



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:09 AM UTC

PDB ID : 5D0F / pdb_00005d0f
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (E564Q) in complex with maltopentaose
Authors : Zhai, L.; Xiang, S.
Deposited on : 2015-08-03
Resolution : 3.30 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:

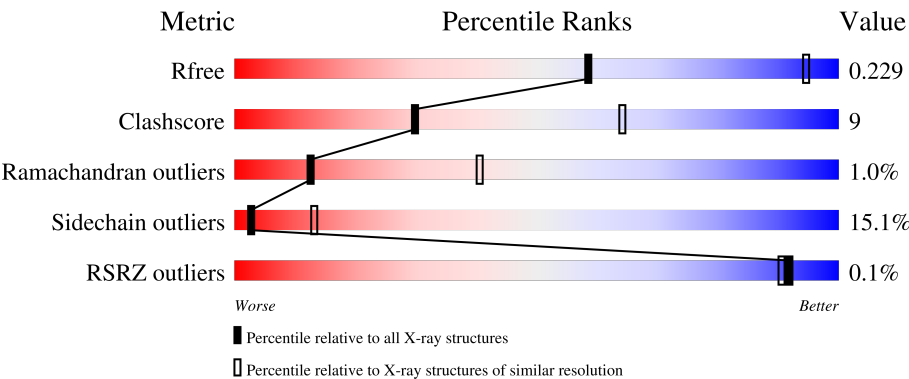
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



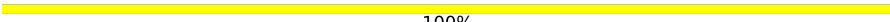
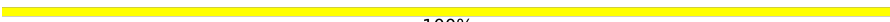
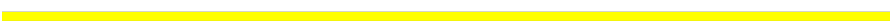
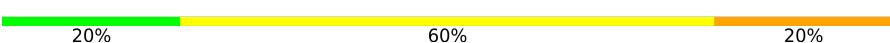
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1528	68%27%5%
1	B	1528	68%27%5%
2	C	4	100%
2	E	4	100%
2	H	4	100%

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Mol	Chain	Length	Quality of chain
2	I	4	 100%
2	K	4	 100%
3	D	5	 100%
3	G	5	 100%
3	J	5	 100%
3	M	5	 20%60%20%
4	F	3	 100%
4	L	3	 67%33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25070 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			

There are 2 discrepancies between the modelled and reference sequences:

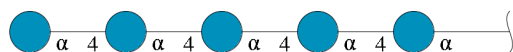
Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLN	GLU	engineered mutation	UNP Q6FSK0
B	564	GLN	GLU	engineered mutation	UNP Q6FSK0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			44	24	20			
2	H	4	Total	C	O	0	0	0
			44	24	20			
2	I	4	Total	C	O	0	0	0
			45	24	21			
2	K	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	5	Total	C	O	0	0	0
			56	30	26			
3	G	5	Total	C	O	0	0	0
			56	30	26			
3	J	5	Total	C	O	0	0	0
			56	30	26			
3	M	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

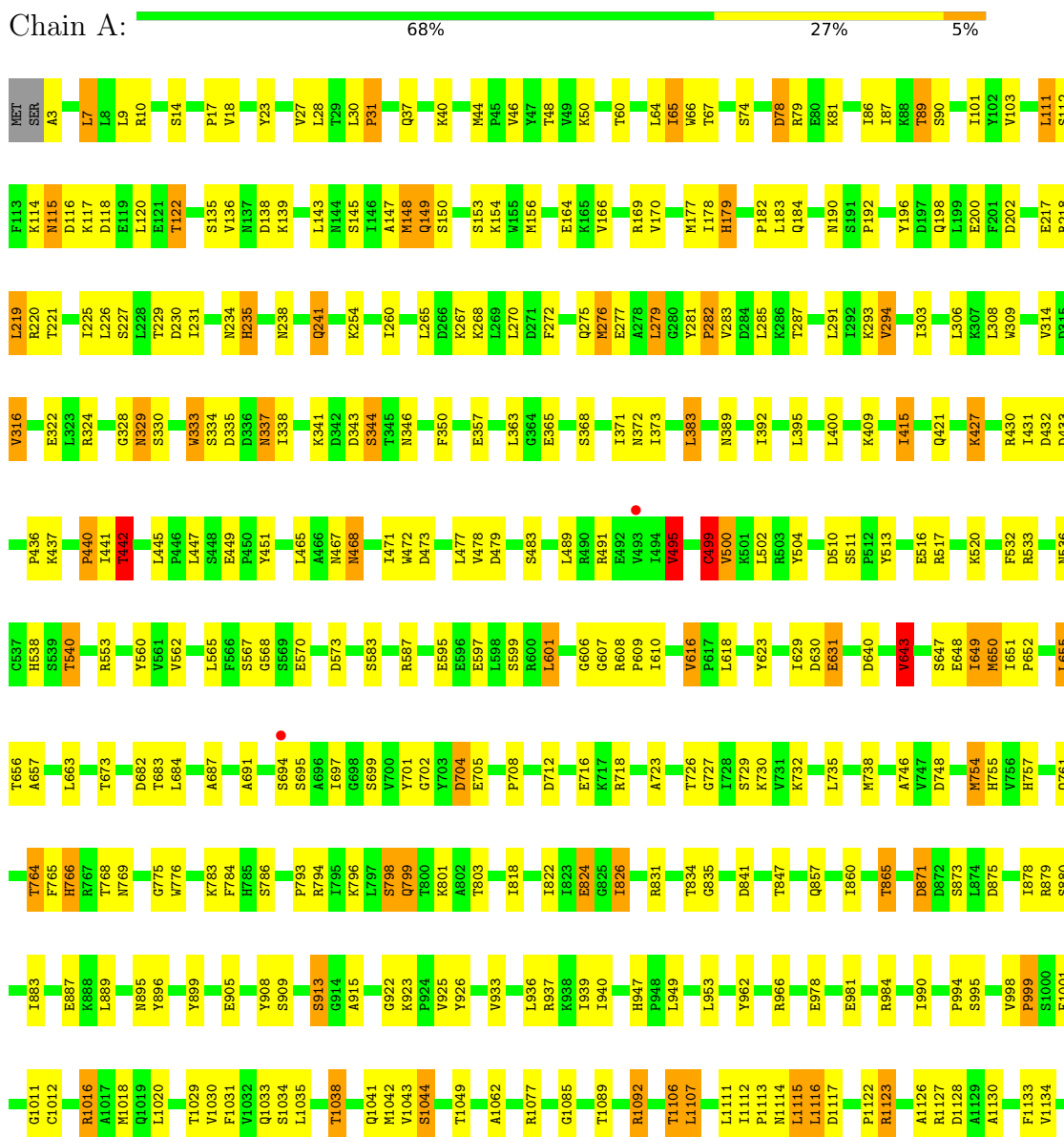


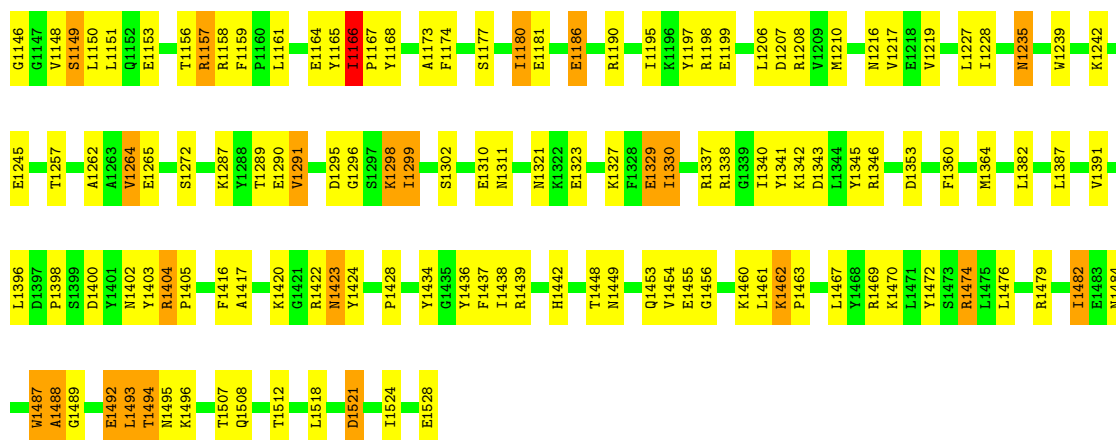
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	3	Total	C	O	0	0	0
			34	18	16			
4	L	3	Total	C	O	0	0	0
			34	18	16			

3 Residue-property plots

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

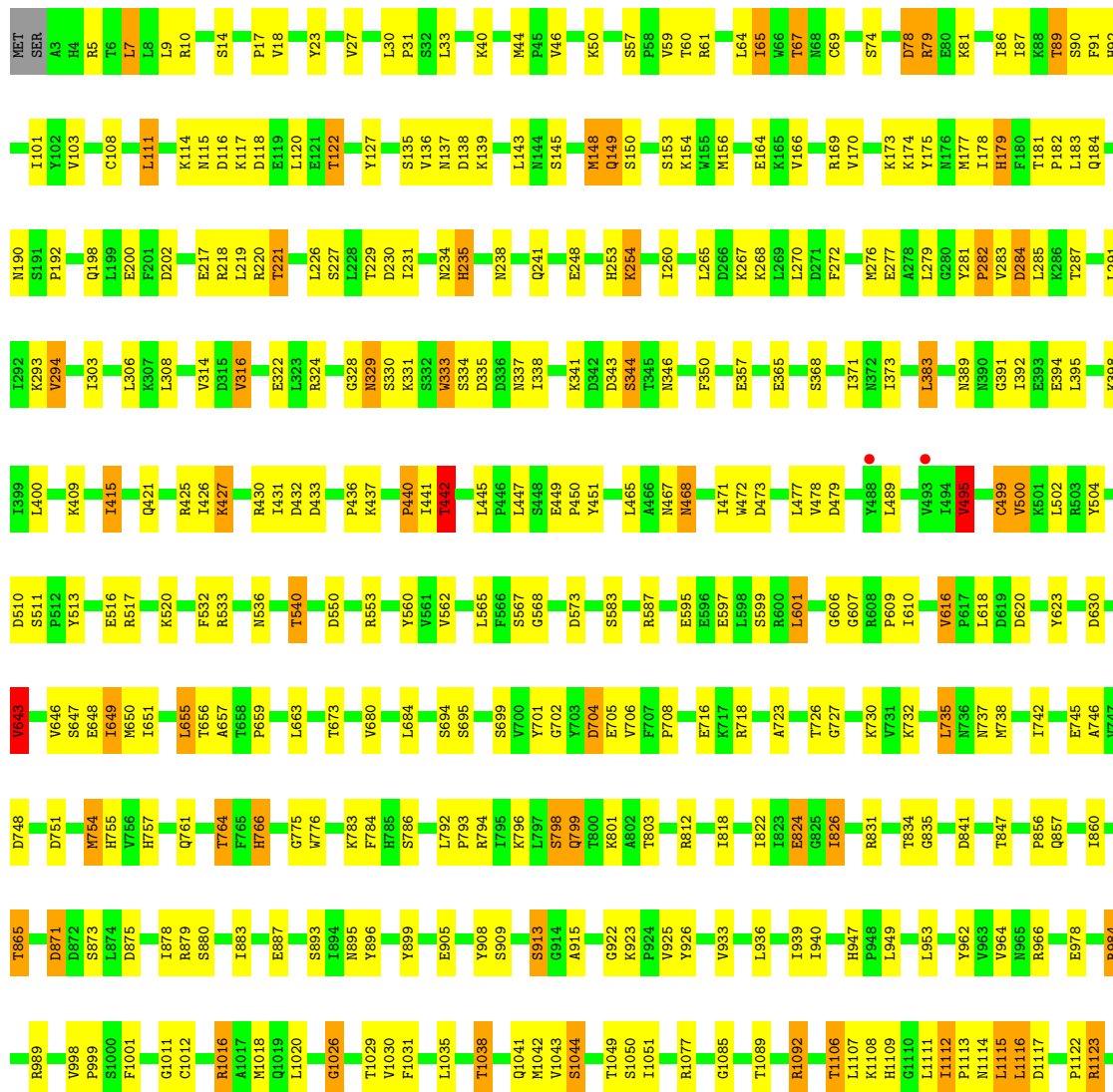
- Molecule 1: Uncharacterized protein

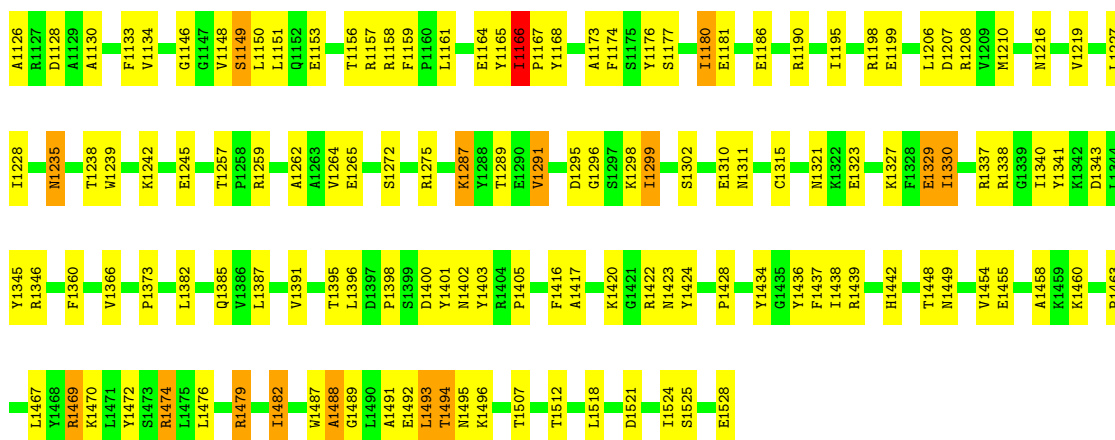




• Molecule 1: Uncharacterized protein

Chain B: 68% 27% 5%





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  100%

GLC1
GLC2
GLC3
GLC4

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

GLC1
GLC2
GLC3
GLC4
GLC5

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:  100%

GLC1
GLC2
GLC3
GLC4
GLC5

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  100%

GLC1
GLC2
GLC3
GLC4
GLC5

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  20% 60% 20%

GLC1
GLC2
GLC3
GLC4
GLC5

- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  100%

GLC1
GLC2
GLC3

- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  67% 33%

GLC1
GLC2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.07Å 202.01Å 135.24Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	49.05 – 3.30 49.05 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.05-3.30) 95.8 (49.05-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.228 0.197 , 0.229	Depositor DCC
R_{free} test set	3073 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: GLC

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	1.10	9/12589 (0.1%)	1.22	57/17071 (0.3%)
1	B	1.09	14/12589 (0.1%)	1.23	60/17071 (0.4%)
All	All	1.09	23/25178 (0.1%)	1.23	117/34142 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	812	ARG	CA-C	7.38	1.62	1.52
1	B	122	THR	CA-C	6.69	1.60	1.52
1	B	659	PRO	CA-C	-6.20	1.46	1.52
1	B	655	LEU	C-O	-6.17	1.16	1.23
1	A	695	SER	C-O	-6.12	1.17	1.23
1	B	1491	ALA	CA-C	-6.09	1.45	1.53
1	A	769	ASN	N-CA	5.99	1.53	1.46
1	A	1462	LYS	N-CA	5.96	1.50	1.45
1	A	122	THR	CA-C	5.91	1.59	1.52
1	A	1484	ASN	CA-C	-5.91	1.44	1.52
1	B	1469	ARG	C-O	-5.61	1.17	1.24
1	A	48	THR	N-CA	-5.41	1.39	1.46
1	B	646	VAL	C-O	-5.35	1.18	1.24
1	A	608	ARG	CA-C	-5.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	SER	N-CA	5.23	1.52	1.45
1	B	695	SER	C-O	-5.21	1.18	1.23
1	A	643	VAL	C-O	-5.21	1.19	1.24
1	B	67	THR	C-O	-5.17	1.17	1.23
1	B	92	HIS	C-O	-5.14	1.17	1.24
1	B	59	VAL	N-CA	-5.13	1.40	1.46
1	B	1479	ARG	N-CA	-5.10	1.40	1.46
1	B	1488	ALA	N-CA	5.02	1.52	1.46
1	B	1026	GLY	C-O	-5.00	1.17	1.23

