



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:17 PM UTC

PDB ID : 5AWC / pdb_00005awc
Title : Crystal structure of human TLR8 in complex with MB-564
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2015-07-03
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:

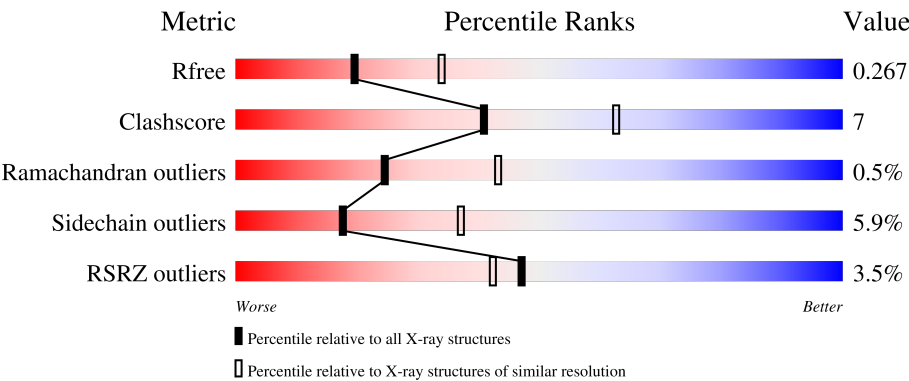
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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.



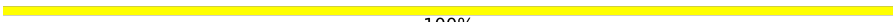
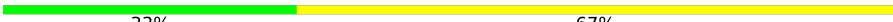
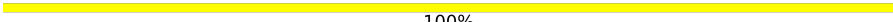
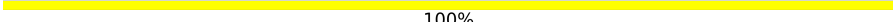
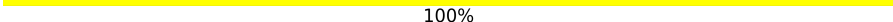
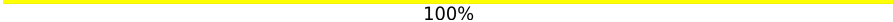
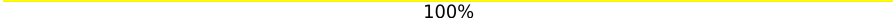
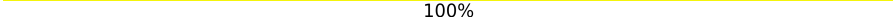
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	811	% 79%12%8%
1	B	811	2% 78%13%9%
1	C	811	2% 76%13%10%
1	D	811	8% 64%21%11%
2	E	3	33%67%

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24478 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			6035	3862	1023	1131	19			
1	B	742	Total	C	N	O	S	0	0	0
			5979	3828	1015	1117	19			
1	C	727	Total	C	N	O	S	0	0	0
			5871	3760	998	1094	19			
1	D	724	Total	C	N	O	S	0	0	0
			5836	3735	990	1092	19			

There are 40 discrepancies between the modelled and reference sequences:

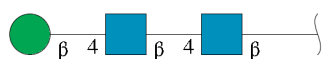
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97
C	23	ARG	-	expression tag	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP Q9NR97
C	832	PRO	-	expression tag	UNP Q9NR97
C	833	ARG	-	expression tag	UNP Q9NR97
D	23	ARG	-	expression tag	UNP Q9NR97
D	24	SER	-	expression tag	UNP Q9NR97
D	25	PRO	-	expression tag	UNP Q9NR97
D	26	TRP	-	expression tag	UNP Q9NR97
D	828	GLU	-	expression tag	UNP Q9NR97
D	829	PHE	-	expression tag	UNP Q9NR97
D	830	LEU	-	expression tag	UNP Q9NR97
D	831	VAL	-	expression tag	UNP Q9NR97
D	832	PRO	-	expression tag	UNP Q9NR97
D	833	ARG	-	expression tag	UNP Q9NR97

- 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.



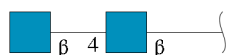
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3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

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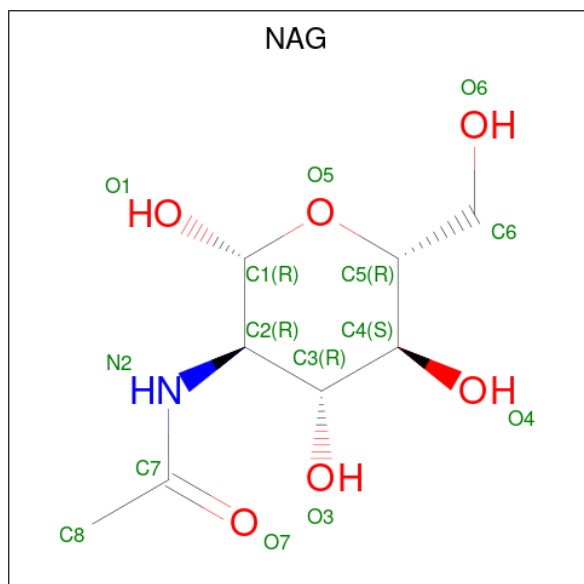
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	I	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			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



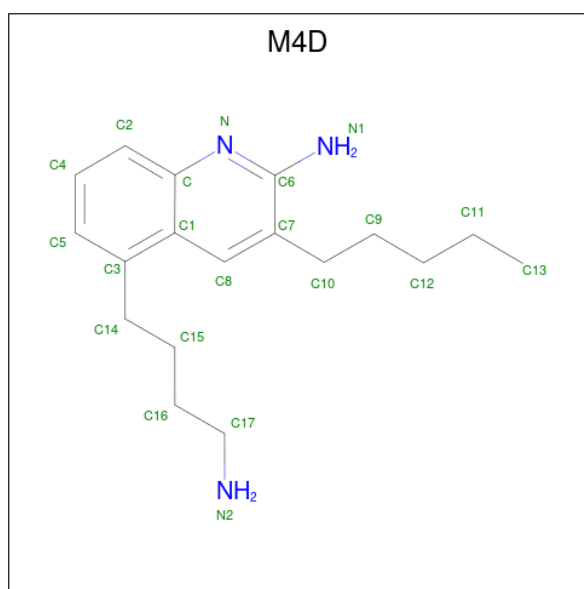
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 5-(4-azanylbutyl)-3-pentyl-quinolin-2-amine (CCD ID: M4D) (formula: $C_{18}H_{27}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			21	18	3		
5	B	1	Total	C	N	0	0
			21	18	3		
5	C	1	Total	C	N	0	0
			21	18	3		

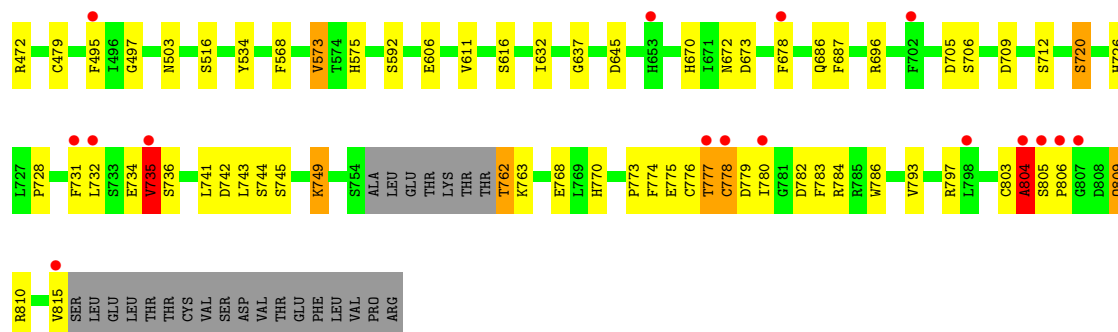
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	N	0	0
			21	18	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		
6	B	42	Total	O	0	0
			42	42		
6	C	21	Total	O	0	0
			21	21		
6	D	22	Total	O	0	0
			22	22		



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

Chain E: 33% 67%



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

Chain G: 100%



- 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: 33% 67%



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

Chain J: 100%



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

Chain K: 100%



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

Chain M:  100%

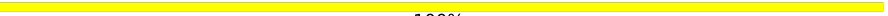
MAG1
MAG2
BMA3

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

Chain P:  100%

MAG1
MAG2
BMA3

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

Chain F:  100%

MAG1
MAG2

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

Chain I:  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:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40Å 140.18Å 169.60Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	47.48 – 2.50 47.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.48-2.50) 94.9 (47.48-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.269 0.212 , 0.267	Depositor DCC
R_{free} test set	6666 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24478	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: NAG, M4D, 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	0.85	4/6159 (0.1%)	0.95	5/8351 (0.1%)
1	B	0.79	0/6102	0.93	2/8272 (0.0%)
1	C	0.72	0/5992	0.90	6/8122 (0.1%)
1	D	0.77	1/5956 (0.0%)	0.97	21/8076 (0.3%)
All	All	0.78	5/24209 (0.0%)	0.94	34/32821 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	4
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	216	VAL	C-N	8.29	1.40	1.33
1	A	566	HIS	CG-ND1	-6.32	1.31	1.38
1	A	268	VAL	C-N	5.62	1.40	1.33
1	A	269	PRO	N-CD	5.16	1.54	1.47
1	A	421	GLU	CA-C	5.05	1.59	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	804	ALA	N-CA-C	-9.38	95.14	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	VAL	CA-C-N	-8.33	113.58	119.66
1	D	216	VAL	C-N-CA	-8.33	113.58	119.66
1	D	363	PHE	N-CA-C	-7.94	100.05	110.53
1	B	736	SER	N-CA-C	7.74	119.72	111.28
1	A	270	CYS	N-CA-C	-7.11	101.12	110.43
1	D	217	PRO	O-C-N	6.89	124.48	121.31
1	A	268	VAL	CA-C-N	-6.70	113.74	120.31
1	A	268	VAL	C-N-CA	-6.70	113.74	120.31
1	D	470	PHE	N-CA-C	-6.70	100.57	110.48
1	C	213	LEU	N-CA-C	-6.16	100.24	109.96
1	C	140	ILE	N-CA-C	-6.10	103.38	108.63
1	D	148	LEU	N-CA-C	6.03	119.21	110.28
1	D	220	LEU	CA-C-N	5.94	127.27	119.84
1	D	220	LEU	C-N-CA	5.94	127.27	119.84
1	A	735	VAL	CB-CA-C	5.71	120.66	111.29
1	C	59	GLN	N-CA-C	-5.68	106.95	112.97
1	D	144	LEU	CA-C-N	5.61	125.62	119.90
1	D	144	LEU	C-N-CA	5.61	125.62	119.90
1	A	268	VAL	CB-CA-C	-5.59	104.32	110.52
1	D	218	PRO	CA-N-CD	-5.54	104.24	112.00
1	C	257	CYS	CA-C-N	5.46	125.77	119.92
1	C	257	CYS	C-N-CA	5.46	125.77	119.92
1	D	809	GLN	N-CA-C	5.41	118.96	111.55
1	B	519	GLN	N-CA-C	5.37	118.38	110.59
1	D	777	THR	CA-C-N	5.30	131.25	121.70
1	D	777	THR	C-N-CA	5.30	131.25	121.70
1	D	687	PHE	CA-C-N	5.26	124.87	119.56
1	D	687	PHE	C-N-CA	5.26	124.87	119.56
1	C	284	GLN	N-CA-C	5.17	117.66	111.71
1	D	162	THR	N-CA-C	5.14	118.01	111.69
1	D	793	VAL	N-CA-C	5.11	113.96	106.55
1	D	217	PRO	CA-N-CD	-5.05	104.93	112.00
1	D	89	LEU	N-CA-C	5.00	117.05	108.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	779	ASP	Peptide
1	C	242	PHE	Peptide
1	D	161	ILE	Peptide
1	D	201	THR	Peptide

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Mol	Chain	Res	Type	Group
1	D	803	CYS	Peptide
1	D	804	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6035	0	6028	63	1
1	B	5979	0	5969	60	1
1	C	5871	0	5857	40	0
1	D	5836	0	5817	154	0
2	E	39	0	34	2	0
2	G	39	0	34	0	0
2	H	39	0	34	0	0
2	J	39	0	34	0	0
2	K	39	0	34	0	0
2	M	39	0	34	0	0
2	N	39	0	34	1	0
2	P	39	0	34	0	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
3	L	28	0	25	0	0
3	O	28	0	25	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	21	0	0	1	0
5	B	21	0	0	1	0
5	C	21	0	0	1	0
5	D	21	0	0	0	0
6	A	38	0	0	2	0
6	B	42	0	0	0	0
6	C	21	0	0	0	0
6	D	22	0	0	0	0
All	All	24478	0	24160	315	1

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 7.

