



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 3SAJ / pdb_00003saj
Title : Crystal Structure of glutamate receptor GluA1 Amino Terminal Domain
Authors : Jin, R.; Zong, Y.; Yao, G.; Gu, S.
Deposited on : 2011-06-02
Resolution : 2.50 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:

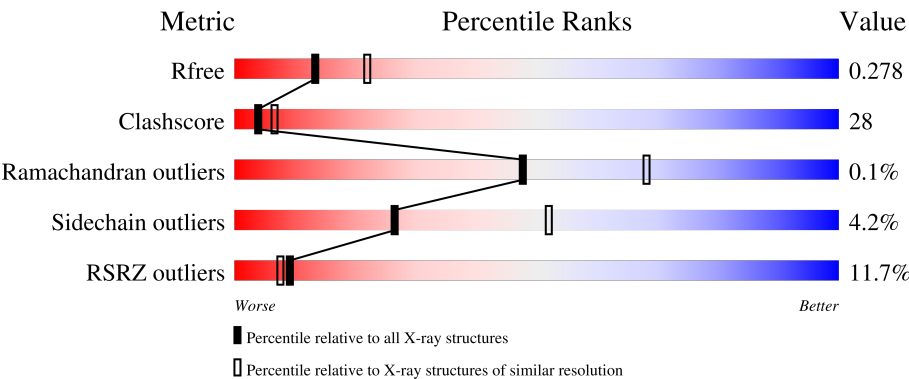
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.50 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.



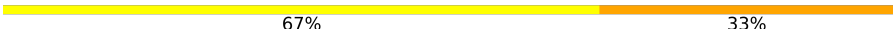
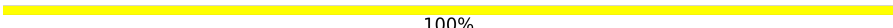
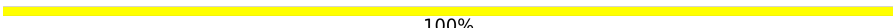
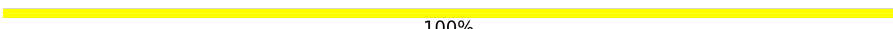
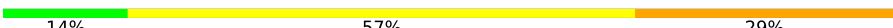
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	384	
1	B	384	
1	C	384	
1	D	384	
2	E	3	

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Mol	Chain	Length	Quality of chain
2	H	3	 67% 33%
2	N	3	 67% 33%
3	F	2	 50% 50%
3	G	2	 50% 50%
3	I	2	 50% 50%
3	J	2	 100%
3	K	2	 100%
3	L	2	 100%
3	O	2	 100%
3	P	2	 100%
4	M	7	 14% 57% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12534 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2987	1899	525	550	13			
1	B	366	Total	C	N	O	S	0	0	0
			2959	1882	518	546	13			
1	C	372	Total	C	N	O	S	0	0	0
			3016	1918	530	555	13			
1	D	367	Total	C	N	O	S	0	0	0
			2963	1884	519	547	13			

There are 52 discrepancies between the modelled and reference sequences:

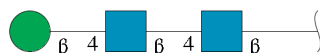
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ILE	-	expression tag	UNP P19490
A	-2	GLU	-	expression tag	UNP P19490
A	-1	GLU	-	expression tag	UNP P19490
A	0	ARG	-	expression tag	UNP P19490
A	1	GLY	-	expression tag	UNP P19490
A	2	ALA	-	expression tag	UNP P19490
A	3	MET	-	expression tag	UNP P19490
A	375	LEU	-	expression tag	UNP P19490
A	376	GLU	-	expression tag	UNP P19490
A	377	VAL	-	expression tag	UNP P19490
A	378	LEU	-	expression tag	UNP P19490
A	379	PHE	-	expression tag	UNP P19490
A	380	GLN	-	expression tag	UNP P19490
B	-3	ILE	-	expression tag	UNP P19490
B	-2	GLU	-	expression tag	UNP P19490
B	-1	GLU	-	expression tag	UNP P19490
B	0	ARG	-	expression tag	UNP P19490
B	1	GLY	-	expression tag	UNP P19490
B	2	ALA	-	expression tag	UNP P19490
B	3	MET	-	expression tag	UNP P19490
B	375	LEU	-	expression tag	UNP P19490

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Chain	Residue	Modelled	Actual	Comment	Reference
B	376	GLU	-	expression tag	UNP P19490
B	377	VAL	-	expression tag	UNP P19490
B	378	LEU	-	expression tag	UNP P19490
B	379	PHE	-	expression tag	UNP P19490
B	380	GLN	-	expression tag	UNP P19490
C	-3	ILE	-	expression tag	UNP P19490
C	-2	GLU	-	expression tag	UNP P19490
C	-1	GLU	-	expression tag	UNP P19490
C	0	ARG	-	expression tag	UNP P19490
C	1	GLY	-	expression tag	UNP P19490
C	2	ALA	-	expression tag	UNP P19490
C	3	MET	-	expression tag	UNP P19490
C	375	LEU	-	expression tag	UNP P19490
C	376	GLU	-	expression tag	UNP P19490
C	377	VAL	-	expression tag	UNP P19490
C	378	LEU	-	expression tag	UNP P19490
C	379	PHE	-	expression tag	UNP P19490
C	380	GLN	-	expression tag	UNP P19490
D	-3	ILE	-	expression tag	UNP P19490
D	-2	GLU	-	expression tag	UNP P19490
D	-1	GLU	-	expression tag	UNP P19490
D	0	ARG	-	expression tag	UNP P19490
D	1	GLY	-	expression tag	UNP P19490
D	2	ALA	-	expression tag	UNP P19490
D	3	MET	-	expression tag	UNP P19490
D	375	LEU	-	expression tag	UNP P19490
D	376	GLU	-	expression tag	UNP P19490
D	377	VAL	-	expression tag	UNP P19490
D	378	LEU	-	expression tag	UNP P19490
D	379	PHE	-	expression tag	UNP P19490
D	380	GLN	-	expression tag	UNP P19490

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



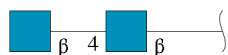
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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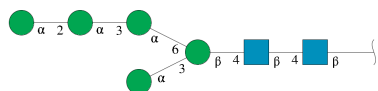
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



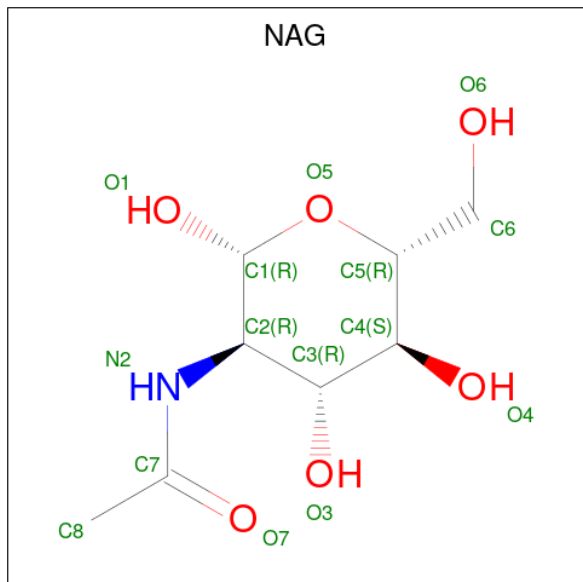
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
4	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

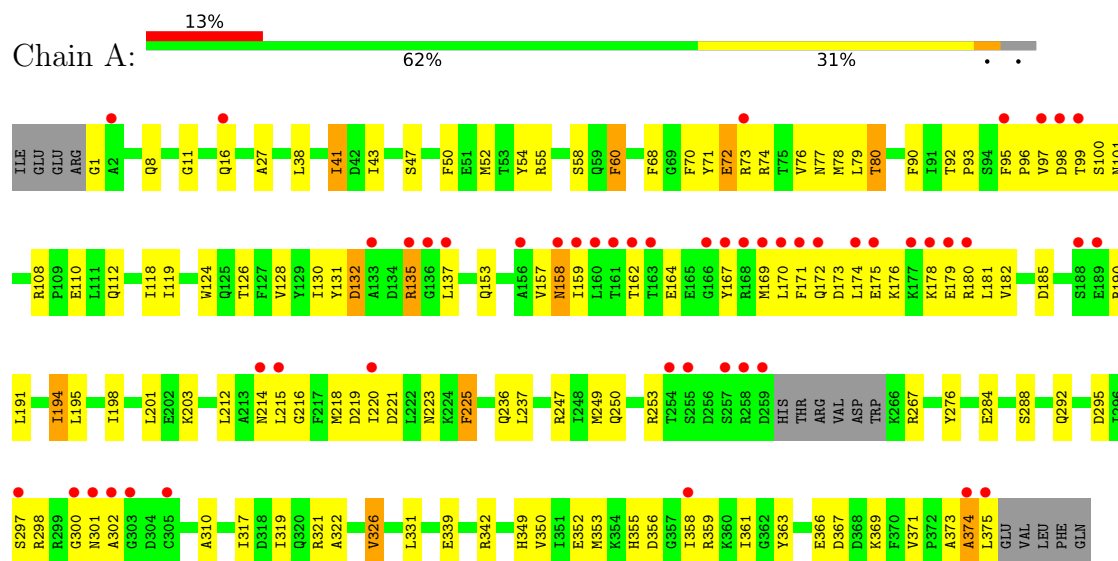
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	29	Total	O	0	0
			29	29		
6	C	41	Total	O	0	0
			41	41		
6	D	24	Total	O	0	0
			24	24		

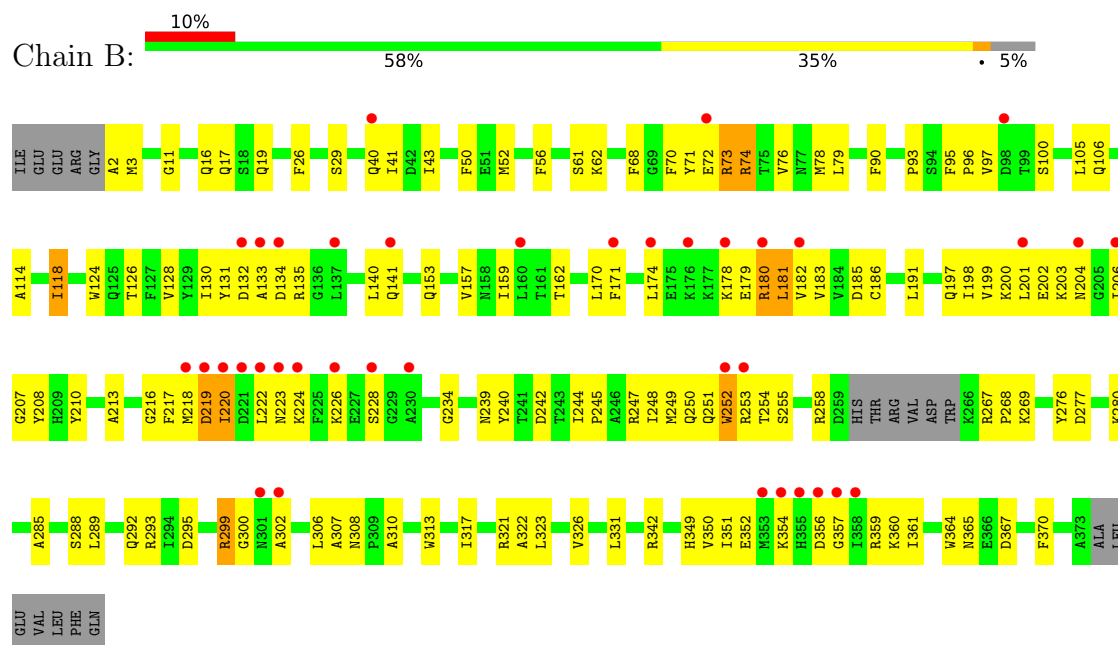
3 Residue-property plots [i](#)

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

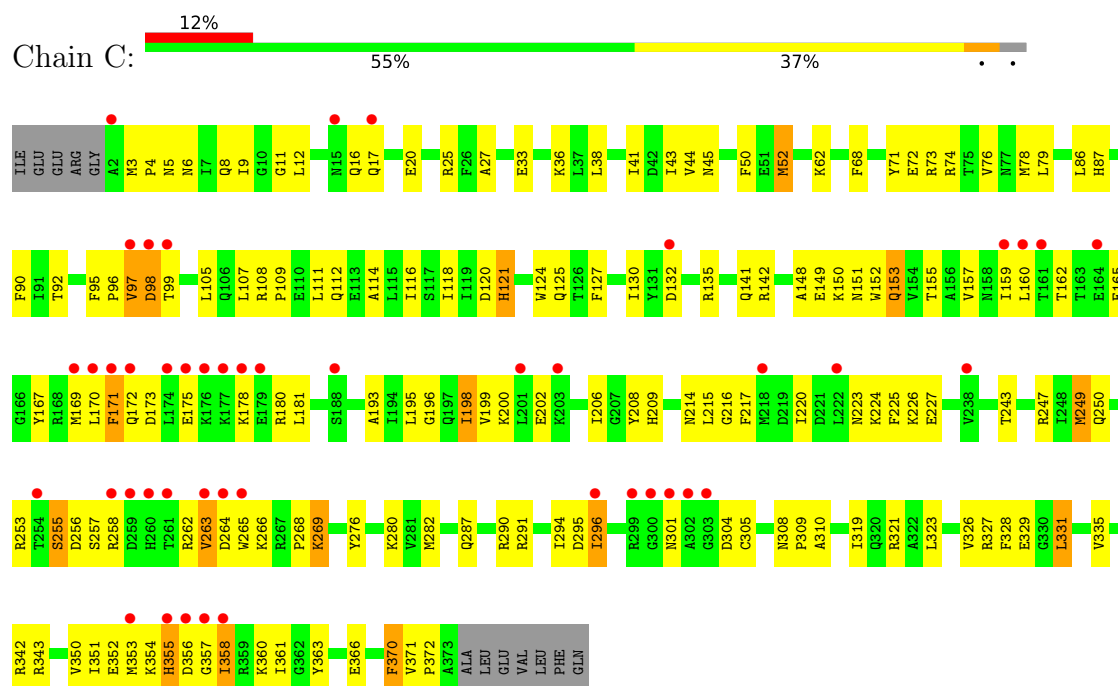
• Molecule 1: Glutamate receptor 1



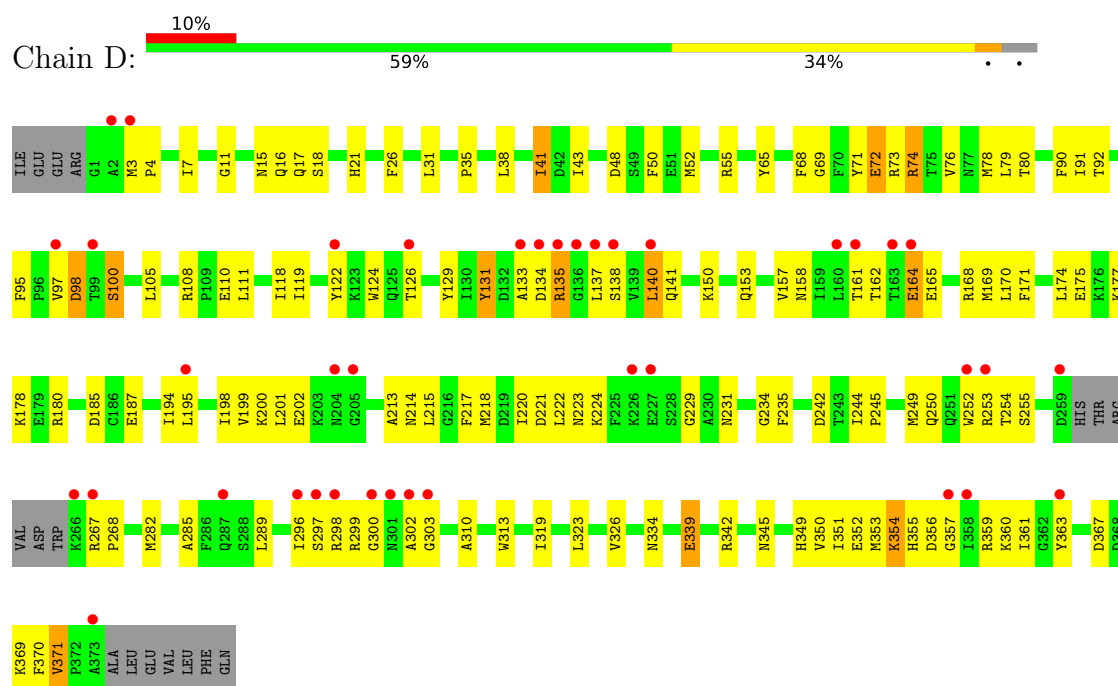
• Molecule 1: Glutamate receptor 1



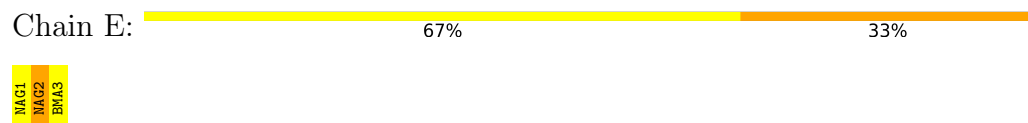
- Molecule 1: Glutamate receptor 1



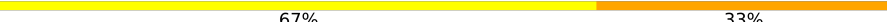
- Molecule 1: Glutamate receptor 1



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



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

Chain H:  67% 33%

MAG1
MAG2
BMA3

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

Chain N:  67% 33%

MAG1
MAG2
BMA3

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  50% 50%

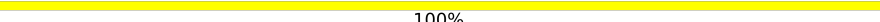
MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

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

Chain P:  100%MAG1
MAG2

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  14% 57% 29%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.59Å 94.42Å 186.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.18 – 2.50 93.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (93.18-2.50) 99.3 (93.18-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.286 0.234 , 0.278	Depositor DCC
R_{free} test set	2894 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12534	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: NAG, MAN, BMA

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	0.69	0/3049	0.96	11/4122 (0.3%)
1	B	0.64	1/3021 (0.0%)	1.02	7/4085 (0.2%)
1	C	0.65	1/3082 (0.0%)	1.00	9/4171 (0.2%)
1	D	0.64	2/3025 (0.1%)	0.95	10/4090 (0.2%)
All	All	0.65	4/12177 (0.0%)	0.98	37/16468 (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
1	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	LEU	CA-C	-7.18	1.43	1.52
1	B	308	ASN	C-O	-5.84	1.18	1.25
1	D	41	ILE	CA-C	-5.84	1.45	1.52
1	C	268	PRO	N-CD	5.08	1.54	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ASP	N-CA-C	9.59	123.61	111.24
1	D	100	SER	N-CA-C	-8.32	96.59	108.07
1	A	300	GLY	N-CA-C	-8.30	105.54	114.67
1	A	367	ASP	N-CA-C	8.04	119.83	111.14
1	D	178	LYS	N-CA-C	7.97	119.97	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASN	N-CA-C	-7.79	96.58	108.96
1	C	294	ILE	N-CA-C	-7.79	96.32	108.23
1	C	193	ALA	N-CA-C	7.69	119.74	111.36
1	C	305	CYS	N-CA-C	7.64	119.24	111.07
1	B	186	CYS	N-CA-C	7.49	118.49	108.38
1	A	369	LYS	CB-CA-C	-7.19	108.28	116.63
1	C	171	PHE	N-CA-C	7.07	121.95	113.12
1	D	367	ASP	N-CA-C	7.00	118.70	111.14
1	A	164	GLU	N-CA-C	6.97	119.72	111.71
1	B	220	ILE	N-CA-C	6.56	119.49	113.20
1	D	41	ILE	N-CA-C	6.51	119.06	108.97
1	A	132	ASP	N-CA-C	-6.26	101.25	110.52
1	C	172	GLN	N-CA-C	-6.08	104.96	112.38
1	A	100	SER	N-CA-C	-5.99	102.80	110.53
1	B	133	ALA	N-CA-C	5.95	117.77	111.28
1	A	225	PHE	N-CA-C	5.78	117.66	111.36
1	C	358	ILE	N-CA-C	-5.71	99.53	107.80
1	B	367	ASP	N-CA-C	5.69	117.57	111.36
1	B	61	SER	N-CA-C	5.61	117.48	111.36
1	A	215	LEU	N-CA-C	-5.58	103.12	110.43
1	B	180	ARG	N-CA-C	5.46	117.58	110.53
1	D	98	ASP	N-CA-C	5.46	117.04	111.14
1	C	370	PHE	N-CA-C	5.44	117.76	108.90
1	C	243	THR	N-CA-C	5.39	116.85	110.97
1	A	374	ALA	N-CA-C	-5.37	105.43	111.28
1	D	300	GLY	N-CA-C	-5.27	106.60	115.62
1	D	80	THR	N-CA-C	-5.21	105.60	111.28
1	A	60	PHE	N-CA-C	5.19	116.62	111.07
1	C	366	GLU	N-CA-C	5.16	117.64	111.71
1	D	131	TYR	N-CA-C	5.15	116.81	109.14
1	D	31	LEU	N-CA-C	5.14	117.48	110.24
1	D	69	GLY	N-CA-C	5.07	117.95	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	299	ARG	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	2987	0	2956	164	0
1	B	2959	0	2920	179	0
1	C	3016	0	2973	200	0
1	D	2963	0	2925	164	0
2	E	39	0	34	2	0
2	H	39	0	34	2	0
2	N	39	0	34	2	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	3	0
3	L	28	0	25	0	0
3	O	28	0	25	4	0
3	P	28	0	25	0	0
4	M	83	0	70	1	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
5	D	14	0	13	4	0
6	A	49	0	0	3	0
6	B	29	0	0	3	0
6	C	41	0	0	5	0
6	D	24	0	0	1	0
All	All	12534	0	12185	693	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 28.