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	651	ILE	CA-C-N	-10.38	110.24	120.52
1	B	651	ILE	C-N-CA	-10.38	110.24	120.52
1	A	651	ILE	CA-C-N	-8.74	111.87	120.52
1	A	651	ILE	C-N-CA	-8.74	111.87	120.52
1	B	1489	GLY	N-CA-C	8.60	125.98	112.31
1	B	984	ARG	N-CA-CB	8.17	121.86	110.01
1	A	922	GLY	N-CA-C	-7.57	102.77	111.85
1	A	1489	GLY	N-CA-C	7.29	125.84	112.27
1	A	46	VAL	N-CA-C	-7.27	104.12	110.74
1	B	1298	LYS	N-CA-C	7.17	120.09	108.34
1	B	922	GLY	N-CA-C	-7.16	103.26	111.85
1	A	30	LEU	CA-C-N	7.06	128.66	119.84
1	A	30	LEU	C-N-CA	7.06	128.66	119.84
1	A	1423	ASN	N-CA-C	6.75	120.38	111.75
1	A	392	ILE	N-CA-C	-6.72	104.30	110.82
1	A	998	VAL	CA-C-N	-6.70	111.47	119.84
1	A	998	VAL	C-N-CA	-6.70	111.47	119.84
1	B	680	VAL	CB-CA-C	-6.67	102.32	112.05
1	B	1448	THR	N-CA-C	6.58	119.05	111.02
1	A	880	SER	N-CA-C	6.58	119.06	109.07
1	B	998	VAL	CA-C-N	-6.58	111.62	119.84
1	B	998	VAL	C-N-CA	-6.58	111.62	119.84
1	A	570	GLU	N-CA-C	-6.46	104.15	111.07
1	A	1448	THR	N-CA-C	6.44	118.87	111.02
1	B	1423	ASN	N-CA-C	6.43	119.98	111.75
1	A	923	LYS	N-CA-C	6.42	117.90	109.93
1	B	880	SER	N-CA-C	6.42	118.83	109.07
1	A	495	VAL	N-CA-C	6.39	117.07	107.80
1	B	923	LYS	N-CA-C	6.36	117.81	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1311	ASN	N-CA-C	6.22	119.04	111.82
1	B	495	VAL	N-CA-C	6.20	116.79	107.80
1	A	78	ASP	N-CA-C	-6.20	97.72	108.69
1	A	1298	LYS	N-CA-C	6.18	118.47	108.34
1	A	746	ALA	N-CA-C	6.16	118.64	109.59
1	A	1488	ALA	N-CA-C	-6.15	104.49	111.07
1	A	1488	ALA	N-CA-CB	6.14	118.91	110.01
1	B	1330	ILE	N-CA-C	6.06	121.94	109.34
1	B	824	GLU	N-CA-C	6.06	118.62	109.41
1	B	1449	ASN	N-CA-C	6.03	117.26	109.72
1	B	643	VAL	N-CA-CB	6.02	117.50	110.82
1	B	78	ASP	N-CA-C	-6.02	98.04	108.69
1	A	1330	ILE	N-CA-C	6.00	121.82	109.34
1	B	392	ILE	N-CA-C	-5.98	105.02	110.82
1	A	796	LYS	N-CA-C	5.96	118.12	108.41
1	B	826	ILE	CA-C-N	5.95	126.26	119.83
1	B	826	ILE	C-N-CA	5.95	126.26	119.83
1	A	294	VAL	CB-CA-C	-5.94	104.02	112.22
1	B	504	TYR	N-CA-C	-5.94	102.86	110.53
1	A	643	VAL	N-CA-CB	5.90	117.37	110.82
1	A	1235	ASN	N-CA-C	5.86	118.19	108.99
1	A	650	MET	N-CA-C	5.82	120.64	112.72
1	B	316	VAL	N-CA-CB	5.79	117.33	110.55
1	B	50	LYS	CB-CA-C	-5.78	100.82	110.29
1	B	1315	CYS	N-CA-C	5.77	117.57	111.28
1	A	824	GLU	N-CA-C	5.76	118.44	109.52
1	B	1525	SER	N-CA-C	5.75	117.55	111.28
1	B	46	VAL	N-CA-C	-5.75	105.51	110.74
1	B	746	ALA	N-CA-C	5.74	118.03	109.59
1	B	1311	ASN	N-CA-C	5.72	118.46	111.82
1	B	468	ASN	CB-CA-C	5.72	119.23	109.80
1	B	1235	ASN	N-CA-C	5.69	117.93	108.99
1	B	1488	ALA	N-CA-CB	5.68	118.47	110.12
1	B	23	TYR	N-CA-C	-5.65	105.59	112.88
1	B	30	LEU	CA-C-N	5.64	126.89	119.84
1	B	30	LEU	C-N-CA	5.64	126.89	119.84
1	B	1208	ARG	CB-CG-CD	5.61	124.21	111.30
1	A	316	VAL	N-CA-CB	5.61	117.12	110.55
1	A	504	TYR	N-CA-C	-5.61	102.61	110.35
1	A	1487	TRP	CA-C-N	-5.59	113.17	120.44
1	A	1487	TRP	C-N-CA	-5.59	113.17	120.44
1	A	499	CYS	N-CA-C	5.58	117.87	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	796	LYS	N-CA-C	5.57	117.60	108.52
1	A	495	VAL	CB-CA-C	-5.57	102.83	110.96
1	A	607	GLY	N-CA-C	-5.56	102.49	110.38
1	B	272	PHE	N-CA-C	5.53	117.17	111.03
1	B	607	GLY	N-CA-C	-5.53	102.53	110.38
1	B	91	PHE	N-CA-C	-5.52	106.38	113.23
1	A	652	PRO	N-CA-C	5.47	119.28	111.13
1	B	314	VAL	N-CA-CB	5.43	116.45	110.53
1	B	5	ARG	N-CA-C	5.42	116.95	110.44
1	B	495	VAL	CB-CA-C	-5.42	103.05	110.96
1	B	601	LEU	CB-CA-C	-5.42	101.47	110.68
1	A	225	ILE	N-CA-C	5.39	115.74	107.77
1	B	1115	LEU	N-CA-C	-5.37	100.95	109.76
1	A	314	VAL	CB-CA-C	-5.36	103.73	111.34
1	A	50	LYS	CB-CA-C	-5.34	101.53	110.29
1	A	90	SER	N-CA-C	-5.33	101.27	109.52
1	A	89	THR	CB-CA-C	-5.32	102.50	110.16
1	B	989	ARG	CG-CD-NE	-5.30	100.33	112.00
1	A	138	ASP	N-CA-C	-5.29	104.26	111.56
1	B	89	THR	CB-CA-C	-5.29	102.55	110.16
1	A	468	ASN	CB-CA-C	5.28	118.51	109.80
1	B	90	SER	N-CA-C	-5.26	101.36	109.52
1	A	23	TYR	N-CA-C	-5.26	106.10	112.88
1	A	768	THR	N-CA-C	5.24	117.44	110.53
1	B	499	CYS	N-CA-C	5.23	117.95	109.06
1	B	138	ASP	N-CA-C	-5.21	104.20	110.88
1	A	601	LEU	CB-CA-C	-5.19	101.86	110.68
1	B	294	VAL	CB-CA-C	-5.19	105.06	112.22
1	A	272	PHE	N-CA-C	5.17	116.77	111.03
1	A	616	VAL	CB-CA-C	-5.16	101.98	111.36
1	A	826	ILE	CA-C-N	5.15	125.96	119.98
1	A	826	ILE	C-N-CA	5.15	125.96	119.98
1	A	1449	ASN	N-CA-C	5.13	116.13	109.72
1	A	768	THR	CA-CB-CG2	5.12	119.21	110.50
1	B	33	LEU	CA-C-N	-5.10	113.47	119.84
1	B	33	LEU	C-N-CA	-5.10	113.47	119.84
1	B	1385	GLN	CB-CA-C	-5.09	101.59	110.09
1	A	235	HIS	N-CA-C	5.08	116.97	108.99
1	B	751	ASP	N-CA-C	5.07	119.50	112.45
1	A	687	ALA	N-CA-C	5.05	117.51	111.71
1	B	235	HIS	N-CA-C	5.05	116.91	108.99
1	B	616	VAL	CB-CA-C	-5.04	102.18	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1264	VAL	CB-CA-C	-5.04	105.42	112.02
1	B	69	CYS	CA-C-N	-5.01	116.00	119.66
1	B	69	CYS	C-N-CA	-5.01	116.00	119.66
1	A	768	THR	N-CA-CB	-5.00	103.21	110.36

