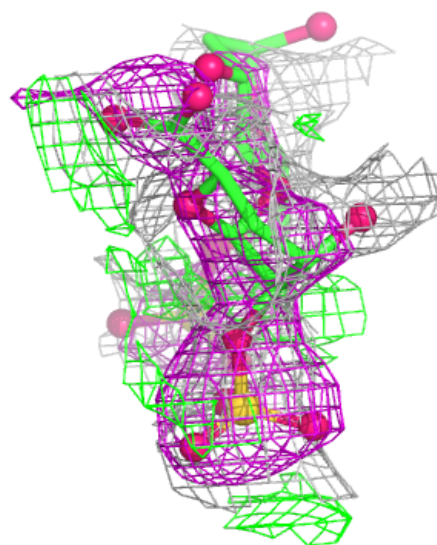
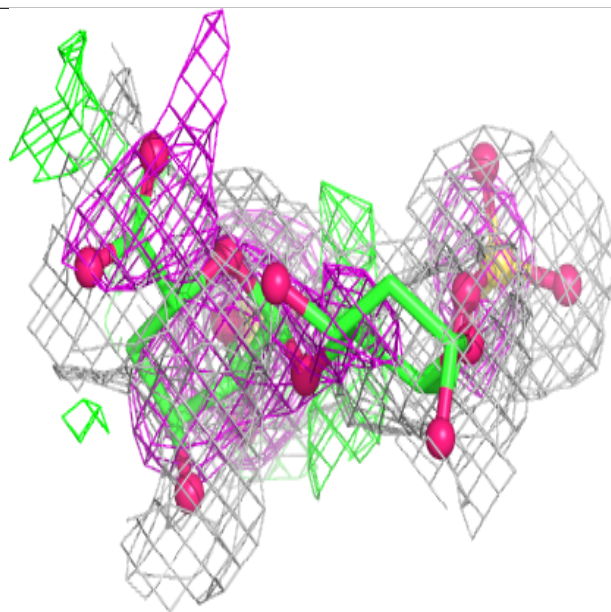
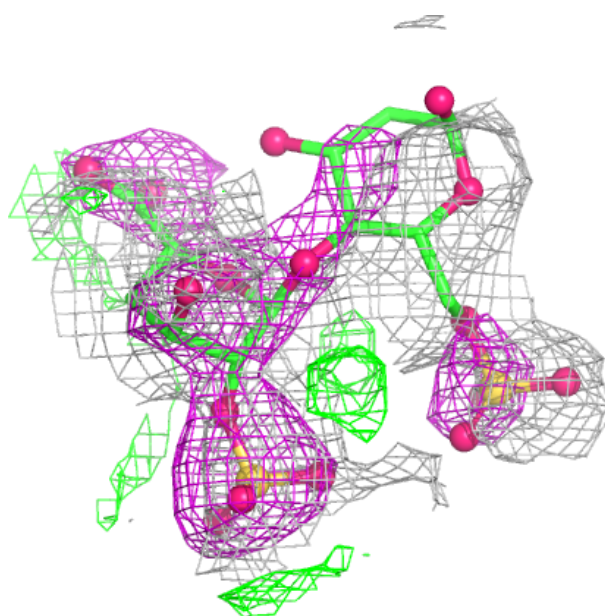
Electron density around Chain O:

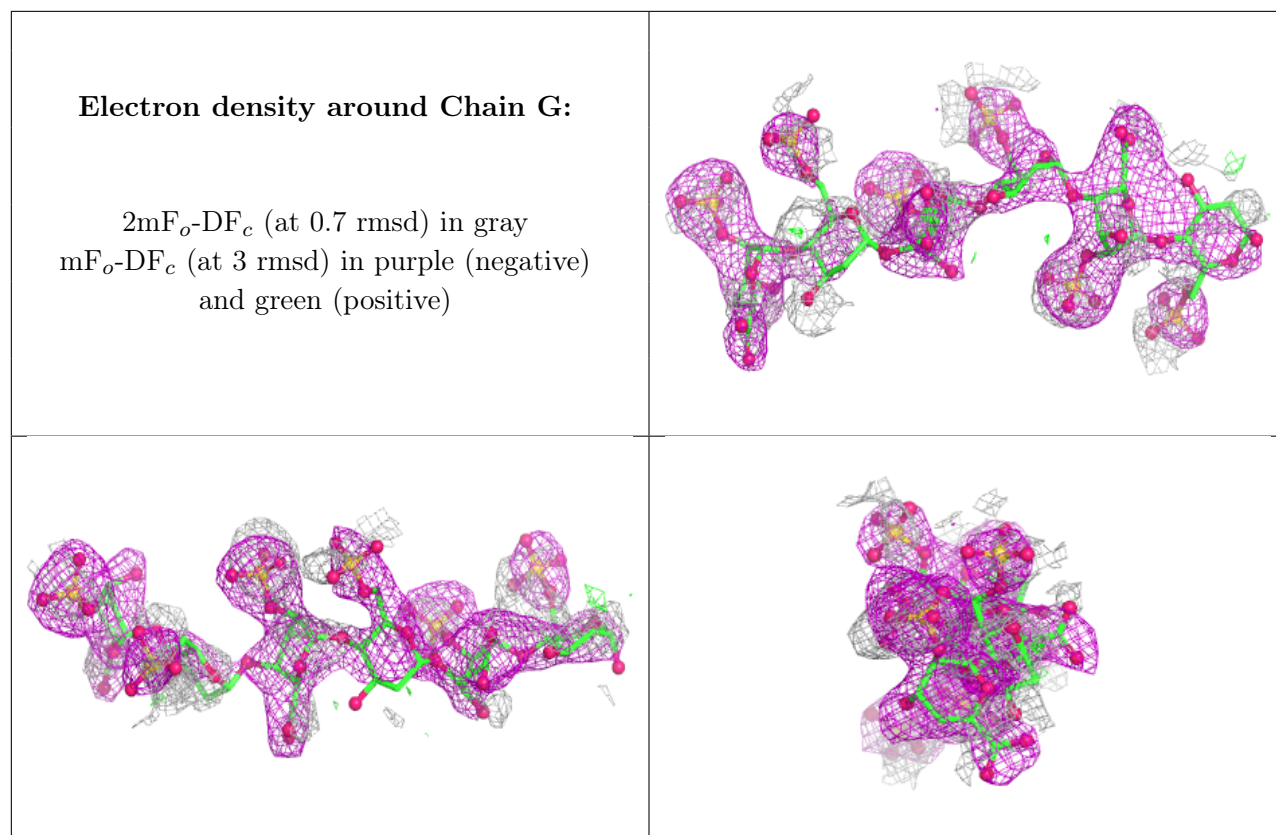
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.