



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:31 AM BST

PDB ID : 1SFY
Title : Crystal structure of recombinant Erythrina corallodendron Lectin
Authors : Kulkarni, K.A.; Srivastava, A.; Mitra, N.; Surolia, A.; Vijayan, M.; Suguna, K.
Deposited on : 2004-02-21
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

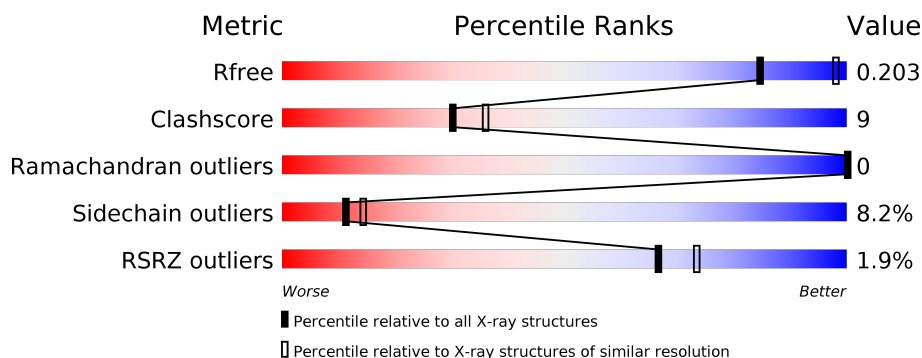
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	239	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div> </div>
1	B	239	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div></div> </div> </div>
1	C	239	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>5%</div> </div> </div>
1	D	239	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div> </div>
1	E	239	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>6%</div> </div> </div>
1	F	239	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12073 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 Lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1843	1178	298	364	3			
1	B	239	Total	C	N	O	S	0	0	0
			1839	1175	297	364	3			
1	C	239	Total	C	N	O	S	0	0	0
			1837	1175	295	364	3			
1	D	239	Total	C	N	O	S	0	0	0
			1840	1176	297	364	3			
1	E	239	Total	C	N	O	S	0	0	0
			1836	1174	296	363	3			
1	F	239	Total	C	N	O	S	0	0	0
			1835	1174	296	362	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	ALA	SEE REMARK 999	UNP P16404
A	134	GLN	PRO	SEE REMARK 999	UNP P16404
A	178	LEU	ILE	SEE REMARK 999	UNP P16404
B	24	SER	ALA	SEE REMARK 999	UNP P16404
B	134	GLN	PRO	SEE REMARK 999	UNP P16404
B	178	LEU	ILE	SEE REMARK 999	UNP P16404
C	24	SER	ALA	SEE REMARK 999	UNP P16404
C	134	GLN	PRO	SEE REMARK 999	UNP P16404
C	178	LEU	ILE	SEE REMARK 999	UNP P16404
D	24	SER	ALA	SEE REMARK 999	UNP P16404
D	134	GLN	PRO	SEE REMARK 999	UNP P16404
D	178	LEU	ILE	SEE REMARK 999	UNP P16404
E	24	SER	ALA	SEE REMARK 999	UNP P16404
E	134	GLN	PRO	SEE REMARK 999	UNP P16404
E	178	LEU	ILE	SEE REMARK 999	UNP P16404
F	24	SER	ALA	SEE REMARK 999	UNP P16404
F	134	GLN	PRO	SEE REMARK 999	UNP P16404

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Chain	Residue	Modelled	Actual	Comment	Reference
F	178	LEU	ILE	SEE REMARK 999	UNP P16404

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

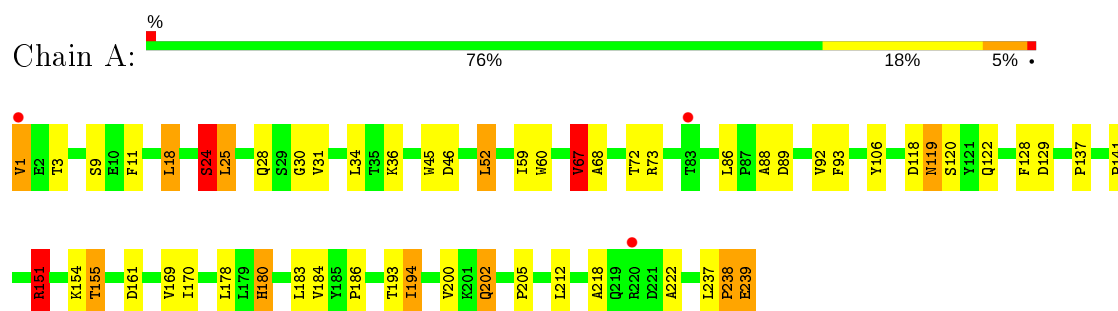
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	168	Total O 168 168	0	0
5	B	139	Total O 139 139	0	0
5	C	166	Total O 166 166	0	0
5	D	152	Total O 152 152	0	0
5	E	142	Total O 142 142	0	0
5	F	126	Total O 126 126	0	0

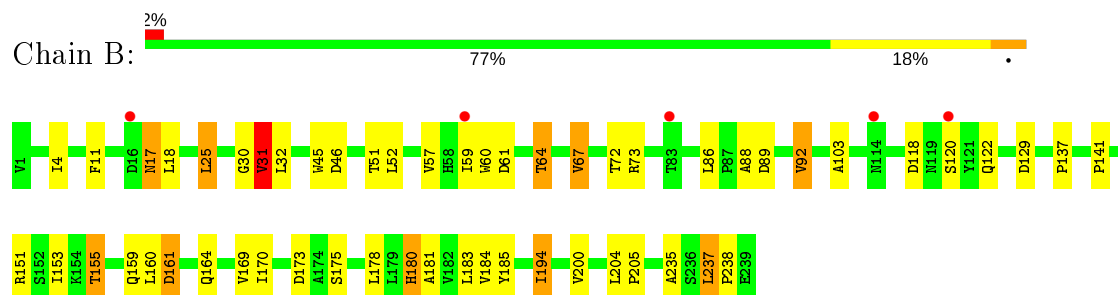
3 Residue-property plots [i](#)

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

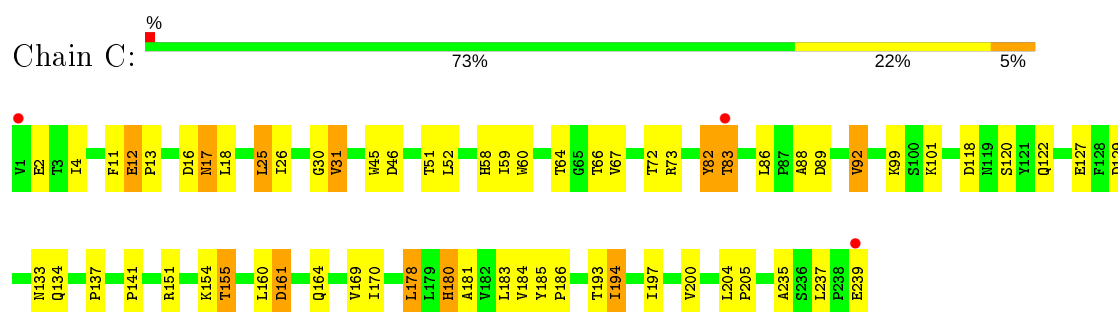
• Molecule 1: Lectin



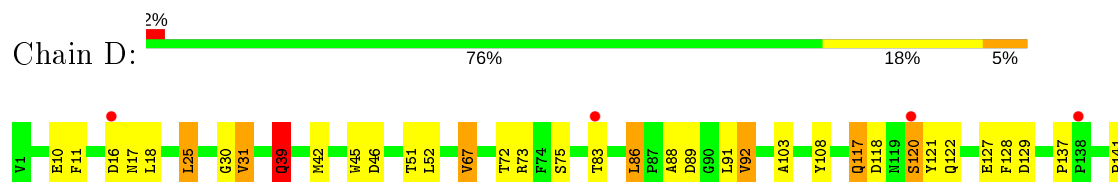
• Molecule 1: Lectin

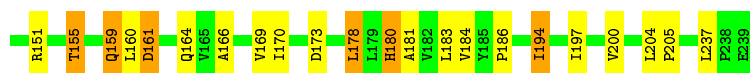


• Molecule 1: Lectin

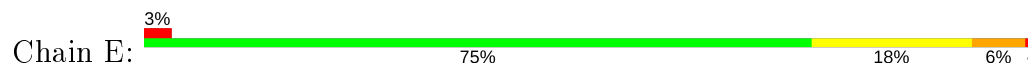


• Molecule 1: Lectin

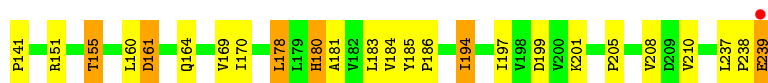
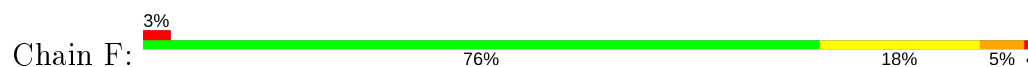




- Molecule 1: Lectin



- Molecule 1: Lectin



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

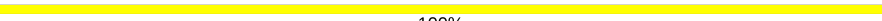


- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%

BG1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:  100%

BG1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.24Å 144.89Å 127.66Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	17.66 – 2.55 17.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	92.4 (17.66-2.55) 92.5 (17.66-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.55Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.208 0.177 , 0.203	Depositor DCC
R_{free} test set	1229 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.0	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	0.95	EDS
Total number of atoms	12073	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: CA, BGC, GAL, MN

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	0.39	0/1893	0.99	20/2587 (0.8%)
1	B	0.37	0/1889	0.79	5/2583 (0.2%)
1	C	0.37	0/1887	1.22	22/2580 (0.9%)
1	D	0.37	0/1890	0.91	13/2585 (0.5%)
1	E	0.38	0/1886	1.07	23/2580 (0.9%)
1	F	0.37	0/1885	0.91	15/2577 (0.6%)
All	All	0.38	0/11330	0.99	98/15492 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	4
All	All	0	7