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1492	GLU	Peptide
1	A	306	LEU	Peptide
1	A	442	THR	Peptide
1	B	1492	GLU	Peptide
1	B	241	GLN	Peptide
1	B	306	LEU	Peptide
1	B	442	THR	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	12278	0	11962	214	0
1	B	12278	0	11962	208	0
2	C	45	0	39	0	0
2	E	44	0	37	0	0
2	H	44	0	37	0	0
2	I	45	0	39	0	0
2	K	44	0	37	0	0
3	D	56	0	48	0	0
3	G	56	0	48	0	0
3	J	56	0	48	0	0
3	M	56	0	48	1	0
4	F	34	0	30	0	0
4	L	34	0	30	1	0
All	All	25070	0	24365	421	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 (421) 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:1158:ARG:O	1:B:1159:PHE:HD2	1.38	1.04
1:B:1158:ARG:O	1:B:1159:PHE:CD2	2.17	0.97
1:A:1062:ALA:O	1:A:1508:GLN:OE1	1.92	0.86
1:A:230:ASP:OD1	1:A:533:ARG:HD3	1.77	0.84
1:B:230:ASP:OD1	1:B:533:ARG:HD3	1.79	0.83
1:B:757:HIS:HB3	1:B:764:THR:HG22	1.62	0.82
1:B:1482:ILE:HG12	1:B:1488:ALA:O	1.82	0.80
1:A:1482:ILE:HG12	1:A:1488:ALA:O	1.82	0.79
1:A:757:HIS:HB3	1:A:764:THR:HG22	1.66	0.78
1:A:738:MET:HE2	1:A:776:TRP:CZ2	2.19	0.78
1:B:871:ASP:OD1	1:B:871:ASP:N	2.20	0.75
1:B:1041:GLN:NE2	1:B:1488:ALA:HB3	2.07	0.70
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	1.91	0.69
1:A:282:PRO:HB3	1:A:294:VAL:HG22	1.74	0.69
1:B:282:PRO:HB3	1:B:294:VAL:HG22	1.75	0.68
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	1.94	0.68
1:B:964:VAL:HG11	1:B:984:ARG:HB3	1.75	0.68
1:A:629:ILE:HD13	1:A:631:GLU:HG2	1.76	0.67
1:A:1041:GLN:NE2	1:A:1488:ALA:HB3	2.09	0.67
1:A:1470:LYS:O	1:A:1474:ARG:HG3	1.94	0.67
1:A:871:ASP:OD1	1:A:871:ASP:N	2.28	0.66
1:B:1470:LYS:O	1:B:1474:ARG:HG3	1.97	0.65
1:A:3:ALA:HB3	1:A:640:ASP:HB3	1.77	0.65
1:B:783:LYS:HG2	1:B:857:GLN:HB3	1.80	0.64
1:A:1165:TYR:O	1:A:1167:PRO:CD	2.46	0.64
1:A:783:LYS:HG2	1:A:857:GLN:HB3	1.78	0.64
1:A:66:TRP:CZ3	1:B:1458:ALA:HB2	2.32	0.64
1:A:1018:MET:HE2	1:A:1018:MET:HA	1.80	0.64
1:A:148:MET:HA	1:A:177:MET:O	1.98	0.63
1:A:705:GLU:OE1	1:A:705:GLU:N	2.31	0.63
1:B:1018:MET:HA	1:B:1018:MET:HE2	1.81	0.63
1:B:1165:TYR:O	1:B:1167:PRO:CD	2.46	0.63
1:B:148:MET:HA	1:B:177:MET:O	1.98	0.63
1:A:704:ASP:OD2	1:A:732:LYS:HG3	1.99	0.63
1:B:115:ASN:HB3	1:B:117:LYS:H	1.64	0.63
1:B:1041:GLN:HE22	1:B:1488:ALA:HB3	1.64	0.63
1:B:656:THR:HG22	1:B:657:ALA:N	2.15	0.62
1:A:115:ASN:HB3	1:A:117:LYS:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HB2	1:A:368:SER:HB3	1.82	0.61
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.01	0.61
1:A:915:ALA:HA	1:A:962:TYR:OH	2.00	0.61
1:B:365:GLU:HB2	1:B:368:SER:HB3	1.83	0.61
1:A:738:MET:HE2	1:A:776:TRP:CE2	2.36	0.61
1:B:1085:GLY:O	1:B:1089:THR:HB	2.01	0.61
1:A:1041:GLN:HE22	1:A:1488:ALA:HB3	1.65	0.60
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.34	0.60
1:B:684:LEU:HD11	1:B:860:ILE:HD12	1.83	0.60
1:B:1146:GLY:O	1:B:1149:SER:OG	2.20	0.60
1:B:79:ARG:HH21	1:B:550:ASP:CG	2.10	0.60
1:B:1472:TYR:OH	1:B:1479:ARG:NH1	2.34	0.60
1:A:9:LEU:HD11	1:A:17:PRO:HB3	1.83	0.59
1:A:283:VAL:HA	1:A:441:ILE:HD11	1.85	0.59
1:B:757:HIS:HB3	1:B:764:THR:CG2	2.31	0.59
1:A:1085:GLY:O	1:A:1089:THR:HB	2.02	0.59
1:B:705:GLU:N	1:B:705:GLU:OE1	2.35	0.59
1:A:1165:TYR:O	1:A:1167:PRO:HD3	2.03	0.59
1:B:915:ALA:HA	1:B:962:TYR:OH	2.03	0.59
1:A:1157:ARG:NH2	1:A:1186:GLU:OE2	2.36	0.58
1:A:182:PRO:HG2	1:A:192:PRO:O	2.03	0.58
1:A:467:ASN:HB2	1:A:499:CYS:O	2.03	0.58
1:A:647:SER:OG	1:A:648:GLU:N	2.36	0.58
1:B:1038:THR:HG21	1:B:1512:THR:OG1	2.03	0.58
1:A:1038:THR:HG21	1:A:1512:THR:OG1	2.03	0.57
1:B:1340:ILE:HG22	1:B:1341:TYR:C	2.29	0.57
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	1.86	0.57
1:B:182:PRO:HG2	1:B:192:PRO:O	2.05	0.57
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.34	0.57
1:B:432:ASP:HB2	1:B:436:PRO:HB3	1.86	0.57
1:B:1165:TYR:O	1:B:1167:PRO:HD3	2.04	0.57
1:B:283:VAL:HA	1:B:441:ILE:HD11	1.86	0.57
1:A:1340:ILE:HG22	1:A:1341:TYR:C	2.30	0.57
1:B:430:ARG:NH1	1:B:440:PRO:O	2.38	0.56
1:A:432:ASP:HB2	1:A:436:PRO:HB3	1.87	0.56
1:A:1158:ARG:O	1:A:1159:PHE:CD2	2.58	0.56
1:A:684:LEU:HD11	1:A:860:ILE:HD12	1.88	0.56
1:B:467:ASN:HB2	1:B:499:CYS:O	2.05	0.56
1:A:1146:GLY:O	1:A:1149:SER:OG	2.23	0.56
1:A:1493:LEU:HD23	1:A:1494:THR:N	2.21	0.56
1:A:798:SER:O	1:A:799:GLN:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.88	0.56
1:A:1492:GLU:HG3	1:A:1508:GLN:HG3	1.88	0.56
1:B:798:SER:O	1:B:799:GLN:C	2.49	0.56
1:B:1396:LEU:HD21	1:B:1400:ASP:CB	2.36	0.56
1:A:1472:TYR:OH	1:A:1479:ARG:NH1	2.39	0.55
1:A:1038:THR:HG21	1:A:1512:THR:CB	2.37	0.55
1:A:1456:GLY:HA3	1:A:1462:LYS:HG3	1.88	0.55
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.89	0.55
1:A:430:ARG:NH1	1:A:440:PRO:O	2.39	0.55
1:B:925:VAL:CG1	1:B:1487:TRP:CE2	2.90	0.55
1:A:656:THR:HG22	1:A:657:ALA:N	2.22	0.54
1:B:630:ASP:O	1:B:648:GLU:HG2	2.07	0.54
1:A:1106:THR:HG21	1:A:1113:PRO:HG3	1.90	0.54
1:A:1123:ARG:NH2	1:A:1207:ASP:OD2	2.41	0.54
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.22	0.54
1:A:630:ASP:O	1:A:648:GLU:HG2	2.06	0.54
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.90	0.54
1:B:1405:PRO:HA	1:B:1428:PRO:HD3	1.89	0.54
1:A:606:GLY:O	1:A:694:SER:HB3	2.08	0.54
1:A:303:ILE:HG13	1:A:415:ILE:HD11	1.90	0.54
1:B:647:SER:OG	1:B:648:GLU:N	2.41	0.53
1:A:196:TYR:OH	1:A:241:GLN:NE2	2.42	0.53
1:A:1396:LEU:HD21	1:A:1400:ASP:CB	2.38	0.53
1:B:303:ILE:HG13	1:B:415:ILE:HD11	1.91	0.53
1:B:1029:THR:HG22	1:B:1030:VAL:N	2.23	0.53
1:A:757:HIS:HB3	1:A:764:THR:CG2	2.37	0.53
1:B:1106:THR:HG21	1:B:1113:PRO:HG3	1.90	0.53
1:A:1156:THR:CG2	1:A:1174:PHE:HA	2.39	0.53
1:A:1168:TYR:CD1	1:A:1168:TYR:C	2.86	0.52
1:B:1123:ARG:NH2	1:B:1207:ASP:OD2	2.42	0.52
1:B:1108:LYS:HE2	1:B:1159:PHE:CD1	2.45	0.52
1:B:60:THR:HG22	1:B:87:ILE:HG21	1.91	0.52
1:A:738:MET:HB3	1:A:776:TRP:CH2	2.45	0.52
1:B:606:GLY:O	1:B:694:SER:HB3	2.10	0.52
1:B:1038:THR:HG21	1:B:1512:THR:CB	2.40	0.52
1:B:560:TYR:CE2	1:B:562:VAL:CG2	2.93	0.52
1:A:60:THR:HG22	1:A:87:ILE:HG21	1.92	0.52
1:B:905:GLU:OE1	1:B:966:ARG:NH1	2.43	0.52
1:B:1128:ASP:OD2	1:B:1239:TRP:N	2.43	0.52
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.92	0.51
1:B:735:LEU:HD12	1:B:738:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1198:ARG:O	1:B:1199:GLU:C	2.53	0.51
1:A:177:MET:HE3	1:A:226:LEU:HB2	1.91	0.51
1:A:1029:THR:HG22	1:A:1030:VAL:N	2.26	0.51
1:B:925:VAL:CG1	1:B:1487:TRP:CD2	2.93	0.51
1:B:1168:TYR:CD1	1:B:1168:TYR:C	2.87	0.51
1:A:281:TYR:N	1:A:282:PRO:HD3	2.25	0.51
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.43	0.51
1:B:1156:THR:CG2	1:B:1174:PHE:HA	2.39	0.51
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.93	0.51
1:A:287:THR:O	1:A:291:LEU:HG	2.11	0.51
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.11	0.51
1:B:9:LEU:HD11	1:B:17:PRO:HB3	1.92	0.51
1:B:177:MET:HE3	1:B:226:LEU:HB2	1.92	0.51
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.92	0.51
1:A:909:SER:CB	1:A:913:SER:HB2	2.41	0.51
1:A:1404:ARG:O	1:A:1423:ASN:OD1	2.29	0.51
1:A:1195:ILE:HG12	1:A:1219:VAL:HB	1.93	0.50
1:B:1035:LEU:O	1:B:1038:THR:HG22	2.12	0.50
1:A:1405:PRO:HA	1:A:1428:PRO:HD3	1.92	0.50
1:B:148:MET:HE3	1:B:663:LEU:HD21	1.93	0.50
1:B:177:MET:HA	1:B:226:LEU:O	2.12	0.50
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.94	0.50
1:B:925:VAL:HG11	1:B:1487:TRP:CD2	2.46	0.50
1:A:231:ILE:HD12	1:A:532:PHE:CD1	2.47	0.50
1:A:282:PRO:CB	1:A:294:VAL:HG22	2.40	0.50
1:A:754:MET:HE3	1:A:754:MET:O	2.12	0.50
1:A:925:VAL:CG1	1:A:1487:TRP:CD2	2.95	0.50
1:A:1264:VAL:HG11	1:A:1360:PHE:HA	1.93	0.50
1:A:1156:THR:HG21	1:A:1174:PHE:HA	1.94	0.50
1:A:1181:GLU:OE1	1:A:1287:LYS:HG3	2.12	0.50
1:A:1291:VAL:CG2	1:A:1299:ILE:O	2.60	0.50
1:B:1166:ILE:HD11	1:B:1168:TYR:HB2	1.94	0.50
1:A:1128:ASP:OD2	1:A:1239:TRP:N	2.44	0.50
1:A:1495:ASN:O	1:A:1496:LYS:C	2.53	0.50
1:B:834:THR:HG22	1:B:835:GLY:N	2.27	0.49
1:A:834:THR:HG22	1:A:835:GLY:N	2.28	0.49
1:B:775:GLY:O	1:B:776:TRP:HD1	1.94	0.49
1:A:761:GLN:NE2	1:A:857:GLN:OE1	2.44	0.49
1:A:896:TYR:O	1:A:966:ARG:NH2	2.40	0.49
1:A:925:VAL:HG11	1:A:1487:TRP:CD2	2.48	0.49
1:A:1166:ILE:HD11	1:A:1168:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1195:ILE:HG12	1:B:1219:VAL:HB	1.93	0.49
1:A:1035:LEU:O	1:A:1038:THR:HG22	2.11	0.49
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.95	0.49
1:B:287:THR:O	1:B:291:LEU:HG	2.12	0.49
1:B:282:PRO:CB	1:B:294:VAL:HG22	2.41	0.49
1:B:1041:GLN:OE1	1:B:1507:THR:HG21	2.13	0.49
1:A:925:VAL:CG1	1:A:1487:TRP:CE2	2.95	0.49
1:B:766:HIS:CE1	1:B:865:THR:HG21	2.48	0.49
1:A:441:ILE:HG22	1:A:442:THR:N	2.27	0.49
1:B:896:TYR:O	1:B:966:ARG:NH2	2.43	0.49
1:B:1198:ARG:HA	1:B:1216:ASN:HA	1.94	0.48
1:B:1434:TYR:OH	1:B:1474:ARG:HB3	2.13	0.48
1:B:478:VAL:O	1:B:479:ASP:C	2.56	0.48
1:B:909:SER:CB	1:B:913:SER:HB2	2.43	0.48
1:B:567:SER:OG	1:B:568:GLY:N	2.46	0.48
1:A:136:VAL:HG12	1:A:139:LYS:HB2	1.94	0.48
1:A:595:GLU:HG3	1:A:784:PHE:CD2	2.48	0.48
1:B:656:THR:CG2	1:B:657:ALA:N	2.77	0.48
1:A:148:MET:HE3	1:A:663:LEU:HD21	1.96	0.48
1:A:467:ASN:HA	1:A:500:VAL:HA	1.95	0.48
1:A:513:TYR:CE2	1:A:517:ARG:HD2	2.48	0.48
1:B:101:ILE:HD12	1:B:101:ILE:N	2.29	0.48
1:B:253:HIS:CD2	1:B:254:LYS:N	2.82	0.48
1:A:177:MET:HA	1:A:226:LEU:O	2.13	0.48
1:B:441:ILE:HG22	1:B:442:THR:N	2.29	0.48
1:B:1108:LYS:CE	1:B:1159:PHE:CD1	2.96	0.48
1:A:478:VAL:O	1:A:479:ASP:C	2.57	0.48
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.96	0.48
1:B:754:MET:HE3	1:B:754:MET:O	2.13	0.48
1:B:899:TYR:CD1	1:B:1041:GLN:HG2	2.49	0.48
1:B:1156:THR:HG21	1:B:1174:PHE:HA	1.95	0.48
1:B:595:GLU:HG3	1:B:784:PHE:CD2	2.49	0.48
1:A:560:TYR:CE2	1:A:562:VAL:CG2	2.96	0.47
1:A:775:GLY:O	1:A:776:TRP:HD1	1.97	0.47
1:B:1108:LYS:HE2	1:B:1159:PHE:HD1	1.78	0.47
1:B:1291:VAL:CG2	1:B:1299:ILE:O	2.61	0.47
1:B:1416:PHE:CE2	1:B:1422:ARG:NH2	2.81	0.47
1:A:1198:ARG:O	1:A:1199:GLU:C	2.58	0.47
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.49	0.47
1:A:899:TYR:CD1	1:A:1041:GLN:HG2	2.49	0.47
1:B:1168:TYR:CD1	1:B:1168:TYR:O	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1417:ALA:O	1:B:1422:ARG:HB2	2.15	0.47
1:A:427:LYS:HE2	1:A:433:ASP:OD2	2.14	0.47
1:A:610:ILE:HD12	1:A:755:HIS:HB2	1.95	0.47
1:B:7:LEU:HD22	1:B:643:VAL:HG21	1.96	0.47
1:A:28:LEU:HB3	1:A:655:LEU:HD11	1.96	0.47
1:A:1011:GLY:O	1:A:1012:CYS:C	2.55	0.47
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.50	0.47
1:B:1165:TYR:O	1:B:1167:PRO:HD2	2.14	0.47
1:A:101:ILE:N	1:A:101:ILE:HD12	2.29	0.47
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.47	0.47
1:B:766:HIS:HE1	1:B:865:THR:HG21	1.79	0.47
1:B:150:SER:OG	1:B:179:HIS:HD2	1.98	0.47
1:B:757:HIS:CB	1:B:764:THR:HG22	2.39	0.47
1:B:136:VAL:HG12	1:B:139:LYS:HG3	1.97	0.47
1:A:766:HIS:HE1	1:A:865:THR:HG21	1.79	0.47
1:B:1018:MET:HE2	1:B:1018:MET:CA	2.45	0.47
1:A:1168:TYR:CD1	1:A:1168:TYR:O	2.67	0.46
1:B:648:GLU:HB3	1:B:883:ILE:HD12	1.98	0.46
1:B:1038:THR:O	1:B:1042:MET:HG2	2.15	0.46
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.48	0.46
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.50	0.46
1:A:1198:ARG:HA	1:A:1216:ASN:HA	1.97	0.46
1:A:623:TYR:CD2	1:A:649:ILE:HD11	2.50	0.46
1:A:1016:ARG:O	1:A:1020:LEU:HG	2.16	0.46
1:A:1165:TYR:O	1:A:1167:PRO:HD2	2.14	0.46
1:A:277:GLU:OE2	1:A:283:VAL:HG22	2.15	0.46
1:A:1038:THR:O	1:A:1042:MET:HG2	2.15	0.46
1:B:925:VAL:HG13	1:B:1487:TRP:CZ2	2.50	0.46
1:A:1077:ARG:NH1	1:A:1114:ASN:OD1	2.49	0.46
1:B:281:TYR:N	1:B:282:PRO:HD3	2.31	0.46
1:B:775:GLY:O	1:B:776:TRP:CD1	2.69	0.46
1:B:925:VAL:HG11	1:B:1487:TRP:CE2	2.50	0.46
1:A:154:LYS:NZ	1:A:190:ASN:O	2.49	0.46
1:A:841:ASP:C	1:A:841:ASP:OD1	2.58	0.46
1:B:1016:ARG:O	1:B:1020:LEU:HG	2.16	0.46
1:A:947:HIS:HD2	1:A:949:LEU:H	1.64	0.46
1:A:1106:THR:CG2	1:A:1113:PRO:HG3	2.46	0.46
1:A:1434:TYR:OH	1:A:1474:ARG:HB3	2.16	0.46
1:B:623:TYR:CD2	1:B:649:ILE:HD11	2.50	0.46
1:A:567:SER:HB3	1:A:573:ASP:OD1	2.16	0.46
1:B:1264:VAL:HG11	1:B:1360:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:ARG:NH1	1:B:1114:ASN:OD1	2.49	0.46
1:B:1438:ILE:HG23	1:B:1518:LEU:HD22	1.98	0.46
1:A:235:HIS:HA	1:A:502:LEU:HG	1.97	0.46
1:A:567:SER:OG	1:A:568:GLY:N	2.48	0.46
1:B:149:GLN:HA	1:B:699:SER:O	2.16	0.46
1:B:235:HIS:HA	1:B:502:LEU:HG	1.97	0.46
1:A:1417:ALA:O	1:A:1422:ARG:HB2	2.15	0.45
1:B:154:LYS:NZ	1:B:190:ASN:O	2.49	0.45
1:B:513:TYR:CE2	1:B:517:ARG:HD2	2.51	0.45
1:B:567:SER:HB3	1:B:573:ASP:OD1	2.17	0.45
1:B:793:PRO:O	1:B:794:ARG:C	2.59	0.45
1:B:1405:PRO:HA	1:B:1428:PRO:CD	2.46	0.45
1:A:648:GLU:HB3	1:A:883:ILE:HD12	1.98	0.45
1:A:936:LEU:O	1:A:940:ILE:HG13	2.16	0.45
1:B:427:LYS:HE2	1:B:433:ASP:OD2	2.16	0.45
1:A:702:GLY:HA2	1:A:705:GLU:HB2	1.98	0.45
1:A:834:THR:HG22	1:A:835:GLY:H	1.81	0.45
1:A:1151:LEU:HA	1:A:1180:ILE:HG22	1.97	0.45
1:B:1030:VAL:O	1:B:1031:PHE:C	2.60	0.45
1:B:1158:ARG:HD3	1:B:1173:ALA:HB1	1.99	0.45
1:A:1416:PHE:CE2	1:A:1422:ARG:NH2	2.85	0.45
1:A:231:ILE:HD12	1:A:532:PHE:CG	2.51	0.45
1:B:1106:THR:CG2	1:B:1113:PRO:HG3	2.47	0.45
1:A:1438:ILE:HG23	1:A:1518:LEU:HD22	1.98	0.45
1:A:218:ARG:O	1:A:219:LEU:C	2.59	0.45
1:A:7:LEU:HD22	1:A:643:VAL:HG21	1.99	0.45
1:A:895:ASN:CG	1:A:1044:SER:HB3	2.42	0.45
1:A:309:TRP:N	1:A:309:TRP:CD1	2.85	0.44
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.50	0.44
1:B:742:ILE:HD12	1:B:776:TRP:CH2	2.51	0.44
1:B:702:GLY:HA2	1:B:705:GLU:HB2	1.99	0.44
1:A:149:GLN:HA	1:A:699:SER:O	2.18	0.44
1:A:202:ASP:OD1	1:A:202:ASP:C	2.61	0.44
1:B:277:GLU:OE2	1:B:283:VAL:HG22	2.16	0.44
1:B:1495:ASN:O	1:B:1496:LYS:C	2.58	0.44
1:A:234:ASN:OD1	1:A:540:THR:OG1	2.33	0.44
1:B:1151:LEU:HA	1:B:1180:ILE:HG22	1.99	0.44
1:A:618:LEU:HD22	1:A:933:VAL:HG13	1.99	0.44
1:A:793:PRO:O	1:A:794:ARG:C	2.61	0.44
1:A:1043:VAL:HB	1:A:1092:ARG:HH22	1.82	0.44
1:A:1508:GLN:OE1	1:A:1508:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:O	1:A:472:TRP:C	2.61	0.44
1:A:765:PHE:C	1:A:765:PHE:CD1	2.96	0.44
1:A:1116:LEU:HA	1:A:1122:PRO:HB3	1.99	0.44
1:A:1290:GLU:HG2	1:A:1298:LYS:NZ	2.33	0.44
1:B:231:ILE:HD12	1:B:532:PHE:CD1	2.53	0.44
1:B:338:ILE:HG21	1:B:383:LEU:HG	2.00	0.44
1:B:738:MET:HE3	1:B:776:TRP:CZ3	2.53	0.44
1:B:761:GLN:NE2	1:B:857:GLN:OE1	2.51	0.44
1:B:322:GLU:HB3	1:B:373:ILE:HD13	1.99	0.44
1:B:467:ASN:HA	1:B:500:VAL:HA	2.00	0.44
1:B:156:MET:HG2	1:B:166:VAL:HG21	2.00	0.43
1:B:328:GLY:C	1:B:329:ASN:HD22	2.26	0.43
1:B:738:MET:HB3	1:B:776:TRP:CH2	2.53	0.43
1:B:1219:VAL:HG13	1:B:1228:ILE:HG23	2.01	0.43
1:A:322:GLU:HB3	1:A:373:ILE:HD13	1.99	0.43
1:B:149:GLN:HG2	1:B:170:VAL:HG11	1.98	0.43
1:A:281:TYR:N	1:A:282:PRO:CD	2.82	0.43
1:A:1492:GLU:HA	1:A:1508:GLN:CG	2.49	0.43
1:B:173:LYS:HE3	1:B:175:TYR:HE1	1.84	0.43
1:B:231:ILE:HD12	1:B:532:PHE:CG	2.53	0.43
1:B:234:ASN:OD1	1:B:540:THR:OG1	2.33	0.43
1:B:716:GLU:OE2	1:B:718:ARG:NH1	2.51	0.43
1:B:899:TYR:O	1:B:926:TYR:HB3	2.18	0.43
1:A:656:THR:CG2	1:A:657:ALA:N	2.82	0.43
1:A:716:GLU:OE2	1:A:718:ARG:NH1	2.52	0.43
1:A:899:TYR:O	1:A:926:TYR:HB3	2.19	0.43
1:B:1043:VAL:HB	1:B:1092:ARG:HH22	1.83	0.43
1:A:338:ILE:HG21	1:A:383:LEU:HG	2.00	0.43
1:A:436:PRO:O	1:A:437:LYS:HG2	2.19	0.43
1:A:1018:MET:HE2	1:A:1018:MET:CA	2.47	0.43
1:A:1033:GLN:O	1:A:1034:SER:C	2.61	0.43
1:A:981:GLU:OE1	1:A:984:ARG:NH1	2.52	0.43
1:A:1405:PRO:HA	1:A:1428:PRO:CD	2.48	0.43
1:B:953:LEU:HD13	1:B:999:PRO:HA	2.00	0.43
1:A:111:LEU:HD23	1:A:111:LEU:N	2.33	0.43
1:B:170:VAL:HG21	1:B:178:ILE:HD11	2.01	0.43
1:B:174:LYS:HG3	1:B:737:ASN:OD1	2.18	0.43
1:B:610:ILE:HD12	1:B:755:HIS:HB2	2.01	0.43
1:B:1108:LYS:CE	1:B:1159:PHE:HD1	2.31	0.43
1:B:1116:LEU:HA	1:B:1122:PRO:HB3	1.99	0.43
1:B:1130:ALA:O	1:B:1133:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG21	1:A:178:ILE:HD11	2.00	0.43
1:A:328:GLY:C	1:A:329:ASN:HD22	2.27	0.43
1:A:775:GLY:HA3	1:A:865:THR:CG2	2.49	0.43
1:A:1042:MET:CE	1:A:1507:THR:HG22	2.48	0.43
1:B:618:LEU:HD22	1:B:933:VAL:HG13	2.00	0.42
1:B:1011:GLY:O	1:B:1012:CYS:C	2.60	0.42
1:B:471:ILE:O	1:B:472:TRP:C	2.62	0.42
1:B:893:SER:HA	1:B:896:TYR:CD2	2.54	0.42
1:B:1181:GLU:OE1	1:B:1287:LYS:HG3	2.19	0.42
1:A:765:PHE:C	1:A:765:PHE:HD1	2.27	0.42
1:A:939:ILE:HD11	1:A:947:HIS:CD2	2.54	0.42
1:B:1329:GLU:O	1:B:1330:ILE:HG23	2.20	0.42
1:A:451:TYR:CE1	1:A:495:VAL:HG21	2.55	0.42
1:A:925:VAL:HG11	1:A:1487:TRP:CE2	2.54	0.42
1:A:1436:TYR:O	1:A:1437:PHE:C	2.63	0.42
1:A:1158:ARG:HD3	1:A:1173:ALA:HB1	2.01	0.42
1:A:1329:GLU:O	1:A:1330:ILE:HG23	2.20	0.42
1:B:391:GLY:HA2	1:B:394:GLU:OE1	2.18	0.42
1:B:878:ILE:HD13	1:B:1001:PHE:HD1	1.85	0.42
1:B:1157:ARG:HG2	1:B:1176:TYR:OH	2.19	0.42
1:A:775:GLY:O	1:A:776:TRP:CD1	2.72	0.42
1:A:1130:ALA:O	1:A:1133:PHE:HB3	2.19	0.42
1:B:436:PRO:O	1:B:437:LYS:HG2	2.20	0.42
1:B:775:GLY:HA3	1:B:865:THR:CG2	2.50	0.42
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.02	0.42
1:A:436:PRO:O	1:A:437:LYS:CG	2.67	0.42
1:B:202:ASP:OD1	1:B:202:ASP:C	2.62	0.42
1:B:217:GLU:O	1:B:221:THR:HG23	2.19	0.42
1:B:834:THR:HG22	1:B:835:GLY:H	1.84	0.42
1:A:217:GLU:O	1:A:221:THR:HG23	2.19	0.42
1:A:1360:PHE:CD1	1:A:1364:MET:HE3	2.55	0.42
1:B:343:ASP:O	1:B:344:SER:C	2.63	0.42
1:B:875:ASP:OD2	1:B:879:ARG:HD2	2.19	0.42
1:A:1115:LEU:HD23	1:A:1115:LEU:C	2.45	0.42
1:A:1493:LEU:HD23	1:A:1493:LEU:C	2.45	0.42
1:B:1108:LYS:HD2	1:B:1109:HIS:CD2	2.55	0.42
1:A:147:ALA:HA	1:A:697:ILE:O	2.19	0.42
1:A:783:LYS:HG2	1:A:857:GLN:CB	2.46	0.42
1:B:148:MET:HG3	1:B:177:MET:HG2	2.01	0.42
1:B:939:ILE:HD11	1:B:947:HIS:CD2	2.55	0.42
1:A:994:PRO:O	1:A:995:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:VAL:HG13	1:A:1228:ILE:HG23	2.01	0.41
1:B:57:SER:O	1:B:60:THR:OG1	2.37	0.41
1:B:1050:SER:OG	1:B:1051:ILE:N	2.52	0.41
1:B:1238:THR:HG21	1:B:1259:ARG:NH1	2.35	0.41
1:B:1275:ARG:NH2	1:B:1366:VAL:O	2.53	0.41
1:B:1493:LEU:HD23	1:B:1493:LEU:C	2.45	0.41
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.55	0.41
1:B:218:ARG:O	1:B:219:LEU:C	2.62	0.41
1:B:1112:ILE:HD13	1:B:1133:PHE:CG	2.55	0.41
1:A:372:ASN:O	1:A:373:ILE:C	2.62	0.41
1:A:1030:VAL:O	1:A:1031:PHE:C	2.64	0.41
1:A:618:LEU:HD12	1:A:937:ARG:HG3	2.03	0.41
1:B:284:ASP:OD1	1:B:284:ASP:N	2.54	0.41
1:B:1042:MET:CE	1:B:1507:THR:HG22	2.50	0.41
1:A:276:MET:O	1:A:279:LEU:O	2.38	0.41
1:A:937:ARG:NH1	1:A:937:ARG:HG2	2.36	0.41
1:A:1264:VAL:HG23	1:A:1343:ASP:O	2.20	0.41
1:A:691:ALA:HA	1:A:697:ILE:HD13	2.03	0.41
1:B:792:LEU:HA	1:B:793:PRO:HD3	1.91	0.41
1:A:149:GLN:OE1	1:A:701:TYR:HA	2.21	0.41
1:A:150:SER:OG	1:A:179:HIS:HD2	2.04	0.41
1:A:230:ASP:OD1	1:A:533:ARG:CD	2.60	0.41
1:A:878:ILE:HD13	1:A:1001:PHE:HD1	1.85	0.41
1:A:1329:GLU:C	1:A:1330:ILE:HG23	2.46	0.41
1:A:1492:GLU:HB2	1:A:1508:GLN:HG2	2.03	0.41
1:B:436:PRO:O	1:B:437:LYS:CG	2.69	0.41
1:B:620:ASP:OD1	1:B:620:ASP:N	2.53	0.41
1:B:895:ASN:CG	1:B:1044:SER:HB3	2.46	0.41
1:B:1329:GLU:C	1:B:1330:ILE:HG23	2.46	0.41
1:B:1400:ASP:HA	4:L:1:GLC:O6	2.21	0.41
1:B:1436:TYR:O	1:B:1437:PHE:C	2.64	0.41
1:A:682:ASP:O	1:A:683:THR:C	2.62	0.41
1:A:875:ASP:OD2	1:A:879:ARG:HD2	2.21	0.41
1:A:1453:GLN:NE2	1:A:1461:LEU:HD21	2.36	0.41
1:B:425:ARG:NE	3:M:4:GLC:O6	2.54	0.41
1:B:856:PRO:O	1:B:857:GLN:C	2.63	0.41
1:A:156:MET:HG2	1:A:166:VAL:HG21	2.03	0.40
1:A:333:TRP:CH2	1:A:350:PHE:HZ	2.38	0.40
1:A:337:ASN:OD1	1:A:337:ASN:N	2.54	0.40
1:B:451:TYR:CE1	1:B:495:VAL:HG21	2.55	0.40
1:B:1264:VAL:HG23	1:B:1343:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:O	1:A:344:SER:C	2.64	0.40
1:A:1197:TYR:CE1	1:A:1217:VAL:HG23	2.56	0.40
1:A:1342:LYS:HB2	1:A:1353:ASP:O	2.21	0.40
1:B:136:VAL:HG13	1:B:137:ASN:N	2.35	0.40
1:B:230:ASP:OD1	1:B:533:ARG:CD	2.61	0.40
1:B:936:LEU:O	1:B:940:ILE:HG13	2.21	0.40
1:B:947:HIS:HD2	1:B:949:LEU:H	1.68	0.40
1:A:729:SER:O	1:A:730:LYS:C	2.62	0.40
1:A:947:HIS:CD2	1:A:949:LEU:H	2.39	0.40
1:A:953:LEU:HD13	1:A:999:PRO:HA	2.03	0.40
1:B:181:THR:HB	1:B:182:PRO:HD2	2.03	0.40
1:B:333:TRP:CH2	1:B:350:PHE:HZ	2.39	0.40
1:B:841:ASP:OD1	1:B:841:ASP:C	2.65	0.40
1:B:111:LEU:HD23	1:B:111:LEU:N	2.36	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	1524/1528 (100%)	1314 (86%)	195 (13%)	15 (1%)	12	40
1	B	1524/1528 (100%)	1321 (87%)	188 (12%)	15 (1%)	12	40
All	All	3048/3056 (100%)	2635 (86%)	383 (13%)	30 (1%)	12	40