All (315) 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:197:PHE:O	1:D:200:LEU:CD2	1.64	1.43
1:D:197:PHE:O	1:D:200:LEU:HD22	1.15	1.15
1:D:181:CYS:SG	1:D:187:CYS:CB	2.36	1.14
1:D:162:THR:HG1	1:D:164:GLU:HG2	1.01	1.09
1:D:177:LEU:O	1:D:208:LEU:HA	1.52	1.09
1:D:200:LEU:HD22	1:D:200:LEU:H	1.17	1.07
1:D:209:SER:OG	1:D:230:SER:N	1.89	1.04
1:D:162:THR:OG1	1:D:165:GLY:N	1.90	1.03
1:D:162:THR:CB	1:D:165:GLY:H	1.70	1.02
1:A:257:CYS:CB	1:A:270:CYS:SG	2.48	1.00
1:D:162:THR:OG1	1:D:164:GLU:HG2	1.64	0.98
1:D:162:THR:HG21	1:D:165:GLY:CA	1.93	0.97
1:D:257:CYS:O	1:D:298:SER:OG	1.85	0.94
1:B:734:GLU:OE2	1:B:736:SER:OG	1.85	0.94
1:D:137:LEU:O	1:D:157:ASN:O	1.89	0.91
1:A:735:VAL:HB	1:A:736:SER:HA	1.52	0.90
1:A:735:VAL:HG12	1:A:736:SER:C	1.99	0.87
1:A:735:VAL:HG13	1:A:738:LEU:CB	2.04	0.86
1:A:735:VAL:CB	1:A:736:SER:HA	2.05	0.86
1:B:731:PHE:O	1:B:735:VAL:CG2	2.24	0.84
1:D:197:PHE:O	1:D:200:LEU:HD23	1.75	0.84
1:D:197:PHE:HA	1:D:200:LEU:HD21	1.60	0.82
1:D:182:TYR:O	1:D:185:LYS:HB3	1.80	0.81
1:D:162:THR:HG1	1:D:164:GLU:CG	1.90	0.80
1:D:152:SER:OG	1:D:176:TYR:HB2	1.82	0.79
1:A:708:SER:OG	1:A:734:GLU:OE1	1.99	0.79
1:B:731:PHE:O	1:B:735:VAL:HG22	1.83	0.79
1:D:199:THR:OG1	1:D:200:LEU:HD13	1.82	0.78
1:D:197:PHE:C	1:D:200:LEU:CD2	2.56	0.78
1:D:162:THR:HG21	1:D:165:GLY:N	2.00	0.77
1:D:201:THR:OG1	1:D:202:ASN:N	2.14	0.76
1:D:162:THR:OG1	1:D:164:GLU:CG	2.33	0.74
1:D:207:SER:HB2	1:D:228:PHE:HB2	1.70	0.73
1:A:735:VAL:HG12	1:A:736:SER:CA	2.18	0.73
1:D:162:THR:CG2	1:D:165:GLY:N	2.51	0.73
1:D:193:GLU:OE2	1:D:193:GLU:HA	1.85	0.73
1:B:732:LEU:HD12	1:B:756:LEU:HD23	1.69	0.73
1:D:162:THR:CB	1:D:165:GLY:N	2.49	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:VAL:CG1	1:A:738:LEU:H	2.03	0.72
1:D:200:LEU:CD2	1:D:200:LEU:H	1.96	0.70
1:B:779:ASP:N	1:B:781:GLY:H	1.89	0.70
1:D:216:VAL:HG11	1:D:241:ASP:HB3	1.73	0.70
1:B:731:PHE:O	1:B:735:VAL:HG21	1.91	0.69
1:D:209:SER:HG	1:D:230:SER:H	1.37	0.68
1:B:734:GLU:O	1:B:735:VAL:HG22	1.92	0.68
1:A:735:VAL:HG13	1:A:738:LEU:HB3	1.74	0.67
1:B:779:ASP:CA	1:B:781:GLY:H	2.08	0.67
1:D:749:LYS:HA	1:D:773:PRO:O	1.94	0.67
1:D:364:SER:HA	1:D:393:LEU:HD21	1.77	0.66
1:D:162:THR:OG1	1:D:164:GLU:N	2.28	0.66
1:A:735:VAL:HG12	1:A:738:LEU:H	1.61	0.66
1:A:338:ARG:NH2	1:A:340:GLU:OE2	2.29	0.65
1:C:532:VAL:HB	1:C:553:LEU:HD22	1.78	0.65
1:D:181:CYS:SG	1:D:187:CYS:HB2	2.35	0.65
1:B:235:LYS:HD3	1:B:270:CYS:SG	2.37	0.64
1:D:197:PHE:CA	1:D:200:LEU:HD21	2.28	0.64
1:D:192:ILE:HD12	1:D:192:ILE:O	1.99	0.63
1:D:162:THR:OG1	1:D:164:GLU:CA	2.47	0.63
1:D:212:SER:O	1:D:213:LEU:HD23	1.99	0.63
1:C:77:HIS:CD2	1:C:115:ASN:HB3	2.34	0.62
1:D:200:LEU:HD22	1:D:200:LEU:N	2.01	0.62
1:D:158:ILE:CG2	1:D:160:ASN:HB2	2.29	0.62
1:A:735:VAL:CG1	1:A:738:LEU:N	2.63	0.62
1:D:259:ARG:NH1	1:D:321:ASN:O	2.33	0.62
1:A:576:HIS:HB3	1:A:578:GLU:OE1	1.99	0.61
1:D:79:THR:HA	1:D:120:ALA:HB1	1.82	0.61
1:D:162:THR:HG21	1:D:165:GLY:C	2.25	0.61
1:D:162:THR:HG21	1:D:165:GLY:HA3	1.78	0.61
1:D:606:GLU:HG2	1:D:637:GLY:HA3	1.83	0.61
1:B:779:ASP:HA	1:B:781:GLY:N	2.16	0.60
1:A:516:SER:OG	1:B:516:SER:OG	2.02	0.60
1:C:764:LEU:O	1:C:793:VAL:HG22	2.01	0.60
1:A:735:VAL:HG13	1:A:738:LEU:HB2	1.83	0.60
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.84	0.60
1:D:775:GLU:O	1:D:780:ILE:HG21	2.02	0.59
1:A:735:VAL:HG12	1:A:737:SER:N	2.17	0.59
1:D:368:SER:HA	1:D:395:ASN:HD22	1.68	0.59
1:D:361:ARG:O	1:D:363:PHE:O	2.20	0.59
1:A:467:PHE:HB3	2:E:1:NAG:H81	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:PHE:O	1:D:285:ASN:N	2.36	0.58
1:A:211:ASN:O	1:A:232:THR:HA	2.03	0.58
1:D:161:ILE:HG22	1:D:193:GLU:HB2	1.86	0.58
1:A:338:ARG:HD3	6:A:1132:HOH:O	2.03	0.57
1:D:158:ILE:HG22	1:D:160:ASN:HB2	1.86	0.57
1:D:51:ASN:ND2	1:D:51:ASN:O	2.35	0.57
1:A:283:PHE:HA	1:A:286:LEU:HD22	1.85	0.57
1:A:706:SER:HB3	1:A:709:ASP:OD2	2.05	0.57
1:D:208:LEU:O	1:D:211:ASN:ND2	2.35	0.57
1:C:47:ALA:HB3	1:C:68:LEU:HD12	1.87	0.57
1:D:161:ILE:CG2	1:D:193:GLU:H	2.17	0.57
1:D:176:TYR:CE2	1:D:205:LEU:HD21	2.40	0.57
1:D:357:ILE:HG13	1:D:377:TYR:CZ	2.40	0.56
1:A:496:ILE:N	1:A:519:GLN:OE1	2.36	0.56
1:B:732:LEU:O	1:B:735:VAL:HG23	2.04	0.56
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.24	0.56
1:A:735:VAL:CG1	1:A:736:SER:HA	2.34	0.56
1:D:161:ILE:HG21	1:D:193:GLU:H	1.71	0.56
1:D:573:VAL:O	1:D:575:HIS:CE1	2.58	0.55
1:A:545:ASP:CG	1:A:545:ASP:O	2.47	0.55
1:D:77:HIS:HB3	1:D:115:ASN:HB3	1.89	0.55
1:D:162:THR:HG21	1:D:166:ILE:N	2.22	0.55
1:C:764:LEU:HD23	1:C:793:VAL:HG13	1.89	0.55
1:D:34:TYR:O	1:D:60:THR:O	2.25	0.55
1:B:732:LEU:HB2	1:B:755:ALA:O	2.07	0.54
1:C:670:HIS:HA	1:C:694:ASP:HB3	1.88	0.54
1:A:257:CYS:CA	1:A:270:CYS:SG	2.95	0.54
1:A:735:VAL:CG1	1:A:736:SER:CA	2.85	0.54
1:C:278:ILE:HB	1:C:306:TRP:CZ2	2.43	0.54
1:C:516:SER:OG	1:D:516:SER:OG	2.12	0.53
1:D:195:GLY:HA3	1:D:219:LYS:HG3	1.89	0.53
1:D:202:ASN:N	1:D:223:SER:OG	2.41	0.53
1:D:212:SER:C	1:D:213:LEU:HD23	2.33	0.53
1:C:250:LEU:C	1:C:250:LEU:HD23	2.34	0.53
1:D:735:VAL:HG13	1:D:736:SER:N	2.22	0.53
1:B:296:SER:HA	1:B:320:PHE:O	2.10	0.52
1:C:557:GLU:OE1	1:C:587:LYS:HE2	2.10	0.52
1:D:249:THR:O	1:D:290:ARG:N	2.28	0.52
1:B:160:ASN:N	1:B:160:ASN:HD22	2.06	0.52
1:B:310:MET:O	1:B:310:MET:HG2	2.10	0.52
1:A:764:LEU:O	1:A:793:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ASP:OD1	1:B:706:SER:OG	2.28	0.52
1:C:317:ASP:OD1	1:C:319:GLU:OE1	2.28	0.52
1:D:163:LYS:HG3	1:D:196:VAL:HG23	1.92	0.52
1:D:741:LEU:HD21	1:D:743:LEU:HD11	1.92	0.51
1:D:259:ARG:NH2	1:D:348:TYR:O	2.30	0.51
1:A:735:VAL:CB	1:A:736:SER:CA	2.84	0.51
1:B:779:ASP:H	1:B:781:GLY:H	1.55	0.51
1:D:192:ILE:HD12	1:D:192:ILE:C	2.36	0.51
1:D:466:ASN:OD1	1:D:467:PHE:N	2.43	0.51
1:A:744:SER:O	1:A:745:SER:C	2.53	0.51
1:C:717:LEU:HD21	1:C:719:LEU:HD11	1.92	0.51
1:D:195:GLY:HA2	1:D:219:LYS:HB2	1.93	0.51
1:D:720:SER:HB3	1:D:744:SER:OG	2.11	0.51
1:B:779:ASP:HA	1:B:781:GLY:H	1.74	0.51
1:C:205:LEU:C	1:C:205:LEU:HD23	2.36	0.51
1:C:620:LEU:HD11	1:C:646:LEU:HD22	1.92	0.51
1:C:619:ARG:NH2	1:C:621:ASP:OD2	2.39	0.50
1:D:200:LEU:O	1:D:202:ASN:HB2	2.11	0.50
1:B:592:SER:HA	1:B:616:SER:O	2.11	0.50
1:A:735:VAL:HG13	1:A:738:LEU:H	1.77	0.50
1:D:36:CYS:HA	1:D:48:GLU:O	2.12	0.50
1:C:628:ASP:OD2	1:C:630:ARG:NH2	2.45	0.49
1:D:275:SER:HA	1:D:298:SER:HB2	1.94	0.49
1:C:388:GLN:N	1:C:389:PRO:CD	2.75	0.49
1:C:565:SER:O	1:C:566:HIS:C	2.55	0.49
1:D:156:ASN:O	1:D:180:ASN:OD1	2.30	0.49
1:D:235:LYS:HD2	1:D:270:CYS:SG	2.52	0.49
1:D:216:VAL:HB	1:D:241:ASP:OD1	2.13	0.49
1:A:52:ARG:HB3	1:A:54:LEU:HG	1.95	0.49
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.94	0.49
1:C:781:GLY:HA2	1:C:784:ARG:HB2	1.95	0.48
1:D:34:TYR:CD1	1:D:35:PRO:HA	2.48	0.48
1:B:756:LEU:HD13	1:B:786:TRP:HB2	1.95	0.48
1:B:804:ALA:HA	1:B:810:ARG:NH1	2.27	0.48
1:D:201:THR:HA	1:D:221:PRO:HB3	1.94	0.48
1:C:234:ILE:O	1:C:256:ASN:HB3	2.14	0.48
1:A:735:VAL:HG13	1:A:738:LEU:N	2.28	0.48
