



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 PM UTC

PDB ID : 1CKL / pdb_00001ckl
Title : N-TERMINAL TWO DOMAINS OF HUMAN CD46 (MEMBRANE COFACTOR PROTEIN, MCP)
Authors : Casasnovas, J.; Larvie, M.; Stehle, T.
Deposited on : 1999-04-22
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

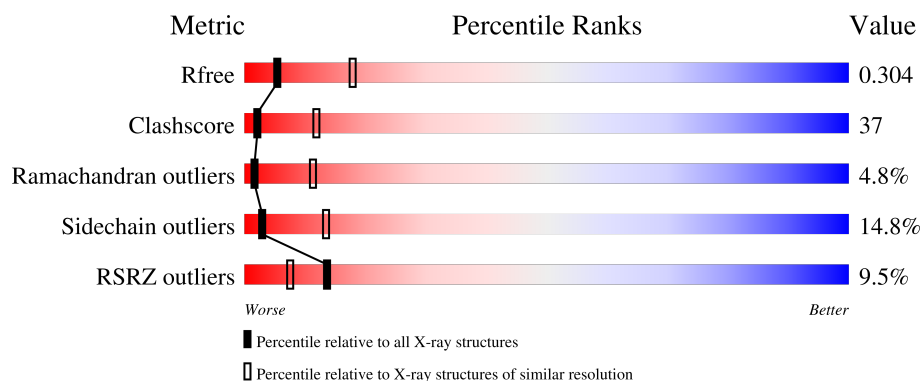
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	126	20% 32% 43% 24% .
1	B	126	8% 41% 43% 13% .
1	C	126	14% 32% 48% 18% .
1	D	126	6% 29% 51% 15% 6%
1	E	126	9% 38% 48% 10% .

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Mol	Chain	Length	Quality of chain
1	F	126	
2	G	8	
3	H	4	
4	I	3	
4	J	3	
4	O	3	
5	K	2	
5	L	2	
5	M	2	
6	N	5	
6	R	5	
7	P	8	
8	Q	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CL	D	4042	-	-	X	-
6	BMA	R	3	-	-	X	-
6	MAN	R	4	-	-	X	-
7	MAN	P	4	-	-	X	-
7	MAN	P	5	-	-	X	-
7	MAN	P	6	-	-	X	-
8	MAN	Q	4	-	-	X	-

2 Entry composition [i](#)

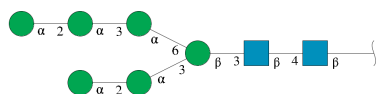
There are 11 unique types of molecules in this entry. The entry contains 6764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CD46).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			
1	B	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			
1	C	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			
1	D	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			
1	E	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			
1	F	126	Total	C	N	O	S	0	0	0
			1018	659	160	189	10			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



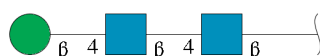
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



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

- Molecule 4 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.



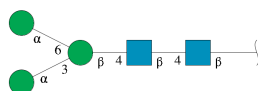
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



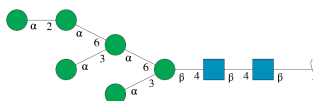
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-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.



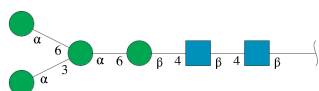
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
7	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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
8	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Ca 1	0	0
9	D	1	Total 1	Ca 1	0	0
9	E	1	Total 1	Ca 1	0	0
9	F	1	Total 1	Ca 1	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	Cl 1	0	0
10	B	1	Total 1	Cl 1	0	0
10	D	1	Total 1	Cl 1	0	0
10	E	1	Total 1	Cl 1	0	0
10	F	1	Total 1	Cl 1	0	0

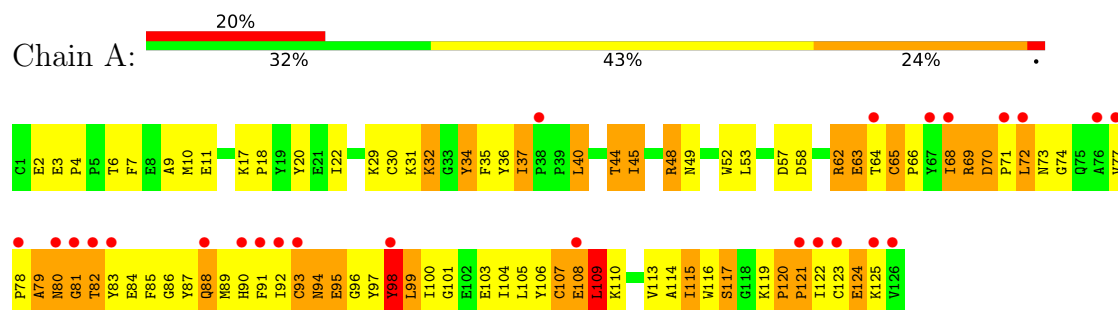
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	2	Total 2	O 2	0	0
11	C	3	Total 3	O 3	0	0
11	D	1	Total 1	O 1	0	0
11	E	2	Total 2	O 2	0	0
11	F	4	Total 4	O 4	0	0

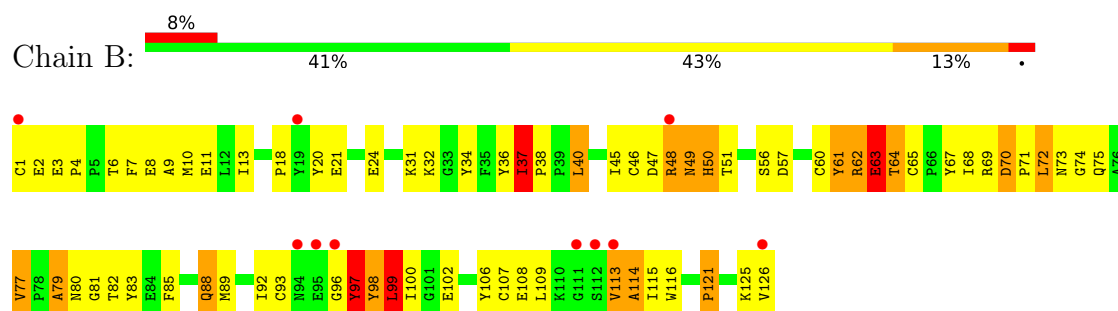
3 Residue-property plots

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.

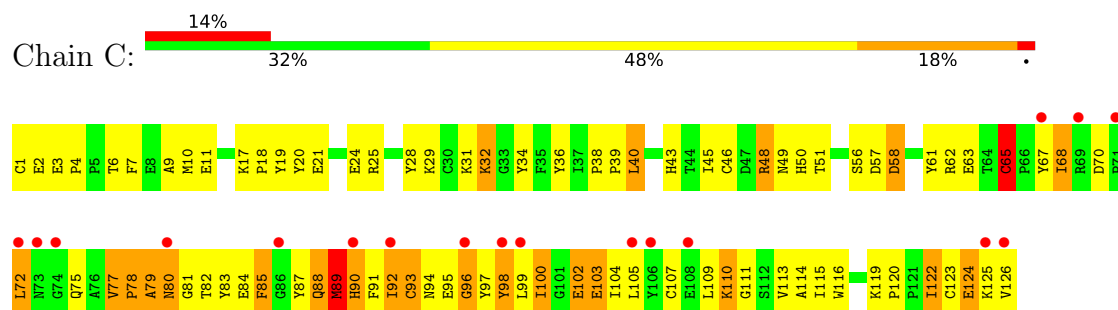
• Molecule 1: PROTEIN (CD46)



• Molecule 1: PROTEIN (CD46)



• Molecule 1: PROTEIN (CD46)



• Molecule 1: PROTEIN (CD46)



MAG1
MAG2
BMA3

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

Chain J:  67% 33%

MAG1
MAG2
BMA3

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

Chain O:  33% 67%

MAG1
MAG2
BMA3

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  50% 50%

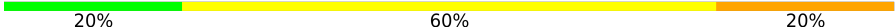
MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

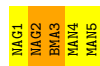
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  20% 60% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

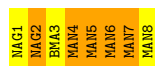
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  60% 40%



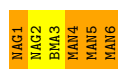
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  38% 62%



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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 Q:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.82Å 111.20Å 136.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.6 (20.00-3.10) 91.8 (20.00-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.09Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.244 , 0.298 0.253 , 0.304	Depositor DCC
R_{free} test set	765 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CL, NAG, CA, MAN

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	0.84	1/1052 (0.1%)	1.51	18/1432 (1.3%)
1	B	0.73	1/1052 (0.1%)	1.35	16/1432 (1.1%)
1	C	0.88	3/1052 (0.3%)	1.54	21/1432 (1.5%)
1	D	0.81	2/1052 (0.2%)	1.57	22/1432 (1.5%)
1	E	0.81	1/1052 (0.1%)	1.40	14/1432 (1.0%)
1	F	0.71	0/1052	1.40	19/1432 (1.3%)
All	All	0.80	8/6312 (0.1%)	1.46	110/8592 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	F	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	VAL	CA-CB	7.64	1.60	1.54
1	E	77	VAL	CA-CB	7.46	1.61	1.53
1	A	92	ILE	CA-CB	7.37	1.62	1.53
1	C	124	GLU	CA-C	5.88	1.59	1.53
1	D	100	ILE	CA-CB	5.78	1.59	1.53
1	D	88	GLN	CD-NE2	-5.49	1.21	1.33
1	C	125	LYS	CA-C	5.26	1.59	1.52
1	C	89	MET	SD-CE	-5.04	1.67	1.79

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	VAL	N-CA-C	14.68	122.58	107.76
1	C	124	GLU	N-CA-C	14.65	135.72	107.44
1	A	80	ASN	N-CA-C	-13.79	93.45	111.92
1	D	125	LYS	N-CA-C	13.17	128.78	110.35
1	A	99	LEU	N-CA-C	13.10	131.97	109.96
1	F	124	GLU	N-CA-C	10.41	125.95	109.50
1	D	77	VAL	N-CA-C	10.30	119.31	107.77
1	C	93	CYS	N-CA-C	-10.25	92.53	109.24
1	F	111	GLY	N-CA-C	-10.11	93.77	112.37
1	C	98	TYR	N-CA-C	9.84	123.92	110.35
1	C	88	GLN	N-CA-C	9.64	123.32	108.96
1	D	58	ASP	N-CA-C	9.56	124.34	112.87
1	C	78	PRO	N-CA-C	9.53	125.85	110.21
1	D	100	ILE	N-CA-C	9.28	119.61	106.53
1	D	94	ASN	N-CA-C	9.15	124.65	109.46
1	C	68	ILE	N-CA-C	8.94	119.91	106.42
1	B	79	ALA	N-CA-C	-8.72	99.01	110.43
1	A	79	ALA	N-CA-C	-8.27	96.50	109.72
1	F	101	GLY	N-CA-C	-8.25	98.97	111.42
1	D	98	TYR	N-CA-C	8.24	121.41	110.53
1	A	101	GLY	N-CA-C	-8.20	99.79	110.45
1	D	79	ALA	N-CA-C	-8.13	99.78	110.43
1	A	120	PRO	N-CA-C	8.04	120.50	110.70
1	D	59	ALA	N-CA-C	-7.96	103.29	113.16
1	E	112	SER	N-CA-C	7.79	121.37	112.57
1	A	34	TYR	N-CA-C	7.64	121.67	110.59
1	D	91	PHE	N-CA-C	7.60	121.71	110.46
1	F	47	ASP	N-CA-C	7.58	120.31	110.53
1	F	79	ALA	N-CA-C	-7.54	100.56	110.43
1	E	79	ALA	N-CA-C	-7.52	100.39	110.55
1	D	74	GLY	N-CA-C	-7.40	95.64	113.18
1	D	99	LEU	N-CA-C	7.33	120.36	108.34
1	C	92	ILE	N-CA-C	7.32	118.36	106.72
1	E	100	ILE	N-CA-C	7.27	118.23	108.27
1	B	125	LYS	N-CA-C	7.21	119.87	110.43
1	E	70	ASP	N-CA-C	-7.08	99.65	109.71
1	B	34	TYR	N-CA-C	7.06	120.92	109.40
1	C	110	LYS	N-CA-C	-6.96	98.73	109.24
1	A	109	LEU	N-CA-C	6.86	120.18	109.96
1	A	121	PRO	N-CA-C	6.82	122.22	111.38
1	F	37	ILE	CA-C-N	6.81	127.40	120.38
1	F	37	ILE	C-N-CA	6.81	127.40	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	ILE	N-CA-C	-6.75	99.42	108.06
1	A	68	ILE	N-CA-C	6.69	117.36	106.72
1	A	117	SER	N-CA-C	6.69	120.19	108.56
1	F	41	ALA	N-CA-C	6.66	120.89	110.17
1	C	65	CYS	CA-C-N	6.62	128.12	119.84
1	C	65	CYS	C-N-CA	6.62	128.12	119.84
1	D	34	TYR	N-CA-C	-6.59	99.55	110.17
1	C	102	GLU	N-CA-C	-6.58	101.22	110.50
1	A	108	GLU	N-CA-C	6.55	117.78	108.74
1	A	125	LYS	N-CA-C	6.55	119.85	109.50
1	A	40	LEU	N-CA-C	6.51	124.66	110.80
1	E	99	LEU	N-CA-C	6.46	119.25	109.23
1	D	62	ARG	CA-CB-CG	6.36	126.83	114.10
1	B	99	LEU	N-CA-C	6.30	119.85	110.52
1	E	93	CYS	CA-CB-SG	-6.25	100.04	114.40
1	F	97	TYR	N-CA-C	6.24	119.67	109.24
1	D	96	GLY	N-CA-C	6.13	127.70	113.18
1	F	107	CYS	N-CA-C	-6.11	99.28	109.24
1	C	124	GLU	CB-CA-C	-6.08	102.59	111.23
1	B	64	THR	N-CA-C	6.06	118.28	108.41
1	C	79	ALA	N-CA-C	-6.03	99.37	108.96
1	D	97	TYR	CA-CB-CG	5.99	124.68	113.90
1	E	109	LEU	N-CA-C	5.97	119.68	110.42
1	B	32	LYS	N-CA-C	5.97	123.51	110.80
1	F	32	LYS	N-CA-C	5.87	123.30	110.80
1	B	61	TYR	N-CA-C	5.71	118.26	109.07
1	D	93	CYS	N-CA-C	-5.69	100.43	109.76
1	F	124	GLU	CA-C-N	5.69	132.41	121.54
1	F	124	GLU	C-N-CA	5.69	132.41	121.54
1	A	98	TYR	N-CA-C	5.68	118.87	110.46
1	E	48	ARG	N-CA-C	5.62	122.77	110.80
1	B	97	TYR	N-CA-C	5.60	118.82	110.14
1	A	65	CYS	N-CA-C	-5.57	102.60	110.29
1	C	58	ASP	N-CA-C	5.54	122.61	110.80
1	C	90	HIS	N-CA-C	-5.49	101.06	109.41
1	A	88	GLN	N-CA-C	5.46	117.98	109.52
1	D	120	PRO	N-CA-C	5.43	117.32	110.70
1	B	92	ILE	N-CA-C	-5.40	100.06	108.81
1	C	125	LYS	N-CA-C	5.40	117.52	109.25
1	C	123	CYS	N-CA-C	5.34	118.00	110.14
1	C	38	PRO	N-CA-C	5.31	117.18	110.70
1	D	122	ILE	N-CA-C	5.31	117.20	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	77	VAL	N-CA-C	5.30	120.33	108.88
1	C	32	LYS	N-CA-C	5.26	122.00	110.80
1	A	74	GLY	N-CA-C	-5.23	100.79	113.18
1	B	37	ILE	CA-C-N	5.19	125.73	120.38
1	B	37	ILE	C-N-CA	5.19	125.73	120.38
1	F	62	ARG	N-CA-C	-5.19	102.37	110.42
1	C	122	ILE	N-CA-C	-5.18	101.23	108.80
1	B	47	ASP	N-CA-C	5.18	117.35	109.63
1	F	111	GLY	CA-C-N	-5.18	111.64	121.54
1	F	111	GLY	C-N-CA	-5.18	111.64	121.54
1	E	88	GLN	N-CA-C	5.14	117.00	109.24
1	E	97	TYR	N-CA-C	-5.13	101.39	109.50
1	D	47	ASP	N-CA-C	5.13	118.31	110.36
1	A	77	VAL	N-CA-C	5.12	119.94	108.88
1	E	72	LEU	N-CA-C	-5.11	99.91	110.80
1	B	88	GLN	N-CA-C	5.10	116.95	109.24
1	E	41	ALA	N-CA-C	5.09	118.25	110.20
1	B	63	GLU	N-CA-C	5.08	121.61	110.80
1	D	93	CYS	CA-C-N	-5.06	115.05	122.19
1	D	93	CYS	C-N-CA	-5.06	115.05	122.19
1	F	88	GLN	N-CA-C	5.04	116.86	109.24
1	B	114	ALA	N-CA-C	-5.04	100.20	108.41
1	E	123	CYS	N-CA-C	5.04	118.28	110.17
1	F	96	GLY	N-CA-C	-5.02	108.15	115.63
1	B	69	ARG	N-CA-C	-5.01	102.49	109.96
1	C	119	LYS	N-CA-C	-5.01	98.74	109.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain
1	D	97	TYR	Sidechain
1	F	97	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1018	0	962	81	0
1	B	1018	0	962	68	0
1	C	1018	0	962	88	0
1	D	1018	0	962	82	0
1	E	1018	0	962	83	0
1	F	1018	0	962	70	0
2	G	94	0	79	3	0
3	H	50	0	43	0	0
4	I	39	0	34	0	0
4	J	39	0	34	4	0
4	O	39	0	34	3	0
5	K	28	0	25	1	0
5	L	28	0	25	3	0
5	M	28	0	25	1	0
6	N	61	0	52	1	0
6	R	61	0	52	12	0
7	P	94	0	79	17	0
8	Q	72	0	61	12	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	3	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
11	B	2	0	0	1	0
11	C	3	0	0	0	0
11	D	1	0	0	0	0
11	E	2	0	0	1	0
11	F	4	0	0	0	0
All	All	6764	0	6315	489	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 37.