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	887	GLU
1	B	887	GLU
1	A	440	PRO
1	A	723	ALA

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Mol	Chain	Res	Type
1	A	1424	TYR
1	B	440	PRO
1	B	1424	TYR
1	A	219	LEU
1	A	282	PRO
1	A	308	LEU
1	B	308	LEU
1	B	723	ALA
1	B	727	GLY
1	B	745	GLU
1	B	1026	GLY
1	B	1166	ILE
1	A	31	PRO
1	A	538	HIS
1	A	708	PRO
1	A	1166	ILE
1	A	1521	ASP
1	B	31	PRO
1	B	282	PRO
1	A	115	ASN
1	A	727	GLY
1	B	708	PRO
1	A	511	SER
1	B	511	SER
1	B	450	PRO
1	B	1373	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	1344/1346 (100%)	1139 (85%)	205 (15%)	3	13
1	B	1344/1346 (100%)	1144 (85%)	200 (15%)	3	13
All	All	2688/2692 (100%)	2283 (85%)	405 (15%)	3	13

All (405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	ARG
1	A	14	SER
1	A	18	VAL
1	A	27	VAL
1	A	31	PRO
1	A	37	GLN
1	A	40	LYS
1	A	44	MET
1	A	64	LEU
1	A	65	ILE
1	A	67	THR
1	A	74	SER
1	A	78	ASP
1	A	79	ARG
1	A	81	LYS
1	A	86	ILE
1	A	89	THR
1	A	103	VAL
1	A	111	LEU
1	A	114	LYS
1	A	116	ASP
1	A	118	ASP
1	A	120	LEU
1	A	122	THR
1	A	135	SER
1	A	143	LEU
1	A	145	SER
1	A	148	MET
1	A	149	GLN
1	A	153	SER
1	A	164	GLU
1	A	179	HIS
1	A	183	LEU
1	A	184	GLN
1	A	198	GLN
1	A	200	GLU
1	A	220	ARG
1	A	227	SER
1	A	229	THR
1	A	238	ASN
1	A	241	GLN
1	A	254	LYS

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Mol	Chain	Res	Type
1	A	260	ILE
1	A	265	LEU
1	A	267	LYS
1	A	268	LYS
1	A	270	LEU
1	A	275	GLN
1	A	276	MET
1	A	279	LEU
1	A	285	LEU
1	A	293	LYS
1	A	316	VAL
1	A	324	ARG
1	A	329	ASN
1	A	330	SER
1	A	333	TRP
1	A	334	SER
1	A	335	ASP
1	A	337	ASN
1	A	341	LYS
1	A	344	SER
1	A	346	ASN
1	A	357	GLU
1	A	363	LEU
1	A	371	ILE
1	A	383	LEU
1	A	389	ASN
1	A	395	LEU
1	A	400	LEU
1	A	409	LYS
1	A	415	ILE
1	A	421	GLN
1	A	427	LYS
1	A	431	ILE
1	A	442	THR
1	A	445	LEU
1	A	447	LEU
1	A	449	GLU
1	A	465	LEU
1	A	468	ASN
1	A	473	ASP
1	A	477	LEU
1	A	483	SER

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Mol	Chain	Res	Type
1	A	489	LEU
1	A	491	ARG
1	A	495	VAL
1	A	499	CYS
1	A	500	VAL
1	A	510	ASP
1	A	516	GLU
1	A	520	LYS
1	A	536	ASN
1	A	540	THR
1	A	553	ARG
1	A	565	LEU
1	A	583	SER
1	A	587	ARG
1	A	597	GLU
1	A	599	SER
1	A	601	LEU
1	A	609	PRO
1	A	616	VAL
1	A	631	GLU
1	A	643	VAL
1	A	649	ILE
1	A	650	MET
1	A	655	LEU
1	A	673	THR
1	A	704	ASP
1	A	712	ASP
1	A	726	THR
1	A	735	LEU
1	A	748	ASP
1	A	754	MET
1	A	764	THR
1	A	766	HIS
1	A	786	SER
1	A	798	SER
1	A	799	GLN
1	A	801	LYS
1	A	803	THR
1	A	818	ILE
1	A	822	ILE
1	A	824	GLU
1	A	826	ILE

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Mol	Chain	Res	Type
1	A	831	ARG
1	A	847	THR
1	A	865	THR
1	A	871	ASP
1	A	873	SER
1	A	889	LEU
1	A	908	TYR
1	A	913	SER
1	A	978	GLU
1	A	990	ILE
1	A	999	PRO
1	A	1016	ARG
1	A	1038	THR
1	A	1044	SER
1	A	1049	THR
1	A	1092	ARG
1	A	1106	THR
1	A	1107	LEU
1	A	1111	LEU
1	A	1112	ILE
1	A	1115	LEU
1	A	1116	LEU
1	A	1117	ASP
1	A	1123	ARG
1	A	1127	ARG
1	A	1134	VAL
1	A	1148	VAL
1	A	1149	SER
1	A	1150	LEU
1	A	1153	GLU
1	A	1157	ARG
1	A	1161	LEU
1	A	1164	GLU
1	A	1166	ILE
1	A	1177	SER
1	A	1180	ILE
1	A	1186	GLU
1	A	1190	ARG
1	A	1206	LEU
1	A	1208	ARG
1	A	1210	MET
1	A	1227	LEU

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Mol	Chain	Res	Type
1	A	1235	ASN
1	A	1242	LYS
1	A	1245	GLU
1	A	1257	THR
1	A	1265	GLU
1	A	1272	SER
1	A	1289	THR
1	A	1291	VAL
1	A	1299	ILE
1	A	1302	SER
1	A	1310	GLU
1	A	1321	ASN
1	A	1323	GLU
1	A	1327	LYS
1	A	1329	GLU
1	A	1337	ARG
1	A	1338	ARG
1	A	1346	ARG
1	A	1382	LEU
1	A	1387	LEU
1	A	1391	VAL
1	A	1402	ASN
1	A	1404	ARG
1	A	1420	LYS
1	A	1442	HIS
1	A	1454	VAL
1	A	1455	GLU
1	A	1460	LYS
1	A	1469	ARG
1	A	1474	ARG
1	A	1476	LEU
1	A	1482	ILE
1	A	1493	LEU
1	A	1494	THR
1	A	1524	ILE
1	A	1528	GLU
1	B	7	LEU
1	B	10	ARG
1	B	14	SER
1	B	18	VAL
1	B	27	VAL
1	B	40	LYS

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Mol	Chain	Res	Type
1	B	44	MET
1	B	61	ARG
1	B	64	LEU
1	B	65	ILE
1	B	67	THR
1	B	74	SER
1	B	78	ASP
1	B	79	ARG
1	B	81	LYS
1	B	86	ILE
1	B	89	THR
1	B	103	VAL
1	B	111	LEU
1	B	114	LYS
1	B	116	ASP
1	B	118	ASP
1	B	120	LEU
1	B	122	THR
1	B	135	SER
1	B	143	LEU
1	B	145	SER
1	B	148	MET
1	B	149	GLN
1	B	153	SER
1	B	164	GLU
1	B	179	HIS
1	B	183	LEU
1	B	184	GLN
1	B	198	GLN
1	B	200	GLU
1	B	220	ARG
1	B	221	THR
1	B	227	SER
1	B	229	THR
1	B	238	ASN
1	B	248	GLU
1	B	254	LYS
1	B	260	ILE
1	B	265	LEU
1	B	267	LYS
1	B	268	LYS
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	276	MET
1	B	279	LEU
1	B	284	ASP
1	B	285	LEU
1	B	293	LYS
1	B	316	VAL
1	B	324	ARG
1	B	329	ASN
1	B	330	SER
1	B	331	LYS
1	B	333	TRP
1	B	334	SER
1	B	335	ASP
1	B	337	ASN
1	B	341	LYS
1	B	344	SER
1	B	346	ASN
1	B	357	GLU
1	B	371	ILE
1	B	383	LEU
1	B	389	ASN
1	B	395	LEU
1	B	398	LYS
1	B	400	LEU
1	B	409	LYS
1	B	415	ILE
1	B	421	GLN
1	B	426	ILE
1	B	427	LYS
1	B	431	ILE
1	B	442	THR
1	B	445	LEU
1	B	447	LEU
1	B	449	GLU
1	B	465	LEU
1	B	468	ASN
1	B	473	ASP
1	B	477	LEU
1	B	489	LEU
1	B	495	VAL
1	B	500	VAL
1	B	510	ASP

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Mol	Chain	Res	Type
1	B	516	GLU
1	B	520	LYS
1	B	536	ASN
1	B	540	THR
1	B	553	ARG
1	B	565	LEU
1	B	583	SER
1	B	587	ARG
1	B	597	GLU
1	B	599	SER
1	B	601	LEU
1	B	609	PRO
1	B	616	VAL
1	B	643	VAL
1	B	649	ILE
1	B	650	MET
1	B	655	LEU
1	B	673	THR
1	B	704	ASP
1	B	706	VAL
1	B	726	THR
1	B	730	LYS
1	B	735	LEU
1	B	748	ASP
1	B	754	MET
1	B	764	THR
1	B	766	HIS
1	B	786	SER
1	B	798	SER
1	B	799	GLN
1	B	801	LYS
1	B	803	THR
1	B	818	ILE
1	B	822	ILE
1	B	824	GLU
1	B	826	ILE
1	B	831	ARG
1	B	847	THR
1	B	865	THR
1	B	871	ASP
1	B	873	SER
1	B	908	TYR