1:D:774:PHE:O	1:D:804:ALA:C	2.57	0.48
1:D:784:ARG:NH1	1:D:815:VAL:O	2.46	0.48
1:D:182:TYR:N	1:D:182:TYR:CD1	2.81	0.47
1:D:162:THR:OG1	1:D:164:GLU:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:SER:O	1:B:549:ALA:C	2.56	0.47
1:D:79:THR:HA	1:D:120:ALA:CB	2.42	0.47
1:D:249:THR:C	1:D:289:LEU:HD12	2.39	0.47
1:C:742:ASP:HA	1:C:768:GLU:HB2	1.96	0.47
1:D:357:ILE:HG13	1:D:377:TYR:CE1	2.49	0.47
1:B:205:LEU:C	1:B:205:LEU:HD23	2.38	0.47
1:B:211:ASN:O	1:B:232:THR:HA	2.14	0.47
1:D:160:ASN:C	1:D:161:ILE:HD13	2.39	0.47
1:D:185:LYS:O	1:D:187:CYS:SG	2.73	0.47
1:D:568:PHE:HA	1:D:575:HIS:CD2	2.49	0.47
1:D:216:VAL:HG21	1:D:241:ASP:CG	2.40	0.47
1:B:119:GLY:O	1:B:120:ALA:C	2.58	0.46
1:B:616:SER:HA	1:B:647:SER:O	2.14	0.46
1:D:201:THR:O	1:D:203:LEU:HB2	2.16	0.46
1:D:777:THR:OG1	1:D:778:CYS:HA	2.15	0.46
1:D:696:ARG:HG2	1:D:720:SER:OG	2.15	0.46
1:B:720:SER:HA	1:B:744:SER:O	2.16	0.46
1:D:289:LEU:HD23	1:D:310:MET:SD	2.55	0.46
1:A:536:ASP:OD1	1:A:538:THR:HG23	2.16	0.46
1:B:287:THR:HA	1:B:309:ASN:O	2.15	0.46
1:B:428:ASN:C	1:B:491:ASN:OD1	2.58	0.46
1:D:177:LEU:HB2	1:D:208:LEU:HD23	1.98	0.46
1:B:487:ASP:OD1	1:B:489:SER:OG	2.32	0.46
1:B:779:ASP:CA	1:B:781:GLY:N	2.73	0.46
1:D:728:PRO:O	1:D:731:PHE:HB2	2.15	0.46
1:C:692:LEU:HD23	1:C:693:LEU:N	2.31	0.45
1:D:762:THR:OG1	1:D:763:LYS:N	2.49	0.45
1:A:275:SER:OG	1:A:276:ILE:O	2.33	0.45
1:B:223:SER:O	1:B:225:ARG:NH1	2.50	0.45
1:B:734:GLU:C	1:B:735:VAL:CG2	2.89	0.45
1:D:363:PHE:O	1:D:364:SER:CB	2.64	0.45
1:B:388:GLN:N	1:B:389:PRO:CD	2.80	0.45
1:A:786:TRP:NE1	1:A:790:HIS:CE1	2.85	0.45
1:B:732:LEU:HD12	1:B:756:LEU:CD2	2.42	0.45
1:D:302:ILE:N	1:D:326:GLU:OE2	2.42	0.45
1:B:732:LEU:O	1:B:762:THR:HG22	2.17	0.45
1:D:135:ASN:HB2	1:D:137:LEU:HG	1.98	0.45
1:D:202:ASN:HD22	1:D:202:ASN:HA	1.60	0.45
1:D:183:PHE:CZ	1:D:265:PHE:HB2	2.51	0.45
1:D:67:GLU:HG2	1:D:91:LYS:HB2	1.99	0.45
1:D:215:HIS:N	1:D:215:HIS:CD2	2.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:HA	1:B:395:ASN:O	2.18	0.44
1:A:84:GLN:HG2	1:A:85:GLY:H	1.83	0.44
1:C:311:PRO:O	1:C:338:ARG:HD2	2.17	0.44
1:C:415:GLN:C	1:C:417:PHE:H	2.25	0.44
1:C:58:PRO:C	1:C:60:THR:H	2.25	0.44
1:C:586:LEU:O	1:C:610:LEU:HA	2.18	0.44
1:D:197:PHE:CA	1:D:200:LEU:CD2	2.92	0.44
1:B:278:ILE:HB	1:B:306:TRP:CZ2	2.52	0.44
1:D:162:THR:CG2	1:D:165:GLY:CA	2.79	0.44
1:A:257:CYS:HA	1:A:270:CYS:SG	2.58	0.44
1:B:183:PHE:HB3	1:B:266:PRO:HG2	2.00	0.44
1:D:205:LEU:HA	1:D:226:LYS:O	2.17	0.44
1:D:645:ASP:HA	1:D:670:HIS:HB2	2.00	0.44
1:D:197:PHE:C	1:D:200:LEU:HD21	2.39	0.44
1:B:600:THR:O	1:B:602:LYS:N	2.47	0.44
1:A:584:THR:O	1:A:609:SER:HB3	2.18	0.43
1:D:97:ASN:HA	1:D:98:PRO:HA	1.85	0.43
1:A:166:ILE:CG2	1:A:200:LEU:HD11	2.48	0.43
1:A:805:SER:HB2	1:A:806:PRO:HA	2.00	0.43
1:B:734:GLU:C	1:B:735:VAL:HG22	2.43	0.43
1:C:384:GLU:HA	1:C:413:LEU:HB3	2.01	0.43
1:D:466:ASN:OD1	1:D:466:ASN:C	2.60	0.43
1:D:672:ASN:O	1:D:673:ASP:C	2.61	0.43
1:D:705:ASP:N	1:D:705:ASP:OD1	2.51	0.43
1:D:749:LYS:H	1:D:749:LYS:HD2	1.83	0.43
1:B:31:SER:HA	1:B:791:LEU:HD13	2.01	0.43
1:B:235:LYS:CD	1:B:270:CYS:SG	3.05	0.43
1:D:57:VAL:HG23	1:D:78:ILE:HD12	2.00	0.43
1:D:90:THR:HG22	1:D:126:ASN:O	2.18	0.43
1:D:203:LEU:O	1:D:224:LEU:HA	2.18	0.43
1:D:326:GLU:O	1:D:327:ILE:C	2.61	0.43
1:C:620:LEU:HA	1:C:623:LEU:HD12	1.99	0.43
1:B:552:GLU:OE1	1:B:552:GLU:N	2.42	0.43
1:B:685:GLN:HG3	1:B:710:PHE:HA	1.99	0.43
1:C:303:ASN:HB3	1:C:306:TRP:CE2	2.53	0.43
1:C:543:ASP:OD2	5:C:1011:M4D:N	2.51	0.43
1:A:375:ARG:HA	1:A:402:GLY:O	2.19	0.43
1:B:732:LEU:HA	1:B:735:VAL:HG21	2.01	0.43
1:D:495:PHE:CE2	1:D:497:GLY:HA2	2.53	0.43
1:D:412:LYS:HA	1:D:503:ASN:O	2.19	0.43
1:A:336:LEU:N	1:A:337:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HD13	1:B:302:ILE:CD1	2.49	0.43
1:C:512:LEU:HB2	1:C:537:LEU:HD23	2.01	0.43
1:D:156:ASN:O	1:D:180:ASN:HA	2.19	0.43
1:D:177:LEU:O	1:D:208:LEU:CA	2.44	0.43
1:A:523:GLY:O	1:A:552:GLU:HB3	2.19	0.42
1:C:705:ASP:HA	1:C:728:PRO:HB3	2.00	0.42
1:C:805:SER:HB2	1:C:806:PRO:HA	2.01	0.42
1:D:806:PRO:HG2	1:D:809:GLN:H	1.84	0.42
1:C:663:PRO:O	1:C:666:LEU:HG	2.20	0.42
1:D:71:SER:OG	1:D:93:ASN:OD1	2.33	0.42
1:A:616:SER:HA	1:A:647:SER:O	2.19	0.42
1:A:695:LEU:HD12	1:A:719:LEU:HD21	2.01	0.42
1:D:770:HIS:CD2	1:D:797:ARG:HH11	2.37	0.42
1:D:742:ASP:HA	1:D:768:GLU:HB2	2.01	0.42
1:A:333:LEU:HD22	1:A:366:LEU:HD11	2.02	0.42
1:B:59:GLN:HG3	1:B:60:THR:HG23	2.01	0.42
1:D:326:GLU:O	1:D:329:SER:N	2.52	0.42
1:D:185:LYS:CG	1:D:187:CYS:SG	3.07	0.42
1:A:485:ALA:HA	1:A:509:CYS:O	2.20	0.42
1:D:353:TYR:CZ	1:D:380:GLN:HG2	2.55	0.42
1:B:238:SER:N	1:B:241:ASP:OD2	2.47	0.42
1:D:36:CYS:N	1:D:49:CYS:SG	2.92	0.42
1:A:650:ARG:HA	1:A:675:MET:HE3	2.02	0.42
1:D:160:ASN:O	1:D:161:ILE:HD13	2.20	0.42
1:D:245:LEU:O	1:D:247:ASN:N	2.53	0.42
1:A:378:VAL:HG11	5:B:901:M4D:C14	2.50	0.41
1:A:543:ASP:OD2	5:A:1012:M4D:N	2.53	0.41
1:B:431:SER:HB2	1:B:432:PRO:CD	2.50	0.41
1:A:372:LEU:HD21	1:A:374:LEU:HD11	2.02	0.41
1:A:708:SER:CB	1:A:734:GLU:OE1	2.67	0.41
1:D:211:ASN:O	1:D:232:THR:HA	2.20	0.41
1:A:160:ASN:ND2	6:A:1108:HOH:O	2.53	0.41
1:B:471:THR:HG22	1:B:471:THR:O	2.20	0.41
1:C:32:ARG:NH2	1:C:790:HIS:O	2.54	0.41
1:A:402:GLY:HA2	1:A:426:SER:O	2.20	0.41
1:A:735:VAL:HG13	1:A:738:LEU:CA	2.49	0.41
1:D:189:LYS:O	1:D:190:THR:O	2.39	0.41
1:D:706:SER:HB3	1:D:709:ASP:OD2	2.20	0.41
1:A:336:LEU:N	1:A:337:PRO:HD3	2.36	0.41
1:A:741:LEU:HD21	1:A:743:LEU:HD11	2.02	0.41
1:C:672:ASN:O	1:C:673:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:CYS:SG	1:D:534:TYR:HB3	2.60	0.41
1:B:731:PHE:C	1:B:735:VAL:HG22	2.43	0.41
1:D:176:TYR:CE2	1:D:205:LEU:CD2	3.03	0.41
1:D:467:PHE:HB3	2:N:1:NAG:H81	2.02	0.41
1:A:573:VAL:O	1:A:575:HIS:CE1	2.74	0.41
1:A:592:SER:HA	1:A:616:SER:O	2.21	0.41
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.02	0.41
1:B:565:SER:O	1:B:566:HIS:C	2.64	0.41
1:B:715:ARG:NH1	1:B:739:LYS:HD3	2.35	0.41
1:C:592:SER:HA	1:C:616:SER:O	2.20	0.41
1:D:56:GLU:O	1:D:57:VAL:C	2.63	0.41
1:D:79:THR:O	1:D:80:ASN:C	2.62	0.41
1:D:257:CYS:SG	1:D:275:SER:O	2.79	0.41
1:A:458:ASP:OD1	1:A:458:ASP:N	2.53	0.41
1:D:118:ASP:OD1	1:D:118:ASP:N	2.54	0.41
1:D:152:SER:OG	1:D:176:TYR:CB	2.62	0.41
1:D:592:SER:HA	1:D:616:SER:O	2.21	0.41
1:C:589:LEU:HD23	1:C:613:LEU:HD13	2.03	0.40
1:D:329:SER:OG	1:D:330:GLY:N	2.54	0.40
1:D:783:PHE:O	1:D:786:TRP:HB3	2.22	0.40
1:A:226:LYS:NZ	2:E:2:NAG:O7	2.50	0.40
1:B:310:MET:N	1:B:311:PRO:HD3	2.36	0.40
1:D:159:TYR:HB3	1:D:190:THR:HA	2.03	0.40
1:D:73:ASN:O	1:D:98:PRO:HA	2.22	0.40
1:D:732:LEU:C	1:D:762:THR:HG21	2.46	0.40
1:C:490:LEU:HD23	1:C:514:ALA:HB1	2.03	0.40
1:C:744:SER:O	1:C:745:SER:C	2.64	0.40
1:D:249:THR:HA	1:D:289:LEU:HA	2.03	0.40
1:D:804:ALA:HB1	1:D:805:SER:HB3	2.02	0.40
1:B:356:HIS:CD2	1:B:383:ARG:NE	2.89	0.40
1:B:538:THR:HB	1:B:539:ASN:ND2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ASP:OD1	1:B:338:ARG:NH2[2_546]	2.13	0.07