All (489) 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)
7:P:4:MAN:C6	7:P:5:MAN:H3	1.38	1.50
7:P:4:MAN:H61	7:P:5:MAN:C3	1.49	1.41
1:D:41:ALA:HA	10:D:4042:CL:CL	1.82	1.17
1:D:48:ARG:HB3	1:F:61:TYR:HE1	1.01	1.12
1:D:97:TYR:HA	1:D:126:VAL:HG23	1.31	1.12
1:C:17:LYS:HE2	1:E:17:LYS:HE2	1.32	1.09
1:D:48:ARG:HB3	1:F:61:TYR:CE1	1.87	1.08
8:Q:4:MAN:H2	8:Q:5:MAN:H2	1.42	1.02
1:F:37:ILE:HB	1:F:61:TYR:HE2	1.24	1.00
5:L:1:NAG:H5	5:L:2:NAG:O5	1.60	0.99
1:D:97:TYR:HB2	1:D:125:LYS:HA	1.45	0.98
8:Q:4:MAN:C2	8:Q:5:MAN:H2	1.93	0.98
1:F:37:ILE:HB	1:F:61:TYR:CE2	1.99	0.96
1:C:65:CYS:SG	1:C:114:ALA:HB1	2.08	0.93
1:A:90:HIS:HB3	1:A:104:ILE:HG12	1.48	0.93
1:A:89:MET:HB2	1:A:116:TRP:CZ3	2.05	0.91
8:Q:4:MAN:H61	8:Q:6:MAN:H3	1.56	0.88
1:C:107:CYS:SG	1:C:114:ALA:HB1	2.14	0.88
1:B:37:ILE:HG13	1:B:61:TYR:HD2	1.38	0.88
1:C:21:GLU:HG3	1:E:14:GLY:HA2	1.54	0.87
1:A:44:THR:HG22	1:A:52:TRP:HE3	1.38	0.87
7:P:5:MAN:C4	7:P:6:MAN:H3	2.04	0.87
1:C:80:ASN:HB3	1:C:87:TYR:HD2	1.40	0.86
1:C:11:GLU:HG3	1:C:31:LYS:HG2	1.55	0.86
1:B:11:GLU:HG3	1:B:31:LYS:HG2	1.59	0.83
1:A:44:THR:HG21	1:A:52:TRP:HB3	1.59	0.83
1:B:70:ASP:HB3	1:B:75:GLN:HA	1.57	0.83
8:Q:4:MAN:H2	8:Q:5:MAN:C2	2.10	0.82
1:B:37:ILE:HG13	1:B:61:TYR:CD2	2.14	0.81
1:C:96:GLY:O	1:C:97:TYR:HD1	1.63	0.81
1:D:11:GLU:HG3	1:D:31:LYS:HG2	1.62	0.81
1:D:85:PHE:HA	1:D:107:CYS:HB3	1.62	0.81
1:A:69:ARG:H	1:A:69:ARG:HD3	1.46	0.80
1:D:10:MET:SD	1:D:57:ASP:HA	2.21	0.80
1:A:107:CYS:HA	1:A:116:TRP:HA	1.63	0.79
1:E:11:GLU:HG3	1:E:31:LYS:HG2	1.62	0.79
1:D:98:TYR:CE1	1:D:126:VAL:HG22	2.17	0.79
1:A:11:GLU:HG3	1:A:31:LYS:HG2	1.65	0.79
1:A:80:ASN:HB3	1:A:87:TYR:CD1	2.18	0.78
1:F:9:ALA:HB3	1:F:57:ASP:HB2	1.65	0.78
1:C:97:TYR:HB2	1:C:124:GLU:O	1.83	0.78
1:A:22:ILE:HD13	1:A:48:ARG:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ALA:CA	10:D:4042:CL:CL	2.67	0.77
1:A:89:MET:HB2	1:A:116:TRP:CE3	2.20	0.76
1:D:42:THR:N	10:D:4042:CL:CL	2.55	0.76
1:E:73:ASN:HB3	1:E:97:TYR:CE2	2.21	0.76
6:R:3:BMA:C2	6:R:4:MAN:H2	2.16	0.76
1:D:97:TYR:CB	1:D:125:LYS:HA	2.15	0.75
1:F:21:GLU:HB2	1:F:24:GLU:HG3	1.67	0.75
1:F:70:ASP:HB3	1:F:75:GLN:HA	1.67	0.75
6:R:3:BMA:H2	6:R:4:MAN:H2	1.70	0.74
7:P:5:MAN:C3	7:P:6:MAN:H3	2.19	0.72
7:P:5:MAN:H4	7:P:6:MAN:H3	1.71	0.72
1:D:95:GLU:OE1	1:D:95:GLU:HA	1.88	0.72
1:F:113:VAL:HG22	1:F:115:ILE:HG12	1.71	0.71
1:F:104:ILE:HD13	6:R:2:NAG:H83	1.73	0.70
8:Q:4:MAN:O2	8:Q:5:MAN:H2	1.91	0.70
1:F:22:ILE:HD13	1:F:48:ARG:HA	1.73	0.70
1:E:11:GLU:HG3	1:E:31:LYS:CG	2.22	0.70
1:D:100:ILE:HG12	1:D:100:ILE:O	1.91	0.69
1:B:48:ARG:C	1:B:50:HIS:H	1.98	0.69
1:E:37:ILE:HD13	1:E:61:TYR:HE1	1.56	0.69
1:A:78:PRO:HG2	1:A:83:TYR:CE1	2.28	0.69
1:D:21:GLU:HB2	1:D:24:GLU:HG3	1.73	0.68
5:L:1:NAG:C5	5:L:2:NAG:O5	2.37	0.68
1:A:93:CYS:HB3	1:A:97:TYR:O	1.94	0.68
1:A:48:ARG:HB2	1:C:82:THR:OG1	1.93	0.68
1:C:79:ALA:HB1	5:L:2:NAG:O6	1.93	0.68
1:C:110:LYS:HB3	1:C:115:ILE:HG12	1.76	0.68
1:E:96:GLY:O	1:E:125:LYS:HD3	1.94	0.67
1:A:113:VAL:HG22	1:A:114:ALA:H	1.59	0.67
1:A:69:ARG:HD3	1:A:69:ARG:N	2.09	0.67
1:E:9:ALA:HB3	1:E:57:ASP:HB2	1.76	0.67
1:C:1:CYS:N	1:C:50:HIS:ND1	2.41	0.67
7:P:4:MAN:O2	7:P:7:MAN:C1	2.42	0.67
1:D:44:THR:HG23	1:D:52:TRP:CE3	2.30	0.67
1:C:79:ALA:O	1:C:80:ASN:HB2	1.96	0.66
1:C:70:ASP:OD1	1:C:75:GLN:HA	1.94	0.66
1:B:8:GLU:O	1:B:31:LYS:HD2	1.95	0.66
1:B:93:CYS:SG	1:B:99:LEU:HD12	2.36	0.66
1:A:100:ILE:HB	1:A:122:ILE:HB	1.78	0.66
1:D:97:TYR:HB3	1:D:126:VAL:H	1.59	0.66
1:C:21:GLU:HB2	1:C:24:GLU:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ILE:CD1	1:E:23:GLY:HA3	2.26	0.66
1:C:10:MET:SD	1:C:57:ASP:HA	2.36	0.66
1:C:65:CYS:SG	1:C:114:ALA:CB	2.84	0.65
1:A:44:THR:HG22	1:A:52:TRP:CE3	2.28	0.65
1:A:93:CYS:SG	1:A:99:LEU:HD21	2.36	0.65
1:F:8:GLU:O	1:F:31:LYS:HD2	1.97	0.65
1:F:11:GLU:HG3	1:F:31:LYS:HG2	1.78	0.65
1:F:125:LYS:HG3	1:F:126:VAL:H	1.62	0.65
1:F:98:TYR:CE2	1:F:126:VAL:HG21	2.32	0.64
1:A:64:THR:HG22	1:A:84:GLU:HA	1.78	0.64
1:F:10:MET:SD	1:F:57:ASP:HA	2.37	0.64
1:B:85:PHE:CZ	1:B:109:LEU:HD22	2.32	0.64
1:F:44:THR:HG23	1:F:52:TRP:CE3	2.32	0.64
1:E:73:ASN:HB3	1:E:97:TYR:HE2	1.61	0.64
7:P:5:MAN:O3	7:P:6:MAN:H3	1.97	0.64
1:B:21:GLU:HB2	1:B:24:GLU:HG3	1.80	0.64
1:B:10:MET:SD	1:B:57:ASP:HA	2.38	0.63
1:E:115:ILE:HG22	1:E:116:TRP:N	2.13	0.63
1:D:106:TYR:O	1:D:116:TRP:HA	1.99	0.63
1:C:80:ASN:HB3	1:C:87:TYR:CD2	2.30	0.63
1:C:85:PHE:O	1:C:87:TYR:HD1	1.81	0.62
1:B:96:GLY:C	1:B:97:TYR:HD1	2.07	0.62
1:B:113:VAL:HG13	1:B:115:ILE:HG13	1.81	0.62
1:D:108:GLU:HB2	1:D:110:LYS:HE3	1.80	0.62
1:E:104:ILE:HD13	7:P:2:NAG:C8	2.29	0.62
1:E:37:ILE:CD1	1:E:61:TYR:HE1	2.12	0.62
1:E:101:GLY:HA3	1:E:121:PRO:HB3	1.81	0.62
7:P:5:MAN:O3	7:P:6:MAN:H2	2.00	0.62
1:D:73:ASN:O	1:D:123:CYS:SG	2.56	0.62
1:D:119:LYS:HB3	1:D:120:PRO:HD2	1.82	0.62
4:O:2:NAG:H61	4:O:3:BMA:O2	1.99	0.62
1:B:61:TYR:HE1	1:C:48:ARG:HG3	1.64	0.61
1:D:82:THR:HA	1:E:48:ARG:HB3	1.82	0.61
1:D:72:LEU:HD12	1:D:122:ILE:HG23	1.82	0.61
1:C:96:GLY:O	1:C:97:TYR:CD1	2.52	0.61
1:E:72:LEU:O	1:E:73:ASN:HB2	1.99	0.61
1:E:77:VAL:HG13	1:E:90:HIS:HB2	1.81	0.61
1:E:76:ALA:HA	1:E:91:PHE:HD1	1.66	0.61
1:F:124:GLU:OE1	1:F:125:LYS:HG2	2.01	0.61
1:A:89:MET:HE3	1:A:89:MET:HA	1.82	0.60
1:E:76:ALA:HA	1:E:91:PHE:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:C	1:B:50:HIS:N	2.56	0.60
1:C:11:GLU:HG3	1:C:31:LYS:CG	2.28	0.60
4:J:1:NAG:O3	4:J:2:NAG:C1	2.48	0.60
1:B:1:CYS:N	1:B:20:TYR:O	2.33	0.60
1:F:85:PHE:HB2	1:F:108:GLU:HA	1.83	0.60
1:A:78:PRO:HG3	1:A:89:MET:HE1	1.84	0.60
1:E:21:GLU:HB2	1:E:24:GLU:HG3	1.82	0.60
1:C:99:LEU:HD13	1:C:103:GLU:HB2	1.83	0.60
1:D:48:ARG:CB	1:F:61:TYR:HE1	1.94	0.60
1:D:97:TYR:HA	1:D:126:VAL:CG2	2.19	0.59
1:D:119:LYS:O	1:D:121:PRO:HD3	2.02	0.59
1:D:80:ASN:O	1:D:82:THR:HG22	2.03	0.59
1:D:37:ILE:HD13	1:E:23:GLY:HA3	1.83	0.58
1:F:89:MET:HB2	1:F:116:TRP:CH2	2.38	0.58
1:E:85:PHE:CE1	1:E:109:LEU:HD22	2.38	0.58
7:P:4:MAN:O2	7:P:7:MAN:C2	2.50	0.58
1:A:97:TYR:CD2	1:A:124:GLU:O	2.57	0.58
1:C:100:ILE:HD11	1:C:124:GLU:HG2	1.84	0.58
1:F:98:TYR:HE2	1:F:126:VAL:HG21	1.66	0.58
1:C:110:LYS:O	1:C:111:GLY:C	2.46	0.58
1:E:70:ASP:HB3	1:E:74:GLY:O	2.03	0.58
1:E:91:PHE:CE2	1:E:121:PRO:HD2	2.38	0.58
1:B:61:TYR:HE1	1:C:48:ARG:CG	2.17	0.58
1:E:71:PRO:O	1:E:73:ASN:N	2.37	0.58
1:A:79:ALA:CB	1:A:90:HIS:CE1	2.87	0.58
1:C:68:ILE:HG21	1:C:91:PHE:HZ	1.68	0.58
1:E:85:PHE:CD1	1:E:109:LEU:HD22	2.39	0.58
1:A:7:PHE:HB3	1:A:57:ASP:HB3	1.86	0.57
1:F:80:ASN:O	1:F:82:THR:HG22	2.04	0.57
1:B:61:TYR:CE1	1:C:48:ARG:CG	2.87	0.57
1:C:17:LYS:HE2	1:E:17:LYS:CE	2.21	0.57
1:C:7:PHE:HB3	1:C:57:ASP:HB3	1.86	0.57
1:C:90:HIS:ND1	1:C:104:ILE:HG12	2.20	0.57
1:A:94:ASN:O	1:A:96:GLY:N	2.38	0.56
1:D:101:GLY:HA3	1:D:121:PRO:HG3	1.87	0.56
1:D:100:ILE:O	1:D:121:PRO:HA	2.05	0.56
1:C:45:ILE:HG22	1:C:46:CYS:N	2.20	0.56
1:C:110:LYS:HB3	1:C:115:ILE:CG1	2.35	0.56
4:O:2:NAG:H61	4:O:3:BMA:C2	2.35	0.56
1:B:61:TYR:CE1	1:C:48:ARG:HG2	2.39	0.56
1:D:9:ALA:HB3	1:D:57:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HG22	1:F:24:GLU:HG2	1.87	0.56
1:D:93:CYS:SG	1:D:99:LEU:CD2	2.94	0.56
1:F:101:GLY:HA3	1:F:121:PRO:HB3	1.87	0.56
1:D:49:ASN:HB2	1:F:81:GLY:O	2.06	0.56
1:B:70:ASP:OD2	1:B:75:GLN:HG3	2.06	0.56
1:E:80:ASN:O	1:E:82:THR:HG22	2.06	0.56
1:E:44:THR:HG23	1:E:52:TRP:CE3	2.41	0.56
1:E:68:ILE:HD12	1:E:89:MET:HE3	1.88	0.56
1:B:73:ASN:HB3	1:B:97:TYR:CE2	2.42	0.55
1:F:37:ILE:CB	1:F:61:TYR:CE2	2.82	0.55
1:F:36:TYR:O	1:F:37:ILE:HD13	2.06	0.55
6:R:2:NAG:H62	6:R:3:BMA:H2	1.87	0.55
1:B:80:ASN:O	1:B:82:THR:HG22	2.06	0.55
1:D:68:ILE:HD12	1:D:89:MET:HE3	1.88	0.55
1:E:61:TYR:HB3	1:F:48:ARG:HH11	1.72	0.55
6:R:3:BMA:H2	6:R:4:MAN:C2	2.37	0.55
1:B:97:TYR:HD1	1:B:97:TYR:N	2.05	0.55
1:C:63:GLU:O	1:C:84:GLU:HA	2.07	0.55
1:C:80:ASN:OD1	1:C:87:TYR:HA	2.07	0.55
8:Q:4:MAN:H61	8:Q:6:MAN:C3	2.27	0.55
1:A:30:CYS:HB3	1:A:34:TYR:HB2	1.89	0.55
1:C:79:ALA:HB2	1:C:90:HIS:CD2	2.42	0.55
1:D:8:GLU:O	1:D:31:LYS:HD2	2.06	0.55
1:D:97:TYR:CA	1:D:126:VAL:HG23	2.21	0.55
1:F:65:CYS:HB3	1:F:116:TRP:CD1	2.42	0.55
1:A:62:ARG:HH21	1:A:86:GLY:HA3	1.72	0.54
1:D:64:THR:HG21	1:E:22:ILE:HD12	1.89	0.54
1:C:96:GLY:C	1:C:97:TYR:HD1	2.14	0.54
1:F:34:TYR:HA	1:F:61:TYR:O	2.08	0.54
1:B:73:ASN:CB	1:B:97:TYR:CE2	2.90	0.54
1:A:44:THR:CG2	1:A:45:ILE:N	2.70	0.54
1:D:74:GLY:HA3	1:D:93:CYS:HA	1.90	0.54
1:C:65:CYS:HB2	1:C:116:TRP:NE1	2.23	0.54
1:E:39:PRO:HD3	1:F:53:LEU:HD13	1.88	0.54
1:A:17:LYS:HE2	1:D:17:LYS:HE2	1.89	0.54
1:B:97:TYR:N	1:B:97:TYR:CD1	2.76	0.54
1:C:93:CYS:SG	1:C:98:TYR:O	2.66	0.54
1:E:88:GLN:HB2	1:E:105:LEU:O	2.08	0.54
1:A:81:GLY:C	1:A:82:THR:HG22	2.32	0.54
1:E:104:ILE:HD13	7:P:2:NAG:H82	1.89	0.54
1:F:35:PHE:N	1:F:35:PHE:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:HD2	1:F:61:TYR:CE1	2.44	0.53
1:F:64:THR:HG22	1:F:83:TYR:C	2.33	0.53
1:F:68:ILE:HD12	1:F:89:MET:HE3	1.91	0.53
1:A:79:ALA:HB3	1:A:90:HIS:CE1	2.44	0.52
1:C:97:TYR:CE2	1:C:126:VAL:HG12	2.44	0.52
7:P:5:MAN:O3	7:P:6:MAN:C3	2.56	0.52
1:A:107:CYS:HB2	1:A:116:TRP:CD2	2.44	0.52
1:D:67:TYR:HA	1:D:83:TYR:CE2	2.44	0.52
1:B:106:TYR:N	1:B:106:TYR:CD1	2.77	0.52
6:R:3:BMA:C2	6:R:4:MAN:C2	2.86	0.52
1:D:98:TYR:CD1	1:D:126:VAL:HG22	2.44	0.52
1:C:85:PHE:HB3	1:C:114:ALA:HB2	1.90	0.52
1:B:36:TYR:C	1:B:37:ILE:HG12	2.35	0.52
1:D:62:ARG:HB2	1:D:85:PHE:CE2	2.44	0.52
1:E:67:TYR:HA	1:E:83:TYR:CE2	2.45	0.52
1:A:110:LYS:HG3	1:A:115:ILE:HG13	1.91	0.52
1:B:115:ILE:HG22	1:B:116:TRP:N	2.24	0.51
1:B:64:THR:HA	1:B:83:TYR:O	2.11	0.51
1:A:65:CYS:SG	1:A:114:ALA:C	2.93	0.51
1:B:49:ASN:HB3	1:B:51:THR:HG23	1.93	0.51
1:E:109:LEU:H	1:E:109:LEU:HD23	1.75	0.51
1:F:67:TYR:HA	1:F:83:TYR:CE2	2.45	0.51
1:B:62:ARG:HB2	1:B:85:PHE:CE2	2.46	0.51
1:C:85:PHE:O	1:C:87:TYR:CD1	2.64	0.51
1:F:100:ILE:N	1:F:100:ILE:HD12	2.26	0.51
4:J:2:NAG:O3	4:J:3:BMA:O5	2.28	0.51
8:Q:4:MAN:H4	8:Q:6:MAN:H2	1.92	0.51
1:E:49:ASN:O	1:E:50:HIS:HB2	2.10	0.51
2:G:2:NAG:O4	2:G:3:BMA:C1	2.59	0.51
1:C:65:CYS:HB2	1:C:116:TRP:CE2	2.46	0.51
1:D:89:MET:HB2	1:D:116:TRP:CZ3	2.46	0.51
1:F:97:TYR:HA	1:F:124:GLU:O	2.11	0.51
6:R:2:NAG:C6	6:R:3:BMA:H2	2.41	0.51
1:B:79:ALA:HB1	4:J:1:NAG:H62	1.92	0.51
1:A:48:ARG:HB2	1:C:82:THR:HG1	1.75	0.51
1:B:37:ILE:HB	1:B:61:TYR:CE2	2.46	0.51
1:C:79:ALA:O	1:C:80:ASN:CB	2.59	0.51
1:E:45:ILE:HG22	1:E:46:CYS:N	2.25	0.51
1:F:98:TYR:CE2	1:F:126:VAL:CG2	2.94	0.51
4:J:2:NAG:C3	4:J:3:BMA:O5	2.58	0.51
1:A:79:ALA:O	1:A:80:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:CB	1:B:75:GLN:HA	2.33	0.50