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Mol	Chain	Res	Type
1	B	913	SER
1	B	978	GLU
1	B	1016	ARG
1	B	1038	THR
1	B	1044	SER
1	B	1049	THR
1	B	1092	ARG
1	B	1106	THR
1	B	1107	LEU
1	B	1111	LEU
1	B	1112	ILE
1	B	1115	LEU
1	B	1116	LEU
1	B	1117	ASP
1	B	1123	ARG
1	B	1134	VAL
1	B	1148	VAL
1	B	1149	SER
1	B	1150	LEU
1	B	1153	GLU
1	B	1161	LEU
1	B	1164	GLU
1	B	1166	ILE
1	B	1177	SER
1	B	1180	ILE
1	B	1186	GLU
1	B	1190	ARG
1	B	1206	LEU
1	B	1210	MET
1	B	1227	LEU
1	B	1235	ASN
1	B	1242	LYS
1	B	1245	GLU
1	B	1257	THR
1	B	1265	GLU
1	B	1272	SER
1	B	1287	LYS
1	B	1289	THR
1	B	1291	VAL
1	B	1299	ILE
1	B	1302	SER
1	B	1310	GLU

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Mol	Chain	Res	Type
1	B	1321	ASN
1	B	1323	GLU
1	B	1327	LYS
1	B	1329	GLU
1	B	1337	ARG
1	B	1338	ARG
1	B	1346	ARG
1	B	1382	LEU
1	B	1387	LEU
1	B	1391	VAL
1	B	1395	THR
1	B	1401	TYR
1	B	1402	ASN
1	B	1420	LYS
1	B	1442	HIS
1	B	1454	VAL
1	B	1455	GLU
1	B	1460	LYS
1	B	1469	ARG
1	B	1474	ARG
1	B	1476	LEU
1	B	1482	ILE
1	B	1493	LEU
1	B	1494	THR
1	B	1524	ILE
1	B	1528	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	92	HIS
1	A	179	HIS
1	A	246	HIS
1	A	253	HIS
1	A	329	ASN
1	A	346	ASN
1	A	354	ASN
1	A	384	HIS
1	A	467	ASN
1	A	536	ASN
1	A	538	HIS

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Mol	Chain	Res	Type
1	A	605	HIS
1	A	686	ASN
1	A	766	HIS
1	A	790	GLN
1	A	866	GLN
1	A	947	HIS
1	A	1056	ASN
1	A	1250	ASN
1	A	1409	ASN
1	A	1442	HIS
1	A	1453	GLN
1	B	92	HIS
1	B	179	HIS
1	B	238	ASN
1	B	246	HIS
1	B	253	HIS
1	B	329	ASN
1	B	346	ASN
1	B	354	ASN
1	B	467	ASN
1	B	536	ASN
1	B	538	HIS
1	B	564	GLN
1	B	686	ASN
1	B	766	HIS
1	B	790	GLN
1	B	947	HIS
1	B	1056	ASN
1	B	1235	ASN
1	B	1311	ASN
1	B	1409	ASN
1	B	1442	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 ⓘ

46 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	GLC	C	1	2	12,12,12	0.86	0	17,17,17	1.38	1 (5%)
2	GLC	C	2	2	11,11,12	0.94	1 (9%)	15,15,17	1.20	1 (6%)
2	GLC	C	3	2	11,11,12	1.20	3 (27%)	15,15,17	1.26	2 (13%)
2	GLC	C	4	2	11,11,12	1.84	3 (27%)	15,15,17	1.37	2 (13%)
3	GLC	D	1	3	12,12,12	0.97	0	17,17,17	1.18	3 (17%)
3	GLC	D	2	3	11,11,12	1.56	2 (18%)	15,15,17	1.43	2 (13%)
3	GLC	D	3	3	11,11,12	0.84	0	15,15,17	1.15	1 (6%)
3	GLC	D	4	3	11,11,12	0.67	0	15,15,17	1.45	3 (20%)
3	GLC	D	5	3	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
2	GLC	E	1	2	11,11,12	1.16	1 (9%)	15,15,17	1.84	5 (33%)
2	GLC	E	2	2	11,11,12	0.87	0	15,15,17	1.07	1 (6%)
2	GLC	E	3	2	11,11,12	0.98	0	15,15,17	1.28	2 (13%)
2	GLC	E	4	2	11,11,12	1.07	1 (9%)	15,15,17	2.08	1 (6%)
4	GLC	F	1	4	12,12,12	0.97	0	17,17,17	0.98	1 (5%)
4	GLC	F	2	4	11,11,12	1.57	2 (18%)	15,15,17	2.65	3 (20%)
4	GLC	F	3	4	11,11,12	0.88	1 (9%)	15,15,17	1.53	1 (6%)
3	GLC	G	1	3	12,12,12	0.96	0	17,17,17	1.00	1 (5%)
3	GLC	G	2	3	11,11,12	1.06	1 (9%)	15,15,17	1.06	1 (6%)
3	GLC	G	3	3	11,11,12	0.86	0	15,15,17	1.14	1 (6%)
3	GLC	G	4	3	11,11,12	0.85	0	15,15,17	1.30	1 (6%)
3	GLC	G	5	3	11,11,12	1.29	2 (18%)	15,15,17	1.59	4 (26%)
2	GLC	H	1	2	11,11,12	1.25	1 (9%)	15,15,17	1.01	1 (6%)
2	GLC	H	2	2	11,11,12	1.57	3 (27%)	15,15,17	1.77	3 (20%)
2	GLC	H	3	2	11,11,12	1.20	2 (18%)	15,15,17	1.88	1 (6%)
2	GLC	H	4	2	11,11,12	0.96	0	15,15,17	1.37	1 (6%)
2	GLC	I	1	2	12,12,12	1.08	0	17,17,17	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	I	2	2	11,11,12	0.90	0	15,15,17	1.75	4 (26%)
2	GLC	I	3	2	11,11,12	1.26	1 (9%)	15,15,17	2.43	2 (13%)
2	GLC	I	4	2	11,11,12	1.62	2 (18%)	15,15,17	1.67	2 (13%)
3	GLC	J	1	3	12,12,12	1.24	2 (16%)	17,17,17	1.04	1 (5%)
3	GLC	J	2	3	11,11,12	2.04	3 (27%)	15,15,17	2.69	1 (6%)
3	GLC	J	3	3	11,11,12	0.81	0	15,15,17	1.47	3 (20%)
3	GLC	J	4	3	11,11,12	0.91	1 (9%)	15,15,17	1.11	2 (13%)
3	GLC	J	5	3	11,11,12	0.95	1 (9%)	15,15,17	1.23	1 (6%)
2	GLC	K	1	2	11,11,12	1.31	3 (27%)	15,15,17	2.91	6 (40%)
2	GLC	K	2	2	11,11,12	0.82	1 (9%)	15,15,17	1.15	3 (20%)
2	GLC	K	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.62	3 (20%)
2	GLC	K	4	2	11,11,12	1.19	2 (18%)	15,15,17	1.76	1 (6%)
4	GLC	L	1	4	12,12,12	0.78	0	17,17,17	0.87	1 (5%)
4	GLC	L	2	4	11,11,12	0.89	0	15,15,17	1.90	2 (13%)
4	GLC	L	3	4	11,11,12	0.71	0	15,15,17	1.74	1 (6%)
3	GLC	M	1	3	12,12,12	0.72	0	17,17,17	0.88	1 (5%)
3	GLC	M	2	3	11,11,12	0.88	0	15,15,17	0.92	0
3	GLC	M	3	3	11,11,12	0.85	0	15,15,17	0.90	1 (6%)
3	GLC	M	4	3	11,11,12	0.85	0	15,15,17	1.62	1 (6%)
3	GLC	M	5	3	11,11,12	1.03	0	15,15,17	1.21	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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	2/2/19/22	0/1/1/1
3	GLC	D	4	3	-	1/2/19/22	0/1/1/1
3	GLC	D	5	3	-	2/2/19/22	0/1/1/1
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	1/2/19/22	0/1/1/1
4	GLC	F	1	4	-	1/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1
4	GLC	F	3	4	-	1/2/19/22	0/1/1/1
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	0/2/19/22	0/1/1/1
3	GLC	G	4	3	-	0/2/19/22	0/1/1/1
3	GLC	G	5	3	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	2/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	GLC	J	2	3	-	1/2/19/22	0/1/1/1
3	GLC	J	3	3	-	2/2/19/22	0/1/1/1
3	GLC	J	4	3	-	2/2/19/22	0/1/1/1
3	GLC	J	5	3	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	1/2/19/22	0/1/1/1
4	GLC	L	1	4	-	0/2/22/22	0/1/1/1
4	GLC	L	2	4	-	1/2/19/22	0/1/1/1
4	GLC	L	3	4	-	2/2/19/22	0/1/1/1
3	GLC	M	1	3	-	2/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	3	3	-	2/2/19/22	0/1/1/1
3	GLC	M	4	3	-	1/2/19/22	0/1/1/1
3	GLC	M	5	3	-	0/2/19/22	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	GLC	O5-C1	4.05	1.50	1.43
3	J	2	GLC	O5-C5	4.03	1.51	1.43
2	I	4	GLC	O5-C1	3.86	1.50	1.43
4	F	2	GLC	O5-C5	3.71	1.50	1.43
2	C	4	GLC	O5-C5	3.67	1.50	1.43
3	D	2	GLC	O5-C1	3.52	1.49	1.43
2	C	4	GLC	O5-C1	3.41	1.49	1.43
2	I	4	GLC	O5-C5	2.94	1.49	1.43
2	I	3	GLC	O5-C5	2.84	1.49	1.43
2	E	4	GLC	O5-C1	2.82	1.48	1.43
2	C	4	GLC	C2-C3	2.82	1.56	1.52
3	D	2	GLC	O5-C5	2.78	1.48	1.43
3	G	5	GLC	C4-C5	2.74	1.58	1.53
2	H	3	GLC	O5-C1	2.73	1.48	1.43
2	H	2	GLC	O5-C1	2.68	1.48	1.43
3	J	2	GLC	C4-C5	2.67	1.58	1.53
2	K	1	GLC	O4-C4	2.65	1.49	1.43
2	H	1	GLC	C4-C5	2.48	1.58	1.53
2	H	2	GLC	C1-C2	2.48	1.58	1.52
2	K	4	GLC	O5-C1	2.47	1.47	1.43
3	J	1	GLC	C4-C5	2.43	1.58	1.53
2	K	3	GLC	O5-C1	2.40	1.47	1.43
4	F	2	GLC	O5-C1	2.38	1.47	1.43
2	C	3	GLC	C1-C2	2.36	1.57	1.52
3	J	1	GLC	O4-C4	2.33	1.48	1.43
3	G	2	GLC	O5-C1	2.31	1.47	1.43
2	C	2	GLC	O4-C4	2.27	1.48	1.43
2	K	4	GLC	O5-C5	2.27	1.47	1.43
3	J	4	GLC	O5-C1	2.26	1.47	1.43
2	C	3	GLC	C2-C3	2.23	1.55	1.52
2	K	1	GLC	C4-C3	2.21	1.58	1.52
4	F	3	GLC	O5-C1	2.14	1.47	1.43
3	J	5	GLC	O5-C1	2.13	1.47	1.43
2	C	3	GLC	O4-C4	2.13	1.48	1.43
2	H	3	GLC	O5-C5	2.12	1.47	1.43
2	H	2	GLC	O4-C4	2.10	1.48	1.43
3	G	5	GLC	C4-C3	2.10	1.57	1.52
2	K	2	GLC	O4-C4	2.10	1.48	1.43
2	E	1	GLC	C4-C5	2.09	1.57	1.53
2	K	1	GLC	C2-C3	2.02	1.55	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	GLC	C1-O5-C5	9.71	125.20	112.19
4	F	2	GLC	C1-O5-C5	9.02	124.28	112.19
2	I	3	GLC	C1-O5-C5	8.64	123.77	112.19
2	E	4	GLC	C1-O5-C5	7.08	121.67	112.19
2	K	1	GLC	C1-O5-C5	6.72	121.20	112.19
2	H	3	GLC	C1-O5-C5	6.50	120.89	112.19
4	L	2	GLC	C1-O5-C5	6.20	120.50	112.19
2	K	4	GLC	C1-O5-C5	6.06	120.31	112.19
4	L	3	GLC	C1-O5-C5	5.75	119.90	112.19
3	M	4	GLC	C1-O5-C5	5.57	119.65	112.19
2	K	1	GLC	O5-C5-C6	5.46	118.29	107.66
2	H	2	GLC	C1-O5-C5	5.36	119.37	112.19
2	I	4	GLC	C1-O5-C5	5.34	119.34	112.19
4	F	3	GLC	C1-O5-C5	5.22	119.18	112.19
2	I	2	GLC	C1-O5-C5	4.41	118.10	112.19
2	K	1	GLC	C2-C3-C4	4.36	118.53	110.86
2	K	3	GLC	O5-C5-C6	4.33	116.08	107.66
2	H	4	GLC	O5-C5-C6	3.98	115.41	107.66
2	E	1	GLC	O5-C5-C6	3.90	115.26	107.66
3	D	4	GLC	C1-O5-C5	3.77	117.24	112.19
3	G	5	GLC	C3-C4-C5	3.67	116.88	110.23
3	D	2	GLC	C1-O5-C5	3.66	117.09	112.19
3	G	4	GLC	C1-O5-C5	3.60	117.01	112.19
3	J	3	GLC	O5-C5-C6	3.57	114.62	107.66
2	E	1	GLC	C1-O5-C5	3.54	116.94	112.19
2	C	1	GLC	O5-C5-C4	3.52	116.04	109.70
2	K	1	GLC	C1-C2-C3	3.47	114.69	109.64
2	C	2	GLC	C3-C4-C5	-3.44	104.00	110.23
2	E	3	GLC	C1-O5-C5	3.40	116.75	112.19
4	F	2	GLC	O5-C5-C6	3.25	114.00	107.66
2	C	4	GLC	C1-O5-C5	3.17	116.44	112.19
2	C	4	GLC	O5-C5-C6	3.16	113.81	107.66
2	C	3	GLC	C1-C2-C3	3.13	114.20	109.64
3	D	2	GLC	O5-C5-C6	3.04	113.58	107.66
2	C	3	GLC	C3-C4-C5	-2.86	105.04	110.23
3	J	3	GLC	C1-O5-C5	2.86	116.02	112.19
3	G	5	GLC	C1-O5-C5	2.86	116.01	112.19
2	H	2	GLC	C1-C2-C3	2.78	113.69	109.64
3	J	4	GLC	C1-O5-C5	2.77	115.90	112.19
3	G	3	GLC	C3-C4-C5	2.72	115.17	110.23
2	K	3	GLC	C3-C4-C5	-2.69	105.36	110.23
2	K	2	GLC	C3-C4-C5	-2.59	105.54	110.23
2	I	2	GLC	O5-C5-C6	-2.58	102.65	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	GLC	C3-C4-C5	-2.56	105.59	110.23
3	D	4	GLC	C2-C3-C4	-2.51	106.45	110.86
2	I	2	GLC	C2-C3-C4	-2.49	106.47	110.86
2	K	1	GLC	C3-C4-C5	2.49	114.75	110.23
3	M	1	GLC	O5-C5-C6	2.46	112.53	106.44
3	D	1	GLC	C1-O5-C5	2.44	118.36	113.65
4	F	2	GLC	C6-C5-C4	-2.41	107.11	113.02
2	E	3	GLC	O5-C5-C6	2.39	112.31	107.66
4	L	1	GLC	O6-C6-C5	-2.38	103.23	111.33
3	M	5	GLC	C1-C2-C3	2.34	113.06	109.64
3	G	1	GLC	C6-C5-C4	-2.34	107.27	113.02
2	E	1	GLC	C2-C3-C4	2.33	114.96	110.86
2	I	2	GLC	C3-C4-C5	-2.33	106.01	110.23
2	I	1	GLC	O5-C5-C4	2.31	113.87	109.70
3	D	3	GLC	C3-C4-C5	2.30	114.41	110.23
3	D	1	GLC	O5-C5-C4	2.30	113.85	109.70
2	I	1	GLC	C3-C4-C5	2.29	114.39	110.23
2	E	1	GLC	C6-C5-C4	-2.28	107.43	113.02
2	E	1	GLC	C3-C4-C5	2.27	114.35	110.23
2	K	1	GLC	O3-C3-C2	-2.27	105.42	110.05
3	J	3	GLC	C6-C5-C4	-2.25	107.49	113.02
3	D	1	GLC	C6-C5-C4	-2.23	107.54	113.02
2	K	2	GLC	C1-C2-C3	2.23	112.89	109.64
3	M	3	GLC	O4-C4-C3	-2.22	105.14	110.38
2	H	1	GLC	O4-C4-C3	-2.17	105.25	110.38
2	H	2	GLC	O4-C4-C5	2.17	114.67	109.32
3	G	2	GLC	O4-C4-C3	-2.13	105.35	110.38
3	J	1	GLC	C3-C4-C5	-2.12	106.38	110.23
4	F	1	GLC	C3-C4-C5	-2.11	106.40	110.23
3	G	5	GLC	O5-C5-C4	2.10	115.94	110.83
3	D	5	GLC	C2-C3-C4	-2.09	107.18	110.86
3	G	5	GLC	O6-C6-C5	-2.08	104.25	111.33
2	I	3	GLC	C2-C3-C4	-2.08	107.20	110.86
3	M	5	GLC	C3-C4-C5	2.08	114.00	110.23
3	J	5	GLC	C3-C4-C5	-2.07	106.47	110.23
3	J	4	GLC	O5-C5-C6	2.07	111.69	107.66
2	K	3	GLC	C2-C3-C4	-2.05	107.25	110.86
4	L	2	GLC	C6-C5-C4	-2.04	108.00	113.02
2	I	4	GLC	O6-C6-C5	-2.03	104.41	111.33
2	K	2	GLC	C1-O5-C5	2.02	114.89	112.19
2	E	2	GLC	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	GLC	C4-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6
3	J	3	GLC	O5-C5-C6-O6
3	D	3	GLC	O5-C5-C6-O6
2	I	3	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
3	J	5	GLC	C4-C5-C6-O6
3	D	5	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
4	L	3	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	I	3	GLC	C4-C5-C6-O6
3	D	3	GLC	C4-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
3	J	3	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
3	D	5	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
3	J	5	GLC	O5-C5-C6-O6
4	L	3	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
3	M	1	GLC	O5-C5-C6-O6
3	M	3	GLC	C4-C5-C6-O6
3	M	3	GLC	O5-C5-C6-O6
3	J	4	GLC	O5-C5-C6-O6
4	F	1	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
4	F	3	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	K	4	GLC	O5-C5-C6-O6
2	I	4	GLC	O5-C5-C6-O6

