



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 AM UTC

PDB ID : 1MPM / pdb_00001mpm
Title : MALTOPORIN MALTOSE COMPLEX
Authors : Dutzler, R.; Schirmer, T.
Deposited on : 1996-01-11
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

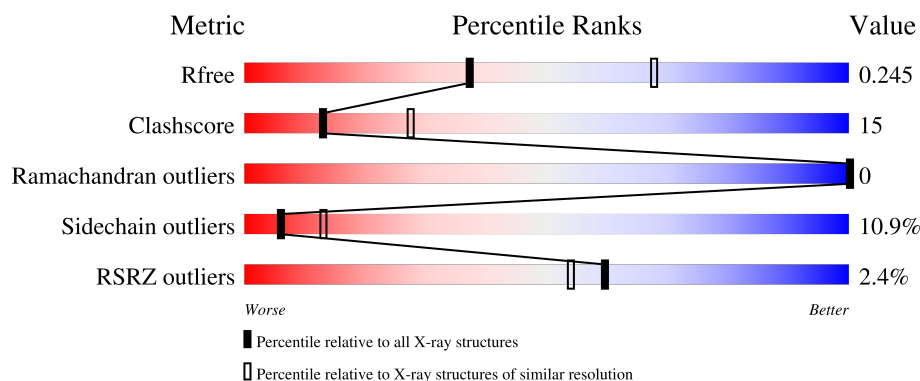
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	421	
1	B	421	
1	C	421	
2	D	2	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	100%
2	I	2	50% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10662 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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	124	0	0
			3350	2110	571	655	14			
1	B	421	Total	C	N	O	S	124	0	0
			3350	2110	571	655	14			
1	C	421	Total	C	N	O	S	124	0	0
			3350	2110	571	655	14			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
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			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

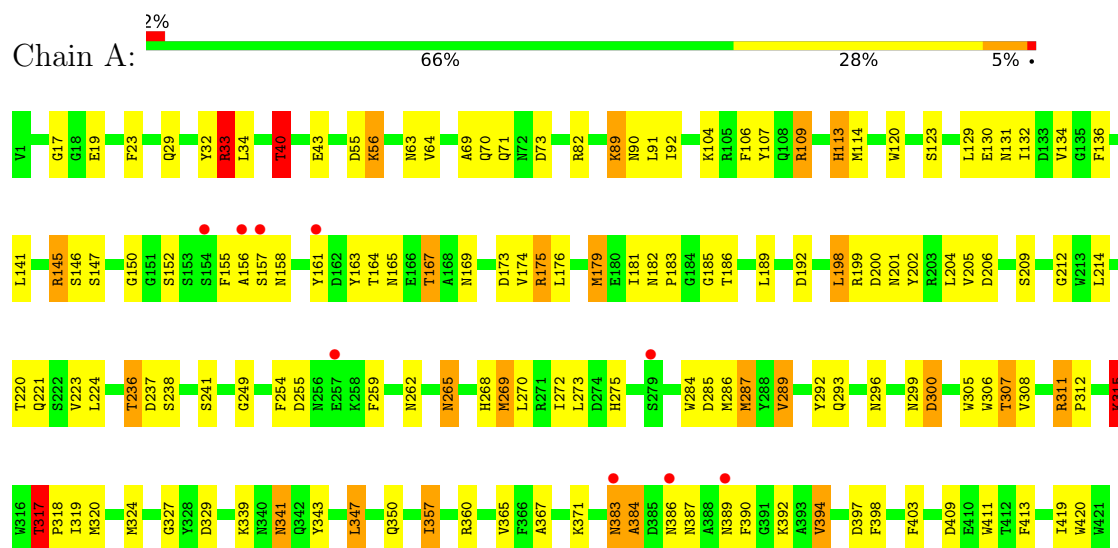
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total 161	O 161	0	0
4	B	155	Total 155	O 155	0	0
4	C	155	Total 155	O 155	0	0

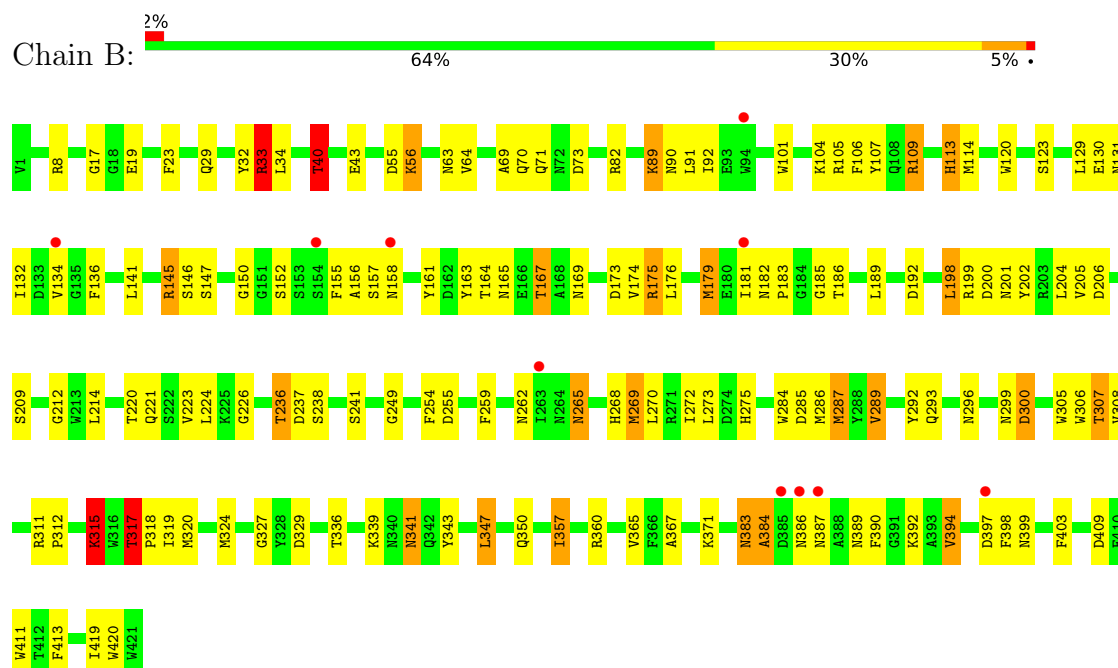
3 Residue-property plots

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

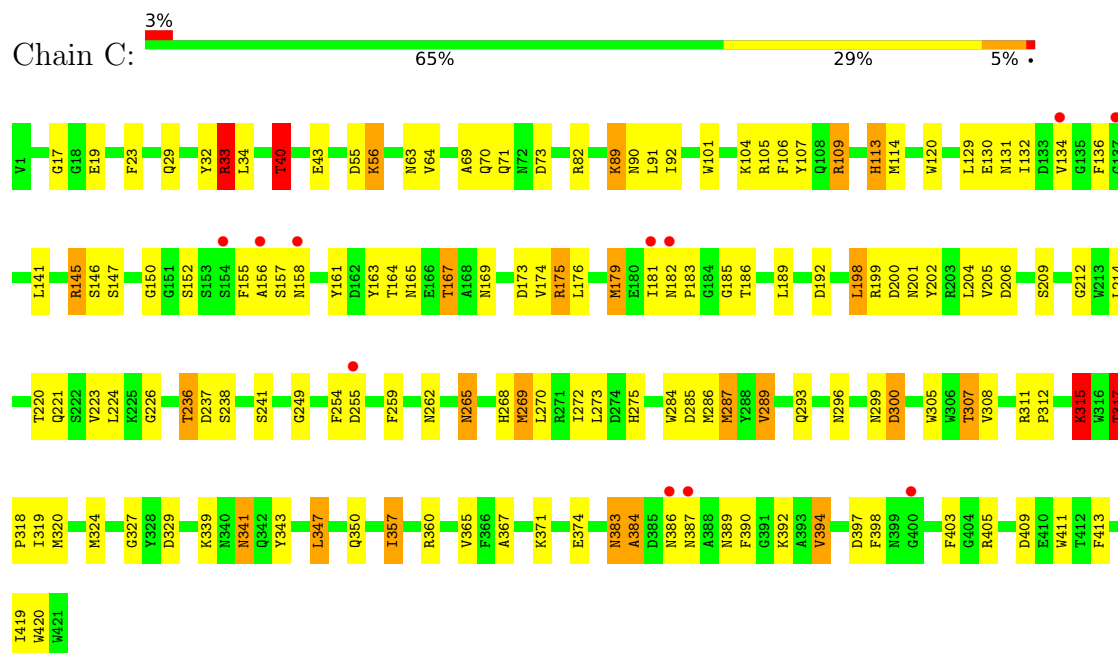
• Molecule 1: MALTOPORIN



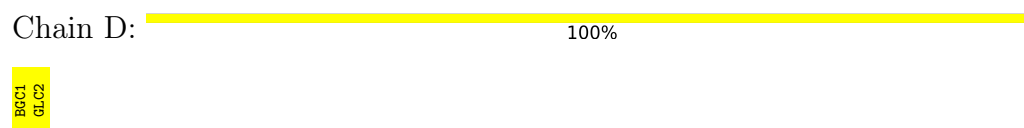
• Molecule 1: MALTOPORIN



- Molecule 1: MALTOPORIN



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



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



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



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



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



BGC1
GLC2

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

Chain I:

50%

50%

BGC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.80Å 211.70Å 218.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.5 (8.00-2.60) 85.6 (8.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.226 , 0.243 0.227 , 0.245	Depositor DCC
R_{free} test set	4108 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 98.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10662	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, BGC, MG