All (693) 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:D:73:ARG:HB2	1:D:134:ASP:O	1.25	1.29
1:C:352:GLU:HB2	1:C:361:ILE:CD1	1.65	1.25
1:D:26:PHE:CZ	1:D:252:TRP:HB3	1.72	1.23
1:C:11:GLY:HA3	1:C:41:ILE:HG22	1.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:HG22	1:A:153:GLN:HB2	1.22	1.17
1:D:133:ALA:HB2	1:D:158:ASN:HD21	1.09	1.17
1:C:226:LYS:HG2	1:C:356:ASP:OD1	1.44	1.16
1:C:352:GLU:CB	1:C:361:ILE:HD11	1.74	1.15
1:D:3:MET:HG2	1:D:4:PRO:CD	1.77	1.15
1:B:197:GLN:O	1:B:201:LEU:HG	1.47	1.15
1:B:203:LYS:HD2	1:B:208:TYR:CZ	1.81	1.15
1:B:349:HIS:HD2	1:B:360:LYS:HE2	1.11	1.14
1:B:203:LYS:HD2	1:B:208:TYR:CE2	1.84	1.12
1:D:11:GLY:HA3	1:D:41:ILE:HG22	1.24	1.10
1:D:133:ALA:HB2	1:D:158:ASN:ND2	1.65	1.10
1:A:128:VAL:HG21	1:A:180:ARG:HH21	0.98	1.10
1:B:349:HIS:CD2	1:B:360:LYS:HE2	1.86	1.10
1:B:255:SER:HA	1:B:258:ARG:HD2	1.27	1.09
1:D:91:ILE:HD13	1:D:282:MET:HE3	1.08	1.07
1:A:249:MET:O	1:A:253:ARG:HG2	1.53	1.07
1:B:76:VAL:HG21	1:B:97:VAL:HG11	1.34	1.06
1:C:353:MET:HE2	1:C:358:ILE:HD11	1.37	1.06
1:A:174:LEU:O	1:A:174:LEU:HG	1.56	1.06
1:A:16:GLN:HB2	1:A:43:ILE:HD11	1.39	1.04
1:A:374:ALA:O	1:A:375:LEU:HD13	1.56	1.04
1:B:203:LYS:CD	1:B:208:TYR:CE2	2.41	1.04
1:B:216:GLY:O	1:B:219:ASP:HB2	1.56	1.03
1:D:3:MET:CG	1:D:4:PRO:HD2	1.89	1.03
1:B:252:TRP:HA	1:B:255:SER:HB3	1.41	1.02
1:D:3:MET:HG2	1:D:4:PRO:HD2	1.02	1.01
1:C:353:MET:HE2	1:C:358:ILE:CD1	1.91	1.01
1:D:133:ALA:CB	1:D:158:ASN:HD21	1.73	1.01
1:D:71:TYR:CD1	1:D:76:VAL:HG12	1.94	1.01
1:A:126:THR:CG2	1:A:153:GLN:HB2	1.91	1.00
1:B:249:MET:HB3	1:B:253:ARG:NH1	1.74	1.00
1:D:126:THR:HG22	1:D:153:GLN:HB3	1.44	1.00
1:B:132:ASP:HB2	6:B:406:HOH:O	1.61	0.99
1:C:96:PRO:HD3	1:C:108:ARG:HD2	1.41	0.99
1:A:135:ARG:CG	1:A:135:ARG:HH11	1.76	0.98
1:B:349:HIS:CD2	1:B:360:LYS:CE	2.46	0.98
1:C:3:MET:SD	1:C:296:ILE:HD11	2.04	0.97
1:C:352:GLU:HB2	1:C:361:ILE:HD11	1.00	0.97
1:D:353:MET:HA	1:D:357:GLY:O	1.64	0.97
1:C:263:VAL:HG12	1:C:264:ASP:H	1.29	0.97
1:A:135:ARG:HH11	1:A:135:ARG:HG3	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLU:OE2	1:C:354:LYS:HE3	1.64	0.95
1:A:128:VAL:HG21	1:A:180:ARG:NH2	1.80	0.95
1:B:249:MET:CB	1:B:253:ARG:NH1	2.30	0.95
1:B:170:LEU:O	1:B:174:LEU:HG	1.66	0.95
1:C:199:VAL:O	1:C:202:GLU:HG2	1.67	0.94
1:B:157:VAL:HG13	1:B:162:THR:HG21	1.49	0.94
1:D:71:TYR:CE1	1:D:76:VAL:HG12	2.02	0.94
1:B:174:LEU:CD2	1:B:180:ARG:HD3	1.98	0.94
1:A:131:TYR:CZ	1:A:158:ASN:HB2	2.03	0.93
1:B:349:HIS:HD2	1:B:360:LYS:CE	1.82	0.93
1:C:44:VAL:HG11	1:C:52:MET:HE1	1.50	0.93
1:D:126:THR:HG22	1:D:153:GLN:CB	1.98	0.93
1:D:26:PHE:CE1	1:D:252:TRP:HB3	2.04	0.93
1:C:44:VAL:HG21	1:C:52:MET:HE3	1.48	0.93
1:A:159:ILE:HD12	1:A:167:TYR:OH	1.70	0.92
1:B:174:LEU:HD23	1:B:180:ARG:HD3	1.52	0.91
1:B:203:LYS:HD2	1:B:208:TYR:OH	1.68	0.91
1:C:165:GLU:O	1:C:169:MET:HG2	1.68	0.91
1:A:374:ALA:O	1:A:375:LEU:CD1	2.19	0.90
1:B:26:PHE:CE1	1:B:252:TRP:HB3	2.06	0.90
1:D:249:MET:HE1	1:D:268:PRO:CD	2.01	0.90
1:D:91:ILE:CD1	1:D:282:MET:HE3	1.99	0.90
1:D:91:ILE:HD13	1:D:282:MET:CE	2.01	0.90
1:D:3:MET:CG	1:D:4:PRO:CD	2.47	0.89
1:A:1:GLY:N	1:A:295:ASP:HB2	1.87	0.89
1:A:190:ARG:HG2	1:A:194:ILE:HD12	1.54	0.88
1:C:181:LEU:HD23	1:C:209:HIS:HB2	1.55	0.88
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.35	0.88
1:A:169:MET:O	1:A:169:MET:SD	2.32	0.88
1:A:99:THR:HG22	1:A:99:THR:O	1.71	0.88
1:C:130:ILE:HD11	1:C:167:TYR:HE1	1.39	0.88
1:A:170:LEU:HD12	1:A:180:ARG:HH22	1.39	0.87
1:B:350:VAL:O	1:B:361:ILE:HG22	1.73	0.87
1:C:353:MET:CE	1:C:358:ILE:CD1	2.51	0.87
1:A:170:LEU:CD1	1:A:180:ARG:HH22	1.88	0.87
1:C:52:MET:HE2	1:C:52:MET:HA	1.54	0.87
1:B:106:GLN:NE2	1:B:342:ARG:HD3	1.90	0.86
1:B:216:GLY:HA3	1:B:219:ASP:OD2	1.75	0.86
1:A:175:GLU:O	1:A:176:LYS:HB2	1.75	0.85
1:B:52:MET:HE3	1:B:79:LEU:HD11	1.56	0.85
1:D:135:ARG:HH11	1:D:135:ARG:CG	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:O	1:A:158:ASN:HA	1.76	0.85
1:A:353:MET:HB2	1:A:358:ILE:HG22	1.59	0.85
1:C:99:THR:HG22	1:C:99:THR:O	1.77	0.84
1:A:195:LEU:HD23	1:A:225:PHE:CE2	2.12	0.84
1:B:204:ASN:O	1:B:228:SER:HB3	1.78	0.84
1:C:181:LEU:CD2	1:C:209:HIS:HB2	2.07	0.84
1:D:95:PHE:CD2	1:D:135:ARG:HB2	2.11	0.84
1:B:239:ASN:HB3	1:B:242:ASP:OD2	1.77	0.84
1:B:249:MET:HB2	1:B:253:ARG:HH12	1.41	0.84
1:A:220:ILE:HG22	1:A:221:ASP:N	1.93	0.83
1:A:363:TYR:CZ	1:A:371:VAL:HG21	2.13	0.83
1:C:121:HIS:ND1	1:C:121:HIS:C	2.36	0.83
1:A:159:ILE:HG23	1:A:167:TYR:OH	1.77	0.83
1:A:352:GLU:OE1	1:A:361:ILE:HG21	1.79	0.83
1:A:11:GLY:HA2	1:A:68:PHE:O	1.80	0.82
1:D:65:TYR:HE1	1:D:296:ILE:HG22	1.43	0.82
1:B:240:TYR:CD1	1:B:249:MET:HE3	2.15	0.82
1:C:217:PHE:O	1:C:220:ILE:HG12	1.79	0.82
1:D:133:ALA:HB2	1:D:158:ASN:CG	2.04	0.82
1:A:97:VAL:HG12	1:A:98:ASP:N	1.95	0.82
1:A:236:GLN:OE1	1:A:267:ARG:NH2	2.13	0.81
1:C:44:VAL:CG2	1:C:52:MET:HE3	2.09	0.81
1:C:263:VAL:HG12	1:C:264:ASP:N	1.95	0.81
1:C:124:TRP:CD1	1:C:181:LEU:HD13	2.16	0.81
1:B:249:MET:CB	1:B:253:ARG:HH12	1.92	0.80
1:D:296:ILE:HD13	1:D:319:ILE:HD11	1.63	0.80
1:C:226:LYS:CG	1:C:356:ASP:OD1	2.29	0.80
1:C:9:ILE:HG23	1:C:282:MET:HE1	1.64	0.80
1:C:223:ASN:O	1:C:227:GLU:HG3	1.81	0.80
1:A:71:TYR:CE2	1:A:92:THR:HG21	2.17	0.80
1:B:128:VAL:HG21	1:B:174:LEU:HD21	1.64	0.80
1:B:203:LYS:CD	1:B:208:TYR:HE2	1.95	0.80
1:D:11:GLY:CA	1:D:41:ILE:HG22	2.09	0.80
1:B:285:ALA:CB	1:B:323:LEU:HD23	2.12	0.79
1:C:124:TRP:CG	1:C:181:LEU:HD13	2.16	0.79
1:A:374:ALA:O	1:A:375:LEU:HB2	1.82	0.79
1:C:352:GLU:CG	1:C:361:ILE:HD11	2.12	0.79
1:D:363:TYR:CZ	1:D:371:VAL:HG21	2.18	0.79
1:B:40:GLN:OE1	1:B:62:LYS:HD3	1.82	0.79
1:A:191:LEU:HD21	1:A:212:LEU:HD13	1.64	0.79
1:D:73:ARG:CB	1:D:134:ASP:O	2.20	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PHE:CD1	1:C:180:ARG:HD3	2.19	0.78
1:B:240:TYR:HD1	1:B:249:MET:HE3	1.48	0.78
1:A:135:ARG:HG3	1:A:135:ARG:NH1	1.97	0.78
1:B:124:TRP:CZ2	1:B:181:LEU:HB3	2.19	0.78
1:B:203:LYS:HD3	1:B:208:TYR:CE2	2.18	0.78
1:D:26:PHE:CE2	1:D:252:TRP:HB3	2.19	0.78
1:C:71:TYR:HD2	1:C:90:PHE:HE2	1.30	0.77
1:C:44:VAL:HG11	1:C:52:MET:CE	2.13	0.77
1:A:220:ILE:HG22	1:A:221:ASP:H	1.45	0.77
1:C:72:GLU:HG2	1:C:73:ARG:H	1.48	0.77
1:C:372:PRO:HB2	6:C:408:HOH:O	1.83	0.77
1:C:363:TYR:CZ	1:C:371:VAL:HG21	2.20	0.77
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.50	0.76
1:B:220:ILE:HG22	1:B:220:ILE:O	1.84	0.76
1:A:50:PHE:CE2	1:C:310:ALA:HB2	2.21	0.76
1:C:132:ASP:OD1	1:C:159:ILE:HD11	1.85	0.76
1:B:285:ALA:HB2	1:B:323:LEU:HD23	1.66	0.76
1:A:220:ILE:CG2	1:A:221:ASP:H	1.99	0.76
1:D:296:ILE:CD1	1:D:319:ILE:HD11	2.16	0.75
1:A:126:THR:HG22	1:A:153:GLN:CB	2.09	0.75
1:B:203:LYS:HD3	1:B:208:TYR:HE2	1.51	0.75
1:C:71:TYR:HD2	1:C:90:PHE:CE2	2.04	0.75
1:D:249:MET:HE1	1:D:268:PRO:CG	2.17	0.75
1:B:50:PHE:CE2	1:D:310:ALA:HB2	2.22	0.75
1:A:172:GLN:OE1	1:C:151:ASN:HB2	1.87	0.75
1:B:247:ARG:O	1:B:251:GLN:HG3	1.87	0.75
5:A:900:NAG:O6	6:A:417:HOH:O	2.04	0.75
1:B:249:MET:HB3	1:B:253:ARG:HH11	1.51	0.75
1:D:71:TYR:HD2	1:D:90:PHE:HE2	1.35	0.75
1:B:131:TYR:OH	1:D:141:GLN:NE2	2.20	0.74
1:D:360:LYS:HD2	5:D:900:NAG:O3	1.87	0.74
1:C:71:TYR:CD2	1:C:90:PHE:HE2	2.04	0.74
1:B:220:ILE:O	1:B:220:ILE:CG2	2.36	0.74
1:C:155:THR:OG1	1:C:170:LEU:HD21	1.88	0.74
1:C:178:LYS:O	1:C:206:ILE:HG13	1.86	0.74
1:A:71:TYR:HE2	1:A:92:THR:HG21	1.51	0.73
1:A:373:ALA:O	1:A:375:LEU:HD12	1.88	0.73
1:D:11:GLY:HA3	1:D:41:ILE:CG2	2.10	0.73
1:B:302:ALA:HB3	1:C:5:ASN:HB3	1.70	0.73
1:C:352:GLU:HB2	1:C:361:ILE:CG1	2.17	0.73
1:D:135:ARG:NH1	1:D:185:ASP:OD2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:CD1	1:A:180:ARG:NH2	2.51	0.73
1:A:1:GLY:H3	1:A:295:ASP:HB2	1.51	0.73
1:A:352:GLU:HB2	1:A:361:ILE:HD13	1.71	0.73
1:C:124:TRP:HZ2	1:C:209:HIS:HB3	1.53	0.73
1:C:4:PRO:HD2	1:C:296:ILE:CD1	2.19	0.72
1:D:218:MET:O	1:D:267:ARG:NH2	2.22	0.72
1:A:71:TYR:HD2	1:A:90:PHE:HE2	1.37	0.72
1:C:11:GLY:CA	1:C:41:ILE:HG22	2.13	0.72
1:C:199:VAL:HA	1:C:202:GLU:OE2	1.88	0.72
1:B:141:GLN:NE2	1:D:131:TYR:OH	2.22	0.72
1:D:65:TYR:HE1	1:D:296:ILE:CG2	2.03	0.72
1:B:248:ILE:HG21	1:B:331:LEU:HD21	1.72	0.72
1:B:242:ASP:HB2	1:B:245:PRO:HG2	1.70	0.71
1:C:71:TYR:CE2	1:C:92:THR:HG21	2.25	0.71
1:D:164:GLU:CD	1:D:164:GLU:H	1.96	0.71
1:C:124:TRP:CZ2	1:C:181:LEU:HD22	2.26	0.71
1:C:353:MET:CE	1:C:358:ILE:HD12	2.20	0.71
1:B:130:ILE:HG22	1:B:159:ILE:HD11	1.71	0.71
1:B:217:PHE:CD1	1:B:234:GLY:HA3	2.25	0.71
1:D:168:ARG:HD2	1:D:201:LEU:HD11	1.72	0.71
1:A:1:GLY:H2	1:A:295:ASP:HB2	1.56	0.71
1:D:71:TYR:CD2	1:D:90:PHE:HE2	2.09	0.70
1:D:352:GLU:OE2	3:O:1:NAG:C1	2.39	0.70
1:A:130:ILE:CG2	1:A:159:ILE:HD11	2.20	0.70
1:D:285:ALA:HB2	1:D:323:LEU:HD23	1.72	0.70
1:C:124:TRP:CE2	1:C:181:LEU:HD22	2.26	0.70
1:B:171:PHE:CD1	1:B:174:LEU:HD12	2.26	0.70
1:C:52:MET:HB3	1:C:78:MET:HE1	1.74	0.69
1:A:171:PHE:CZ	1:A:203:LYS:HE2	2.27	0.69
1:C:124:TRP:CZ3	1:C:181:LEU:HB3	2.27	0.69
1:C:130:ILE:HD11	1:C:167:TYR:CE1	2.26	0.69
1:A:310:ALA:HB2	1:C:50:PHE:CE2	2.28	0.69
1:A:374:ALA:C	1:A:375:LEU:CD1	2.65	0.69
1:B:70:PHE:CE1	1:B:93:PRO:HG2	2.27	0.69
1:A:124:TRP:CG	1:A:181:LEU:HD13	2.27	0.68
1:B:354:LYS:O	1:B:357:GLY:N	2.26	0.68
1:D:71:TYR:HD2	1:D:90:PHE:CE2	2.11	0.68
1:A:97:VAL:HG12	1:A:98:ASP:H	1.57	0.68
1:B:174:LEU:HD22	1:B:180:ARG:HD3	1.74	0.68
1:B:307:ALA:HB2	1:C:38:LEU:HD12	1.75	0.68
1:C:263:VAL:CG1	1:C:264:ASP:H	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:CD1	1:D:323:LEU:HB3	2.24	0.68
1:C:253:ARG:NH2	1:C:266:LYS:O	2.27	0.68
1:B:52:MET:CE	1:B:79:LEU:HD11	2.23	0.68
1:B:72:GLU:CD	1:B:73:ARG:N	2.51	0.68
1:C:353:MET:HE3	1:C:358:ILE:HD12	1.76	0.68
1:A:374:ALA:O	1:A:375:LEU:CB	2.42	0.68
1:A:95:PHE:CD2	1:A:135:ARG:O	2.47	0.67
1:B:11:GLY:HA3	1:B:41:ILE:HG22	1.76	0.67
1:A:167:TYR:HB2	1:A:201:LEU:HD13	1.75	0.67
1:D:249:MET:HE1	1:D:268:PRO:HD3	1.74	0.67
1:C:8:GLN:HG3	1:C:38:LEU:HD23	1.76	0.67
1:A:11:GLY:HA3	1:A:41:ILE:HG22	1.77	0.67
1:C:3:MET:HE3	1:C:290:ARG:HB2	1.75	0.67
1:B:52:MET:HB3	1:B:78:MET:HE2	1.76	0.67
1:C:9:ILE:CG2	1:C:282:MET:HE1	2.24	0.67
1:D:126:THR:HG22	1:D:153:GLN:HB2	1.77	0.67
1:A:52:MET:HB3	1:A:78:MET:HE1	1.76	0.66
1:B:26:PHE:CZ	1:B:252:TRP:HB3	2.29	0.66
1:B:179:GLU:HB2	1:B:207:GLY:O	1.95	0.66
1:A:80:THR:O	1:A:101:ASN:ND2	2.27	0.66
1:B:299:ARG:HD2	1:B:313:TRP:CE2	2.30	0.66
1:C:11:GLY:HA2	1:C:68:PHE:O	1.95	0.66
1:C:352:GLU:OE2	1:C:354:LYS:CE	2.42	0.66
1:B:130:ILE:CG2	1:B:159:ILE:HD11	2.26	0.66
1:C:226:LYS:HE2	1:C:356:ASP:CG	2.20	0.66
1:C:124:TRP:CH2	1:C:181:LEU:HB3	2.31	0.66
1:C:4:PRO:HD2	1:C:296:ILE:HD12	1.78	0.66
1:C:74:ARG:NH1	3:K:2:NAG:O7	2.28	0.66
1:A:363:TYR:CZ	1:A:371:VAL:CG2	2.79	0.66
1:B:52:MET:CB	1:B:78:MET:HE2	2.26	0.65
1:D:165:GLU:O	1:D:169:MET:HG2	1.95	0.65
1:B:321:ARG:HG2	1:C:258:ARG:NE	2.11	0.65
1:C:175:GLU:OE2	1:C:178:LYS:NZ	2.27	0.65
1:C:180:ARG:NE	1:C:206:ILE:HD13	2.12	0.65
1:D:289:LEU:HD13	1:D:296:ILE:HD11	1.78	0.65
1:B:239:ASN:HB3	1:B:242:ASP:CG	2.20	0.65
1:D:17:GLN:HE22	3:K:1:NAG:H81	1.61	0.65
1:A:130:ILE:HG23	1:A:159:ILE:HD11	1.78	0.65
1:D:72:GLU:OE2	1:D:74:ARG:HD3	1.97	0.64
1:C:180:ARG:CD	1:C:206:ILE:HD13	2.28	0.64
1:C:352:GLU:CD	1:C:361:ILE:HD11	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ALA:HB2	1:D:50:PHE:CE2	2.32	0.64
1:A:130:ILE:HG23	1:A:159:ILE:CG1	2.27	0.64
1:C:9:ILE:HD12	1:C:282:MET:HE2	1.77	0.64
1:A:130:ILE:HG23	1:A:159:ILE:HG12	1.78	0.64
1:A:132:ASP:C	1:A:132:ASP:OD1	2.40	0.64
1:B:254:THR:O	1:B:258:ARG:HG3	1.97	0.64
1:C:71:TYR:HE2	1:C:92:THR:HG21	1.61	0.64
1:D:71:TYR:CD1	1:D:76:VAL:CG1	2.78	0.64
1:A:71:TYR:CB	1:A:79:LEU:HD12	2.28	0.64
1:A:97:VAL:CG1	1:A:98:ASP:N	2.60	0.64
1:C:44:VAL:HG21	1:C:52:MET:CE	2.26	0.64
1:B:216:GLY:O	1:B:219:ASP:CB	2.42	0.64
1:D:135:ARG:HG3	1:D:135:ARG:NH1	2.08	0.64
1:B:74:ARG:HH21	2:H:2:NAG:H83	1.63	0.63
1:A:169:MET:HE2	1:C:148:ALA:O	1.97	0.63
1:B:72:GLU:CD	1:B:73:ARG:H	2.06	0.63
1:A:130:ILE:HG23	1:A:159:ILE:CD1	2.28	0.63
1:A:74:ARG:NH1	2:E:2:NAG:H83	2.13	0.63
1:A:95:PHE:CE2	1:A:135:ARG:O	2.51	0.63
1:B:132:ASP:OD1	1:B:135:ARG:NH2	2.32	0.63
1:C:178:LYS:O	1:C:206:ILE:CG1	2.46	0.63
1:A:97:VAL:CG1	1:A:98:ASP:H	2.11	0.63
1:A:159:ILE:CD1	1:A:167:TYR:OH	2.44	0.63
1:C:351:ILE:CD1	1:C:360:LYS:HG3	2.29	0.63
1:D:133:ALA:HB2	1:D:158:ASN:OD1	1.99	0.63
1:D:73:ARG:HD3	1:D:137:LEU:HD23	1.81	0.62
1:D:352:GLU:OE2	3:O:1:NAG:N2	2.30	0.62
1:D:15:ASN:O	1:D:21:HIS:NE2	2.31	0.62
1:B:157:VAL:CG1	1:B:162:THR:HG21	2.25	0.62
1:C:301:ASN:O	1:C:304:ASP:HB2	2.00	0.62
1:D:52:MET:HB3	1:D:78:MET:CE	2.28	0.62
1:A:124:TRP:CD1	1:A:181:LEU:HD13	2.34	0.62
1:C:363:TYR:CZ	1:C:371:VAL:CG2	2.83	0.62
1:A:71:TYR:HB3	1:A:79:LEU:CD1	2.30	0.62
1:A:135:ARG:HH21	1:A:214:ASN:HB2	1.64	0.62
1:B:307:ALA:HB2	1:C:38:LEU:CD1	2.30	0.62
1:A:110:GLU:CD	1:A:112:GLN:HE22	2.08	0.62
1:A:131:TYR:CE1	1:A:158:ASN:HB2	2.34	0.62
1:D:17:GLN:NE2	3:K:1:NAG:H81	2.15	0.62
1:A:249:MET:O	1:A:253:ARG:CG	2.42	0.62
1:C:199:VAL:O	1:C:202:GLU:CG	2.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD12	1:A:180:ARG:NH2	2.12	0.62
1:A:374:ALA:C	1:A:375:LEU:HD12	2.24	0.62
1:C:12:LEU:HD22	1:C:52:MET:HE1	1.82	0.61
1:B:354:LYS:HB2	3:I:1:NAG:O7	2.00	0.61
1:B:40:GLN:HE22	1:B:62:LYS:HE2	1.63	0.61
1:B:200:LYS:C	1:B:202:GLU:H	2.04	0.61
1:C:196:GLY:O	1:C:200:LYS:HE3	2.00	0.61
1:B:248:ILE:CG2	1:B:331:LEU:HD21	2.31	0.61
1:A:170:LEU:HD13	1:A:180:ARG:NH2	2.14	0.61
1:A:353:MET:CB	1:A:358:ILE:HG22	2.29	0.61
1:C:16:GLN:HG3	1:C:43:ILE:HD11	1.82	0.61
1:B:52:MET:HB3	1:B:78:MET:CE	2.31	0.60
1:A:72:GLU:HG2	1:A:73:ARG:H	1.65	0.60
1:C:352:GLU:CD	1:C:354:LYS:HE3	2.25	0.60
1:B:106:GLN:HE21	1:B:342:ARG:HD3	1.65	0.60
1:B:197:GLN:O	1:B:201:LEU:CG	2.37	0.60
1:D:371:VAL:CG2	1:D:371:VAL:O	2.48	0.60
1:C:52:MET:HA	1:C:52:MET:CE	2.30	0.60
1:B:217:PHE:C	1:B:219:ASP:H	2.09	0.60
1:B:95:PHE:CD1	1:B:96:PRO:HD2	2.37	0.59
1:C:72:GLU:HG2	1:C:73:ARG:N	2.17	0.59
1:B:71:TYR:HD2	1:B:90:PHE:HE2	1.50	0.59
1:C:195:LEU:HB3	1:C:225:PHE:CZ	2.36	0.59
1:C:206:ILE:HG23	1:C:208:TYR:CE1	2.37	0.59
1:D:11:GLY:HA2	1:D:68:PHE:O	2.02	0.59
1:D:65:TYR:CE1	1:D:296:ILE:CG2	2.84	0.59
1:A:191:LEU:HD23	1:A:220:ILE:HG13	1.85	0.59
1:C:76:VAL:HG21	1:C:97:VAL:HG11	1.84	0.59
1:D:111:LEU:HD13	1:D:215:LEU:HD21	1.83	0.59
1:D:352:GLU:HB2	1:D:361:ILE:HD11	1.84	0.59
1:A:288:SER:O	1:A:292:GLN:HB2	2.03	0.59
1:B:114:ALA:O	1:B:118:ILE:HG12	2.03	0.59
1:B:124:TRP:CD1	1:B:181:LEU:HD13	2.37	0.59
1:A:52:MET:CE	1:A:79:LEU:HD11	2.33	0.59
1:C:124:TRP:CE3	1:C:181:LEU:HB3	2.38	0.59
1:C:157:VAL:HG13	1:C:162:THR:OG1	2.03	0.59
1:A:52:MET:HB2	1:A:78:MET:HE2	1.84	0.58
1:C:52:MET:HB3	1:C:78:MET:CE	2.32	0.58
1:A:52:MET:HB2	1:A:78:MET:CE	2.33	0.58
1:A:157:VAL:HG13	1:A:162:THR:HG21	1.85	0.58
1:B:350:VAL:C	1:B:361:ILE:HG22	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:MET:CE	1:C:331:LEU:HD11	2.33	0.58
1:C:159:ILE:HG13	1:C:160:LEU:HG	1.84	0.58
1:A:247:ARG:O	1:A:250:GLN:HB3	2.03	0.58
1:B:128:VAL:CG2	1:B:174:LEU:HD21	2.33	0.58
1:D:16:GLN:HG3	1:D:43:ILE:CD1	2.33	0.58
1:B:242:ASP:OD1	5:B:900:NAG:O5	2.22	0.58
1:A:178:LYS:C	1:A:179:GLU:HG2	2.26	0.58
1:A:342:ARG:HG3	1:A:342:ARG:NH1	2.16	0.58
1:C:111:LEU:HD21	1:C:215:LEU:HG	1.86	0.58
1:C:6:ASN:HD22	1:C:36:LYS:HB3	1.69	0.58
1:C:263:VAL:O	1:C:264:ASP:HB2	2.04	0.57
1:A:96:PRO:HD3	1:A:108:ARG:HD2	1.86	0.57
1:B:17:GLN:HG3	1:B:17:GLN:O	2.04	0.57
1:C:223:ASN:O	1:C:227:GLU:CG	2.52	0.57
1:D:16:GLN:HA	1:D:43:ILE:HD11	1.85	0.57