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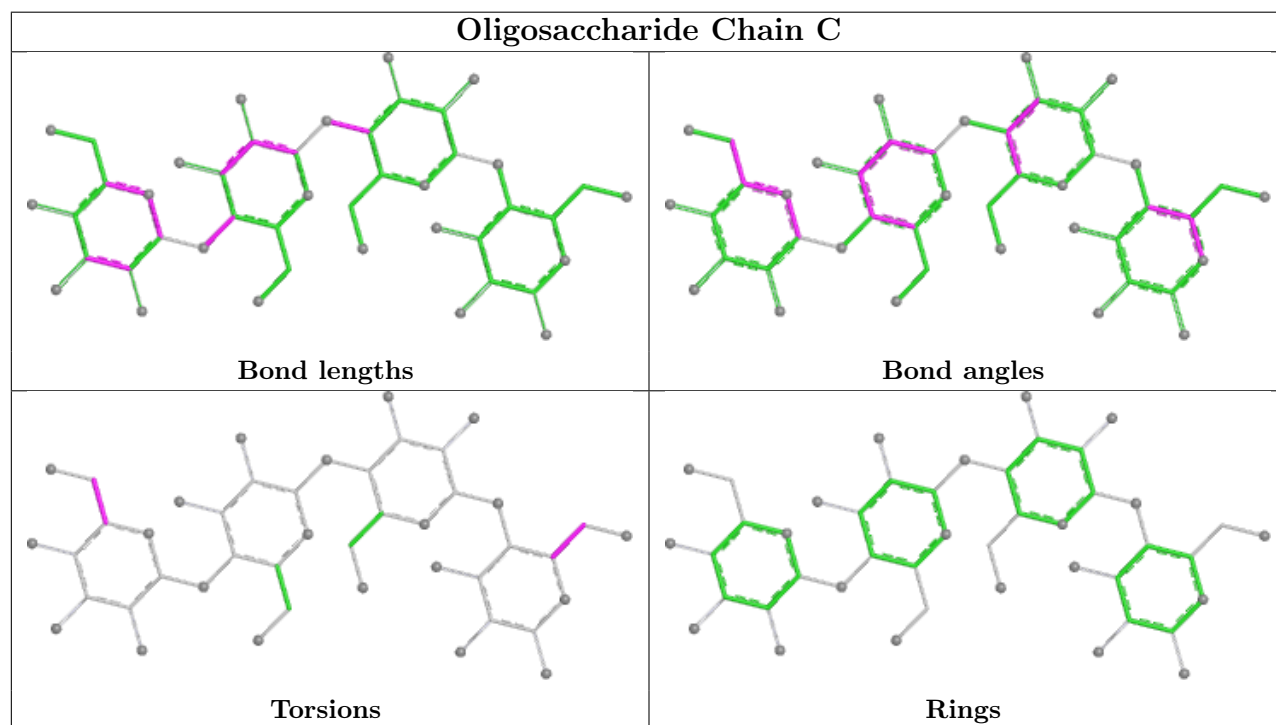
Mol	Chain	Res	Type	Atoms
2	E	4	GLC	O5-C5-C6-O6
3	M	1	GLC	C4-C5-C6-O6
3	D	4	GLC	O5-C5-C6-O6
3	J	4	GLC	C4-C5-C6-O6
3	J	2	GLC	C4-C5-C6-O6
4	L	2	GLC	C4-C5-C6-O6
3	M	4	GLC	O5-C5-C6-O6

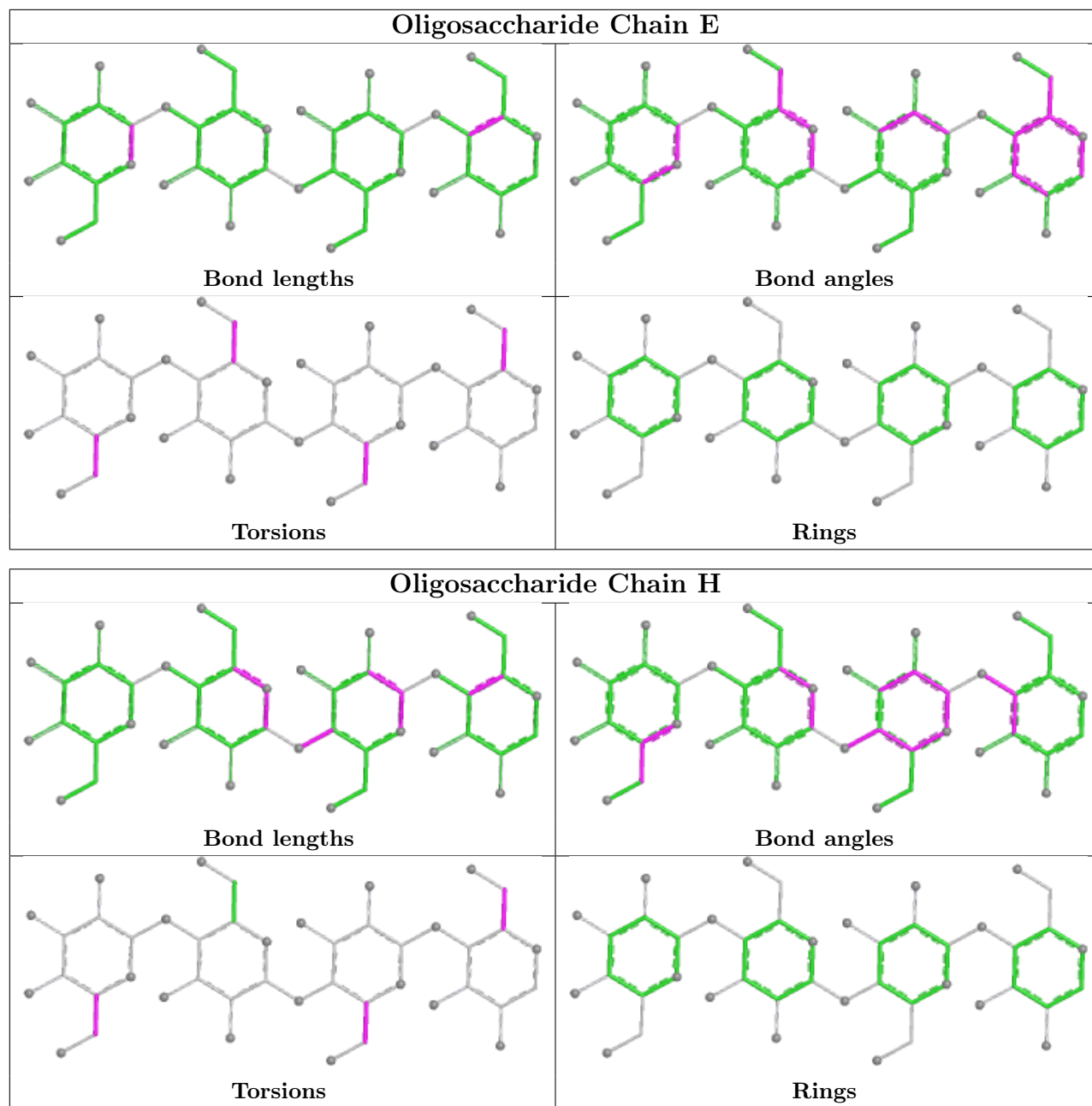
There are no ring outliers.

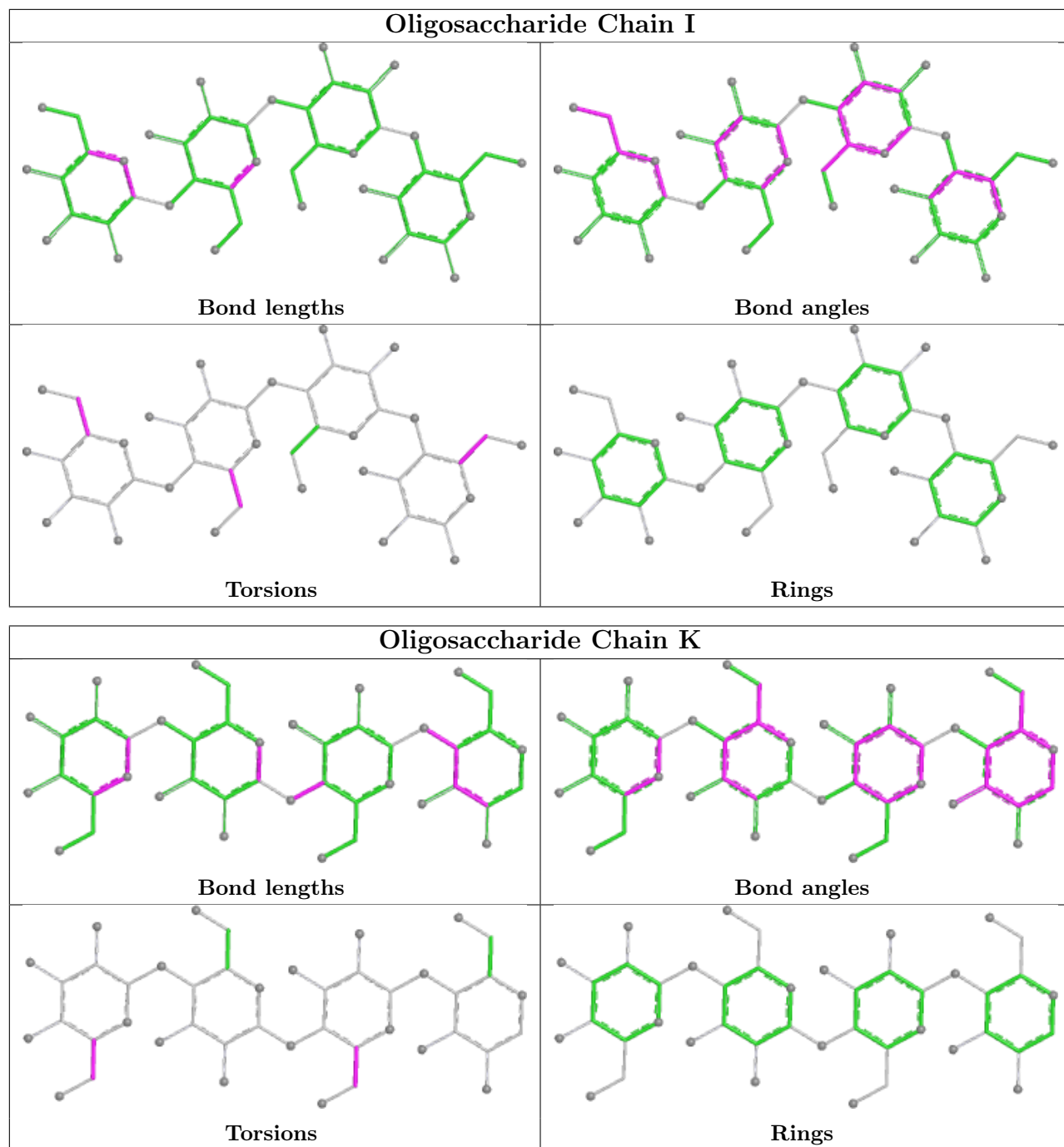
2 monomers are involved in 2 short contacts:

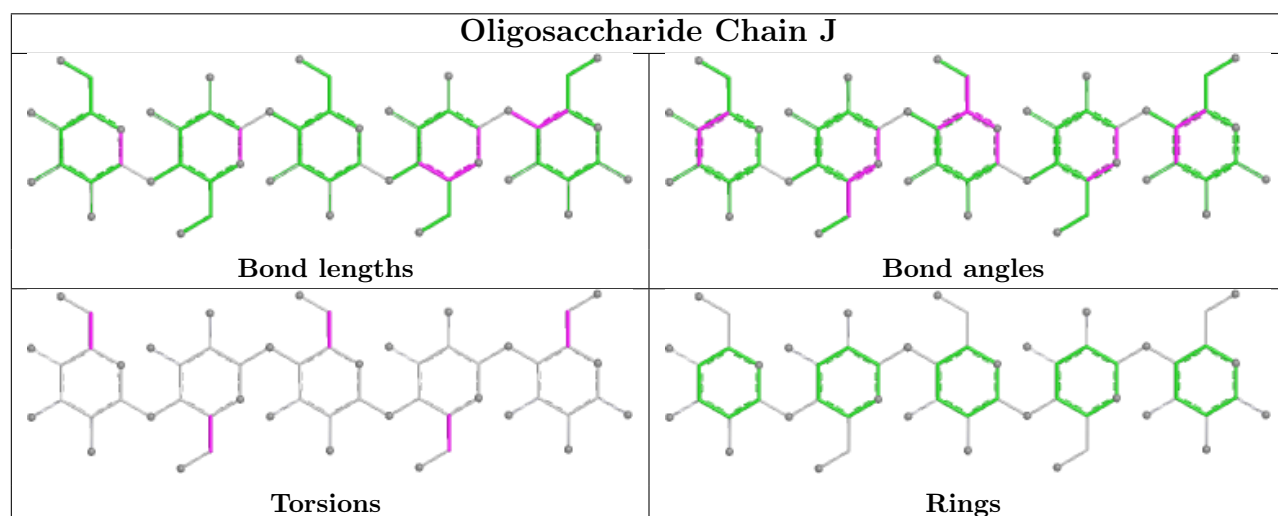
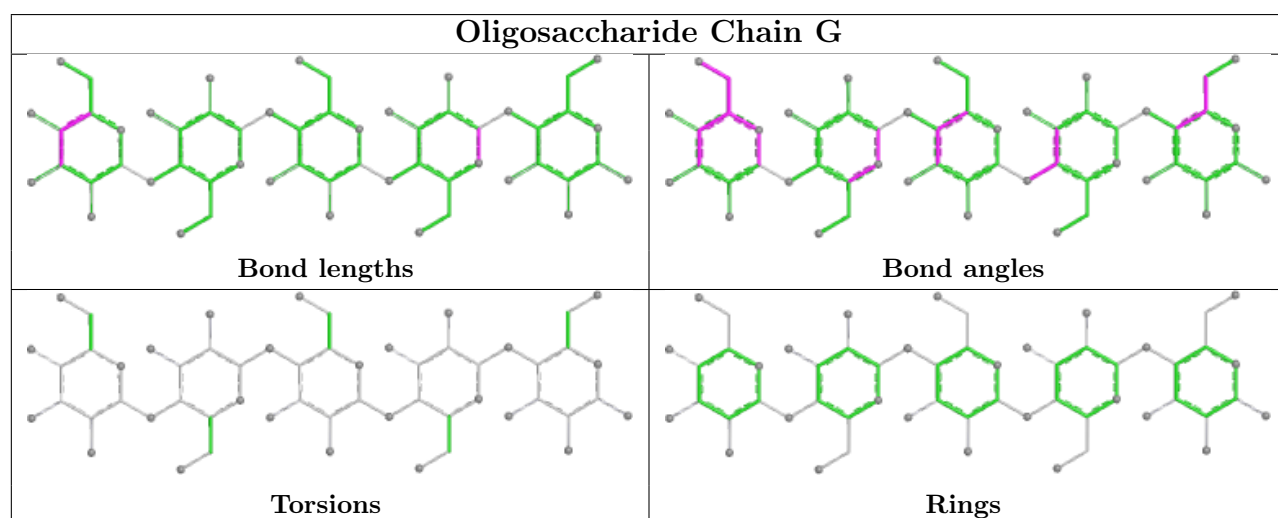
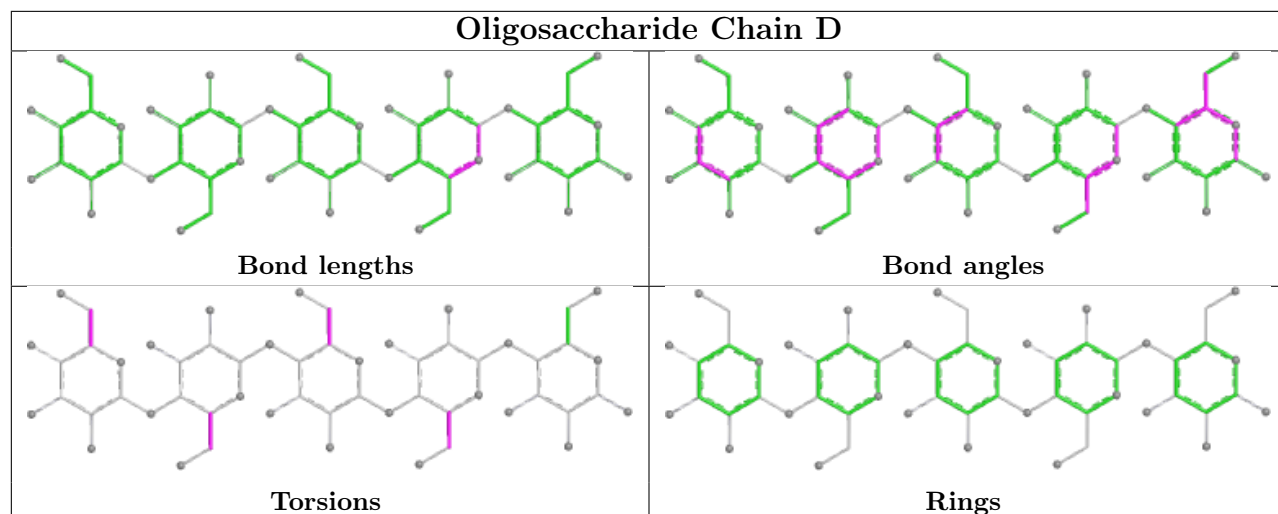
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	GLC	1	0
3	M	4	GLC	1	0