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	1.04	5/3443 (0.1%)	1.28	30/4668 (0.6%)
1	B	1.04	5/3443 (0.1%)	1.28	30/4668 (0.6%)
1	C	1.04	5/3443 (0.1%)	1.28	29/4668 (0.6%)
All	All	1.04	15/10329 (0.1%)	1.28	89/14004 (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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	VAL	CA-CB	-6.66	1.45	1.54
1	C	365	VAL	CA-CB	-6.65	1.45	1.54
1	B	365	VAL	CA-CB	-6.65	1.45	1.54
1	B	179	MET	SD-CE	-6.28	1.63	1.79
1	A	179	MET	SD-CE	-6.26	1.63	1.79
1	C	179	MET	SD-CE	-6.25	1.64	1.79
1	C	367	ALA	CA-CB	-5.51	1.44	1.53
1	A	367	ALA	CA-CB	-5.49	1.44	1.53
1	B	367	ALA	CA-CB	-5.48	1.44	1.53
1	B	409	ASP	CB-CG	-5.26	1.38	1.52
1	A	409	ASP	CB-CG	-5.26	1.39	1.52
1	C	409	ASP	CB-CG	-5.24	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ILE	CA-CB	5.11	1.59	1.53
1	C	92	ILE	CA-CB	5.11	1.59	1.53
1	B	92	ILE	CA-CB	5.06	1.59	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ARG	N-CA-C	12.10	124.47	111.28
1	B	33	ARG	N-CA-C	12.07	124.44	111.28
1	A	33	ARG	N-CA-C	12.07	124.43	111.28
1	C	158	ASN	N-CA-C	-8.10	103.19	113.72
1	A	158	ASN	N-CA-C	-8.08	103.22	113.72
1	B	158	ASN	N-CA-C	-8.08	103.22	113.72
1	C	384	ALA	N-CA-C	-7.60	103.27	112.54
1	B	384	ALA	N-CA-C	-7.59	103.28	112.54
1	A	384	ALA	N-CA-C	-7.59	103.28	112.54
1	A	289	VAL	CB-CA-C	-7.45	97.37	110.71
1	C	289	VAL	CB-CA-C	-7.45	97.37	110.71
1	B	289	VAL	CB-CA-C	-7.45	97.38	110.71
1	B	113	HIS	N-CA-C	6.79	118.33	111.07
1	A	113	HIS	N-CA-C	6.77	118.32	111.07
1	C	113	HIS	N-CA-C	6.77	118.31	111.07
1	B	317	THR	CA-C-N	-6.76	112.83	119.87
1	B	317	THR	C-N-CA	-6.76	112.83	119.87
1	A	317	THR	CA-C-N	-6.73	112.88	119.87
1	A	317	THR	C-N-CA	-6.73	112.88	119.87
1	C	317	THR	CA-C-N	-6.71	112.90	119.87
1	C	317	THR	C-N-CA	-6.71	112.90	119.87
1	B	181	ILE	N-CA-C	-6.68	102.70	111.05
1	A	181	ILE	N-CA-C	-6.68	102.70	111.05
1	C	181	ILE	N-CA-C	-6.68	102.70	111.05
1	C	82	ARG	N-CA-C	6.59	121.40	113.23
1	A	82	ARG	N-CA-C	6.58	121.39	113.23
1	B	82	ARG	N-CA-C	6.58	121.39	113.23
1	B	365	VAL	N-CA-C	-6.36	98.36	107.77
1	C	365	VAL	N-CA-C	-6.35	98.37	107.77
1	A	365	VAL	N-CA-C	-6.34	98.38	107.77
1	A	134	VAL	N-CA-C	-6.33	106.34	112.29
1	B	134	VAL	N-CA-C	-6.32	106.34	112.29
1	C	134	VAL	N-CA-C	-6.32	106.34	112.29
1	B	350	GLN	N-CA-C	6.28	118.95	109.41
1	B	317	THR	N-CA-CB	-6.27	103.39	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	THR	N-CA-CB	-6.26	103.40	111.35
1	A	317	THR	N-CA-CB	-6.26	103.41	111.35
1	A	350	GLN	N-CA-C	6.25	118.92	109.41
1	C	23	PHE	N-CA-C	6.25	118.95	108.02
1	C	350	GLN	N-CA-C	6.25	118.90	109.41
1	A	23	PHE	N-CA-C	6.23	118.93	108.02
1	B	23	PHE	N-CA-C	6.21	118.89	108.02
1	B	198	LEU	N-CA-C	6.12	119.33	110.28
1	A	198	LEU	N-CA-C	6.09	119.29	110.28
1	C	198	LEU	N-CA-C	6.09	119.29	110.28
1	C	107	TYR	N-CA-C	5.97	118.02	108.41
1	A	107	TYR	N-CA-C	5.96	118.00	108.41
1	B	107	TYR	N-CA-C	5.96	118.00	108.41
1	A	131	ASN	N-CA-C	5.84	119.30	111.24
1	B	131	ASN	N-CA-C	5.84	119.30	111.24
1	C	131	ASN	N-CA-C	5.84	119.30	111.24
1	B	238	SER	N-CA-C	5.74	119.76	112.87
1	A	238	SER	N-CA-C	5.73	119.75	112.87
1	C	284	TRP	N-CA-C	5.73	118.45	108.76
1	A	284	TRP	N-CA-C	5.72	118.43	108.76
1	C	238	SER	N-CA-C	5.72	119.74	112.87
1	C	315	LYS	N-CA-C	5.68	117.56	108.41
1	B	315	LYS	N-CA-C	5.67	117.54	108.41
1	A	315	LYS	N-CA-C	5.67	117.54	108.41
1	B	284	TRP	N-CA-C	5.50	118.43	108.69
1	A	409	ASP	CB-CA-C	-5.48	98.66	111.09
1	B	409	ASP	CB-CA-C	-5.47	98.67	111.09
1	C	409	ASP	CB-CA-C	-5.46	98.70	111.09
1	C	56	LYS	N-CA-C	5.45	118.51	109.46
1	B	56	LYS	N-CA-C	5.45	118.50	109.46
1	A	56	LYS	N-CA-C	5.44	118.49	109.46
1	C	262	ASN	N-CA-C	5.42	117.08	108.67
1	B	262	ASN	N-CA-C	5.40	117.03	108.67
1	A	262	ASN	N-CA-C	5.39	117.03	108.67
1	B	40	THR	N-CA-C	-5.37	99.97	108.73
1	A	40	THR	N-CA-C	-5.36	99.99	108.73
1	C	40	THR	N-CA-C	-5.36	100.00	108.73
1	C	357	ILE	N-CA-C	-5.28	106.14	113.00
1	A	357	ILE	N-CA-C	-5.27	106.15	113.00
1	C	130	GLU	N-CA-C	5.26	118.64	110.17
1	A	130	GLU	N-CA-C	5.25	118.61	110.17
1	B	357	ILE	N-CA-C	-5.24	106.19	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	GLU	N-CA-C	5.23	118.59	110.17
1	B	389	ASN	N-CA-C	-5.23	106.48	112.92
1	C	389	ASN	N-CA-C	-5.22	106.50	112.92
1	A	389	ASN	N-CA-C	-5.20	106.53	112.92
1	A	265	ASN	N-CA-C	5.15	118.87	112.59
1	C	265	ASN	N-CA-C	5.11	118.82	112.59
1	B	265	ASN	N-CA-C	5.10	118.82	112.59
1	B	339	LYS	N-CA-C	5.08	117.68	108.69
1	A	339	LYS	N-CA-C	5.08	117.67	108.69
1	C	339	LYS	N-CA-C	5.07	117.67	108.69
1	B	123	SER	N-CA-C	5.01	117.00	110.43
1	A	123	SER	N-CA-C	5.00	116.98	110.43

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	TYR	Sidechain
1	B	32	TYR	Sidechain
1	C	32	TYR	Sidechain

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	3350	0	3070	98	0
1	B	3350	0	3070	101	3
1	C	3350	0	3070	98	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
2	F	23	0	21	1	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	161	0	0	14	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	155	0	0	14	1
4	C	155	0	0	14	0
All	All	10662	0	9336	279	4

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 15.