1:C:25:ARG:NH2	1:C:262:ARG:NH1	2.52	0.57
1:C:11:GLY:HA3	1:C:41:ILE:CG2	2.15	0.57
1:C:180:ARG:HG3	1:C:206:ILE:HD11	1.87	0.57
1:D:129:TYR:CE2	1:D:131:TYR:HB3	2.40	0.56
1:A:157:VAL:CG1	1:A:162:THR:HG21	2.35	0.56
1:C:17:GLN:NE2	2:N:1:NAG:H81	2.20	0.56
1:D:252:TRP:HA	1:D:255:SER:HB2	1.87	0.56
1:C:9:ILE:HD12	1:C:282:MET:CE	2.36	0.56
1:C:71:TYR:HB3	1:C:79:LEU:CD1	2.35	0.56
1:C:249:MET:HE3	1:C:331:LEU:HD11	1.86	0.56
1:B:199:VAL:HG12	1:B:204:ASN:HD22	1.70	0.56
1:D:249:MET:HE1	1:D:268:PRO:HG2	1.86	0.56
1:C:253:ARG:HH22	1:C:266:LYS:C	2.13	0.56
1:A:218:MET:HG2	1:A:236:GLN:NE2	2.21	0.56
1:A:363:TYR:CE2	1:A:371:VAL:CG2	2.88	0.56
1:C:112:GLN:HG3	1:C:142:ARG:HG2	1.88	0.56
1:C:321:ARG:CZ	6:C:411:HOH:O	2.53	0.56
1:A:71:TYR:HD2	1:A:90:PHE:CE2	2.21	0.55
1:B:302:ALA:CB	1:C:5:ASN:HB3	2.35	0.55
1:A:52:MET:CB	1:A:78:MET:CE	2.85	0.55
1:B:171:PHE:CD2	1:B:201:LEU:HD13	2.41	0.55
1:C:124:TRP:CD2	1:C:181:LEU:HD13	2.41	0.55
1:D:194:ILE:HG22	1:D:198:ILE:HD12	1.89	0.55
1:B:95:PHE:CD2	1:B:134:ASP:HB3	2.41	0.55
1:C:180:ARG:NE	1:C:206:ILE:CD1	2.69	0.55
1:D:363:TYR:CZ	1:D:371:VAL:CG2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:O	1:B:17:GLN:CG	2.55	0.55
1:D:351:ILE:HD11	5:D:900:NAG:H81	1.87	0.55
1:C:353:MET:HE3	1:C:358:ILE:CD1	2.33	0.55
1:A:169:MET:SD	1:A:169:MET:C	2.89	0.55
1:B:131:TYR:CZ	1:B:140:LEU:HD22	2.42	0.55
1:B:40:GLN:OE1	1:B:62:LYS:CD	2.54	0.55
1:B:200:LYS:C	1:B:202:GLU:N	2.64	0.55
1:B:306:LEU:O	6:B:391:HOH:O	2.18	0.55
1:D:285:ALA:CB	1:D:323:LEU:HD23	2.36	0.55
1:C:16:GLN:HG3	1:C:43:ILE:CD1	2.37	0.55
1:B:293:ARG:HA	6:B:402:HOH:O	2.06	0.54
1:C:321:ARG:NH2	6:C:411:HOH:O	2.39	0.54
1:D:222:LEU:HD13	1:D:353:MET:HE1	1.88	0.54
1:C:62:LYS:NZ	6:C:419:HOH:O	2.38	0.54
1:A:71:TYR:HB3	1:A:79:LEU:HD12	1.90	0.54
1:C:98:ASP:HA	1:C:342:ARG:NH2	2.23	0.54
1:D:71:TYR:CE1	1:D:76:VAL:CG1	2.86	0.54
1:B:130:ILE:CG2	1:B:159:ILE:CD1	2.85	0.54
1:D:224:LYS:NZ	6:D:387:HOH:O	2.41	0.53
1:B:185:ASP:HA	1:B:213:ALA:HB3	1.90	0.53
1:D:71:TYR:CE2	1:D:92:THR:HG21	2.43	0.53
1:C:52:MET:CB	1:C:78:MET:CE	2.86	0.53
3:F:1:NAG:H61	3:F:2:NAG:C7	2.38	0.53
1:A:27:ALA:HB2	1:A:276:TYR:CD1	2.43	0.53
1:A:71:TYR:HB2	1:A:79:LEU:HD12	1.88	0.53
1:A:99:THR:O	1:A:99:THR:CG2	2.45	0.53
1:A:135:ARG:HH11	1:A:135:ARG:HG2	1.69	0.53
1:B:124:TRP:CE2	1:B:181:LEU:HB3	2.43	0.53
1:C:99:THR:O	1:C:99:THR:CG2	2.50	0.53
1:B:19:GLN:OE1	1:B:269:LYS:HE3	2.09	0.53
1:D:137:LEU:HD12	1:D:137:LEU:C	2.34	0.53
1:B:74:ARG:NH2	2:H:2:NAG:H83	2.23	0.53
1:B:365:ASN:OD1	1:B:365:ASN:C	2.52	0.53
1:D:371:VAL:O	1:D:371:VAL:HG23	2.09	0.53
1:A:363:TYR:CE2	1:A:371:VAL:HG21	2.43	0.52
1:D:174:LEU:HD23	1:D:177:LYS:NZ	2.24	0.52
1:A:322:ALA:O	6:A:409:HOH:O	2.19	0.52
1:B:252:TRP:H	1:B:252:TRP:HD1	1.57	0.52
1:B:288:SER:O	1:B:292:GLN:HG3	2.09	0.52
1:B:349:HIS:CD2	1:B:360:LYS:HE3	2.42	0.52
1:D:195:LEU:HD11	1:D:220:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASN:O	1:D:235:PHE:HB2	2.10	0.52
1:D:361:ILE:CG2	1:D:370:PHE:HZ	2.22	0.52
1:B:179:GLU:HG3	1:B:207:GLY:HA3	1.92	0.52
1:D:98:ASP:O	1:D:342:ARG:NH2	2.43	0.52
1:A:153:GLN:OE1	1:C:153:GLN:HG3	2.10	0.52
1:C:125:GLN:O	1:C:152:TRP:HA	2.10	0.52
1:D:185:ASP:HA	1:D:213:ALA:HB3	1.92	0.52
1:C:114:ALA:O	1:C:118:ILE:HG12	2.10	0.51
1:A:153:GLN:OE1	1:C:153:GLN:CG	2.58	0.51
1:B:171:PHE:HA	1:B:174:LEU:HD12	1.91	0.51
1:C:256:ASP:HB3	1:C:265:TRP:NE1	2.24	0.51
1:D:16:GLN:HG3	1:D:43:ILE:HD11	1.91	0.51
1:A:78:MET:SD	1:A:78:MET:C	2.93	0.51
1:B:78:MET:SD	1:B:78:MET:C	2.93	0.51
1:A:52:MET:CB	1:A:78:MET:HE1	2.40	0.51
1:D:3:MET:CG	1:D:4:PRO:HD3	2.39	0.51
1:B:201:LEU:O	1:B:203:LYS:HG2	2.10	0.51
1:B:252:TRP:H	1:B:252:TRP:CD1	2.27	0.51
1:C:124:TRP:CZ2	1:C:209:HIS:HB3	2.41	0.51
1:B:364:TRP:HD1	1:B:370:PHE:HB2	1.76	0.51
1:A:47:SER:OG	1:A:72:GLU:OE1	2.25	0.51
1:C:95:PHE:CE1	1:C:135:ARG:NH2	2.79	0.51
1:C:124:TRP:CZ2	1:C:181:LEU:HB3	2.45	0.51
1:D:126:THR:CG2	1:D:153:GLN:HB3	2.31	0.51
1:B:249:MET:HB2	1:B:253:ARG:NH1	2.07	0.51
1:B:26:PHE:O	1:B:29:SER:OG	2.29	0.51
1:C:171:PHE:C	1:C:173:ASP:N	2.66	0.51
1:C:295:ASP:O	1:C:296:ILE:HG23	2.11	0.51
1:D:108:ARG:HH12	1:D:187:GLU:CD	2.19	0.51
1:D:72:GLU:O	1:D:76:VAL:HG13	2.11	0.50
1:D:52:MET:CB	1:D:78:MET:CE	2.88	0.50
1:B:16:GLN:HA	1:B:43:ILE:CD1	2.41	0.50
1:B:204:ASN:O	1:B:204:ASN:OD1	2.30	0.50
1:D:352:GLU:HB2	1:D:361:ILE:CD1	2.41	0.50
1:A:236:GLN:HB3	1:A:349:HIS:HB2	1.93	0.50
1:B:40:GLN:NE2	1:B:62:LYS:HE2	2.27	0.50
1:A:128:VAL:HB	1:A:182:VAL:HG22	1.93	0.50
1:D:252:TRP:HA	1:D:255:SER:CB	2.41	0.50
1:D:79:LEU:HD23	1:D:90:PHE:CE2	2.46	0.50
1:A:71:TYR:O	1:A:71:TYR:CD1	2.65	0.50
1:B:255:SER:O	1:B:258:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:TYR:CE2	1:D:371:VAL:HG21	2.47	0.50
1:A:132:ASP:OD1	1:A:132:ASP:O	2.30	0.50
1:D:352:GLU:OE2	3:O:1:NAG:C2	2.60	0.50
1:B:97:VAL:CG2	1:B:100:SER:HB3	2.41	0.49
1:D:108:ARG:NH1	1:D:187:GLU:OE2	2.39	0.49
1:C:226:LYS:HE2	1:C:356:ASP:OD1	2.12	0.49
1:A:218:MET:CG	1:A:236:GLN:NE2	2.76	0.49
1:D:171:PHE:O	1:D:175:GLU:HG2	2.12	0.49
1:D:352:GLU:O	1:D:357:GLY:O	2.30	0.49
1:B:239:ASN:CB	1:B:242:ASP:OD2	2.53	0.49
1:B:276:TYR:CE2	1:B:280:LYS:HD2	2.47	0.49
1:C:296:ILE:HG21	1:C:319:ILE:HD11	1.93	0.49
1:D:105:LEU:HD13	1:D:323:LEU:HB3	1.95	0.49
1:D:168:ARG:HA	1:D:201:LEU:HD21	1.94	0.49
1:D:356:ASP:OD1	1:D:356:ASP:O	2.30	0.49
1:B:72:GLU:CG	1:B:73:ARG:H	2.25	0.49
1:B:130:ILE:HG22	1:B:159:ILE:CD1	2.40	0.49
1:C:121:HIS:CD2	1:C:370:PHE:CE2	2.99	0.49
1:A:131:TYR:HA	1:A:185:ASP:O	2.13	0.49
1:D:242:ASP:HB3	1:D:245:PRO:HG2	1.93	0.49
1:D:361:ILE:HG22	1:D:370:PHE:HZ	1.75	0.49
1:B:317:ILE:O	1:B:317:ILE:HG13	2.12	0.49
1:B:199:VAL:O	1:B:202:GLU:HA	2.13	0.49
1:C:180:ARG:HD2	1:C:206:ILE:HD13	1.94	0.49
1:B:124:TRP:CH2	1:B:181:LEU:HB3	2.47	0.48
1:C:72:GLU:CG	1:C:73:ARG:N	2.76	0.48
1:C:121:HIS:CD2	1:C:370:PHE:HE2	2.31	0.48
1:A:130:ILE:CG2	1:A:159:ILE:CG1	2.91	0.48
1:B:97:VAL:HG23	1:B:100:SER:HB3	1.95	0.48
1:D:65:TYR:CE1	1:D:296:ILE:HG22	2.34	0.48
1:D:296:ILE:HG22	1:D:297:SER:N	2.26	0.48
1:D:52:MET:HB3	1:D:78:MET:HE1	1.94	0.48
1:B:106:GLN:HE22	1:B:342:ARG:HD3	1.74	0.48
1:B:199:VAL:O	1:B:202:GLU:N	2.46	0.48
1:C:16:GLN:HA	1:C:43:ILE:HD11	1.94	0.48
1:C:181:LEU:HD22	1:C:209:HIS:HB2	1.90	0.48
1:A:353:MET:HA	1:A:358:ILE:HA	1.95	0.48
1:B:182:VAL:HG12	1:B:183:VAL:N	2.29	0.48
1:C:157:VAL:CG1	1:C:162:THR:OG1	2.62	0.48
1:D:334:ASN:ND2	1:D:345:ASN:HB3	2.29	0.48
1:A:135:ARG:CG	1:A:135:ARG:NH1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:O	1:C:343:ARG:NH1	2.45	0.48
1:C:216:GLY:O	1:C:220:ILE:HG23	2.13	0.48
1:C:6:ASN:ND2	1:C:36:LYS:HB3	2.28	0.48
1:D:229:GLY:O	1:D:354:LYS:HE3	2.14	0.48
1:B:11:GLY:HA2	1:B:68:PHE:O	2.13	0.48
1:C:226:LYS:HE3	1:C:356:ASP:C	2.39	0.47
1:D:339:GLU:CD	1:D:339:GLU:H	2.22	0.47
1:A:124:TRP:CE2	1:A:181:LEU:HB3	2.49	0.47
1:C:363:TYR:CE2	1:C:371:VAL:CG2	2.97	0.47
1:D:349:HIS:HB2	5:D:900:NAG:H82	1.95	0.47
1:A:47:SER:CB	1:A:72:GLU:OE1	2.62	0.47
1:B:135:ARG:NE	1:B:185:ASP:OD1	2.47	0.47
1:B:226:LYS:HD3	1:B:356:ASP:OD1	2.15	0.47
1:B:354:LYS:O	1:B:357:GLY:CA	2.62	0.47
1:D:194:ILE:HG22	1:D:198:ILE:CD1	2.44	0.47
1:A:301:ASN:OD1	1:A:302:ALA:N	2.47	0.47
1:B:3:MET:HE1	1:B:289:LEU:HB2	1.96	0.47
1:B:106:GLN:NE2	1:B:342:ARG:CD	2.70	0.47
1:C:171:PHE:CE1	1:C:180:ARG:HB3	2.49	0.47
1:A:159:ILE:HD12	1:A:167:TYR:CZ	2.47	0.47
1:C:124:TRP:CD2	1:C:181:LEU:HB3	2.49	0.47
1:C:195:LEU:O	1:C:198:ILE:HG22	2.14	0.47
1:D:249:MET:CE	1:D:268:PRO:CD	2.85	0.47
1:A:119:ILE:HG23	1:A:124:TRP:HB2	1.97	0.47
1:D:122:TYR:HB3	3:O:2:NAG:H81	1.96	0.47
1:D:218:MET:C	1:D:267:ARG:HH22	2.23	0.47
1:D:289:LEU:HD13	1:D:296:ILE:CD1	2.44	0.47
1:A:190:ARG:HG2	1:A:194:ILE:CD1	2.36	0.47
1:C:105:LEU:HD21	1:C:323:LEU:HB3	1.95	0.47
1:C:263:VAL:CG1	1:C:264:ASP:N	2.67	0.47
1:D:199:VAL:HG23	1:D:200:LYS:N	2.29	0.47
1:A:52:MET:HE3	1:A:79:LEU:HD11	1.97	0.47
1:C:124:TRP:CE2	1:C:181:LEU:HB3	2.50	0.47
1:D:48:ASP:O	1:D:52:MET:HG2	2.14	0.47
1:D:105:LEU:CD1	1:D:323:LEU:CB	2.93	0.47
1:D:119:ILE:HG23	1:D:124:TRP:HB2	1.97	0.47
1:D:199:VAL:HA	1:D:202:GLU:HG2	1.97	0.47
1:A:54:TYR:O	1:A:58:SER:HB2	2.15	0.47
1:C:149:GLU:HG3	1:C:150:LYS:HG3	1.97	0.46
1:C:304:ASP:OD2	6:C:406:HOH:O	2.20	0.46
1:B:26:PHE:CD1	1:B:252:TRP:HB3	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:CG1	1:C:52:MET:CE	2.89	0.46
1:C:280:LYS:HE3	1:C:328:PHE:HE1	1.80	0.46
1:D:354:LYS:O	1:D:357:GLY:N	2.49	0.46
1:A:8:GLN:HE21	1:A:38:LEU:HD23	1.79	0.46
1:A:355:HIS:O	1:A:356:ASP:HB2	2.15	0.46
1:B:126:THR:HG22	1:B:153:GLN:HB2	1.97	0.46
1:C:12:LEU:HD22	1:C:52:MET:CE	2.45	0.46
1:C:287:GLN:O	1:C:291:ARG:HG2	2.15	0.46
1:D:158:ASN:HB3	1:D:161:THR:HG22	1.96	0.46
1:C:20:GLU:OE1	1:C:20:GLU:N	2.34	0.46
1:A:76:VAL:HG13	1:A:77:ASN:N	2.31	0.46
1:A:130:ILE:HG21	1:A:159:ILE:HD11	1.94	0.46
1:B:277:ASP:OD1	1:B:280:LYS:NZ	2.40	0.46
1:C:108:ARG:HA	1:C:109:PRO:HD3	1.81	0.46
1:D:231:ASN:HA	1:D:354:LYS:HG3	1.98	0.46
1:C:105:LEU:CD2	1:C:323:LEU:HB3	2.45	0.46
1:D:250:GLN:O	1:D:254:THR:HG23	2.16	0.46
1:D:296:ILE:CG2	1:D:297:SER:N	2.79	0.46
1:D:55:ARG:HA	1:D:55:ARG:HD3	1.75	0.46
1:B:52:MET:HB2	1:B:78:MET:HE2	1.98	0.45
1:B:70:PHE:HE1	1:B:93:PRO:HG2	1.77	0.45
1:B:206:ILE:H	1:B:206:ILE:HG13	1.57	0.45
1:C:224:LYS:NZ	1:C:225:PHE:CE1	2.83	0.45
1:C:280:LYS:HE3	1:C:328:PHE:CE1	2.51	0.45
1:B:217:PHE:C	1:B:219:ASP:N	2.74	0.45
1:C:71:TYR:CD2	1:C:90:PHE:CE2	2.88	0.45
1:C:276:TYR:CE2	1:C:280:LYS:CD	2.98	0.45
1:C:249:MET:HE1	1:C:331:LEU:HD21	1.98	0.45
1:D:129:TYR:CD2	1:D:140:LEU:HD13	2.51	0.45
1:B:72:GLU:CG	1:B:73:ARG:N	2.80	0.45
1:D:170:LEU:HD12	1:D:170:LEU:C	2.41	0.45
1:D:354:LYS:O	1:D:355:HIS:C	2.59	0.45
1:B:222:LEU:O	1:B:223:ASN:OD1	2.34	0.45
1:B:267:ARG:HA	1:B:268:PRO:HD3	1.77	0.45
1:A:130:ILE:CG2	1:A:159:ILE:CD1	2.91	0.45
1:B:354:LYS:HE2	1:B:359:ARG:HH12	1.82	0.45
1:B:71:TYR:CD2	1:B:90:PHE:HE2	2.32	0.45
1:C:352:GLU:OE1	1:C:361:ILE:CD1	2.65	0.45
1:D:361:ILE:HG22	1:D:370:PHE:CZ	2.52	0.45
1:A:219:ASP:OD1	1:A:267:ARG:NH1	2.50	0.44
1:B:239:ASN:ND2	1:B:242:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LYS:C	1:C:355:HIS:CG	2.94	0.44
1:D:26:PHE:CE2	1:D:252:TRP:CB	2.98	0.44
1:C:86:LEU:O	1:C:87:HIS:HB2	2.16	0.44
1:D:71:TYR:CD2	1:D:90:PHE:CE2	2.94	0.44
1:B:56:PHE:CD2	1:B:56:PHE:C	2.95	0.44
1:B:174:LEU:HD23	1:B:180:ARG:CD	2.37	0.44
1:A:319:ILE:N	1:A:319:ILE:HD12	2.32	0.44
1:A:366:GLU:OE2	6:A:398:HOH:O	2.21	0.44
1:D:26:PHE:CZ	1:D:252:TRP:CB	2.68	0.44
1:D:135:ARG:CG	1:D:135:ARG:NH1	2.61	0.44
1:A:60:PHE:O	1:A:298:ARG:NH2	2.50	0.44
1:B:249:MET:O	1:B:253:ARG:HG3	2.18	0.44
1:C:25:ARG:NH2	1:C:262:ARG:HH12	2.14	0.44
1:D:157:VAL:HG13	1:D:162:THR:HG21	2.00	0.44
1:C:121:HIS:HD2	1:C:370:PHE:CE2	2.35	0.44
1:D:97:VAL:CG2	1:D:100:SER:HB3	2.47	0.44
1:A:373:ALA:O	1:A:375:LEU:CD1	2.62	0.43
1:C:124:TRP:HZ2	1:C:209:HIS:CB	2.28	0.43
1:A:70:PHE:CE1	1:A:93:PRO:HG2	2.53	0.43
1:B:3:MET:HE1	1:B:289:LEU:CB	2.47	0.43
1:A:55:ARG:HA	1:A:55:ARG:HD3	1.81	0.43
1:B:71:TYR:HD2	1:B:90:PHE:CE2	2.31	0.43
1:B:78:MET:CE	1:B:79:LEU:HG	2.49	0.43
1:B:250:GLN:CA	1:B:253:ARG:NH2	2.82	0.43
1:B:352:GLU:OE1	1:B:361:ILE:HD13	2.19	0.43
1:C:255:SER:C	1:C:257:SER:H	2.26	0.43
1:D:369:LYS:HA	1:D:369:LYS:HD3	1.75	0.43
1:C:3:MET:HG3	1:C:4:PRO:O	2.18	0.43
1:C:353:MET:HA	1:C:357:GLY:O	2.17	0.43
1:D:195:LEU:HD11	1:D:220:ILE:HG23	2.00	0.43
1:B:322:ALA:O	1:B:326:VAL:HG23	2.19	0.43
1:C:200:LYS:H	1:C:200:LYS:HG3	1.66	0.43
4:M:3:BMA:H4	4:M:4:MAN:H2	2.00	0.43
1:D:16:GLN:HA	1:D:43:ILE:CD1	2.48	0.43
1:C:45:ASN:OD1	1:C:45:ASN:C	2.62	0.43
1:C:171:PHE:C	1:C:173:ASP:H	2.24	0.43
1:C:276:TYR:CE2	1:C:280:LYS:HD2	2.54	0.43
1:C:352:GLU:OE1	1:C:361:ILE:HG12	2.18	0.43
1:A:76:VAL:HG21	1:A:97:VAL:HG21	2.00	0.43
1:C:20:GLU:OE2	1:C:269:LYS:NZ	2.51	0.43
1:D:71:TYR:HE2	1:D:92:THR:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:HIS:CB	5:D:900:NAG:H82	2.49	0.43
1:A:169:MET:CE	1:C:148:ALA:O	2.65	0.43
1:A:371:VAL:O	1:A:371:VAL:HG23	2.19	0.43
1:C:352:GLU:HB2	1:C:361:ILE:HG13	2.01	0.43
1:B:16:GLN:HA	1:B:43:ILE:HD11	2.01	0.42
1:D:7:ILE:HG12	1:D:35:PRO:HB2	2.01	0.42
1:A:216:GLY:O	1:A:220:ILE:HG12	2.19	0.42
1:A:71:TYR:CD1	1:A:71:TYR:C	2.97	0.42
1:A:175:GLU:O	1:A:176:LYS:CB	2.51	0.42
1:A:194:ILE:O	1:A:198:ILE:HG12	2.20	0.42
1:C:17:GLN:HE22	2:N:1:NAG:C8	2.32	0.42
1:C:355:HIS:HB2	1:C:356:ASP:H	1.68	0.42
1:D:180:ARG:N	1:D:180:ARG:HD2	2.34	0.42
1:A:135:ARG:NH2	1:A:185:ASP:OD1	2.52	0.42
1:C:247:ARG:O	1:C:250:GLN:HB2	2.20	0.42
1:C:327:ARG:HA	1:C:335:VAL:O	2.20	0.42
1:A:169:MET:C	1:A:169:MET:HE3	2.45	0.42
1:D:249:MET:O	1:D:253:ARG:HB2	2.19	0.42
1:A:191:LEU:HD23	1:A:220:ILE:CG1	2.47	0.42
1:D:26:PHE:CE2	1:D:252:TRP:CG	3.07	0.42
1:D:363:TYR:CE2	1:D:371:VAL:CG2	3.02	0.42
1:B:128:VAL:HB	1:B:182:VAL:HG13	2.02	0.42
1:B:131:TYR:HD1	1:B:132:ASP:O	2.02	0.42
1:A:137:LEU:HD11	1:C:141:GLN:OE1	2.19	0.42
1:A:218:MET:HG3	1:A:236:GLN:CD	2.45	0.42
1:B:299:ARG:O	1:B:300:GLY:C	2.62	0.42
1:D:137:LEU:HD12	1:D:138:SER:N	2.34	0.42
1:B:2:ALA:O	1:B:295:ASP:HA	2.20	0.42
1:C:96:PRO:CD	1:C:108:ARG:HD2	2.30	0.42
1:A:135:ARG:HG3	1:A:135:ARG:O	2.19	0.41
1:C:25:ARG:CZ	1:C:262:ARG:HH12	2.33	0.41
1:D:18:SER:OG	1:D:21:HIS:HD2	2.03	0.41
1:B:178:LYS:HB3	1:B:179:GLU:H	1.61	0.41
1:C:27:ALA:HB2	1:C:276:TYR:CD1	2.55	0.41
1:A:71:TYR:CD2	1:A:90:PHE:HE2	2.27	0.41
1:B:171:PHE:CG	1:B:174:LEU:HD12	2.56	0.41
1:D:65:TYR:CE1	1:D:296:ILE:HG21	2.54	0.41
1:B:352:GLU:CD	1:B:361:ILE:HD13	2.44	0.41
1:D:122:TYR:OH	1:D:361:ILE:HD13	2.20	0.41
1:C:124:TRP:CE2	1:C:181:LEU:HD13	2.55	0.41
1:D:16:GLN:C	1:D:17:GLN:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ASP:OD2	1:D:223:ASN:ND2	2.53	0.41
1:D:298:ARG:HD2	1:D:313:TRP:CE2	2.55	0.41
1:A:284:GLU:HB3	1:A:326:VAL:HG22	2.03	0.41
1:B:11:GLY:HA3	1:B:41:ILE:CG2	2.48	0.41
1:B:208:TYR:HB3	1:B:210:TYR:CE2	2.55	0.41
1:C:121:HIS:ND1	1:C:121:HIS:O	2.53	0.41
1:C:308:ASN:HA	1:C:309:PRO:HA	1.81	0.41
1:D:217:PHE:CD1	1:D:234:GLY:HA3	2.55	0.41
1:B:350:VAL:HB	1:B:361:ILE:CG2	2.49	0.41
1:C:132:ASP:HB3	1:C:135:ARG:HG2	2.03	0.41
1:D:319:ILE:N	1:D:319:ILE:HD12	2.36	0.41
1:A:47:SER:HB3	1:A:72:GLU:OE1	2.21	0.41
1:A:195:LEU:CD2	1:A:225:PHE:CE2	2.94	0.41
1:A:350:VAL:HG23	1:A:363:TYR:HA	2.01	0.41
1:B:3:MET:CE	1:B:289:LEU:HB3	2.51	0.41
1:B:106:GLN:HE22	1:B:342:ARG:CD	2.32	0.41
1:B:350:VAL:HB	1:B:361:ILE:HG23	2.02	0.41
1:D:26:PHE:CE1	1:D:252:TRP:CB	2.90	0.41
1:B:276:TYR:O	1:B:280:LYS:HD3	2.21	0.41
1:D:302:ALA:O	1:D:303:GLY:C	2.64	0.41
1:A:74:ARG:NH1	2:E:2:NAG:C8	2.82	0.40
1:A:124:TRP:CZ2	1:A:181:LEU:HB3	2.56	0.40
1:A:317:ILE:O	1:A:321:ARG:HG3	2.21	0.40
1:A:171:PHE:HA	1:A:174:LEU:HB3	2.01	0.40
1:C:33:GLU:HB2	1:C:287:GLN:NE2	2.35	0.40
1:B:198:ILE:O	1:B:201:LEU:HB2	2.22	0.40
1:C:121:HIS:HD2	1:C:370:PHE:HE2	1.68	0.40
1:D:352:GLU:OE1	1:D:359:ARG:NH2	2.54	0.40
1:A:73:ARG:O	1:A:76:VAL:HG12	2.21	0.40
1:A:173:ASP:OD2	1:A:173:ASP:N	2.54	0.40
1:B:199:VAL:C	1:B:202:GLU:H	2.29	0.40
1:D:118:ILE:HD11	1:D:350:VAL:HG21	2.03	0.40
1:C:127:PHE:HB2	1:C:181:LEU:O	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	366/384 (95%)	354 (97%)	12 (3%)	0	100	100
1	B	362/384 (94%)	341 (94%)	20 (6%)	1 (0%)	36	55
1	C	370/384 (96%)	350 (95%)	19 (5%)	1 (0%)	36	55
1	D	363/384 (94%)	342 (94%)	21 (6%)	0	100	100
All	All	1461/1536 (95%)	1387 (95%)	72 (5%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	MET
1	C	263	VAL

