



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:19 PM EDT

PDB ID : 5AB2 / pdb_00005ab2
Title : Crystal structure of aminopeptidase ERAP2 with ligand
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Mavridis, I.M.; Stratikos, E.
Deposited on : 2015-07-31
Resolution : 2.73 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:

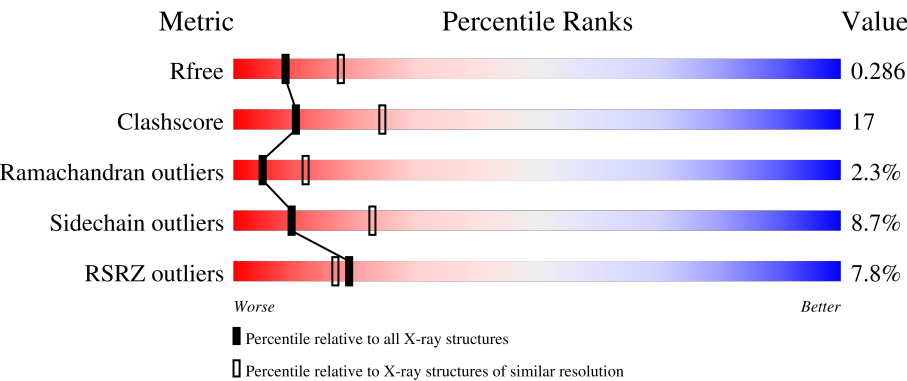
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.73 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.



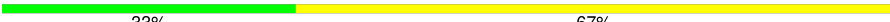
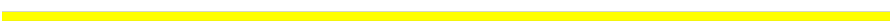
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	967	67% 23% • 7%
1	B	967	12% 51% 33% 6% • 9%
2	C	6	83% 50% 33% 17%
2	D	6	83% 33% 50% 17%
3	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	G	3	 33%67%
4	F	2	 50%50%
4	H	2	 50%50%
4	I	2	 100%
4	J	2	 50%50%
4	K	2	 50%50%
4	M	2	 100%
4	N	2	 50%50%
5	L	4	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15144 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 ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C	N	O	S	0	8	1
			7344	4737	1217	1361	29			
1	B	879	Total	C	N	O	S	0	0	1
			7156	4617	1188	1323	28			

There are 14 discrepancies between the modelled and reference sequences:

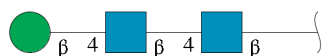
Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	cloning artifact	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

- Molecule 2 is a protein called GPI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	5	0
			80	52	17	11			
2	D	6	Total	C	N	O	0	0	0
			42	27	9	6			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



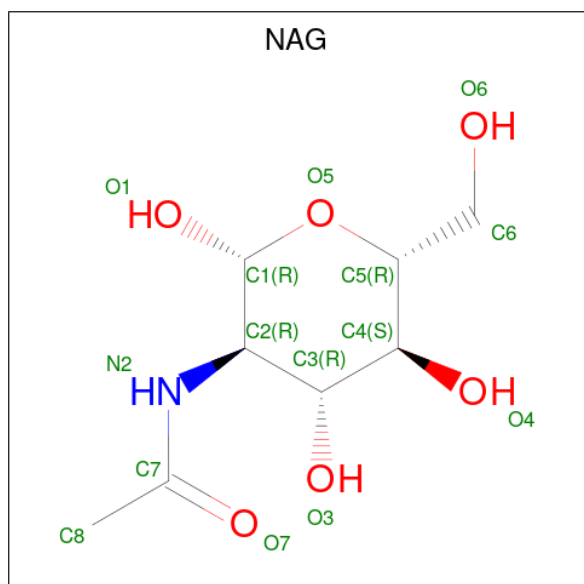
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2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

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

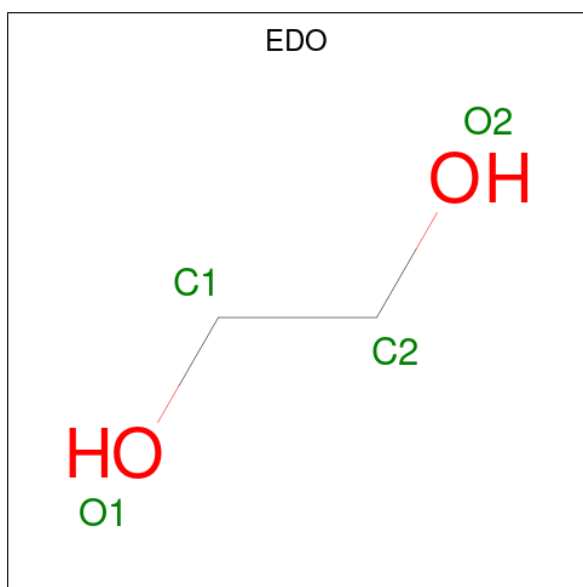


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

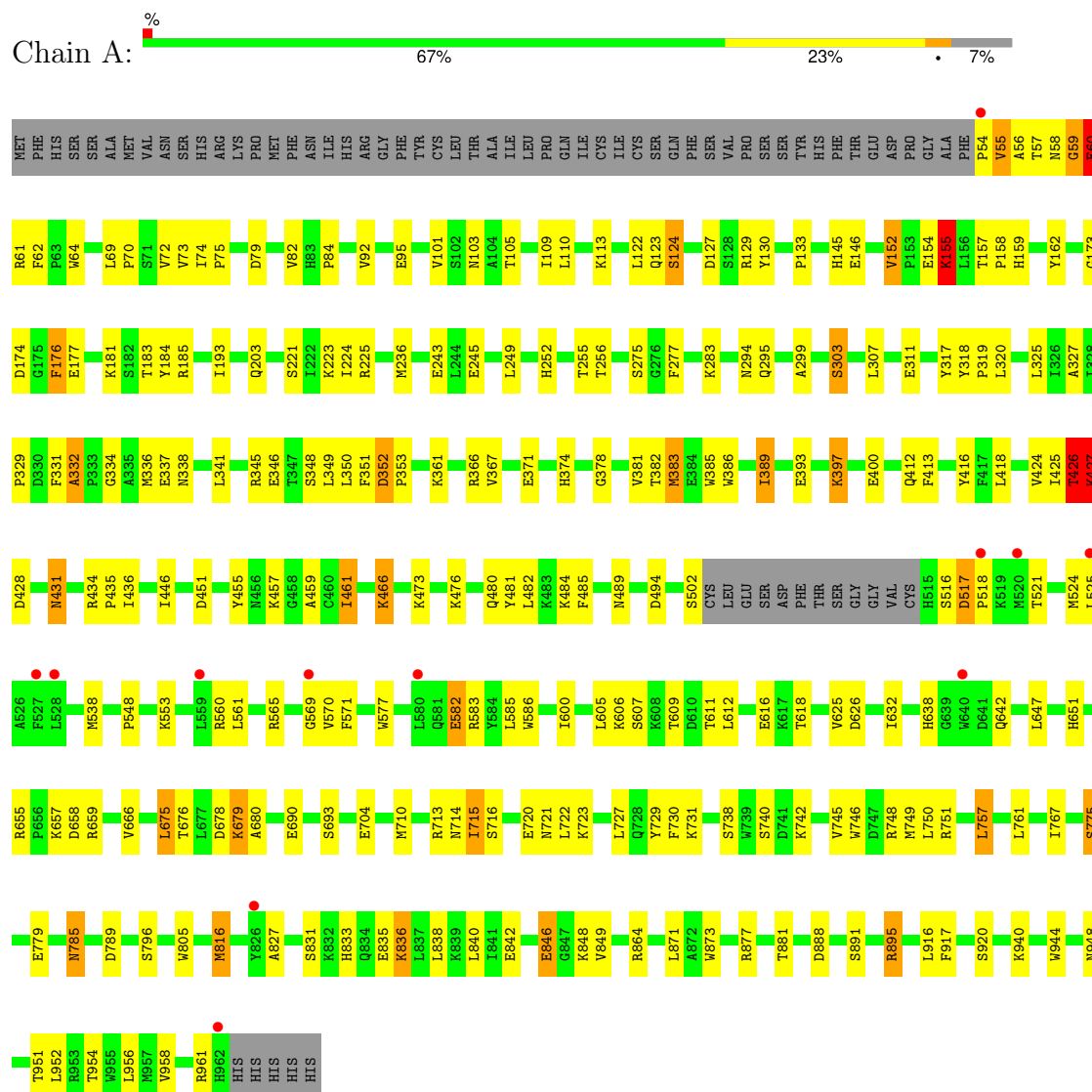
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	82	Total O 82 82	0	0
9	B	20	Total O 20 20	0	0

3 Residue-property plots

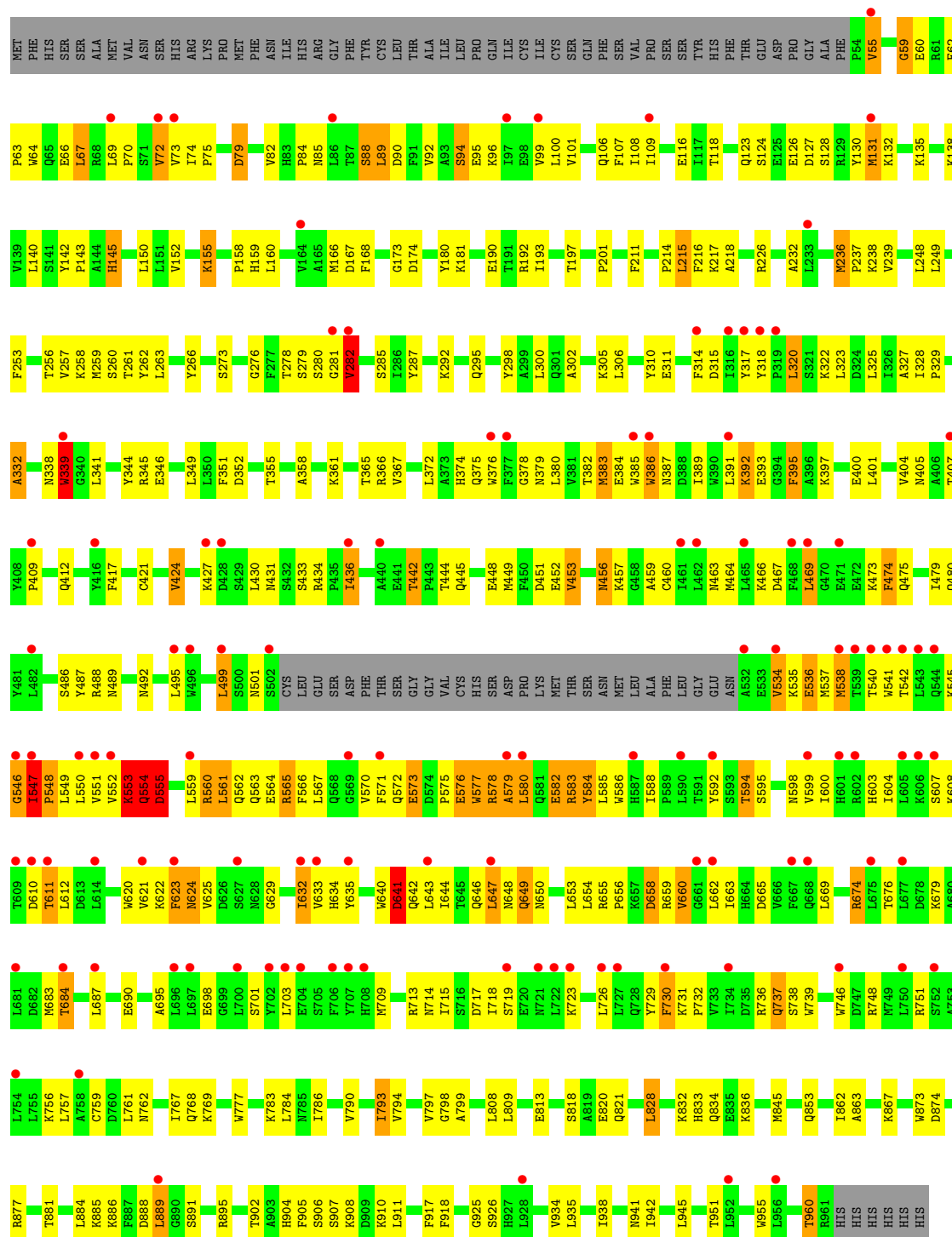
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2

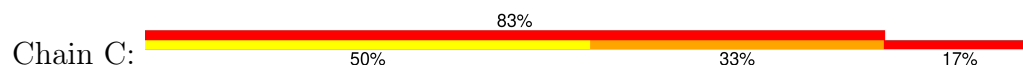


• Molecule 1: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2

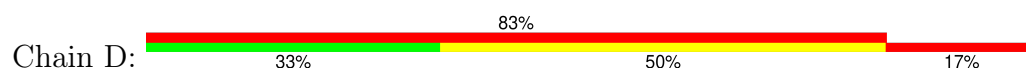




• Molecule 2: GPI



• Molecule 2: GPI



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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

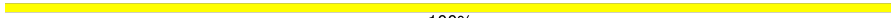


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

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

Chain N:  50% 50%

NAG1
NAG2

- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

NAG1
NAG2
BMA3
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 135.47Å 128.21Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	49.01 – 2.73 49.01 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.01-2.73) 98.6 (49.01-2.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.223 , 0.286 0.227 , 0.286	Depositor DCC
R_{free} test set	3395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15144	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, EDO, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	1/7550 (0.0%)	0.97	7/10229 (0.1%)
1	B	0.51	2/7334 (0.0%)	0.91	23/9939 (0.2%)
2	C	0.65	0/82	0.99	0/106
2	D	0.70	0/43	1.44	1/56 (1.8%)
All	All	0.63	3/15009 (0.0%)	0.94	31/20330 (0.2%)

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
2	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	C-N	-10.18	1.19	1.33
1	B	548	PRO	N-CD	5.26	1.55	1.47
1	B	547	ILE	C-N	5.17	1.40	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	GLY	N-CA-C	9.27	125.26	112.57
1	A	176	PHE	N-CA-C	-7.95	101.62	112.03
1	B	578	ARG	N-CA-C	-7.76	102.76	111.07
1	B	579	ALA	N-CA-C	-7.16	100.89	110.55
1	B	332	ALA	CA-C-N	-6.36	114.22	120.52
1	B	332	ALA	C-N-CA	-6.36	114.22	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	ILE	CA-C-N	-6.23	113.36	119.78
1	B	547	ILE	C-N-CA	-6.23	113.36	119.78
1	B	236	MET	CA-C-N	-6.12	114.23	120.85
1	B	236	MET	C-N-CA	-6.12	114.23	120.85
1	A	58	ASN	N-CA-C	-5.98	105.65	113.12
1	B	352	ASP	CA-C-N	5.78	127.07	119.84
1	B	352	ASP	C-N-CA	5.78	127.07	119.84
1	B	282	VAL	N-CA-C	5.76	121.33	109.34
1	A	569	GLY	N-CA-C	-5.75	106.81	115.32
1	B	555	ASP	N-CA-C	5.67	117.90	108.20
1	B	641	ASP	N-CA-C	-5.61	104.25	113.50
1	A	332	ALA	CA-C-N	-5.55	112.90	119.84
1	A	332	ALA	C-N-CA	-5.55	112.90	119.84
2	D	4	ARG	N-CA-C	5.31	118.33	110.48
1	A	55	VAL	N-CA-C	5.21	115.15	107.75
1	B	62	PHE	CA-C-N	5.19	126.33	119.84
1	B	62	PHE	C-N-CA	5.19	126.33	119.84
1	B	553	LYS	N-CA-C	5.15	116.03	107.73
1	B	142	TYR	CA-C-N	5.13	126.25	119.84
1	B	142	TYR	C-N-CA	5.13	126.25	119.84
1	B	577	TRP	CA-C-N	-5.05	113.88	120.44
1	B	577	TRP	C-N-CA	-5.05	113.88	120.44
1	A	60	GLU	N-CA-C	5.04	121.54	110.80
1	B	59	GLY	CA-C-N	5.01	130.72	121.70
1	B	59	GLY	C-N-CA	5.01	130.72	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	3[A]	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7344	0	7298	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7156	0	7112	344	0
2	C	80	0	79	11	0
2	D	42	0	42	6	0
3	E	39	0	34	0	0
3	G	39	0	34	0	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
4	K	28	0	25	1	0
4	M	28	0	25	1	0
4	N	28	0	25	1	0
5	L	50	0	43	6	0
6	A	28	0	26	0	0
6	B	42	0	39	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	12	0	18	0	0
8	B	12	0	18	0	0
9	A	82	0	0	9	0
9	B	20	0	0	8	0
All	All	15144	0	14918	513	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 17.