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ARG	NE-CZ-NH1	-24.49	108.05	120.30
1	C	151	ARG	NE-CZ-NH2	22.56	131.58	120.30
1	C	82	TYR	O-C-N	-14.15	100.06	122.70
1	C	83	THR	O-C-N	13.74	144.69	122.70
1	E	67	VAL	CA-CB-CG1	-13.01	91.38	110.90
1	E	83	THR	N-CA-CB	-11.58	88.30	110.30
1	C	133	ASN	O-C-N	-10.54	105.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	THR	CA-C-N	-10.52	94.06	117.20
1	E	220	ARG	CA-CB-CG	10.10	135.62	113.40
1	E	151	ARG	CD-NE-CZ	10.02	137.63	123.60
1	A	151	ARG	CG-CD-NE	9.67	132.10	111.80
1	D	42	MET	CG-SD-CE	9.32	115.12	100.20
1	A	238	PRO	O-C-N	-9.24	107.91	122.70
1	C	83	THR	C-N-CA	-9.09	98.97	121.70
1	E	223	ALA	N-CA-CB	-9.00	97.50	110.10
1	E	159	GLN	N-CA-CB	8.99	126.78	110.60
1	E	238	PRO	CA-C-N	8.95	136.90	117.20
1	F	201	LYS	CA-CB-CG	8.94	133.06	113.40
1	F	12	GLU	CA-CB-CG	8.88	132.94	113.40
1	D	108	TYR	CA-CB-CG	8.84	130.19	113.40
1	A	193	THR	N-CA-CB	-8.83	93.53	110.30
1	E	238	PRO	O-C-N	-8.78	108.66	122.70
1	A	24	SER	N-CA-CB	8.71	123.57	110.50
1	E	239	GLU	CB-CG-CD	8.51	137.17	114.20
1	F	86	LEU	N-CA-CB	-8.38	93.64	110.40
1	F	3	THR	CA-CB-CG2	-8.25	100.86	112.40
1	A	119	ASN	CB-CA-C	8.18	126.76	110.40
1	D	108	TYR	CB-CA-C	8.04	126.49	110.40
1	C	134	GLN	CA-C-N	-8.04	99.51	117.20
1	D	39	GLN	CA-CB-CG	7.92	130.82	113.40
1	C	133	ASN	CA-C-N	7.78	134.32	117.20
1	E	83	THR	CA-CB-CG2	-7.73	101.58	112.40
1	D	159	GLN	CB-CG-CD	7.66	131.52	111.60
1	B	31	VAL	CA-CB-CG1	-7.62	99.47	110.90
1	A	200	VAL	CB-CA-C	7.48	125.61	111.40
1	D	121	TYR	N-CA-CB	7.34	123.82	110.60
1	E	3	THR	CA-CB-CG2	-7.33	102.14	112.40
1	A	222	ALA	CB-CA-C	7.31	121.06	110.10
1	A	238	PRO	C-N-CA	7.29	139.92	121.70
1	F	16	ASP	CB-CA-C	-7.24	95.93	110.40
1	E	71	GLU	CA-CB-CG	7.16	129.14	113.40
1	C	134	GLN	C-N-CA	-7.06	104.04	121.70
1	A	222	ALA	N-CA-CB	6.93	119.81	110.10
1	E	67	VAL	N-CA-CB	6.92	126.72	111.50
1	C	83	THR	CA-CB-OG1	-6.79	94.73	109.00
1	C	134	GLN	O-C-N	6.73	133.47	122.70
1	B	67	VAL	CA-CB-CG1	-6.69	100.86	110.90
1	B	103	ALA	CB-CA-C	6.65	120.08	110.10
1	A	1	VAL	O-C-N	-6.49	112.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	VAL	CB-CA-C	-6.49	99.07	111.40
1	C	31	VAL	CA-CB-CG1	-6.47	101.20	110.90
1	C	83	THR	N-CA-CB	-6.43	98.08	110.30
1	A	202	GLN	CB-CG-CD	6.43	128.32	111.60
1	A	28	GLN	CB-CG-CD	6.40	128.24	111.60
1	C	133	ASN	C-N-CA	6.35	137.56	121.70
1	C	82	TYR	CA-C-N	6.33	131.13	117.20
1	C	64	THR	CA-CB-CG2	-6.30	103.58	112.40
1	A	200	VAL	N-CA-CB	-6.23	97.80	111.50
1	C	193	THR	N-CA-CB	-6.18	98.55	110.30
1	A	67	VAL	CA-CB-CG1	-6.16	101.66	110.90
1	E	154	LYS	CA-CB-CG	6.08	126.78	113.40
1	A	238	PRO	CA-C-N	6.06	130.54	117.20
1	E	59	ILE	CB-CA-C	6.05	123.70	111.60
1	B	173	ASP	N-CA-CB	6.04	121.48	110.60
1	E	33	GLN	CB-CG-CD	6.03	127.27	111.60
1	F	25	LEU	CA-CB-CG	6.00	129.10	115.30
1	E	238	PRO	C-N-CA	5.96	136.60	121.70
1	E	71	GLU	CB-CG-CD	5.89	130.11	114.20
1	D	117	GLN	CA-CB-CG	5.88	126.33	113.40
1	D	103	ALA	CB-CA-C	5.86	118.89	110.10
1	E	95	MET	CG-SD-CE	5.83	109.53	100.20
1	A	52	LEU	CB-CA-C	-5.83	99.13	110.20
1	C	12	GLU	CB-CA-C	5.82	122.05	110.40
1	C	101	LYS	CG-CD-CE	5.82	129.36	111.90
1	C	82	TYR	C-N-CA	5.78	136.14	121.70
1	E	28	GLN	CB-CG-CD	5.69	126.39	111.60
1	F	98	THR	O-C-N	5.65	131.74	122.70
1	F	210	VAL	CB-CA-C	5.60	122.03	111.40
1	D	10	GLU	CA-CB-CG	5.54	125.58	113.40
1	C	151	ARG	CD-NE-CZ	-5.51	115.88	123.60
1	F	199	ASP	N-CA-CB	5.43	120.38	110.60
1	A	202	GLN	CB-CA-C	-5.43	99.54	110.40
1	A	67	VAL	N-CA-CB	5.37	123.32	111.50
1	F	64	THR	CA-CB-CG2	-5.37	104.89	112.40
1	F	52	LEU	CB-CA-C	-5.32	100.09	110.20
1	A	119	ASN	N-CA-CB	-5.31	101.05	110.60
1	A	151	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	86	LEU	CA-CB-CG	5.22	127.31	115.30
1	E	25	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	67	VAL	N-CA-CB	5.21	122.97	111.50
1	D	151	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	THR	CA-CB-CG2	-5.17	105.17	112.40
1	E	151	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	F	208	VAL	CB-CA-C	-5.12	101.67	111.40
1	D	31	VAL	CB-CA-C	-5.11	101.69	111.40
1	E	25	LEU	CB-CA-C	-5.09	100.52	110.20
1	F	12	GLU	N-CA-CB	5.01	119.62	110.60
1	F	151	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	151	ARG	Sidechain
1	C	82	TYR	Mainchain
1	E	151	ARG	Sidechain
1	E	220	ARG	Sidechain
1	E	238	PRO	Mainchain,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	1843	0	1760	31	0
1	B	1839	0	1749	34	0
1	C	1837	0	1749	44	0
1	D	1840	0	1750	31	0
1	E	1836	0	1744	35	0
1	F	1835	0	1748	36	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	168	0	0	5	0
5	B	139	0	0	2	0
5	C	166	0	0	1	0
5	D	152	0	0	1	0
5	E	142	0	0	3	0
5	F	126	0	0	0	0
All	All	12073	0	10626	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HG3	1:A:194:ILE:HD11	1.35	1.07
1:B:61:ASP:OD2	1:B:64:THR:HG23	1.75	0.87
1:C:181:ALA:HB3	1:C:194:ILE:HD13	1.58	0.86
1:F:181:ALA:HB3	1:F:194:ILE:HD13	1.59	0.85
1:B:181:ALA:HB3	1:B:194:ILE:HD13	1.58	0.84
1:E:181:ALA:HB3	1:E:194:ILE:HD13	1.59	0.83
1:F:61:ASP:OD2	1:F:64:THR:HG23	1.79	0.82
1:C:66:THR:HG21	1:C:239:GLU:HB2	1.58	0.82
1:D:181:ALA:HB3	1:D:194:ILE:HD13	1.60	0.82
1:F:118:ASP:OD1	1:F:120:SER:HB2	1.82	0.80
1:F:118:ASP:OD1	1:F:120:SER:CB	2.30	0.79
1:C:4:ILE:HG22	1:C:235:ALA:HB3	1.65	0.79
1:C:181:ALA:HB3	1:C:194:ILE:CD1	2.13	0.77
1:F:181:ALA:HB3	1:F:194:ILE:CD1	2.15	0.76
1:E:181:ALA:HB3	1:E:194:ILE:CD1	2.16	0.76
1:D:181:ALA:HB3	1:D:194:ILE:CD1	2.15	0.76
1:B:181:ALA:HB3	1:B:194:ILE:CD1	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASP:OD2	1:C:120:SER:HB3	1.87	0.75
1:D:39:GLN:H	1:D:39:GLN:NE2	1.86	0.73
1:D:173:ASP:HB3	5:D:4594:HOH:O	1.89	0.72
1:C:25:LEU:HD23	1:C:25:LEU:C	2.10	0.71
1:C:17:ASN:HD22	1:C:17:ASN:N	1.88	0.70
1:A:118:ASP:OD1	1:A:120:SER:HB3	1.93	0.69
1:B:118:ASP:OD2	1:B:120:SER:HB3	1.94	0.67
1:C:25:LEU:HD23	1:C:26:ILE:N	2.09	0.67
1:F:137:PRO:HG3	1:F:155:THR:HG21	1.78	0.66
1:D:137:PRO:HG3	1:D:155:THR:HG21	1.78	0.65
1:D:39:GLN:H	1:D:39:GLN:CD	2.00	0.65
1:B:137:PRO:HG3	1:B:155:THR:HG21	1.79	0.65
1:B:31:VAL:HG23	1:B:32:LEU:N	2.12	0.64
1:A:137:PRO:HG3	1:A:155:THR:HG21	1.80	0.64
1:C:66:THR:HG21	1:C:239:GLU:CB	2.28	0.62
1:C:137:PRO:HG3	1:C:155:THR:HG21	1.80	0.62
1:E:178:LEU:HD21	1:F:178:LEU:HD21	1.82	0.60
1:A:118:ASP:OD1	1:A:120:SER:CB	2.50	0.60
1:B:237:LEU:HD23	1:B:238:PRO:HD2	1.83	0.60
1:E:183:LEU:HD23	1:E:184:VAL:N	2.19	0.57
1:C:25:LEU:CD2	1:C:25:LEU:C	2.73	0.57
1:C:178:LEU:HD21	1:D:178:LEU:HD21	1.87	0.56
1:E:166:ALA:HB1	1:E:183:LEU:HD21	1.87	0.56
1:E:95:MET:HG2	1:E:210:VAL:HG12	1.86	0.56
1:C:183:LEU:HD23	1:C:184:VAL:N	2.20	0.56
1:D:183:LEU:HD23	1:D:184:VAL:N	2.21	0.56
1:E:122:GLN:HB3	1:E:205:PRO:HD3	1.88	0.55
1:C:122:GLN:HB3	1:C:205:PRO:HD3	1.88	0.55
1:B:4:ILE:HG22	1:B:235:ALA:HB3	1.88	0.55
1:F:183:LEU:HD23	1:F:184:VAL:N	2.22	0.55
1:B:183:LEU:HD23	1:B:184:VAL:N	2.21	0.54
1:A:128:PHE:CE1	1:A:183:LEU:HD12	2.43	0.54
1:E:197:ILE:HD11	1:F:197:ILE:HD11	1.90	0.54
1:A:25:LEU:C	1:A:25:LEU:HD23	2.29	0.53
1:A:36:LYS:HE2	5:A:1519:HOH:O	2.08	0.53
1:C:4:ILE:CG2	1:C:235:ALA:HB3	2.37	0.53
1:A:238:PRO:O	1:A:239:GLU:HB2	2.07	0.53
1:E:71:GLU:OE1	1:E:73:ARG:NH2	2.39	0.53