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	322/336 (96%)	309 (96%)	13 (4%)	28	54
1	B	320/336 (95%)	309 (97%)	11 (3%)	32	60
1	C	326/336 (97%)	308 (94%)	18 (6%)	19	40
1	D	320/336 (95%)	308 (96%)	12 (4%)	29	56
All	All	1288/1344 (96%)	1234 (96%)	54 (4%)	26	52

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	72	GLU
1	A	80	THR
1	A	118	ILE
1	A	135	ARG
1	A	194	ILE
1	A	223	ASN
1	A	237	LEU
1	A	297	SER
1	A	326	VAL
1	A	331	LEU
1	A	339	GLU
1	A	359	ARG
1	B	73	ARG
1	B	74	ARG
1	B	105	LEU
1	B	118	ILE
1	B	181	LEU
1	B	191	LEU
1	B	224	LYS
1	B	244	ILE
1	B	252	TRP
1	B	299	ARG
1	B	351	ILE
1	C	52	MET
1	C	97	VAL
1	C	98	ASP
1	C	116	ILE
1	C	120	ASP
1	C	121	HIS
1	C	153	GLN
1	C	198	ILE
1	C	214	ASN
1	C	249	MET
1	C	255	SER
1	C	269	LYS
1	C	296	ILE
1	C	326	VAL
1	C	329	GLU
1	C	331	LEU
1	C	350	VAL
1	C	355	HIS
1	D	38	LEU

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Mol	Chain	Res	Type
1	D	72	GLU
1	D	74	ARG
1	D	110	GLU
1	D	135	ARG
1	D	150	LYS
1	D	164	GLU
1	D	244	ILE
1	D	326	VAL
1	D	339	GLU
1	D	354	LYS
1	D	371	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	17	GLN
1	A	40	GLN
1	A	77	ASN
1	A	106	GLN
1	A	287	GLN
1	A	324	GLN
1	B	141	GLN
1	B	158	ASN
1	B	192	ASN
1	B	197	GLN
1	B	204	ASN
1	B	209	HIS
1	B	325	GLN
1	B	336	GLN
1	B	349	HIS
1	B	355	HIS
1	C	6	ASN
1	C	17	GLN
1	C	192	ASN
1	C	324	GLN
1	C	355	HIS
1	D	17	GLN
1	D	59	GLN
1	D	141	GLN
1	D	197	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 ⓘ

32 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	NAG	E	1	2,1	14,14,15	0.82	0	17,19,21	1.56	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	2.26	2 (11%)
2	BMA	E	3	2	11,11,12	0.52	0	15,15,17	1.44	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.63	0	17,19,21	0.68	0
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	2.18	7 (41%)
3	NAG	G	1	1,3	14,14,15	0.74	0	17,19,21	1.01	0
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	1.11	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	1.34	3 (17%)
2	BMA	H	3	2	11,11,12	0.56	0	15,15,17	1.23	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.63	0	17,19,21	2.34	4 (23%)
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	1.03	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.68	0	17,19,21	1.45	2 (11%)
3	NAG	J	2	3	14,14,15	0.41	0	17,19,21	1.91	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.69	0	17,19,21	1.40	3 (17%)
3	NAG	K	2	3	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.61	0	17,19,21	1.11	2 (11%)
3	NAG	L	2	3	14,14,15	0.57	0	17,19,21	1.39	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	1	4,1	14,14,15	0.65	0	17,19,21	1.34	2 (11%)
4	NAG	M	2	4	14,14,15	0.70	0	17,19,21	1.00	0
4	BMA	M	3	4	11,11,12	0.48	0	15,15,17	1.05	1 (6%)
4	MAN	M	4	4	11,11,12	0.71	0	15,15,17	1.97	5 (33%)
4	MAN	M	5	4	11,11,12	0.75	0	15,15,17	1.50	4 (26%)
4	MAN	M	6	4	11,11,12	0.58	0	15,15,17	0.89	1 (6%)
4	MAN	M	7	4	11,11,12	0.58	0	15,15,17	1.10	1 (6%)
2	NAG	N	1	2,1	14,14,15	0.67	0	17,19,21	2.00	4 (23%)
2	NAG	N	2	2	14,14,15	0.68	0	17,19,21	1.66	8 (47%)
2	BMA	N	3	2	11,11,12	0.60	0	15,15,17	1.54	2 (13%)
3	NAG	O	1	1,3	14,14,15	1.46	1 (7%)	17,19,21	1.29	1 (5%)
3	NAG	O	2	3	14,14,15	0.80	0	17,19,21	2.03	4 (23%)
3	NAG	P	1	1,3	14,14,15	1.44	1 (7%)	17,19,21	1.22	2 (11%)
3	NAG	P	2	3	14,14,15	0.62	0	17,19,21	1.06	1 (5%)