All (513) 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:566:PHE:CE1	1:B:567:LEU:O	1.72	1.40
1:B:554:GLN:CG	1:B:560:ARG:HD2	1.59	1.31
1:B:566:PHE:CD1	1:B:567:LEU:N	2.10	1.18
1:B:554:GLN:HG2	1:B:560:ARG:HD2	1.32	1.12
1:B:554:GLN:HG2	1:B:560:ARG:CD	1.88	1.03
1:B:634:HIS:CD2	1:B:635:TYR:H	1.76	1.02
1:B:566:PHE:HE1	1:B:567:LEU:O	1.43	1.00
1:B:554:GLN:CB	1:B:560:ARG:HD2	1.90	0.99
1:B:634:HIS:HB2	1:B:669:LEU:HD22	1.47	0.95
1:B:550:LEU:HB3	1:B:633:VAL:HG12	1.45	0.95
1:B:554:GLN:CG	1:B:560:ARG:CD	2.44	0.94
1:B:566:PHE:HD1	1:B:567:LEU:H	1.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LEU:HD12	1:B:550:LEU:N	1.84	0.91
1:A:236:MET:HE3	1:A:256:THR:HA	1.53	0.91
1:B:550:LEU:CB	1:B:633:VAL:HG12	2.01	0.90
1:B:552:VAL:N	1:B:634:HIS:O	2.05	0.89
1:B:573:GLU:HB3	1:B:674:ARG:NH2	1.87	0.88
1:B:634:HIS:CD2	1:B:635:TYR:N	2.42	0.87
1:A:426:THR:O	1:A:428:ASP:N	2.07	0.86
1:B:383:MET:HE1	1:B:392:LYS:HD3	1.59	0.85
1:B:566:PHE:O	1:B:567:LEU:HG	1.75	0.84
1:B:554:GLN:HB2	1:B:560:ARG:HG3	1.59	0.84
1:B:554:GLN:HG2	1:B:560:ARG:NE	1.93	0.83
1:B:59:GLY:HA3	1:B:60:GLU:HB2	1.59	0.83
1:B:552:VAL:HB	1:B:635:TYR:CD2	2.15	0.82
1:A:961:ARG:O	9:A:2074:HOH:O	1.97	0.82
1:B:554:GLN:CB	1:B:560:ARG:CD	2.57	0.81
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.61	0.81
1:B:573:GLU:HB3	1:B:674:ARG:HH21	1.45	0.81
1:B:576:GLU:O	1:B:579:ALA:O	2.00	0.80
1:B:383:MET:HE3	1:B:383:MET:H	1.46	0.80
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.17	0.80
1:B:549:LEU:HD12	1:B:550:LEU:H	1.44	0.79
1:B:549:LEU:HD13	1:B:632:ILE:HG22	1.64	0.79
1:B:215:LEU:O	1:B:217:LYS:N	2.17	0.78
1:B:553:LYS:O	1:B:560:ARG:HG3	1.84	0.77
1:B:554:GLN:CD	1:B:560:ARG:HD2	2.09	0.77
1:B:248:LEU:HD21	5:L:1:NAG:H61	1.67	0.77
1:B:600:ILE:HG12	1:B:625:VAL:HG21	1.65	0.76
1:B:550:LEU:O	1:B:633:VAL:HA	1.85	0.76
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.67	0.76
1:B:554:GLN:HB2	1:B:560:ARG:HD2	1.68	0.74
1:B:554:GLN:HB2	1:B:560:ARG:CG	2.18	0.74
1:B:551:VAL:O	1:B:561:LEU:HD13	1.88	0.74
1:B:769:LYS:NZ	9:B:2014:HOH:O	2.21	0.74
1:B:565:ARG:HD2	1:B:566:PHE:O	1.87	0.73
1:B:298:TYR:HH	1:B:365:THR:HG1	1.32	0.73
1:A:55:VAL:HB	1:A:62:PHE:H	1.53	0.73
1:B:108:ILE:HG23	1:B:150:LEU:HB2	1.69	0.73
1:B:486:SER:HB3	1:B:487:TYR:HD1	1.53	0.72
1:B:907:SER:HB2	1:B:910:LYS:HB2	1.70	0.72
1:B:60:GLU:HG2	1:B:140:LEU:HD11	1.72	0.72
1:B:374:HIS:HE1	1:B:392:LYS:HG2	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:MET:O	9:B:2002:HOH:O	2.07	0.71
1:B:236:MET:HE3	1:B:256:THR:HA	1.73	0.71
1:B:634:HIS:HD2	1:B:635:TYR:H	1.36	0.71
1:B:548:PRO:HG3	1:B:586:TRP:CE3	2.26	0.71
1:B:549:LEU:HB3	1:B:564:GLU:O	1.91	0.71
1:B:577:TRP:C	1:B:579:ALA:O	2.34	0.70
1:B:552:VAL:CG1	1:B:635:TYR:CD2	2.74	0.70
1:A:221:SER:HG	1:A:255:THR:HG1	1.39	0.70
1:B:552:VAL:HG11	1:B:635:TYR:CD2	2.26	0.70
1:B:592:TYR:HB3	1:B:623:PHE:HE1	1.56	0.69
1:B:550:LEU:HD23	1:B:562:GLN:O	1.93	0.69
1:A:895:ARG:HG3	1:A:895:ARG:HH11	1.58	0.68
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.75	0.68
1:B:553:LYS:O	1:B:554:GLN:HB2	1.92	0.68
2:C:2[A]:PRO:HB2	2:C:4[A]:ARG:HG3	1.74	0.68
1:A:236:MET:HE1	1:A:320:LEU:HD22	1.75	0.68
1:B:124:SER:HB2	1:B:130:TYR:HB2	1.76	0.68
1:B:106:GLN:HB3	1:B:155:LYS:HG2	1.76	0.67
1:A:838:LEU:HD13	1:A:871:LEU:HD11	1.75	0.67
1:B:436:ILE:HG22	1:B:453:VAL:HG12	1.77	0.67
1:B:554:GLN:HB2	1:B:560:ARG:CD	2.24	0.67
1:B:659:ARG:NH1	1:B:690:GLU:OE2	2.27	0.67
1:B:69:LEU:HD23	1:B:211:PHE:HD1	1.60	0.67
1:B:552:VAL:CB	1:B:635:TYR:CD2	2.77	0.67
1:A:659:ARG:NH1	1:A:690:GLU:OE1	2.28	0.66
2:D:4:ARG:H	2:D:4:ARG:HD2	1.61	0.66
1:B:95:GLU:O	9:B:2002:HOH:O	2.12	0.65
1:B:550:LEU:N	1:B:632:ILE:O	2.28	0.65
1:B:566:PHE:CD1	1:B:567:LEU:O	2.45	0.65
1:A:714:ASN:O	1:A:716:SER:N	2.30	0.65
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.78	0.65
1:B:595:SER:HB3	1:B:620:TRP:CE2	2.32	0.65
1:A:334:GLY:HA3	2:C:4[A]:ARG:H	1.63	0.64
1:B:563:GLN:OE1	1:B:586:TRP:N	2.23	0.64
1:B:566:PHE:CG	1:B:567:LEU:N	2.65	0.64
1:B:70:PRO:HB2	1:B:72:VAL:HG23	1.80	0.64
1:B:620:TRP:NE1	1:B:646:GLN:OE1	2.26	0.64
1:A:658:ASP:OD2	9:A:2049:HOH:O	2.15	0.64
1:B:552:VAL:HG11	1:B:635:TYR:CE2	2.33	0.64
1:A:553:LYS:HD2	1:A:560:ARG:HH21	1.62	0.63
1:A:397:LYS:HB3	1:A:459:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD2	1:B:109:ILE:HG21	1.80	0.63
1:B:64:TRP:NE1	1:B:70:PRO:HD3	2.13	0.62
1:B:562:GLN:HE21	1:B:608:LYS:CD	2.12	0.62
1:B:237:PRO:HG3	1:B:322:LYS:HG2	1.81	0.62
1:B:292:LYS:HG2	1:B:295:GLN:HE21	1.62	0.62
1:B:560:ARG:C	1:B:561:LEU:HD22	2.25	0.62
1:B:583:ARG:O	1:B:585:LEU:N	2.33	0.62
1:B:138:LYS:NZ	9:B:2005:HOH:O	2.33	0.62
1:A:836:LYS:NZ	9:A:2065:HOH:O	2.33	0.62
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.65	0.62
1:B:273:SER:HB3	1:B:287:TYR:CE1	2.35	0.62
1:B:280:SER:OG	1:B:281:GLY:N	2.32	0.61
1:A:954:THR:O	1:A:958:VAL:HG23	2.01	0.61
1:A:295:GLN:HG2	1:A:352:ASP:HB2	1.83	0.61
1:A:275:SER:OG	9:A:2030:HOH:O	2.16	0.61
1:B:292:LYS:NZ	1:B:346:GLU:OE1	2.32	0.61
1:B:551:VAL:HG12	1:B:553:LYS:HG2	1.81	0.61
1:B:560:ARG:O	1:B:561:LEU:HD22	2.00	0.60
1:A:517:ASP:HB2	1:A:518:PRO:HD3	1.82	0.60
1:B:173:GLY:H	1:B:180:TYR:HA	1.66	0.60
1:B:655:ARG:HB2	1:B:658:ASP:HB2	1.84	0.60
2:C:3[A]:GLY:O	2:C:4[A]:ARG:HB2	2.01	0.60
1:B:310:TYR:O	1:B:314:PHE:HB2	2.02	0.60
1:B:579:ALA:C	1:B:580:LEU:HD23	2.26	0.60
1:B:738:SER:OG	1:B:751:ARG:NH1	2.35	0.60
1:B:332:ALA:O	1:B:345:ARG:NH2	2.35	0.59
1:B:118:THR:HB	1:B:167:ASP:HB2	1.84	0.59
1:B:549:LEU:CD1	1:B:632:ILE:HG22	2.31	0.59
1:B:397:LYS:HB3	1:B:459:ALA:HB2	1.85	0.59
4:J:1:NAG:H3	4:J:1:NAG:H83	1.85	0.59
1:B:684:THR:O	1:B:684:THR:OG1	2.18	0.59
1:A:184:TYR:HB3	1:A:329:PRO:HG2	1.84	0.58
1:B:563:GLN:OE1	1:B:585:LEU:HA	2.03	0.58
1:B:874:ASP:OD1	1:B:877:ARG:NH2	2.34	0.58
1:A:59:GLY:O	1:A:60:GLU:O	2.21	0.58
1:B:594:THR:HG22	1:B:621:VAL:HG23	1.84	0.58
1:A:397:LYS:HD3	1:A:455:TYR:HB3	1.85	0.58
1:A:723:LYS:HG3	1:A:761:LEU:HB3	1.85	0.58
1:B:302:ALA:O	1:B:306:LEU:HB2	2.03	0.58
1:B:738:SER:O	1:B:751:ARG:HD2	2.02	0.58
1:B:257:VAL:HG12	4:N:2:NAG:H81	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:VAL:HG21	1:B:635:TYR:CE2	2.38	0.58
1:A:72:VAL:HG23	1:A:73:VAL:HG23	1.85	0.58
1:B:486:SER:HB3	1:B:487:TYR:CD1	2.37	0.58
1:B:565:ARG:HD2	1:B:566:PHE:N	2.19	0.58
1:B:226:ARG:HH12	1:B:249:LEU:HD12	1.68	0.58
1:B:881:THR:HG22	1:B:885:LYS:HE3	1.85	0.58
1:A:366:ARG:HH11	1:A:416:TYR:HE2	1.50	0.58
1:A:338:ASN:HB2	1:A:341:LEU:O	2.04	0.58
1:B:338:ASN:HB2	1:B:341:LEU:O	2.04	0.57
1:B:582:GLU:C	1:B:584:TYR:H	2.12	0.57
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.85	0.57
1:B:375:GLN:O	1:B:379:ASN:HB2	2.03	0.57
1:B:376:TRP:HA	1:B:380:LEU:HD12	1.87	0.57
1:B:576:GLU:HB3	1:B:580:LEU:HG	1.87	0.57
1:B:611:THR:O	1:B:611:THR:OG1	2.17	0.57
1:A:236:MET:HE3	1:A:256:THR:CA	2.31	0.57
1:B:214:PRO:HA	1:B:260:SER:HB3	1.85	0.57
1:B:259:MET:HE2	1:B:339:TRP:CD1	2.40	0.57
1:A:722:LEU:HG	1:A:956:LEU:HD11	1.86	0.57
1:B:88:SER:OG	1:B:90:ASP:OD1	2.22	0.57
1:B:550:LEU:HD22	1:B:561:LEU:HD12	1.86	0.57
1:B:818:SER:HA	1:B:821:GLN:HB2	1.87	0.56
1:B:886:LYS:NZ	9:B:2019:HOH:O	2.30	0.56
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.40	0.56
1:B:640:TRP:CD1	1:B:643:LEU:HD13	2.40	0.56
1:B:547:ILE:HG23	1:B:547:ILE:O	2.05	0.56
1:A:944:TRP:O	1:A:948:ASN:HB2	2.05	0.56
1:B:576:GLU:O	1:B:579:ALA:C	2.49	0.56
1:A:158:PRO:HB2	1:A:159:HIS:ND1	2.21	0.55
1:B:217:LYS:HD2	1:B:382:THR:OG1	2.06	0.55
1:A:473:LYS:HG3	1:A:502:SER:HB3	1.88	0.55
5:L:1:NAG:HO6	5:L:2:NAG:HO6	1.52	0.55
1:B:59:GLY:CA	1:B:60:GLU:HB2	2.35	0.55
1:B:756:LYS:HG3	1:B:793:ILE:HG23	1.86	0.55
1:B:634:HIS:CG	1:B:635:TYR:N	2.73	0.55
1:A:348:SER:HB3	1:A:367:VAL:HG11	1.88	0.55
1:B:566:PHE:O	1:B:567:LEU:CG	2.51	0.55
1:B:833:HIS:HB2	1:B:836:LYS:HB2	1.88	0.55
1:A:332:ALA:O	1:A:345:ARG:NH1	2.39	0.55
1:A:466:LYS:O	1:A:466:LYS:HG2	2.07	0.55
1:B:541:TRP:CZ3	1:B:548:PRO:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:TYR:HB3	1:B:623:PHE:CE1	2.39	0.55
1:B:622:LYS:HE2	1:B:662:LEU:HG	1.88	0.55
1:A:366:ARG:HD2	1:A:413:PHE:CE1	2.42	0.55
1:A:434:ARG:NH1	1:A:435:PRO:O	2.39	0.55
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.42	0.55
1:A:738:SER:O	1:A:751:ARG:HD3	2.06	0.55
1:B:732:PRO:O	1:B:736:ARG:HB2	2.06	0.54
1:B:550:LEU:HB2	1:B:633:VAL:HG12	1.84	0.54
1:A:176:PHE:CG	1:A:332:ALA:HB2	2.42	0.54
1:B:88:SER:HB3	5:L:1:NAG:H82	1.89	0.54
1:A:366:ARG:NH1	1:A:416:TYR:HE2	2.05	0.54
1:B:554:GLN:CB	1:B:560:ARG:CG	2.85	0.54
1:B:445:GLN:HA	1:B:448:GLU:HB2	1.90	0.54
1:A:383:MET:HG2	1:A:389:ILE:HA	1.90	0.54
1:B:594:THR:HA	1:B:621:VAL:HA	1.89	0.54
1:A:451:ASP:HA	2:C:4[A]:ARG:HH22	1.73	0.54
1:A:585:LEU:HD21	1:A:606:LYS:O	2.07	0.54
1:A:659:ARG:HH11	1:A:690:GLU:CD	2.16	0.54
1:B:552:VAL:CG1	1:B:635:TYR:HD2	2.20	0.54
1:B:660:VAL:HG13	1:B:695:ALA:HA	1.90	0.54
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.89	0.54
1:B:395:PHE:HE2	1:B:495:LEU:HD21	1.73	0.54
1:B:570:VAL:HG11	1:B:577:TRP:HB2	1.90	0.54
1:B:355:THR:HB	1:B:820:GLU:HB2	1.90	0.53
1:B:563:GLN:HB3	1:B:608:LYS:HB3	1.89	0.53
1:B:541:TRP:HH2	1:B:548:PRO:HG2	1.73	0.53
1:B:541:TRP:HH2	1:B:548:PRO:CD	2.22	0.53
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.43	0.53
1:B:375:GLN:HA	1:B:379:ASN:ND2	2.24	0.53
1:B:918:PHE:HE2	1:B:934:VAL:HB	1.73	0.53
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.74	0.53
1:A:710:MET:HE3	1:A:952:LEU:HD23	1.90	0.53
1:B:565:ARG:HG2	1:B:584:TYR:CD2	2.43	0.53
1:B:748:ARG:HG2	1:B:751:ARG:HH21	1.74	0.53
1:B:634:HIS:HB2	1:B:669:LEU:CD2	2.33	0.52
1:B:676:THR:HG23	1:B:679:LYS:HG2	1.91	0.52
1:B:375:GLN:HA	1:B:379:ASN:HD22	1.75	0.52
1:B:480:GLN:NE2	1:B:501:ASN:O	2.43	0.52
1:B:623:PHE:HD2	1:B:633:VAL:HG11	1.74	0.52
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.10	0.52
1:A:54:PRO:HG2	1:A:55:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5[A]:ALA:O	2:C:6[A]:PHE:HB2	2.08	0.52
1:A:647:LEU:HD21	1:A:659:ARG:HG2	1.92	0.52
1:A:704:GLU:HG3	1:A:757:LEU:HD12	1.91	0.52
1:B:537:MET:O	1:B:540:THR:OG1	2.26	0.52
1:B:580:LEU:N	1:B:580:LEU:CD2	2.73	0.52
1:B:552:VAL:O	1:B:635:TYR:HA	2.09	0.52
1:B:566:PHE:HD1	1:B:567:LEU:N	1.78	0.52
1:B:451:ASP:C	2:D:4:ARG:HH22	2.18	0.51
1:B:845:MET:O	1:B:886:LYS:HE2	2.11	0.51
1:A:223:LYS:HE2	1:A:252:HIS:CD2	2.46	0.51
1:B:124:SER:OG	1:B:127:ASP:HB3	2.11	0.51
1:B:634:HIS:CD2	1:B:669:LEU:HD13	2.46	0.51
4:M:1:NAG:O3	4:M:2:NAG:O5	2.24	0.51
1:B:474:PHE:HB3	1:B:499:LEU:HD21	1.92	0.51
1:B:809:LEU:HB2	1:B:828:LEU:HD21	1.92	0.51
1:B:256:THR:HB	1:B:259:MET:HE3	1.92	0.51
1:B:278:THR:OG1	1:B:279:SER:N	2.39	0.51
1:B:541:TRP:CH2	1:B:548:PRO:CD	2.94	0.51
1:B:217:LYS:HE3	1:B:259:MET:HA	1.92	0.51
1:B:541:TRP:CH2	1:B:548:PRO:HG2	2.46	0.50
1:B:808:LEU:HB2	1:B:828:LEU:HD11	1.93	0.50
1:B:442:THR:HG22	1:B:444:THR:H	1.76	0.50
1:B:448:GLU:HA	1:B:895:ARG:NH1	2.26	0.50
1:B:572:GLN:O	1:B:573:GLU:HG3	2.11	0.50
1:A:69:LEU:HD22	1:A:109:ILE:HG22	1.93	0.50
1:B:79:ASP:HB2	1:B:96:LYS:HG3	1.93	0.50
1:B:599:VAL:HG22	1:B:600:ILE:H	1.77	0.50
1:B:566:PHE:CZ	1:B:567:LEU:O	2.52	0.50
1:A:775:SER:O	1:A:779:GLU:HG2	2.11	0.50
1:B:579:ALA:O	1:B:580:LEU:HB2	2.11	0.50
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.47	0.49
1:B:85:ASN:ND2	9:B:2001:HOH:O	2.46	0.49
1:A:54:PRO:C	1:A:55:VAL:HG13	2.36	0.49
1:A:676:THR:OG1	1:A:678:ASP:OD1	2.27	0.49
1:B:127:ASP:OD1	1:B:128:SER:N	2.46	0.49
1:B:647:LEU:HD13	1:B:654:LEU:HD23	1.93	0.49
1:B:717:ASP:OD1	1:B:718:ILE:N	2.45	0.49
1:B:762:ASN:HA	1:B:767:ILE:HD11	1.94	0.49
5:L:3:BMA:H61	5:L:4:BMA:H2	1.65	0.49
1:B:158:PRO:HB2	1:B:159:HIS:ND1	2.27	0.49