1:B:98:TYR:C	1:B:98:TYR:CD1	2.89	0.50
1:D:44:THR:HG23	1:D:52:TRP:HE3	1.73	0.50
1:D:93:CYS:SG	1:D:99:LEU:HD21	2.52	0.50
1:C:77:VAL:C	1:C:89:MET:HE2	2.35	0.50
1:D:73:ASN:HB3	1:D:97:TYR:OH	2.11	0.50
1:C:36:TYR:CD2	1:D:36:TYR:CD2	2.99	0.50
1:C:49:ASN:O	1:C:51:THR:HG23	2.11	0.50
7:P:4:MAN:O2	7:P:7:MAN:O2	2.26	0.50
1:B:67:TYR:HA	1:B:83:TYR:CE2	2.46	0.50
1:B:68:ILE:HD12	1:B:89:MET:HE3	1.93	0.50
1:D:85:PHE:HA	1:D:107:CYS:CB	2.34	0.50
1:D:93:CYS:HB2	1:D:99:LEU:HD21	1.94	0.50
1:C:10:MET:HA	1:C:29:LYS:O	2.12	0.49
1:C:72:LEU:O	1:C:72:LEU:HG	2.12	0.49
1:B:48:ARG:O	1:B:50:HIS:N	2.46	0.49
1:C:93:CYS:HB2	1:C:97:TYR:O	2.12	0.49
1:A:78:PRO:HG2	1:A:83:TYR:HE1	1.73	0.49
1:A:100:ILE:O	1:A:122:ILE:HD12	2.11	0.49
1:B:65:CYS:HB3	1:B:116:TRP:CD1	2.47	0.49
1:D:71:PRO:HB2	1:D:74:GLY:O	2.11	0.49
1:E:85:PHE:HB2	1:E:108:GLU:HA	1.94	0.49
1:F:99:LEU:C	1:F:100:ILE:HD12	2.36	0.49
1:E:93:CYS:HB2	1:E:99:LEU:HD22	1.94	0.49
1:F:65:CYS:HB3	1:F:116:TRP:NE1	2.28	0.49
1:F:37:ILE:CB	1:F:61:TYR:HE2	2.12	0.49
1:A:11:GLU:HG3	1:A:31:LYS:CG	2.40	0.49
1:D:1:CYS:HB2	1:D:20:TYR:HB2	1.94	0.49
1:D:97:TYR:CB	1:D:126:VAL:H	2.25	0.49
1:B:108:GLU:O	1:B:114:ALA:HA	2.13	0.49
1:E:72:LEU:HD23	1:E:72:LEU:N	2.28	0.49
1:E:78:PRO:HD2	8:Q:1:NAG:H62	1.95	0.49
1:F:99:LEU:HD23	1:F:121:PRO:HB2	1.95	0.49
1:F:125:LYS:CG	1:F:126:VAL:H	2.26	0.49
1:B:49:ASN:HD22	1:B:51:THR:HG21	1.77	0.49
1:C:98:TYR:CE1	1:C:124:GLU:HG3	2.47	0.48
1:E:107:CYS:HB2	1:E:116:TRP:CZ3	2.48	0.48
4:O:2:NAG:H61	4:O:3:BMA:H2	1.93	0.48
1:A:91:PHE:CD2	1:A:121:PRO:HG2	2.49	0.48
1:B:72:LEU:HD23	1:B:72:LEU:N	2.29	0.48
1:E:115:ILE:CG2	1:E:116:TRP:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:MET:HA	1:A:29:LYS:O	2.13	0.48
1:A:91:PHE:CG	1:A:121:PRO:HG2	2.48	0.48
1:B:98:TYR:C	1:B:98:TYR:HD1	2.20	0.48
1:C:100:ILE:O	1:C:100:ILE:HG22	2.13	0.48
1:A:89:MET:HB3	1:A:105:LEU:HB2	1.95	0.48
1:E:8:GLU:O	1:E:31:LYS:HD2	2.14	0.48
1:A:89:MET:O	1:A:104:ILE:HA	2.13	0.48
1:F:88:GLN:OE1	6:R:2:NAG:H82	2.14	0.48
1:F:100:ILE:HD13	1:F:124:GLU:HG2	1.96	0.48
1:A:79:ALA:HB2	1:A:90:HIS:CE1	2.49	0.48
1:F:93:CYS:HB3	1:F:97:TYR:HB2	1.96	0.48
1:B:83:TYR:CZ	1:B:89:MET:HE1	2.48	0.47
1:E:83:TYR:CZ	1:E:89:MET:HE1	2.49	0.47
1:F:26:VAL:CG2	1:F:44:THR:HG22	2.44	0.47
1:A:45:ILE:HB	1:A:53:LEU:HD12	1.96	0.47
1:B:37:ILE:CG1	1:B:61:TYR:CD2	2.94	0.47
1:C:1:CYS:HB3	1:C:50:HIS:O	2.15	0.47
1:B:98:TYR:CE1	1:B:100:ILE:HD11	2.49	0.47
7:P:4:MAN:H61	7:P:5:MAN:C4	2.33	0.47
1:C:19:TYR:HE2	1:C:21:GLU:OE2	1.96	0.47
1:F:45:ILE:HB	1:F:53:LEU:HD12	1.96	0.47
1:F:49:ASN:HD22	8:Q:1:NAG:C7	2.27	0.47
1:B:72:LEU:HD23	1:B:72:LEU:H	1.78	0.47
1:A:62:ARG:NH2	1:A:86:GLY:HA3	2.30	0.47
1:A:99:LEU:HD22	1:A:123:CYS:HA	1.97	0.47
8:Q:4:MAN:H2	8:Q:5:MAN:C3	2.44	0.47
1:B:11:GLU:HG3	1:B:31:LYS:CG	2.36	0.47
1:B:71:PRO:O	1:B:74:GLY:O	2.32	0.47
1:C:97:TYR:CD2	1:C:126:VAL:HG12	2.50	0.47
1:C:21:GLU:CG	1:E:14:GLY:HA2	2.36	0.47
1:F:83:TYR:CZ	1:F:89:MET:HE1	2.50	0.47
1:A:62:ARG:HG2	1:A:84:GLU:OE2	2.15	0.47
1:B:85:PHE:HA	1:B:107:CYS:HB3	1.97	0.47
1:C:9:ALA:HB3	1:C:57:ASP:HB2	1.96	0.47
1:D:37:ILE:HG21	1:D:61:TYR:CE1	2.50	0.47
1:A:36:TYR:O	1:A:37:ILE:HD13	2.15	0.46
1:A:91:PHE:CG	1:A:121:PRO:CG	2.98	0.46
1:A:98:TYR:C	1:A:99:LEU:HD23	2.39	0.46
1:D:83:TYR:CZ	1:D:89:MET:HE1	2.50	0.46
1:E:37:ILE:CD1	1:E:61:TYR:CE1	2.96	0.46
1:E:75:GLN:NE2	11:E:5070:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:CYS:HB2	1:E:99:LEU:CD2	2.46	0.46
1:A:105:LEU:O	1:A:116:TRP:HE3	1.98	0.46
1:A:109:LEU:HD22	1:A:109:LEU:HA	1.79	0.46
1:C:81:GLY:O	1:C:82:THR:HB	2.16	0.46
1:C:95:GLU:O	1:C:96:GLY:O	2.34	0.46
1:F:73:ASN:O	1:F:94:ASN:HB2	2.16	0.46
1:A:49:ASN:OD1	1:C:78:PRO:HG3	2.15	0.46
1:C:61:TYR:N	1:C:61:TYR:CD1	2.83	0.46
6:R:3:BMA:H3	6:R:4:MAN:H3	1.98	0.46
1:B:93:CYS:SG	1:B:99:LEU:CD1	3.02	0.46
1:D:45:ILE:HD13	1:F:38:PRO:HG2	1.98	0.46
1:D:89:MET:HE2	1:D:116:TRP:CH2	2.50	0.46
1:E:4:PRO:HD3	1:E:20:TYR:CE2	2.51	0.46
1:A:85:PHE:HB3	1:A:114:ALA:CB	2.45	0.46
1:B:116:TRP:HA	1:B:116:TRP:CE3	2.50	0.46
1:C:85:PHE:CD1	1:C:85:PHE:C	2.93	0.46
1:E:31:LYS:O	1:E:32:LYS:C	2.58	0.46
1:E:61:TYR:HB3	1:F:48:ARG:NH1	2.31	0.46
1:F:3:GLU:OE2	1:F:18:PRO:HA	2.16	0.46
1:A:35:PHE:CE2	1:A:63:GLU:HG2	2.51	0.45
1:A:106:TYR:O	1:A:117:SER:N	2.49	0.45
1:C:31:LYS:O	1:C:34:TYR:HB2	2.16	0.45
1:E:3:GLU:OE2	1:E:18:PRO:HA	2.16	0.45
1:C:97:TYR:CB	1:C:124:GLU:O	2.59	0.45
1:F:44:THR:HG23	1:F:52:TRP:HE3	1.79	0.45
1:A:94:ASN:O	1:A:95:GLU:C	2.59	0.45
1:C:79:ALA:O	1:C:88:GLN:HG3	2.15	0.45
1:D:7:PHE:HB3	1:D:57:ASP:HB3	1.98	0.45
1:E:22:ILE:HD13	1:E:48:ARG:HA	1.97	0.45
7:P:5:MAN:H4	7:P:6:MAN:H5	1.98	0.45
1:B:4:PRO:HD3	1:B:20:TYR:CE2	2.52	0.45
1:E:85:PHE:CE2	1:E:109:LEU:HD13	2.52	0.45
1:A:4:PRO:HD3	1:A:20:TYR:CE2	2.51	0.45
1:D:37:ILE:HD11	1:E:23:GLY:HA3	1.97	0.45
1:E:125:LYS:HD2	1:E:126:VAL:H	1.81	0.45
6:R:3:BMA:H2	6:R:4:MAN:H3	1.99	0.45
1:C:65:CYS:CB	1:C:116:TRP:NE1	2.79	0.45
1:E:124:GLU:HG3	1:E:125:LYS:O	2.16	0.45
1:E:37:ILE:HG22	1:E:37:ILE:O	2.17	0.45
1:A:99:LEU:CD2	1:A:123:CYS:HA	2.46	0.45
1:A:105:LEU:HD11	1:A:120:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:THR:C	1:E:45:ILE:HG13	2.41	0.45
1:F:4:PRO:HD3	1:F:20:TYR:CE2	2.52	0.45
7:P:5:MAN:O3	7:P:6:MAN:C2	2.64	0.45
1:B:9:ALA:HB1	1:B:60:CYS:HB2	1.99	0.45
1:E:81:GLY:O	1:F:49:ASN:HB2	2.17	0.45
1:B:36:TYR:O	1:B:37:ILE:HG12	2.17	0.44
1:B:3:GLU:OE2	1:B:18:PRO:HA	2.17	0.44
1:B:102:GLU:O	1:B:121:PRO:HG3	2.18	0.44
1:D:91:PHE:CD1	1:D:91:PHE:N	2.85	0.44
1:A:35:PHE:HE2	1:A:63:GLU:HG2	1.81	0.44
1:D:115:ILE:HG22	1:D:116:TRP:N	2.32	0.44
1:B:37:ILE:HA	1:B:38:PRO:HD2	1.65	0.44
1:C:105:LEU:HD11	1:C:120:PRO:HA	1.99	0.44
1:A:68:ILE:HD13	1:A:89:MET:HG2	1.99	0.44
1:A:85:PHE:HA	1:A:107:CYS:SG	2.58	0.44
1:C:4:PRO:HD3	1:C:20:TYR:CE2	2.53	0.44
1:D:4:PRO:HD3	1:D:20:TYR:CE2	2.53	0.44
1:D:49:ASN:ND2	5:M:1:NAG:O7	2.50	0.44
1:E:35:PHE:O	1:E:60:CYS:HA	2.17	0.44
1:F:37:ILE:HA	1:F:38:PRO:HD2	1.66	0.44
1:C:3:GLU:OE2	1:C:18:PRO:HA	2.18	0.44
1:D:105:LEU:HA	1:D:105:LEU:HD23	1.50	0.44
1:F:98:TYR:HE2	1:F:126:VAL:CG2	2.28	0.44
1:B:93:CYS:HB3	1:B:97:TYR:HB2	1.99	0.43
1:E:71:PRO:HD2	1:E:75:GLN:C	2.43	0.43
1:A:3:GLU:OE2	1:A:18:PRO:HA	2.18	0.43
1:E:24:GLU:O	1:E:45:ILE:HG23	2.19	0.43
1:E:68:ILE:HD11	1:E:116:TRP:CE2	2.53	0.43
1:A:105:LEU:O	1:A:116:TRP:CE3	2.71	0.43
1:D:63:GLU:OE1	1:D:85:PHE:HE2	2.01	0.43
1:B:61:TYR:CE1	1:C:48:ARG:HG3	2.48	0.43
1:D:97:TYR:CG	1:D:125:LYS:HA	2.54	0.43
8:Q:4:MAN:C5	8:Q:6:MAN:H2	2.48	0.43
1:B:2:GLU:O	1:B:20:TYR:HD2	2.00	0.43
1:D:3:GLU:OE2	1:D:18:PRO:HA	2.18	0.43
1:E:64:THR:HA	1:E:83:TYR:O	2.19	0.43
1:E:101:GLY:CA	1:E:121:PRO:HB3	2.46	0.43
1:A:95:GLU:HG3	1:A:95:GLU:O	2.18	0.43
1:A:9:ALA:HB3	1:A:57:ASP:HB2	2.00	0.43
1:B:45:ILE:HG22	1:B:46:CYS:N	2.33	0.43
1:A:64:THR:HG22	1:A:84:GLU:CA	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:O	1:A:72:LEU:C	2.61	0.43
1:D:90:HIS:HB2	1:D:103:GLU:O	2.19	0.43
2:G:4:MAN:H2	2:G:5:MAN:C5	2.49	0.43
1:C:99:LEU:CD1	1:C:103:GLU:HB2	2.46	0.43
1:F:2:GLU:O	1:F:20:TYR:HD2	2.02	0.43
7:P:4:MAN:H61	7:P:5:MAN:H3	0.54	0.43
1:C:63:GLU:CB	1:C:85:PHE:HD2	2.32	0.43
1:A:89:MET:O	1:A:105:LEU:N	2.50	0.42
1:E:35:PHE:N	1:E:35:PHE:CD1	2.86	0.42
1:E:97:TYR:CD1	1:E:125:LYS:HB2	2.54	0.42
1:F:109:LEU:HD12	1:F:113:VAL:C	2.45	0.42
1:C:40:LEU:HD23	1:C:40:LEU:HA	1.70	0.42
1:D:10:MET:HE3	1:D:28:TYR:HB2	2.02	0.42
1:E:82:THR:HA	1:F:48:ARG:O	2.19	0.42
1:C:102:GLU:HB2	1:C:105:LEU:HD21	2.02	0.42
1:E:120:PRO:HA	1:E:121:PRO:HD2	1.86	0.42
1:F:64:THR:HG22	1:F:83:TYR:O	2.19	0.42
1:C:2:GLU:O	1:C:20:TYR:HD2	2.03	0.42
1:E:37:ILE:HD12	1:E:37:ILE:HA	1.85	0.42
1:F:11:GLU:HG3	1:F:31:LYS:CG	2.45	0.42
8:Q:4:MAN:O5	8:Q:6:MAN:H2	2.19	0.42
1:B:7:PHE:HB3	1:B:57:ASP:HB3	2.01	0.42
1:B:75:GLN:NE2	11:B:2070:HOH:O	2.51	0.42
1:C:91:PHE:HD2	1:C:103:GLU:O	2.02	0.42
1:A:69:ARG:O	1:A:70:ASP:C	2.62	0.42
1:D:15:LYS:HA	1:D:16:PRO:HD3	1.94	0.42
1:A:34:TYR:CD1	1:A:34:TYR:N	2.88	0.42
1:A:2:GLU:O	1:A:20:TYR:HD2	2.03	0.42
1:C:45:ILE:CG2	1:C:46:CYS:N	2.82	0.42
1:C:83:TYR:CD2	1:C:116:TRP:HZ2	2.37	0.42
1:C:89:MET:HE3	1:C:89:MET:HA	2.01	0.42
1:C:100:ILE:HD12	1:C:122:ILE:C	2.44	0.42
1:D:49:ASN:ND2	1:D:51:THR:CG2	2.83	0.42
1:E:73:ASN:CB	1:E:97:TYR:HE2	2.30	0.42
1:B:98:TYR:HD1	1:B:98:TYR:O	2.03	0.41
1:C:89:MET:HG2	1:C:91:PHE:CZ	2.55	0.41
1:D:26:VAL:CG2	1:D:44:THR:HG22	2.50	0.41
1:F:37:ILE:HG12	1:F:61:TYR:CD2	2.55	0.41
1:F:99:LEU:HD21	1:F:121:PRO:HG3	2.01	0.41
6:R:3:BMA:O2	6:R:4:MAN:H2	2.20	0.41
1:D:30:CYS:HB3	1:D:34:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:GLY:CA	1:F:121:PRO:HB3	2.50	0.41
1:E:101:GLY:HA3	1:E:121:PRO:CB	2.48	0.41
6:R:3:BMA:H2	6:R:4:MAN:C3	2.49	0.41
1:D:62:ARG:HD2	1:D:85:PHE:CZ	2.55	0.41
1:D:98:TYR:O	1:D:99:LEU:HD23	2.20	0.41
1:B:37:ILE:CG1	1:B:61:TYR:HD2	2.20	0.41
1:B:72:LEU:H	1:B:72:LEU:CD2	2.32	0.41
1:E:2:GLU:O	1:E:20:TYR:HD2	2.03	0.41
1:E:71:PRO:HD2	1:E:76:ALA:N	2.36	0.41
1:A:44:THR:HG23	1:A:53:LEU:H	1.85	0.41
1:A:79:ALA:O	1:A:80:ASN:CB	2.68	0.41
1:D:2:GLU:O	1:D:20:TYR:HD2	2.03	0.41
1:D:88:GLN:HB2	1:D:105:LEU:O	2.21	0.41
1:E:125:LYS:HG3	1:E:126:VAL:N	2.36	0.41
2:G:2:NAG:O4	2:G:3:BMA:O5	2.35	0.41
1:C:10:MET:HE3	1:C:28:TYR:HB2	2.02	0.41
1:E:31:LYS:O	1:E:34:TYR:HB2	2.21	0.41
1:A:88:GLN:C	1:A:116:TRP:HZ3	2.28	0.41
1:C:25:ARG:CZ	1:C:43:HIS:CD2	3.04	0.41
1:C:68:ILE:HG22	1:C:68:ILE:O	2.20	0.41
1:A:31:LYS:O	1:A:32:LYS:C	2.64	0.41
1:C:61:TYR:N	1:C:61:TYR:HD1	2.19	0.41
6:N:3:BMA:O2	6:N:4:MAN:C1	2.66	0.41
1:D:10:MET:HA	1:D:29:LYS:O	2.22	0.40
1:D:37:ILE:CG2	1:D:61:TYR:CE1	3.05	0.40
1:D:47:ASP:OD1	1:D:51:THR:O	2.39	0.40
1:E:70:ASP:O	1:E:71:PRO:C	2.64	0.40
1:B:21:GLU:CB	1:B:24:GLU:HG3	2.50	0.40
1:C:45:ILE:HG22	1:C:46:CYS:H	1.83	0.40
1:A:113:VAL:HG22	1:A:114:ALA:N	2.33	0.40
1:F:37:ILE:HB	1:F:61:TYR:CD2	2.52	0.40
1:D:31:LYS:O	1:D:33:GLY:N	2.54	0.40
1:E:97:TYR:HD1	1:E:125:LYS:HB2	1.86	0.40
1:E:105:LEU:HD22	1:E:117:SER:HB2	2.03	0.40
1:F:47:ASP:OD1	1:F:49:ASN:HB3	2.21	0.40
5:K:1:NAG:O3	5:K:2:NAG:C1	2.69	0.40
1:A:103:GLU:HG2	1:A:104:ILE:HG13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	124/126 (98%)	94 (76%)	21 (17%)	9 (7%)	1	5
1	B	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	2	13
1	C	124/126 (98%)	96 (77%)	21 (17%)	7 (6%)	1	8
1	D	124/126 (98%)	99 (80%)	17 (14%)	8 (6%)	1	6
1	E	124/126 (98%)	101 (82%)	18 (14%)	5 (4%)	2	13
1	F	124/126 (98%)	106 (86%)	16 (13%)	2 (2%)	7	30
All	All	744/756 (98%)	604 (81%)	104 (14%)	36 (5%)	2	11