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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	MAN	M	5	4	-	0/2/19/22	0/1/1/1
4	MAN	M	6	4	-	0/2/19/22	0/1/1/1
4	MAN	M	7	4	-	2/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	O5-C1	-5.20	1.35	1.43
3	P	1	NAG	O5-C1	-5.10	1.35	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	8.30	123.31	112.19
3	J	2	NAG	C1-O5-C5	6.39	120.75	112.19
3	I	1	NAG	C1-O5-C5	5.81	119.98	112.19
4	M	4	MAN	C3-C4-C5	4.73	118.80	110.23
3	O	2	NAG	C2-N2-C7	4.61	129.07	122.90
2	N	1	NAG	O4-C4-C5	-4.41	98.47	109.32
3	F	2	NAG	C1-O5-C5	4.37	118.05	112.19
3	I	1	NAG	C4-C3-C2	4.35	117.40	111.02
3	O	2	NAG	C4-C3-C2	4.33	117.37	111.02
2	N	1	NAG	O5-C1-C2	-4.10	104.94	111.29
3	F	2	NAG	C3-C4-C5	-3.98	103.02	110.23
2	E	1	NAG	C4-C3-C2	3.98	116.84	111.02
3	L	2	NAG	C1-O5-C5	3.62	117.03	112.19
2	N	1	NAG	C6-C5-C4	-3.55	104.30	113.02
2	E	1	NAG	C1-C2-N2	-3.47	104.96	110.43
3	J	1	NAG	C1-C2-N2	-3.44	105.02	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-C2-C3	3.44	114.65	109.64
3	O	1	NAG	O5-C1-C2	-3.41	106.02	111.29
2	N	1	NAG	C1-O5-C5	3.36	116.68	112.19
4	M	4	MAN	C2-C3-C4	3.28	116.63	110.86
4	M	4	MAN	C1-O5-C5	3.28	116.58	112.19
4	M	5	MAN	C2-C3-C4	3.24	116.56	110.86
2	N	2	NAG	O5-C5-C4	-3.24	102.94	110.83
2	N	3	BMA	O5-C5-C4	-3.20	103.05	110.83
2	H	3	BMA	C2-C3-C4	3.16	116.42	110.86
3	O	2	NAG	O7-C7-N2	3.15	127.54	121.98
3	K	1	NAG	C3-C4-C5	-3.11	104.58	110.23
3	I	1	NAG	O7-C7-C8	-3.10	116.54	122.05
2	H	2	NAG	C8-C7-N2	2.99	121.08	116.12
3	I	1	NAG	C2-N2-C7	2.97	126.88	122.90
3	K	1	NAG	O5-C5-C6	2.97	113.44	107.66
3	F	2	NAG	O3-C3-C2	2.94	115.51	109.40
3	F	2	NAG	O4-C4-C5	2.93	116.55	109.32
4	M	5	MAN	C3-C4-C5	2.92	115.52	110.23
2	E	2	NAG	C4-C3-C2	-2.91	106.75	111.02
3	F	2	NAG	C4-C3-C2	-2.88	106.80	111.02
2	H	1	NAG	O5-C5-C6	2.82	113.16	107.66
3	J	2	NAG	C4-C3-C2	-2.71	107.05	111.02
2	N	3	BMA	O2-C2-C1	-2.58	103.31	109.22
3	G	2	NAG	C4-C3-C2	2.53	114.73	111.02
3	F	2	NAG	C1-C2-N2	2.52	114.40	110.43
4	M	5	MAN	C1-C2-C3	2.49	113.27	109.64
3	I	2	NAG	O7-C7-C8	-2.47	117.66	122.05
4	M	7	MAN	C3-C4-C5	2.45	114.67	110.23
3	J	2	NAG	C1-C2-N2	2.43	114.26	110.43
2	H	3	BMA	C3-C4-C5	2.32	114.45	110.23
4	M	1	NAG	C4-C3-C2	2.29	114.38	111.02
2	H	1	NAG	C4-C3-C2	2.29	114.38	111.02
3	P	1	NAG	C1-O5-C5	-2.29	109.12	112.19
3	L	1	NAG	C1-C2-N2	-2.27	106.85	110.43
3	K	1	NAG	C1-C2-N2	-2.21	106.96	110.43
4	M	5	MAN	C1-O5-C5	2.20	115.13	112.19
3	P	2	NAG	C2-N2-C7	2.19	125.84	122.90
4	M	3	BMA	C1-O5-C5	2.18	115.11	112.19
3	L	2	NAG	C2-N2-C7	2.18	125.82	122.90
3	G	2	NAG	O5-C5-C6	2.17	111.89	107.66
3	F	2	NAG	O5-C5-C6	2.17	111.88	107.66
3	P	1	NAG	O5-C1-C2	-2.16	107.94	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	NAG	C8-C7-N2	-2.16	112.53	116.12
2	N	2	NAG	O4-C4-C5	-2.14	104.05	109.32
4	M	1	NAG	O4-C4-C3	-2.14	105.34	110.38
3	I	2	NAG	C8-C7-N2	2.14	119.66	116.12
2	N	2	NAG	O4-C4-C3	-2.13	105.34	110.38
4	M	6	MAN	C1-O5-C5	2.13	115.04	112.19
2	E	3	BMA	C1-O5-C5	2.13	115.03	112.19
2	N	2	NAG	O3-C3-C2	2.11	113.79	109.40
3	K	2	NAG	O7-C7-C8	-2.11	118.30	122.05
3	J	1	NAG	C2-N2-C7	2.11	125.72	122.90
2	E	3	BMA	O5-C5-C4	-2.08	105.76	110.83
4	M	4	MAN	C1-C2-C3	2.08	112.68	109.64
2	H	2	NAG	O7-C7-C8	-2.07	118.37	122.05
2	N	2	NAG	C8-C7-N2	2.06	119.54	116.12
2	N	2	NAG	O7-C7-C8	-2.06	118.38	122.05
2	N	2	NAG	O3-C3-C4	-2.05	105.55	110.38
2	N	2	NAG	C2-N2-C7	-2.03	120.18	122.90
2	H	2	NAG	O5-C5-C4	-2.02	105.91	110.83
4	M	4	MAN	O5-C5-C4	2.02	115.74	110.83
3	L	1	NAG	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
4	M	7	MAN	O5-C5-C6-O6
4	M	7	MAN	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6

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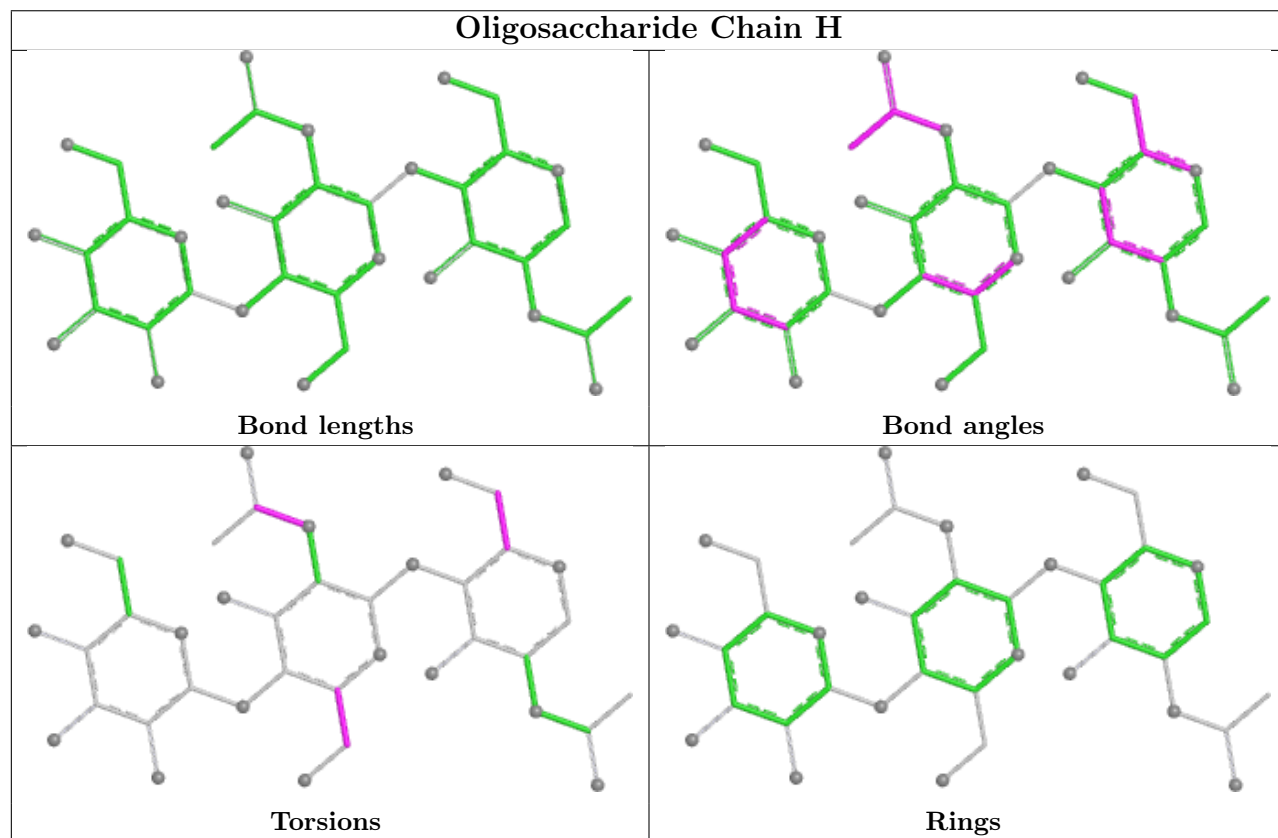
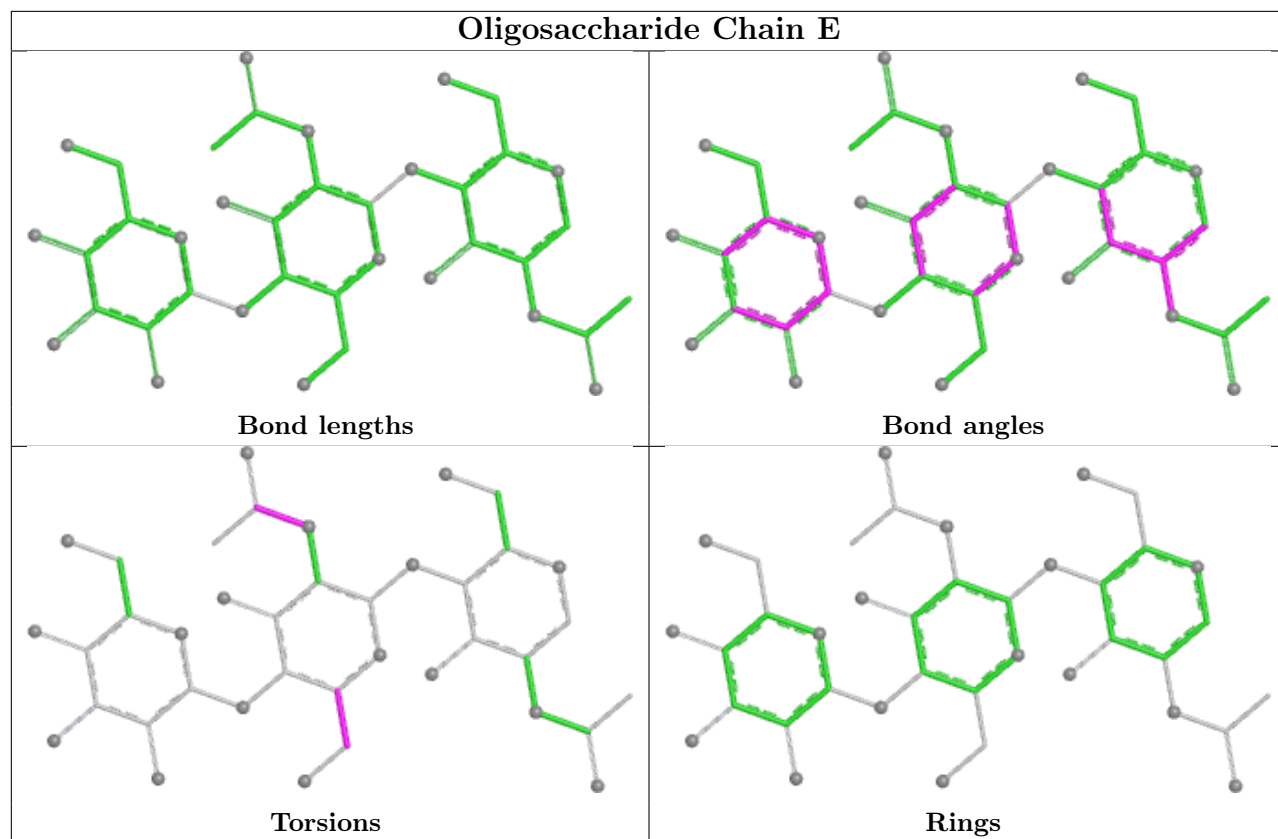
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	J	1	NAG	C4-C5-C6-O6

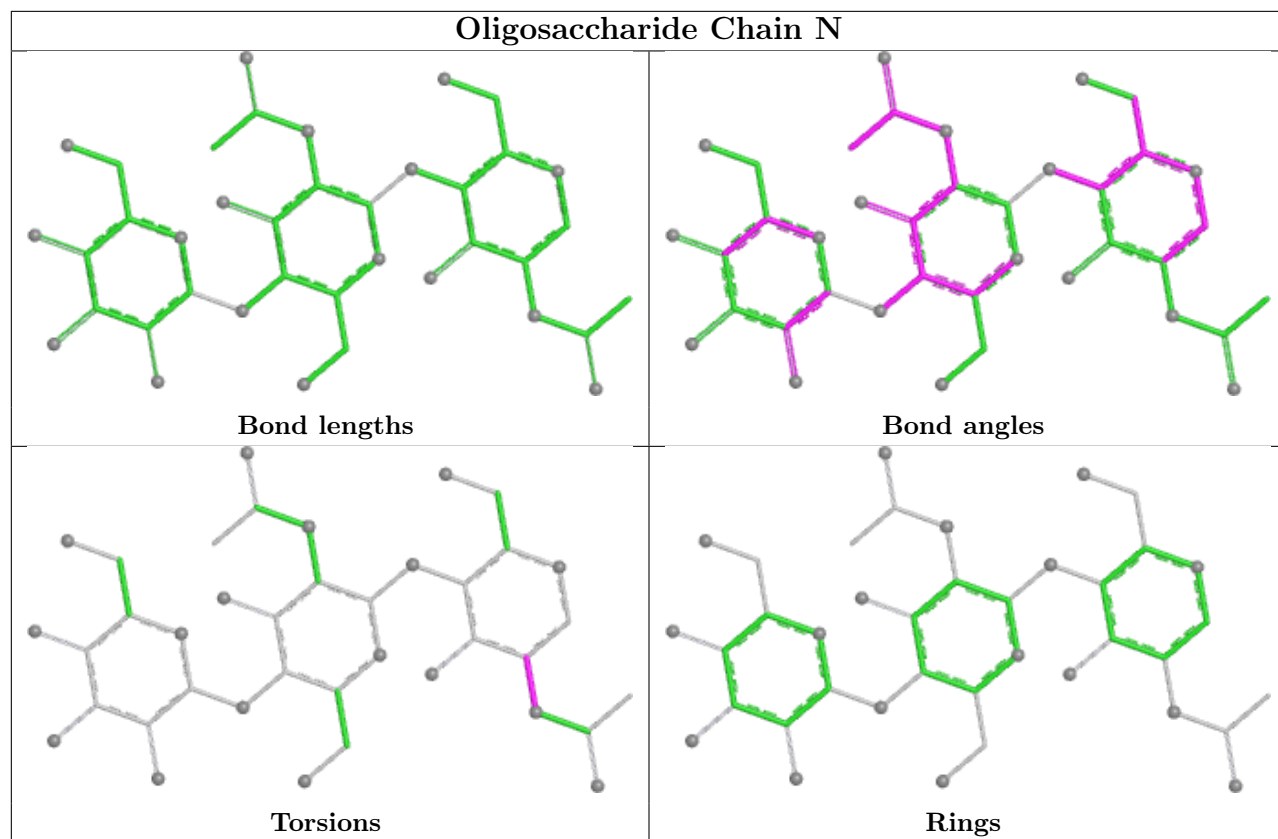
There are no ring outliers.

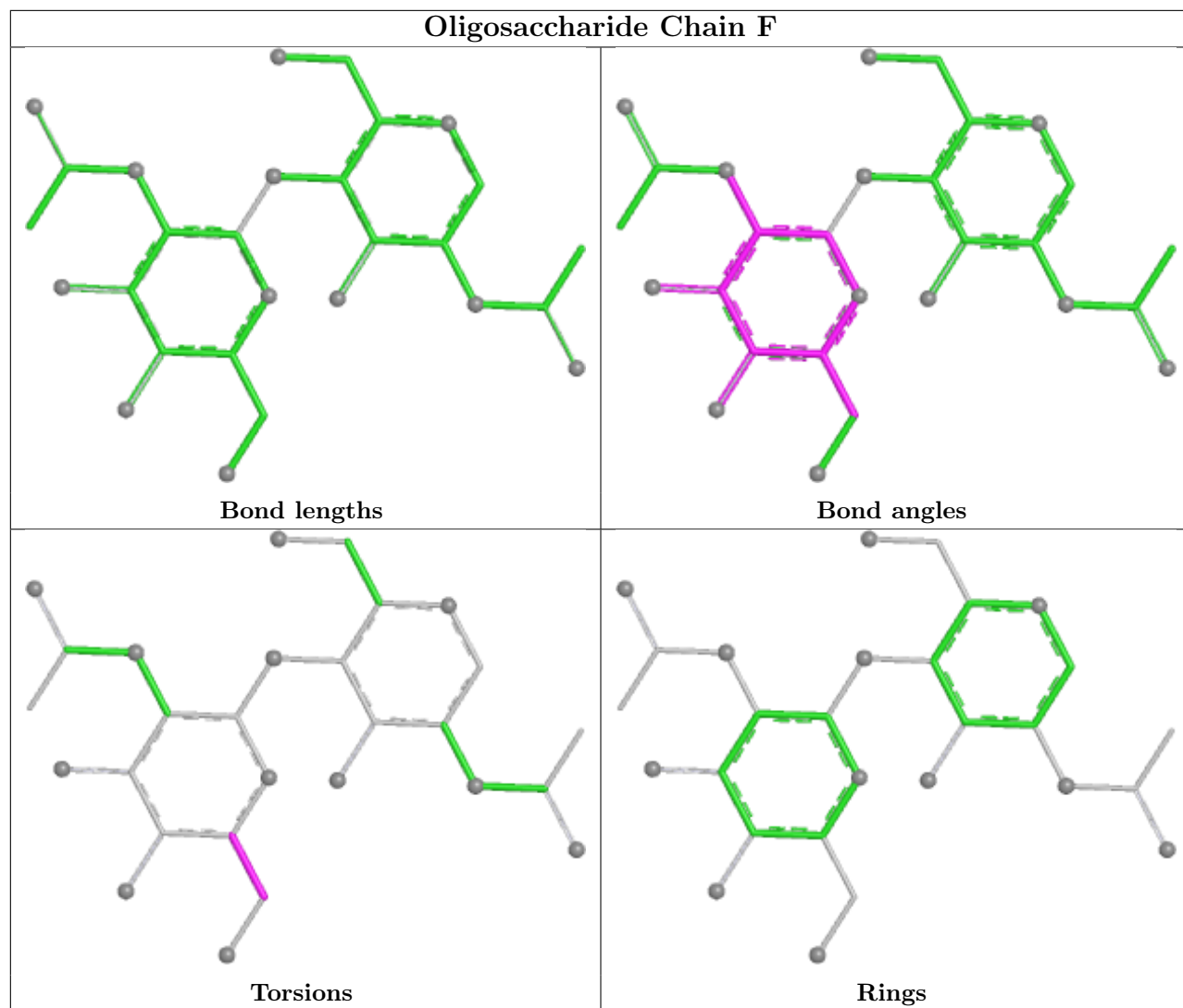
12 monomers are involved in 16 short contacts:

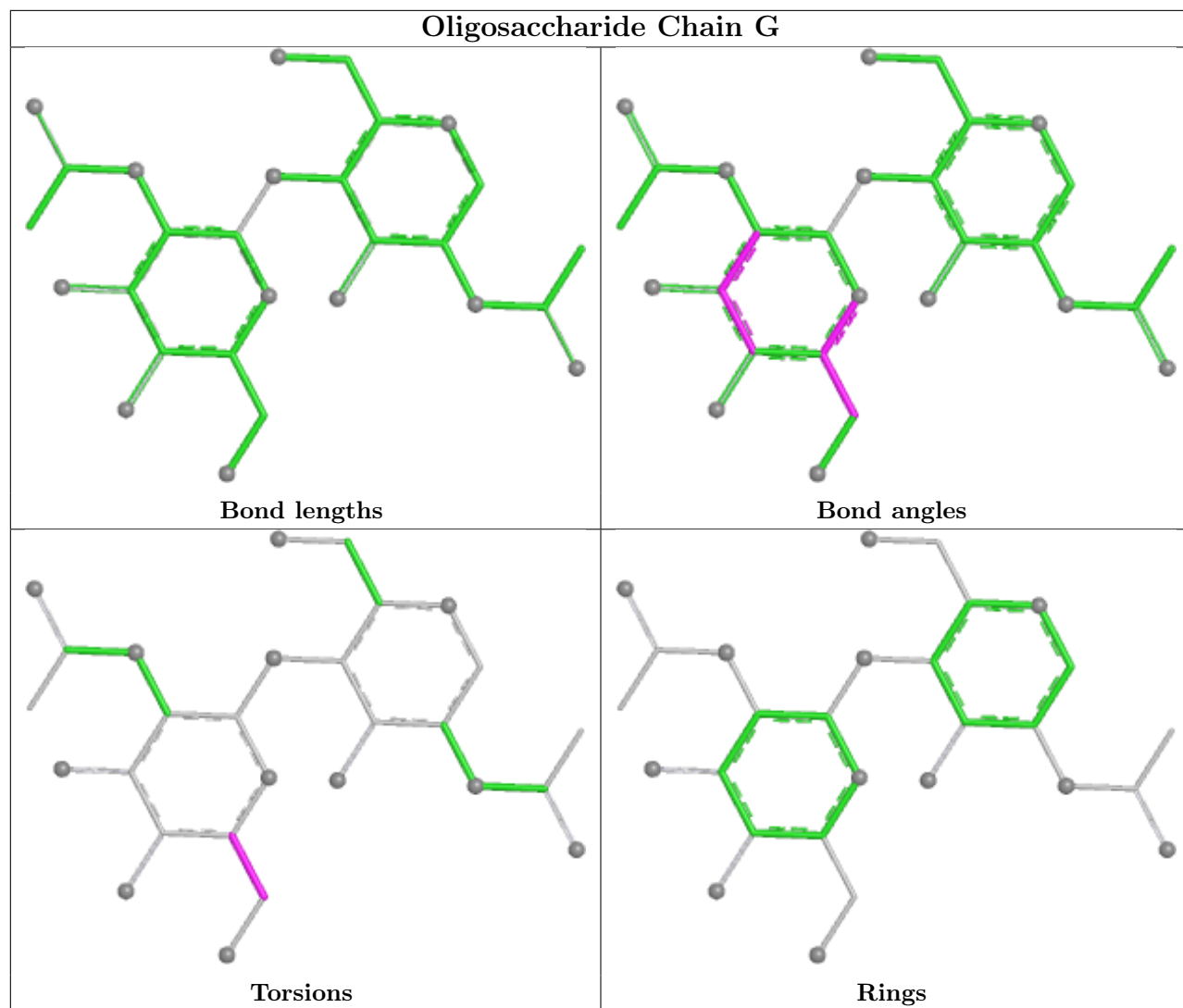
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2	NAG	1	0
3	O	1	NAG	3	0
3	F	1	NAG	1	0
3	F	2	NAG	1	0
2	H	2	NAG	2	0
2	E	2	NAG	2	0
3	K	1	NAG	2	0
3	O	2	NAG	1	0
4	M	4	MAN	1	0
2	N	1	NAG	2	0
4	M	3	BMA	1	0
3	I	1	NAG	1	0

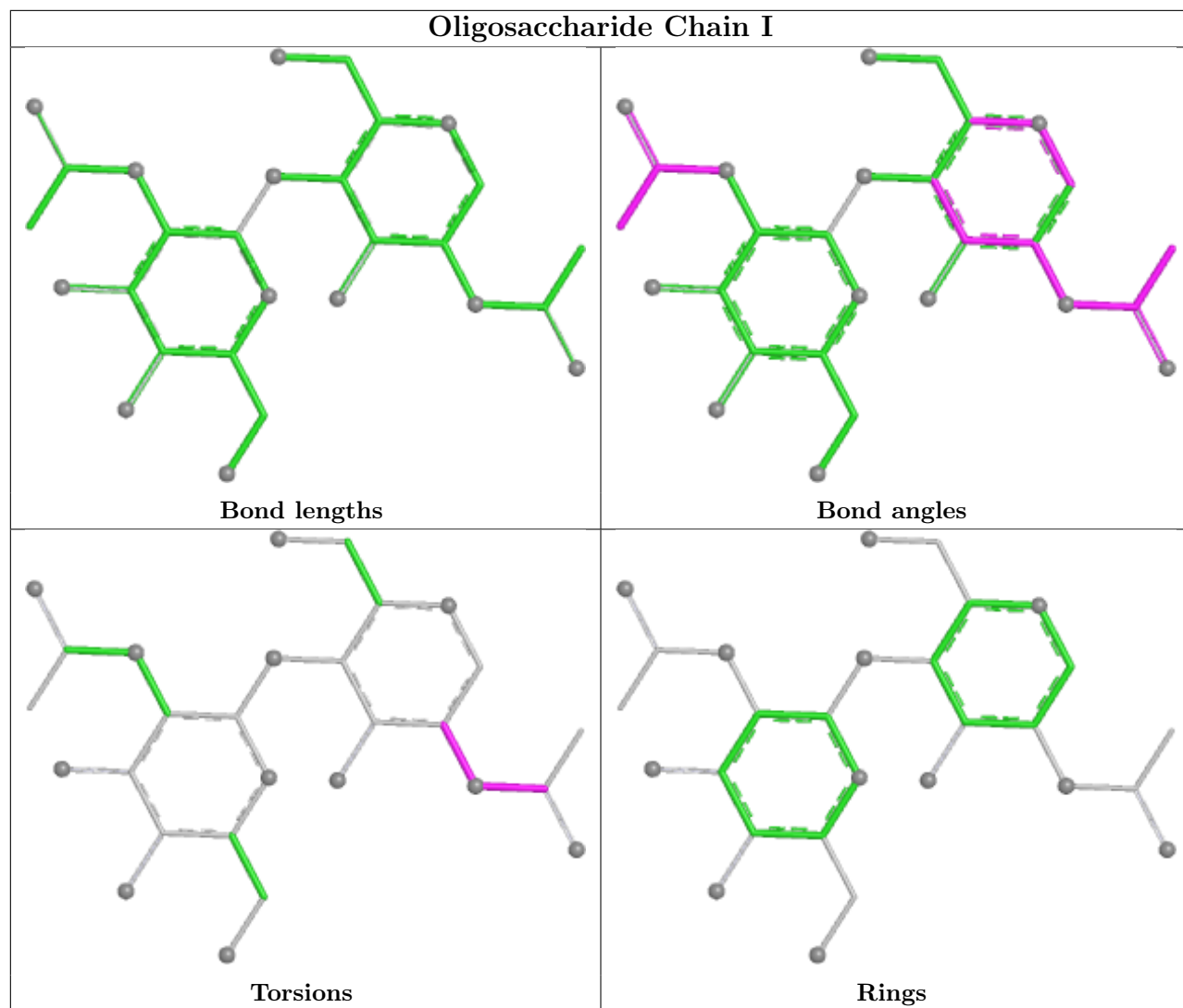
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