1:A:334:GLY:HA3	2:C:4[A]:ARG:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:TRP:HH2	1:B:548:PRO:CG	2.26	0.49
1:B:456:ASN:OD1	1:B:456:ASN:N	2.46	0.49
1:B:644:ILE:HG23	1:B:683:MET:HG2	1.95	0.48
1:B:737:GLN:HG3	1:B:751:ARG:HG3	1.95	0.48
1:B:218:ALA:O	1:B:258:LYS:HA	2.14	0.48
1:B:232:ALA:O	1:B:253:PHE:HZ	1.96	0.48
1:A:82:VAL:HG12	1:A:84:PRO:HD3	1.95	0.48
1:B:385:TRP:CG	1:B:386:TRP:N	2.82	0.48
1:B:911:LEU:HB2	1:B:942:ILE:HD11	1.95	0.48
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.96	0.48
1:A:888:ASP:O	1:A:891:SER:OG	2.29	0.48
1:B:375:GLN:OE1	1:B:379:ASN:ND2	2.46	0.48
1:B:345:ARG:HG3	1:B:853:GLN:HE22	1.78	0.48
1:B:385:TRP:C	1:B:387:ASN:H	2.22	0.48
1:B:665:ASP:O	1:B:669:LEU:HG	2.14	0.48
1:B:687:LEU:HB2	1:B:730:PHE:HE1	1.79	0.48
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.95	0.48
1:A:451:ASP:HA	2:C:4[A]:ARG:NH2	2.28	0.48
1:B:888:ASP:O	1:B:891:SER:N	2.42	0.48
4:J:1:NAG:O3	4:J:2:NAG:H2	2.14	0.48
1:B:832:LYS:O	1:B:867:LYS:HD2	2.14	0.47
1:B:935:LEU:HD23	1:B:935:LEU:HA	1.71	0.47
1:A:346:GLU:HG2	1:A:350:LEU:HD12	1.95	0.47
1:A:877:ARG:HG2	1:A:917:PHE:CD1	2.49	0.47
1:B:393:GLU:CD	2:D:1:GLY:HA3	2.39	0.47
1:A:720:GLU:OE1	9:A:2055:HOH:O	2.20	0.47
1:B:469:LEU:O	1:B:473:LYS:HB2	2.14	0.47
1:B:64:TRP:CE2	1:B:70:PRO:HD3	2.49	0.47
1:B:554:GLN:OE1	1:B:560:ARG:HD2	2.14	0.47
1:A:425:ILE:C	1:A:426:THR:O	2.54	0.47
1:B:190:GLU:OE1	1:B:192:ARG:NH2	2.46	0.47
1:B:401:LEU:HD13	1:B:417:PHE:HB2	1.96	0.47
1:B:554:GLN:HB3	1:B:555:ASP:H	1.52	0.47
1:B:644:ILE:O	1:B:648:ASN:ND2	2.48	0.47
1:A:638:HIS:O	1:A:642:GLN:N	2.35	0.47
1:B:535:LYS:HB2	1:B:535:LYS:HE3	1.72	0.47
1:B:739:TRP:O	9:B:2012:HOH:O	2.20	0.47
5:L:1:NAG:O7	5:L:1:NAG:O3	2.21	0.47
1:A:184:TYR:HB3	1:A:329:PRO:CG	2.44	0.47
1:A:393:GLU:CD	2:C:1:GLY:HA3	2.38	0.47
1:A:693:SER:OG	1:A:750:LEU:HD22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:TYR:HD1	1:B:314:PHE:HE2	1.63	0.47
1:B:731:LYS:N	1:B:732:PRO:HD2	2.29	0.47
1:A:55:VAL:HG21	1:A:61:ARG:HA	1.96	0.46
1:B:318:TYR:CE1	1:B:339:TRP:HZ3	2.32	0.46
2:C:1:GLY:HA2	2:C:2[A]:PRO:HD3	1.57	0.46
1:A:331:PHE:O	1:A:345:ARG:HD2	2.15	0.46
1:A:385:TRP:CG	1:A:386:TRP:N	2.83	0.46
1:B:562:GLN:HE21	1:B:608:LYS:HD3	1.79	0.46
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.31	0.46
1:A:570:VAL:HG12	1:A:577:TRP:HD1	1.80	0.46
1:B:131:MET:HG3	1:B:132:LYS:H	1.80	0.46
1:A:299:ALA:O	1:A:303:SER:OG	2.29	0.46
1:B:566:PHE:C	1:B:567:LEU:HG	2.41	0.46
1:B:698:GLU:O	1:B:701:SER:OG	2.25	0.46
1:A:805:TRP:CD2	1:A:836:LYS:HD3	2.50	0.46
1:B:89:LEU:HD13	1:B:181:LYS:HD3	1.97	0.46
2:D:5:ALA:O	2:D:6:PHE:HB2	2.16	0.46
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.98	0.46
1:B:729:TYR:C	1:B:731:LYS:H	2.24	0.46
1:B:786:ILE:HD13	1:B:794:VAL:HG11	1.96	0.46
1:A:336:MET:HB2	1:A:336:MET:HE2	1.58	0.46
1:B:282:VAL:HG22	1:B:318:TYR:HD2	1.80	0.46
1:B:546:GLY:HA3	1:B:586:TRP:CZ2	2.51	0.46
1:B:729:TYR:O	1:B:731:LYS:N	2.48	0.46
1:A:397:LYS:O	1:A:400:GLU:HG3	2.16	0.46
1:B:292:LYS:HG2	1:B:295:GLN:NE2	2.29	0.46
1:B:306:LEU:O	1:B:310:TYR:HD2	1.99	0.46
1:B:397:LYS:HB3	1:B:397:LYS:HE3	1.83	0.46
1:B:683:MET:HE3	1:B:684:THR:HG22	1.97	0.46
1:A:740:SER:O	1:A:751:ARG:NE	2.49	0.45
1:B:938:ILE:HA	1:B:941:ASN:HB2	1.97	0.45
2:D:4:ARG:H	2:D:4:ARG:CD	2.25	0.45
1:B:655:ARG:O	1:B:659:ARG:HG3	2.16	0.45
1:B:884:LEU:HD13	1:B:889:LEU:HD23	1.98	0.45
1:B:535:LYS:HB3	1:B:536:GLU:H	1.49	0.45
1:A:351:PHE:CZ	1:A:361:LYS:HE3	2.51	0.45
1:B:424:VAL:HG13	1:B:452:GLU:HB3	1.98	0.45
1:B:709:MET:HE3	1:B:709:MET:HB2	1.86	0.45
1:A:385:TRP:CG	1:A:386:TRP:H	2.34	0.45
1:A:481:TYR:O	1:A:485:PHE:HD2	2.00	0.45
1:B:126:GLU:O	1:B:160:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:HD21	1:B:372:LEU:HD22	1.97	0.45
1:B:562:GLN:HG2	1:B:563:GLN:N	2.30	0.45
1:A:424:VAL:O	1:A:428:ASP:HB2	2.17	0.45
1:A:489:ASN:OD1	1:A:489:ASN:N	2.50	0.45
1:A:55:VAL:HG11	1:A:61:ARG:HG3	1.97	0.45
1:B:82:VAL:HG12	1:B:84:PRO:HD3	1.99	0.45
1:B:424:VAL:O	1:B:427:LYS:N	2.46	0.45
1:A:895:ARG:HG3	1:A:895:ARG:NH1	2.29	0.45
1:B:263:LEU:HD23	1:B:338:ASN:HA	1.98	0.45
1:A:55:VAL:O	1:A:56:ALA:HB2	2.16	0.45
1:A:484:LYS:HG2	1:A:485:PHE:CE2	2.51	0.45
1:A:173:GLY:O	1:A:181[A]:LYS:HG2	2.17	0.45
1:A:951:THR:OG1	9:A:2073:HOH:O	2.21	0.45
1:B:464:MET:CG	1:B:629:GLY:HA2	2.47	0.45
1:B:640:TRP:HB2	1:B:642:GLN:H	1.82	0.44
1:A:294:ASN:HD22	4:K:1:NAG:C7	2.30	0.44
1:A:366:ARG:HD2	1:A:413:PHE:HE1	1.82	0.44
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.52	0.44
1:B:649:GLN:HA	1:B:650:ASN:HA	1.72	0.44
1:B:106:GLN:HG3	1:B:107:PHE:H	1.80	0.44
1:A:243:GLU:HA	1:A:249:LEU:HD23	1.99	0.44
1:A:393:GLU:OE2	2:C:1:GLY:HA3	2.18	0.44
1:B:94:SER:HB3	1:B:167:ASP:OD1	2.18	0.44
1:B:400:GLU:O	1:B:404:VAL:HG23	2.17	0.44
1:B:541:TRP:HZ3	1:B:548:PRO:HD3	1.82	0.44
1:B:611:THR:O	1:B:612:LEU:HD23	2.18	0.44
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.52	0.44
1:A:582:GLU:HG3	1:A:583:ARG:HG2	2.00	0.44
1:A:679:LYS:HE2	1:A:679:LYS:HB2	1.91	0.44
1:B:314:PHE:O	1:B:479:ILE:HD12	2.17	0.44
1:B:541:TRP:CH2	1:B:548:PRO:CG	3.00	0.44
1:B:173:GLY:N	1:B:180:TYR:HA	2.32	0.44
1:B:393:GLU:OE2	2:D:1:GLY:HA3	2.18	0.44
1:A:79:ASP:O	1:A:95:GLU:HA	2.17	0.44
1:B:75:PRO:HA	1:B:99:VAL:HA	2.00	0.44
1:B:659:ARG:O	1:B:662:LEU:HB2	2.17	0.44
1:A:427:LYS:HE2	1:A:427:LYS:HB3	1.84	0.44
1:A:561:LEU:HD11	1:A:612:LEU:HD12	1.98	0.44
1:A:727:LEU:O	1:A:731:LYS:HB2	2.18	0.44
1:B:430:LEU:HD12	1:B:431:ASN:H	1.83	0.44
1:A:159:HIS:O	9:A:2011:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLN:OE1	1:A:745:VAL:HB	2.18	0.43
1:A:746:TRP:CE3	1:A:749:MET:HE3	2.52	0.43
1:B:106:GLN:HG3	1:B:107:PHE:CD1	2.53	0.43
1:B:236:MET:HE1	1:B:320:LEU:HD22	1.99	0.43
1:B:436:ILE:CG2	1:B:457:LYS:HD2	2.47	0.43
1:B:634:HIS:CE1	1:B:674:ARG:O	2.70	0.43
1:A:183:THR:HG22	1:A:193:ILE:HG12	1.99	0.43
1:A:655:ARG:HG3	9:A:2049:HOH:O	2.17	0.43
1:B:656:PRO:HA	1:B:659:ARG:NE	2.32	0.43
1:A:655:ARG:HG3	1:A:655:ARG:H	1.58	0.43
1:B:561:LEU:HD13	1:B:561:LEU:HA	1.74	0.43
1:B:391:LEU:O	1:B:395:PHE:HB2	2.19	0.43
1:A:796:SER:HB3	1:A:827:ALA:HA	2.00	0.43
1:B:325:LEU:HG	1:B:344:TYR:HE1	1.83	0.43
1:A:378:GLY:O	1:A:382:THR:OG1	2.23	0.43
1:A:431:ASN:HA	1:A:565:ARG:HH21	1.83	0.43
1:B:64:TRP:NE1	1:B:66:GLU:HB3	2.33	0.43
1:B:863:ALA:O	1:B:904:HIS:NE2	2.52	0.43
1:A:130:TYR:OH	1:A:152:VAL:HG13	2.18	0.43
1:A:742:LYS:O	1:A:751:ARG:NH2	2.52	0.43
1:A:796:SER:HA	1:A:827:ALA:HB1	2.01	0.43
1:B:474:PHE:CD1	1:B:474:PHE:C	2.96	0.43
1:A:600:ILE:HG23	1:A:625:VAL:HG21	2.00	0.43
1:B:374:HIS:CE1	1:B:393:GLU:OE2	2.72	0.43
1:B:640:TRP:HE3	1:B:641:ASP:HA	1.82	0.43
1:B:643:LEU:O	1:B:647:LEU:HB2	2.19	0.43
1:A:327:ALA:HB2	1:A:349:LEU:HD23	2.01	0.43
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.79	0.43
1:B:236:MET:HE3	1:B:256:THR:CA	2.45	0.43
1:B:238:LYS:HB3	1:B:238:LYS:HE2	1.81	0.43
1:B:433:SER:OG	1:B:434:ARG:N	2.48	0.43
1:A:485:PHE:CZ	1:A:494:ASP:HB3	2.54	0.42
1:A:785:ASN:OD1	9:A:2062:HOH:O	2.22	0.42
1:B:358:ALA:HB2	1:B:748:ARG:CZ	2.49	0.42
1:B:383:MET:HE3	1:B:383:MET:N	2.26	0.42
1:B:925:GLY:HA2	1:B:926:SER:HA	1.68	0.42
1:A:381:VAL:HG21	1:A:482:LEU:HA	2.01	0.42
1:B:261:THR:O	1:B:263:LEU:N	2.52	0.42
1:B:374:HIS:NE2	1:B:393:GLU:OE2	2.52	0.42
1:B:421:CYS:O	1:B:424:VAL:HG23	2.19	0.42
1:A:177:GLU:HG2	1:A:203:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:HD3	1:B:488:ARG:HA	2.02	0.42
1:B:310:TYR:HD1	1:B:314:PHE:CE2	2.37	0.42
1:B:378:GLY:CA	1:B:392:LYS:HG3	2.49	0.42
1:B:412:GLN:NE2	1:B:746:TRP:HD1	2.18	0.42
1:B:550:LEU:O	1:B:634:HIS:N	2.50	0.42
1:A:721:ASN:CB	1:A:956:LEU:HD13	2.49	0.42
1:B:88:SER:HG	1:B:90:ASP:CG	2.28	0.42
1:B:389:ILE:H	1:B:389:ILE:HG13	1.57	0.42
1:B:392:LYS:HB3	1:B:392:LYS:HE3	1.84	0.42
1:A:277:PHE:CE2	1:A:283:LYS:HB2	2.55	0.42
1:B:126:GLU:HB2	1:B:160:LEU:HB3	2.00	0.42
1:B:582:GLU:C	1:B:584:TYR:N	2.76	0.42
1:B:723:LYS:HG3	1:B:761:LEU:HB3	2.02	0.42
1:B:729:TYR:HB3	1:B:730:PHE:CD2	2.55	0.42
1:B:328:ILE:HA	1:B:329:PRO:HD3	1.79	0.42
1:B:731:LYS:HE2	1:B:731:LYS:HB3	1.75	0.42
1:B:877:ARG:HG2	1:B:917:PHE:CE1	2.55	0.42
1:B:905:PHE:O	1:B:938:ILE:HG23	2.20	0.42
1:A:55:VAL:HG12	1:A:62:PHE:O	2.19	0.42
1:A:113:LYS:HB2	1:A:146:GLU:HG2	2.01	0.42
1:A:371:GLU:OE2	2:C:2[B]:PRO:HD2	2.19	0.42
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.93	0.42
1:B:305:LYS:HE2	1:B:305:LYS:HB3	1.86	0.42
1:B:563:GLN:O	1:B:563:GLN:HG2	2.19	0.42
1:A:157:THR:HA	1:A:158:PRO:HD2	1.80	0.42
1:A:721:ASN:HB2	1:A:956:LEU:HD13	2.02	0.42
1:B:579:ALA:CB	1:B:580:LEU:HD23	2.50	0.42
1:A:476:LYS:O	1:A:480:GLN:HG3	2.20	0.41
1:B:298:TYR:OH	1:B:365:THR:OG1	2.08	0.41
1:B:449:MET:HE2	1:B:449:MET:HB3	1.89	0.41
1:A:745:VAL:O	1:A:749:MET:HG3	2.20	0.41
1:B:116:GLU:O	1:B:168:PHE:HA	2.20	0.41
1:B:366:ARG:HG2	1:B:400:GLU:OE1	2.20	0.41
1:B:434:ARG:HE	1:B:449:MET:HE3	1.86	0.41
1:B:576:GLU:O	1:B:579:ALA:HB3	2.21	0.41
1:B:577:TRP:O	1:B:578:ARG:C	2.60	0.41
1:A:64:TRP:CE3	1:A:70:PRO:HG3	2.56	0.41
1:A:607:SER:C	1:A:609:THR:H	2.28	0.41
1:B:261:THR:C	1:B:263:LEU:H	2.28	0.41
1:B:545:LYS:O	1:B:545:LYS:HG2	2.20	0.41
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.91	0.41
1:B:580:LEU:HD23	1:B:580:LEU:N	2.36	0.41
1:A:647:LEU:HD23	1:A:651:HIS:HB2	2.01	0.41
1:A:748:ARG:HB3	1:A:789:ASP:OD2	2.20	0.41
1:B:407:THR:C	1:B:409:PRO:HD3	2.45	0.41
1:B:538:MET:CE	1:B:541:TRP:HD1	2.32	0.41
1:A:154:GLU:O	1:A:155:LYS:C	2.63	0.41
1:B:314:PHE:O	1:B:315:ASP:HB3	2.20	0.41
1:A:74:ILE:HA	1:A:75:PRO:HD2	1.95	0.41
1:B:797:VAL:O	1:B:799:ALA:N	2.53	0.41
1:A:729:TYR:O	1:A:730:PHE:HB2	2.20	0.41
1:B:748:ARG:HG2	1:B:751:ARG:NH2	2.36	0.41
1:A:64:TRP:CE2	1:A:70:PRO:HG3	2.56	0.41
1:A:185:ARG:NH1	1:A:816:MET:HE3	2.36	0.41
1:B:351:PHE:CZ	1:B:361:LYS:HD2	2.56	0.41
1:B:372:LEU:HA	1:B:375:GLN:HG2	2.02	0.41
1:B:460:CYS:O	1:B:463:ASN:N	2.54	0.41
1:B:951:THR:O	1:B:955:TRP:HB2	2.21	0.41
1:B:70:PRO:C	1:B:72:VAL:H	2.29	0.41
1:B:385:TRP:O	1:B:387:ASN:N	2.54	0.41
1:B:442:THR:O	1:B:445:GLN:HG2	2.21	0.41
1:B:549:LEU:HD13	1:B:632:ILE:CG2	2.43	0.41
1:B:902:THR:O	1:B:905:PHE:HB2	2.21	0.41
1:B:276:GLY:HA3	1:B:300:LEU:HD11	2.02	0.40
1:B:384:GLU:HA	1:B:489:ASN:HB3	2.02	0.40
1:B:703:LEU:HD13	1:B:726:LEU:HD21	2.02	0.40
1:B:67:LEU:HG	1:B:145:HIS:CD2	2.56	0.40
1:B:226:ARG:NH1	1:B:249:LEU:HD12	2.36	0.40
1:B:464:MET:HG2	1:B:629:GLY:HA2	2.03	0.40
1:B:541:TRP:CH2	1:B:548:PRO:HD3	2.56	0.40
1:B:624:ASN:HD22	1:B:624:ASN:HA	1.63	0.40
1:A:124:SER:OG	1:A:127:ASP:N	2.50	0.40
1:A:318:TYR:HA	1:A:319:PRO:HD3	1.93	0.40
1:A:424:VAL:HG21	1:A:457:LYS:HB2	2.03	0.40
1:A:746:TRP:CZ3	1:A:749:MET:HE3	2.56	0.40
1:B:197:THR:HG23	1:B:266:TYR:O	2.22	0.40
1:B:659:ARG:O	1:B:663:ILE:HG13	2.22	0.40
1:A:325:LEU:N	1:A:325:LEU:HD12	2.36	0.40
1:A:538:MET:HE3	1:A:538:MET:HB3	1.95	0.40
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.69	0.40
1:A:846:GLU:OE1	1:A:848:LYS:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:OE1	1:B:317:TYR:HA	2.21	0.40
1:B:550:LEU:HB2	1:B:632:ILE:O	2.22	0.40
1:B:560:ARG:HB3	1:B:610:ASP:OD2	2.20	0.40
1:B:713:ARG:HB2	1:B:715:ILE:HG13	2.04	0.40
9:B:2001:HOH:O	5:L:1:NAG:C1	2.69	0.40
1:A:457:LYS:O	1:A:461:ILE:HG23	2.21	0.40
1:A:675:LEU:HD12	1:A:675:LEU:HA	1.67	0.40
1:B:436:ILE:HG21	1:B:457:LYS:HD2	2.02	0.40
1:B:575:PRO:HG2	1:B:576:GLU:OE1	2.21	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	901/967 (93%)	814 (90%)	75 (8%)	12 (1%)	9	23
1	B	875/967 (90%)	732 (84%)	117 (13%)	26 (3%)	3	7
2	C	8/6 (133%)	4 (50%)	0	4 (50%)	0	0
2	D	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1788/1946 (92%)	1554 (87%)	192 (11%)	42 (2%)	5	12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	60	GLU
1	A	245	GLU
1	A	582	GLU
1	A	616	GLU
1	B	216	PHE