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	58	ASP
1	A	63	GLU
1	A	66	PRO
1	A	95	GLU
1	B	40	LEU
1	C	58	ASP
1	D	32	LYS
1	D	40	LEU
1	E	73	ASN
1	F	32	LYS
1	A	73	ASN
1	A	81	GLY
1	B	63	GLU
1	B	121	PRO
1	C	32	LYS
1	C	80	ASN
1	C	96	GLY
1	D	73	ASN
1	D	96	GLY

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Mol	Chain	Res	Type
1	E	72	LEU
1	A	72	LEU
1	C	67	TYR
1	C	85	PHE
1	E	40	LEU
1	B	49	ASN
1	D	81	GLY
1	D	95	GLU
1	D	120	PRO
1	E	81	GLY
1	F	81	GLY
1	A	32	LYS
1	B	81	GLY
1	C	48	ARG
1	E	50	HIS
1	D	71	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/110 (100%)	93 (84%)	17 (16%)	2	12
1	B	110/110 (100%)	93 (84%)	17 (16%)	2	12
1	C	110/110 (100%)	95 (86%)	15 (14%)	3	16
1	D	110/110 (100%)	92 (84%)	18 (16%)	2	11
1	E	110/110 (100%)	96 (87%)	14 (13%)	4	18
1	F	110/110 (100%)	93 (84%)	17 (16%)	2	12
All	All	660/660 (100%)	562 (85%)	98 (15%)	3	13

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	37	ILE

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Mol	Chain	Res	Type
1	A	44	THR
1	A	45	ILE
1	A	48	ARG
1	A	62	ARG
1	A	69	ARG
1	A	70	ASP
1	A	82	THR
1	A	93	CYS
1	A	94	ASN
1	A	107	CYS
1	A	108	GLU
1	A	109	LEU
1	A	115	ILE
1	A	119	LYS
1	A	124	GLU
1	B	6	THR
1	B	37	ILE
1	B	40	LEU
1	B	48	ARG
1	B	50	HIS
1	B	56	SER
1	B	62	ARG
1	B	63	GLU
1	B	70	ASP
1	B	72	LEU
1	B	77	VAL
1	B	88	GLN
1	B	97	TYR
1	B	98	TYR
1	B	99	LEU
1	B	113	VAL
1	B	126	VAL
1	C	6	THR
1	C	39	PRO
1	C	40	LEU
1	C	56	SER
1	C	62	ARG
1	C	65	CYS
1	C	72	LEU
1	C	77	VAL
1	C	89	MET
1	C	92	ILE

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Mol	Chain	Res	Type
1	C	94	ASN
1	C	100	ILE
1	C	103	GLU
1	C	109	LEU
1	C	113	VAL
1	D	6	THR
1	D	37	ILE
1	D	40	LEU
1	D	45	ILE
1	D	48	ARG
1	D	72	LEU
1	D	73	ASN
1	D	75	GLN
1	D	77	VAL
1	D	91	PHE
1	D	93	CYS
1	D	95	GLU
1	D	100	ILE
1	D	102	GLU
1	D	108	GLU
1	D	113	VAL
1	D	123	CYS
1	D	124	GLU
1	E	6	THR
1	E	35	PHE
1	E	37	ILE
1	E	49	ASN
1	E	72	LEU
1	E	75	GLN
1	E	88	GLN
1	E	93	CYS
1	E	97	TYR
1	E	99	LEU
1	E	103	GLU
1	E	113	VAL
1	E	123	CYS
1	E	126	VAL
1	F	6	THR
1	F	32	LYS
1	F	35	PHE
1	F	39	PRO
1	F	45	ILE

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Mol	Chain	Res	Type
1	F	47	ASP
1	F	48	ARG
1	F	70	ASP
1	F	77	VAL
1	F	88	GLN
1	F	92	ILE
1	F	99	LEU
1	F	102	GLU
1	F	112	SER
1	F	113	VAL
1	F	125	LYS
1	F	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	94	ASN
1	B	43	HIS
1	B	88	GLN
1	C	43	HIS
1	C	94	ASN
1	D	73	ASN
1	D	75	GLN
1	E	75	GLN
1	E	88	GLN
1	F	75	GLN
1	F	94	ASN

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 ⓘ

51 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	G	1	1,2	14,14,15	0.61	0	17,19,21	1.60	2 (11%)
2	NAG	G	2	2	14,14,15	2.38	6 (42%)	17,19,21	3.49	8 (47%)
2	BMA	G	3	2	11,11,12	3.53	4 (36%)	15,15,17	1.82	4 (26%)
2	MAN	G	4	2	11,11,12	0.93	1 (9%)	15,15,17	1.87	5 (33%)
2	MAN	G	5	2	11,11,12	1.13	1 (9%)	15,15,17	0.97	1 (6%)
2	MAN	G	6	2	11,11,12	0.69	0	15,15,17	1.24	1 (6%)
2	MAN	G	7	2	11,11,12	1.31	2 (18%)	15,15,17	1.76	2 (13%)
2	MAN	G	8	2	11,11,12	0.85	1 (9%)	15,15,17	1.08	2 (13%)
3	NAG	H	1	1,3	14,14,15	1.44	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	H	2	3	14,14,15	3.59	6 (42%)	17,19,21	3.01	7 (41%)
3	BMA	H	3	3	11,11,12	2.76	6 (54%)	15,15,17	1.36	2 (13%)
3	MAN	H	4	3	11,11,12	0.91	0	15,15,17	1.55	2 (13%)
4	NAG	I	1	1,4	14,14,15	0.98	0	17,19,21	1.59	5 (29%)
4	NAG	I	2	4	14,14,15	1.14	1 (7%)	17,19,21	1.29	3 (17%)
4	BMA	I	3	4	11,11,12	0.82	0	15,15,17	0.65	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.81	0	17,19,21	0.92	0
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	2.10	8 (47%)
4	BMA	J	3	4	11,11,12	0.48	0	15,15,17	0.69	0
5	NAG	K	1	1,5	14,14,15	1.22	3 (21%)	17,19,21	2.01	6 (35%)
5	NAG	K	2	5	14,14,15	1.69	2 (14%)	17,19,21	1.01	2 (11%)
5	NAG	L	1	1,5	14,14,15	1.50	1 (7%)	17,19,21	2.81	6 (35%)
5	NAG	L	2	5	14,14,15	0.46	0	17,19,21	0.66	0
5	NAG	M	1	1,5	14,14,15	0.56	0	17,19,21	0.98	1 (5%)
5	NAG	M	2	5	14,14,15	0.63	0	17,19,21	1.36	2 (11%)
6	NAG	N	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	1.37	2 (11%)
6	NAG	N	2	6	14,14,15	0.86	1 (7%)	17,19,21	1.07	1 (5%)
6	BMA	N	3	6	11,11,12	0.86	1 (9%)	15,15,17	1.06	1 (6%)
6	MAN	N	4	6	11,11,12	0.59	0	15,15,17	0.59	0
6	MAN	N	5	6	11,11,12	0.64	0	15,15,17	0.55	0
4	NAG	O	1	1,4	14,14,15	0.77	0	17,19,21	1.22	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	2	4	14,14,15	1.27	1 (7%)	17,19,21	1.42	3 (17%)
4	BMA	O	3	4	11,11,12	0.47	0	15,15,17	0.99	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.72	0	17,19,21	1.65	2 (11%)
7	NAG	P	2	7	14,14,15	1.03	0	17,19,21	1.77	6 (35%)
7	BMA	P	3	7	11,11,12	0.90	0	15,15,17	0.92	1 (6%)
7	MAN	P	4	7	11,11,12	0.78	0	15,15,17	1.95	3 (20%)
7	MAN	P	5	7	11,11,12	1.28	1 (9%)	15,15,17	2.63	3 (20%)
7	MAN	P	6	7	11,11,12	0.89	0	15,15,17	1.11	1 (6%)
7	MAN	P	7	7	11,11,12	0.60	0	15,15,17	1.76	3 (20%)
7	MAN	P	8	7	11,11,12	0.54	0	15,15,17	1.44	4 (26%)
8	NAG	Q	1	1,8	14,14,15	0.44	0	17,19,21	1.85	1 (5%)
8	NAG	Q	2	8	14,14,15	0.89	1 (7%)	17,19,21	2.22	5 (29%)
8	BMA	Q	3	8	11,11,12	0.85	0	15,15,17	1.42	3 (20%)
8	MAN	Q	4	8	11,11,12	1.24	2 (18%)	15,15,17	1.21	1 (6%)
8	MAN	Q	5	8	11,11,12	0.97	1 (9%)	15,15,17	0.86	1 (6%)
8	MAN	Q	6	8	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
6	NAG	R	1	1,6	14,14,15	0.39	0	17,19,21	1.06	1 (5%)
6	NAG	R	2	6	14,14,15	0.79	0	17,19,21	1.67	4 (23%)
6	BMA	R	3	6	11,11,12	0.80	0	15,15,17	1.49	3 (20%)
6	MAN	R	4	6	11,11,12	0.63	0	15,15,17	0.79	0
6	MAN	R	5	6	11,11,12	0.55	0	15,15,17	1.65	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	0/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1
3	NAG	H	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	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	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	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	1/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
7	MAN	P	5	7	-	0/2/19/22	0/1/1/1
7	MAN	P	6	7	-	0/2/19/22	0/1/1/1
7	MAN	P	7	7	-	1/2/19/22	0/1/1/1
7	MAN	P	8	7	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	6	8	-	0/2/19/22	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	2/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C3-C2	10.32	1.74	1.52
2	G	3	BMA	C2-C3	8.00	1.64	1.52
2	G	3	BMA	C1-C2	7.11	1.69	1.52
5	K	2	NAG	C1-C2	5.05	1.59	1.52
3	H	3	BMA	C2-C3	4.99	1.60	1.52
2	G	2	NAG	C1-C2	4.67	1.58	1.52
3	H	3	BMA	O5-C5	4.67	1.52	1.43
3	H	2	NAG	O3-C3	4.66	1.54	1.43
3	H	2	NAG	C1-C2	4.64	1.58	1.52
2	G	2	NAG	C3-C2	4.61	1.62	1.52
5	L	1	NAG	C1-C2	4.13	1.58	1.52
3	H	2	NAG	C8-C7	3.52	1.57	1.50
2	G	2	NAG	C4-C5	-3.33	1.45	1.53
3	H	2	NAG	O5-C1	-3.26	1.38	1.43
2	G	5	MAN	C2-C3	3.19	1.57	1.52
3	H	1	NAG	C4-C5	3.16	1.59	1.53
3	H	3	BMA	O5-C1	3.13	1.49	1.43
3	H	3	BMA	O3-C3	3.13	1.50	1.43
2	G	3	BMA	O3-C3	3.10	1.50	1.43
3	H	3	BMA	C1-C2	3.03	1.59	1.52
3	H	1	NAG	O4-C4	3.00	1.50	1.43
7	P	5	MAN	O2-C2	2.79	1.49	1.43
2	G	2	NAG	C8-C7	2.66	1.56	1.50
4	O	2	NAG	C4-C3	2.65	1.59	1.52
2	G	2	NAG	O3-C3	2.58	1.49	1.43
5	K	2	NAG	C3-C2	2.53	1.57	1.52
3	H	3	BMA	C4-C5	2.40	1.58	1.53
5	K	1	NAG	O4-C4	2.32	1.48	1.43
4	I	2	NAG	C4-C5	2.29	1.57	1.53
2	G	4	MAN	O5-C1	-2.29	1.39	1.43
6	N	1	NAG	C1-C2	2.29	1.55	1.52
3	H	2	NAG	C2-N2	2.26	1.50	1.46
5	K	1	NAG	C4-C5	2.26	1.57	1.53
8	Q	4	MAN	C1-C2	2.23	1.57	1.52
2	G	2	NAG	C2-N2	2.20	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	BMA	O5-C1	-2.15	1.40	1.43
8	Q	5	MAN	C2-C3	2.15	1.55	1.52
2	G	7	MAN	C2-C3	2.15	1.55	1.52
6	N	2	NAG	C1-C2	-2.14	1.49	1.52
2	G	7	MAN	C1-C2	2.13	1.57	1.52
3	H	1	NAG	C4-C3	2.10	1.57	1.52
8	Q	2	NAG	O5-C1	2.06	1.47	1.43
5	K	1	NAG	O5-C5	2.06	1.47	1.43
2	G	8	MAN	C1-C2	2.02	1.57	1.52
8	Q	4	MAN	C2-C3	-2.02	1.49	1.52
6	N	3	BMA	C4-C5	-2.00	1.48	1.53

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	8.59	123.69	112.19
7	P	5	MAN	C1-C2-C3	-8.52	97.24	109.64
5	L	1	NAG	C1-C2-N2	7.04	121.52	110.43
8	Q	1	NAG	C4-C3-C2	-6.32	101.75	111.02
3	H	2	NAG	C3-C4-C5	5.92	120.96	110.23
2	G	2	NAG	C3-C4-C5	5.89	120.91	110.23
2	G	7	MAN	C1-O5-C5	5.69	119.81	112.19
5	K	1	NAG	C3-C4-C5	-5.42	100.41	110.23
8	Q	2	NAG	C1-O5-C5	5.36	119.37	112.19
7	P	1	NAG	C3-C4-C5	5.25	119.74	110.23
3	H	2	NAG	O3-C3-C2	5.23	120.26	109.40
7	P	4	MAN	C1-O5-C5	5.21	119.17	112.19
3	H	2	NAG	C8-C7-N2	5.10	124.58	116.12
6	R	5	MAN	C1-O5-C5	5.03	118.93	112.19
6	R	2	NAG	C4-C3-C2	-4.96	103.75	111.02
2	G	2	NAG	O5-C1-C2	4.92	118.91	111.29
5	L	1	NAG	O5-C1-C2	-4.66	104.08	111.29
3	H	4	MAN	C1-O5-C5	4.61	118.37	112.19
6	R	3	BMA	C1-C2-C3	4.41	116.07	109.64
3	H	2	NAG	C1-C2-N2	-4.36	103.57	110.43
8	Q	2	NAG	O5-C1-C2	4.31	117.97	111.29
2	G	2	NAG	C1-C2-N2	-4.26	103.72	110.43
2	G	4	MAN	C2-C3-C4	4.18	118.22	110.86
5	L	1	NAG	C4-C3-C2	4.11	117.04	111.02
3	H	2	NAG	O7-C7-C8	-4.11	114.74	122.05
2	G	6	MAN	C1-O5-C5	4.06	117.63	112.19
4	J	2	NAG	O5-C1-C2	4.03	117.52	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	7	MAN	C1-C2-C3	4.02	115.49	109.64
2	G	2	NAG	O3-C3-C4	-4.00	100.96	110.38
8	Q	2	NAG	C4-C3-C2	-3.80	105.45	111.02
8	Q	3	BMA	C6-C5-C4	-3.72	103.88	113.02
7	P	2	NAG	C1-C2-N2	-3.72	104.57	110.43
7	P	7	MAN	C1-O5-C5	3.71	117.16	112.19
2	G	3	BMA	C6-C5-C4	3.65	121.99	113.02
6	N	1	NAG	C4-C3-C2	3.59	116.28	111.02
5	L	1	NAG	C8-C7-N2	3.59	122.06	116.12
8	Q	4	MAN	C1-O5-C5	3.52	116.91	112.19
5	M	2	NAG	C4-C3-C2	3.48	116.12	111.02
2	G	1	NAG	C1-O5-C5	3.44	116.80	112.19
7	P	8	MAN	C1-O5-C5	3.43	116.78	112.19
5	L	1	NAG	C2-N2-C7	-3.37	118.39	122.90
4	O	2	NAG	C4-C3-C2	3.36	115.94	111.02
8	Q	2	NAG	C3-C4-C5	-3.35	104.17	110.23
4	I	1	NAG	C4-C3-C2	3.31	115.87	111.02
7	P	2	NAG	C4-C3-C2	3.30	115.86	111.02
2	G	8	MAN	C1-O5-C5	3.24	116.53	112.19
4	J	2	NAG	C2-N2-C7	-3.22	118.58	122.90
3	H	2	NAG	O3-C3-C4	-3.22	102.80	110.38
5	M	2	NAG	C3-C4-C5	3.18	116.01	110.23
7	P	4	MAN	O5-C1-C2	3.18	118.39	110.79
2	G	3	BMA	C2-C3-C4	-3.18	105.27	110.86
5	L	1	NAG	O7-C7-C8	-3.16	116.42	122.05
5	K	1	NAG	C4-C3-C2	-3.15	106.40	111.02
2	G	2	NAG	O3-C3-C2	3.14	115.92	109.40
2	G	3	BMA	O5-C5-C6	-3.06	101.70	107.66
7	P	1	NAG	C1-C2-N2	3.04	115.23	110.43
2	G	2	NAG	C8-C7-N2	3.02	121.13	116.12
4	J	2	NAG	C1-O5-C5	2.98	116.17	112.19
2	G	1	NAG	O4-C4-C5	-2.94	102.09	109.32
6	N	1	NAG	C3-C4-C5	2.91	115.51	110.23
2	G	2	NAG	O7-C7-C8	-2.88	116.92	122.05
4	J	2	NAG	C3-C4-C5	2.86	115.42	110.23
2	G	7	MAN	C1-C2-C3	2.84	113.78	109.64
2	G	3	BMA	O3-C3-C2	2.83	115.83	110.05
5	K	1	NAG	C1-O5-C5	2.83	115.97	112.19
7	P	5	MAN	O3-C3-C2	2.82	115.80	110.05
4	J	2	NAG	C8-C7-N2	2.81	120.77	116.12
3	H	4	MAN	C1-C2-C3	2.80	113.73	109.64
4	J	2	NAG	O4-C4-C5	-2.77	102.50	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	MAN	O5-C1-C2	2.76	117.37	110.79
8	Q	2	NAG	C2-N2-C7	-2.75	119.21	122.90
2	G	4	MAN	C3-C4-C5	-2.75	105.25	110.23
8	Q	6	MAN	C1-C2-C3	2.74	113.63	109.64
5	M	1	NAG	C4-C3-C2	-2.71	107.04	111.02
5	K	2	NAG	C4-C3-C2	2.71	114.98	111.02
4	O	1	NAG	C3-C4-C5	2.69	115.11	110.23
7	P	4	MAN	C1-C2-C3	2.69	113.56	109.64
8	Q	5	MAN	C1-O5-C5	2.69	115.78	112.19
7	P	5	MAN	C1-O5-C5	2.62	115.70	112.19
7	P	7	MAN	O5-C1-C2	2.61	117.01	110.79
6	R	1	NAG	C2-N2-C7	-2.60	119.42	122.90
4	O	3	BMA	C2-C3-C4	-2.56	106.36	110.86
4	I	2	NAG	C4-C3-C2	2.54	114.74	111.02
4	J	2	NAG	O3-C3-C2	-2.54	104.12	109.40
4	I	1	NAG	C3-C4-C5	2.54	114.83	110.23
6	R	2	NAG	O5-C5-C6	-2.52	102.75	107.66
3	H	3	BMA	C2-C3-C4	-2.45	106.56	110.86
3	H	2	NAG	O5-C1-C2	-2.45	107.51	111.29
7	P	2	NAG	C6-C5-C4	2.41	118.94	113.02
6	R	5	MAN	C1-C2-C3	2.40	113.14	109.64
7	P	2	NAG	O5-C5-C4	-2.40	105.00	110.83
6	R	3	BMA	C3-C4-C5	2.40	114.58	110.23
8	Q	3	BMA	C3-C4-C5	2.36	114.52	110.23
3	H	1	NAG	C4-C3-C2	2.36	114.47	111.02
8	Q	3	BMA	C1-C2-C3	-2.35	106.22	109.64
6	R	3	BMA	C6-C5-C4	-2.34	107.27	113.02
4	O	2	NAG	C6-C5-C4	2.33	118.74	113.02
6	R	2	NAG	C1-O5-C5	2.32	115.29	112.19
4	I	1	NAG	C8-C7-N2	2.29	119.92	116.12
7	P	8	MAN	C1-C2-C3	2.29	112.98	109.64
7	P	6	MAN	C1-O5-C5	2.27	115.23	112.19
4	O	1	NAG	C1-C2-N2	-2.27	106.85	110.43
7	P	8	MAN	C3-C4-C5	-2.27	106.11	110.23
6	N	3	BMA	C6-C5-C4	-2.27	107.46	113.02
3	H	3	BMA	C1-C2-C3	2.26	112.94	109.64
7	P	3	BMA	C1-C2-C3	2.25	112.92	109.64
7	P	2	NAG	C8-C7-N2	-2.25	112.39	116.12
6	R	2	NAG	C2-N2-C7	-2.22	119.93	122.90
5	K	1	NAG	C6-C5-C4	2.22	118.46	113.02
4	J	2	NAG	O7-C7-C8	-2.21	118.11	122.05
2	G	4	MAN	C1-O5-C5	2.21	115.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1	NAG	C1-C2-N2	2.21	113.91	110.43
4	O	2	NAG	C3-C4-C5	2.20	114.22	110.23
2	G	4	MAN	C6-C5-C4	2.19	118.40	113.02
2	G	8	MAN	C1-C2-C3	2.19	112.84	109.64
5	K	2	NAG	C1-O5-C5	2.14	115.06	112.19
5	K	1	NAG	O4-C4-C5	2.14	114.60	109.32
2	G	5	MAN	C1-O5-C5	2.13	115.04	112.19
4	O	1	NAG	C1-O5-C5	-2.11	109.36	112.19
4	I	1	NAG	O7-C7-C8	-2.09	118.33	122.05
4	I	2	NAG	C3-C4-C5	2.07	113.99	110.23
4	I	3	BMA	C1-C2-C3	2.07	112.66	109.64
4	I	2	NAG	C1-C2-N2	2.06	113.68	110.43
6	N	2	NAG	O4-C4-C3	-2.05	105.54	110.38
4	I	1	NAG	C2-N2-C7	-2.04	120.17	122.90
7	P	8	MAN	O5-C1-C2	2.00	115.57	110.79
7	P	2	NAG	O7-C7-N2	2.00	125.52	121.98

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
6	N	5	MAN	C4-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
8	Q	4	MAN	C4-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
8	Q	3	BMA	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
7	P	7	MAN	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
6	R	4	MAN	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6

There are no ring outliers.