1:E:67:VAL:HG23	1:E:68:ALA:N	2.24	0.53
1:F:118:ASP:OD1	1:F:120:SER:N	2.40	0.53
1:B:151:ARG:NH1	5:B:2614:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:PRO:O	1:F:239:GLU:OXT	2.28	0.52
1:B:25:LEU:HD23	1:B:25:LEU:C	2.31	0.51
1:A:119:ASN:HD22	1:A:119:ASN:N	2.09	0.51
1:D:25:LEU:HD23	1:D:25:LEU:C	2.30	0.51
1:E:155:THR:HG22	5:E:5592:HOH:O	2.09	0.51
1:E:16:ASP:HA	5:E:5531:HOH:O	2.10	0.50
1:E:51:THR:C	1:E:52:LEU:HD12	2.32	0.50
1:E:161:ASP:HB3	1:E:164:GLN:HB2	1.94	0.50
1:C:161:ASP:HB3	1:C:164:GLN:HB2	1.93	0.49
1:C:16:ASP:OD1	1:E:101:LYS:NZ	2.43	0.49
1:B:4:ILE:HG21	1:B:57:VAL:HB	1.93	0.49
1:F:25:LEU:C	1:F:25:LEU:HD23	2.33	0.49
1:D:122:GLN:HB3	1:D:205:PRO:HD3	1.94	0.49
1:F:73:ARG:HG2	1:F:169:VAL:HG22	1.94	0.49
1:F:25:LEU:HD23	1:F:26:ILE:N	2.27	0.49
1:D:72:THR:HG22	1:D:170:ILE:HB	1.94	0.49
1:F:161:ASP:HB3	1:F:164:GLN:HB2	1.94	0.49
1:B:51:THR:C	1:B:52:LEU:HD12	2.34	0.48
1:D:51:THR:C	1:D:52:LEU:HD12	2.34	0.48
1:F:122:GLN:HB3	1:F:205:PRO:HD3	1.95	0.48
1:E:72:THR:HG22	1:E:170:ILE:HB	1.93	0.48
1:B:160:LEU:HD12	1:B:185:TYR:OH	2.13	0.48
1:B:122:GLN:HB3	1:B:205:PRO:HD3	1.96	0.48
1:B:72:THR:HG22	1:B:170:ILE:HB	1.94	0.48
1:C:66:THR:HG21	1:C:239:GLU:HG3	1.95	0.48
1:E:73:ARG:HG2	1:E:169:VAL:HG22	1.95	0.48
1:F:160:LEU:HD12	1:F:185:TYR:OH	2.12	0.48
1:F:72:THR:HG22	1:F:170:ILE:HB	1.96	0.48
1:D:161:ASP:HB3	1:D:164:GLN:HB2	1.94	0.48
1:F:238:PRO:O	1:F:239:GLU:HB2	2.14	0.47
1:C:92:VAL:HG13	1:C:127:GLU:HB3	1.96	0.47
1:C:160:LEU:HD12	1:C:185:TYR:OH	2.15	0.47
1:D:73:ARG:HG2	1:D:169:VAL:HG22	1.95	0.47
1:F:92:VAL:HG13	1:F:127:GLU:HB3	1.95	0.47
1:C:154:LYS:NZ	5:C:3609:HOH:O	2.46	0.47
1:C:66:THR:CG2	1:C:239:GLU:HG3	2.45	0.47
1:F:11:PHE:O	1:F:30:GLY:HA2	2.14	0.47
1:E:28:GLN:H	1:E:28:GLN:HG2	1.53	0.47
1:C:2:GLU:OE2	1:C:58:HIS:ND1	2.36	0.46
1:B:73:ARG:HG2	1:B:169:VAL:HG22	1.97	0.46
1:C:72:THR:HG22	1:C:170:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:HG13	1:D:204:LEU:HD12	1.97	0.46
1:A:154:LYS:CG	1:A:194:ILE:HD11	2.25	0.46
1:C:51:THR:C	1:C:52:LEU:HD12	2.36	0.46
1:A:11:PHE:O	1:A:30:GLY:HA2	2.15	0.46
1:D:11:PHE:O	1:D:30:GLY:HA2	2.16	0.46
1:E:181:ALA:O	1:E:194:ILE:HD12	2.16	0.46
1:B:11:PHE:O	1:B:30:GLY:HA2	2.16	0.45
1:B:200:VAL:HG13	1:B:204:LEU:HD12	1.97	0.45
1:F:194:ILE:HD12	1:F:194:ILE:H	1.81	0.45
1:D:118:ASP:OD2	1:D:120:SER:HB3	2.17	0.45
1:E:184:VAL:O	1:E:186:PRO:HD3	2.16	0.45
1:C:180:HIS:CD2	1:C:180:HIS:H	2.35	0.45
1:E:11:PHE:O	1:E:30:GLY:HA2	2.15	0.45
1:C:11:PHE:O	1:C:30:GLY:HA2	2.16	0.45
1:C:99:LYS:HE3	1:E:22:GLY:O	2.17	0.45
1:D:118:ASP:OD2	1:D:120:SER:CB	2.65	0.45
1:B:118:ASP:CG	1:B:120:SER:HB3	2.36	0.45
1:B:161:ASP:HB3	1:B:164:GLN:HB2	1.98	0.45
1:C:73:ARG:HG2	1:C:169:VAL:HG22	1.97	0.45
1:D:180:HIS:H	1:D:180:HIS:CD2	2.35	0.45
1:F:119:ASN:HD22	1:F:119:ASN:N	2.14	0.45
1:F:180:HIS:CD2	1:F:180:HIS:H	2.34	0.45
1:F:92:VAL:HG22	1:F:109:LEU:HD13	1.99	0.45
1:A:180:HIS:CD2	1:A:180:HIS:H	2.36	0.44
1:E:88:ALA:HB1	1:E:89:ASP:CG	2.38	0.44
1:D:91:LEU:HG	1:D:128:PHE:HB2	1.99	0.44
1:A:122:GLN:HB3	1:A:205:PRO:HD3	1.99	0.44
1:B:194:ILE:HD12	1:B:194:ILE:H	1.82	0.44
1:E:75:SER:HA	1:E:166:ALA:O	2.18	0.44
1:B:181:ALA:O	1:B:194:ILE:HD12	2.18	0.44
1:C:200:VAL:HG13	1:C:204:LEU:HD12	2.00	0.44
1:D:194:ILE:H	1:D:194:ILE:HD12	1.83	0.44
1:C:183:LEU:HD23	1:C:183:LEU:C	2.38	0.44
1:D:181:ALA:O	1:D:194:ILE:HD12	2.18	0.44
1:A:129:ASP:O	1:A:141:PRO:HA	2.18	0.44
1:E:180:HIS:CD2	1:E:180:HIS:H	2.36	0.44
1:B:153:ILE:HG22	1:E:64:THR:HG22	1.99	0.43
1:E:194:ILE:HD12	1:E:194:ILE:H	1.82	0.43
1:C:12:GLU:HA	1:C:13:PRO:HD3	1.93	0.43
1:C:181:ALA:O	1:C:194:ILE:HD12	2.18	0.43
1:B:180:HIS:H	1:B:180:HIS:CD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HB1	1:B:89:ASP:CG	2.38	0.43
1:C:194:ILE:H	1:C:194:ILE:HD12	1.83	0.43
1:C:88:ALA:HB1	1:C:89:ASP:CG	2.39	0.43
1:E:200:VAL:HG13	1:E:204:LEU:HD12	2.01	0.43
1:D:92:VAL:HG13	1:D:127:GLU:HB3	2.01	0.43
1:F:64:THR:OG1	1:F:66:THR:OG1	2.32	0.43
1:B:89:ASP:OD1	5:B:2503:HOH:O	2.21	0.43
1:D:180:HIS:N	1:D:180:HIS:CD2	2.86	0.43
1:F:129:ASP:O	1:F:141:PRO:HA	2.19	0.43
1:F:180:HIS:CD2	1:F:180:HIS:N	2.86	0.43
1:B:129:ASP:O	1:B:141:PRO:HA	2.19	0.43
1:D:184:VAL:O	1:D:186:PRO:HD3	2.18	0.42
1:C:66:THR:HG21	1:C:239:GLU:CG	2.49	0.42
1:C:180:HIS:CD2	1:C:180:HIS:N	2.86	0.42
1:E:92:VAL:HG13	1:E:127:GLU:HB3	2.00	0.42
1:A:155:THR:HB	5:A:1561:HOH:O	2.20	0.42
1:A:72:THR:HG22	1:A:170:ILE:HB	2.00	0.42
1:A:73:ARG:HG2	1:A:169:VAL:HG22	2.02	0.42
1:A:93:PHE:HA	1:A:212:LEU:HD23	2.02	0.42
1:C:197:ILE:HD11	1:D:197:ILE:HD11	2.01	0.42
1:E:193:THR:HG23	1:F:180:HIS:CE1	2.54	0.42
1:A:118:ASP:CG	1:A:120:SER:HB3	2.40	0.42
1:A:88:ALA:HB1	1:A:89:ASP:CG	2.40	0.42
1:D:88:ALA:HB1	1:D:89:ASP:CG	2.39	0.42
1:E:28:GLN:HG2	5:E:5541:HOH:O	2.19	0.42
1:F:59:ILE:CG2	1:F:60:TRP:HD1	2.33	0.42
1:A:180:HIS:CD2	1:A:180:HIS:N	2.87	0.42
1:A:45:TRP:CE3	1:A:46:ASP:HB2	2.55	0.42
1:C:184:VAL:O	1:C:186:PRO:HD3	2.19	0.42
1:E:129:ASP:O	1:E:141:PRO:HA	2.19	0.42
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.95	0.42
1:B:180:HIS:N	1:B:180:HIS:CD2	2.87	0.42
1:F:181:ALA:O	1:F:194:ILE:HD12	2.20	0.42
1:B:45:TRP:CE3	1:B:46:ASP:HB2	2.55	0.42
1:D:129:ASP:O	1:D:141:PRO:HA	2.19	0.42
1:C:45:TRP:CE3	1:C:46:ASP:HB2	2.55	0.42
1:A:180:HIS:HB2	5:A:1639:HOH:O	2.20	0.41
1:D:45:TRP:CE3	1:D:46:ASP:HB2	2.56	0.41
1:D:183:LEU:HD23	1:D:183:LEU:C	2.41	0.41
1:A:3:THR:HG21	5:A:1664:HOH:O	2.20	0.41
1:E:180:HIS:N	1:E:180:HIS:CD2	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:VAL:O	1:F:186:PRO:HD3	2.20	0.41
1:F:45:TRP:CE3	1:F:46:ASP:HB2	2.56	0.41
1:B:59:ILE:CG2	1:B:60:TRP:HD1	2.34	0.41
1:C:118:ASP:CG	1:C:120:SER:HB3	2.40	0.41
1:E:17:ASN:HD22	1:E:17:ASN:N	2.19	0.41
1:C:59:ILE:CG2	1:C:60:TRP:HD1	2.33	0.41
1:B:183:LEU:HD23	1:B:183:LEU:C	2.41	0.41
1:D:75:SER:HA	1:D:166:ALA:O	2.20	0.41
1:F:88:ALA:HB1	1:F:89:ASP:CG	2.41	0.41
1:A:184:VAL:O	1:A:186:PRO:HD3	2.20	0.41
1:A:59:ILE:CG2	1:A:60:TRP:HD1	2.34	0.41
1:C:129:ASP:O	1:C:141:PRO:HA	2.20	0.41
1:F:183:LEU:HD23	1:F:183:LEU:C	2.42	0.41
1:A:67:VAL:HG23	1:A:68:ALA:N	2.36	0.41
1:C:17:ASN:N	1:C:17:ASN:ND2	2.58	0.40
1:A:24:SER:OG	1:A:34:LEU:HD23	2.21	0.40
1:A:67:VAL:HG11	5:A:1649:HOH:O	2.22	0.40
1:B:17:ASN:HD22	1:B:17:ASN:N	2.20	0.40
1:E:71:GLU:OE1	1:E:73:ARG:NE	2.52	0.40
1:F:194:ILE:N	1:F:194:ILE:HD12	2.36	0.40
1:A:106:TYR:CE1	1:A:218:ALA:HA	2.57	0.40
1:B:4:ILE:CG2	1:B:235:ALA:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
1	B	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
1	C	237/239 (99%)	228 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	237/239 (99%)	226 (95%)	11 (5%)	0	100	100
1	E	237/239 (99%)	228 (96%)	9 (4%)	0	100	100
1	F	237/239 (99%)	226 (95%)	11 (5%)	0	100	100
All	All	1422/1434 (99%)	1366 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	202/205 (98%)	184 (91%)	18 (9%)	9	12
1	B	201/205 (98%)	185 (92%)	16 (8%)	12	15
1	C	201/205 (98%)	187 (93%)	14 (7%)	15	19
1	D	201/205 (98%)	181 (90%)	20 (10%)	7	8
1	E	200/205 (98%)	184 (92%)	16 (8%)	12	15
1	F	200/205 (98%)	185 (92%)	15 (8%)	13	17
All	All	1205/1230 (98%)	1106 (92%)	99 (8%)	11	14