All (279) 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:17:GLY:O	4:A:601:HOH:O	1.69	1.10
1:B:17:GLY:O	4:B:449:HOH:O	1.69	1.09
1:C:17:GLY:O	4:C:450:HOH:O	1.69	1.08
1:C:317:THR:HG21	4:C:573:HOH:O	1.54	1.08
1:B:317:THR:HG21	4:B:573:HOH:O	1.54	1.07
1:A:317:THR:HG21	4:A:566:HOH:O	1.54	1.06
1:B:145:ARG:HD2	1:C:71:GLN:NE2	1.76	1.00
1:A:145:ARG:HD2	1:B:71:GLN:NE2	1.76	1.00
1:A:71:GLN:NE2	1:C:145:ARG:HD2	1.76	1.00
1:B:317:THR:HG22	1:B:319:ILE:H	1.32	0.95
1:A:317:THR:HG22	1:A:319:ILE:H	1.32	0.93
1:C:383:ASN:HB3	1:C:386:ASN:H	1.34	0.93
1:B:383:ASN:HB3	1:B:386:ASN:H	1.34	0.92
1:C:317:THR:HG22	1:C:319:ILE:H	1.32	0.92
1:A:383:ASN:HB3	1:A:386:ASN:H	1.34	0.91
1:B:145:ARG:HD2	1:C:71:GLN:HE22	1.39	0.84
1:A:71:GLN:HE22	1:C:145:ARG:HD2	1.39	0.83
1:A:145:ARG:HD2	1:B:71:GLN:HE22	1.40	0.82
4:A:551:HOH:O	1:B:320:MET:HE2	1.83	0.77
1:C:173:ASP:OD1	1:C:175:ARG:HD2	1.85	0.77
1:B:173:ASP:OD1	1:B:175:ARG:HD2	1.85	0.77
4:B:558:HOH:O	1:C:320:MET:HE2	1.84	0.77
1:A:173:ASP:OD1	1:A:175:ARG:HD2	1.85	0.76
1:A:320:MET:HE2	4:C:558:HOH:O	1.84	0.76
1:C:182:ASN:HB2	1:C:183:PRO:HD2	1.68	0.76
1:A:182:ASN:HB2	1:A:183:PRO:HD2	1.68	0.75
1:B:182:ASN:HB2	1:B:183:PRO:HD2	1.68	0.75
1:B:33:ARG:HD2	1:B:113:HIS:O	1.89	0.73
1:C:33:ARG:HD2	1:C:113:HIS:O	1.89	0.72
1:A:161:TYR:CE1	1:A:259:PHE:HD1	2.08	0.72
1:A:33:ARG:HD2	1:A:113:HIS:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:TYR:CE1	1:C:259:PHE:HD1	2.08	0.71
1:B:161:TYR:CE1	1:B:259:PHE:HD1	2.08	0.71
1:C:169:ASN:HD21	1:C:249:GLY:H	1.40	0.70
1:B:169:ASN:HD21	1:B:249:GLY:H	1.40	0.70
1:A:169:ASN:HD21	1:A:249:GLY:H	1.40	0.68
1:A:324:MET:HE3	1:A:347:LEU:HD23	1.74	0.68
1:B:176:LEU:HG	1:B:179:MET:HE3	1.75	0.68
1:B:324:MET:HE3	1:B:347:LEU:HD23	1.74	0.68
1:A:63:ASN:HD22	1:A:64:VAL:N	1.92	0.68
1:B:63:ASN:HD22	1:B:64:VAL:N	1.92	0.68
1:C:324:MET:HE3	1:C:347:LEU:HD23	1.74	0.68
1:C:176:LEU:HG	1:C:179:MET:HE3	1.75	0.67
1:A:176:LEU:HG	1:A:179:MET:HE3	1.75	0.67
1:A:145:ARG:HH11	1:B:71:GLN:HE22	1.43	0.66
1:B:145:ARG:HH11	1:C:71:GLN:HE22	1.43	0.66
1:C:63:ASN:HD22	1:C:64:VAL:N	1.92	0.66
1:B:317:THR:HG23	1:B:318:PRO:HD2	1.78	0.65
1:A:63:ASN:HD22	1:A:63:ASN:C	2.04	0.65
1:B:63:ASN:HD22	1:B:63:ASN:C	2.04	0.65
1:A:71:GLN:HE22	1:C:145:ARG:HH11	1.43	0.64
1:A:198:LEU:HD11	1:A:204:LEU:HG	1.79	0.64
1:C:317:THR:HG23	1:C:318:PRO:HD2	1.78	0.64
1:B:198:LEU:HD11	1:B:204:LEU:HG	1.79	0.64
1:C:63:ASN:HD22	1:C:63:ASN:C	2.04	0.64
1:C:198:LEU:HD11	1:C:204:LEU:HG	1.79	0.64
1:A:317:THR:HG23	1:A:318:PRO:HD2	1.78	0.64
1:C:255:ASP:CG	1:C:259:PHE:HB2	2.25	0.62
1:A:255:ASP:CG	1:A:259:PHE:HB2	2.25	0.61
1:B:255:ASP:CG	1:B:259:PHE:HB2	2.25	0.61
1:A:315:LYS:HB3	4:A:500:HOH:O	2.00	0.61
1:B:315:LYS:HB3	4:B:507:HOH:O	2.00	0.61
1:C:315:LYS:HB3	4:C:508:HOH:O	2.00	0.61
1:A:275:HIS:HD2	4:A:467:HOH:O	1.85	0.60
1:A:145:ARG:HD2	1:B:71:GLN:HE21	1.66	0.60
1:C:307:THR:HG23	1:C:329:ASP:OD1	2.02	0.59
1:A:307:THR:HG23	1:A:329:ASP:OD1	2.02	0.59
1:B:307:THR:HG23	1:B:329:ASP:OD1	2.02	0.59
1:B:275:HIS:HD2	4:B:474:HOH:O	1.85	0.59
1:C:33:ARG:HG3	1:C:114:MET:O	2.03	0.58
1:B:129:LEU:HG	1:B:132:ILE:HD11	1.85	0.58
1:B:324:MET:CE	1:B:347:LEU:HD23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:HIS:HD2	4:C:475:HOH:O	1.85	0.58
1:A:33:ARG:HG3	1:A:114:MET:O	2.03	0.58
1:C:324:MET:CE	1:C:347:LEU:HD23	2.33	0.58
1:A:129:LEU:HG	1:A:132:ILE:HD11	1.86	0.57
1:C:129:LEU:HG	1:C:132:ILE:HD11	1.86	0.57
1:B:147:SER:HB3	4:C:486:HOH:O	2.05	0.57
1:A:147:SER:HB3	4:B:485:HOH:O	2.05	0.57
1:A:324:MET:CE	1:A:347:LEU:HD23	2.33	0.57
1:B:19:GLU:HG2	4:B:509:HOH:O	2.05	0.57
1:B:33:ARG:HG3	1:B:114:MET:O	2.03	0.57
1:C:69:ALA:O	1:C:70:GLN:HG2	2.05	0.57
1:A:71:GLN:HE21	1:C:145:ARG:HD2	1.66	0.56
1:B:69:ALA:O	1:B:70:GLN:HG2	2.04	0.56
1:A:89:LYS:CB	4:A:497:HOH:O	2.53	0.56
4:A:478:HOH:O	1:C:147:SER:CB	2.54	0.56
1:A:19:GLU:HG2	4:A:502:HOH:O	2.05	0.56
1:A:69:ALA:O	1:A:70:GLN:HG2	2.04	0.56
4:A:478:HOH:O	1:C:147:SER:HB3	2.05	0.56
1:C:89:LYS:CB	4:C:505:HOH:O	2.53	0.56
1:A:147:SER:CB	4:B:485:HOH:O	2.54	0.55
1:C:19:GLU:HG2	4:C:510:HOH:O	2.05	0.55
1:B:147:SER:CB	4:C:486:HOH:O	2.54	0.55
1:B:89:LYS:CB	4:B:504:HOH:O	2.53	0.55
1:C:387:ASN:HB3	1:C:390:PHE:HB2	1.89	0.55
1:B:287:MET:HE2	1:B:357:ILE:HG12	1.89	0.55
1:B:387:ASN:HB3	1:B:390:PHE:HB2	1.89	0.55
1:A:106:PHE:HB3	1:A:109:ARG:HD3	1.89	0.54
1:A:387:ASN:HB3	1:A:390:PHE:HB2	1.89	0.54
1:A:287:MET:HE2	1:A:357:ILE:HG12	1.89	0.54
1:B:145:ARG:HD2	1:C:71:GLN:HE21	1.66	0.54
1:C:287:MET:HE2	1:C:357:ILE:HG12	1.89	0.54
1:B:106:PHE:HB3	1:B:109:ARG:HD3	1.89	0.54
1:C:106:PHE:HB3	1:C:109:ARG:HD3	1.89	0.54
1:B:89:LYS:HB2	4:B:504:HOH:O	2.08	0.53
1:A:89:LYS:HB2	4:A:497:HOH:O	2.08	0.53
1:B:411:TRP:CZ3	1:B:413:PHE:CD1	2.97	0.53
1:C:89:LYS:HB2	4:C:505:HOH:O	2.08	0.53
1:C:411:TRP:CZ3	1:C:413:PHE:CD1	2.97	0.53
1:C:164:THR:HG22	1:C:254:PHE:HE2	1.75	0.52
1:A:411:TRP:CZ3	1:A:413:PHE:CD1	2.97	0.52
1:A:164:THR:HG22	1:A:254:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:MET:HE3	1:B:312:PRO:HB3	1.92	0.52
1:C:286:MET:HE3	1:C:312:PRO:HB3	1.92	0.52
4:B:558:HOH:O	1:C:320:MET:CE	2.51	0.52
1:B:164:THR:HG22	1:B:254:PHE:HE2	1.75	0.51
1:C:150:GLY:O	1:C:167:THR:CG2	2.59	0.51
1:A:29:GLN:HB2	1:A:305:TRP:CZ3	2.45	0.51
1:A:150:GLY:O	1:A:167:THR:CG2	2.59	0.51
1:B:29:GLN:HB2	1:B:305:TRP:CZ3	2.45	0.51
1:C:29:GLN:HB2	1:C:305:TRP:CZ3	2.45	0.51
1:A:286:MET:HE3	1:A:312:PRO:HB3	1.92	0.51
1:B:176:LEU:CG	1:B:179:MET:HE3	2.41	0.51
4:A:551:HOH:O	1:B:320:MET:CE	2.51	0.50
1:B:161:TYR:CE1	1:B:259:PHE:CD1	2.96	0.50
1:B:270:LEU:HD21	1:B:272:ILE:HD11	1.93	0.50
1:C:161:TYR:CE1	1:C:259:PHE:CD1	2.96	0.50
1:B:150:GLY:O	1:B:167:THR:CG2	2.59	0.50
1:C:270:LEU:HD21	1:C:272:ILE:HD11	1.93	0.50
1:C:176:LEU:CG	1:C:179:MET:HE3	2.41	0.50
1:A:341:ASN:C	1:A:341:ASN:ND2	2.70	0.50
1:C:341:ASN:C	1:C:341:ASN:ND2	2.70	0.50
1:A:270:LEU:HD21	1:A:272:ILE:HD11	1.93	0.50
1:A:176:LEU:CG	1:A:179:MET:HE3	2.41	0.50
1:B:341:ASN:C	1:B:341:ASN:ND2	2.70	0.49
1:C:120:TRP:CH2	1:C:175:ARG:HG2	2.47	0.49
1:A:120:TRP:CH2	1:A:175:ARG:HG2	2.47	0.49
1:B:269:MET:HE2	1:B:293:GLN:CD	2.38	0.49
1:C:259:PHE:HB3	1:C:384:ALA:HB3	1.95	0.49
1:C:269:MET:HE2	1:C:293:GLN:CD	2.38	0.49
1:A:161:TYR:CE1	1:A:259:PHE:CD1	2.96	0.49
1:A:269:MET:HE2	1:A:293:GLN:CD	2.38	0.49
1:B:120:TRP:CH2	1:B:175:ARG:HG2	2.48	0.49
1:C:141:LEU:CD2	1:C:174:VAL:HG22	2.43	0.49
1:B:259:PHE:HB3	1:B:384:ALA:HB3	1.95	0.48
1:B:141:LEU:CD2	1:B:174:VAL:HG22	2.43	0.48
1:A:202:TYR:N	1:A:202:TYR:CD1	2.80	0.48
1:A:259:PHE:HB3	1:A:384:ALA:HB3	1.95	0.48
1:A:141:LEU:CD2	1:A:174:VAL:HG22	2.43	0.48
1:C:202:TYR:CD1	1:C:202:TYR:N	2.80	0.48
1:A:192:ASP:HB2	1:A:214:LEU:HB3	1.95	0.48
1:B:192:ASP:HB2	1:B:214:LEU:HB3	1.95	0.48
1:B:202:TYR:N	1:B:202:TYR:CD1	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:CD1	1:A:136:PHE:N	2.81	0.48
1:A:394:VAL:HG13	1:A:398:PHE:CB	2.44	0.48
1:A:155:PHE:CE1	1:A:157:SER:HB2	2.49	0.47
1:A:324:MET:HE3	1:A:347:LEU:CD2	2.43	0.47
1:B:155:PHE:CE1	1:B:157:SER:HB2	2.49	0.47
1:C:394:VAL:HG13	1:C:398:PHE:CB	2.44	0.47
1:C:155:PHE:CE1	1:C:157:SER:HB2	2.49	0.47
1:A:145:ARG:CD	1:B:71:GLN:NE2	2.65	0.47
1:C:192:ASP:HB2	1:C:214:LEU:HB3	1.95	0.47
1:C:185:GLY:HA2	1:C:220:THR:O	2.15	0.47
1:B:221:GLN:HG3	1:B:223:VAL:HG23	1.97	0.47
1:A:320:MET:CE	4:C:558:HOH:O	2.52	0.46
1:B:394:VAL:HG13	1:B:398:PHE:CB	2.44	0.46
1:C:221:GLN:HG3	1:C:223:VAL:HG23	1.97	0.46
1:C:202:TYR:N	1:C:202:TYR:HD1	2.14	0.46
1:A:221:GLN:HG3	1:A:223:VAL:HG23	1.97	0.46
1:B:202:TYR:N	1:B:202:TYR:HD1	2.14	0.46
1:A:71:GLN:O	1:C:146:SER:HA	2.16	0.46
1:A:185:GLY:HA2	1:A:220:THR:O	2.15	0.46
1:B:146:SER:HA	1:C:71:GLN:O	2.16	0.46
1:C:136:PHE:CD1	1:C:136:PHE:N	2.81	0.46
1:C:360:ARG:NH1	1:C:420:TRP:CH2	2.84	0.46
1:A:202:TYR:N	1:A:202:TYR:HD1	2.13	0.45
1:B:185:GLY:HA2	1:B:220:THR:O	2.15	0.45
1:B:152:SER:HB2	1:B:165:ASN:HB2	1.99	0.45
1:B:360:ARG:NH1	1:B:420:TRP:CH2	2.84	0.45
1:C:152:SER:HB2	1:C:165:ASN:HB2	1.99	0.45
1:B:63:ASN:C	1:B:63:ASN:ND2	2.73	0.45
1:A:152:SER:HB2	1:A:165:ASN:HB2	1.99	0.45
1:A:360:ARG:NH1	1:A:420:TRP:CH2	2.84	0.45
1:B:268:HIS:CD2	1:B:268:HIS:C	2.95	0.45
1:B:324:MET:HE3	1:B:347:LEU:CD2	2.43	0.45
1:C:268:HIS:CD2	1:C:268:HIS:C	2.95	0.45
1:A:146:SER:HA	1:B:71:GLN:O	2.16	0.45
1:A:268:HIS:CD2	1:A:268:HIS:C	2.95	0.45
1:A:71:GLN:NE2	1:C:145:ARG:CD	2.65	0.45
1:A:403:PHE:N	1:A:403:PHE:CD1	2.85	0.45
1:B:403:PHE:CD1	1:B:403:PHE:N	2.85	0.45
1:B:317:THR:CG2	1:B:318:PRO:N	2.80	0.44
1:C:317:THR:CG2	1:C:318:PRO:N	2.80	0.44
1:C:403:PHE:CD1	1:C:403:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:C	1:A:341:ASN:HD22	2.25	0.44
1:B:150:GLY:O	1:B:167:THR:HG23	2.18	0.44
1:B:341:ASN:C	1:B:341:ASN:HD22	2.25	0.44
1:B:90:ASN:HA	4:B:527:HOH:O	2.17	0.44
1:B:145:ARG:CD	1:C:71:GLN:NE2	2.64	0.44
1:C:397:ASP:O	1:C:398:PHE:C	2.61	0.44
1:A:90:ASN:HA	4:A:520:HOH:O	2.17	0.44
1:C:150:GLY:O	1:C:167:THR:HG23	2.18	0.44
1:A:397:ASP:O	1:A:398:PHE:C	2.61	0.44
1:A:155:PHE:HD1	1:A:156:ALA:O	2.02	0.43
1:B:155:PHE:HD1	1:B:156:ALA:O	2.02	0.43
1:C:341:ASN:C	1:C:341:ASN:HD22	2.25	0.43
1:A:317:THR:CG2	1:A:318:PRO:N	2.80	0.43
1:A:360:ARG:HG3	1:A:420:TRP:CD2	2.54	0.43
1:B:70:GLN:O	1:B:70:GLN:HG3	2.19	0.43
1:A:109:ARG:H	1:A:109:ARG:HG2	1.65	0.43
1:C:155:PHE:HD1	1:C:156:ALA:O	2.02	0.43
1:C:90:ASN:HA	4:C:527:HOH:O	2.17	0.43
1:C:324:MET:HE3	1:C:347:LEU:CD2	2.43	0.43
1:A:70:GLN:HG3	1:A:70:GLN:O	2.19	0.43
1:A:317:THR:HG23	1:A:318:PRO:CD	2.48	0.43
1:B:360:ARG:HG3	1:B:420:TRP:CD2	2.54	0.43
1:A:150:GLY:O	1:A:167:THR:HG23	2.18	0.42
1:C:360:ARG:HG3	1:C:420:TRP:CD2	2.54	0.42
1:A:383:ASN:H	1:A:386:ASN:HB2	1.84	0.42
1:A:43:GLU:HB3	1:A:63:ASN:HD21	1.84	0.42
1:B:383:ASN:H	1:B:386:ASN:HB2	1.84	0.42
1:C:43:GLU:HB3	1:C:63:ASN:HD21	1.84	0.42
1:C:70:GLN:HG3	1:C:70:GLN:O	2.19	0.42
1:C:200:ASP:O	1:C:201:ASN:HB2	2.20	0.42
1:C:223:VAL:O	1:C:226:GLY:N	2.41	0.42
1:C:299:ASN:O	1:C:300:ASP:HB2	2.20	0.42
1:C:327:GLY:O	1:C:343:TYR:HA	2.20	0.42
1:A:327:GLY:O	1:A:343:TYR:HA	2.20	0.42
1:B:397:ASP:O	1:B:398:PHE:C	2.61	0.42
1:B:40:THR:OG1	1:B:70:GLN:NE2	2.51	0.42
1:B:43:GLU:HB3	1:B:63:ASN:HD21	1.84	0.42
1:B:360:ARG:HB3	1:B:419:ILE:HA	2.02	0.42
1:A:40:THR:OG1	1:A:70:GLN:NE2	2.51	0.42
1:A:360:ARG:HB3	1:A:419:ILE:HA	2.02	0.42
1:B:200:ASP:O	1:B:201:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLY:O	1:B:343:TYR:HA	2.20	0.42
1:A:163:TYR:CD1	1:A:163:TYR:N	2.88	0.42
1:C:163:TYR:CD1	1:C:163:TYR:N	2.88	0.42
1:C:383:ASN:H	1:C:386:ASN:HB2	1.84	0.42
1:A:200:ASP:O	1:A:201:ASN:HB2	2.20	0.42
1:C:317:THR:HG23	1:C:318:PRO:CD	2.48	0.42
1:B:136:PHE:CD1	1:B:136:PHE:N	2.81	0.41
1:B:212:GLY:HA2	1:B:236:THR:HG22	2.02	0.41
1:A:299:ASN:O	1:A:300:ASP:HB2	2.20	0.41
1:A:394:VAL:HG13	1:A:398:PHE:HB2	2.02	0.41
1:B:199:ARG:HA	4:C:450:HOH:O	2.20	0.41
1:B:285:ASP:HB3	1:B:357:ILE:HB	2.02	0.41
1:C:394:VAL:HG13	1:C:398:PHE:HB2	2.03	0.41
1:B:8:ARG:HH12	2:F:1:BGC:HB	1.68	0.41
1:A:199:ARG:HA	4:B:449:HOH:O	2.20	0.41
1:A:223:VAL:HG12	1:A:224:LEU:N	2.35	0.41
1:B:163:TYR:CD1	1:B:163:TYR:N	2.88	0.41
1:B:317:THR:HG23	1:B:318:PRO:CD	2.48	0.41
1:C:40:THR:OG1	1:C:70:GLN:NE2	2.51	0.41
1:A:212:GLY:HA2	1:A:236:THR:HG22	2.02	0.41
1:A:292:TYR:CD1	1:A:306:TRP:CE2	3.09	0.41
1:C:212:GLY:HA2	1:C:236:THR:HG22	2.02	0.41
1:C:223:VAL:HG12	1:C:224:LEU:N	2.35	0.41
1:C:360:ARG:HB3	1:C:419:ILE:HA	2.02	0.41
1:A:209:SER:HB2	1:A:237:ASP:HB3	2.03	0.41
1:A:285:ASP:HB3	1:A:357:ILE:HB	2.02	0.41
1:B:223:VAL:O	1:B:226:GLY:N	2.41	0.41
4:A:601:HOH:O	1:C:199:ARG:HA	2.20	0.41
1:B:223:VAL:HG12	1:B:224:LEU:N	2.35	0.41
1:B:299:ASN:O	1:B:300:ASP:HB2	2.20	0.41
1:C:209:SER:HB2	1:C:237:ASP:HB3	2.03	0.41
1:B:209:SER:HB2	1:B:237:ASP:HB3	2.03	0.41
1:B:394:VAL:HG13	1:B:398:PHE:HB2	2.03	0.41
1:A:89:LYS:HE3	4:A:506:HOH:O	2.21	0.40
1:B:109:ARG:H	1:B:109:ARG:HG2	1.65	0.40
1:B:89:LYS:HE3	4:B:513:HOH:O	2.21	0.40
1:C:285:ASP:HB3	1:C:357:ILE:HB	2.02	0.40
1:B:292:TYR:CD1	1:B:306:TRP:CE2	3.09	0.40
1:B:101:TRP:CG	1:B:105:ARG:HH11	2.39	0.40
1:C:89:LYS:HE3	4:C:514:HOH:O	2.21	0.40
1:C:101:TRP:CG	1:C:105:ARG:HH11	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HA	1:A:324:MET:O	2.22	0.40
1:C:374:GLU:CD	1:C:405:ARG:HB2	2.47	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ASN:ND2	4:A:484:HOH:O[8_456]	0.27	1.93
1:B:399:ASN:CG	4:A:484:HOH:O[8_456]	1.44	0.76
4:A:443:HOH:O	4:B:534:HOH:O[8_556]	1.52	0.68
1:B:336:THR:CB	4:A:527:HOH:O[8_456]	1.93	0.27