28 monomers are involved in 57 short contacts:

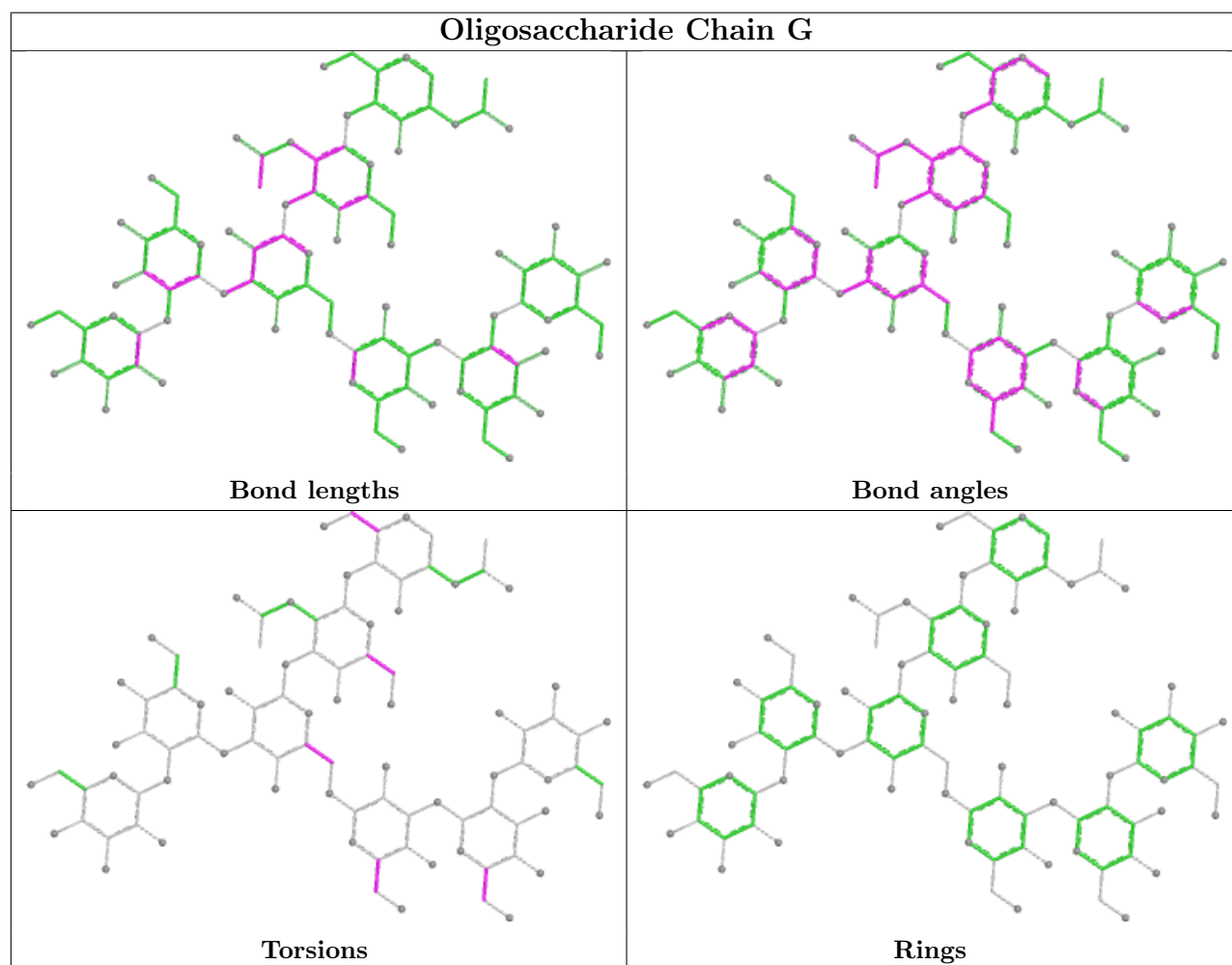
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	3	BMA	3	0
7	P	4	MAN	7	0
7	P	7	MAN	3	0
2	G	5	MAN	1	0
6	R	2	NAG	4	0
4	O	2	NAG	3	0
2	G	4	MAN	1	0
5	L	1	NAG	2	0
7	P	6	MAN	8	0
4	J	1	NAG	2	0
6	R	3	BMA	10	0
5	L	2	NAG	3	0
2	G	3	BMA	2	0

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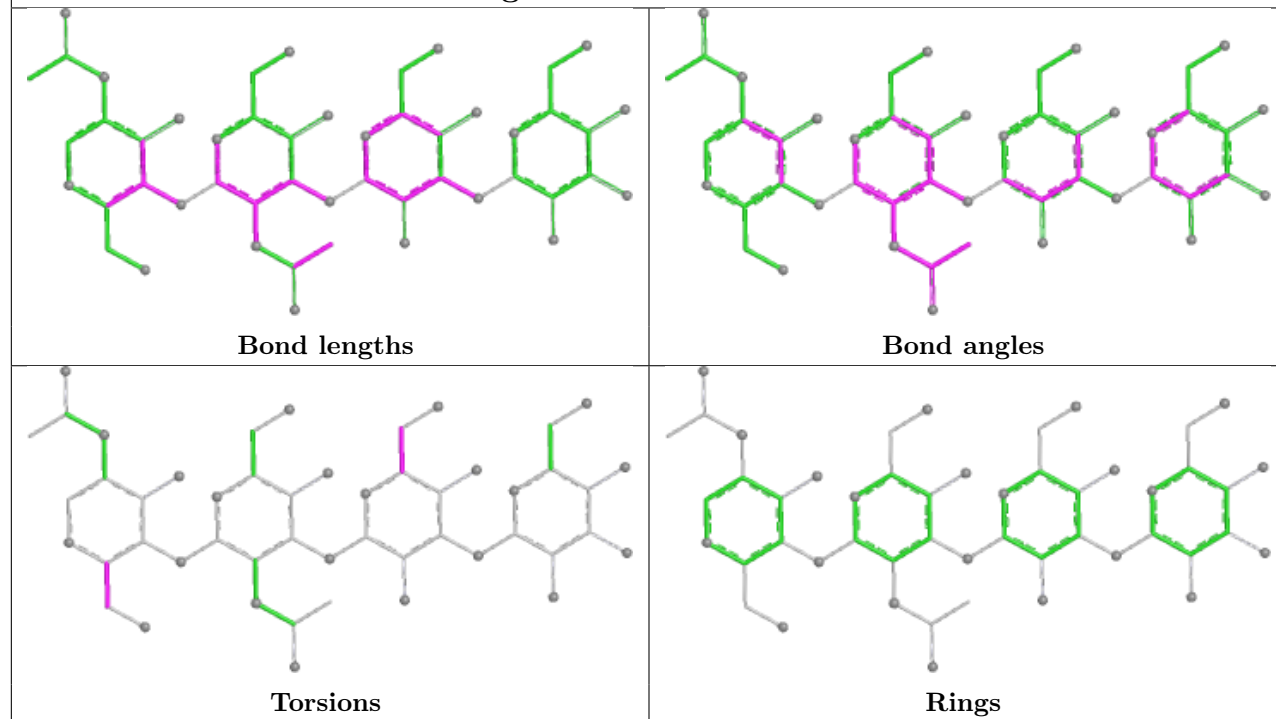
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
8	Q	1	NAG	2	0
4	J	3	BMA	2	0
4	J	2	NAG	3	0
8	Q	6	MAN	5	0
8	Q	4	MAN	10	0
7	P	2	NAG	2	0
2	G	2	NAG	2	0
6	N	3	BMA	1	0
8	Q	5	MAN	5	0
5	K	2	NAG	1	0
6	N	4	MAN	1	0
5	M	1	NAG	1	0
6	R	4	MAN	8	0
7	P	5	MAN	12	0

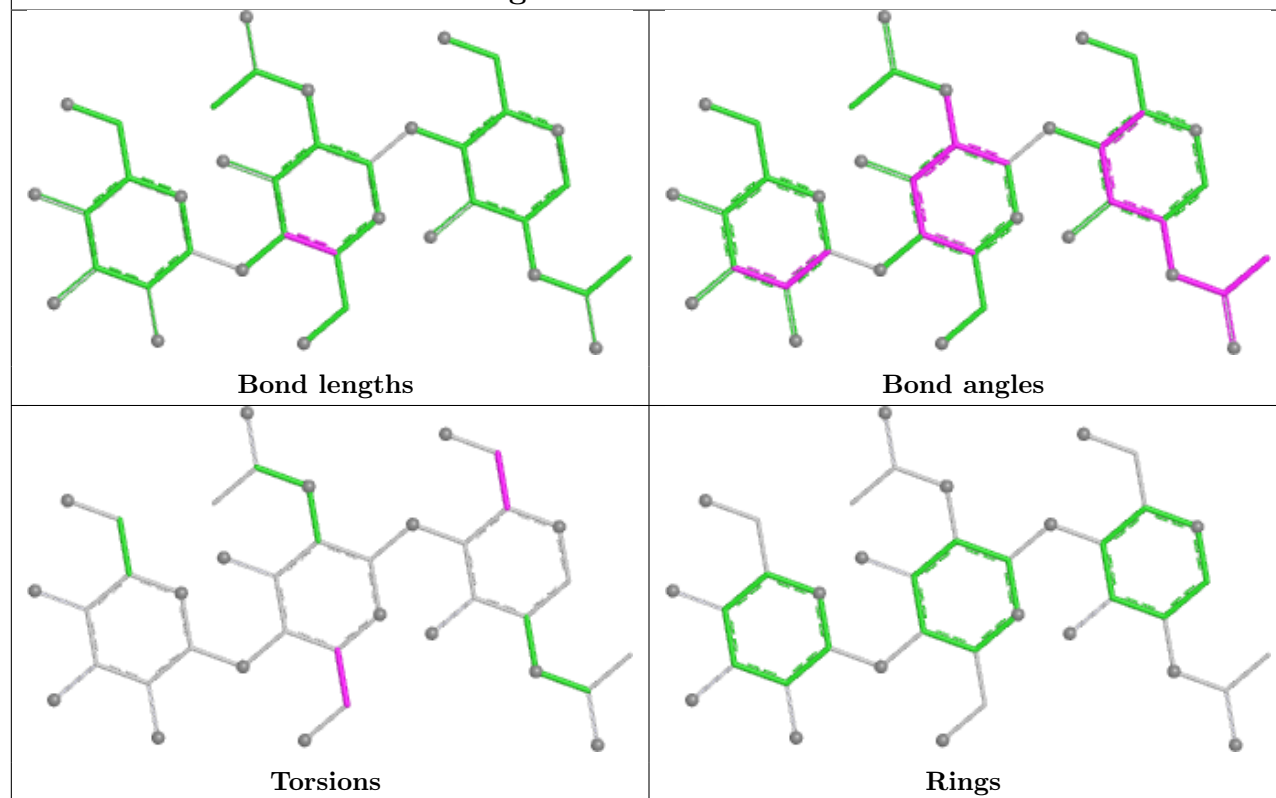
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