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	LEU
1	A	24	SER
1	A	25	LEU
1	A	31	VAL
1	A	52	LEU
1	A	67	VAL
1	A	86	LEU
1	A	92	VAL
1	A	151	ARG

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Mol	Chain	Res	Type
1	A	155	THR
1	A	161	ASP
1	A	178	LEU
1	A	180	HIS
1	A	194	ILE
1	A	202	GLN
1	A	237	LEU
1	A	239	GLU
1	B	17	ASN
1	B	18	LEU
1	B	25	LEU
1	B	31	VAL
1	B	64	THR
1	B	67	VAL
1	B	86	LEU
1	B	92	VAL
1	B	155	THR
1	B	159	GLN
1	B	161	ASP
1	B	175	SER
1	B	178	LEU
1	B	180	HIS
1	B	194	ILE
1	B	237	LEU
1	C	17	ASN
1	C	18	LEU
1	C	25	LEU
1	C	31	VAL
1	C	67	VAL
1	C	83	THR
1	C	86	LEU
1	C	92	VAL
1	C	155	THR
1	C	161	ASP
1	C	178	LEU
1	C	180	HIS
1	C	194	ILE
1	C	237	LEU
1	D	16	ASP
1	D	17	ASN
1	D	18	LEU
1	D	25	LEU

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Mol	Chain	Res	Type
1	D	31	VAL
1	D	39	GLN
1	D	67	VAL
1	D	83	THR
1	D	86	LEU
1	D	92	VAL
1	D	117	GLN
1	D	120	SER
1	D	155	THR
1	D	159	GLN
1	D	160	LEU
1	D	161	ASP
1	D	178	LEU
1	D	180	HIS
1	D	194	ILE
1	D	237	LEU
1	E	17	ASN
1	E	18	LEU
1	E	28	GLN
1	E	31	VAL
1	E	67	VAL
1	E	83	THR
1	E	86	LEU
1	E	92	VAL
1	E	117	GLN
1	E	155	THR
1	E	161	ASP
1	E	178	LEU
1	E	180	HIS
1	E	194	ILE
1	E	237	LEU
1	E	239	GLU
1	F	18	LEU
1	F	25	LEU
1	F	52	LEU
1	F	66	THR
1	F	67	VAL
1	F	92	VAL
1	F	119	ASN
1	F	120	SER
1	F	155	THR
1	F	161	ASP

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Mol	Chain	Res	Type
1	F	178	LEU
1	F	180	HIS
1	F	194	ILE
1	F	237	LEU
1	F	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	39	GLN
1	A	80	GLN
1	A	117	GLN
1	A	119	ASN
1	A	156	GLN
1	A	180	HIS
1	B	17	ASN
1	B	28	GLN
1	B	33	GLN
1	B	80	GLN
1	B	117	GLN
1	B	119	ASN
1	B	180	HIS
1	C	17	ASN
1	C	33	GLN
1	C	80	GLN
1	C	117	GLN
1	C	119	ASN
1	C	156	GLN
1	C	234	GLN
1	D	17	ASN
1	D	33	GLN
1	D	39	GLN
1	D	80	GLN
1	D	117	GLN
1	D	119	ASN
1	D	156	GLN
1	E	80	GLN
1	E	117	GLN
1	E	119	ASN
1	E	156	GLN
1	F	17	ASN

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Mol	Chain	Res	Type
1	F	28	GLN
1	F	33	GLN
1	F	80	GLN
1	F	119	ASN
1	F	156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	BGC	G	1	2	12,12,12	1.32	2 (16%)	17,17,17	1.04	3 (17%)
2	GAL	G	2	2	11,11,12	1.28	1 (9%)	15,15,17	0.98	2 (13%)
2	BGC	H	1	2	12,12,12	1.28	1 (8%)	17,17,17	1.11	3 (17%)
2	GAL	H	2	2	11,11,12	1.18	1 (9%)	15,15,17	0.99	2 (13%)
2	BGC	I	1	2	12,12,12	1.25	1 (8%)	17,17,17	1.14	1 (5%)
2	GAL	I	2	2	11,11,12	1.13	1 (9%)	15,15,17	1.01	2 (13%)
2	BGC	J	1	2	12,12,12	1.31	1 (8%)	17,17,17	1.10	3 (17%)
2	GAL	J	2	2	11,11,12	1.22	1 (9%)	15,15,17	1.01	2 (13%)
2	BGC	K	1	2	12,12,12	1.32	1 (8%)	17,17,17	1.26	4 (23%)
2	GAL	K	2	2	11,11,12	1.20	1 (9%)	15,15,17	1.00	2 (13%)
2	BGC	L	1	2	12,12,12	1.22	1 (8%)	17,17,17	1.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	L	2	2	11,11,12	1.20	1 (9%)	15,15,17	1.01	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	2/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	1	2	-	1/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	L	1	2	-	1/2/22/22	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	BGC	C4-C3	2.65	1.59	1.52
2	K	1	BGC	C4-C3	2.62	1.59	1.52
2	J	2	GAL	C2-C3	2.60	1.56	1.52
2	H	1	BGC	C4-C3	2.59	1.58	1.52
2	G	1	BGC	C4-C3	2.44	1.58	1.52
2	I	1	BGC	C4-C3	2.41	1.58	1.52
2	L	1	BGC	C4-C3	2.37	1.58	1.52
2	K	2	GAL	C2-C3	2.36	1.56	1.52
2	G	2	GAL	C2-C3	2.33	1.55	1.52
2	I	2	GAL	C2-C3	2.29	1.55	1.52
2	L	2	GAL	C2-C3	2.14	1.55	1.52
2	G	1	BGC	C4-C5	2.07	1.57	1.53
2	H	2	GAL	C2-C3	2.05	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	BGC	O6-C6-C5	2.72	120.61	111.29
2	J	2	GAL	C1-O5-C5	2.25	115.25	112.19
2	L	2	GAL	C2-C3-C4	-2.17	107.14	110.89
2	I	2	GAL	C2-C3-C4	-2.16	107.16	110.89
2	K	1	BGC	C4-C3-C2	-2.15	107.07	110.82
2	K	2	GAL	C1-O5-C5	2.15	115.10	112.19
2	I	2	GAL	C1-O5-C5	2.12	115.06	112.19
2	H	2	GAL	C2-C3-C4	-2.12	107.23	110.89
2	J	1	BGC	C4-C3-C2	-2.11	107.13	110.82
2	K	2	GAL	C2-C3-C4	-2.10	107.27	110.89
2	L	2	GAL	C1-O5-C5	2.09	115.02	112.19
2	G	2	GAL	C1-O5-C5	2.08	115.01	112.19
2	I	1	BGC	C4-C3-C2	-2.08	107.20	110.82
2	K	1	BGC	C1-O5-C5	2.07	117.58	113.66
2	J	1	BGC	C1-O5-C5	2.07	117.57	113.66
2	J	2	GAL	C2-C3-C4	-2.07	107.32	110.89
2	H	1	BGC	C1-O5-C5	2.06	117.55	113.66
2	L	1	BGC	C1-O5-C5	2.05	117.54	113.66
2	G	1	BGC	C1-O5-C5	2.05	117.54	113.66
2	L	1	BGC	C4-C3-C2	-2.05	107.24	110.82
2	H	1	BGC	C4-C3-C2	-2.05	107.25	110.82
2	G	2	GAL	C2-C3-C4	-2.03	107.39	110.89
2	G	1	BGC	C6-C5-C4	2.03	117.75	113.00
2	G	1	BGC	C4-C3-C2	-2.02	107.29	110.82
2	J	1	BGC	C6-C5-C4	2.02	117.73	113.00
2	K	1	BGC	C6-C5-C4	2.01	117.71	113.00
2	H	2	GAL	C1-O5-C5	2.01	114.92	112.19
2	H	1	BGC	C6-C5-C4	2.00	117.69	113.00