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Mol	Chain	Res	Type
1	B	536	GLU
1	B	554	GLN
1	B	571	PHE
1	B	584	TYR
1	A	124	SER
1	A	427	LYS
1	A	605	LEU
1	A	715	ILE
1	B	72	VAL
1	B	89	LEU
1	B	131	MET
1	B	143	PRO
1	B	155	LYS
1	B	598	ASN
1	B	960	THR
2	C	4[A]	ARG
2	C	4[B]	ARG
2	C	5[A]	ALA
2	C	5[B]	ALA
1	A	155	LYS
1	A	426	THR
1	B	63	PRO
1	B	649	GLN
1	B	730	PHE
1	B	262	TYR
1	B	453	VAL
1	B	534	VAL
1	B	607	SER
1	B	215	LEU
1	B	339	TRP
1	B	386	TRP
1	B	436	ILE
1	B	798	GLY
1	B	55	VAL
1	A	133	PRO
1	B	201	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	813/870 (93%)	758 (93%)	55 (7%)	14	33
1	B	790/870 (91%)	706 (89%)	84 (11%)	6	16
2	C	6/3 (200%)	4 (67%)	2 (33%)	0	0
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1612/1746 (92%)	1470 (91%)	142 (9%)	9	22

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	101	VAL
1	A	103	ASN
1	A	105	THR
1	A	110	LEU
1	A	123	GLN
1	A	129	ARG
1	A	145	HIS
1	A	152	VAL
1	A	155	LYS
1	A	174	ASP
1	A	224	ILE
1	A	225	ARG
1	A	303	SER
1	A	307	LEU
1	A	352	ASP
1	A	383	MET
1	A	389	ILE
1	A	397	LYS
1	A	426	THR
1	A	427	LYS
1	A	431	ASN
1	A	436	ILE
1	A	461	ILE
1	A	466	LYS
1	A	516	SER
1	A	517	ASP
1	A	521	THR
1	A	524	MET
1	A	525	LEU

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Mol	Chain	Res	Type
1	A	571	PHE
1	A	611	THR
1	A	618	THR
1	A	632	ILE
1	A	675	LEU
1	A	679	LYS
1	A	757	LEU
1	A	767	ILE
1	A	775	SER
1	A	785	ASN
1	A	816	MET
1	A	831	SER
1	A	835	GLU
1	A	836	LYS
1	A	842[A]	GLU
1	A	842[B]	GLU
1	A	846	GLU
1	A	849	VAL
1	A	864	ARG
1	A	873	TRP
1	A	881	THR
1	A	895	ARG
1	A	916	LEU
1	A	920	SER
1	A	940	LYS
1	B	55	VAL
1	B	67	LEU
1	B	73	VAL
1	B	74	ILE
1	B	79	ASP
1	B	88	SER
1	B	92	VAL
1	B	94	SER
1	B	100	LEU
1	B	101	VAL
1	B	123	GLN
1	B	145	HIS
1	B	152	VAL
1	B	174	ASP
1	B	193	ILE
1	B	239	VAL
1	B	282	VAL

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Mol	Chain	Res	Type
1	B	285	SER
1	B	320	LEU
1	B	339	TRP
1	B	367	VAL
1	B	383	MET
1	B	392	LYS
1	B	395	PHE
1	B	405	ASN
1	B	424	VAL
1	B	442	THR
1	B	456	ASN
1	B	466	LYS
1	B	467	ASP
1	B	469	LEU
1	B	474	PHE
1	B	475	GLN
1	B	492	ASN
1	B	499	LEU
1	B	534	VAL
1	B	538	MET
1	B	542	THR
1	B	547	ILE
1	B	553	LYS
1	B	554	GLN
1	B	555	ASP
1	B	559	LEU
1	B	560	ARG
1	B	561	LEU
1	B	565	ARG
1	B	573	GLU
1	B	576	GLU
1	B	580	LEU
1	B	582	GLU
1	B	583	ARG
1	B	588	ILE
1	B	594	THR
1	B	603	HIS
1	B	604	ILE
1	B	611	THR
1	B	623	PHE
1	B	624	ASN
1	B	632	ILE

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Mol	Chain	Res	Type
1	B	641	ASP
1	B	647	LEU
1	B	653	LEU
1	B	658	ASP
1	B	660	VAL
1	B	674	ARG
1	B	684	THR
1	B	714	ASN
1	B	719	SER
1	B	737	GLN
1	B	757	LEU
1	B	759	CYS
1	B	768	GLN
1	B	783	LYS
1	B	790	VAL
1	B	793	ILE
1	B	813	GLU
1	B	828	LEU
1	B	834	GLN
1	B	862	ILE
1	B	889	LEU
1	B	906	SER
1	B	908	LYS
1	B	945	LEU
1	B	960	THR
2	C	4[A]	ARG
2	C	4[B]	ARG
2	D	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	GLN
1	A	651	HIS
1	A	708	HIS
1	A	785	ASN
1	B	295	GLN
1	B	562	GLN
1	B	581	GLN
1	B	624	ASN
1	B	634	HIS
1	B	806	ASN

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Mol	Chain	Res	Type
1	B	879	ASN
1	B	924	GLN
1	B	959	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 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
3	NAG	E	1	1,3	14,14,15	0.49	0	17,19,21	0.54	0
3	NAG	E	2	3	14,14,15	1.27	1 (7%)	17,19,21	1.70	1 (5%)
3	BMA	E	3	3	11,11,12	1.21	2 (18%)	15,15,17	1.33	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.68	1 (7%)	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.47	0	17,19,21	0.46	0
3	NAG	G	1	1,3	14,14,15	1.08	1 (7%)	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	0.66	0
3	BMA	G	3	3	11,11,12	2.05	4 (36%)	15,15,17	2.14	5 (33%)
4	NAG	H	1	1,4	14,14,15	0.32	0	17,19,21	0.76	1 (5%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.38	0
4	NAG	I	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	I	2	4	14,14,15	0.87	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.32	0	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	2	4	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	K	1	1,4	14,14,15	0.93	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	K	2	4	14,14,15	0.46	0	17,19,21	0.36	0
5	NAG	L	1	5,1	14,14,15	0.80	0	17,19,21	1.50	2 (11%)
5	NAG	L	2	5	14,14,15	0.64	0	17,19,21	1.40	1 (5%)
5	BMA	L	3	5	11,11,12	1.58	2 (18%)	15,15,17	1.09	1 (6%)
5	BMA	L	4	5	11,11,12	0.99	0	15,15,17	1.45	2 (13%)
4	NAG	M	1	1,4	14,14,15	0.39	0	17,19,21	0.57	0
4	NAG	M	2	4	14,14,15	0.52	0	17,19,21	0.51	0
4	NAG	N	1	1,4	14,14,15	0.31	0	17,19,21	0.91	0
4	NAG	N	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
5	NAG	L	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	BMA	L	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	4.59	1.51	1.43
5	L	3	BMA	C2-C3	3.98	1.58	1.52
3	G	3	BMA	O5-C5	3.91	1.51	1.43
3	G	3	BMA	C1-C2	3.77	1.61	1.52
3	G	1	NAG	O5-C1	-3.54	1.37	1.43
4	K	1	NAG	O5-C1	-3.21	1.38	1.43
3	G	3	BMA	O5-C1	2.91	1.48	1.43
4	I	2	NAG	O5-C1	2.86	1.48	1.43
4	N	2	NAG	C1-C2	2.54	1.55	1.52
3	E	3	BMA	O5-C5	2.50	1.48	1.43
3	E	3	BMA	C1-C2	2.44	1.58	1.52
4	I	1	NAG	O5-C1	-2.32	1.39	1.43
3	G	3	BMA	C2-C3	2.16	1.55	1.52
4	F	1	NAG	C1-C2	2.01	1.55	1.52
5	L	3	BMA	O5-C5	2.00	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	6.64	121.09	112.19
3	G	3	BMA	C1-O5-C5	6.45	120.83	112.19
5	L	2	NAG	C1-O5-C5	4.84	118.68	112.19
4	J	1	NAG	C2-N2-C7	4.61	129.08	122.90
5	L	1	NAG	O4-C4-C3	-4.04	100.85	110.38
5	L	3	BMA	O3-C3-C2	3.37	116.94	110.05
5	L	1	NAG	C4-C3-C2	3.30	115.85	111.02
4	I	2	NAG	C1-O5-C5	3.09	116.33	112.19
5	L	4	BMA	C1-O5-C5	2.97	116.17	112.19
3	E	3	BMA	C1-O5-C5	2.88	116.04	112.19
4	J	1	NAG	C1-C2-N2	2.43	114.26	110.43
4	K	1	NAG	C3-C4-C5	2.39	114.56	110.23
3	G	3	BMA	O5-C1-C2	2.27	116.20	110.79
3	G	3	BMA	C3-C4-C5	-2.22	106.20	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-C2-C3	2.08	112.68	109.64
4	I	1	NAG	O4-C4-C3	-2.07	105.50	110.38
3	E	3	BMA	C1-C2-C3	2.05	112.64	109.64
3	G	3	BMA	O2-C2-C3	-2.03	105.94	110.15
5	L	4	BMA	O2-C2-C3	-2.01	105.98	110.15
4	H	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1	NAG	C3-C2-N2-C7
4	M	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	K	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C1-C2-N2-C7