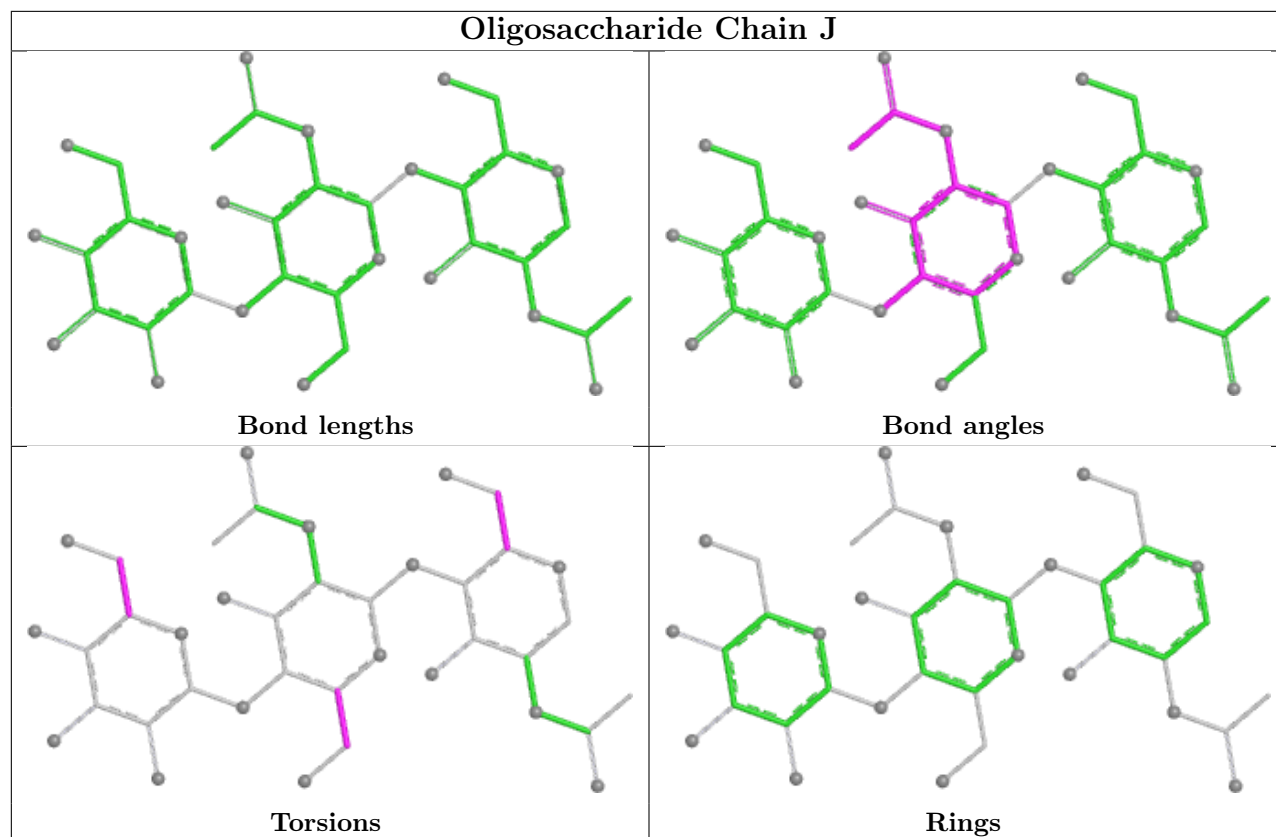
Oligosaccharide Chain H



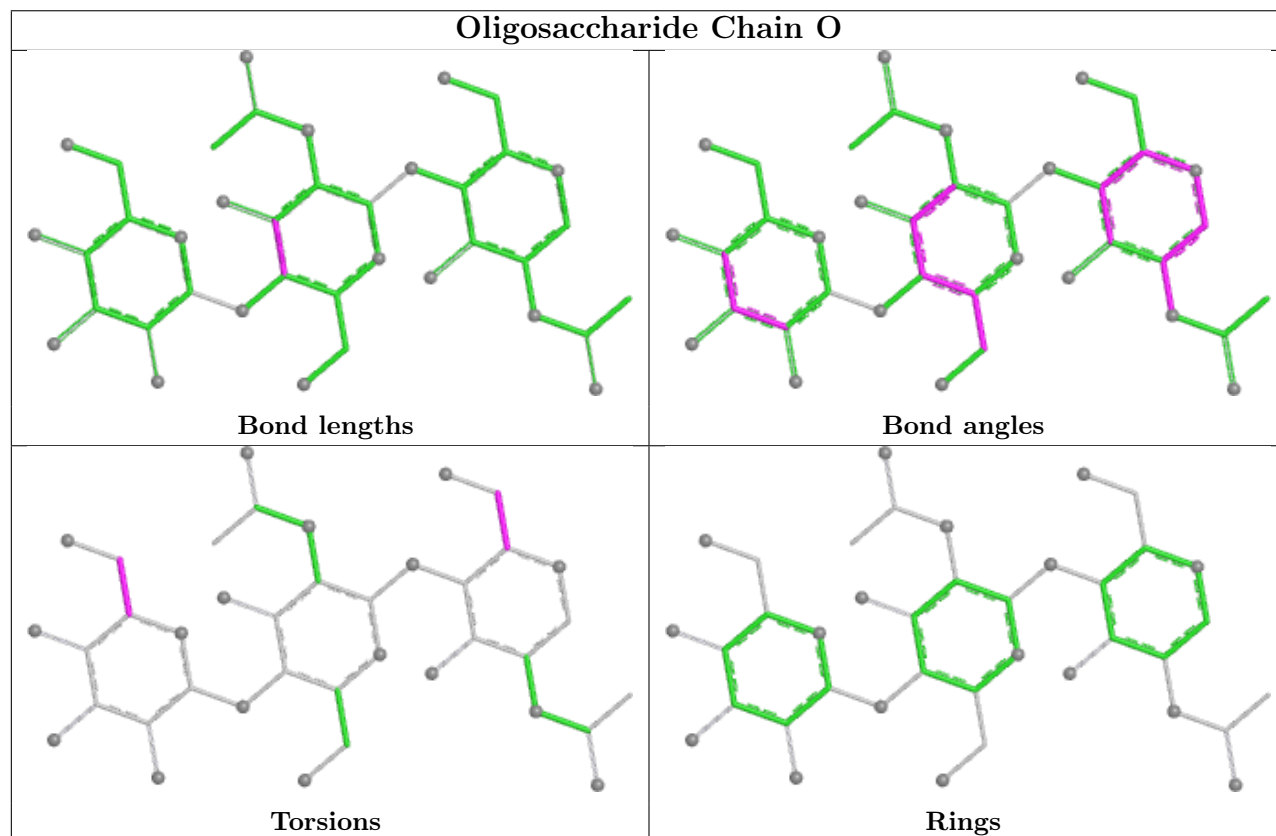
Oligosaccharide Chain I

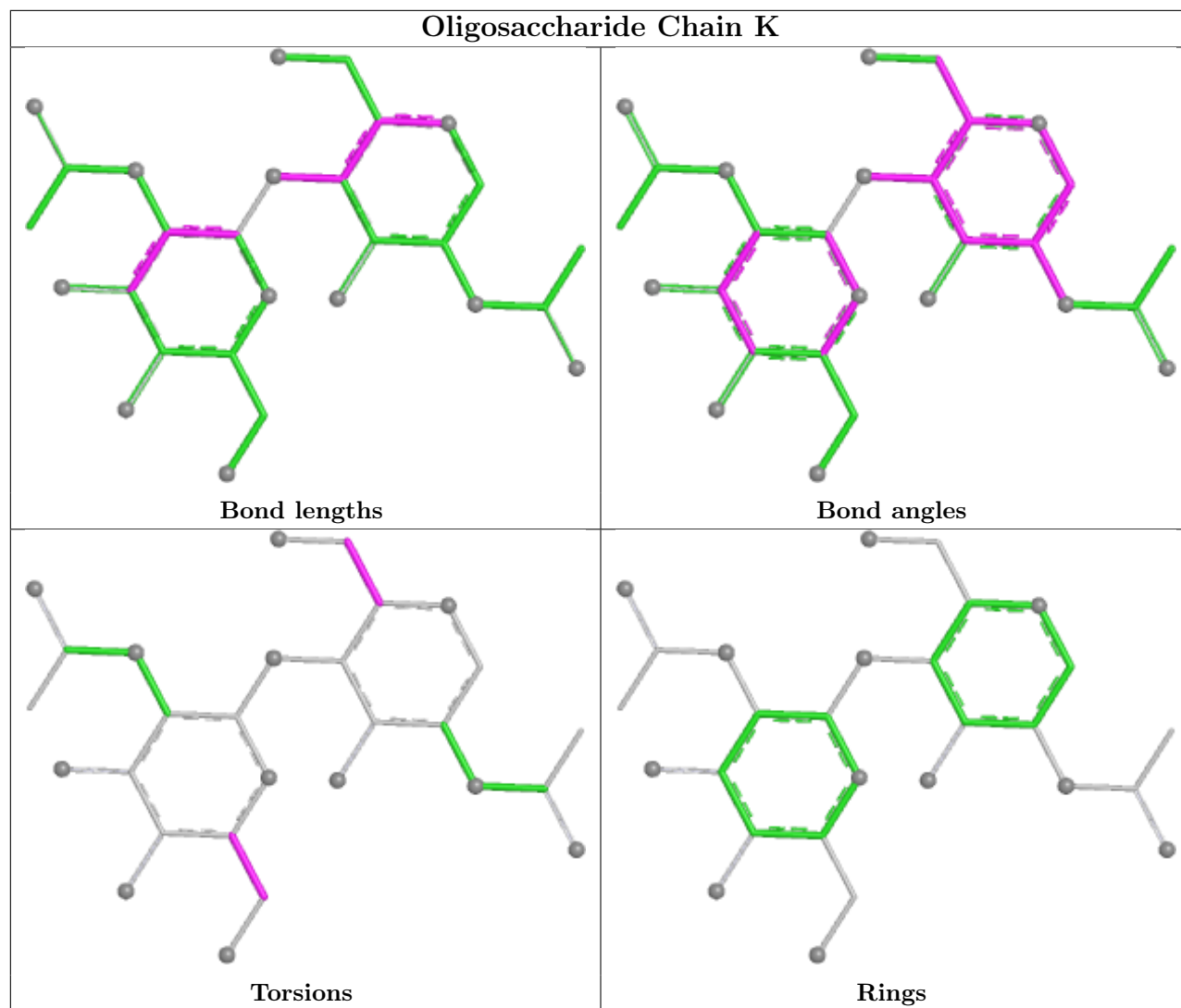


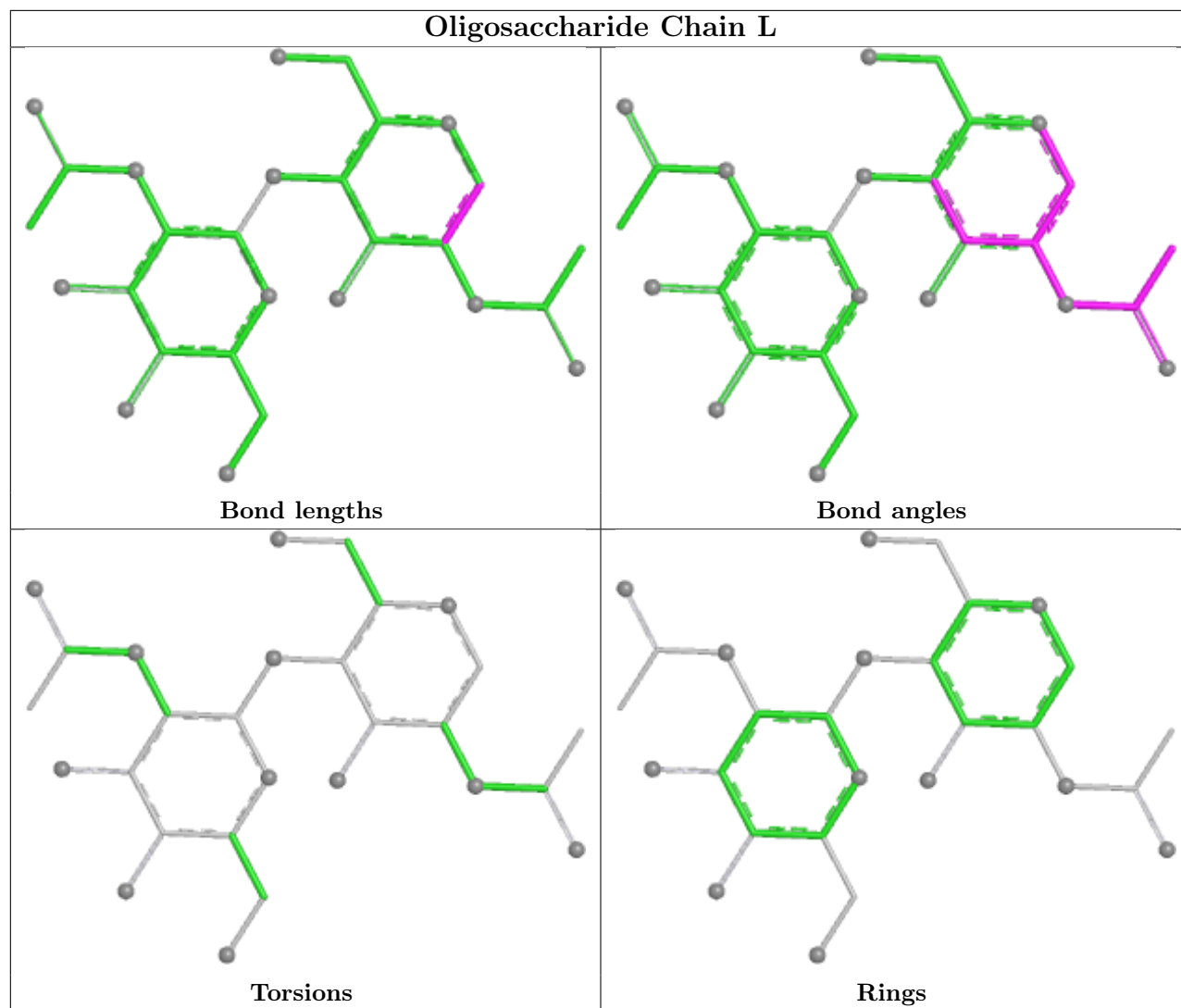
Oligosaccharide Chain J

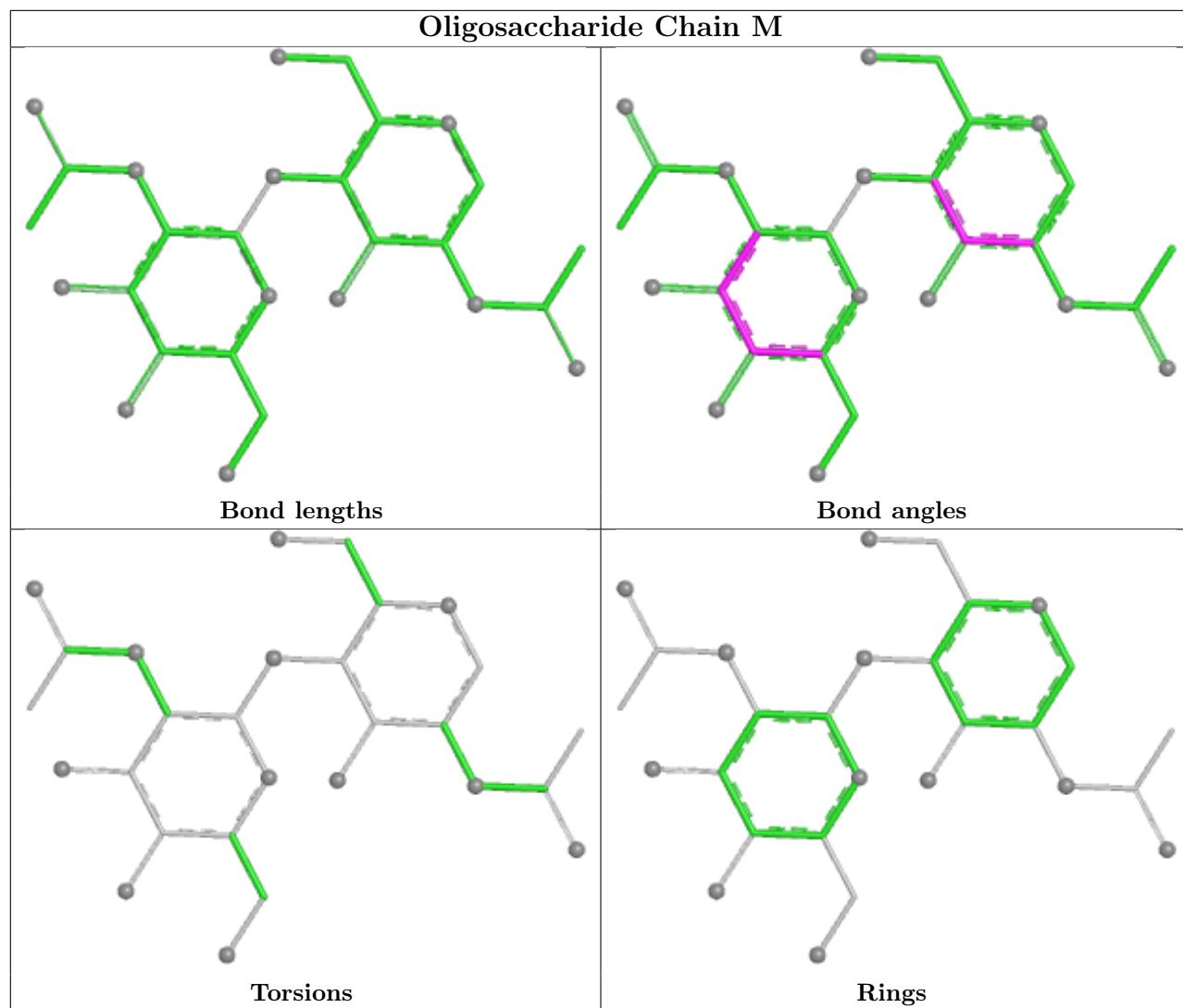


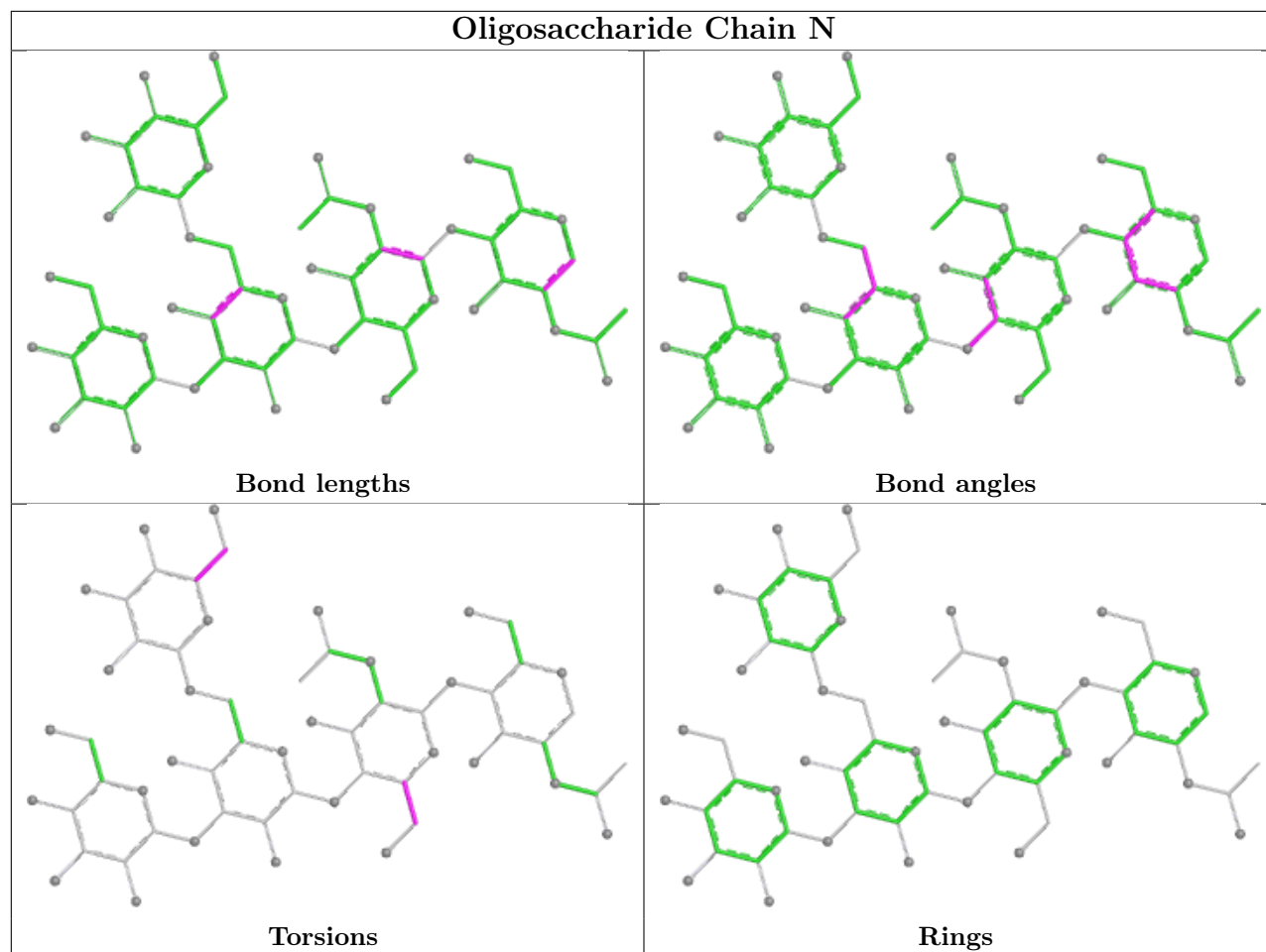
Oligosaccharide Chain O

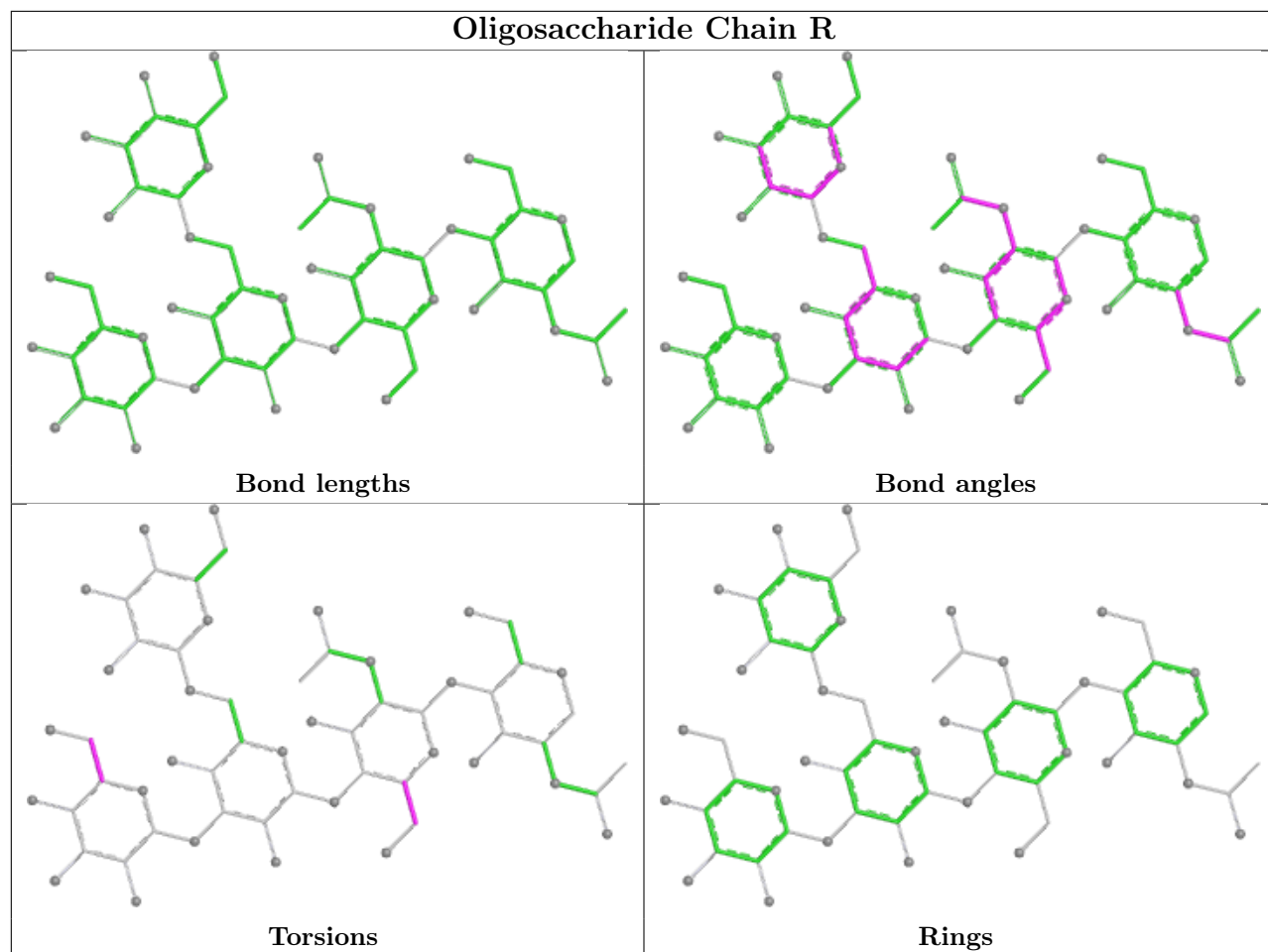


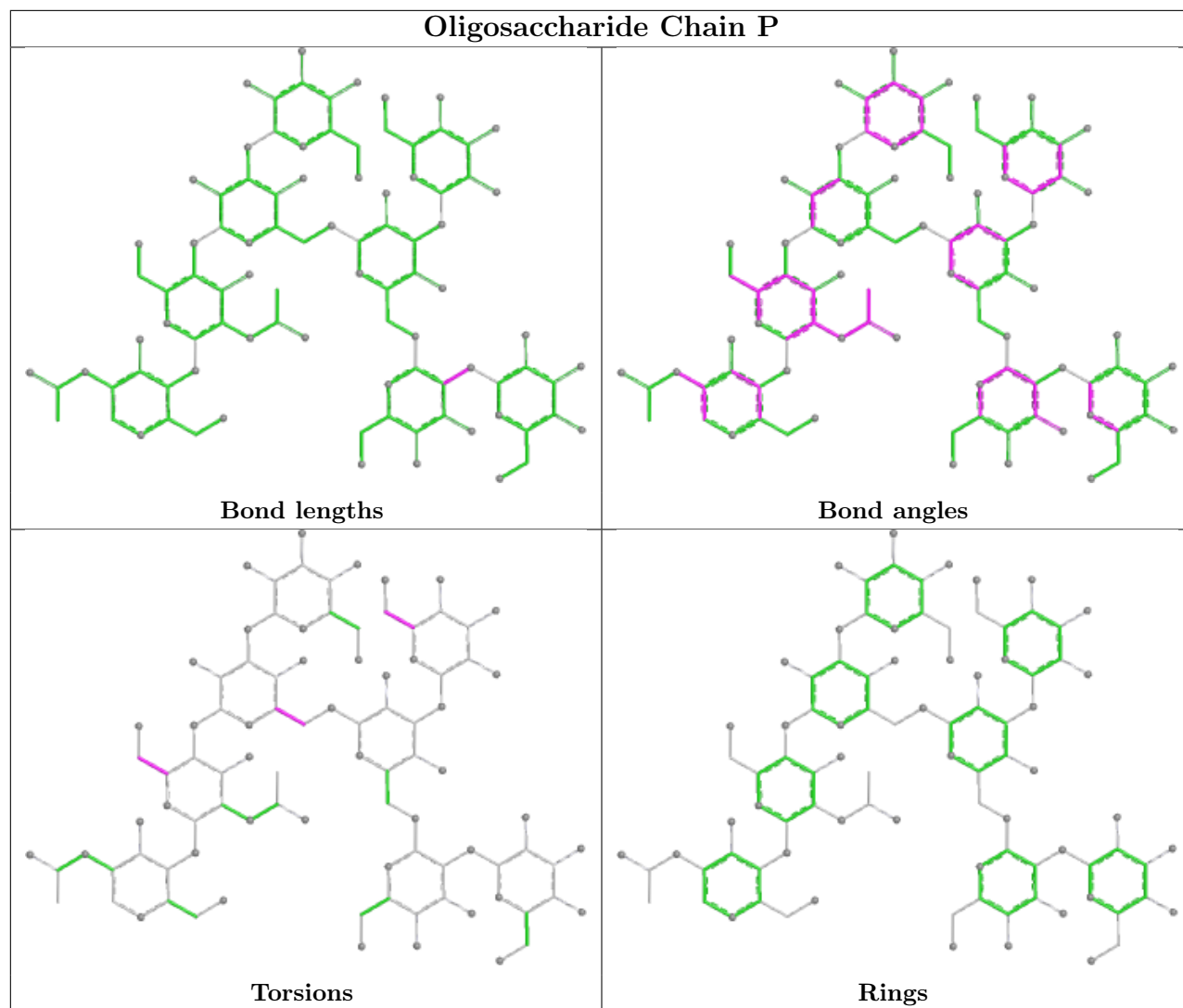


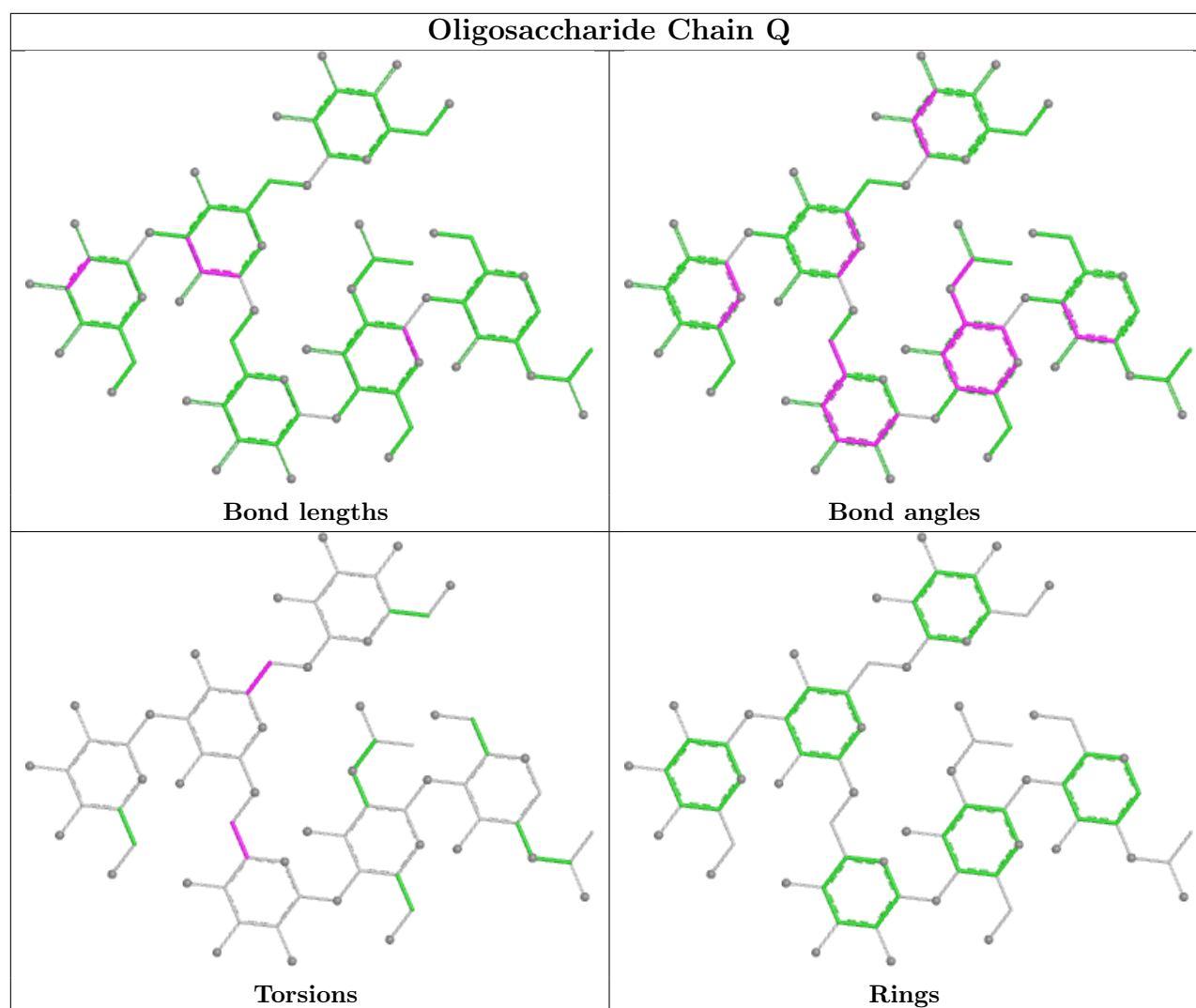












5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	126/126 (100%)	1.38	25 (19%) 3 1	47, 108, 157, 173	0
1	B	126/126 (100%)	0.71	10 (7%) 18 10	35, 70, 105, 122	0
1	C	126/126 (100%)	1.02	18 (14%) 6 3	46, 88, 144, 159	0
1	D	126/126 (100%)	0.68	7 (5%) 30 16	44, 71, 131, 145	0
1	E	126/126 (100%)	0.62	11 (8%) 16 9	34, 69, 120, 133	0
1	F	126/126 (100%)	0.36	1 (0%) 82 65	36, 64, 98, 111	0
All	All	756/756 (100%)	0.80	72 (9%) 14 7	34, 73, 141, 173	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ILE	6.3
1	A	126	VAL	6.1
1	A	68	ILE	4.7
1	A	122	ILE	4.5
1	A	83	TYR	4.4
1	C	126	VAL	4.0
1	C	125	LYS	3.6
1	A	123	CYS	3.5
1	A	98	TYR	3.4
1	A	78	PRO	3.3
1	A	76	ALA	3.2
1	A	125	LYS	3.2
1	A	77	VAL	3.2
1	C	72	LEU	3.2
1	A	91	PHE	3.1
1	B	94	ASN	3.1
1	A	82	THR	3.1
1	A	121	PRO	3.1
1	E	126	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	111	GLY	3.0
1	C	90	HIS	2.9
1	D	122	ILE	2.8
1	B	96	GLY	2.7
1	A	67	TYR	2.7
1	C	73	ASN	2.7
1	D	124	GLU	2.6
1	C	80	ASN	2.6
1	D	91	PHE	2.6
1	E	49	ASN	2.6
1	C	86	GLY	2.6
1	B	113	VAL	2.6
1	B	112	SER	2.5
1	A	64	THR	2.5
1	C	71	PRO	2.5
1	A	90	HIS	2.5
1	E	97	TYR	2.5
1	E	99	LEU	2.5
1	A	80	ASN	2.5
1	C	92	ILE	2.5
1	B	19	TYR	2.5
1	D	69	ARG	2.5
1	A	108	GLU	2.4
1	B	95	GLU	2.4
1	B	111	GLY	2.4
1	D	98	TYR	2.4
1	A	93	CYS	2.4
1	B	126	VAL	2.4
1	B	48	ARG	2.3
1	A	72	LEU	2.3
1	C	99	LEU	2.3
1	C	98	TYR	2.3
1	A	71	PRO	2.3
1	C	74	GLY	2.3
1	A	81	GLY	2.3
1	C	96	GLY	2.3
1	F	124	GLU	2.2
1	A	88	GLN	2.2
1	E	73	ASN	2.2
1	C	69	ARG	2.2
1	C	108	GLU	2.2
1	E	123	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	67	TYR	2.1
1	C	105	LEU	2.1
1	E	72	LEU	2.1
1	D	71	PRO	2.1
1	E	76	ALA	2.1
1	E	91	PHE	2.1
1	B	1	CYS	2.1
1	E	89	MET	2.1
1	A	38	PRO	2.1
1	C	106	TYR	2.0
1	D	75	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	G	4	11/12	-0.04	0.20	145,152,156,156	0
2	MAN	G	5	11/12	0.15	0.16	140,151,156,158	0
2	BMA	G	3	11/12	0.16	0.19	147,150,153,154	0
7	MAN	P	4	11/12	0.17	0.17	143,147,152,153	0
2	MAN	G	6	11/12	0.18	0.16	145,154,156,162	0
4	BMA	J	3	11/12	0.19	0.17	144,152,155,159	0
6	MAN	R	5	11/12	0.21	0.18	149,159,163,163	0
4	BMA	I	3	11/12	0.24	0.17	134,146,150,151	0