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/421 (100%)	398 (95%)	21 (5%)	0	100	100
1	B	419/421 (100%)	398 (95%)	21 (5%)	0	100	100
1	C	419/421 (100%)	398 (95%)	21 (5%)	0	100	100
All	All	1257/1263 (100%)	1194 (95%)	63 (5%)	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	340/340 (100%)	303 (89%)	37 (11%)	6	13
1	B	340/340 (100%)	303 (89%)	37 (11%)	6	13
1	C	340/340 (100%)	303 (89%)	37 (11%)	6	13
All	All	1020/1020 (100%)	909 (89%)	111 (11%)	6	13

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	34	LEU
1	A	40	THR
1	A	55	ASP
1	A	56	LYS
1	A	73	ASP
1	A	89	LYS
1	A	91	LEU
1	A	104	LYS
1	A	109	ARG
1	A	145	ARG
1	A	167	THR
1	A	175	ARG
1	A	186	THR
1	A	189	LEU
1	A	205	VAL
1	A	206	ASP
1	A	236	THR
1	A	241	SER
1	A	265	ASN
1	A	269	MET
1	A	273	LEU
1	A	287	MET
1	A	289	VAL
1	A	296	ASN
1	A	300	ASP
1	A	307	THR
1	A	308	VAL
1	A	311	ARG
1	A	315	LYS
1	A	317	THR
1	A	341	ASN
1	A	347	LEU
1	A	371	LYS

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Mol	Chain	Res	Type
1	A	383	ASN
1	A	392	LYS
1	A	394	VAL
1	B	33	ARG
1	B	34	LEU
1	B	40	THR
1	B	55	ASP
1	B	56	LYS
1	B	73	ASP
1	B	89	LYS
1	B	91	LEU
1	B	104	LYS
1	B	109	ARG
1	B	145	ARG
1	B	167	THR
1	B	175	ARG
1	B	186	THR
1	B	189	LEU
1	B	205	VAL
1	B	206	ASP
1	B	236	THR
1	B	241	SER
1	B	265	ASN
1	B	269	MET
1	B	273	LEU
1	B	287	MET
1	B	289	VAL
1	B	296	ASN
1	B	300	ASP
1	B	307	THR
1	B	308	VAL
1	B	311	ARG
1	B	315	LYS
1	B	317	THR
1	B	341	ASN
1	B	347	LEU
1	B	371	LYS
1	B	383	ASN
1	B	392	LYS
1	B	394	VAL
1	C	33	ARG
1	C	34	LEU