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

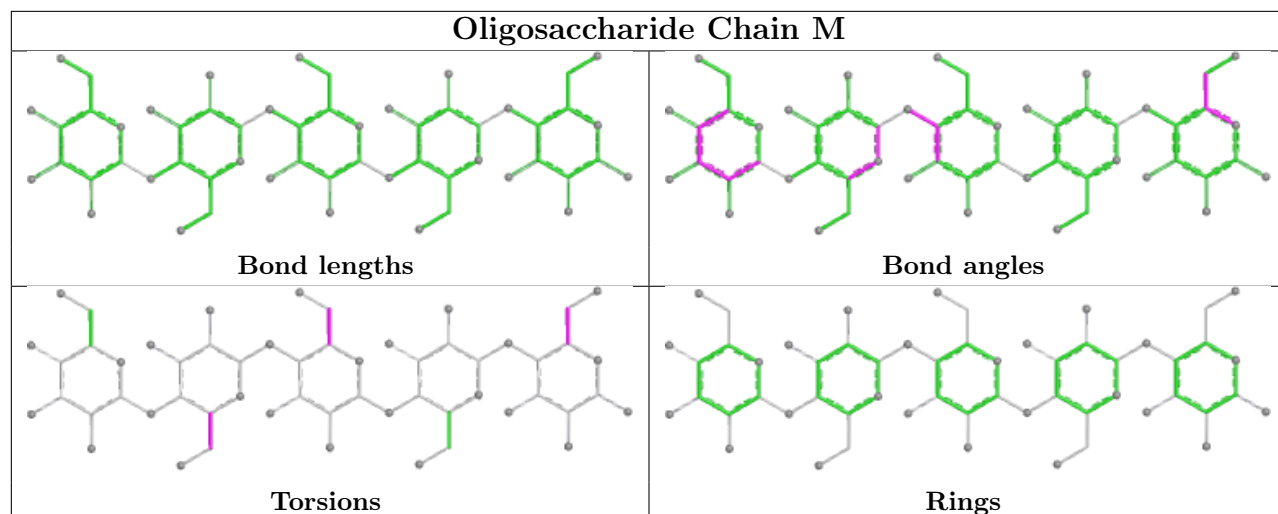




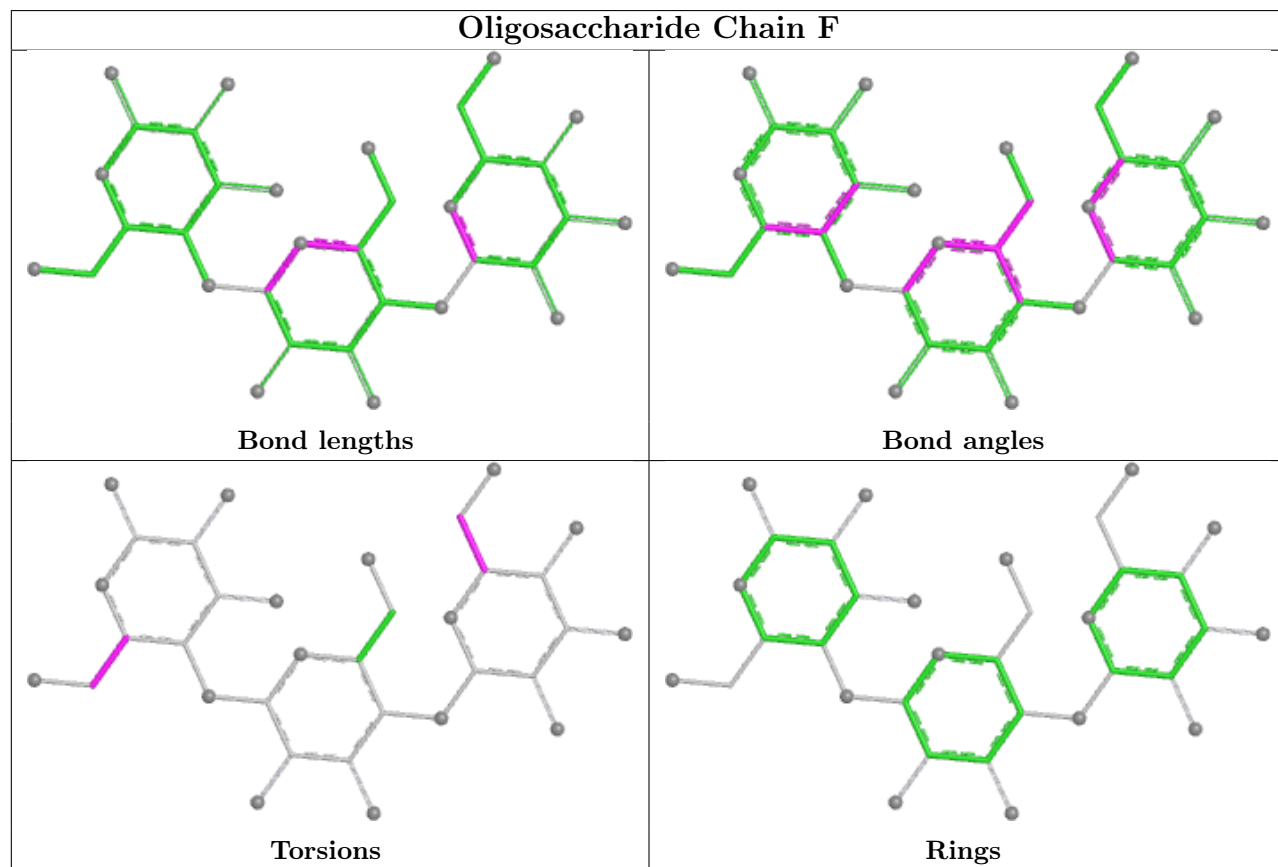


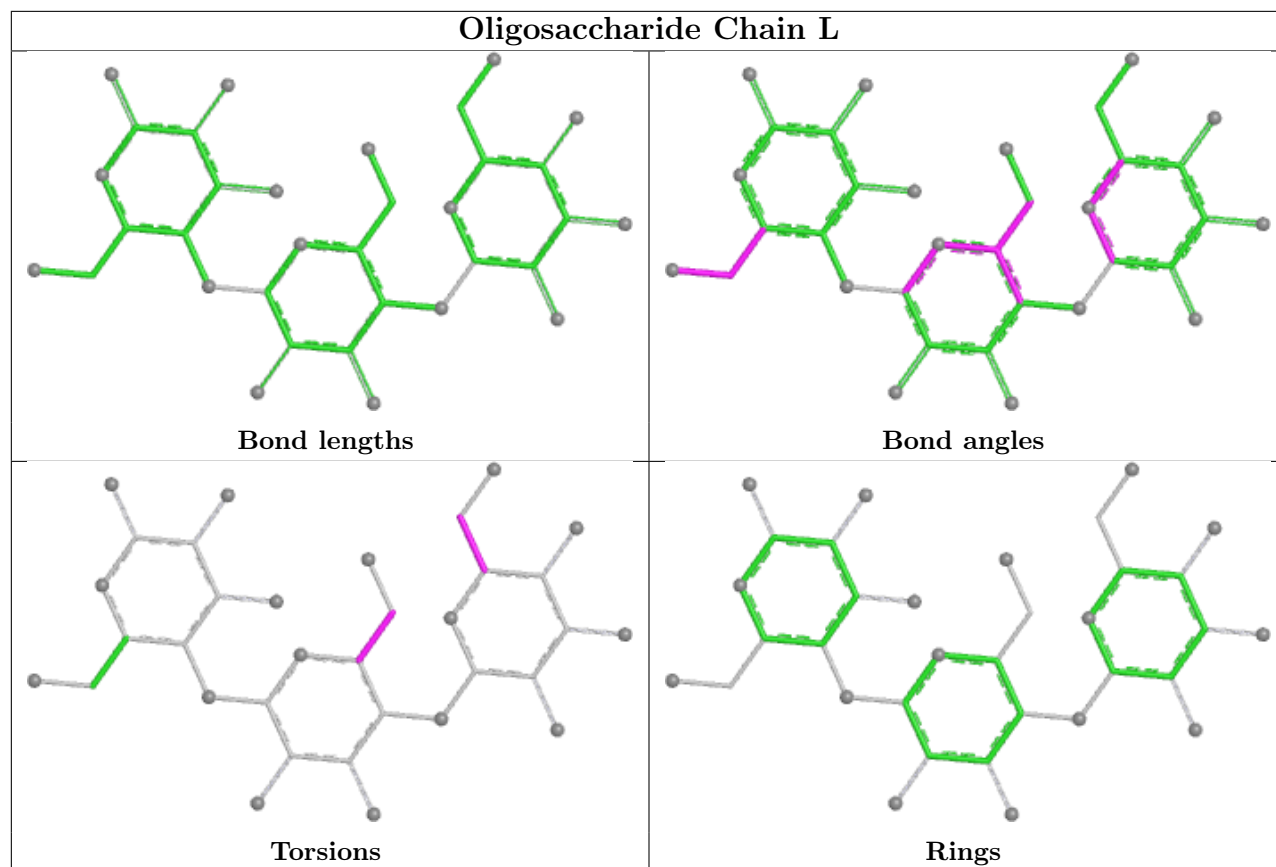


Oligosaccharide Chain M



Oligosaccharide Chain F





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1526/1528 (99%)	-0.45	2 (0%) 92 90	50, 86, 144, 176	0
1	B	1526/1528 (99%)	-0.45	2 (0%) 92 90	50, 83, 146, 190	0
All	All	3052/3056 (99%)	-0.45	4 (0%) 92 90	50, 85, 145, 190	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	493	VAL	2.4
1	A	493	VAL	2.3
1	A	694	SER	2.2
1	B	488	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	M	2	11/12	0.49	0.11	150,177,181,188	0
3	GLC	M	5	11/12	0.50	0.12	186,201,208,211	0
2	GLC	H	1	11/12	0.54	0.10	113,137,147,147	0
3	GLC	D	5	11/12	0.54	0.10	144,152,172,173	0
2	GLC	H	4	11/12	0.57	0.07	154,180,189,196	0

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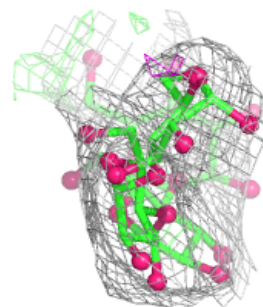
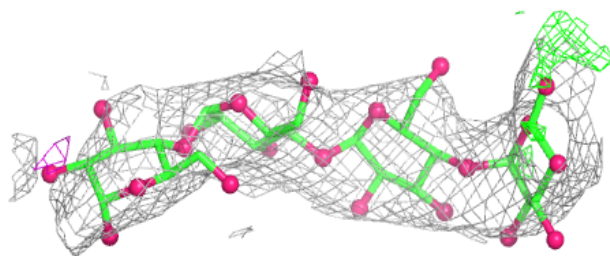
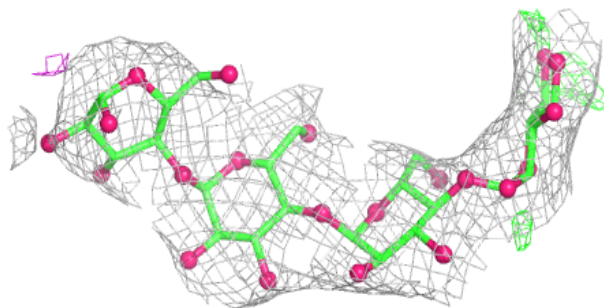
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLC	F	1	12/12	0.63	0.09	157,161,164,164	0
4	GLC	L	3	11/12	0.65	0.08	130,145,159,162	0
4	GLC	F	3	11/12	0.70	0.07	152,169,173,179	0
3	GLC	J	5	11/12	0.71	0.09	121,129,135,137	0
2	GLC	H	3	11/12	0.71	0.09	147,167,186,188	0
2	GLC	H	2	11/12	0.72	0.11	135,152,165,172	0
3	GLC	G	1	12/12	0.73	0.13	131,183,190,194	0
2	GLC	K	1	11/12	0.76	0.09	104,121,127,130	0
4	GLC	F	2	11/12	0.77	0.08	129,167,181,185	0
3	GLC	J	1	12/12	0.78	0.13	129,138,144,145	0
2	GLC	C	4	11/12	0.78	0.13	98,128,136,141	0
3	GLC	M	1	12/12	0.78	0.10	137,168,174,178	0
3	GLC	M	3	11/12	0.79	0.10	146,173,184,185	0
3	GLC	G	5	11/12	0.79	0.08	174,185,191,192	0
3	GLC	J	2	11/12	0.80	0.13	123,129,144,145	0
2	GLC	I	4	11/12	0.81	0.10	110,127,136,153	0
2	GLC	E	1	11/12	0.81	0.09	120,125,132,135	0
4	GLC	L	2	11/12	0.82	0.08	124,134,166,190	0
3	GLC	D	2	11/12	0.82	0.10	126,132,138,142	0
3	GLC	J	3	11/12	0.84	0.09	105,117,120,125	0
3	GLC	J	4	11/12	0.84	0.09	108,120,128,128	0
2	GLC	K	4	11/12	0.84	0.10	108,120,135,136	0
2	GLC	I	1	12/12	0.85	0.12	138,144,158,162	0
3	GLC	D	1	12/12	0.85	0.12	117,135,142,144	0
2	GLC	C	1	12/12	0.86	0.12	124,143,157,171	0
3	GLC	G	2	11/12	0.87	0.08	138,157,166,171	0
3	GLC	M	4	11/12	0.87	0.09	159,174,189,199	0
4	GLC	L	1	12/12	0.87	0.06	114,131,133,141	0
2	GLC	E	2	11/12	0.87	0.09	92,108,117,118	0
2	GLC	E	4	11/12	0.87	0.08	105,119,126,132	0
3	GLC	G	3	11/12	0.88	0.08	151,166,173,187	0
3	GLC	G	4	11/12	0.91	0.10	147,197,208,208	0
2	GLC	I	3	11/12	0.91	0.10	105,118,134,142	0
3	GLC	D	3	11/12	0.91	0.08	112,129,140,143	0
2	GLC	I	2	11/12	0.92	0.07	102,109,115,120	0
2	GLC	C	3	11/12	0.92	0.08	107,113,133,135	0
3	GLC	D	4	11/12	0.93	0.07	123,133,142,148	0
2	GLC	K	3	11/12	0.94	0.08	91,93,100,105	0
2	GLC	E	3	11/12	0.95	0.07	71,78,90,91	0
2	GLC	K	2	11/12	0.95	0.07	112,113,119,119	0
2	GLC	C	2	11/12	0.96	0.09	102,114,121,128	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