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	741/811 (91%)	691 (93%)	47 (6%)	3 (0%)	30	49
1	B	732/811 (90%)	675 (92%)	55 (8%)	2 (0%)	36	55
1	C	715/811 (88%)	655 (92%)	58 (8%)	2 (0%)	36	55
1	D	712/811 (88%)	612 (86%)	93 (13%)	7 (1%)	12	24
All	All	2900/3244 (89%)	2633 (91%)	253 (9%)	14 (0%)	24	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	ILE
1	D	190	THR
1	D	284	GLN
1	B	735	VAL
1	D	246	ILE
1	A	378	VAL
1	A	735	VAL
1	C	378	VAL
1	C	601	ASP
1	A	579	PHE
1	B	378	VAL
1	D	378	VAL
1	D	91	LYS
1	D	735	VAL

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	696/755 (92%)	657 (94%)	39 (6%)	19	39
1	B	689/755 (91%)	652 (95%)	37 (5%)	20	41
1	C	676/755 (90%)	641 (95%)	35 (5%)	21	42
1	D	673/755 (89%)	623 (93%)	50 (7%)	13	27
All	All	2734/3020 (90%)	2573 (94%)	161 (6%)	18	37

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	45	VAL
1	A	49	CYS
1	A	51	ASN
1	A	52	ARG
1	A	81	GLU
1	A	96	HIS
1	A	118	ASP
1	A	150	GLU
1	A	248	LEU
1	A	275	SER
1	A	286	LEU
1	A	296	SER
1	A	302	ILE
1	A	329	SER
1	A	338	ARG
1	A	416	ASN
1	A	419	ASN
1	A	458	ASP
1	A	471	THR
1	A	472	ARG
1	A	569	ARG
1	A	573	VAL
1	A	611	VAL
1	A	625	ASN
1	A	632	ILE
1	A	678	PHE
1	A	686	GLN
1	A	689	ARG
1	A	736	SER
1	A	737	SER
1	A	739	LYS
1	A	753	LYS

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Mol	Chain	Res	Type
1	A	754	SER
1	A	760	THR
1	A	762	THR
1	A	780	ILE
1	A	785	ARG
1	A	817	LEU
1	B	49	CYS
1	B	51	ASN
1	B	79	THR
1	B	100	VAL
1	B	122	LEU
1	B	136	GLN
1	B	142	SER
1	B	150	GLU
1	B	160	ASN
1	B	170	ILE
1	B	173	LYS
1	B	199	THR
1	B	205	LEU
1	B	215	HIS
1	B	235	LYS
1	B	286	LEU
1	B	308	LYS
1	B	408	GLN
1	B	458	ASP
1	B	472	ARG
1	B	502	GLU
1	B	573	VAL
1	B	595	ASN
1	B	611	VAL
1	B	686	GLN
1	B	702	PHE
1	B	727	LEU
1	B	733	SER
1	B	735	VAL
1	B	737	SER
1	B	749	LYS
1	B	756	LEU
1	B	762	THR
1	B	763	LYS
1	B	808	ASP
1	B	815	VAL

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Mol	Chain	Res	Type
1	B	817	LEU
1	C	39	LYS
1	C	49	CYS
1	C	51	ASN
1	C	59	GLN
1	C	60	THR
1	C	76	THR
1	C	122	LEU
1	C	125	LYS
1	C	142	SER
1	C	199	THR
1	C	239	GLU
1	C	240	GLU
1	C	243	LYS
1	C	248	LEU
1	C	286	LEU
1	C	308	LYS
1	C	329	SER
1	C	355	GLN
1	C	385	ASP
1	C	403	ILE
1	C	409	ILE
1	C	412	LYS
1	C	431	SER
1	C	465	SER
1	C	573	VAL
1	C	598	THR
1	C	611	VAL
1	C	643	ARG
1	C	671	ILE
1	C	711	THR
1	C	726	HIS
1	C	753	LYS
1	C	764	LEU
1	C	778	CYS
1	C	812	LYS
1	D	48	GLU
1	D	52	ARG
1	D	59	GLN
1	D	77	HIS
1	D	80	ASN
1	D	126	ASN

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Mol	Chain	Res	Type
1	D	127	LEU
1	D	147	SER
1	D	150	GLU
1	D	160	ASN
1	D	161	ILE
1	D	162	THR
1	D	169	LEU
1	D	185	LYS
1	D	190	THR
1	D	193	GLU
1	D	194	ASP
1	D	200	LEU
1	D	201	THR
1	D	202	ASN
1	D	209	SER
1	D	215	HIS
1	D	221	PRO
1	D	222	SER
1	D	246	ILE
1	D	296	SER
1	D	301	LYS
1	D	338	ARG
1	D	361	ARG
1	D	409	ILE
1	D	471	THR
1	D	472	ARG
1	D	573	VAL
1	D	611	VAL
1	D	632	ILE
1	D	678	PHE
1	D	686	GLN
1	D	712	SER
1	D	720	SER
1	D	726	HIS
1	D	734	GLU
1	D	735	VAL
1	D	745	SER
1	D	749	LYS
1	D	762	THR
1	D	776	CYS
1	D	778	CYS
1	D	779	ASP

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Mol	Chain	Res	Type
1	D	782	ASP
1	D	810	ARG

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

Mol	Chain	Res	Type
1	A	41	GLN
1	A	288	GLN
1	A	309	ASN
1	A	581	GLN
1	A	593	HIS
1	A	653	HIS
1	A	686	GLN
1	A	809	GLN
1	B	51	ASN
1	B	77	HIS
1	B	160	ASN
1	B	231	ASN
1	B	312	HIS
1	B	388	GLN
1	B	416	ASN
1	B	539	ASN
1	B	721	HIS
1	C	55	GLN
1	C	77	HIS
1	C	84	GLN
1	C	160	ASN
1	C	215	HIS
1	C	247	ASN
1	C	284	GLN
1	C	355	GLN
1	C	416	ASN
1	C	419	ASN
1	C	469	HIS
1	C	585	ASN
1	C	653	HIS
1	C	686	GLN
1	D	139	GLN
1	D	202	ASN
1	D	215	HIS
1	D	233	GLN
1	D	303	ASN

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Mol	Chain	Res	Type
1	D	355	GLN
1	D	395	ASN
1	D	531	HIS
1	D	582	ASN
1	D	593	HIS
1	D	595	ASN
1	D	770	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.92	1 (7%)	17,19,21	1.19	1 (5%)
2	NAG	E	2	2	14,14,15	0.88	0	17,19,21	1.40	3 (17%)
2	BMA	E	3	2	11,11,12	0.85	0	15,15,17	1.64	3 (20%)
3	NAG	F	1	3,1	14,14,15	1.04	1 (7%)	17,19,21	1.73	3 (17%)
3	NAG	F	2	3	14,14,15	0.68	0	17,19,21	1.70	3 (17%)
2	NAG	G	1	2,1	14,14,15	0.68	0	17,19,21	1.81	4 (23%)
2	NAG	G	2	2	14,14,15	0.87	1 (7%)	17,19,21	1.30	3 (17%)
2	BMA	G	3	2	11,11,12	0.62	0	15,15,17	1.26	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.74	0	17,19,21	1.51	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	2	2	14,14,15	0.66	0	17,19,21	1.14	0
2	BMA	H	3	2	11,11,12	0.87	0	15,15,17	1.50	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.93	1 (7%)	17,19,21	2.06	4 (23%)
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	1.32	3 (17%)
2	NAG	J	1	2,1	14,14,15	0.67	0	17,19,21	1.37	3 (17%)
2	NAG	J	2	2	14,14,15	0.76	0	17,19,21	1.33	1 (5%)
2	BMA	J	3	2	11,11,12	0.63	0	15,15,17	1.41	3 (20%)
2	NAG	K	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	1.70	3 (17%)
2	NAG	K	2	2	14,14,15	0.68	0	17,19,21	1.47	3 (17%)
2	BMA	K	3	2	11,11,12	0.92	1 (9%)	15,15,17	1.50	4 (26%)
3	NAG	L	1	3,1	14,14,15	0.91	0	17,19,21	1.47	2 (11%)
3	NAG	L	2	3	14,14,15	0.70	0	17,19,21	1.72	5 (29%)
2	NAG	M	1	2,1	14,14,15	0.75	1 (7%)	17,19,21	1.52	4 (23%)
2	NAG	M	2	2	14,14,15	1.12	2 (14%)	17,19,21	1.60	4 (23%)
2	BMA	M	3	2	11,11,12	0.60	0	15,15,17	1.18	2 (13%)
2	NAG	N	1	2,1	14,14,15	0.58	0	17,19,21	1.45	3 (17%)
2	NAG	N	2	2	14,14,15	0.89	1 (7%)	17,19,21	1.38	2 (11%)
2	BMA	N	3	2	11,11,12	0.71	0	15,15,17	1.26	1 (6%)
3	NAG	O	1	3,1	14,14,15	0.78	1 (7%)	17,19,21	1.16	1 (5%)
3	NAG	O	2	3	14,14,15	0.76	0	17,19,21	0.84	0
2	NAG	P	1	2,1	14,14,15	0.61	0	17,19,21	1.54	2 (11%)
2	NAG	P	2	2	14,14,15	0.95	0	17,19,21	1.22	3 (17%)
2	BMA	P	3	2	11,11,12	0.89	0	15,15,17	1.81	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	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	O5-C1	-3.14	1.38	1.43
2	M	2	NAG	O5-C1	-2.88	1.38	1.43
3	F	1	NAG	C1-C2	-2.41	1.49	1.52
2	E	1	NAG	O5-C1	-2.25	1.39	1.43
3	O	1	NAG	O5-C1	-2.22	1.40	1.43
2	M	1	NAG	C1-C2	2.19	1.55	1.52
2	N	2	NAG	O5-C1	-2.13	1.40	1.43
2	M	2	NAG	C2-N2	-2.10	1.42	1.46
2	K	3	BMA	O3-C3	2.08	1.48	1.43
2	G	2	NAG	O5-C1	-2.06	1.40	1.43
3	I	1	NAG	O5-C1	-2.01	1.40	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-C2-N2	-5.85	101.21	110.43
3	F	2	NAG	C1-O5-C5	5.20	119.15	112.19
2	K	1	NAG	O5-C1-C2	-4.85	103.78	111.29
3	F	1	NAG	C1-C2-N2	-4.54	103.27	110.43
2	P	3	BMA	C1-O5-C5	4.42	118.11	112.19
3	L	1	NAG	C1-C2-N2	-3.92	104.25	110.43
2	P	1	NAG	O5-C1-C2	-3.89	105.28	111.29
2	G	1	NAG	O7-C7-N2	3.87	128.83	121.98
2	G	1	NAG	C1-O5-C5	3.71	117.16	112.19
2	N	1	NAG	C1-O5-C5	3.66	117.09	112.19
2	E	3	BMA	C1-O5-C5	3.63	117.05	112.19
2	J	2	NAG	C2-N2-C7	3.61	127.74	122.90
2	M	2	NAG	O5-C1-C2	-3.43	105.98	111.29
2	N	2	NAG	O5-C1-C2	-3.40	106.03	111.29
2	P	1	NAG	C1-O5-C5	3.27	116.57	112.19
2	K	2	NAG	O5-C1-C2	-3.25	106.27	111.29
3	I	1	NAG	C3-C4-C5	-3.21	104.40	110.23
2	G	1	NAG	O7-C7-C8	-3.15	116.44	122.05
3	L	2	NAG	C3-C4-C5	-3.13	104.56	110.23
3	F	2	NAG	O3-C3-C2	-3.13	102.91	109.40
2	J	3	BMA	O3-C3-C4	3.09	117.66	110.38
2	K	3	BMA	C2-C3-C4	-3.00	105.58	110.86
2	K	1	NAG	C3-C4-C5	-2.99	104.82	110.23
3	O	1	NAG	C1-C2-N2	-2.98	105.73	110.43
3	I	2	NAG	C1-O5-C5	2.98	116.18	112.19
2	E	2	NAG	C3-C4-C5	-2.97	104.84	110.23
3	L	1	NAG	C1-O5-C5	2.97	116.17	112.19
2	G	1	NAG	C2-N2-C7	2.90	126.78	122.90
2	H	3	BMA	C2-C3-C4	-2.88	105.80	110.86
2	H	3	BMA	O4-C4-C3	-2.84	103.69	110.38
2	K	2	NAG	C3-C4-C5	-2.83	105.10	110.23
2	J	1	NAG	O4-C4-C3	-2.83	103.71	110.38
2	J	1	NAG	O7-C7-C8	-2.81	117.05	122.05
2	M	1	NAG	O7-C7-C8	-2.79	117.08	122.05
3	I	1	NAG	C1-O5-C5	2.79	115.93	112.19
2	E	3	BMA	O6-C6-C5	2.79	120.83	111.33
3	L	2	NAG	O7-C7-C8	-2.78	117.10	122.05
3	F	1	NAG	O3-C3-C2	-2.78	103.62	109.40
2	H	1	NAG	O4-C4-C5	-2.78	102.48	109.32
2	M	3	BMA	C1-C2-C3	2.77	113.68	109.64
2	G	2	NAG	O5-C1-C2	-2.77	107.01	111.29
2	E	2	NAG	O5-C1-C2	-2.71	107.09	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NAG	O7-C7-N2	2.71	126.78	121.98
2	J	3	BMA	O5-C5-C6	2.71	112.94	107.66
2	P	2	NAG	O7-C7-N2	2.70	126.75	121.98
3	L	2	NAG	O4-C4-C5	2.65	115.85	109.32
2	H	1	NAG	C3-C4-C5	-2.63	105.46	110.23
2	J	1	NAG	C1-O5-C5	2.61	115.69	112.19
3	L	2	NAG	O5-C5-C6	2.61	112.75	107.66
2	K	3	BMA	C1-C2-C3	2.59	113.42	109.64
2	P	3	BMA	O3-C3-C2	2.57	115.29	110.05
2	M	1	NAG	C1-O5-C5	2.55	115.60	112.19
2	G	3	BMA	O4-C4-C3	-2.53	104.42	110.38
2	H	1	NAG	O5-C1-C2	-2.47	107.46	111.29
2	M	2	NAG	O5-C5-C6	-2.46	102.87	107.66
2	P	2	NAG	O5-C1-C2	-2.44	107.52	111.29
3	I	2	NAG	C3-C4-C5	-2.39	105.89	110.23
2	K	1	NAG	O7-C7-C8	-2.37	117.83	122.05
2	E	3	BMA	O4-C4-C3	-2.37	104.79	110.38
3	I	2	NAG	O4-C4-C5	2.36	115.13	109.32
2	N	1	NAG	O5-C1-C2	-2.34	107.66	111.29
2	M	2	NAG	C2-N2-C7	-2.30	119.82	122.90
2	G	2	NAG	O5-C5-C6	-2.28	103.22	107.66
2	G	2	NAG	O6-C6-C5	-2.23	103.74	111.33
2	H	3	BMA	C1-O5-C5	2.22	115.16	112.19
2	M	1	NAG	C3-C4-C5	-2.17	106.31	110.23
2	E	2	NAG	O7-C7-N2	2.16	125.80	121.98
2	M	2	NAG	C4-C3-C2	-2.16	107.86	111.02
3	L	2	NAG	O7-C7-N2	2.16	125.79	121.98
2	K	2	NAG	O6-C6-C5	-2.14	104.03	111.33
2	E	1	NAG	C3-C4-C5	-2.13	106.36	110.23
3	F	1	NAG	C4-C3-C2	-2.12	107.91	111.02
2	N	3	BMA	C1-C2-C3	2.12	112.73	109.64
2	K	3	BMA	O3-C3-C4	2.11	115.36	110.38
2	N	2	NAG	O5-C5-C6	-2.10	103.57	107.66
2	K	3	BMA	O3-C3-C2	2.09	114.32	110.05
3	I	1	NAG	C2-N2-C7	2.08	125.69	122.90
2	P	2	NAG	C1-O5-C5	2.07	114.96	112.19
2	M	3	BMA	C1-O5-C5	2.06	114.95	112.19
2	N	1	NAG	O7-C7-C8	-2.04	118.41	122.05
2	J	3	BMA	O2-C2-C3	2.04	114.38	110.15
3	F	2	NAG	O7-C7-C8	-2.04	118.43	122.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