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Mol	Chain	Res	Type
1	C	40	THR
1	C	55	ASP
1	C	56	LYS
1	C	73	ASP
1	C	89	LYS
1	C	91	LEU
1	C	104	LYS
1	C	109	ARG
1	C	145	ARG
1	C	167	THR
1	C	175	ARG
1	C	186	THR
1	C	189	LEU
1	C	205	VAL
1	C	206	ASP
1	C	236	THR
1	C	241	SER
1	C	265	ASN
1	C	269	MET
1	C	273	LEU
1	C	287	MET
1	C	289	VAL
1	C	296	ASN
1	C	300	ASP
1	C	307	THR
1	C	308	VAL
1	C	311	ARG
1	C	315	LYS
1	C	317	THR
1	C	341	ASN
1	C	347	LEU
1	C	371	LYS
1	C	383	ASN
1	C	392	LYS
1	C	394	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	70	GLN
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	169	ASN
1	A	248	GLN
1	A	265	ASN
1	A	266	ASN
1	A	268	HIS
1	A	275	HIS
1	A	296	ASN
1	A	330	ASN
1	A	341	ASN
1	A	349	GLN
1	B	63	ASN
1	B	70	GLN
1	B	71	GLN
1	B	87	GLN
1	B	159	ASN
1	B	169	ASN
1	B	248	GLN
1	B	265	ASN
1	B	266	ASN
1	B	268	HIS
1	B	275	HIS
1	B	296	ASN
1	B	341	ASN
1	B	349	GLN
1	C	63	ASN
1	C	70	GLN
1	C	71	GLN
1	C	159	ASN
1	C	169	ASN
1	C	228	ASN
1	C	248	GLN
1	C	265	ASN
1	C	266	ASN
1	C	268	HIS
1	C	275	HIS
1	C	296	ASN
1	C	330	ASN
1	C	341	ASN
1	C	349	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	D	1	2	12,12,12	0.42	0	17,17,17	1.23	2 (11%)
2	GLC	D	2	2	11,11,12	0.55	0	15,15,17	0.88	1 (6%)
2	BGC	E	1	2	12,12,12	0.24	0	17,17,17	0.82	0
2	GLC	E	2	2	11,11,12	0.58	0	15,15,17	1.01	1 (6%)
2	BGC	F	1	2	12,12,12	0.41	0	17,17,17	1.22	2 (11%)
2	GLC	F	2	2	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	BGC	G	1	2	12,12,12	0.24	0	17,17,17	0.82	0
2	GLC	G	2	2	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
2	BGC	H	1	2	12,12,12	0.41	0	17,17,17	1.22	2 (11%)
2	GLC	H	2	2	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	BGC	I	1	2	12,12,12	0.24	0	17,17,17	0.82	0
2	GLC	I	2	2	11,11,12	0.57	0	15,15,17	1.02	1 (6%)

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	D	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	BGC	C1-C2-C3	-3.09	104.06	110.36
2	H	1	BGC	C1-C2-C3	-3.08	104.07	110.36
2	D	1	BGC	C1-C2-C3	-3.08	104.07	110.36
2	D	1	BGC	C3-C4-C5	2.55	114.85	110.23
2	F	1	BGC	C3-C4-C5	2.54	114.84	110.23
2	H	1	BGC	C3-C4-C5	2.54	114.84	110.23
2	D	2	GLC	C3-C4-C5	-2.28	106.10	110.23
2	F	2	GLC	C3-C4-C5	-2.28	106.11	110.23
2	H	2	GLC	C3-C4-C5	-2.27	106.12	110.23
2	E	2	GLC	C1-C2-C3	2.09	112.68	109.64
2	G	2	GLC	C1-C2-C3	2.09	112.68	109.64
2	I	2	GLC	C1-C2-C3	2.07	112.66	109.64

There are no chirality outliers.

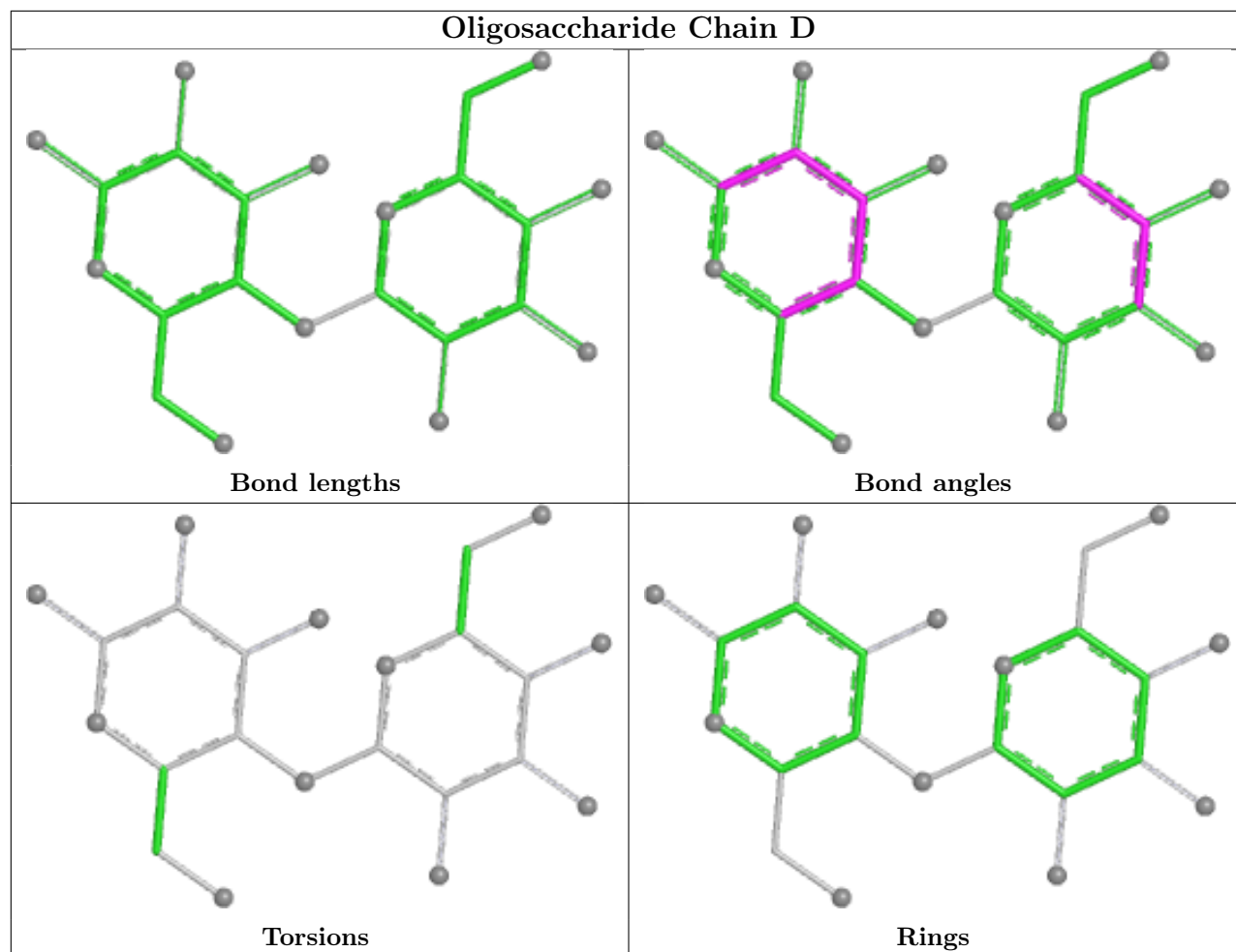
There are no torsion outliers.

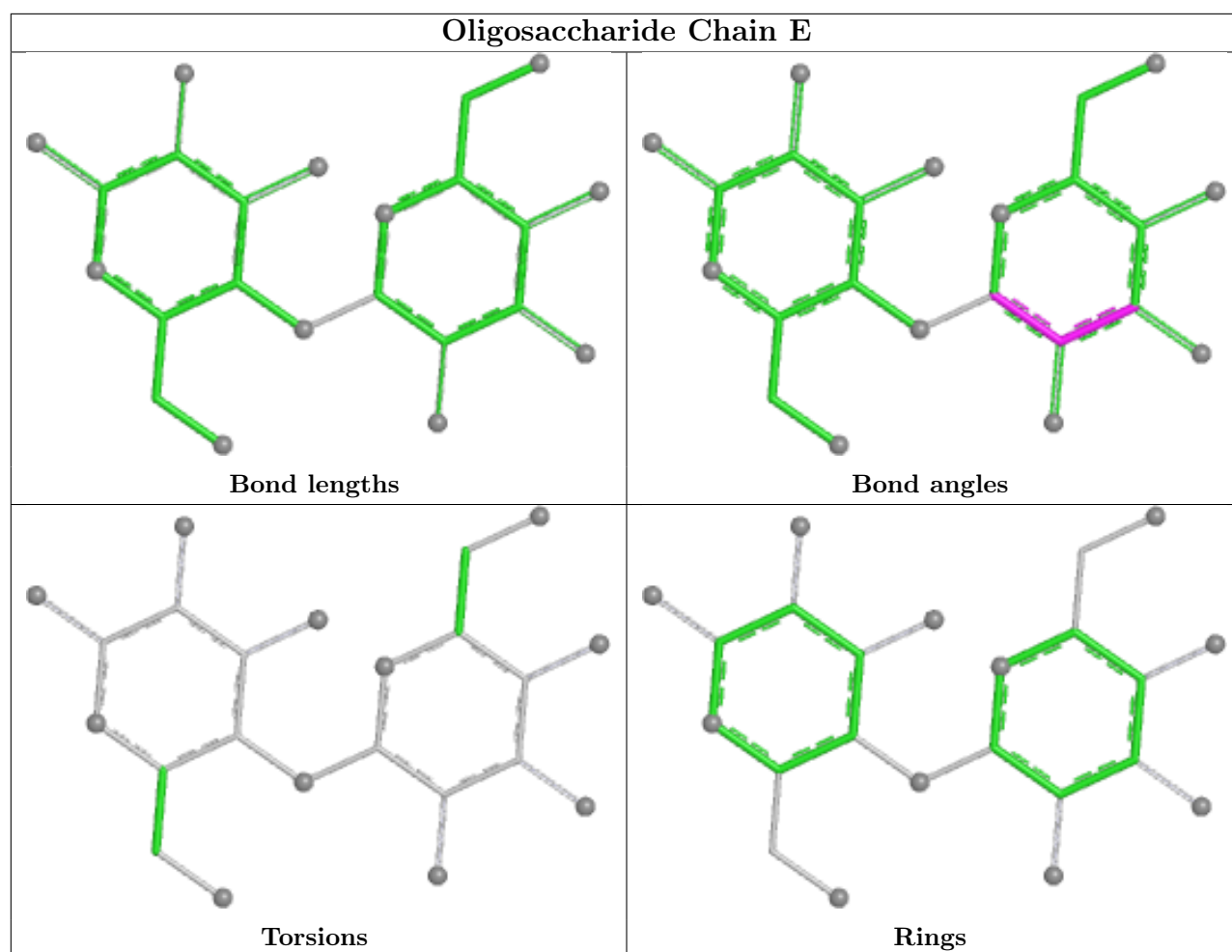
There are no ring outliers.