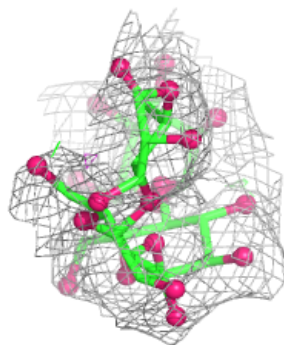
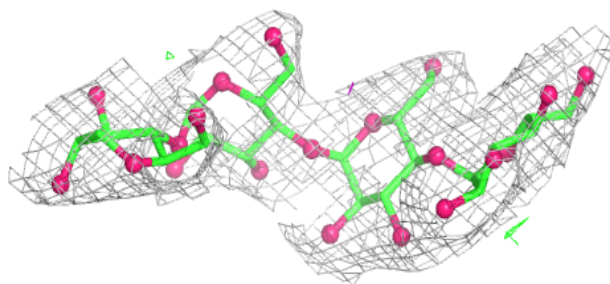
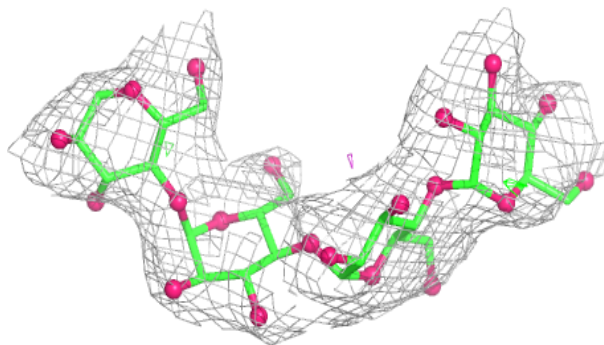
Electron density around Chain C:

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



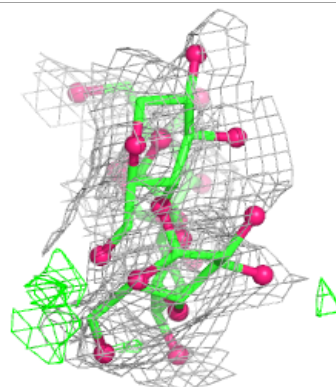
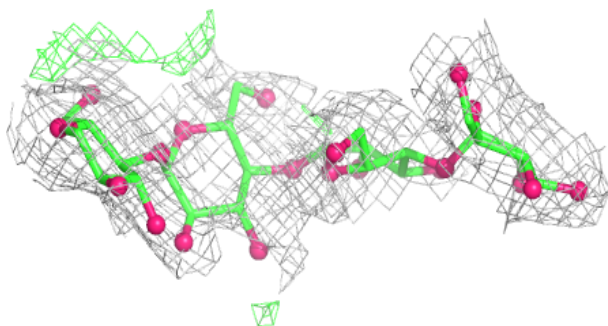
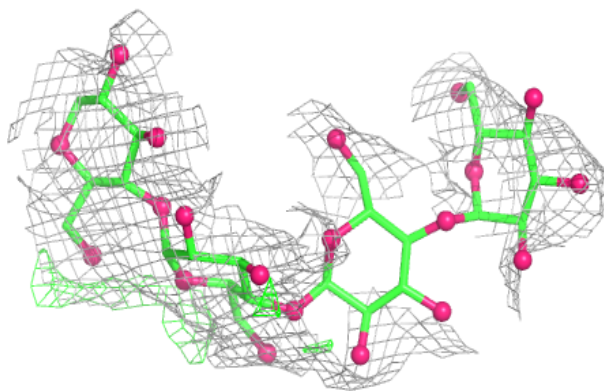
Electron density around Chain E:

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

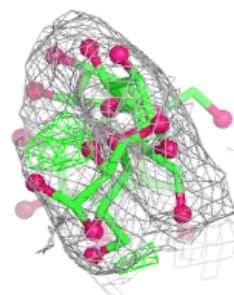
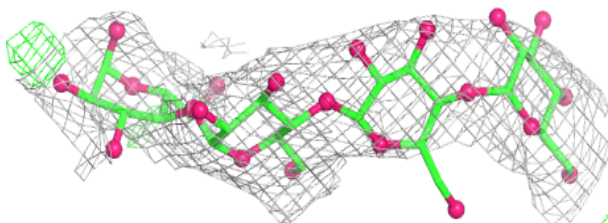
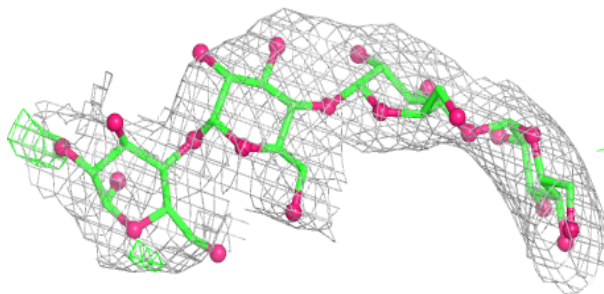


Electron density around Chain H:

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

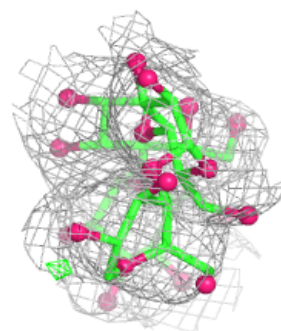
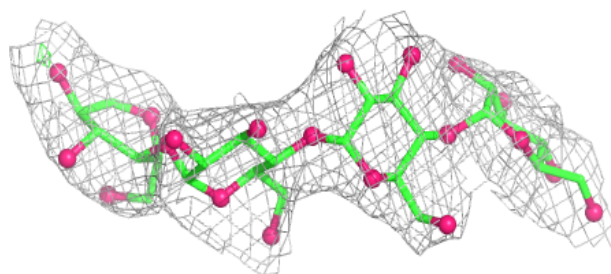
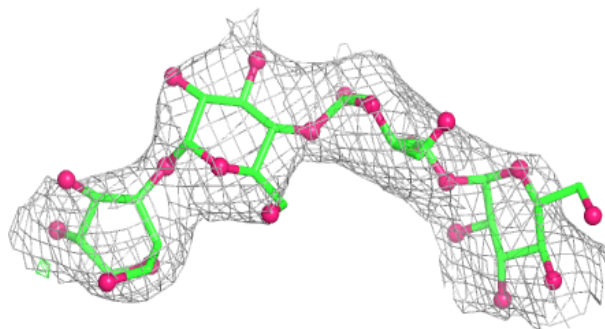
**Electron density around Chain I:**

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

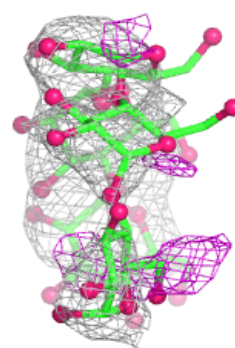
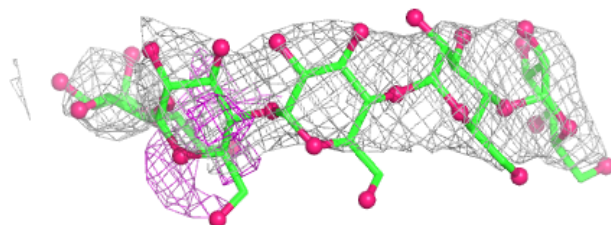
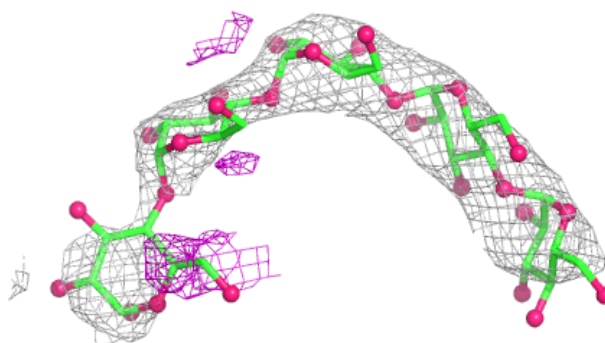


Electron density around Chain K:

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

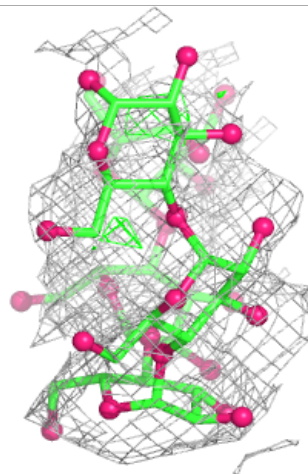
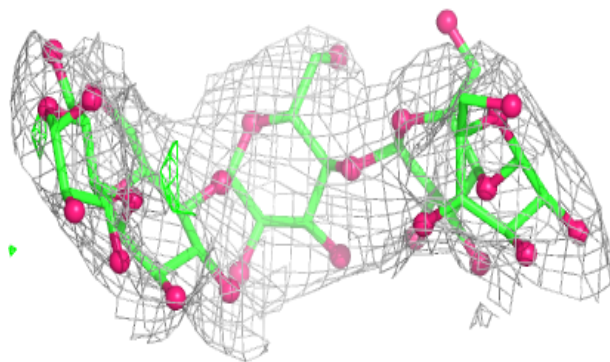
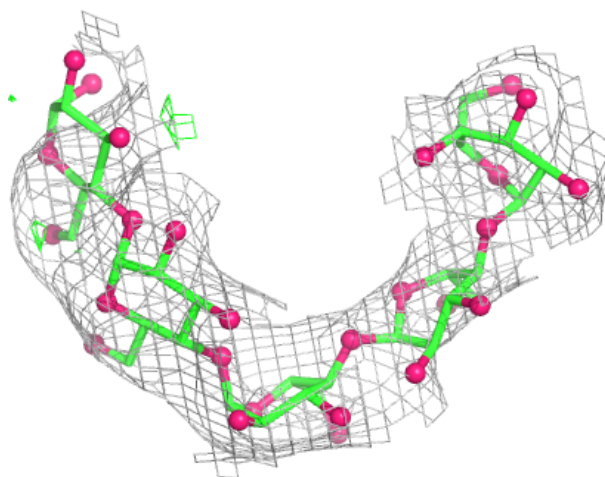
**Electron density around Chain D:**

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



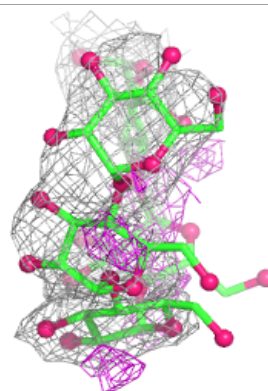
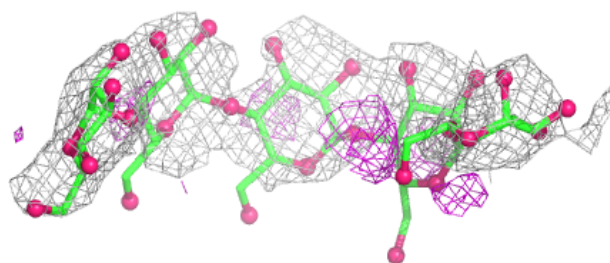
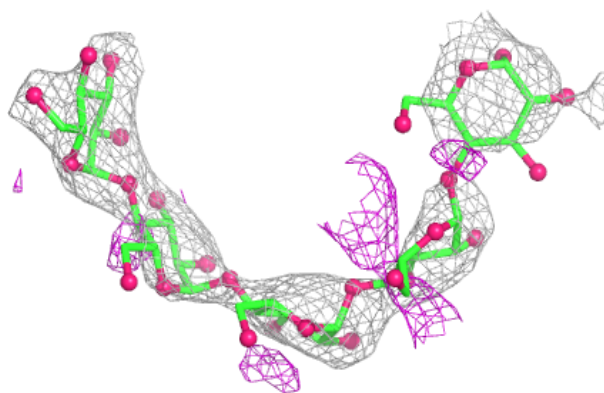
Electron density around Chain G:

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

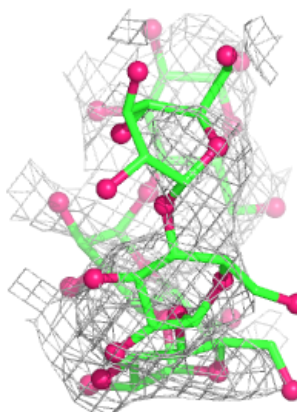
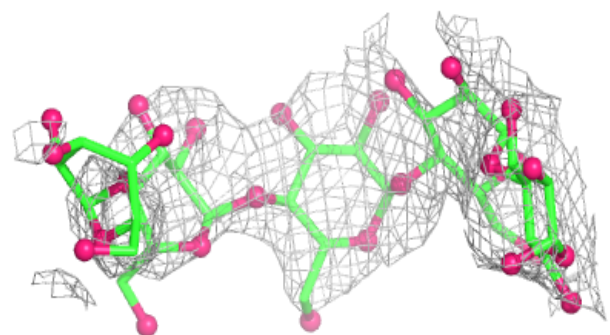
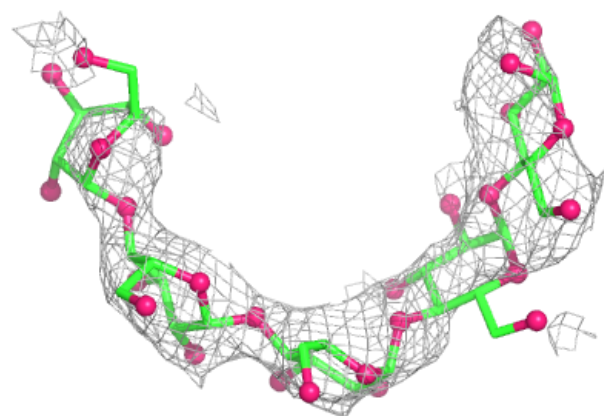


Electron density around Chain J:

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

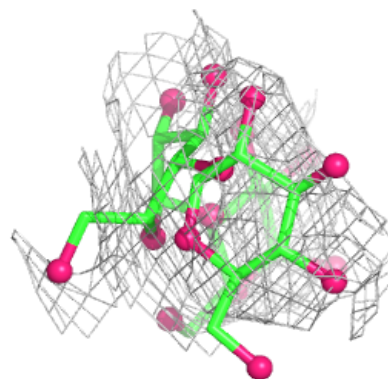
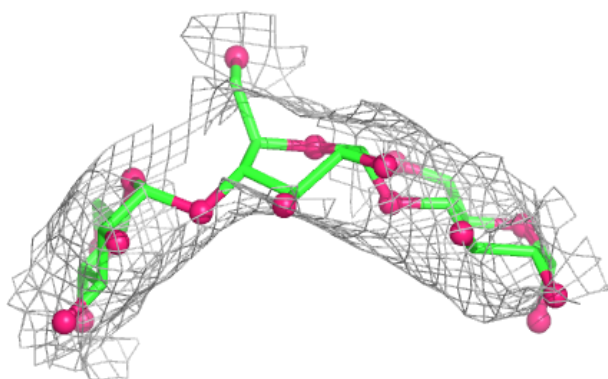
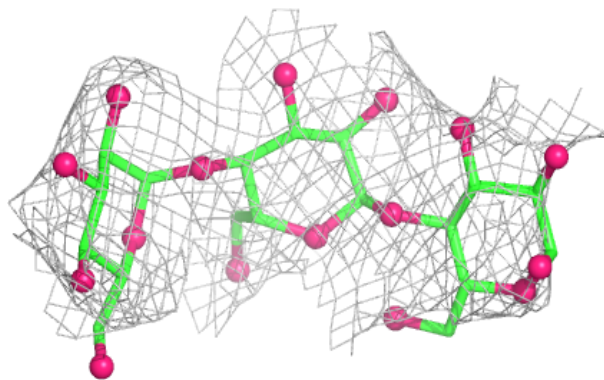
**Electron density around Chain M:**

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

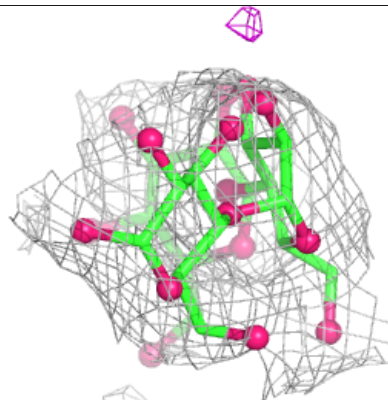
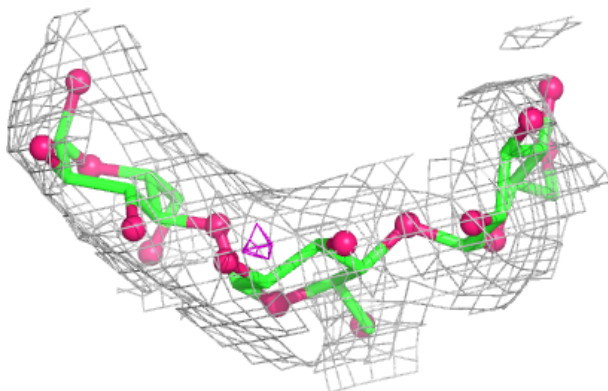
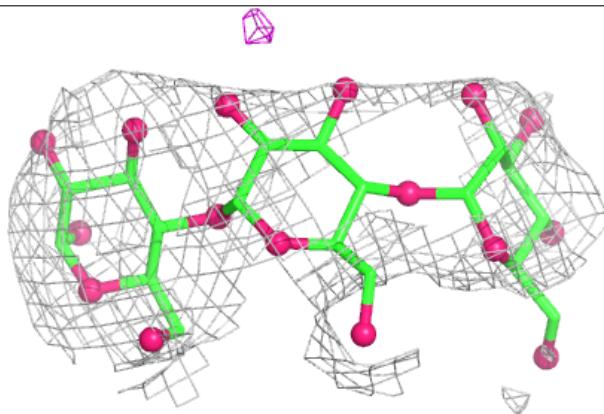


Electron density around Chain F:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.