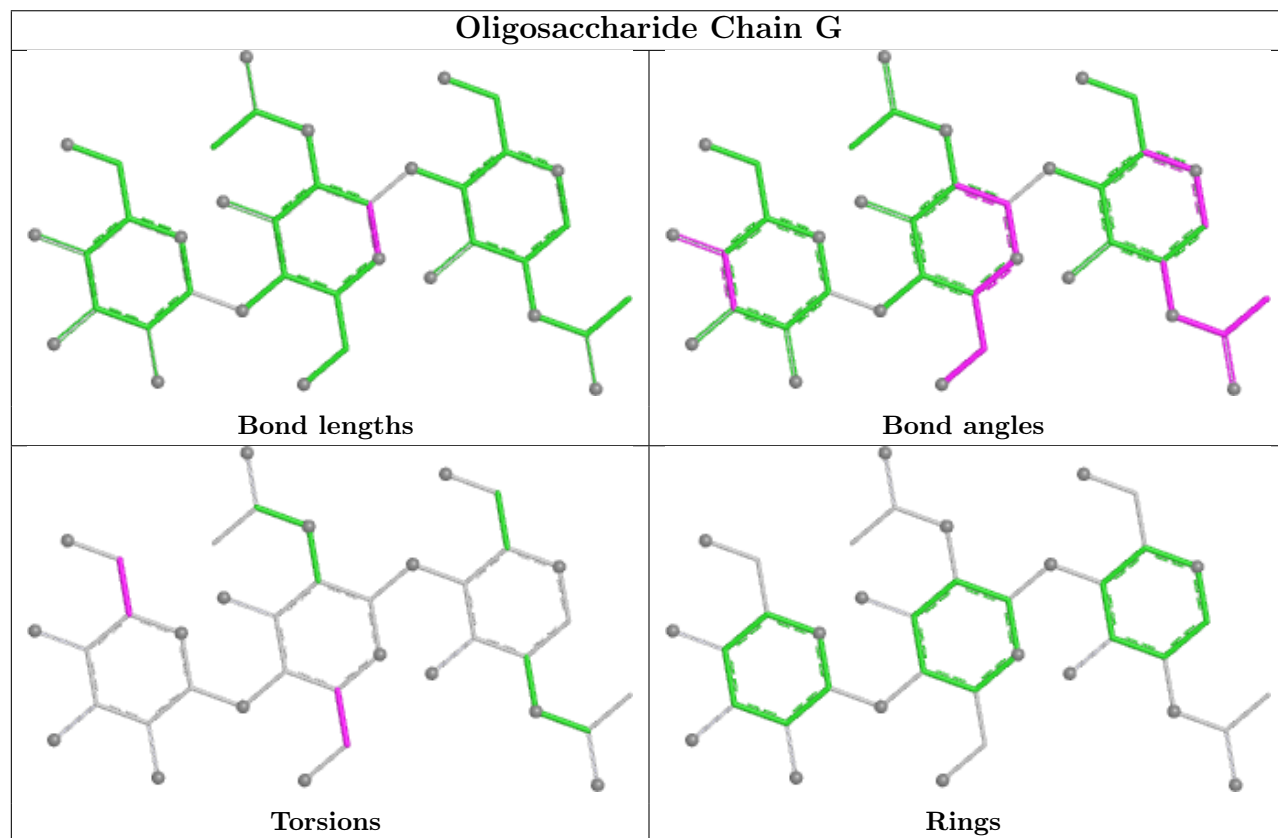
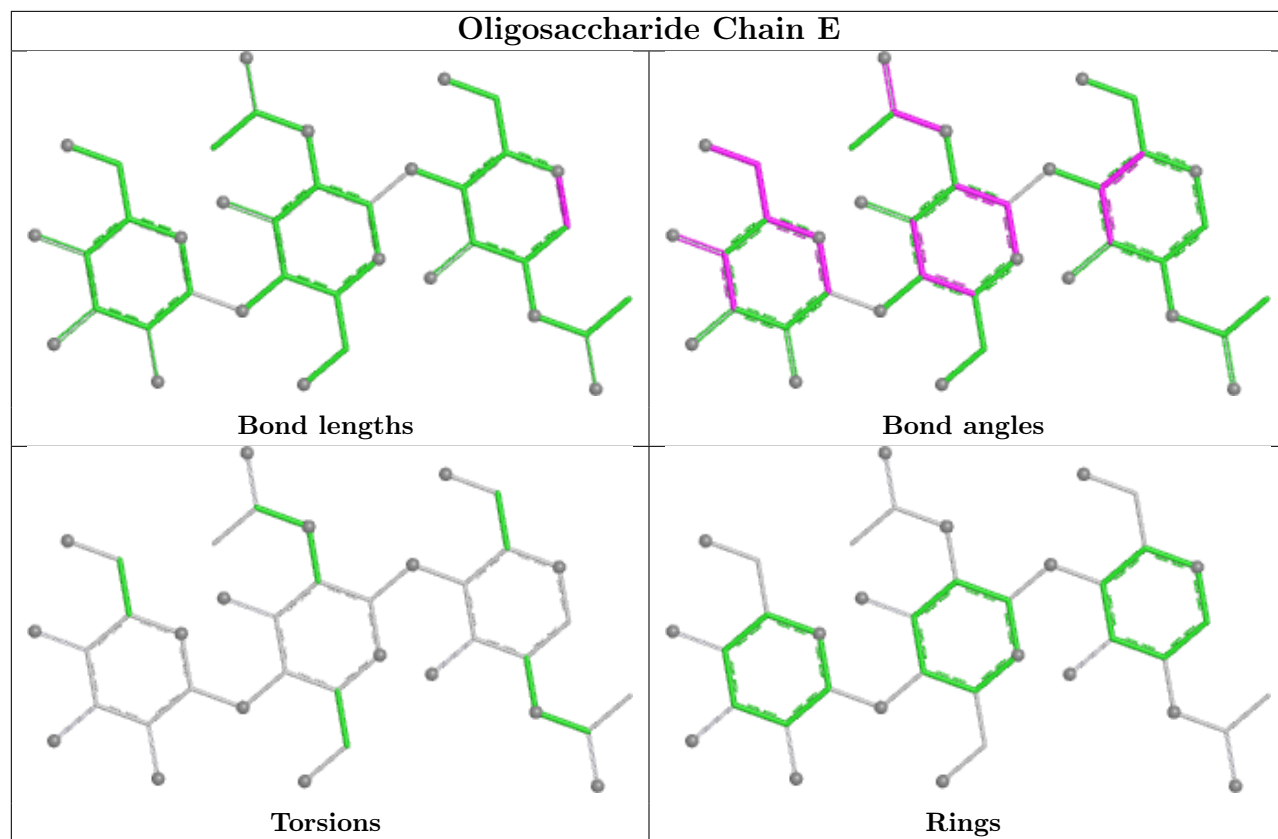
Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6