There are no chirality outliers.

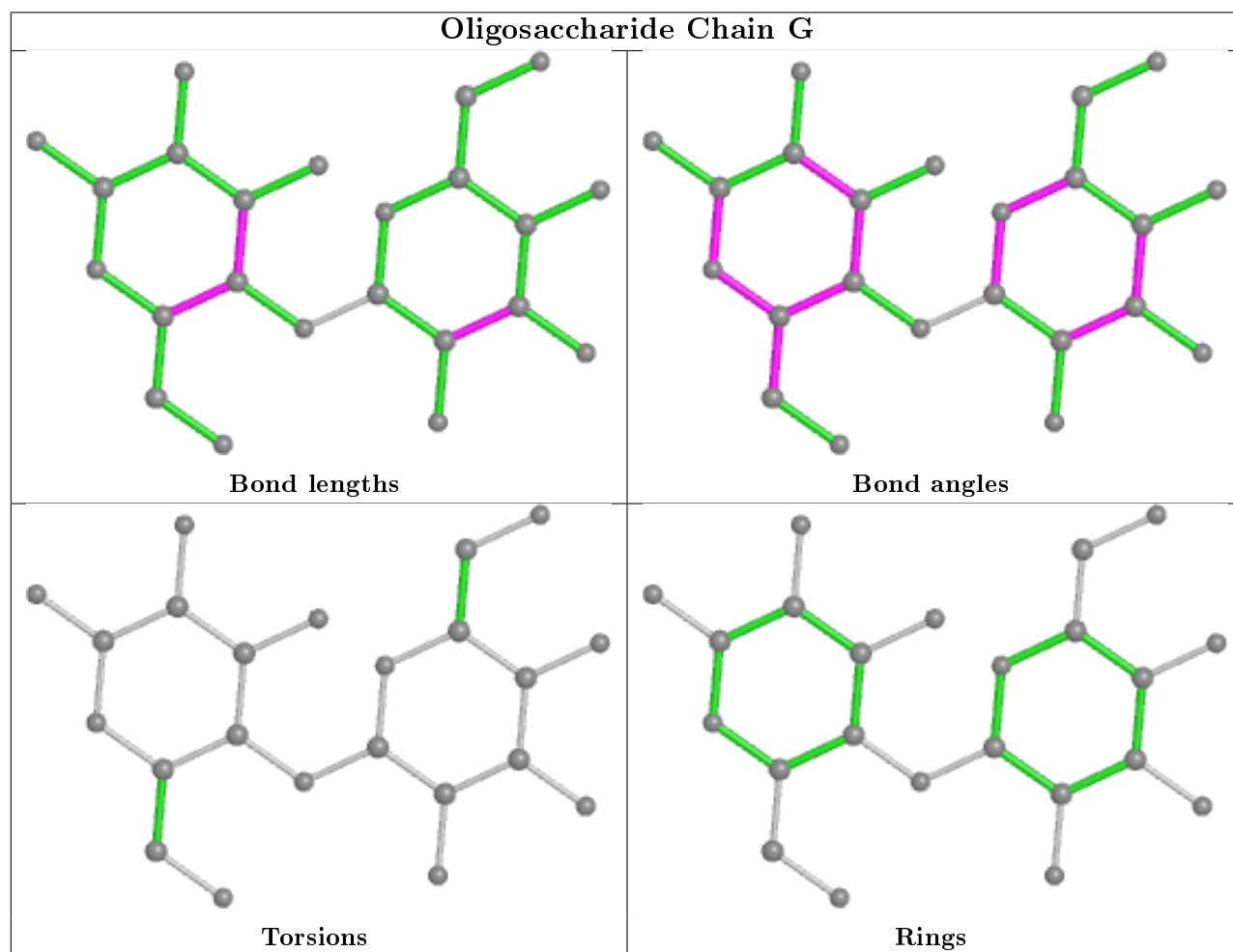
All (6) torsion outliers are listed below:

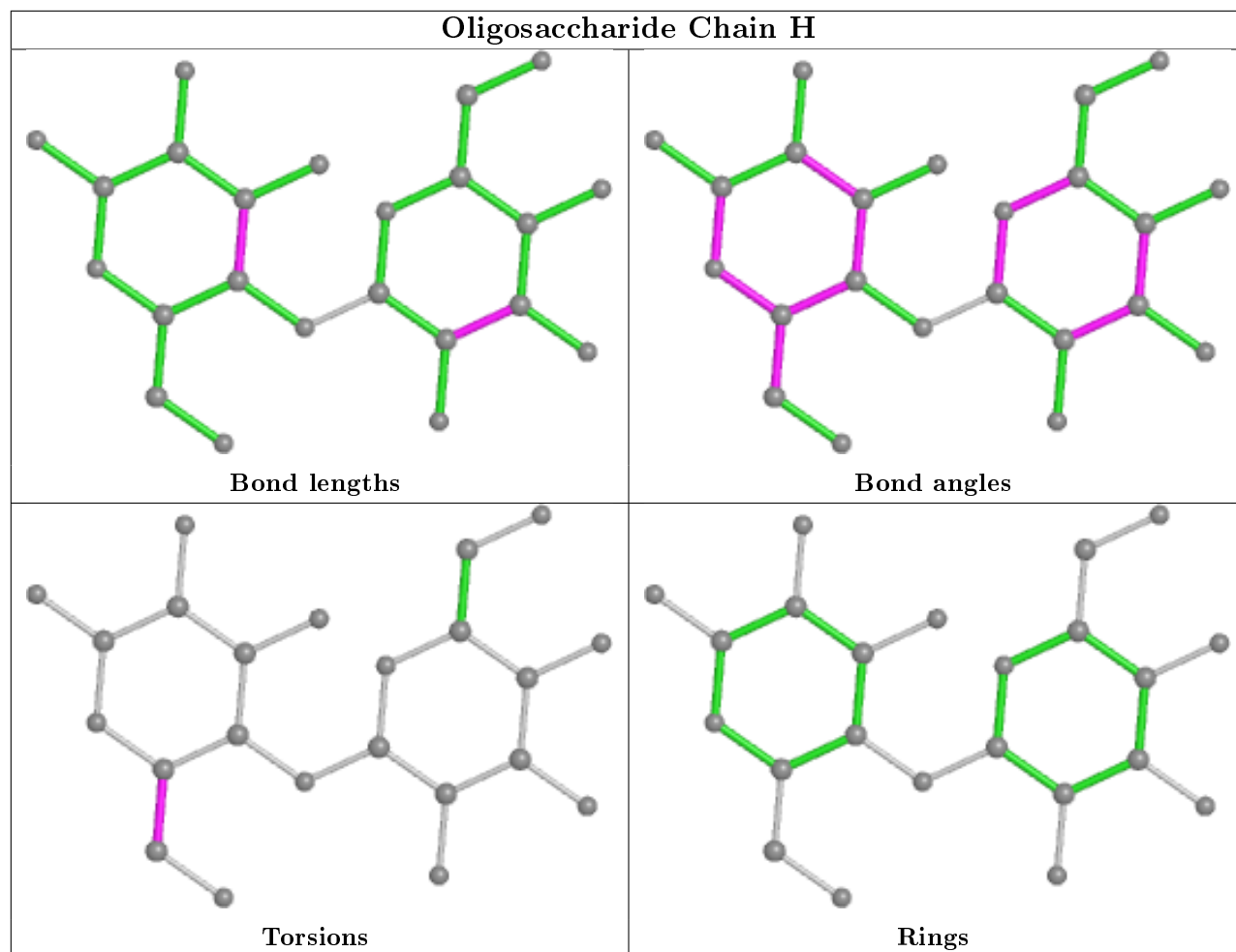
Mol	Chain	Res	Type	Atoms
2	H	1	BGC	C4-C5-C6-O6
2	H	1	BGC	O5-C5-C6-O6
2	I	1	BGC	C4-C5-C6-O6
2	I	1	BGC	O5-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
2	L	1	BGC	C4-C5-C6-O6