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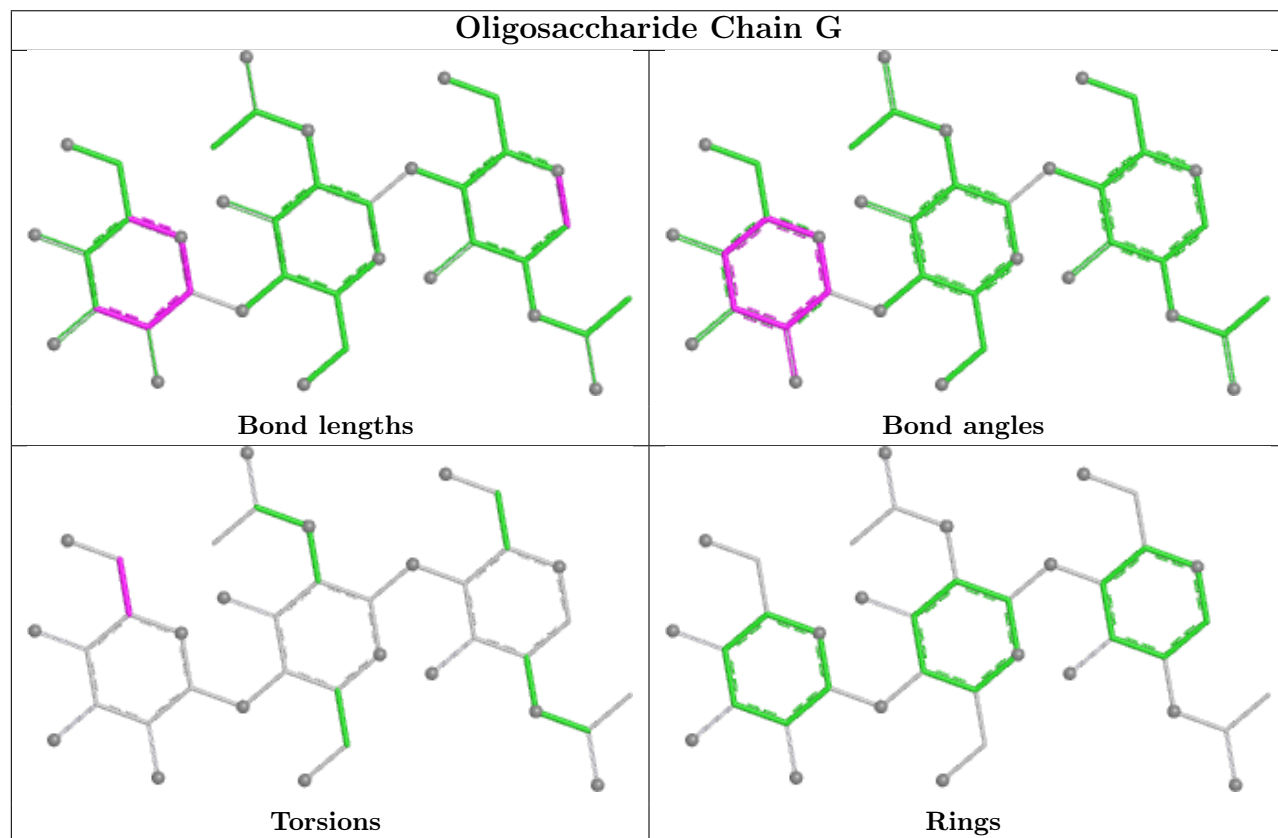
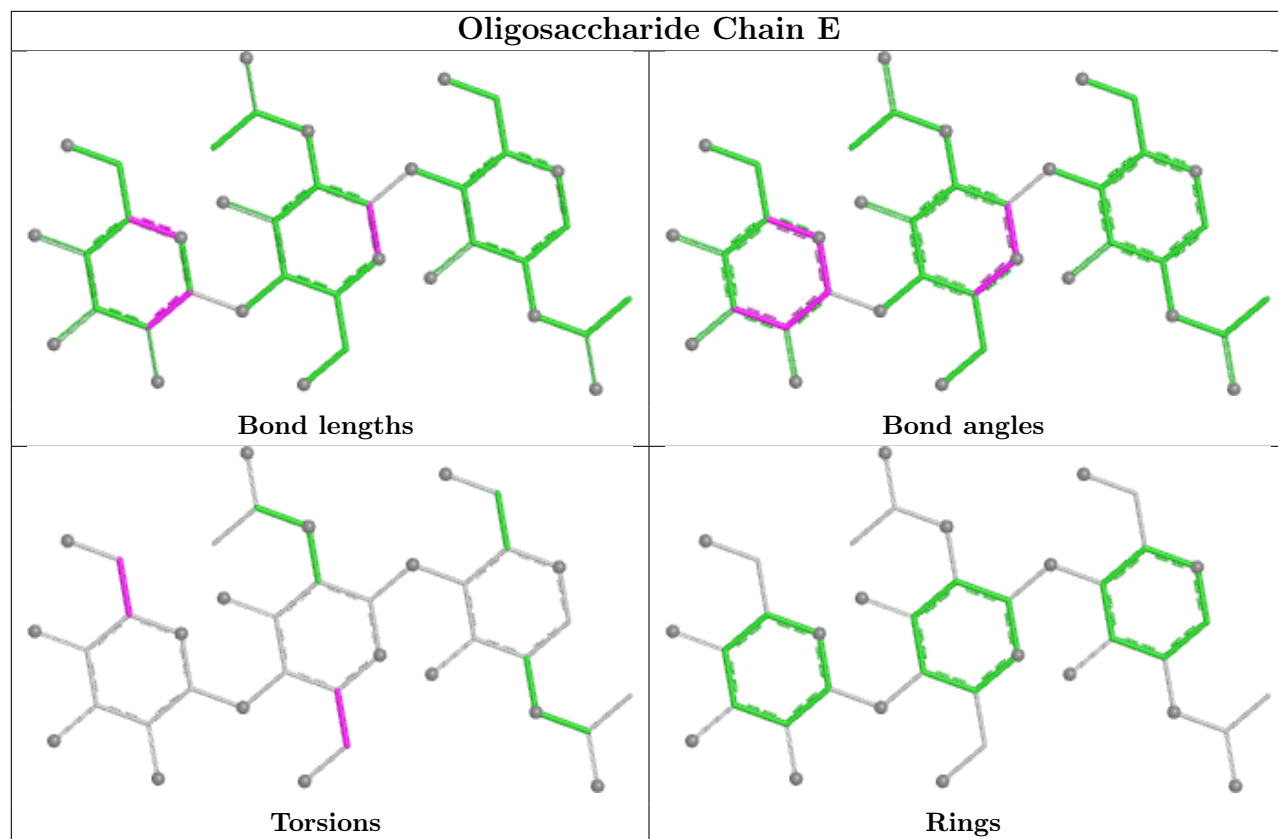
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C3-C2-N2-C7
4	N	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C1-C2-N2-C7
4	N	1	NAG	C3-C2-N2-C7

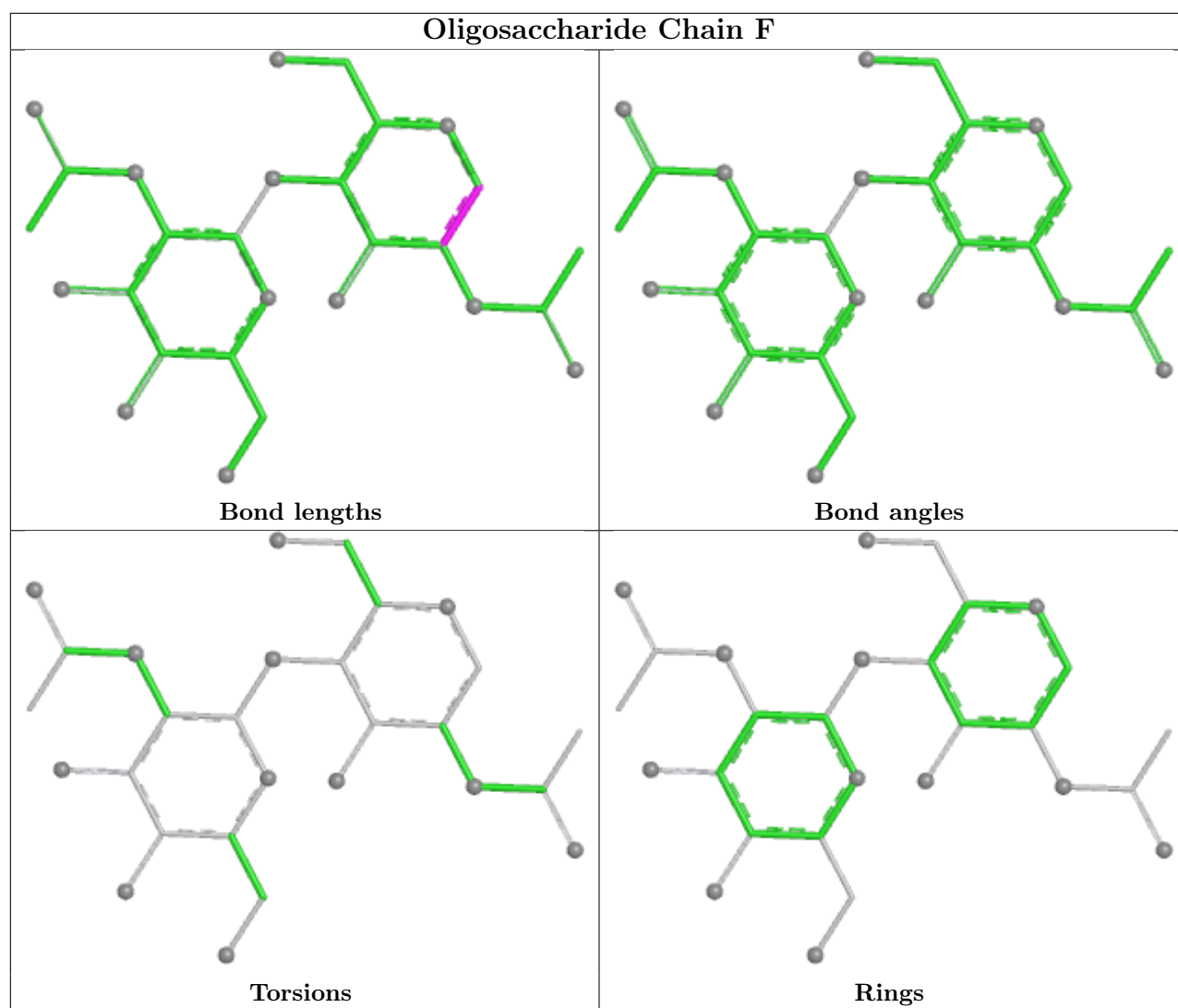
There are no ring outliers.

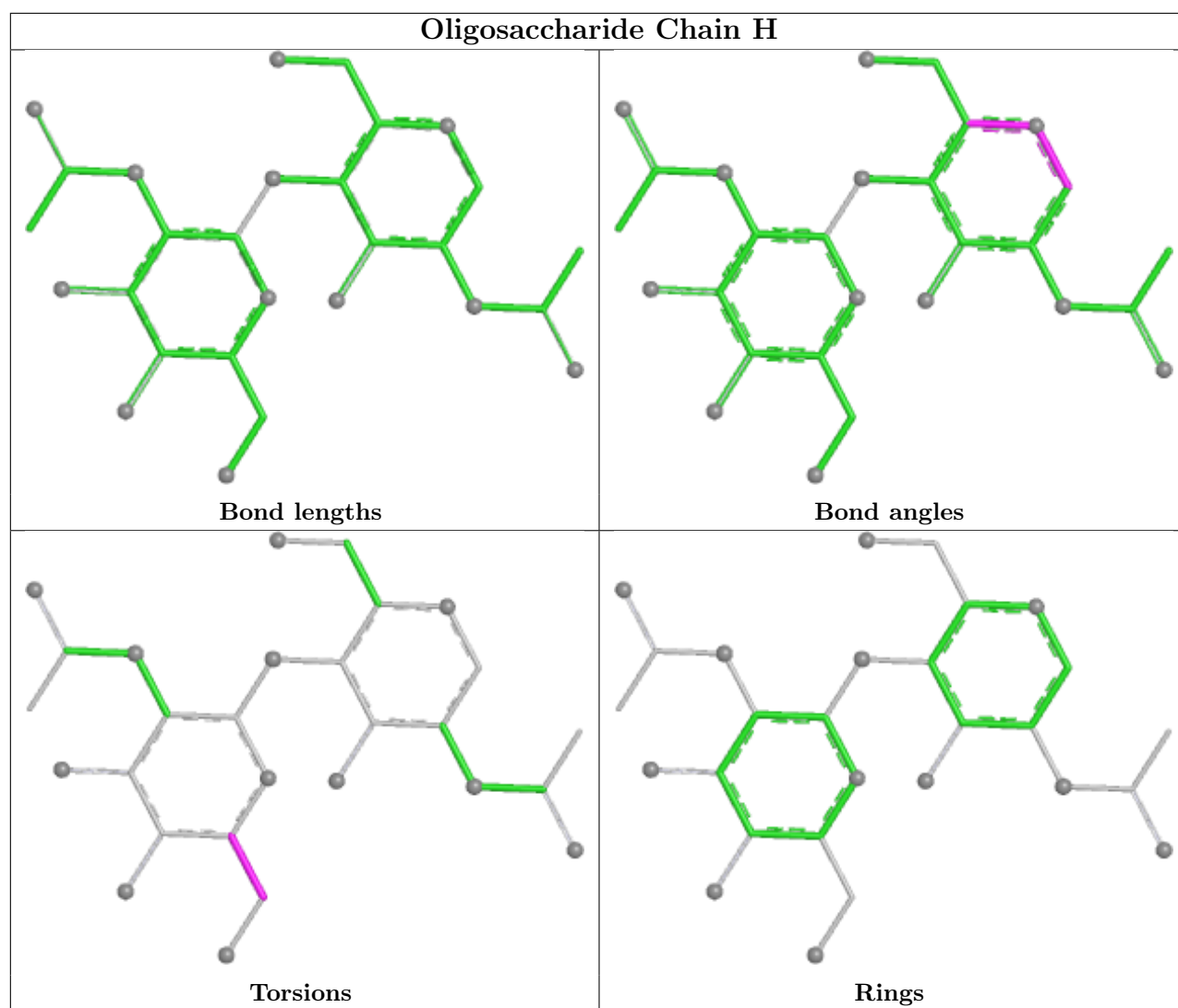
10 monomers are involved in 11 short contacts:

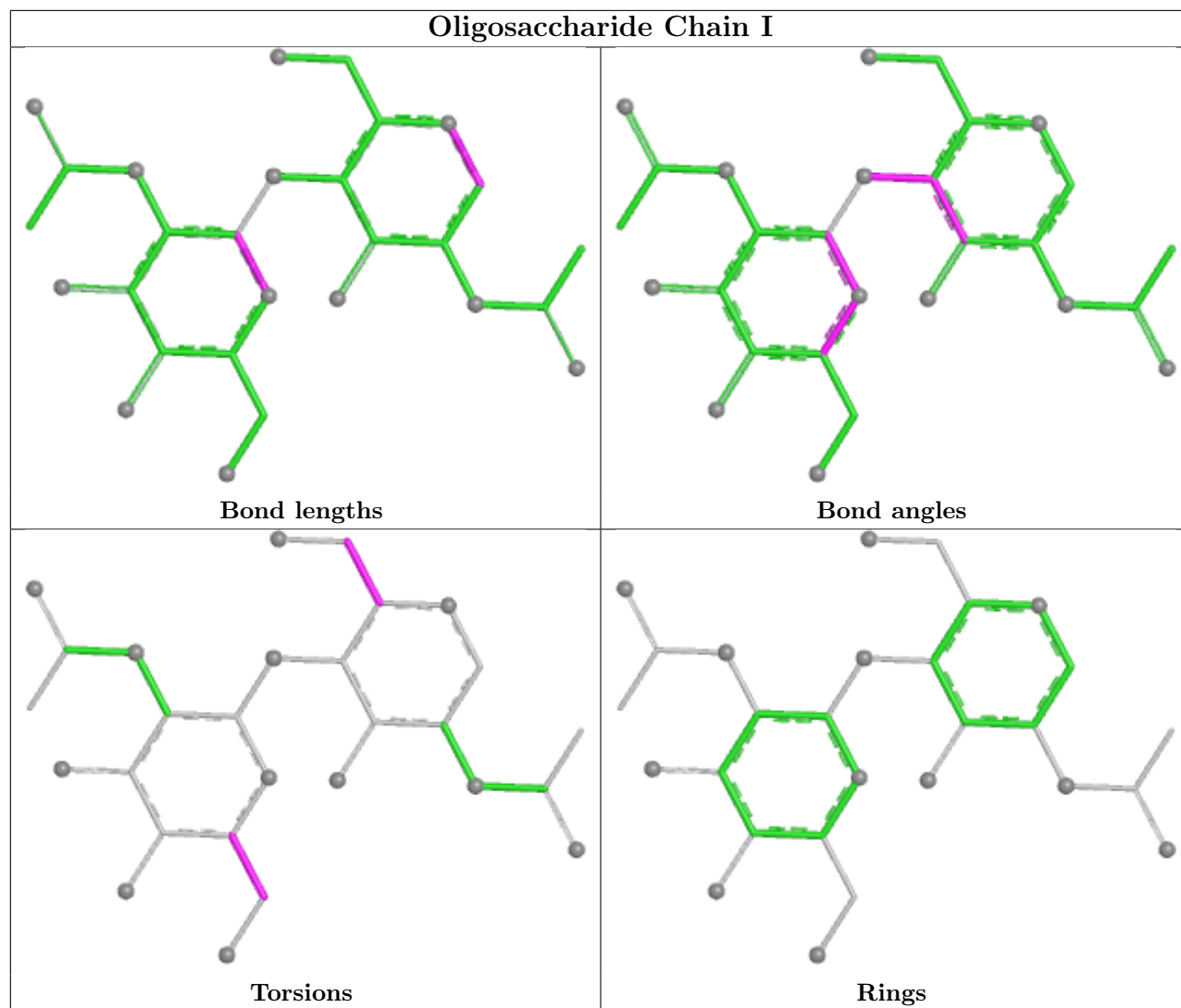
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	N	2	NAG	1	0
5	L	2	NAG	1	0
4	M	1	NAG	1	0
4	J	1	NAG	2	0
5	L	4	BMA	1	0
4	M	2	NAG	1	0
5	L	1	NAG	5	0
5	L	3	BMA	1	0
4	J	2	NAG	1	0