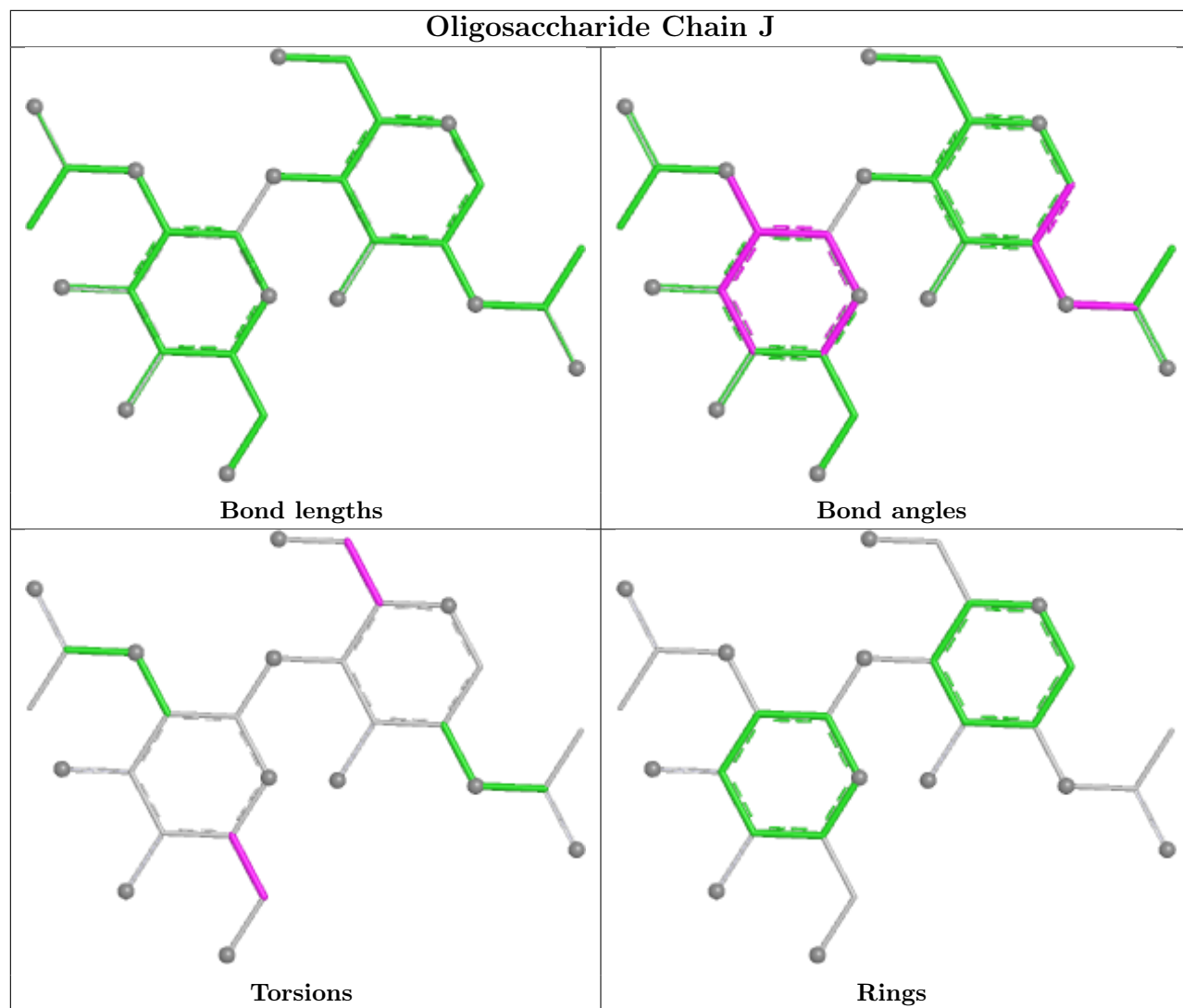


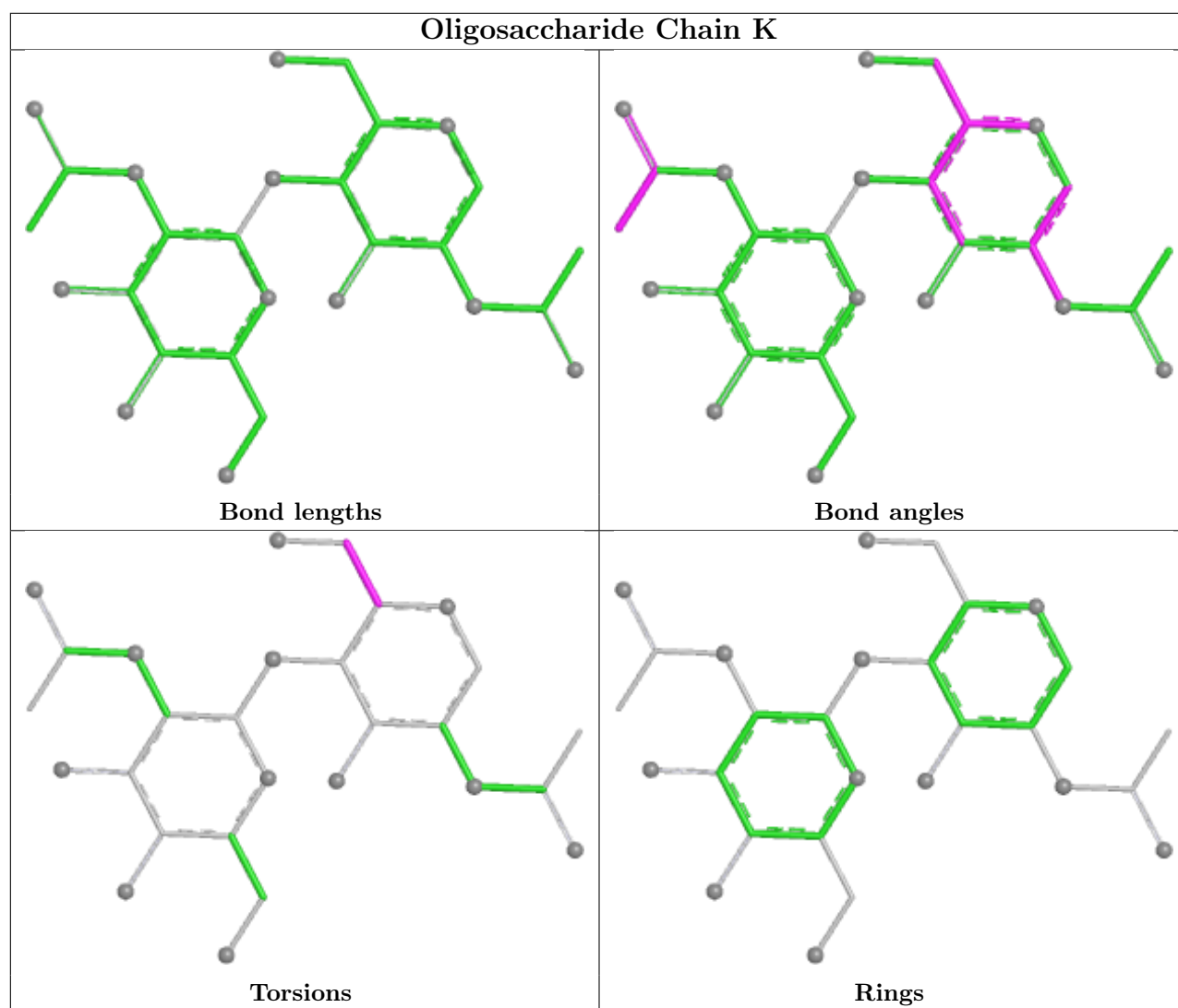


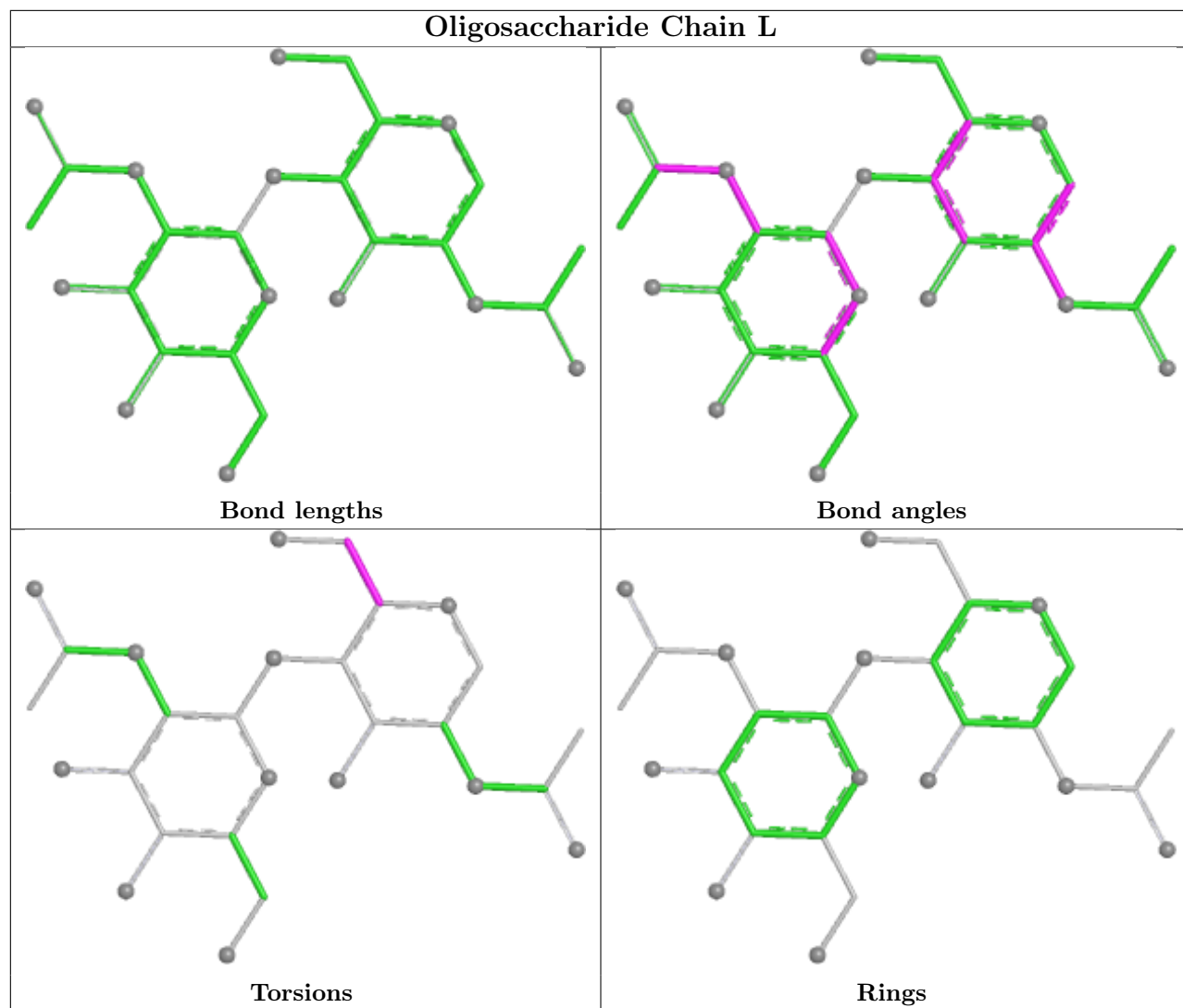


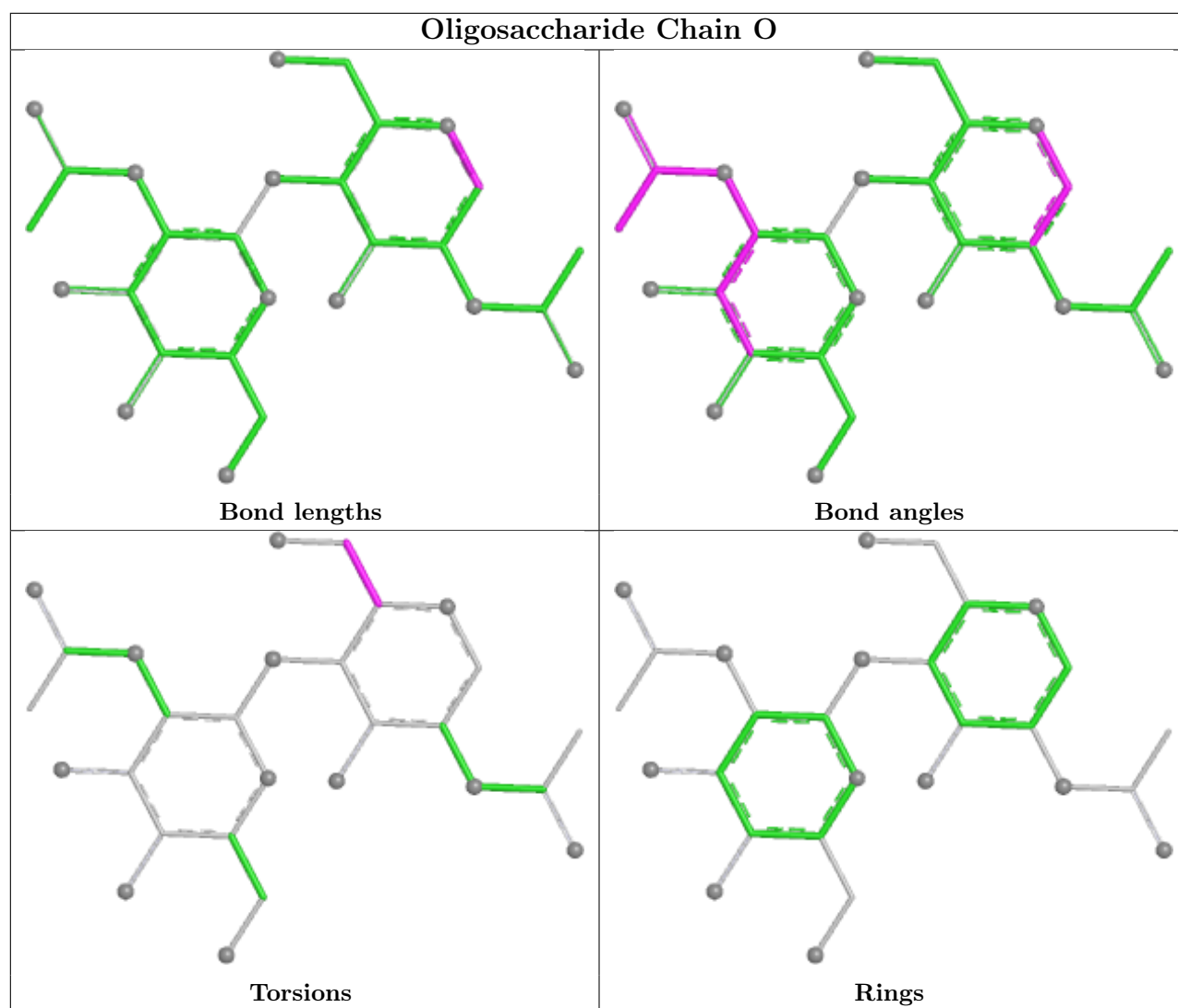


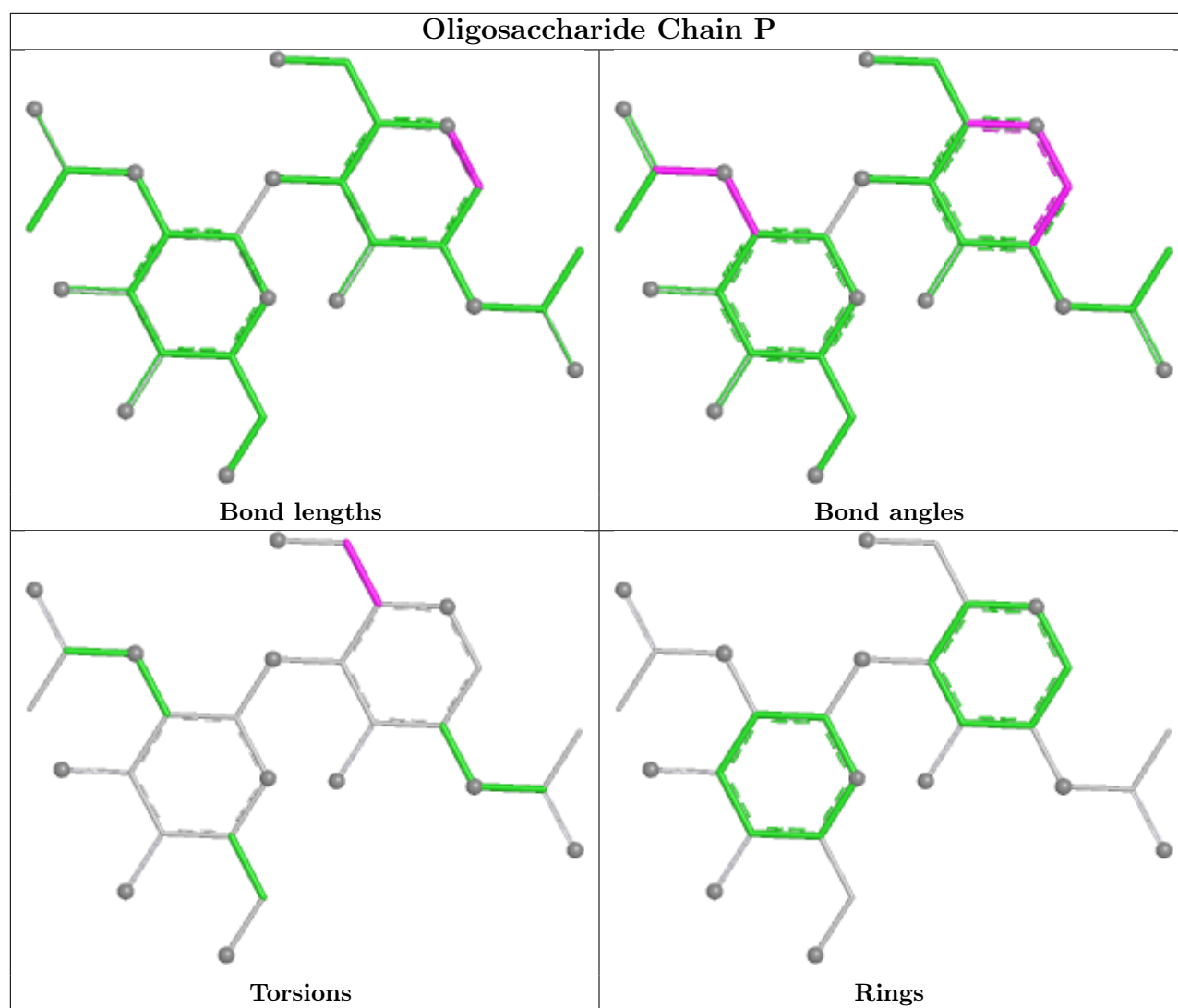


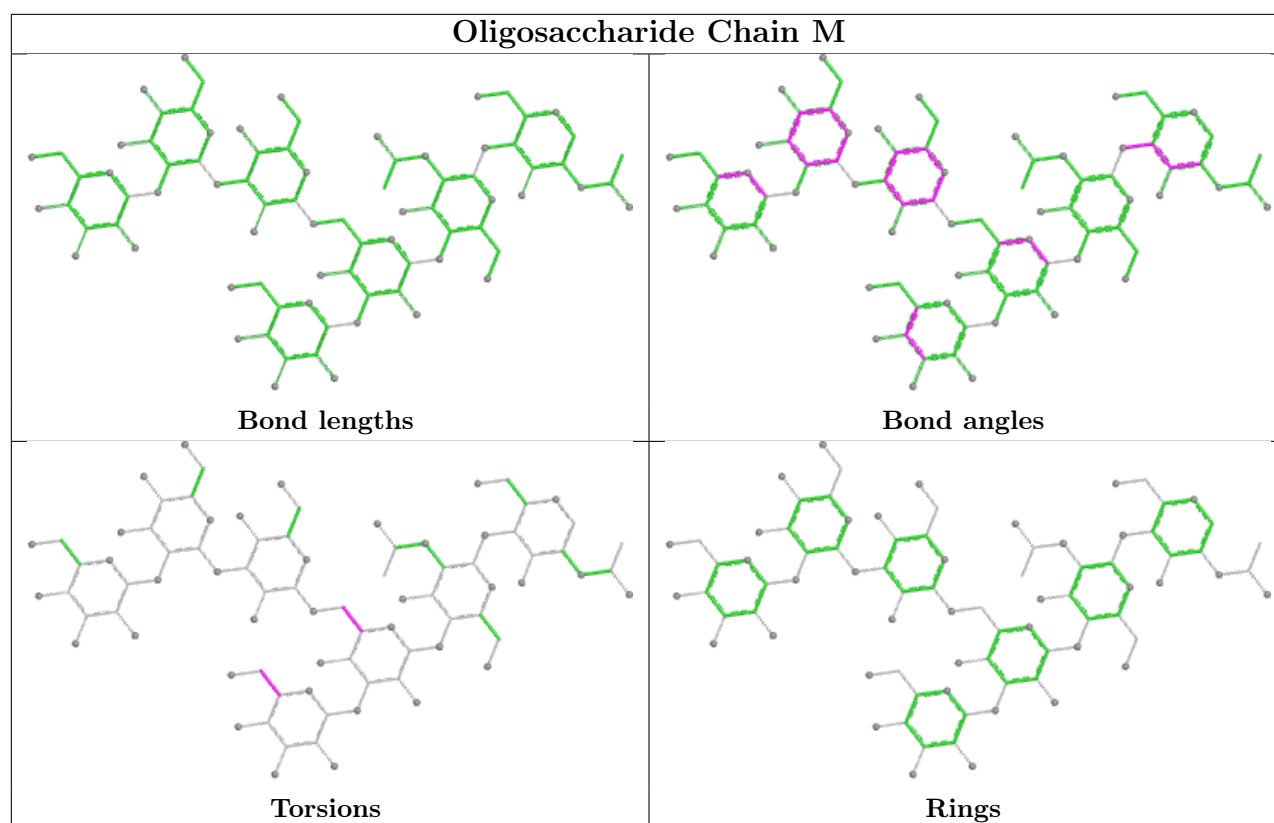












5.6 Ligand geometry [i](#)

3 ligands 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$
5	NAG	A	900	1	14,14,15	0.70	0	17,19,21	2.07	5 (29%)
5	NAG	B	900	1	14,14,15	0.46	0	17,19,21	1.25	2 (11%)
5	NAG	D	900	1	14,14,15	1.32	1 (7%)	17,19,21	3.55	11 (64%)

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
5	NAG	A	900	1	-	2/6/23/26	0/1/1/1
5	NAG	B	900	1	-	2/6/23/26	0/1/1/1
5	NAG	D	900	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	900	NAG	O5-C5	4.69	1.52	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	900	NAG	C2-N2-C7	7.86	133.43	122.90
5	D	900	NAG	O5-C1-C2	-6.38	101.42	111.29
5	D	900	NAG	O5-C5-C6	-5.09	97.76	107.66
5	D	900	NAG	C1-C2-N2	-4.87	102.75	110.43
5	D	900	NAG	O5-C5-C4	-4.56	99.74	110.83
5	A	900	NAG	C1-O5-C5	-4.18	106.58	112.19
5	A	900	NAG	C1-C2-N2	-4.06	104.03	110.43
5	A	900	NAG	O5-C1-C2	-3.70	105.57	111.29
5	D	900	NAG	O4-C4-C5	-3.18	101.49	109.32
5	D	900	NAG	O7-C7-N2	2.46	126.33	121.98
5	D	900	NAG	O4-C4-C3	-2.38	104.77	110.38
5	A	900	NAG	C3-C4-C5	2.32	114.45	110.23
5	B	900	NAG	C4-C3-C2	-2.22	107.76	111.02
5	D	900	NAG	C4-C3-C2	-2.21	107.77	111.02
5	D	900	NAG	C1-O5-C5	2.21	115.14	112.19
5	A	900	NAG	C4-C3-C2	2.16	114.19	111.02
5	B	900	NAG	O4-C4-C5	2.16	114.65	109.32
5	D	900	NAG	C6-C5-C4	-2.04	108.02	113.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	900	NAG	C3-C2-N2-C7
5	A	900	NAG	O5-C5-C6-O6
5	B	900	NAG	O5-C5-C6-O6
5	A	900	NAG	C4-C5-C6-O6
5	B	900	NAG	C4-C5-C6-O6
5	D	900	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	NAG	1	0
5	B	900	NAG	1	0
5	D	900	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	369/384 (96%)	0.63	50 (13%)	7 5	21, 54, 130, 203	1 (0%)
1	B	366/384 (95%)	0.70	38 (10%)	11 10	29, 68, 114, 159	0
1	C	372/384 (96%)	0.77	46 (12%)	8 6	29, 63, 133, 199	0
1	D	367/384 (95%)	0.75	39 (10%)	11 9	30, 67, 103, 124	0
All	All	1474/1536 (95%)	0.71	173 (11%)	9 7	21, 62, 119, 203	1 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	LEU	5.1
1	A	301	ASN	4.8
1	C	265	TRP	4.6
1	B	220	ILE	4.5
1	A	302	ALA	4.5
1	C	263	VAL	4.4
1	B	353	MET	4.4
1	A	167	TYR	4.3
1	A	259	ASP	4.1
1	D	302	ALA	4.1
1	B	218	MET	4.1
1	D	252	TRP	4.0
1	B	230	ALA	4.0
1	A	99	THR	4.0
1	D	137	LEU	3.9
1	A	180	ARG	3.8
1	B	226	LYS	3.8
1	A	177	LYS	3.8
1	D	134	ASP	3.8
1	B	201	LEU	3.7
1	C	302	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	161	THR	3.6
1	C	264	ASP	3.6
1	D	301	ASN	3.6
1	A	375	LEU	3.6
1	D	296	ILE	3.5
1	C	2	ALA	3.4
1	A	133	ALA	3.4
1	B	222	LEU	3.4
1	A	300	GLY	3.4
1	D	2	ALA	3.4
1	A	98	ASP	3.3
1	C	160	LEU	3.3
1	B	206	ILE	3.3
1	B	134	ASP	3.3
1	C	174	LEU	3.3
1	A	188	SER	3.3
1	D	140	LEU	3.3
1	B	252	TRP	3.3
1	A	174	LEU	3.2
1	A	215	LEU	3.2
1	C	99	THR	3.2
1	D	357	GLY	3.2
1	C	261	THR	3.1
1	A	160	LEU	3.1
1	C	97	VAL	3.1
1	A	163	THR	3.1
1	D	160	LEU	3.1
1	D	133	ALA	3.0
1	C	98	ASP	3.0
1	C	188	SER	3.0
1	A	166	GLY	3.0
1	B	221	ASP	2.9
1	D	300	GLY	2.9
1	B	160	LEU	2.9
1	B	358	ILE	2.9
1	D	161	THR	2.9
1	B	219	ASP	2.8
1	B	180	ARG	2.8
1	D	135	ARG	2.8
1	D	267	ARG	2.8
1	C	178	LYS	2.8
1	C	260	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	164	GLU	2.8
1	A	214	ASN	2.7
1	A	254	THR	2.7
1	A	158	ASN	2.7
1	A	374	ALA	2.7
1	B	357	GLY	2.7
1	C	357	GLY	2.7
1	D	204	ASN	2.7
1	C	355	HIS	2.7
1	D	259	ASP	2.6
1	A	189	GLU	2.6
1	B	133	ALA	2.6
1	D	164	GLU	2.6
1	D	373	ALA	2.6
1	B	204	ASN	2.6
1	D	358	ILE	2.5
1	C	171	PHE	2.5
1	D	97	VAL	2.5
1	A	162	THR	2.5
1	C	353	MET	2.5
1	C	238	VAL	2.5
1	A	95	PHE	2.5
1	A	257	SER	2.5
1	B	174	LEU	2.5
1	B	141	GLN	2.5
1	C	17	GLN	2.5
1	A	169	MET	2.5
1	C	259	ASP	2.4
1	C	222	LEU	2.4
1	A	159	ILE	2.4
1	A	358	ILE	2.4
1	C	132	ASP	2.4
1	A	258	ARG	2.4
1	D	163	THR	2.4
1	D	99	THR	2.4
1	A	172	GLN	2.4
1	D	205	GLY	2.3
1	A	137	LEU	2.3
1	C	296	ILE	2.3
1	D	195	LEU	2.3
1	B	171	PHE	2.3
1	B	178	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	266	LYS	2.3
1	A	175	GLU	2.3
1	D	126	THR	2.3
1	D	303	GLY	2.3
1	B	356	ASP	2.3
1	C	356	ASP	2.3
1	C	161	THR	2.3
1	D	136	GLY	2.3
1	B	137	LEU	2.3
1	C	258	ARG	2.3
1	B	40	GLN	2.3
1	B	228	SER	2.3
1	A	170	LEU	2.3
1	C	159	ILE	2.3
1	B	98	ASP	2.3
1	A	179	GLU	2.3
1	A	2	ALA	2.2
1	B	224	LYS	2.2
1	C	218	MET	2.2
1	D	3	MET	2.2
1	A	171	PHE	2.2
1	B	182	VAL	2.2
1	C	299	ARG	2.2
1	B	176	LYS	2.2
1	C	169	MET	2.2
1	C	300	GLY	2.2
1	A	255	SER	2.2
1	A	73	ARG	2.2
1	A	135	ARG	2.2
1	B	223	ASN	2.2
1	B	354	LYS	2.2
1	B	301	ASN	2.2
1	A	220	ILE	2.2
1	C	201	LEU	2.1
1	B	132	ASP	2.1
1	D	138	SER	2.1
1	C	203	LYS	2.1
1	D	226	LYS	2.1
1	A	16	GLN	2.1
1	C	303	GLY	2.1
1	B	72	GLU	2.1
1	B	253	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	122	TYR	2.1
1	A	297	SER	2.1
1	A	178	LYS	2.1
1	C	172	GLN	2.1
1	D	253	ARG	2.1
1	D	227	GLU	2.1
1	C	177	LYS	2.1
1	D	287	GLN	2.1
1	A	156	ALA	2.1
1	A	168	ARG	2.1
1	A	303	GLY	2.1
1	D	298	ARG	2.1
1	C	254	THR	2.1
1	C	358	ILE	2.1
1	D	363	TYR	2.1
1	D	297	SER	2.1
1	A	305	CYS	2.1
1	B	302	ALA	2.0
1	C	15	ASN	2.0
1	C	301	ASN	2.0
1	C	176	LYS	2.0
1	B	355	HIS	2.0
1	A	97	VAL	2.0
1	C	175	GLU	2.0
1	C	179	GLU	2.0
1	A	136	GLY	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
4	MAN	M	4	11/12	0.16	0.16	206,210,211,216	0
2	BMA	H	3	11/12	0.24	0.19	184,186,187,188	0

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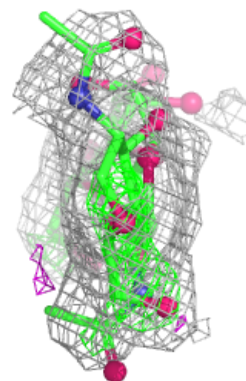
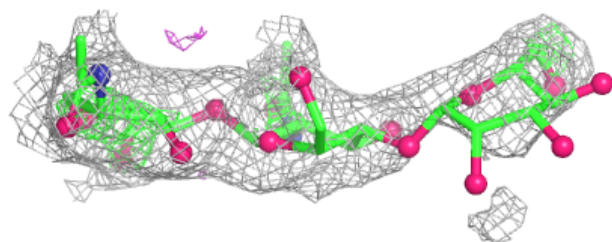
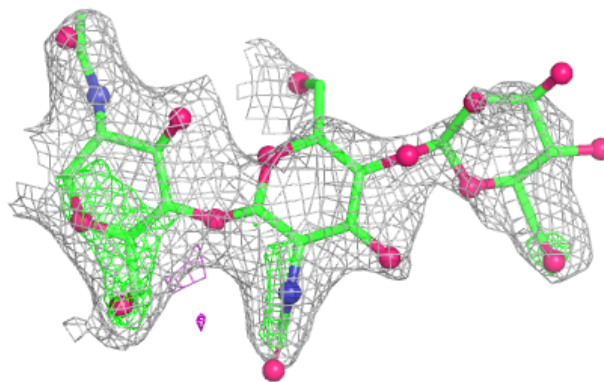
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	E	3	11/12	0.30	0.17	180,183,184,184	0
3	NAG	I	1	14/15	0.36	0.17	129,143,158,168	0
4	MAN	M	7	11/12	0.41	0.19	185,186,187,187	0
3	NAG	I	2	14/15	0.43	0.14	102,175,193,194	0
3	NAG	P	2	14/15	0.44	0.21	175,180,184,184	0
3	NAG	O	2	14/15	0.49	0.21	160,173,175,176	0
4	MAN	M	6	11/12	0.53	0.24	224,224,225,225	0
2	BMA	N	3	11/12	0.53	0.16	136,138,140,142	0
3	NAG	L	1	14/15	0.63	0.27	144,150,157,159	0
4	NAG	M	2	14/15	0.64	0.33	148,152,156,166	0
3	NAG	J	2	14/15	0.64	0.17	168,172,174,174	0
3	NAG	F	2	14/15	0.65	0.22	155,158,160,160	0
4	BMA	M	3	11/12	0.67	0.18	175,181,192,200	0
3	NAG	O	1	14/15	0.69	0.23	150,160,163,167	0
4	MAN	M	5	11/12	0.69	0.19	220,222,223,223	0
3	NAG	L	2	14/15	0.71	0.25	162,164,165,166	0
3	NAG	G	2	14/15	0.72	0.19	162,166,168,169	0
2	NAG	H	2	14/15	0.74	0.23	163,167,174,179	0
3	NAG	F	1	14/15	0.74	0.24	129,137,145,150	0
3	NAG	K	2	14/15	0.75	0.26	152,156,160,161	0
3	NAG	P	1	14/15	0.76	0.24	146,155,160,168	0
2	NAG	E	2	14/15	0.77	0.22	161,166,171,177	0
3	NAG	J	1	14/15	0.77	0.27	139,150,154,161	0
2	NAG	E	1	14/15	0.79	0.26	125,139,144,151	0
2	NAG	N	2	14/15	0.82	0.21	123,126,132,132	0
2	NAG	H	1	14/15	0.85	0.27	130,140,144,154	0
3	NAG	K	1	14/15	0.85	0.30	122,135,144,146	0
3	NAG	G	1	14/15	0.85	0.31	129,137,145,153	0
2	NAG	N	1	14/15	0.87	0.26	109,119,125,127	0
4	NAG	M	1	14/15	0.87	0.28	127,133,139,143	0