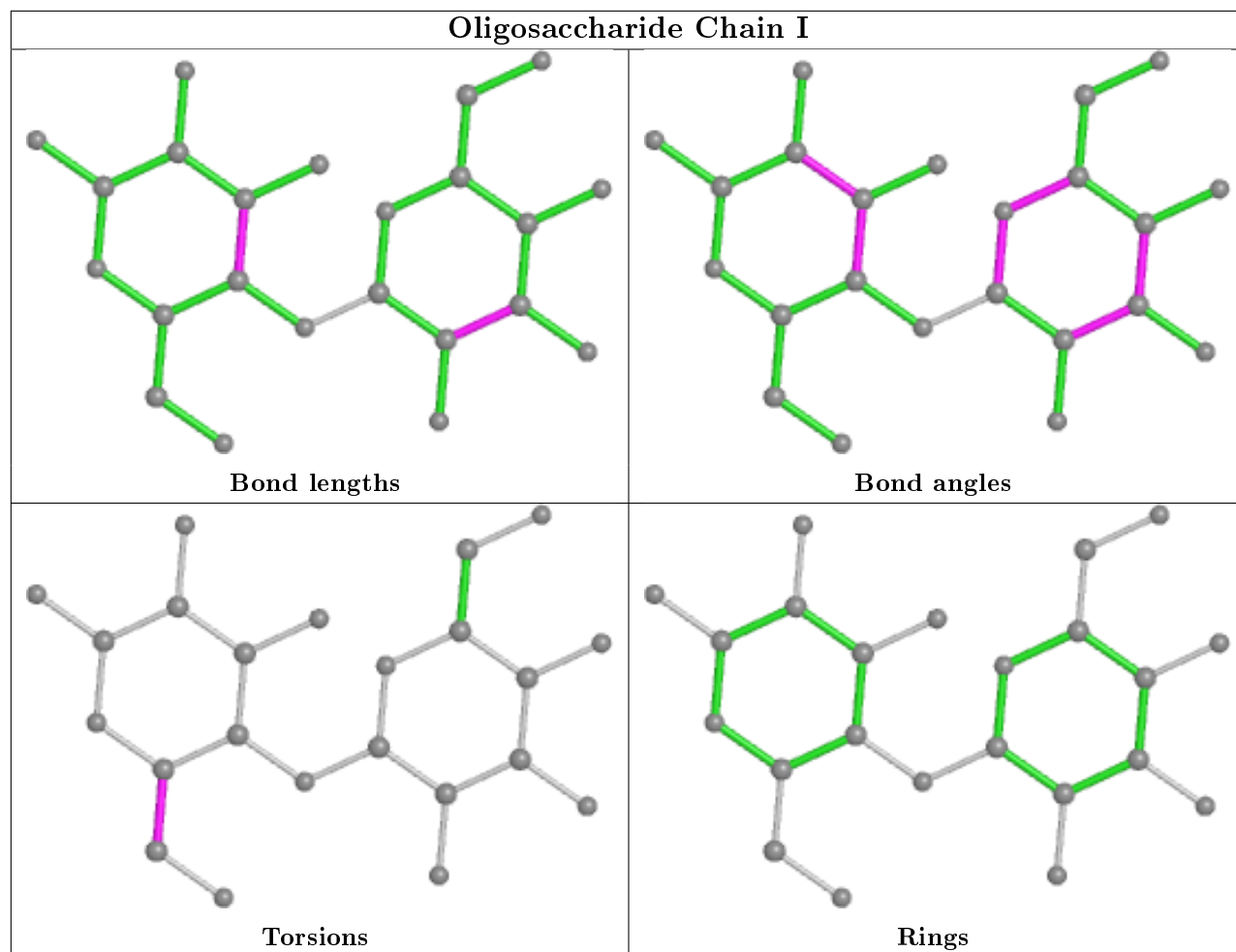
There are no ring outliers.

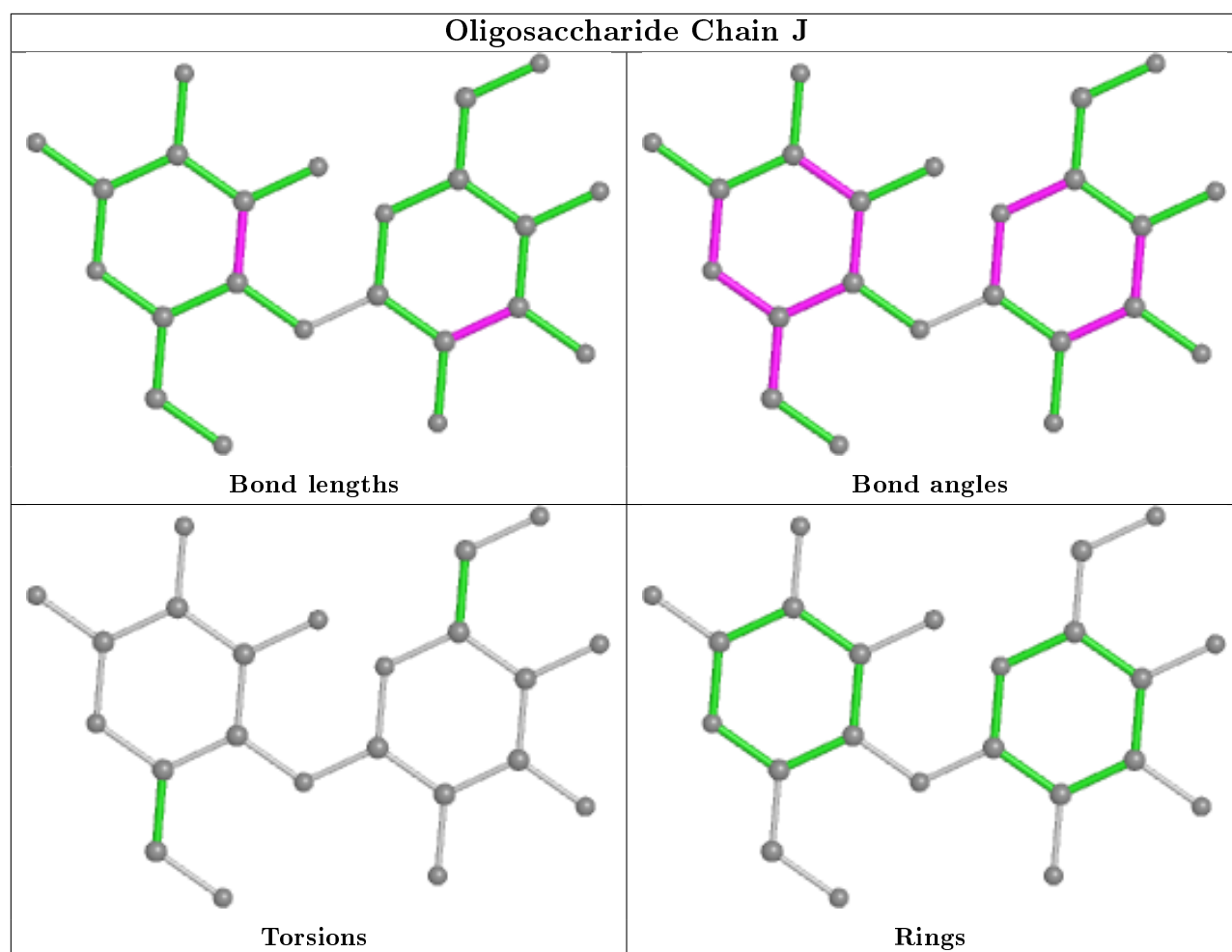
No monomer is involved in short contacts.

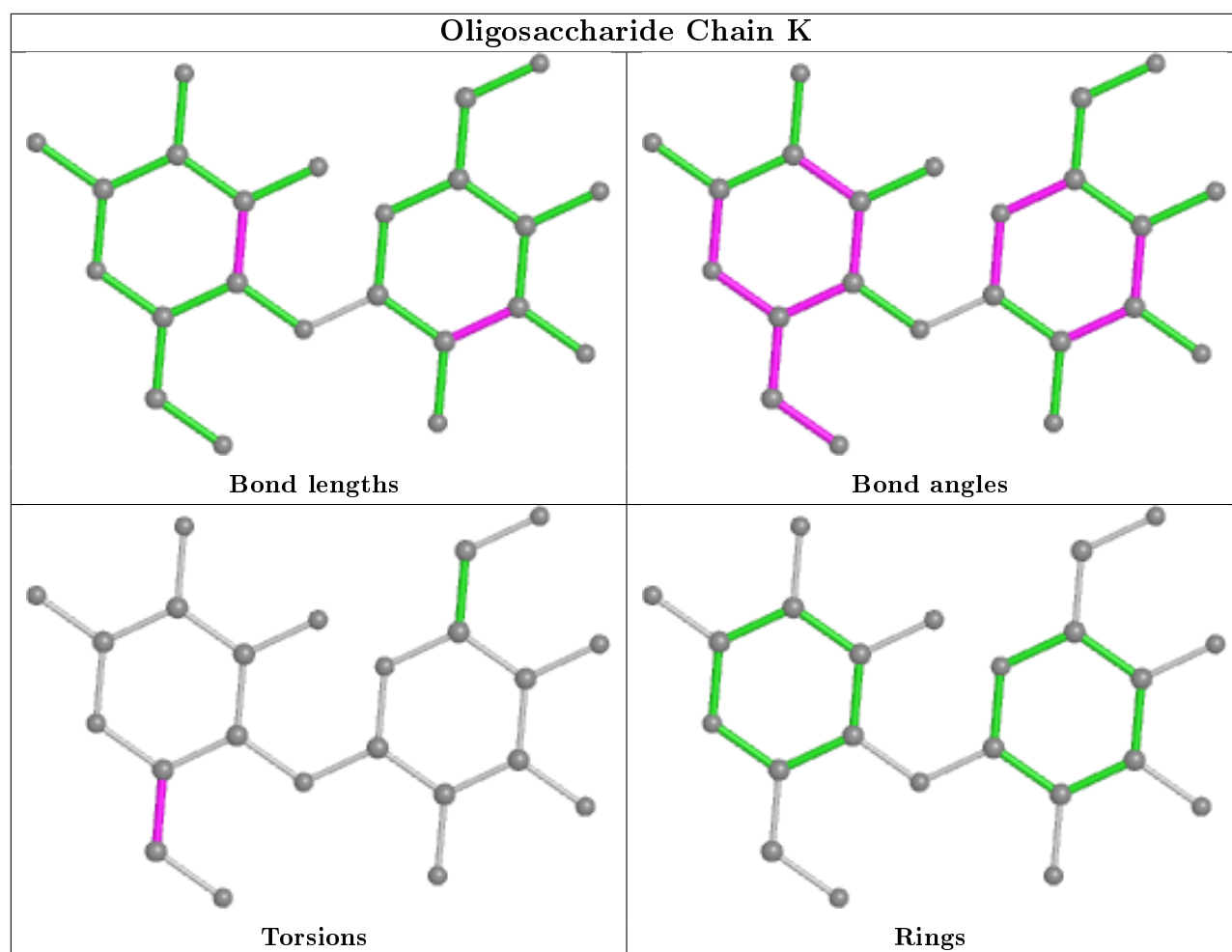
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