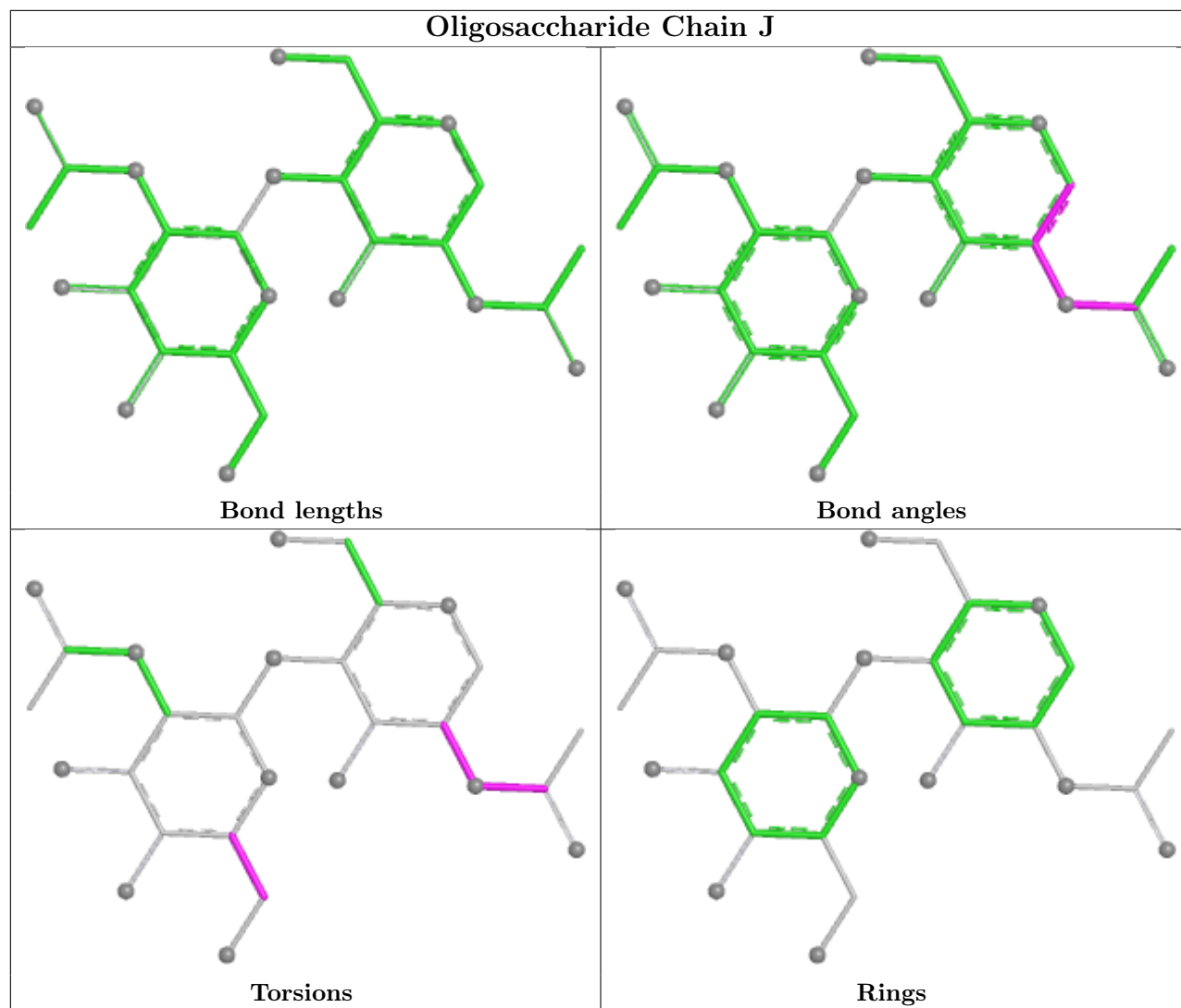
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