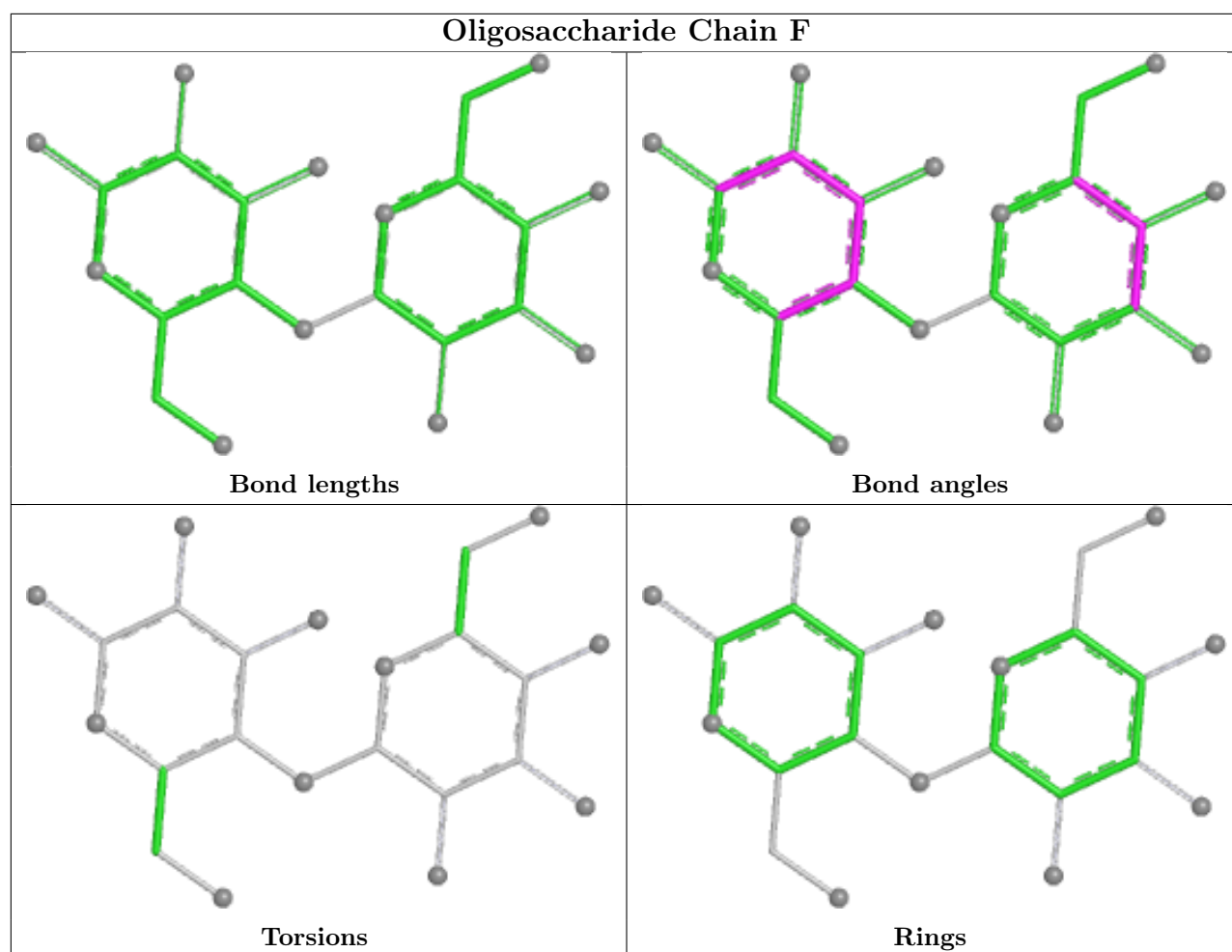
1 monomer is involved in 1 short contact:

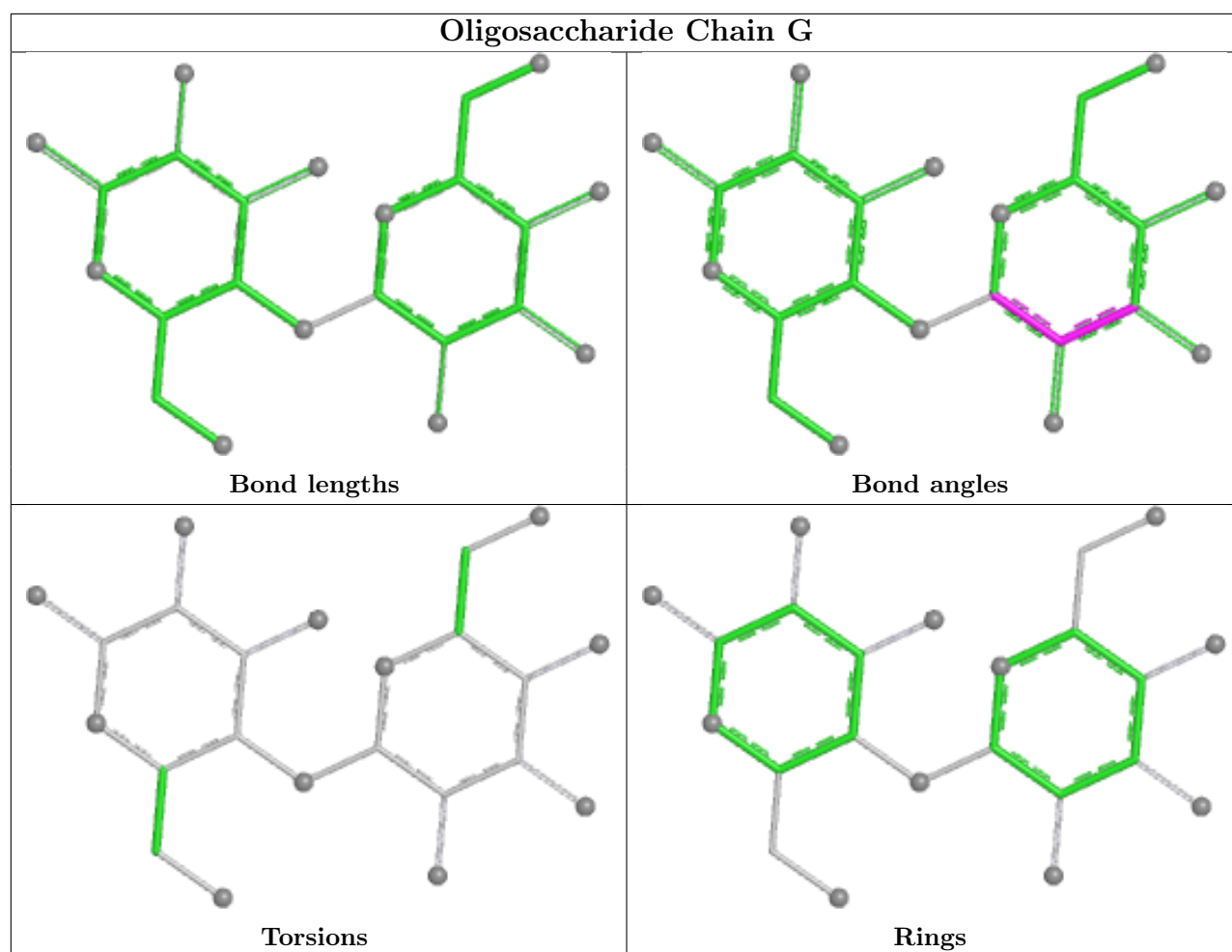
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	BGC	1	0

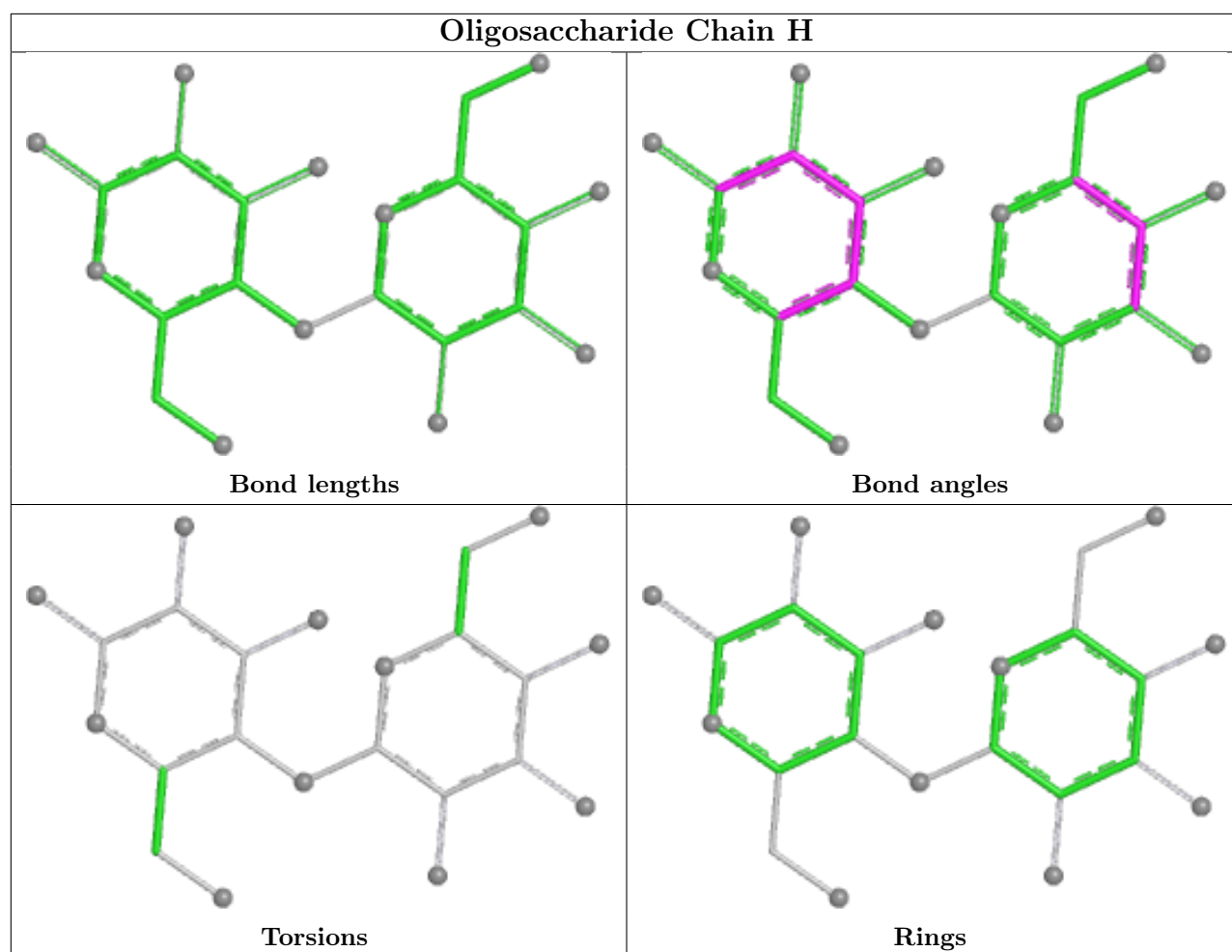
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