7	MAN	P	6	11/12	0.26	0.20	142,152,158,159	0
6	MAN	R	4	11/12	0.28	0.21	137,158,167,171	0
5	NAG	K	2	14/15	0.28	0.20	132,140,147,155	0
3	NAG	H	2	14/15	0.31	0.19	149,154,158,162	0
8	MAN	Q	5	11/12	0.31	0.15	112,121,130,133	0
6	BMA	R	3	11/12	0.32	0.15	137,148,155,158	0
4	NAG	I	2	14/15	0.33	0.18	132,136,144,147	0
4	BMA	O	3	11/12	0.33	0.18	125,147,150,152	0
2	NAG	G	2	14/15	0.33	0.18	144,148,152,154	0

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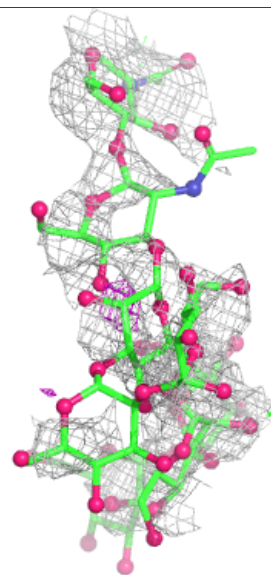
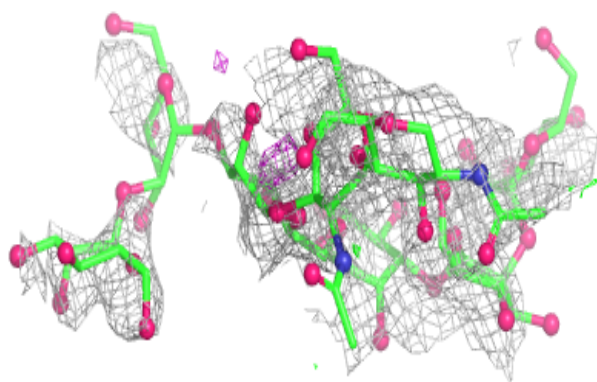
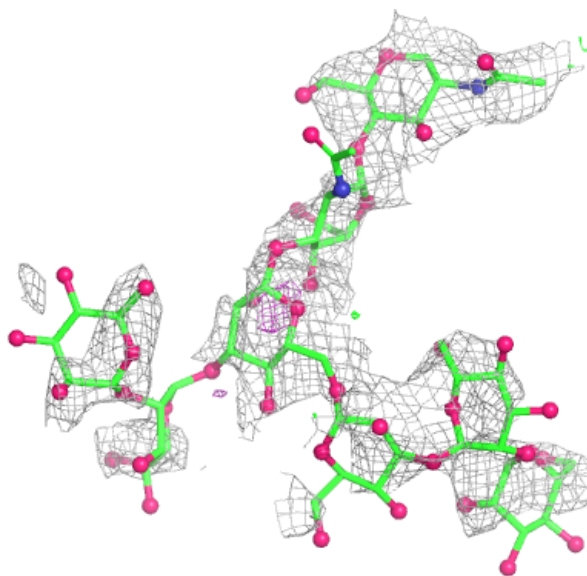
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	1	14/15	0.35	0.19	115,123,131,138	0
2	MAN	G	7	11/12	0.38	0.17	137,148,151,151	0
7	MAN	P	5	11/12	0.41	0.18	130,150,156,159	0
2	MAN	G	8	11/12	0.42	0.16	144,150,154,157	0
3	NAG	H	1	14/15	0.43	0.18	113,142,150,153	0
3	MAN	H	4	11/12	0.44	0.18	162,167,170,174	0
8	MAN	Q	6	11/12	0.44	0.22	159,163,168,169	0
6	MAN	N	5	11/12	0.46	0.16	131,144,153,155	0
6	MAN	N	4	11/12	0.47	0.16	123,137,140,143	0
7	MAN	P	7	11/12	0.48	0.18	136,153,156,158	0
4	NAG	I	1	14/15	0.48	0.18	100,112,123,126	0
5	NAG	L	2	14/15	0.48	0.19	138,141,147,151	0
4	NAG	J	2	14/15	0.52	0.15	106,122,131,143	0
8	BMA	Q	3	11/12	0.53	0.12	136,137,141,143	0
3	BMA	H	3	11/12	0.57	0.11	150,158,165,165	0
7	BMA	P	3	11/12	0.59	0.13	113,122,131,140	0
6	NAG	N	2	14/15	0.59	0.19	99,112,129,142	0
4	NAG	O	1	14/15	0.61	0.17	120,124,127,139	0
7	NAG	P	2	14/15	0.61	0.16	84,113,121,128	0
8	NAG	Q	2	14/15	0.64	0.12	107,111,120,127	0
8	MAN	Q	4	11/12	0.64	0.11	123,136,143,149	0
5	NAG	M	2	14/15	0.65	0.17	101,110,116,118	0
5	NAG	L	1	14/15	0.65	0.17	134,140,143,146	0
5	NAG	K	1	14/15	0.65	0.18	85,97,113,119	0
4	NAG	O	2	14/15	0.66	0.16	143,147,149,151	0
7	MAN	P	8	11/12	0.67	0.14	112,118,132,137	0
7	NAG	P	1	14/15	0.67	0.16	83,93,104,113	0
6	BMA	N	3	11/12	0.68	0.13	127,133,140,141	0
6	NAG	N	1	14/15	0.69	0.18	93,104,108,115	0
4	NAG	J	1	14/15	0.73	0.15	73,86,97,102	0
8	NAG	Q	1	14/15	0.76	0.15	72,81,94,104	0
6	NAG	R	2	14/15	0.80	0.15	92,105,122,126	0
5	NAG	M	1	14/15	0.88	0.12	49,65,87,87	0
6	NAG	R	1	14/15	0.90	0.10	46,64,79,80	0

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

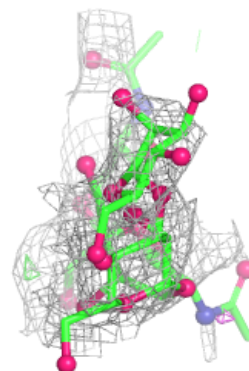
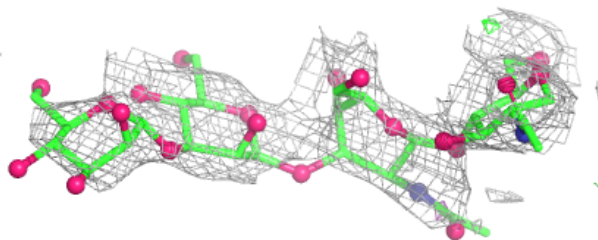
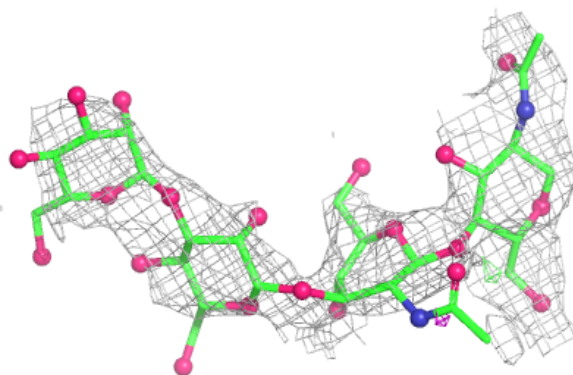
Electron density around Chain G:

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

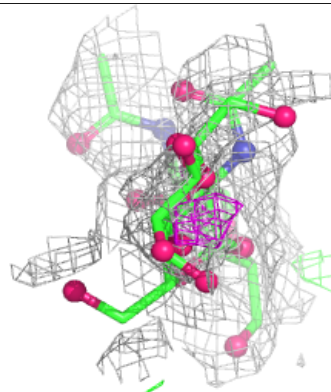
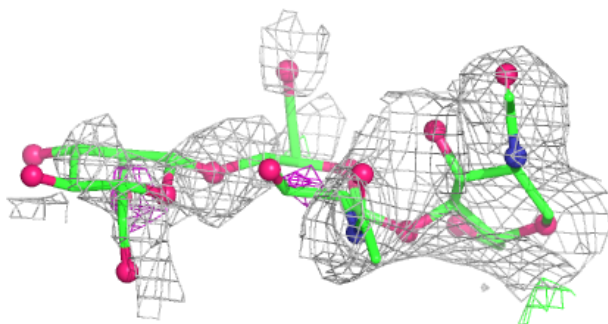
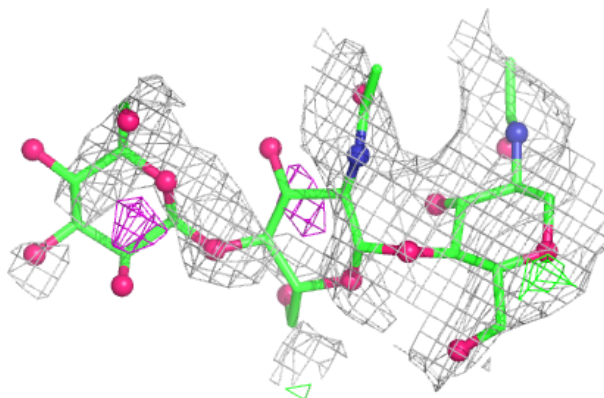


Electron density around Chain H:

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

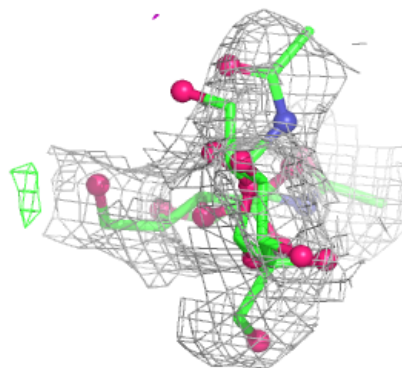
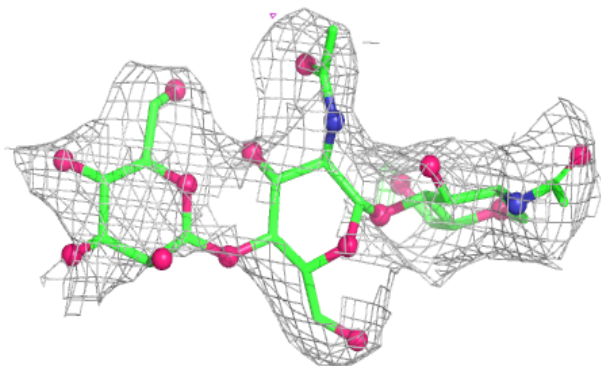
**Electron density around Chain I:**

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

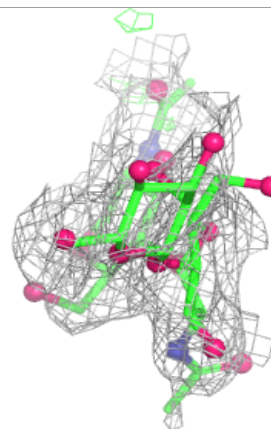
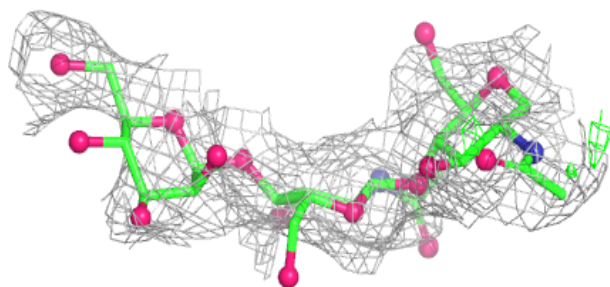
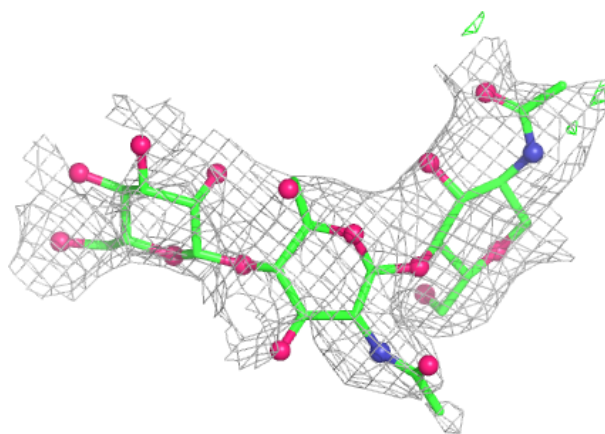


Electron density around Chain J:

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

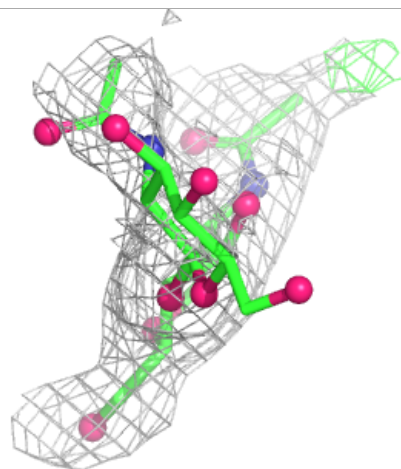
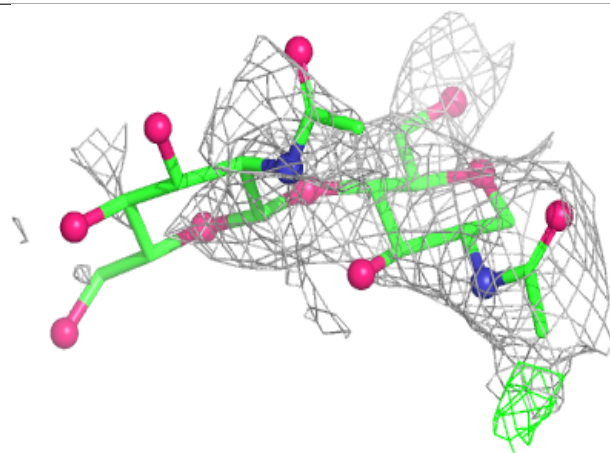
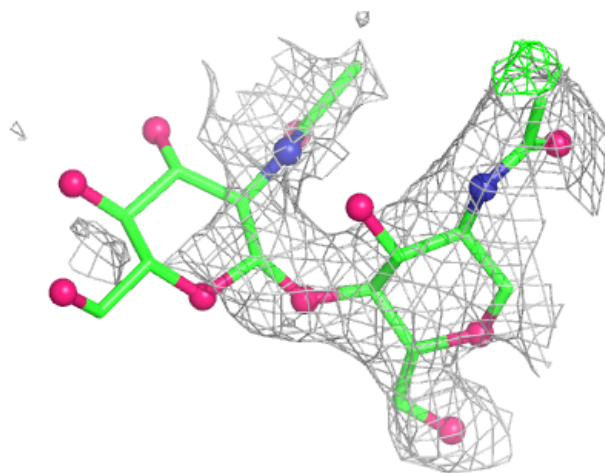
**Electron density around Chain O:**

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



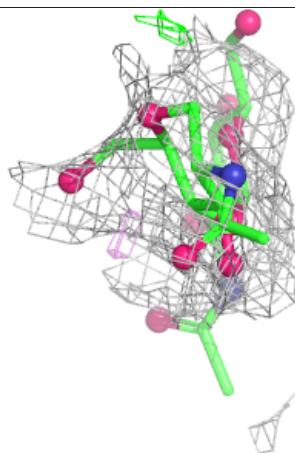
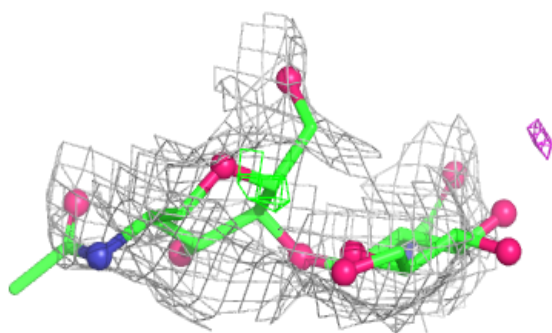
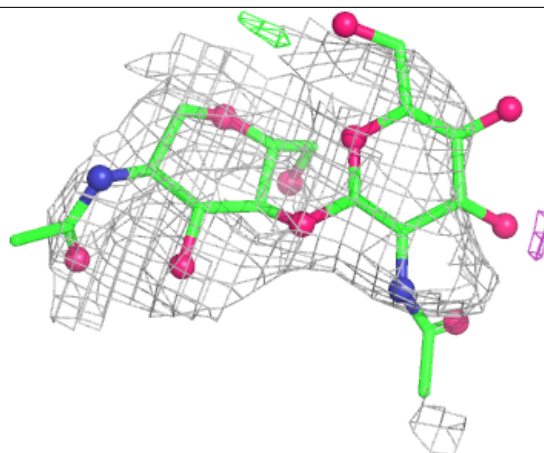
Electron density around Chain K:

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



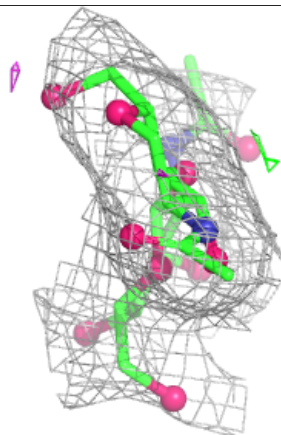
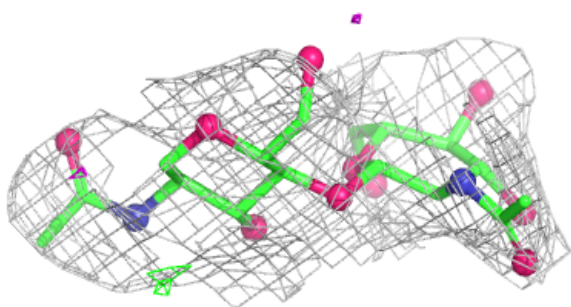
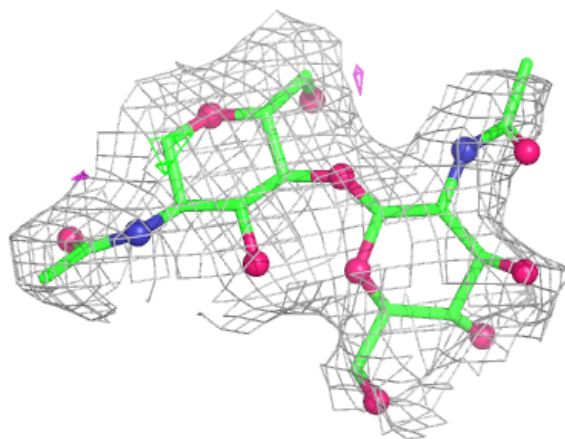
Electron density around Chain L:

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



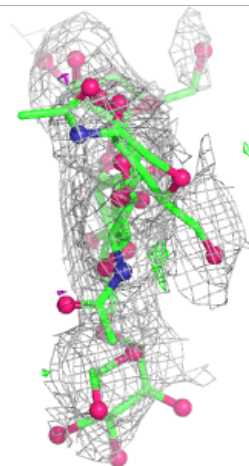
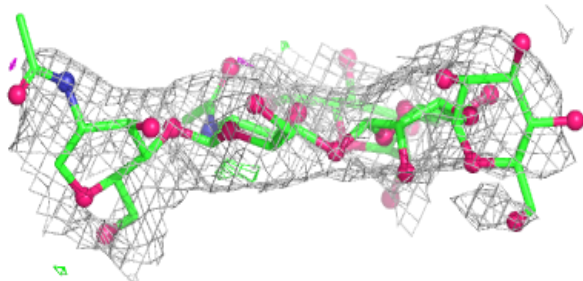
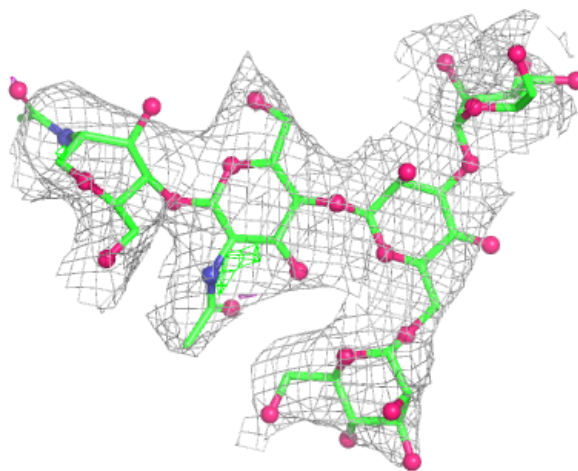
Electron density around Chain M:

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



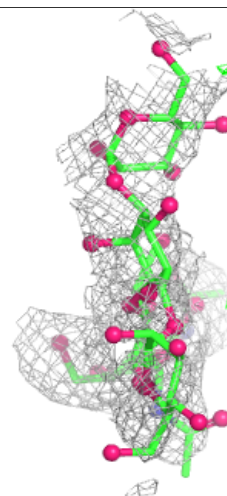
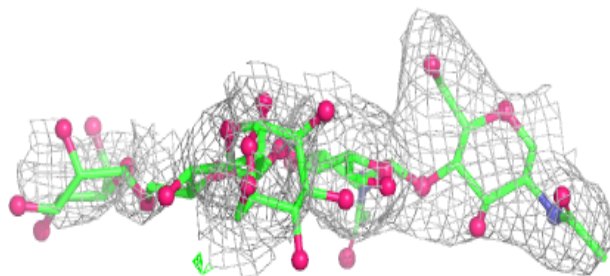
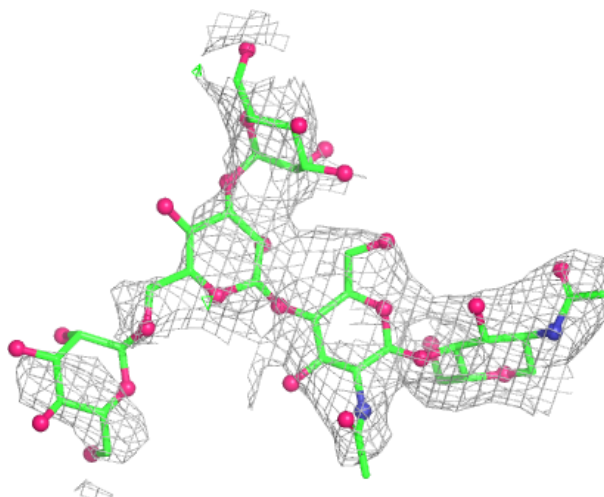
Electron density around Chain N:

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



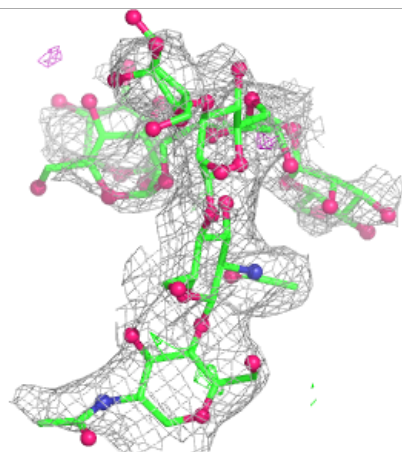
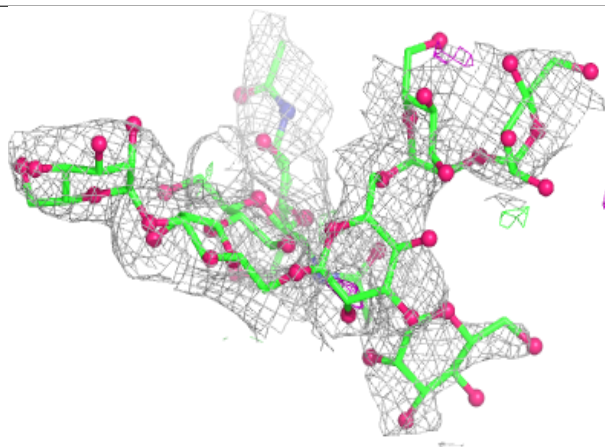
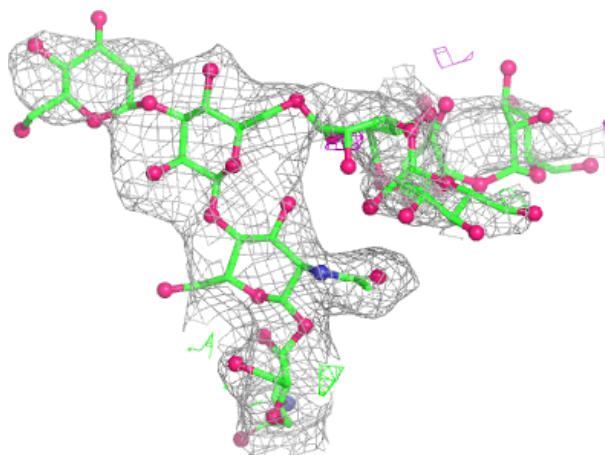
Electron density around Chain R:

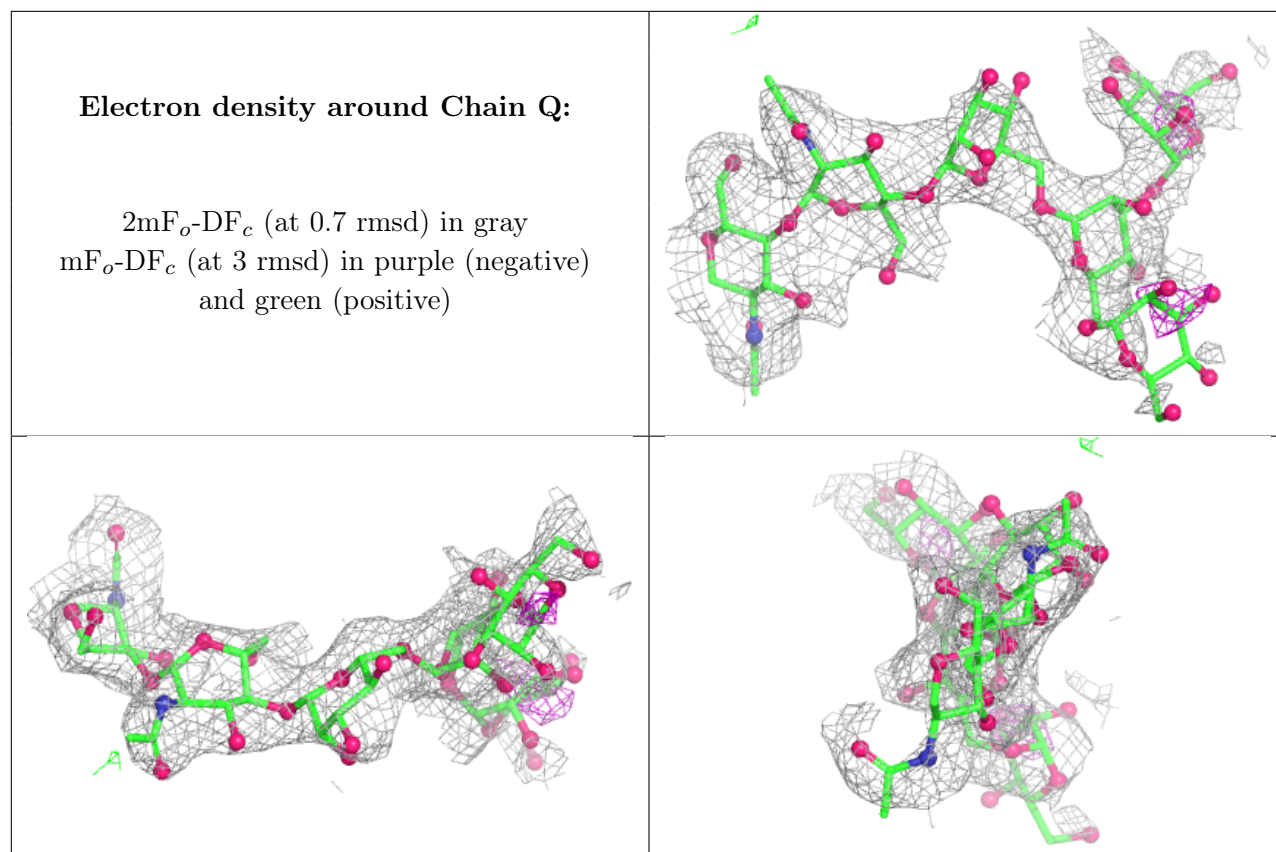
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
9	CA	C	3057	1/1	0.70	0.11	109,109,109,109	0
10	CL	D	4042	1/1	0.80	0.16	104,104,104,104	0
10	CL	A	1042	1/1	0.86	0.12	65,65,65,65	0
9	CA	A	1057	1/1	0.90	0.07	87,87,87,87	0
9	CA	D	4057	1/1	0.91	0.10	89,89,89,89	0
9	CA	F	6057	1/1	0.91	0.08	62,62,62,62	0
9	CA	E	5057	1/1	0.92	0.08	89,89,89,89	0
10	CL	E	5042	1/1	0.94	0.08	57,57,57,57	0
9	CA	B	2057	1/1	0.96	0.05	67,67,67,67	0
10	CL	B	2042	1/1	0.96	0.04	47,47,47,47	0
10	CL	F	6042	1/1	0.98	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.