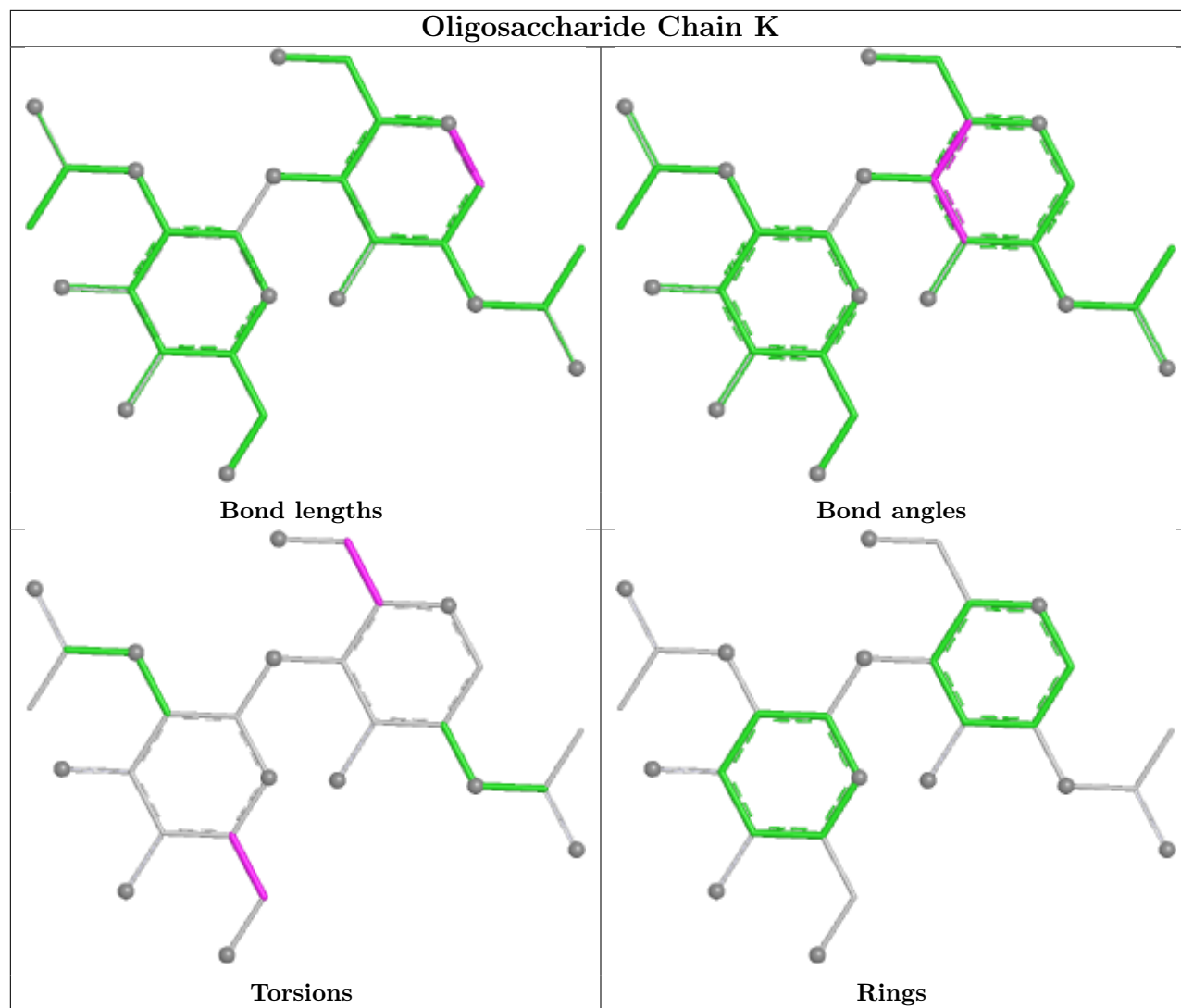


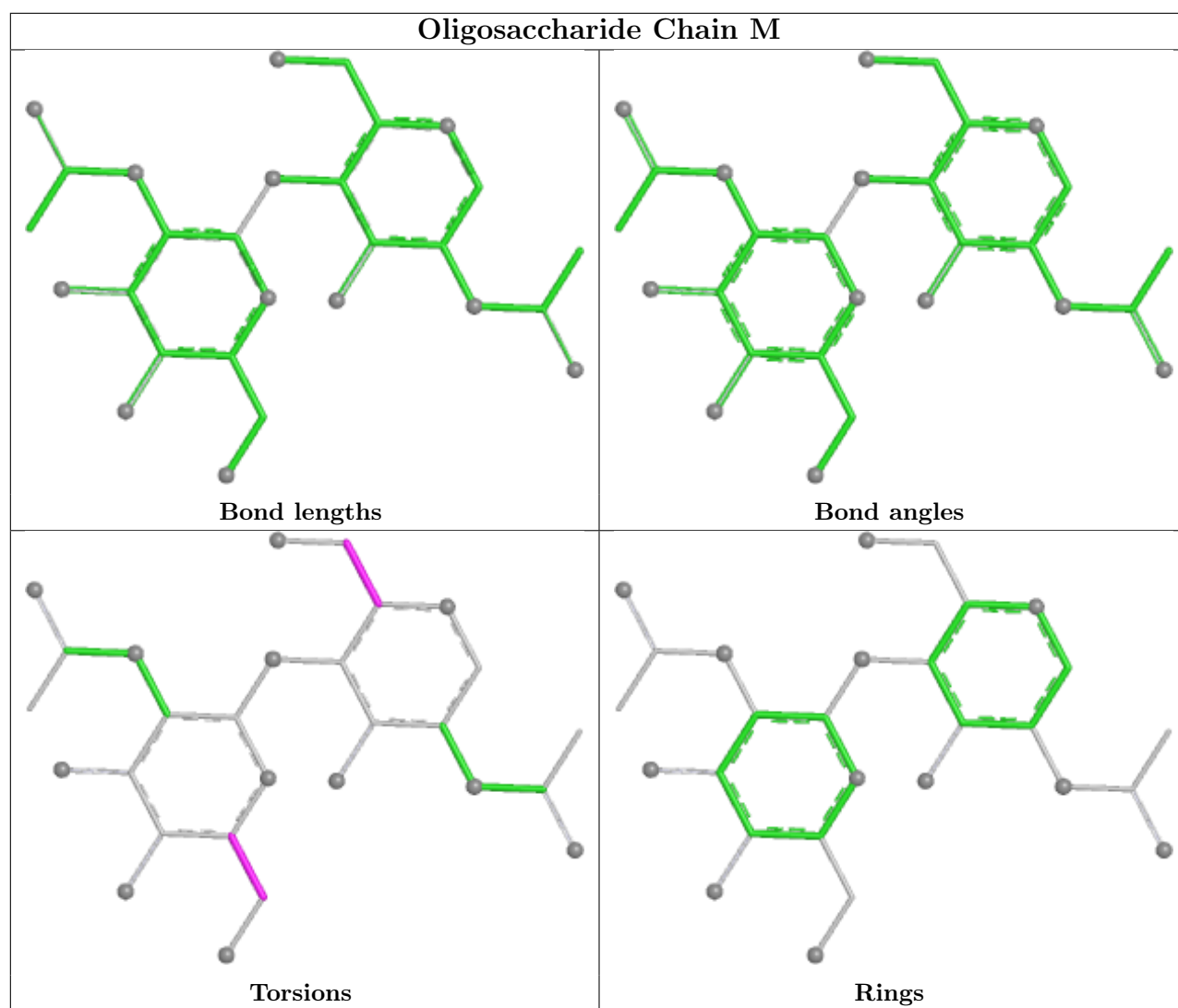


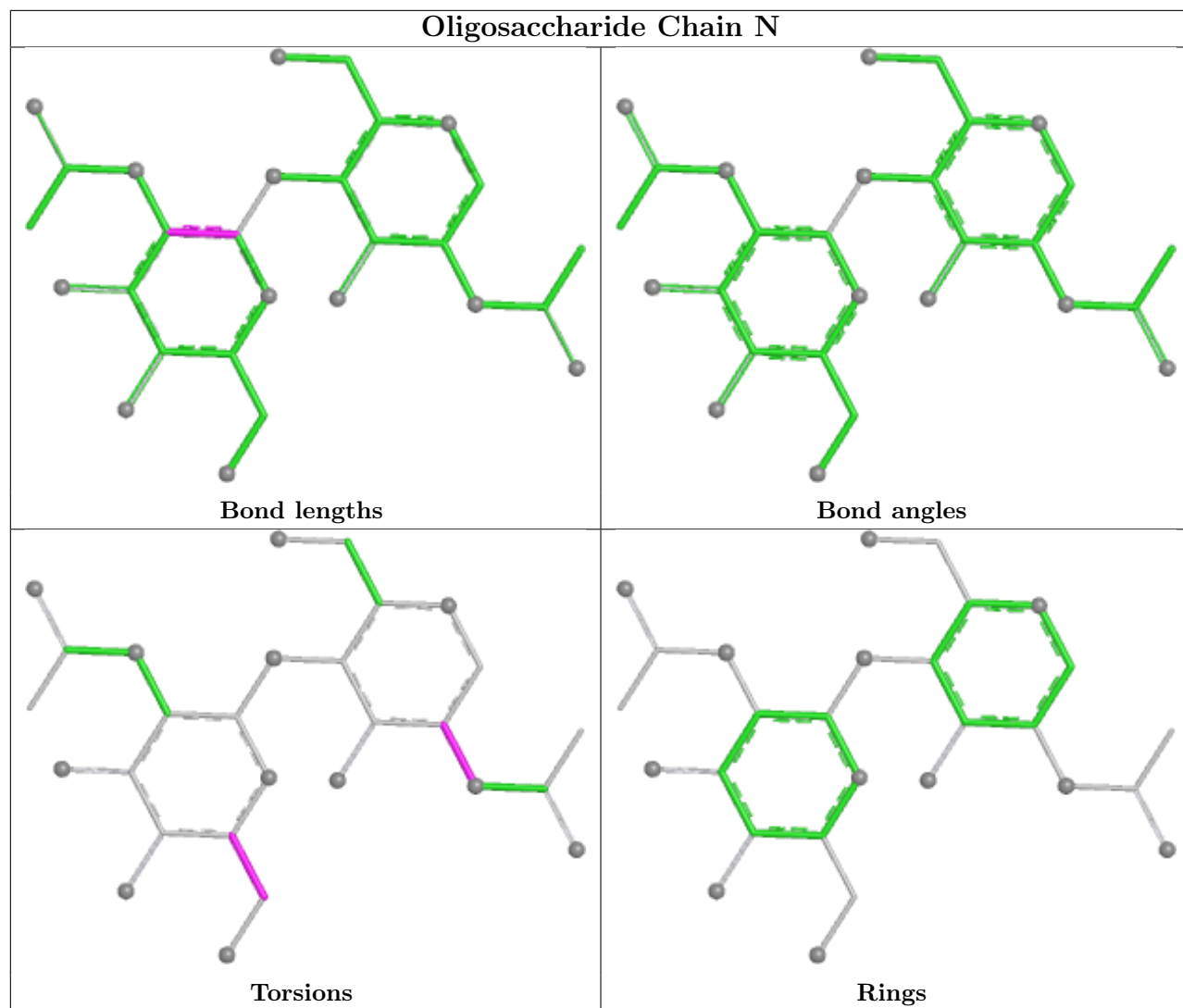


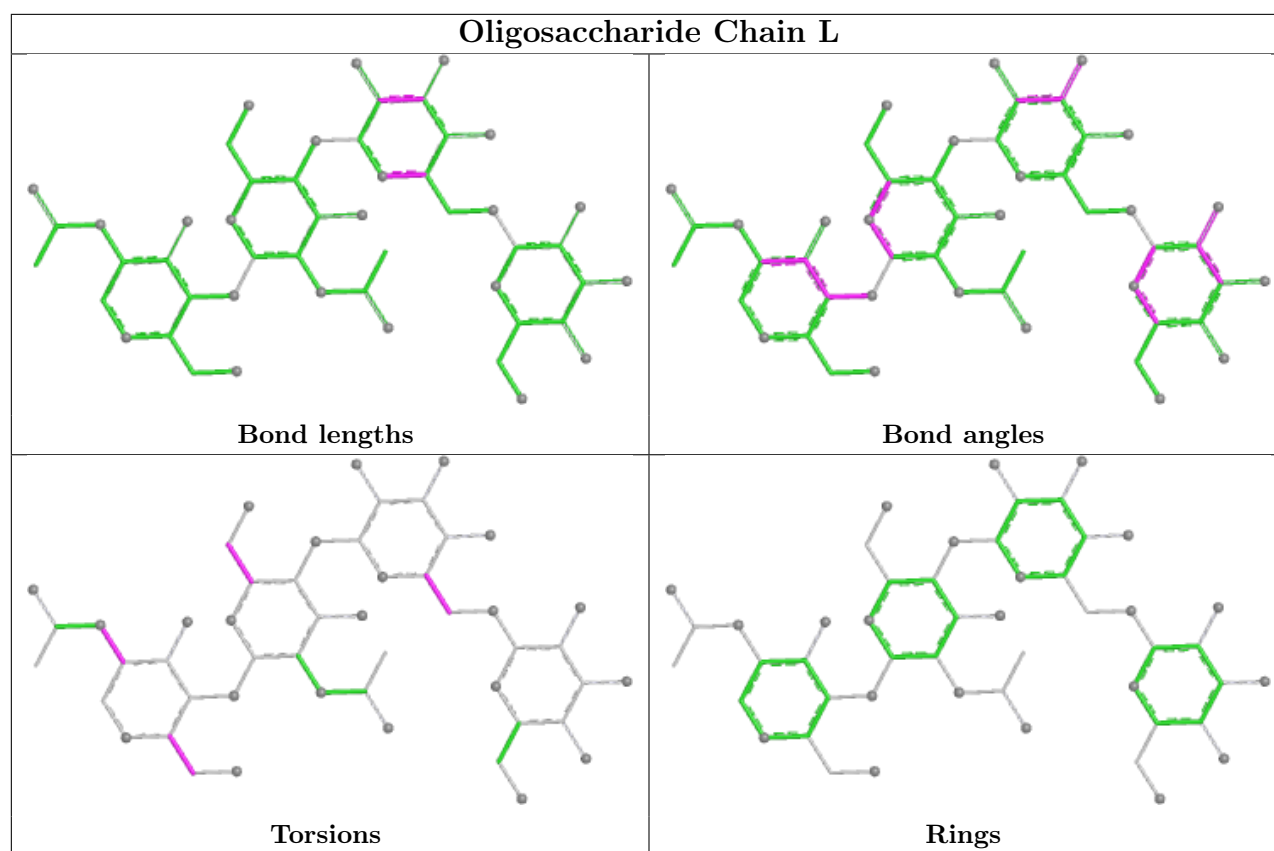












5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
6	NAG	A	1018	1	14,14,15	0.52	0	17,19,21	0.57	0
6	NAG	B	1011	1	14,14,15	0.54	0	17,19,21	0.46	0
8	EDO	A	1964	-	3,3,3	0.51	0	2,2,2	0.25	0
8	EDO	B	1962	-	3,3,3	0.44	0	2,2,2	0.37	0
6	NAG	A	1009	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
6	NAG	B	1005	1	14,14,15	0.54	0	17,19,21	0.62	1 (5%)
8	EDO	B	1961	-	3,3,3	0.48	0	2,2,2	0.20	0
8	EDO	A	1962	-	3,3,3	0.63	0	2,2,2	0.13	0
8	EDO	B	1963	-	3,3,3	0.41	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	1963	-	3,3,3	0.44	0	2,2,2	0.41	0
6	NAG	B	1010	1	14,14,15	0.37	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1018	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1011	1	-	4/6/23/26	0/1/1/1
8	EDO	A	1964	-	-	0/1/1/1	-
8	EDO	B	1962	-	-	0/1/1/1	-
6	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
8	EDO	B	1961	-	-	0/1/1/1	-
8	EDO	A	1962	-	-	1/1/1/1	-
8	EDO	B	1963	-	-	0/1/1/1	-
8	EDO	A	1963	-	-	0/1/1/1	-
6	NAG	B	1010	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1009	NAG	C1-O5-C5	2.31	115.28	112.19
6	B	1005	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1010	NAG	O5-C5-C6-O6
6	A	1018	NAG	O5-C5-C6-O6
6	B	1011	NAG	O5-C5-C6-O6
6	B	1010	NAG	C4-C5-C6-O6
6	A	1018	NAG	C4-C5-C6-O6
6	B	1011	NAG	C4-C5-C6-O6
6	A	1018	NAG	C8-C7-N2-C2
6	A	1018	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	B	1011	NAG	C8-C7-N2-C2
6	B	1011	NAG	O7-C7-N2-C2
6	B	1005	NAG	O5-C5-C6-O6
6	A	1009	NAG	O5-C5-C6-O6
6	A	1009	NAG	C4-C5-C6-O6
8	A	1962	EDO	O1-C1-C2-O2
6	B	1005	NAG	C4-C5-C6-O6

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	59:GLY	C	60:GLU	N	1.19

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	897/967 (92%)	-0.16	12 (1%) 75 73	24, 47, 86, 151	8 (0%)
1	B	879/967 (90%)	0.91	117 (13%) 7 6	30, 100, 150, 170	0
2	C	6/6 (100%)	3.73	5 (83%) 0 0	24, 26, 27, 42	5 (83%)
2	D	6/6 (100%)	5.72	5 (83%) 0 0	57, 59, 64, 68	6 (100%)
All	All	1788/1946 (91%)	0.40	139 (7%) 19 17	24, 66, 137, 170	19 (1%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	5	ALA	8.8
2	D	3	GLY	7.2
2	D	4	ARG	6.7
2	C	6[A]	PHE	6.7
2	D	6	PHE	6.3
1	B	318	TYR	5.7
2	C	3[A]	GLY	5.4
1	A	826[A]	TYR	5.3
1	B	580	LEU	5.0
1	A	962	HIS	4.6
1	B	667	PHE	4.4
1	B	727	LEU	4.3
2	C	5[A]	ALA	4.2
1	B	696	LEU	4.1
1	B	704	GLU	4.1
1	B	687	LEU	4.1
1	B	499	LEU	4.1
1	B	750	LEU	4.1
2	D	2	PRO	4.0
1	B	559	LEU	4.0
1	B	532	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	539	THR	3.8
1	B	681	LEU	3.6
1	B	281	GLY	3.5
1	B	316	ILE	3.5
1	B	543	LEU	3.5
1	B	605	LEU	3.4
1	B	502	SER	3.4
1	A	520	MET	3.4
1	B	416	TYR	3.4
1	B	386	TRP	3.3
1	B	752	SER	3.3
1	B	552	VAL	3.3
1	B	723	LYS	3.2
1	B	587	HIS	3.2
1	B	551	VAL	3.2
1	B	534	VAL	3.2
1	B	233	LEU	3.0
1	B	721	ASN	3.0
1	B	72	VAL	3.0
1	B	609	THR	3.0
1	B	495	LEU	2.9
1	B	722	LEU	2.9
1	B	376	TRP	2.9
1	B	546	GLY	2.9
1	B	469	LEU	2.9
1	B	109	ILE	2.9
1	B	662	LEU	2.9
1	B	956	LEU	2.9
1	B	282	VAL	2.8
1	B	461	ILE	2.8
1	B	952	LEU	2.8
1	B	611	THR	2.8
1	B	627	SER	2.8
1	B	623	PHE	2.8
2	C	4[A]	ARG	2.8
1	A	528	LEU	2.7
1	B	440	ALA	2.7
1	B	677	LEU	2.7
1	B	719	SER	2.7
1	B	707	TYR	2.7
1	A	569	GLY	2.7
1	B	339	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	427	LYS	2.6
1	B	607	SER	2.6
1	B	706	PHE	2.6
1	B	635	TYR	2.6
1	B	73	VAL	2.6
1	B	377	PHE	2.6
1	B	496	TRP	2.6
1	B	703	LEU	2.6
1	A	518	PRO	2.6
1	B	314	PHE	2.6
1	B	590	LEU	2.5
1	B	697	LEU	2.5
1	B	599	VAL	2.5
1	B	547	ILE	2.5
1	B	55	VAL	2.5
1	B	571	PHE	2.5
1	B	69	LEU	2.5
1	B	550	LEU	2.5
1	B	579	ALA	2.5
1	B	684	THR	2.4
1	B	726	LEU	2.4
1	B	734	ILE	2.4
1	B	661	GLY	2.4
1	A	580	LEU	2.4
1	A	54	PRO	2.4
1	B	592	TYR	2.4
1	B	633	VAL	2.4
1	B	700	LEU	2.4
1	B	614	LEU	2.4
1	B	610	ASP	2.4
1	B	465	LEU	2.3
1	B	540	THR	2.3
1	B	541	TRP	2.3
1	B	746	TRP	2.3
2	C	2[A]	PRO	2.3
1	B	544	GLN	2.3
1	B	462	LEU	2.3
1	B	482	LEU	2.3
1	B	164	VAL	2.3
1	A	527	PHE	2.3
1	B	889	LEU	2.3
1	B	436	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	319	PRO	2.3
1	B	601	HIS	2.3
1	B	471	GLU	2.3
1	B	409	PRO	2.3
1	B	407	THR	2.2
1	B	542	THR	2.2
1	B	385	TRP	2.2
1	B	391	LEU	2.2
1	B	730	PHE	2.2
1	B	428	ASP	2.2
1	A	525	LEU	2.2
1	B	758	ALA	2.2
1	B	675	LEU	2.2
1	A	640	TRP	2.2
1	B	97	ILE	2.2
1	B	754	LEU	2.2
1	B	928	LEU	2.2
1	B	632	ILE	2.2
1	B	668	GLN	2.1
1	B	569	GLY	2.1
1	B	99	VAL	2.1
1	B	708	HIS	2.1
1	B	602	ARG	2.1
1	B	621	VAL	2.1
1	B	468	PHE	2.1
1	B	643	LEU	2.1
1	A	559	LEU	2.1
1	B	647	LEU	2.1
1	B	702	TYR	2.1
1	B	131	MET	2.0
1	B	538	MET	2.0
1	B	86	LEU	2.0
1	B	317	TYR	2.0
1	B	606	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

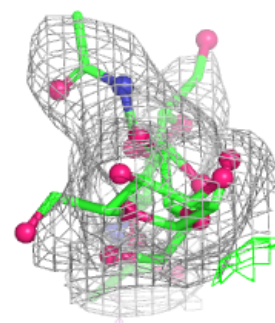
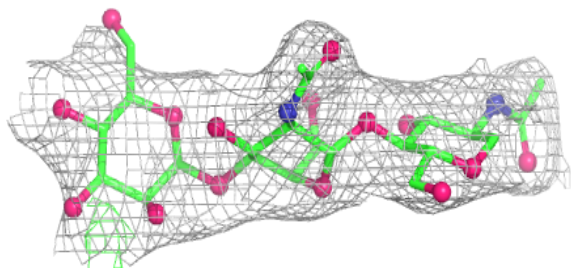
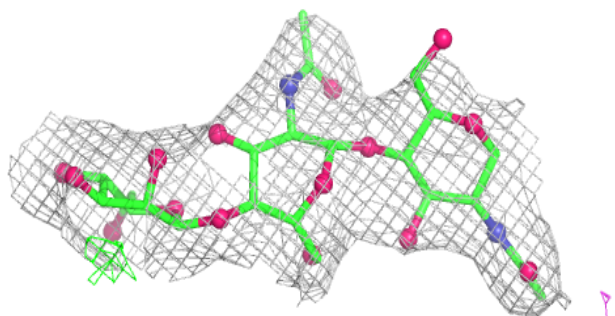
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	M	2	14/15	0.27	0.13	131,158,162,163	0
4	NAG	M	1	14/15	0.40	0.13	138,153,159,164	0
4	NAG	F	2	14/15	0.40	0.12	142,155,160,161	0
4	NAG	J	2	14/15	0.43	0.14	119,132,141,141	0
3	BMA	E	3	11/12	0.45	0.12	109,117,121,122	0
3	BMA	G	3	11/12	0.50	0.14	90,97,105,107	0
4	NAG	I	2	14/15	0.53	0.15	112,122,130,132	0
4	NAG	K	2	14/15	0.57	0.13	115,128,133,139	0
5	BMA	L	4	11/12	0.58	0.15	73,100,109,113	0
4	NAG	J	1	14/15	0.59	0.13	106,127,136,138	0
5	BMA	L	3	11/12	0.61	0.13	73,98,104,104	0
4	NAG	F	1	14/15	0.61	0.11	91,119,136,146	0
4	NAG	H	2	14/15	0.64	0.13	103,114,118,119	0
4	NAG	N	2	14/15	0.66	0.16	121,133,137,140	0
4	NAG	N	1	14/15	0.67	0.14	91,115,128,134	0
4	NAG	K	1	14/15	0.68	0.13	57,92,108,122	0
5	NAG	L	2	14/15	0.83	0.10	50,77,88,88	0
3	NAG	E	2	14/15	0.84	0.09	79,90,107,113	0
4	NAG	I	1	14/15	0.87	0.10	95,103,114,117	0
3	NAG	G	2	14/15	0.87	0.09	46,66,84,88	0
5	NAG	L	1	14/15	0.87	0.13	57,67,76,79	0
4	NAG	H	1	14/15	0.91	0.07	76,84,97,106	0
3	NAG	G	1	14/15	0.92	0.08	41,46,56,62	0
3	NAG	E	1	14/15	0.93	0.09	43,68,77,77	0

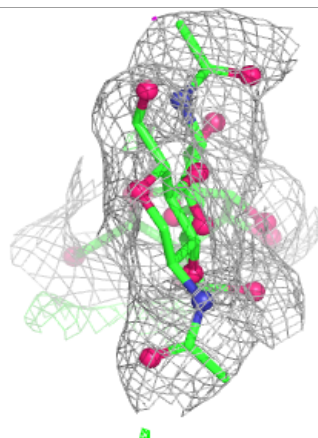
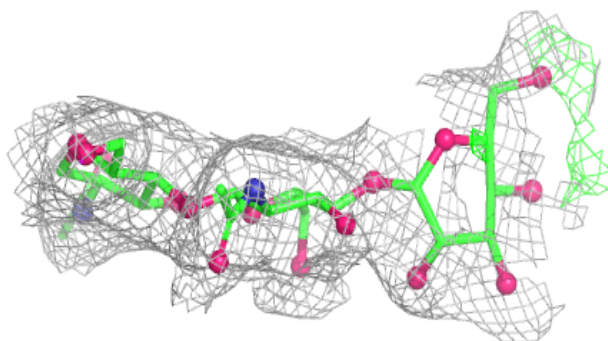
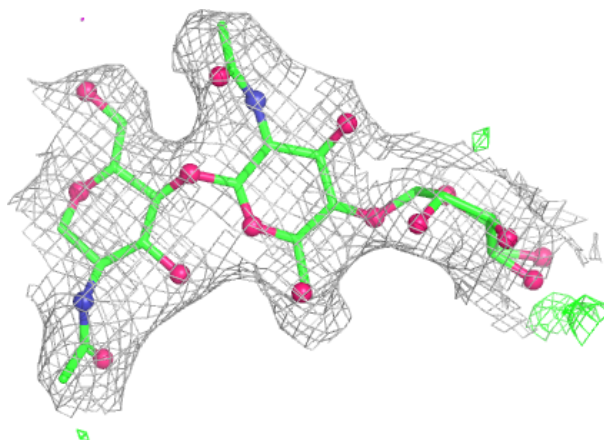
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

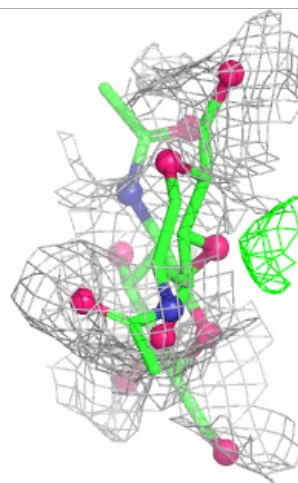
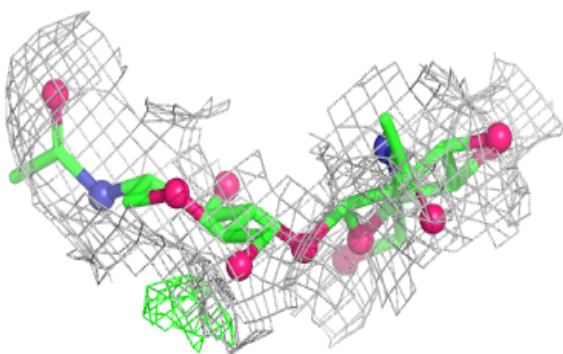
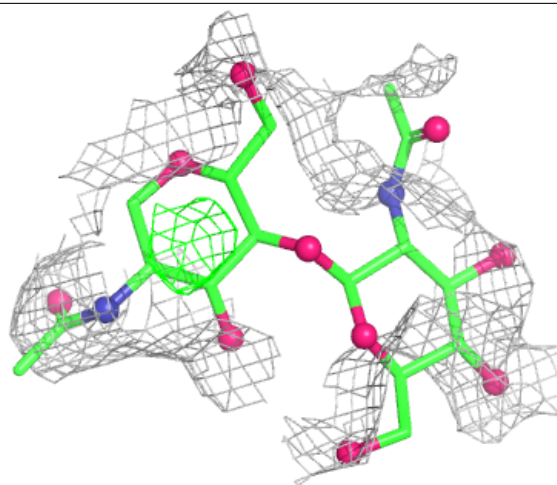
**Electron density around Chain G:**