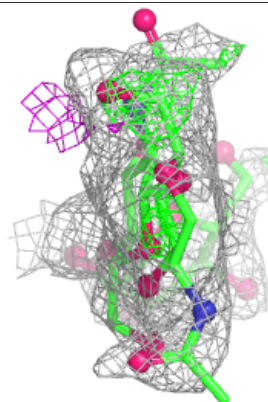
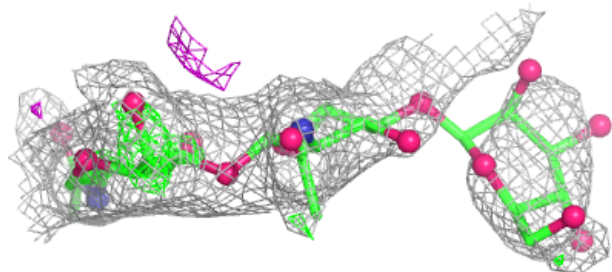
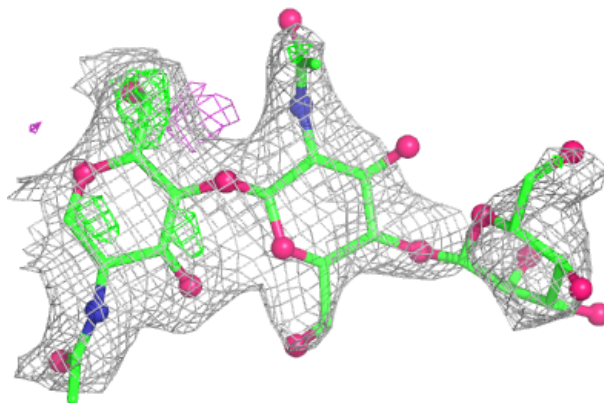
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

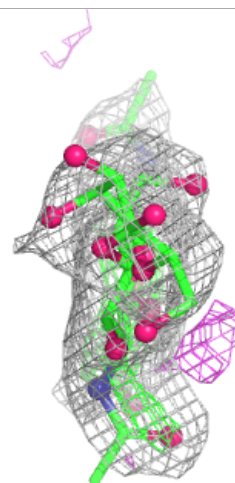
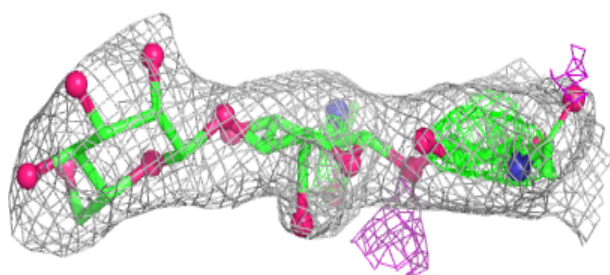
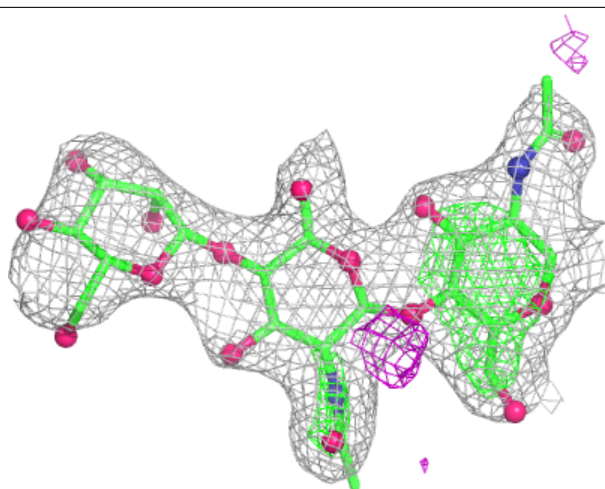
**Electron density around Chain H:**

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



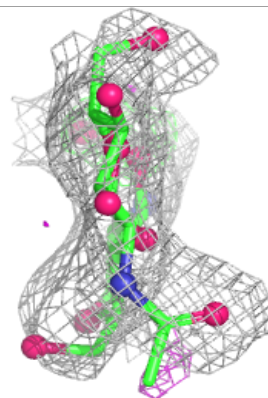
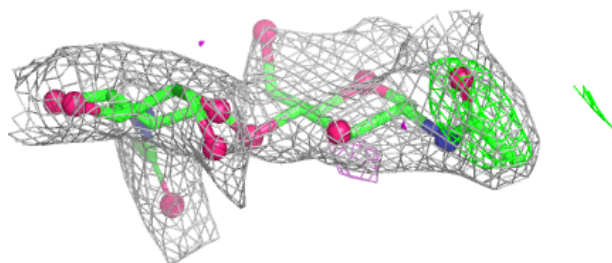
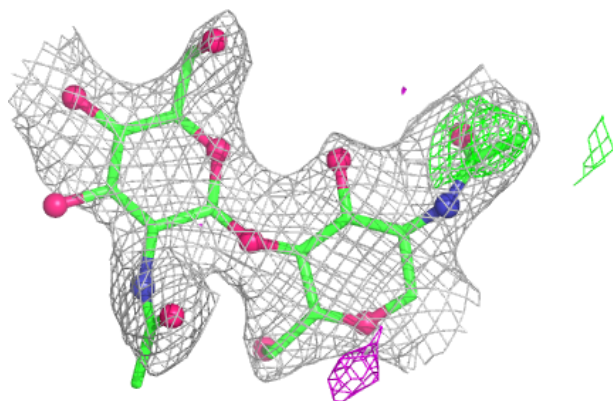
Electron density around Chain N:

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



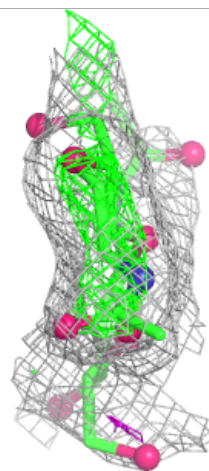
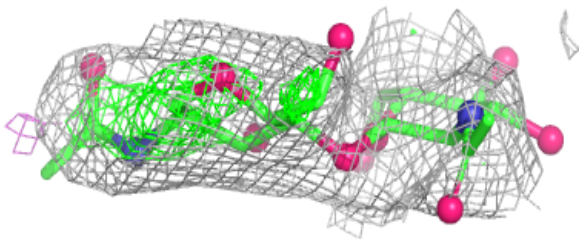
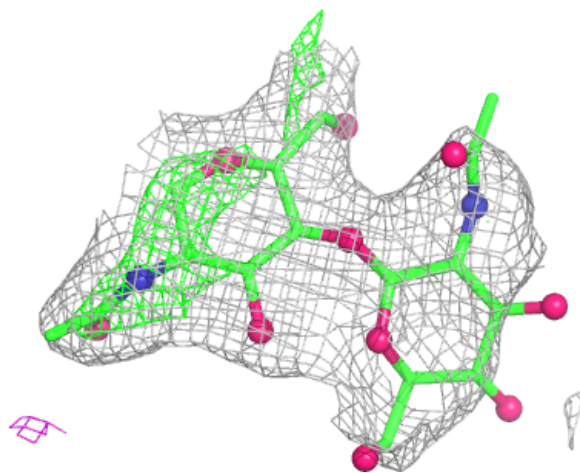
Electron density around Chain F:

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



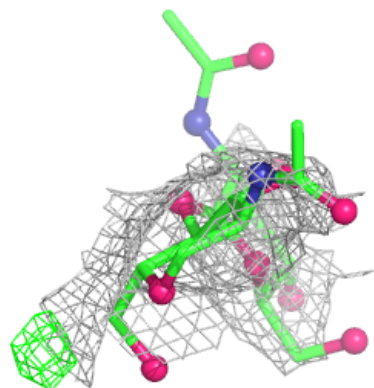
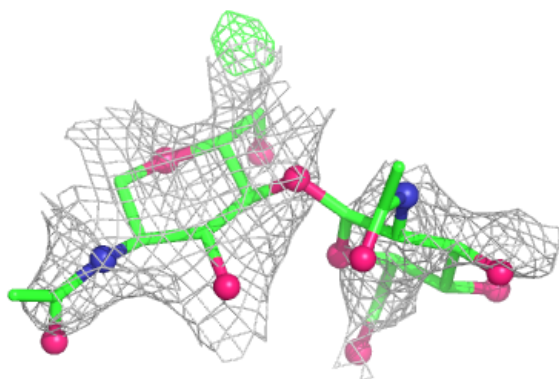
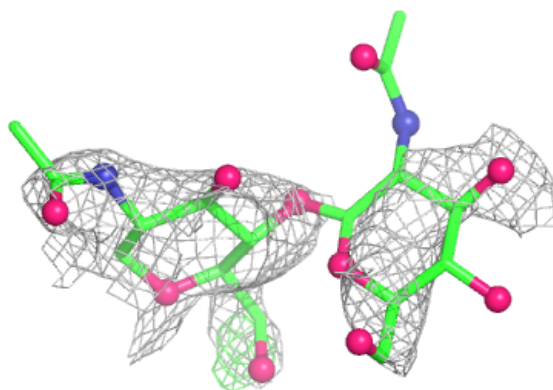
Electron density around Chain G:

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and green (positive)



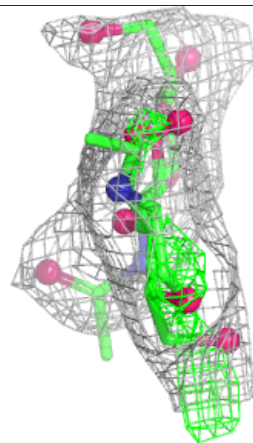
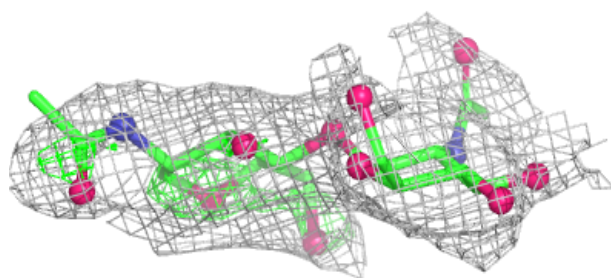
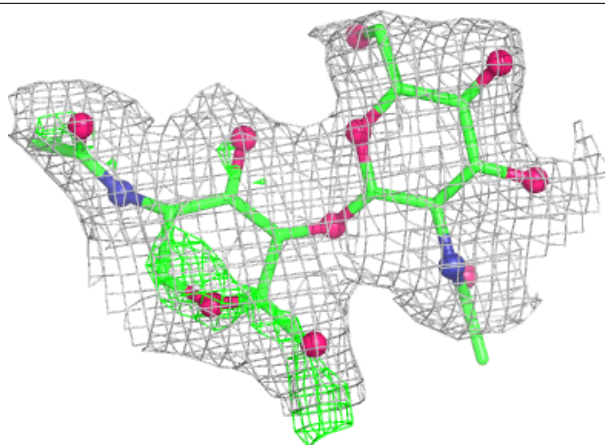
Electron density around Chain I:

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and green (positive)



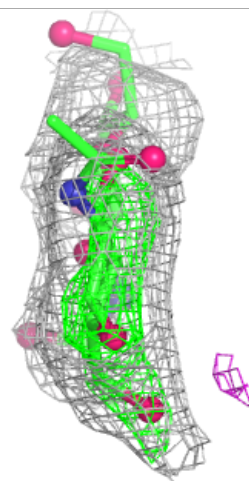
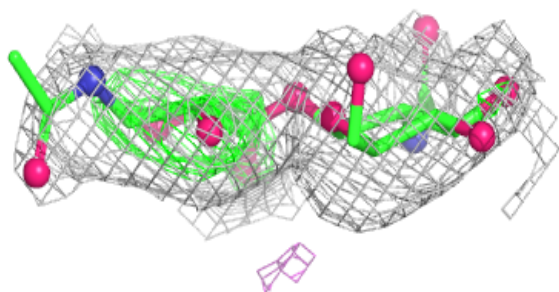
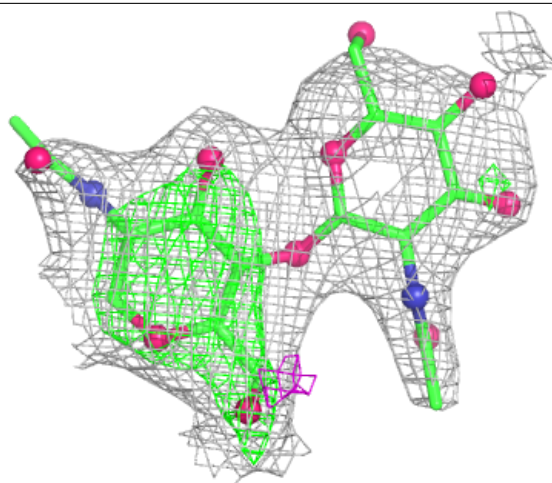
Electron density around Chain J:

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and green (positive)



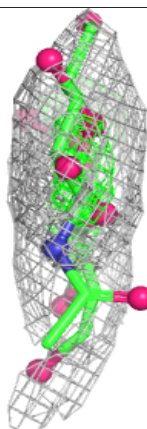
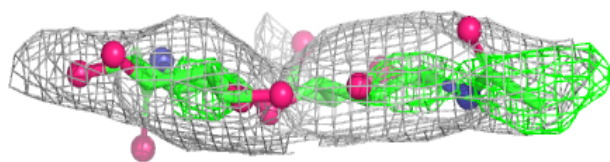
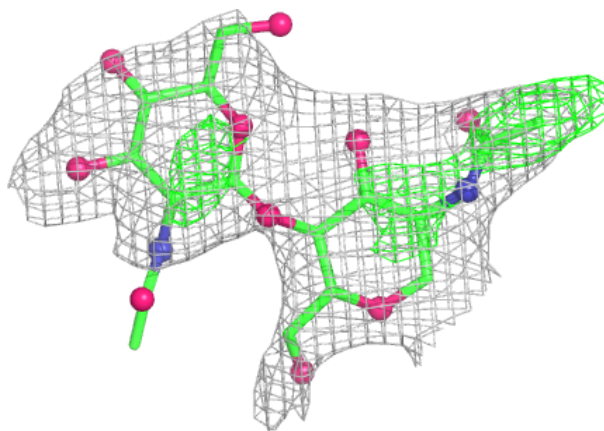
Electron density around Chain K:

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and green (positive)



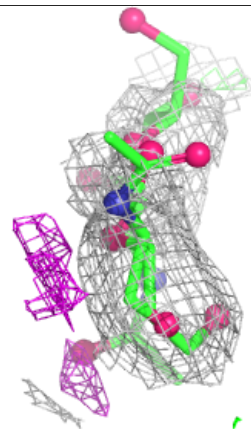
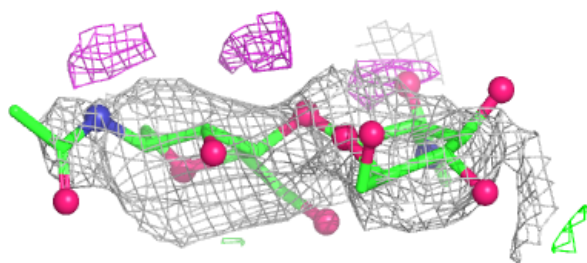
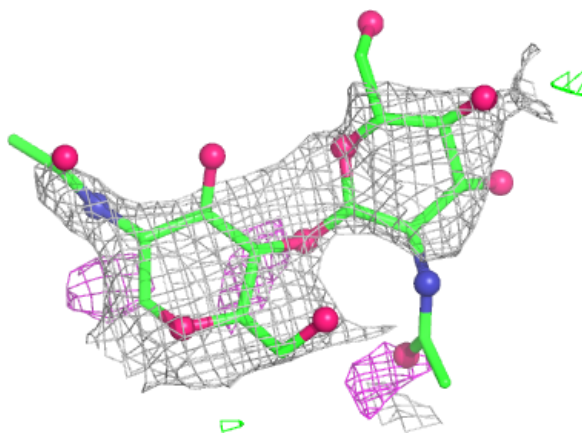
Electron density around Chain L:

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



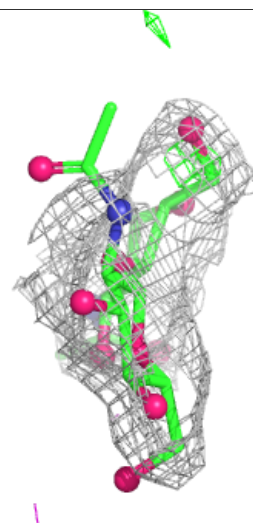
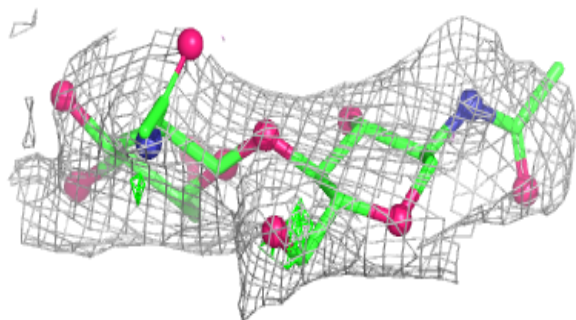
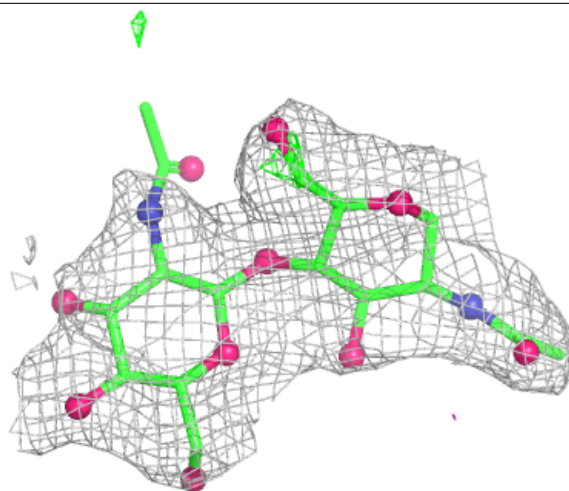
Electron density around Chain O:

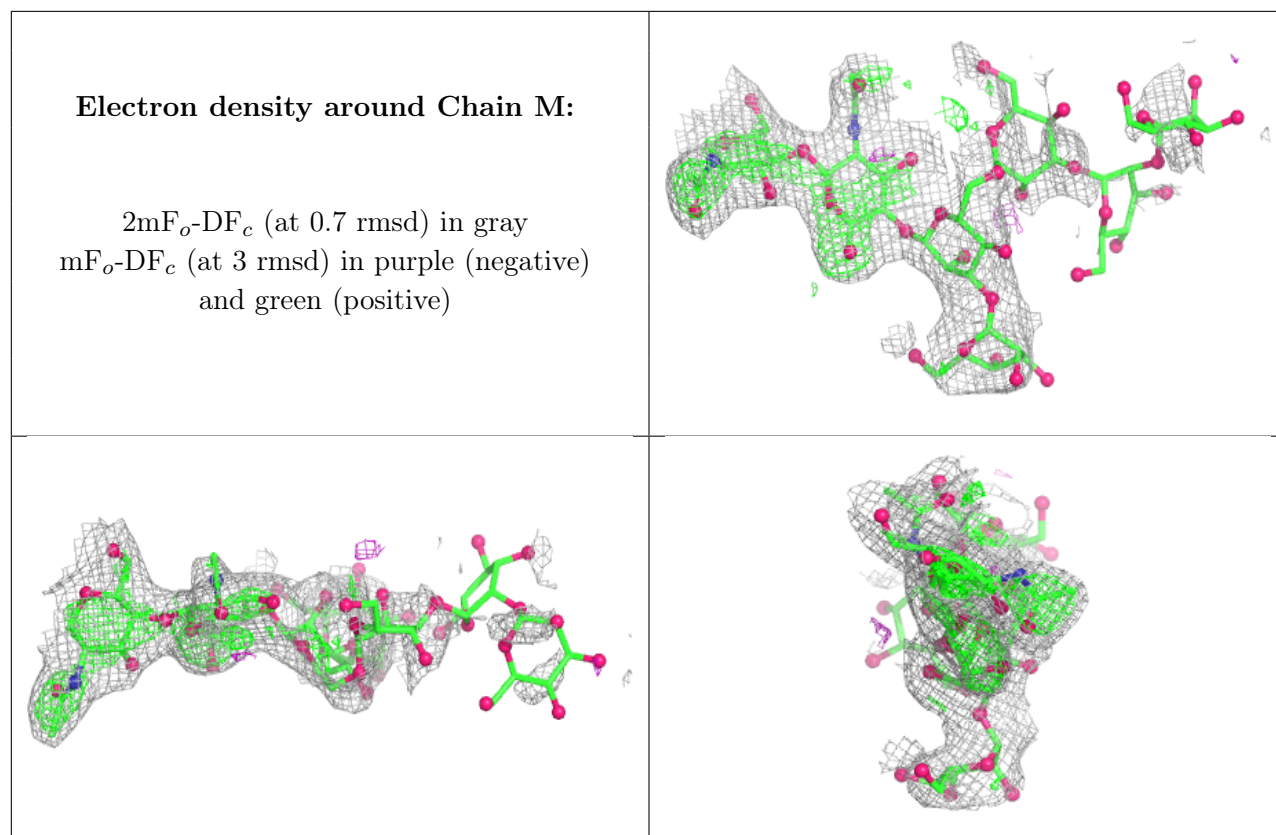
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

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





6.4 Ligands [i](#)

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
5	NAG	D	900	14/15	0.66	0.20	159,166,173,173	0
5	NAG	B	900	14/15	0.69	0.20	156,165,172,172	0
5	NAG	A	900	14/15	0.79	0.20	152,159,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.