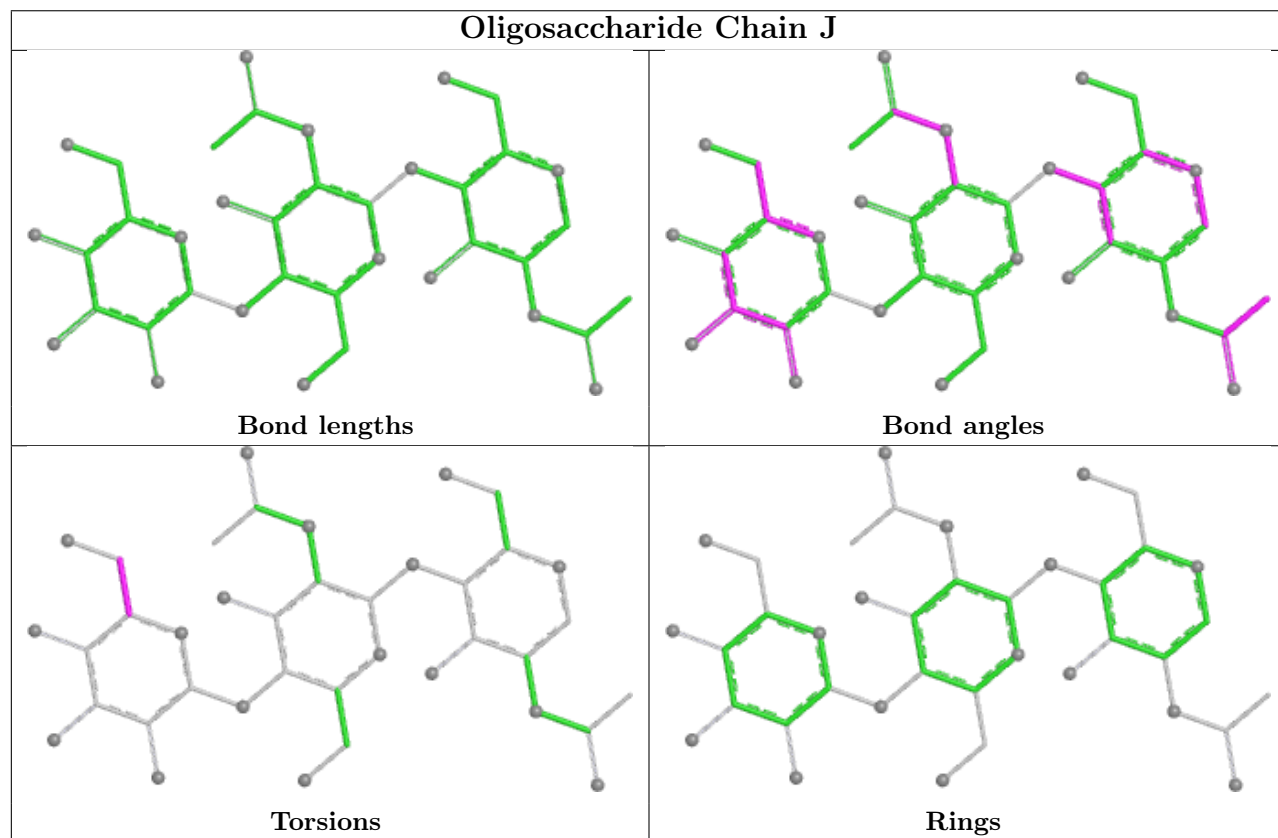
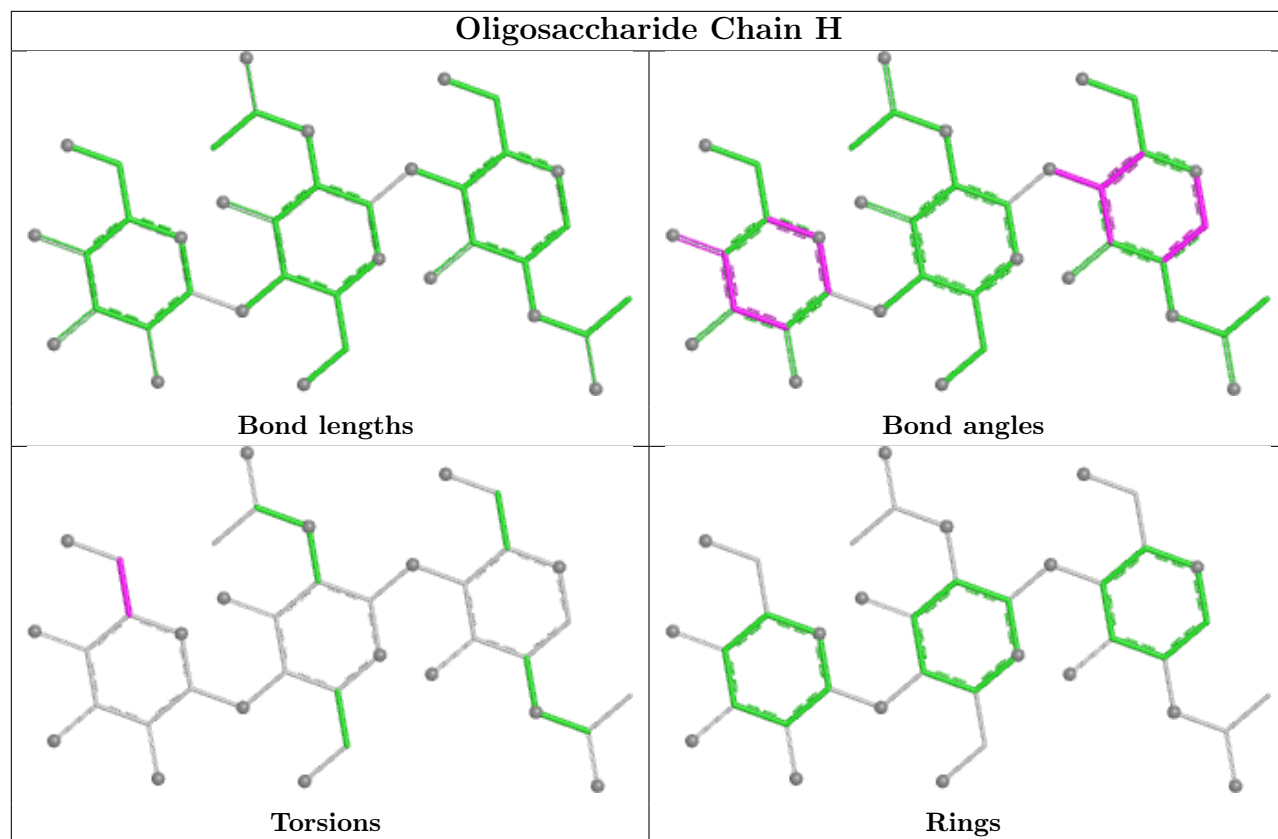
There are no ring outliers.

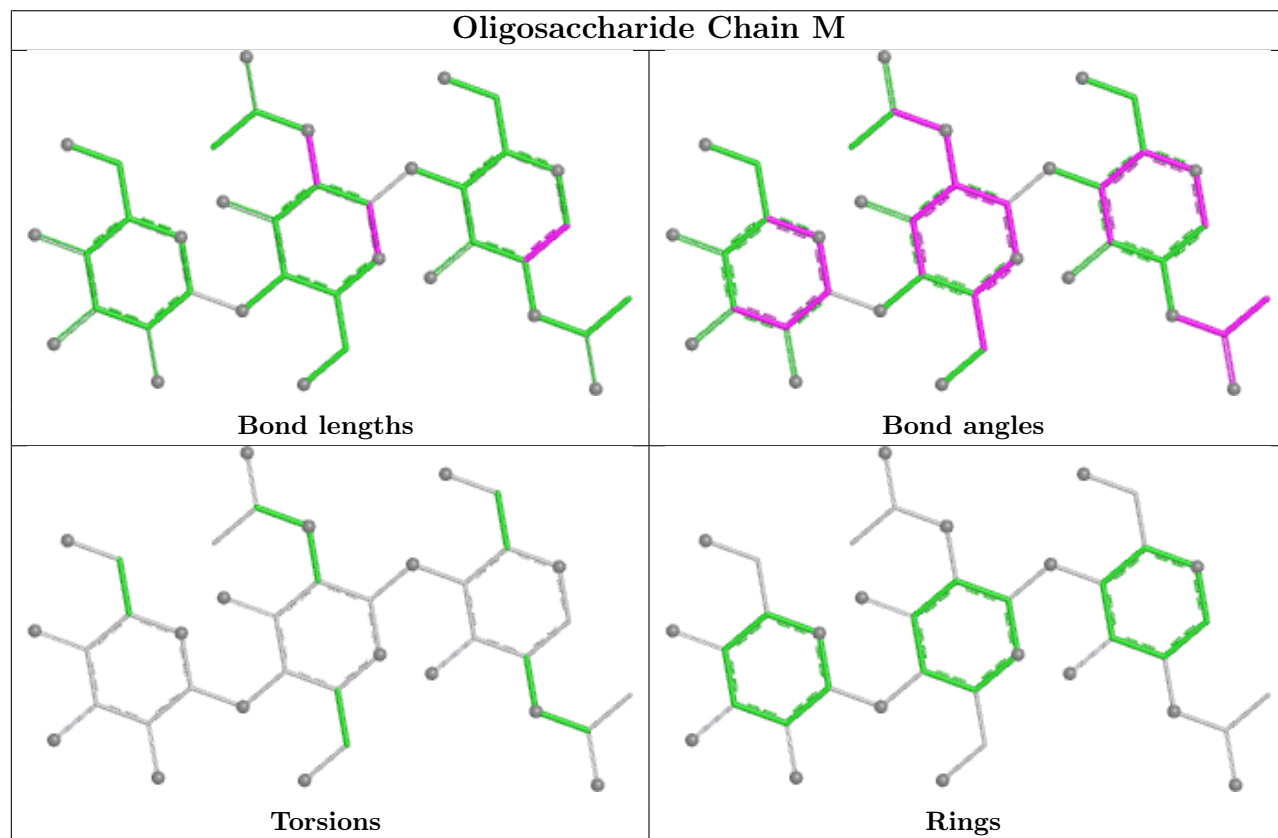
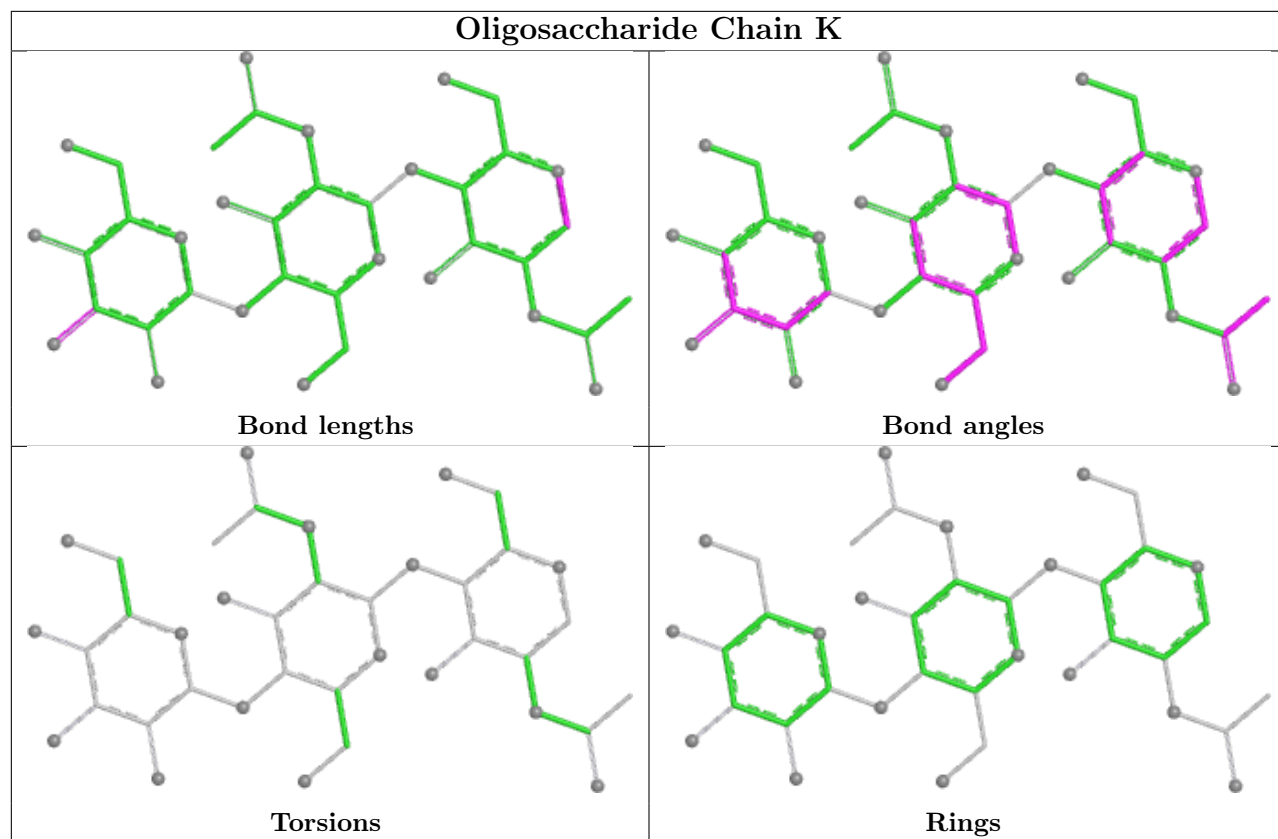
3 monomers are involved in 3 short contacts:

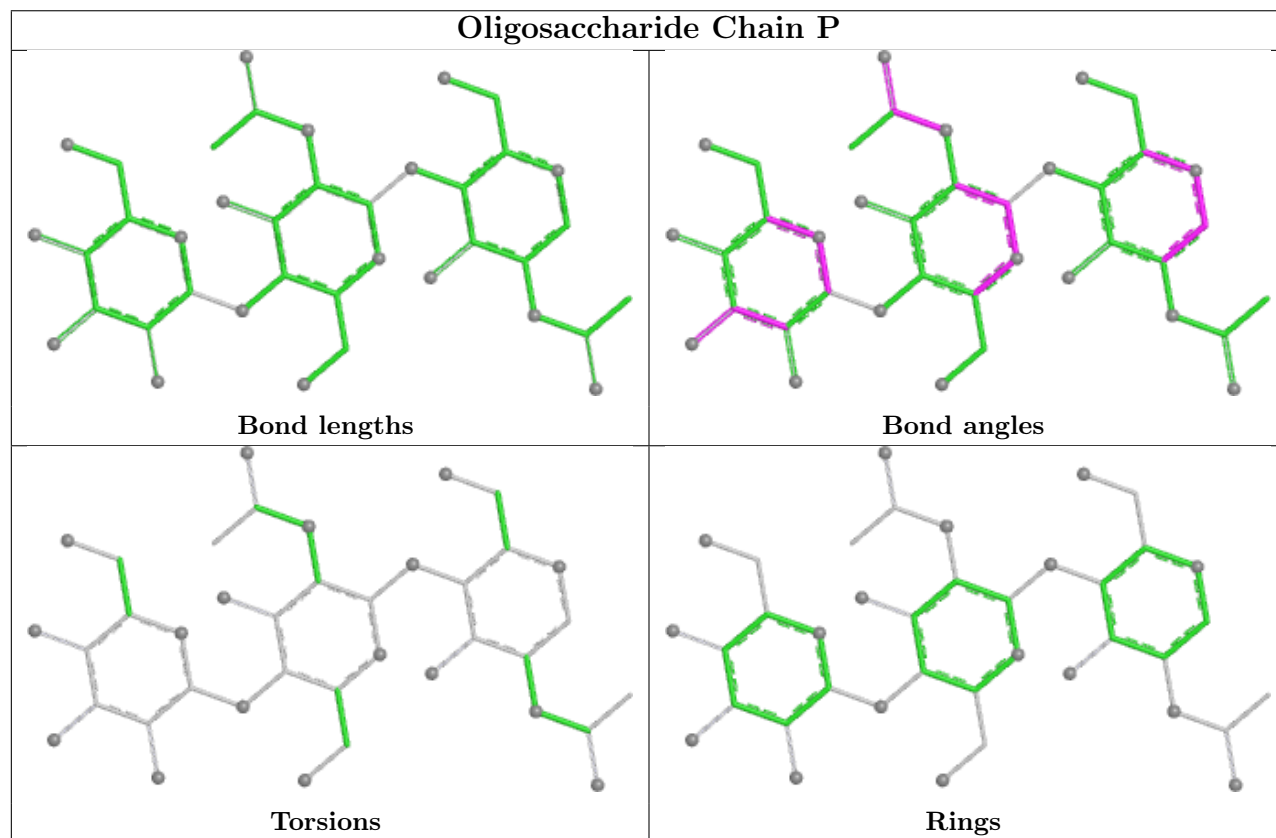
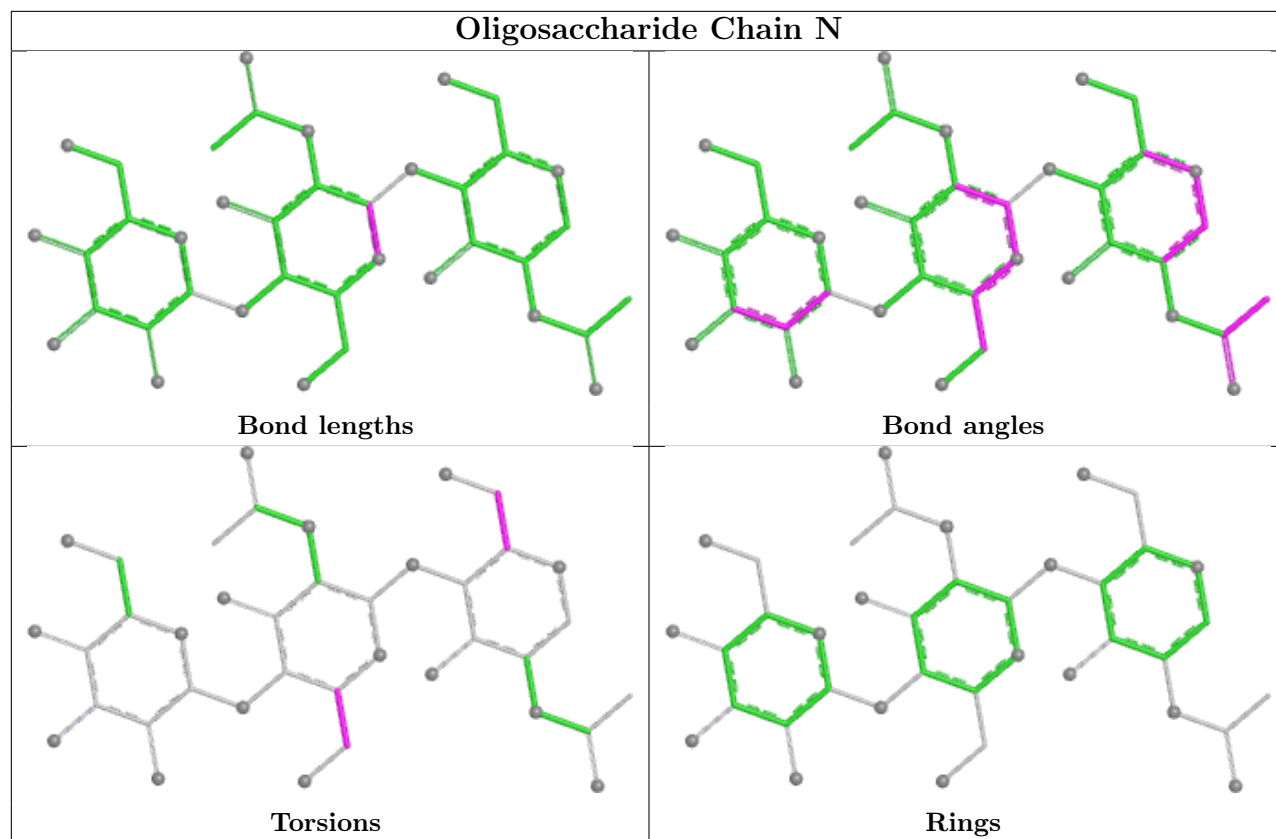
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	N	1	NAG	1	0
2	E	2	NAG	1	0

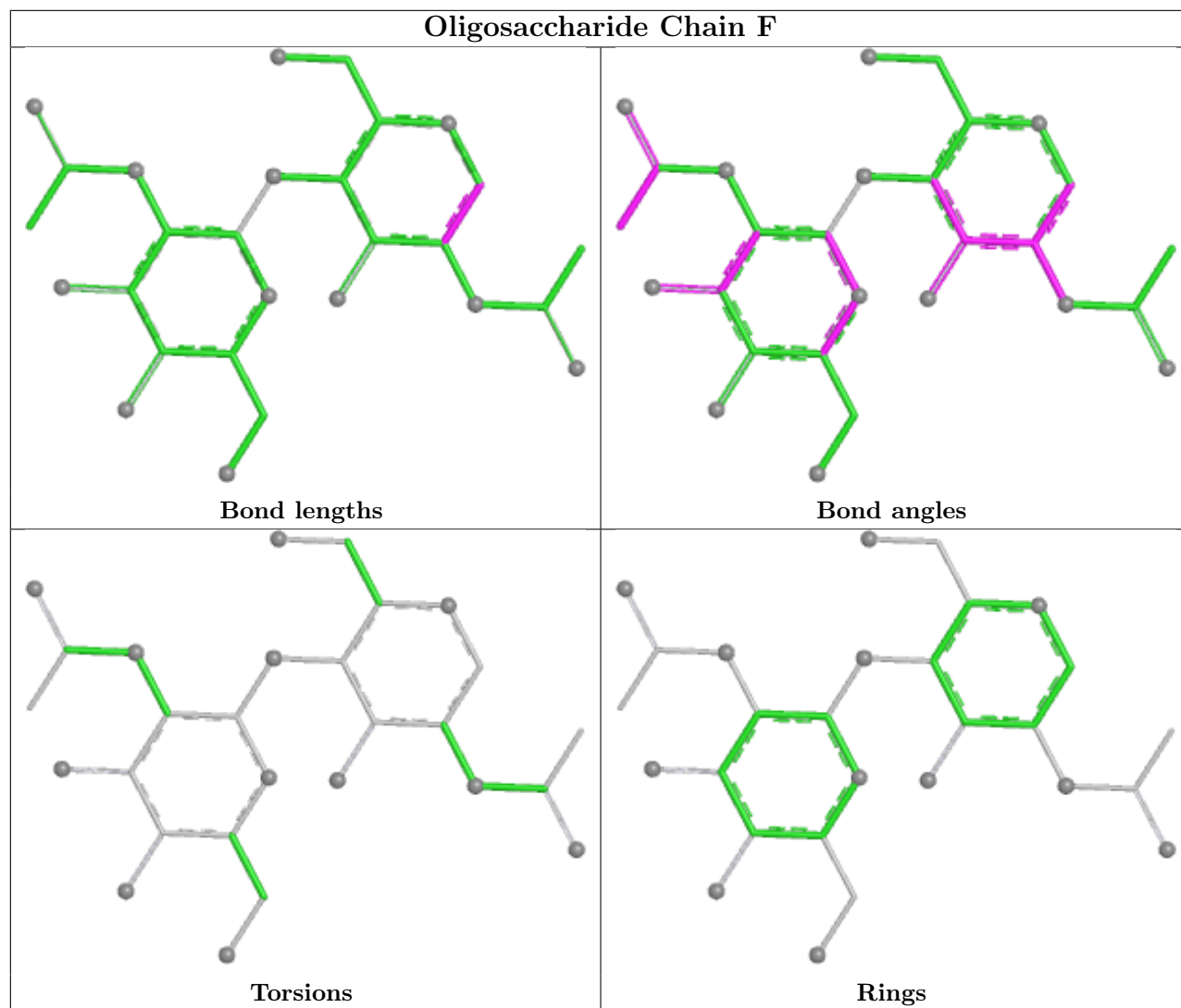
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