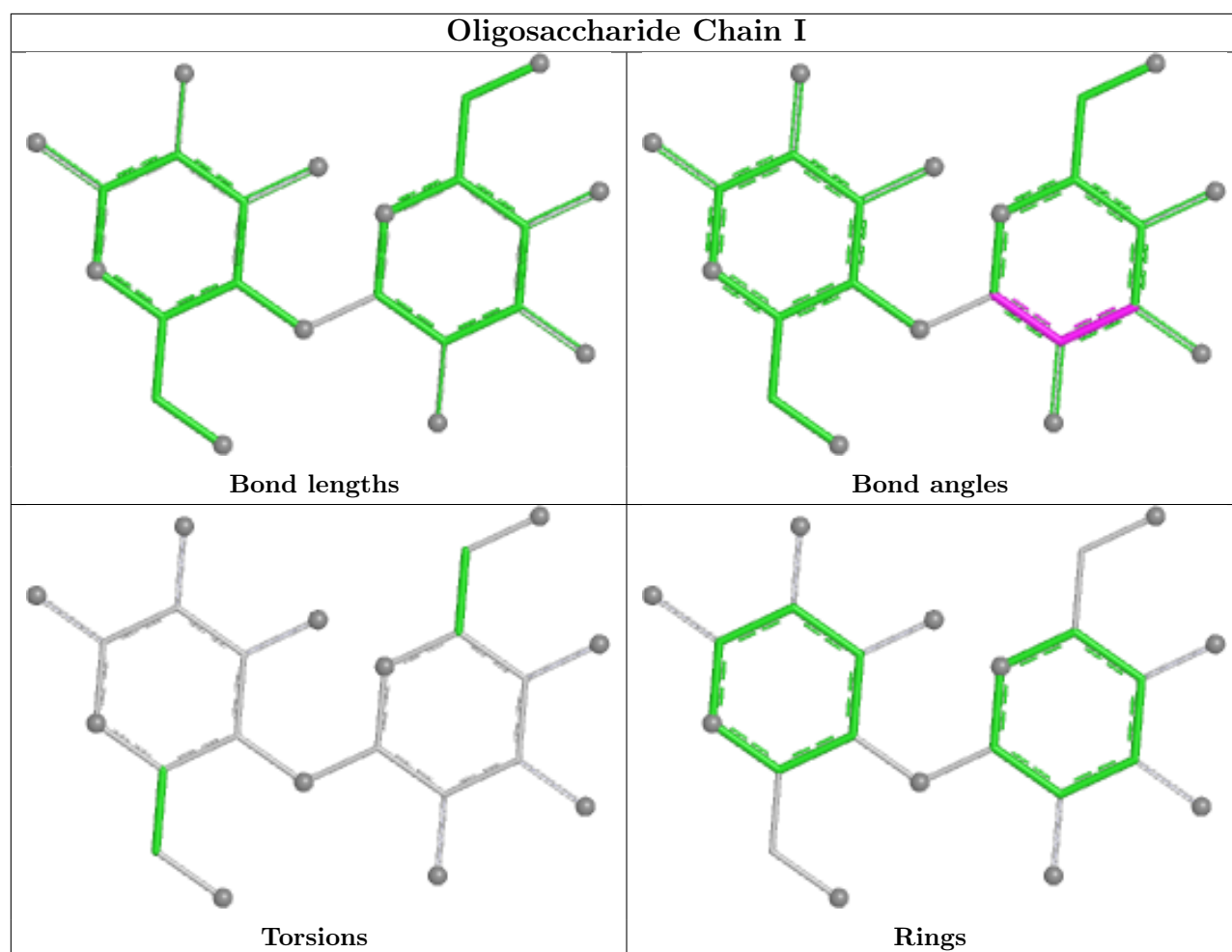












5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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	421/421 (100%)	-0.31	9 (2%) 63 58	16, 32, 47, 63	46 (10%)
1	B	421/421 (100%)	-0.28	10 (2%) 59 54	16, 32, 47, 63	46 (10%)
1	C	421/421 (100%)	-0.28	11 (2%) 57 51	16, 32, 47, 63	46 (10%)
All	All	1263/1263 (100%)	-0.29	30 (2%) 59 54	16, 32, 49, 63	138 (10%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	255	ASP	3.4
1	C	154	SER	3.1
1	B	181	ILE	3.0
1	A	389	ASN	2.9
1	B	397	ASP	2.9
1	B	158	ASN	2.8
1	A	257	GLU	2.8
1	C	387	ASN	2.8
1	A	383	ASN	2.6
1	A	157	SER	2.5
1	A	154	SER	2.4
1	C	181	ILE	2.3
1	B	385	ASP	2.3
1	A	161	TYR	2.2
1	A	386	ASN	2.2
1	C	156	ALA	2.2
1	A	279	SER	2.2
1	B	386	ASN	2.2
1	A	156	ALA	2.2
1	C	386	ASN	2.2
1	B	387	ASN	2.1
1	C	400	GLY	2.1
1	B	94	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	158	ASN	2.1
1	C	182	ASN	2.1
1	B	134	VAL	2.1
1	B	263	ILE	2.1
1	B	154	SER	2.0
1	C	137	GLY	2.0
1	C	134	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

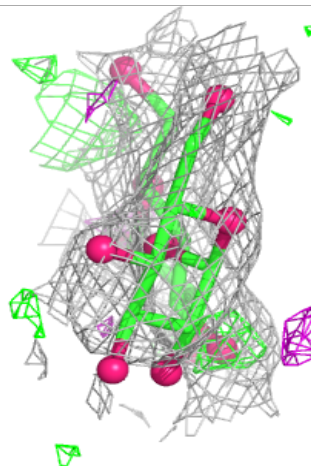
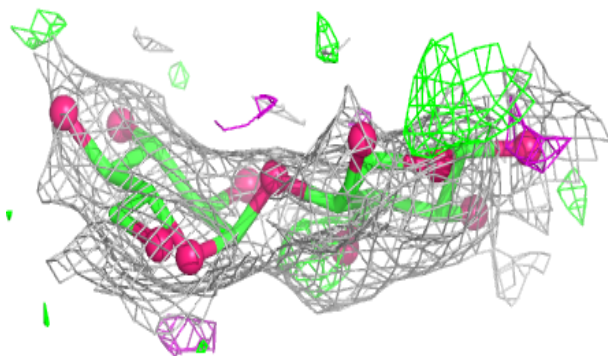
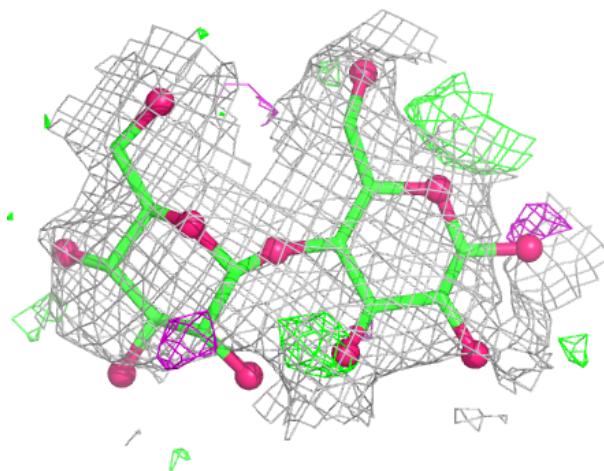
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	D	1	12/12	0.73	0.18	32,32,32,32	12
2	BGC	H	1	12/12	0.82	0.18	32,32,32,32	12
2	GLC	G	2	11/12	0.83	0.17	33,33,33,33	11
2	BGC	E	1	12/12	0.86	0.10	39,39,39,39	12
2	GLC	F	2	11/12	0.87	0.14	37,37,37,37	11
2	GLC	I	2	11/12	0.87	0.15	33,33,33,33	11
2	GLC	D	2	11/12	0.88	0.12	37,37,37,37	11
2	GLC	E	2	11/12	0.89	0.14	33,33,33,33	11
2	GLC	H	2	11/12	0.89	0.13	37,37,37,37	11
2	BGC	F	1	12/12	0.89	0.11	32,32,32,32	12
2	BGC	I	1	12/12	0.90	0.10	39,39,39,39	12
2	BGC	G	1	12/12	0.91	0.11	39,39,39,39	12

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.

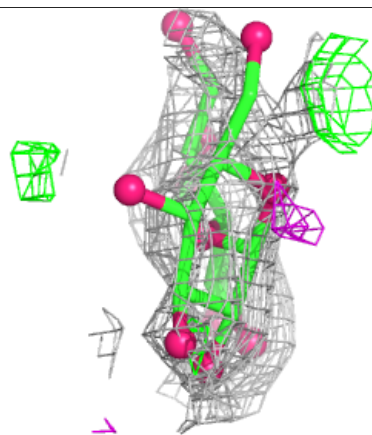
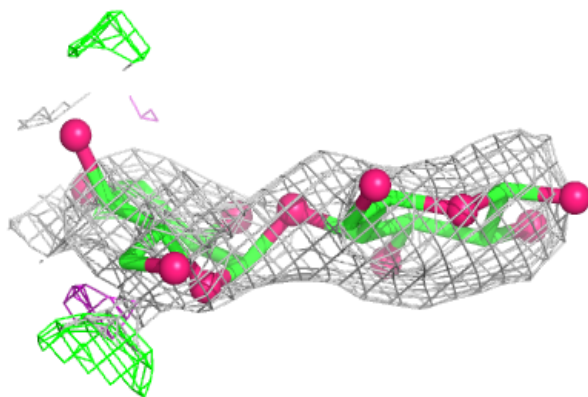
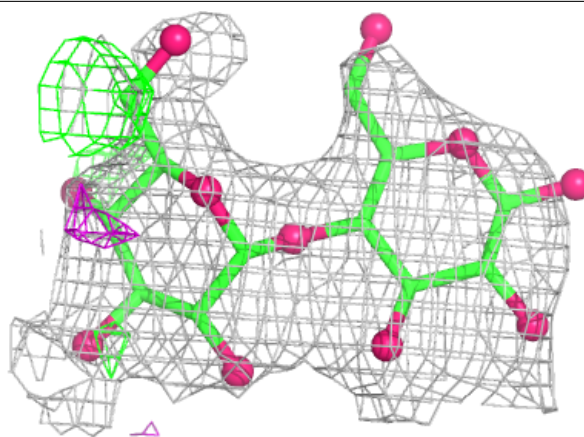
Electron density around Chain D:

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



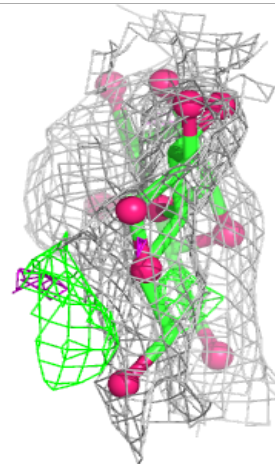
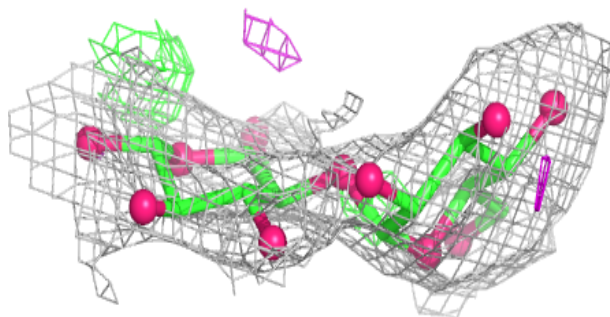
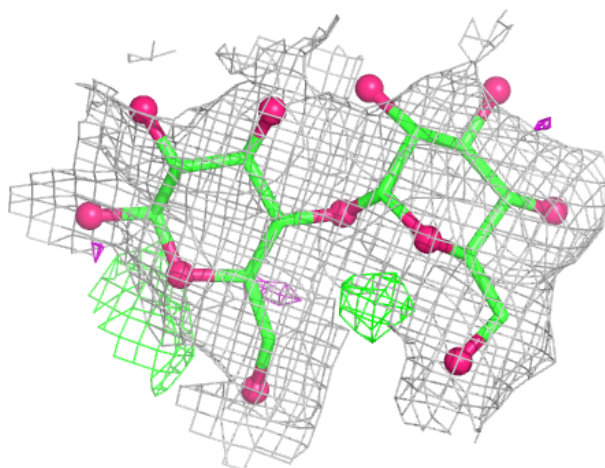
Electron density around Chain E:

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



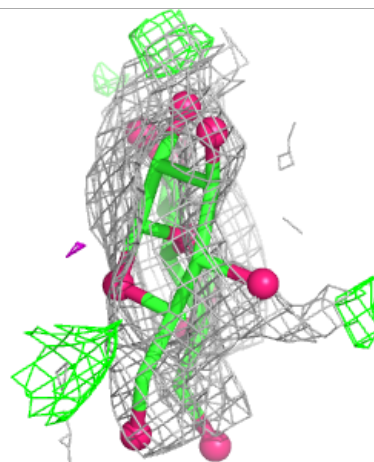
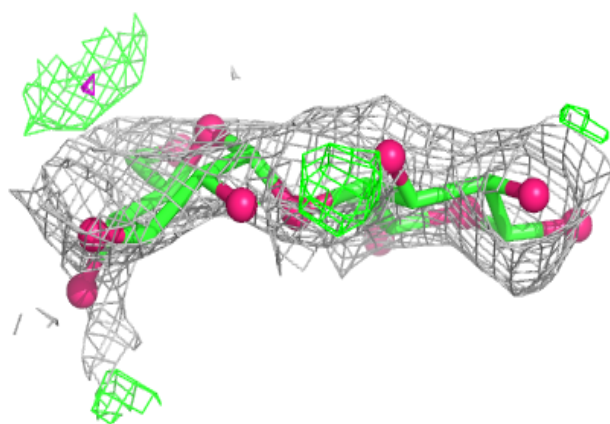
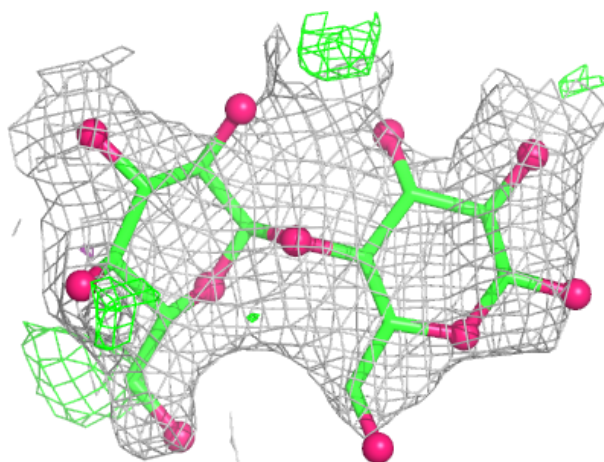
Electron density around Chain F:

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



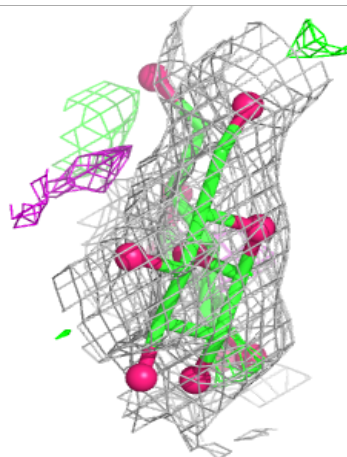
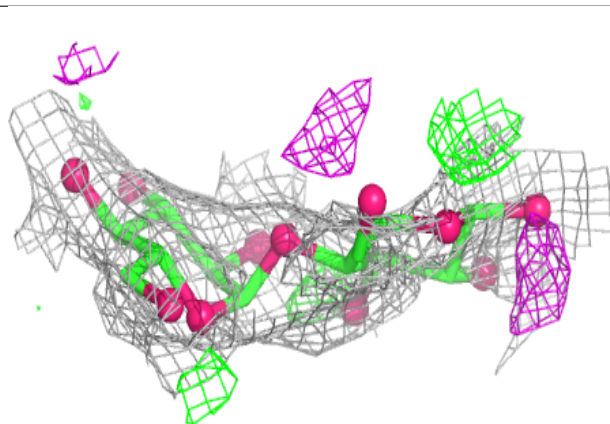
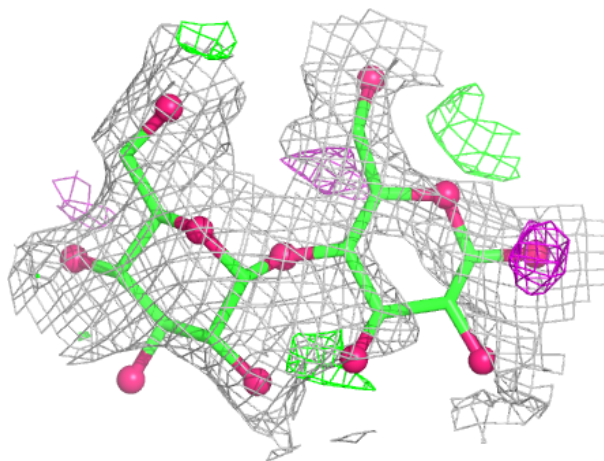
Electron density around Chain G:

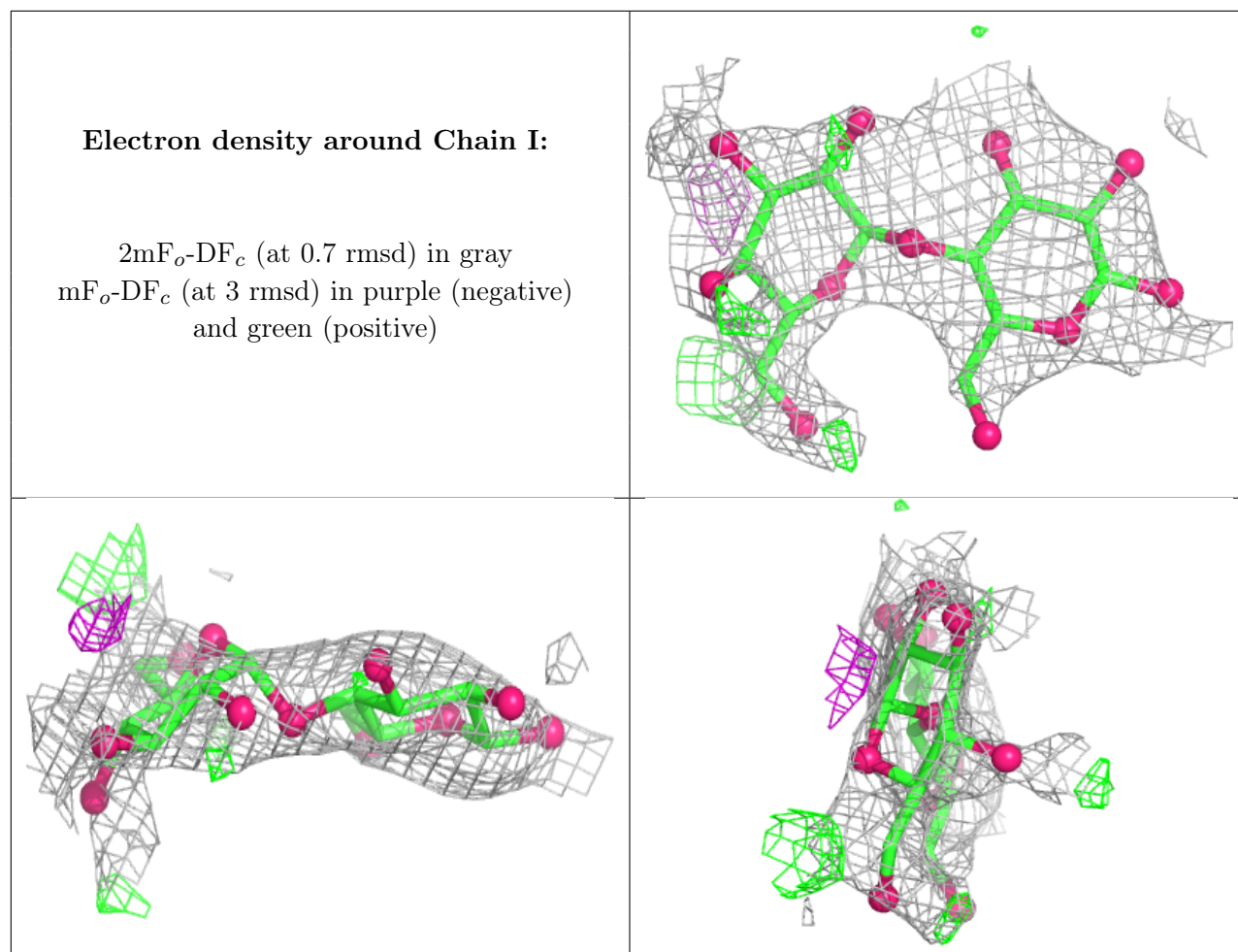
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	422	1/1	0.82	0.29	16,16,16,16	1
3	MG	A	422	1/1	0.88	0.22	16,16,16,16	1
3	MG	A	423	1/1	0.92	0.25	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.