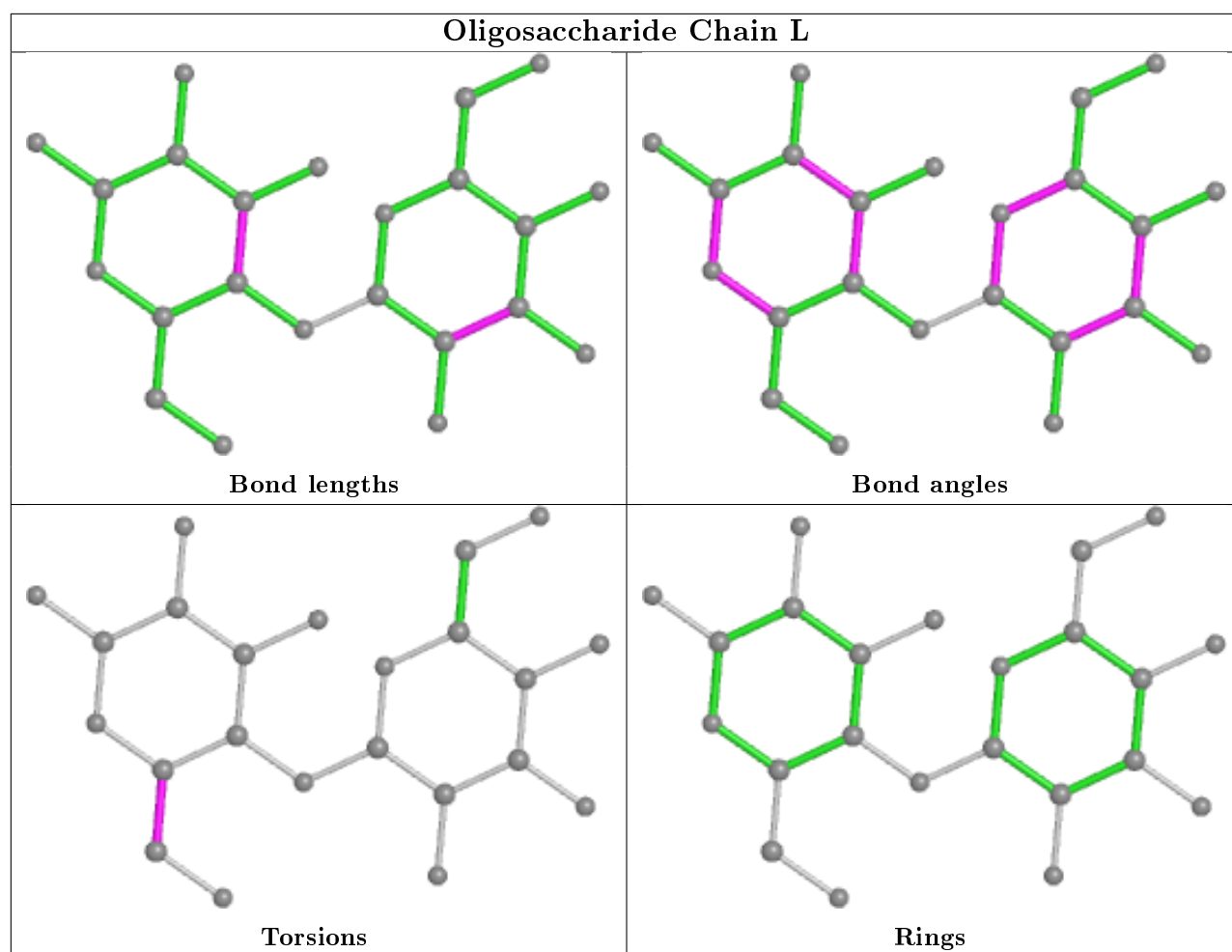












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	239/239 (100%)	-0.30	3 (1%) 77 82	15, 29, 46, 59	0
1	B	239/239 (100%)	-0.32	5 (2%) 63 70	16, 30, 47, 59	0
1	C	239/239 (100%)	-0.33	3 (1%) 77 82	15, 29, 46, 59	1 (0%)
1	D	239/239 (100%)	-0.26	4 (1%) 70 76	16, 30, 48, 60	0
1	E	239/239 (100%)	-0.21	6 (2%) 57 63	17, 31, 50, 67	0
1	F	239/239 (100%)	-0.28	6 (2%) 57 63	17, 31, 49, 63	0
All	All	1434/1434 (100%)	-0.28	27 (1%) 66 73	15, 30, 48, 67	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	VAL	3.6
1	E	120	SER	3.5
1	A	83	THR	3.0
1	B	83	THR	3.0
1	D	120	SER	2.9
1	D	83	THR	2.9
1	C	239	GLU	2.8
1	C	1	VAL	2.7
1	E	101	LYS	2.6
1	F	1	VAL	2.6
1	D	16	ASP	2.6
1	E	115	SER	2.5
1	D	138	PRO	2.4
1	C	83	THR	2.4
1	F	83	THR	2.4
1	F	239	GLU	2.3
1	B	120	SER	2.3
1	F	99	LYS	2.2
1	B	16	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	83	THR	2.2
1	F	62	MET	2.2
1	A	220	ARG	2.1
1	B	59	ILE	2.1
1	E	16	ASP	2.1
1	A	1	VAL	2.0
1	F	120	SER	2.0
1	B	114	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

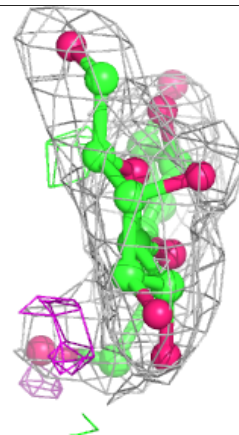
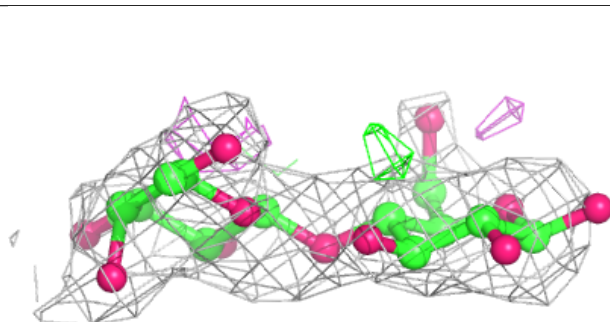
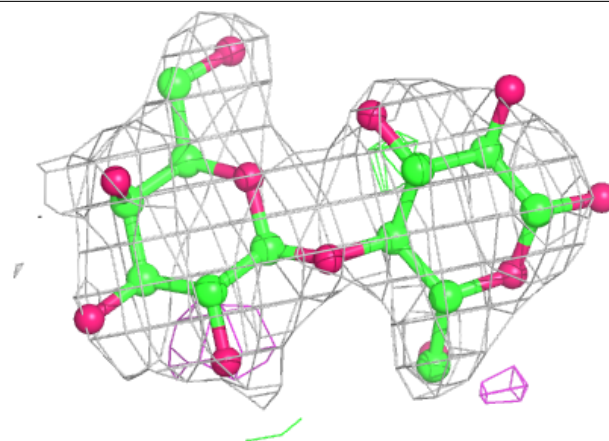
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	L	1	12/12	0.85	0.29	56,61,64,64	0
2	BGC	G	1	12/12	0.85	0.27	55,59,62,62	0
2	BGC	I	1	12/12	0.85	0.23	55,60,62,63	0
2	BGC	K	1	12/12	0.85	0.31	56,60,62,63	0
2	BGC	J	1	12/12	0.86	0.28	55,60,63,64	0
2	BGC	H	1	12/12	0.87	0.29	55,61,62,62	0
2	GAL	J	2	11/12	0.90	0.17	46,48,52,52	0
2	GAL	L	2	11/12	0.91	0.16	48,49,51,52	0
2	GAL	K	2	11/12	0.92	0.14	48,50,52,52	0
2	GAL	H	2	11/12	0.94	0.14	47,49,51,51	0
2	GAL	G	2	11/12	0.95	0.14	44,48,51,51	0
2	GAL	I	2	11/12	0.95	0.15	46,48,50,51	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.

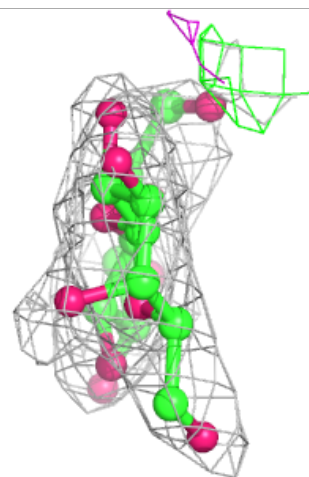
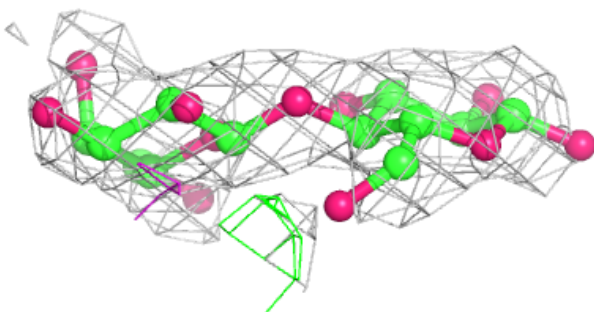
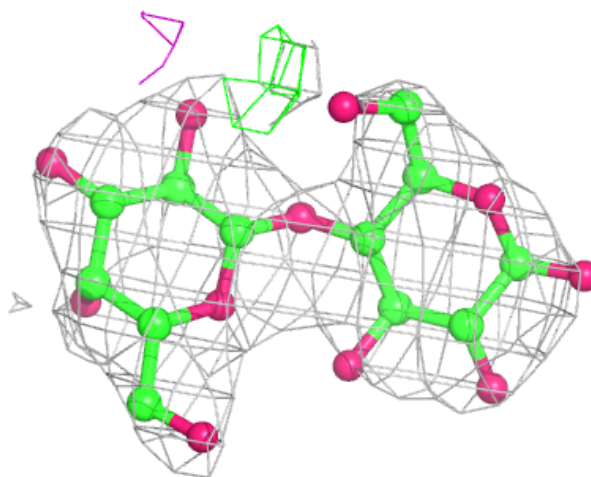
Electron density around Chain G:

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



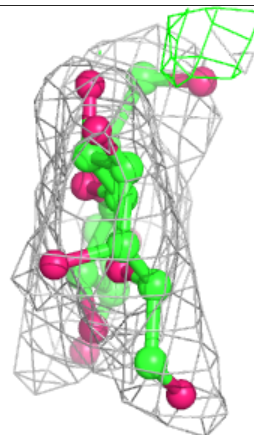
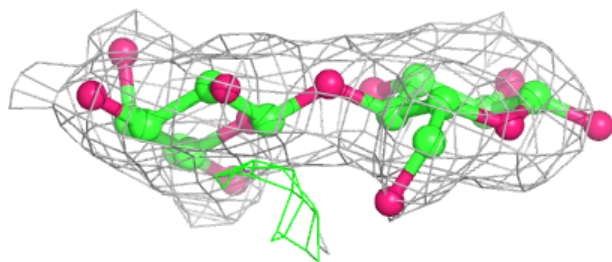
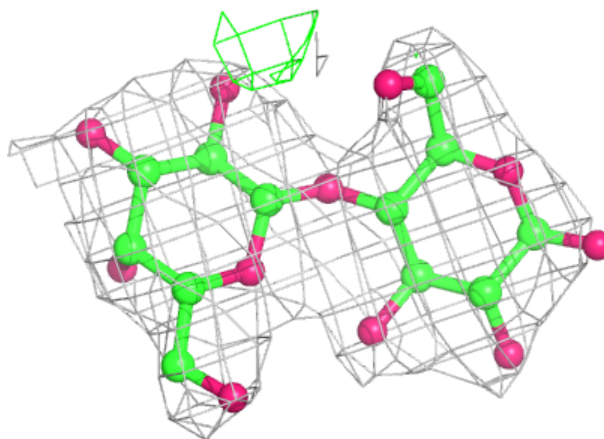
Electron density around Chain H:

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



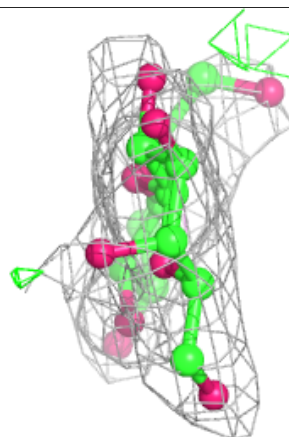
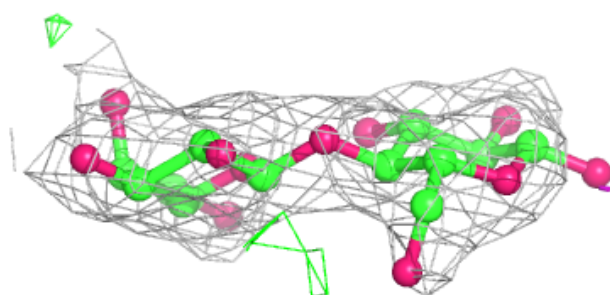
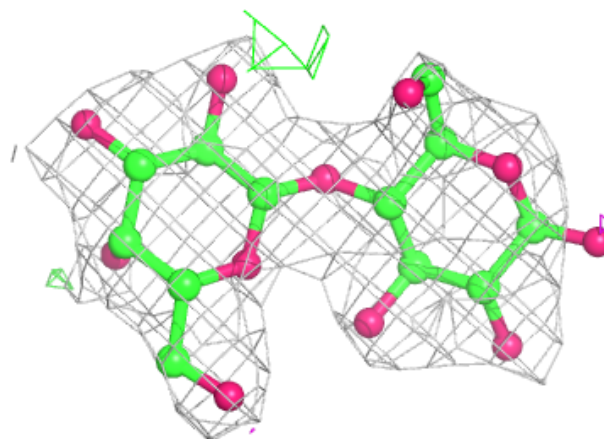
Electron density around Chain I:

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



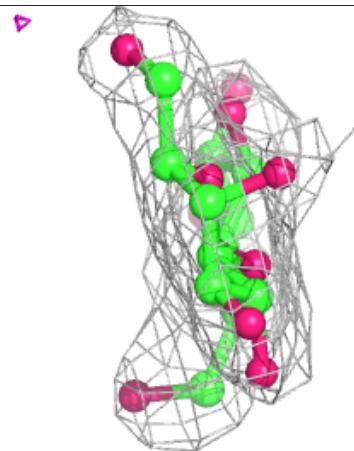
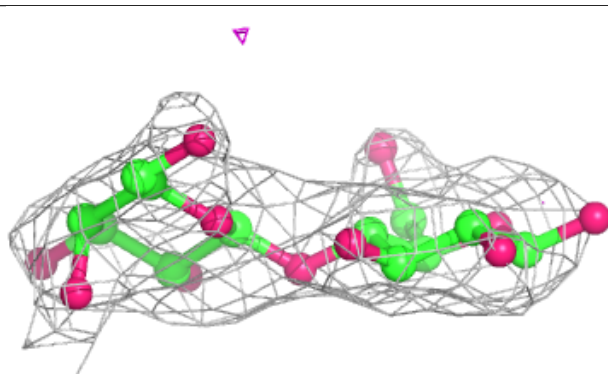
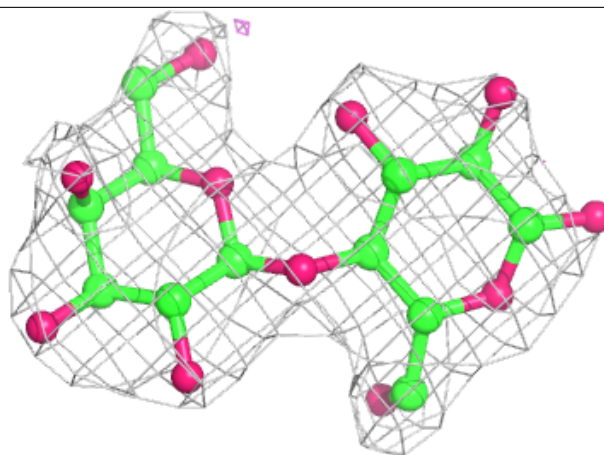
Electron density around Chain J:

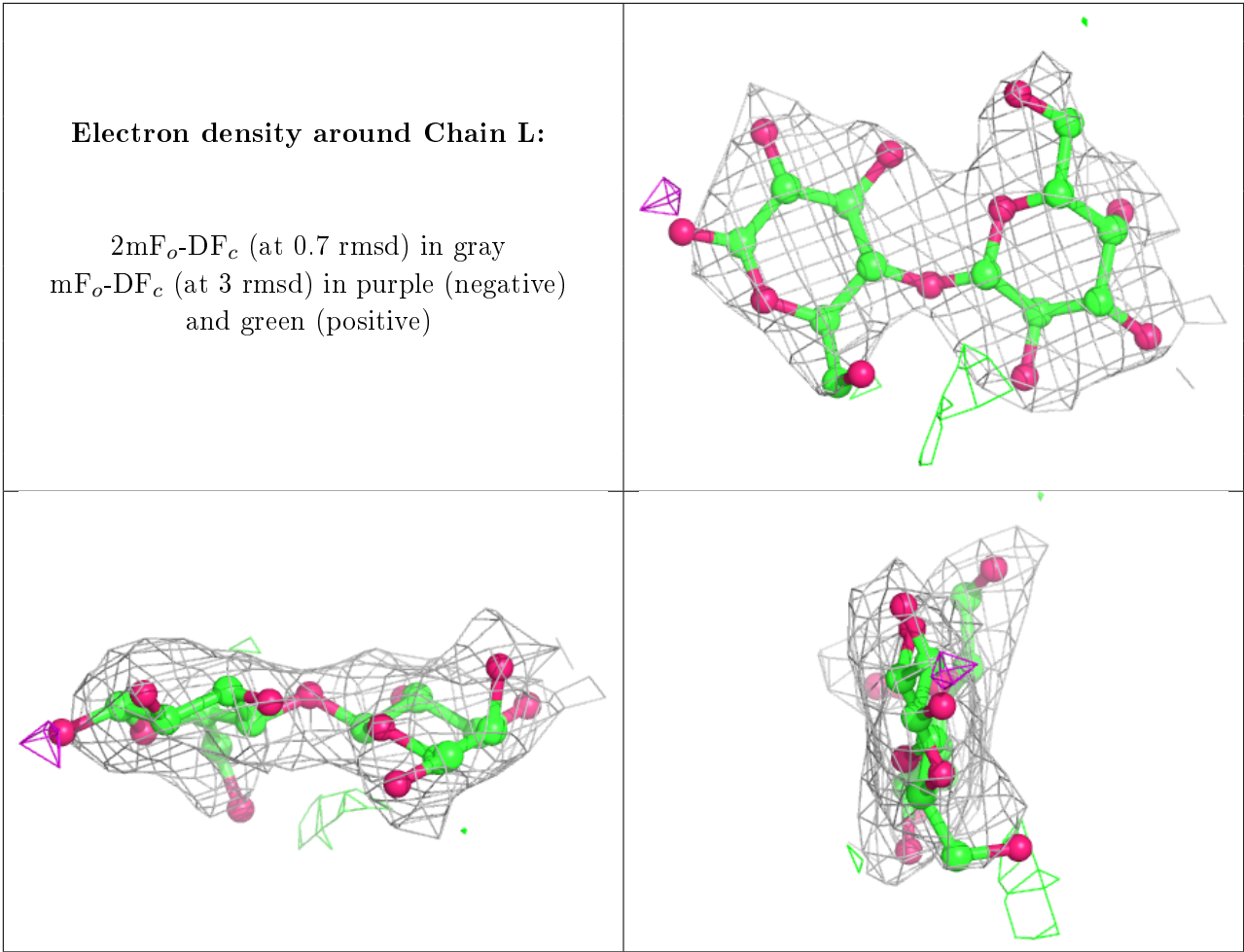
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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
4	CA	A	1290	1/1	0.95	0.18	36,36,36,36	0
4	CA	C	3290	1/1	0.95	0.16	27,27,27,27	0
4	CA	F	6290	1/1	0.97	0.18	33,33,33,33	0
4	CA	E	5290	1/1	0.98	0.21	37,37,37,37	0
4	CA	B	2290	1/1	0.98	0.15	29,29,29,29	0
4	CA	D	4290	1/1	0.98	0.13	31,31,31,31	0
3	MN	A	1289	1/1	0.98	0.06	22,22,22,22	0
3	MN	C	3289	1/1	0.99	0.09	19,19,19,19	0
3	MN	B	2289	1/1	0.99	0.06	25,25,25,25	0
3	MN	F	6289	1/1	0.99	0.08	25,25,25,25	0
3	MN	D	4289	1/1	1.00	0.05	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	E	5289	1/1	1.00	0.07	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.