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



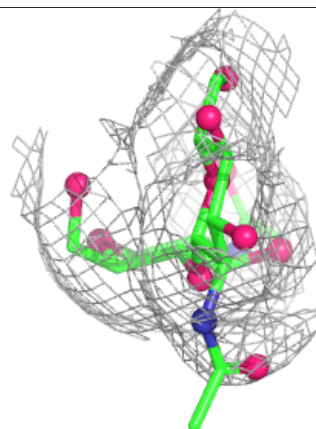
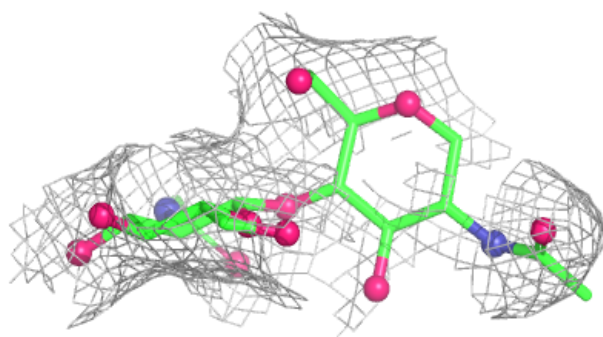
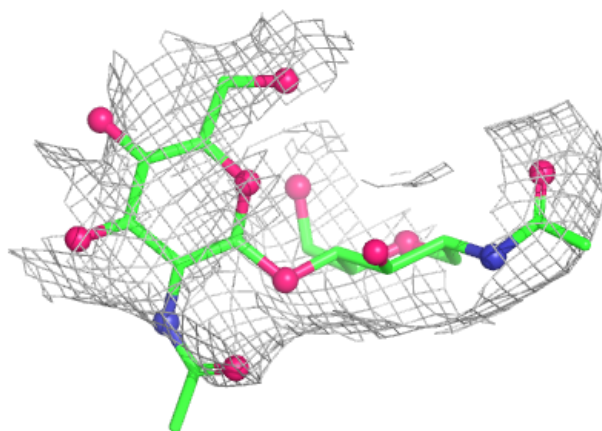
Electron density around Chain F:

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



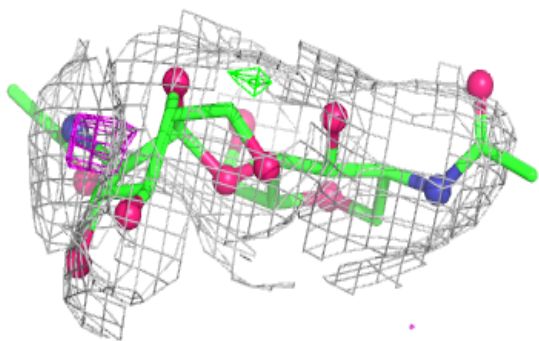
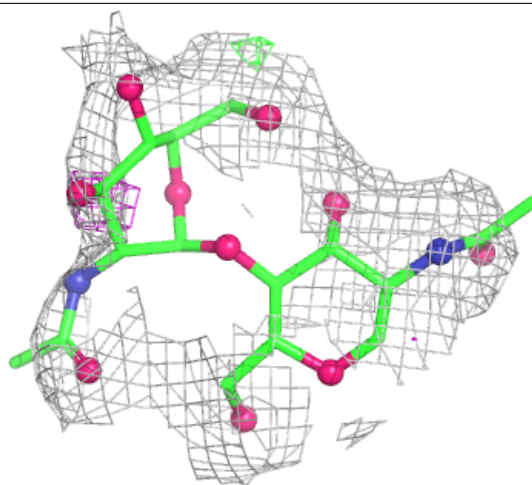
Electron density around Chain H:

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



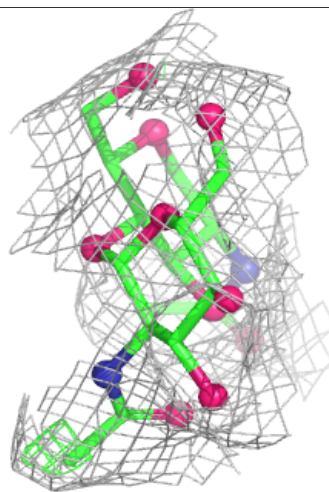
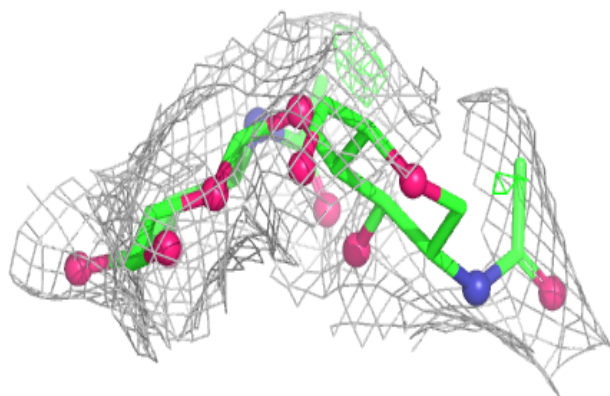
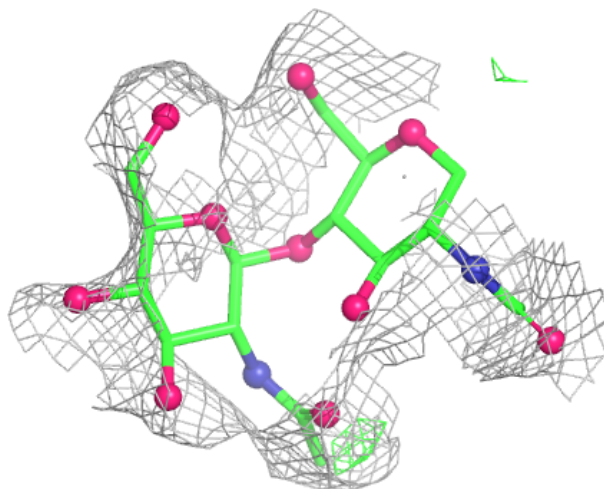
Electron density around Chain I:

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



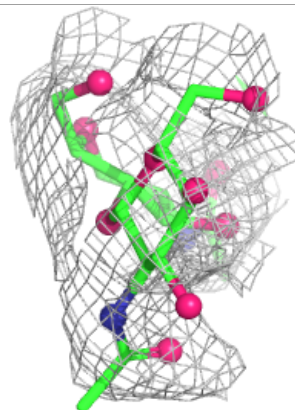
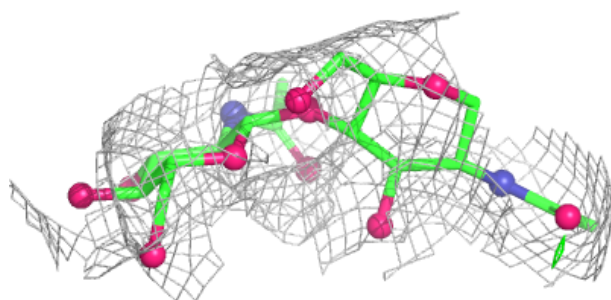
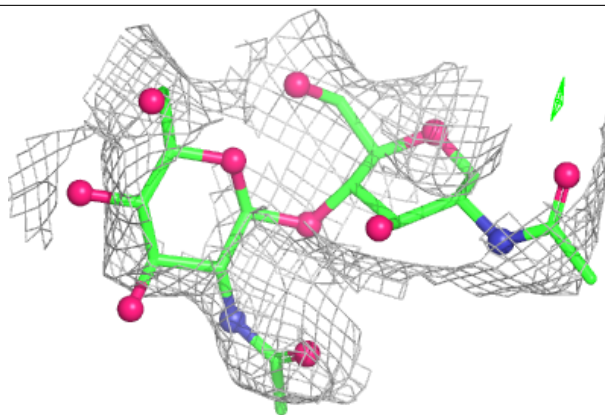
Electron density around Chain J:

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



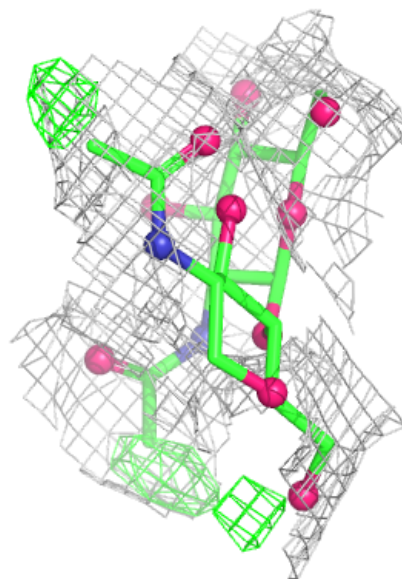
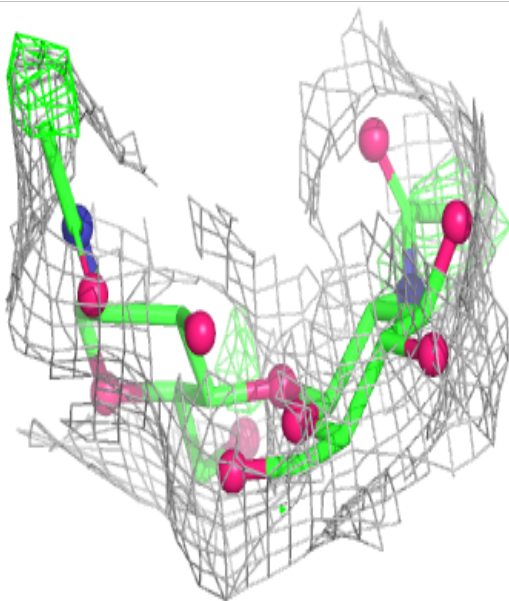
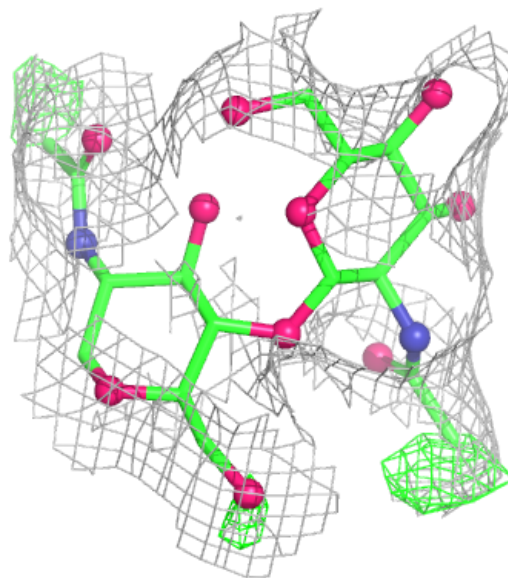
Electron density around Chain K:

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



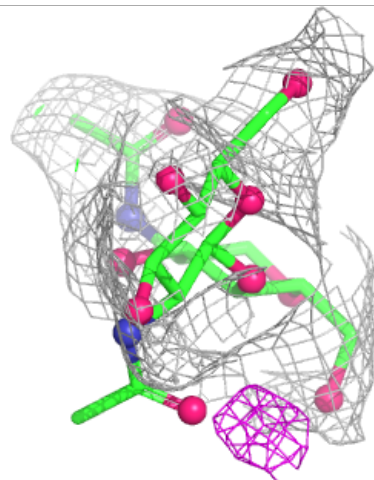
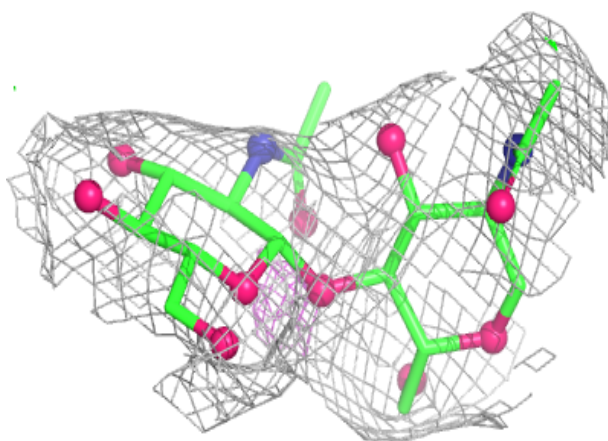
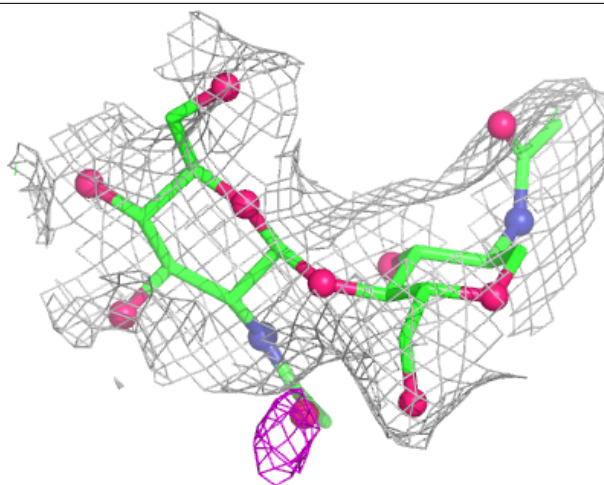
Electron density around Chain M:

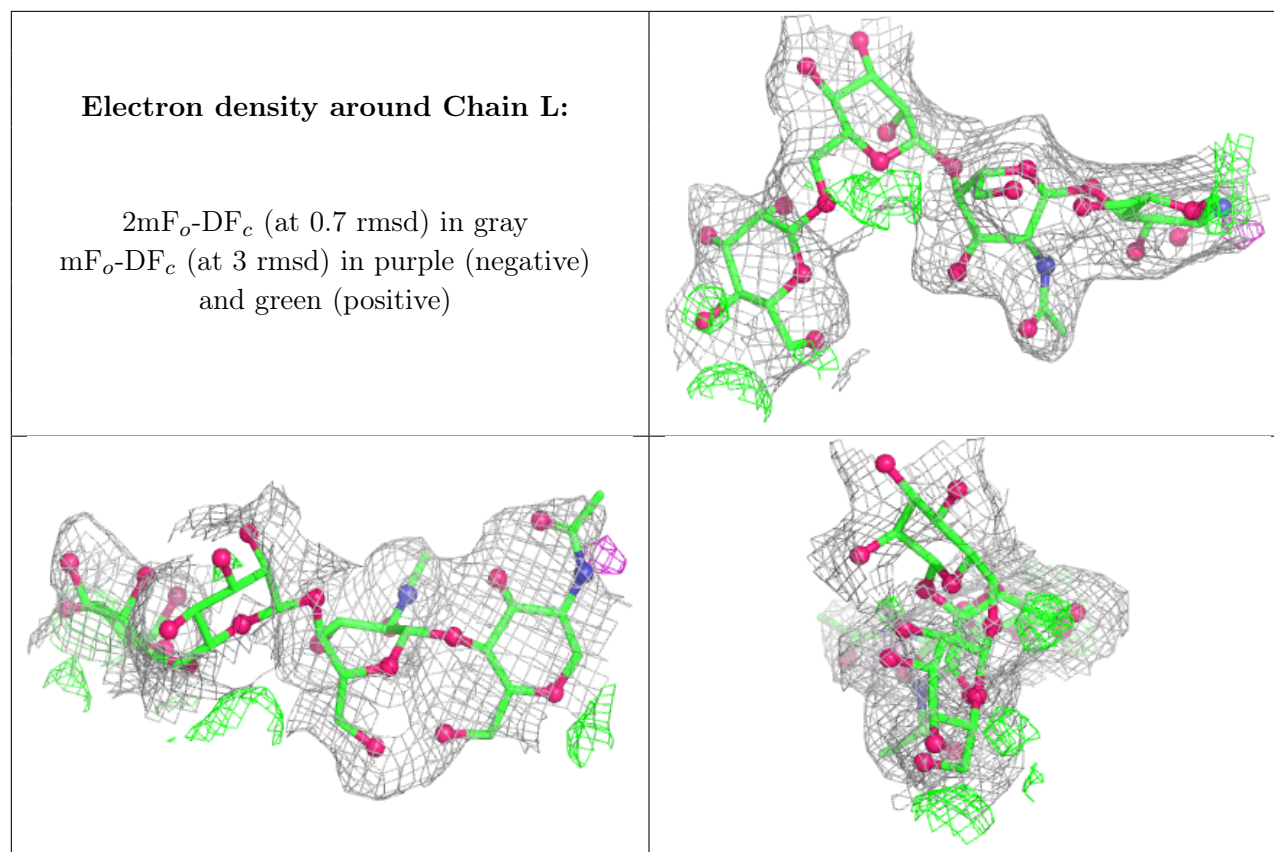
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (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
6	NAG	B	1011	14/15	0.29	0.16	132,143,148,150	0
6	NAG	B	1010	14/15	0.32	0.19	112,136,147,147	0
8	EDO	A	1963	4/4	0.49	0.28	83,89,90,96	0
6	NAG	B	1005	14/15	0.53	0.11	143,151,154,154	0
8	EDO	B	1962	4/4	0.54	0.15	96,99,103,116	0
8	EDO	A	1964	4/4	0.58	0.17	74,80,84,88	0
8	EDO	B	1963	4/4	0.65	0.14	99,99,104,120	0
6	NAG	A	1018	14/15	0.66	0.14	97,110,122,129	0
8	EDO	B	1961	4/4	0.74	0.14	81,93,96,97	0
6	NAG	A	1009	14/15	0.79	0.12	60,84,88,89	0
8	EDO	A	1962	4/4	0.90	0.12	51,56,57,65	0
7	ZN	A	1119	1/1	0.99	0.05	28,28,28,28	0
7	ZN	B	1119	1/1	0.99	0.04	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.