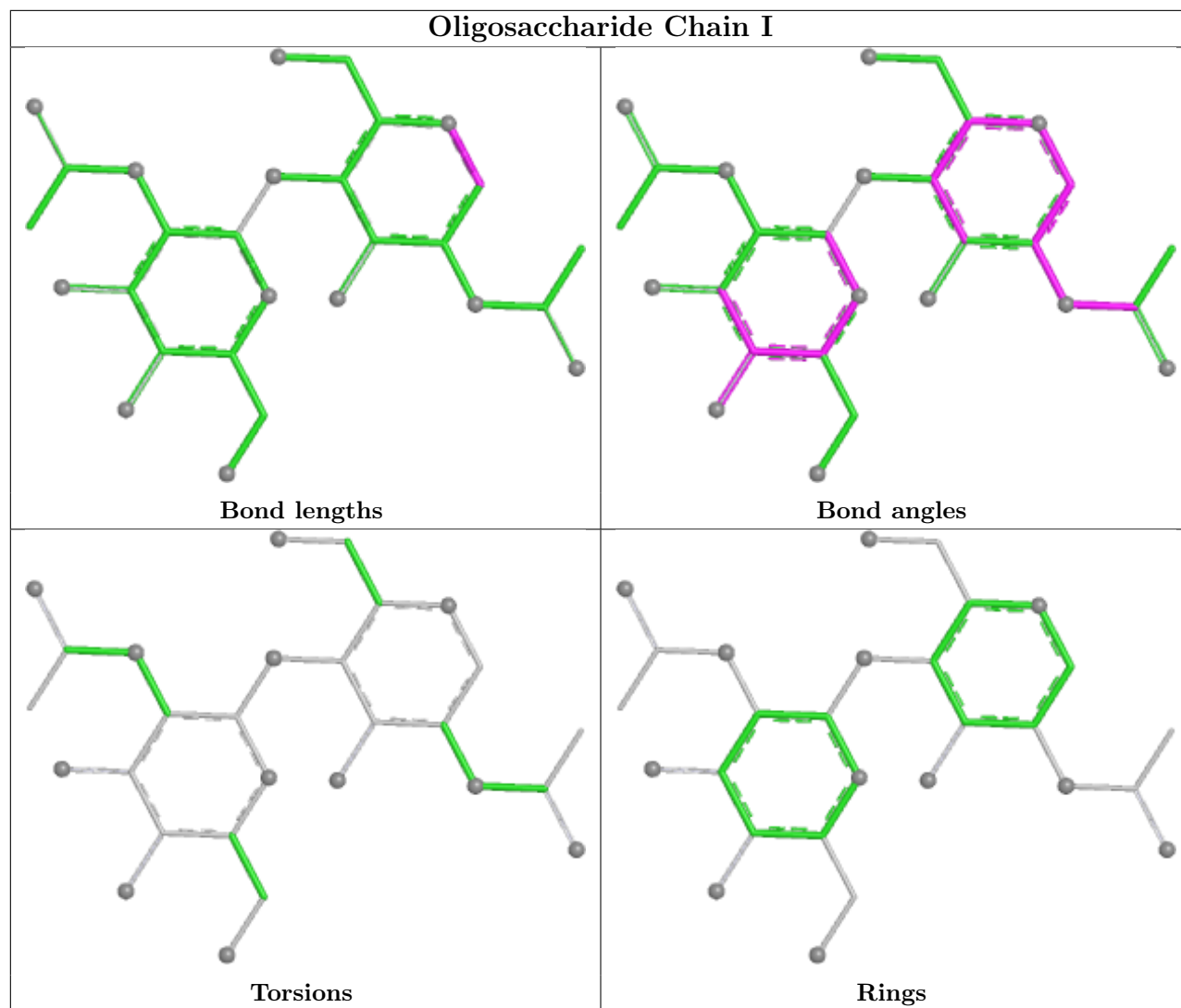


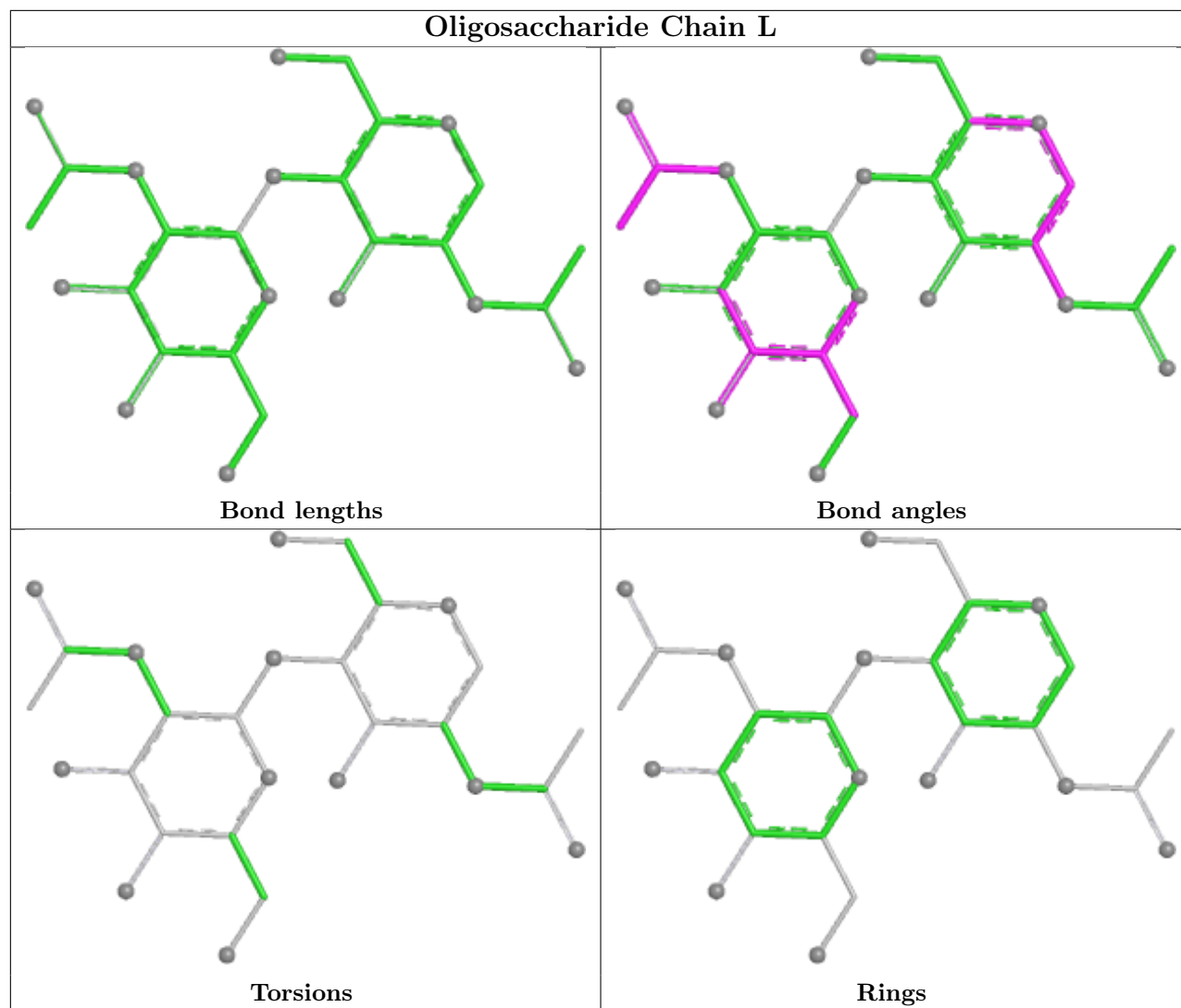


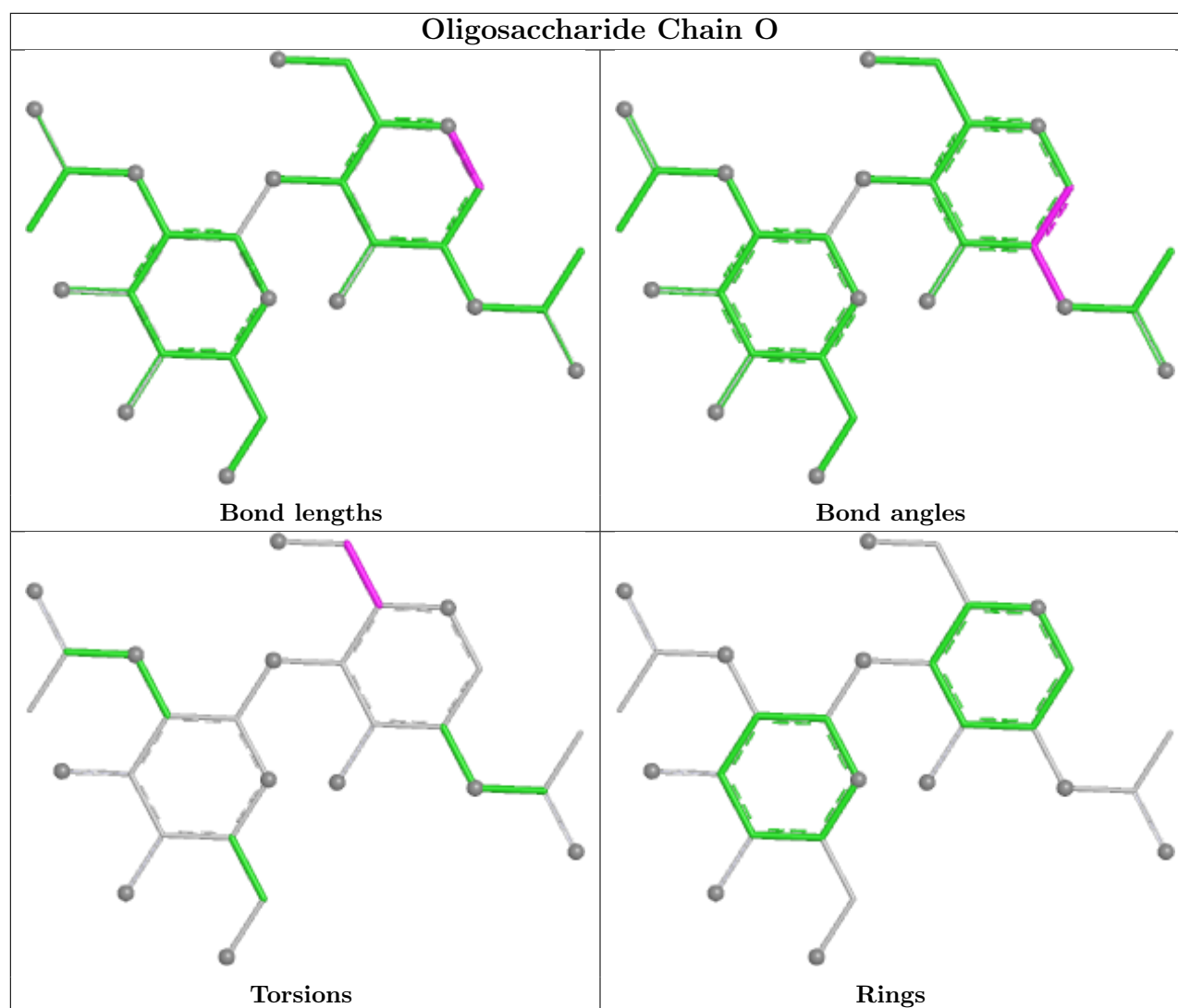












5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
4	NAG	A	1010	1	14,14,15	0.55	0	17,19,21	1.26	2 (11%)
5	M4D	A	1012	-	22,22,22	1.64	2 (9%)	27,28,28	1.20	2 (7%)
5	M4D	B	901	-	22,22,22	1.46	2 (9%)	27,28,28	1.26	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	911	1	14,14,15	0.60	0	17,19,21	1.24	2 (11%)
4	NAG	D	907	1	14,14,15	0.80	0	17,19,21	1.89	4 (23%)
4	NAG	C	1010	1	14,14,15	0.64	0	17,19,21	1.48	2 (11%)
4	NAG	B	907	1	14,14,15	0.74	0	17,19,21	1.32	2 (11%)
5	M4D	D	901	-	22,22,22	1.16	4 (18%)	27,28,28	1.15	2 (7%)
4	NAG	A	1006	1	14,14,15	0.60	0	17,19,21	1.35	3 (17%)
5	M4D	C	1011	-	22,22,22	1.51	3 (13%)	27,28,28	1.17	2 (7%)
4	NAG	A	1011	1	14,14,15	0.80	0	17,19,21	0.90	1 (5%)
4	NAG	C	1006	1	14,14,15	0.58	0	17,19,21	1.69	3 (17%)
4	NAG	D	911	1	14,14,15	0.54	0	17,19,21	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1010	1	-	2/6/23/26	0/1/1/1
5	M4D	A	1012	-	-	2/10/10/10	0/2/2/2
5	M4D	B	901	-	-	0/10/10/10	0/2/2/2
4	NAG	B	911	1	-	0/6/23/26	0/1/1/1
4	NAG	D	907	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	2/6/23/26	0/1/1/1
5	M4D	D	901	-	-	0/10/10/10	0/2/2/2
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
5	M4D	C	1011	-	-	2/10/10/10	0/2/2/2
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1006	1	-	2/6/23/26	0/1/1/1
4	NAG	D	911	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1012	M4D	C7-C6	4.69	1.50	1.42
5	C	1011	M4D	C7-C6	4.38	1.50	1.42
5	B	901	M4D	C7-C6	4.35	1.50	1.42
5	A	1012	M4D	C1-C	4.16	1.49	1.42
5	C	1011	M4D	C1-C	3.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	M4D	C1-C	3.39	1.47	1.42
5	C	1011	M4D	C3-C1	2.49	1.48	1.42
5	D	901	M4D	C3-C1	2.39	1.48	1.42
5	D	901	M4D	C7-C6	2.34	1.46	1.42
5	D	901	M4D	C-N	-2.27	1.34	1.37
5	D	901	M4D	C2-C	-2.17	1.38	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	907	NAG	O5-C1-C2	-5.58	102.66	111.29
5	A	1012	M4D	C8-C7-C6	3.95	119.96	116.42
4	C	1006	NAG	C8-C7-N2	3.83	122.47	116.12
4	B	911	NAG	C1-O5-C5	3.82	117.31	112.19
5	C	1011	M4D	C8-C7-C6	3.77	119.80	116.42
4	C	1010	NAG	C1-O5-C5	3.50	116.88	112.19
5	B	901	M4D	C8-C7-C6	3.31	119.39	116.42
5	B	901	M4D	C1-C-N	-3.19	119.42	122.80
4	B	907	NAG	O5-C1-C2	-3.18	106.37	111.29
5	D	901	M4D	C1-C-N	-3.12	119.50	122.80
4	D	907	NAG	C1-C2-N2	3.03	115.21	110.43
4	C	1006	NAG	O5-C1-C2	-2.72	107.08	111.29
5	D	901	M4D	C8-C7-C6	2.71	118.85	116.42
4	D	907	NAG	O4-C4-C3	-2.69	104.03	110.38
4	A	1010	NAG	O5-C5-C6	2.67	112.85	107.66
4	C	1010	NAG	C4-C3-C2	-2.64	107.14	111.02
4	C	1006	NAG	C1-O5-C5	2.61	115.69	112.19
4	A	1006	NAG	C4-C3-C2	-2.41	107.49	111.02
4	B	907	NAG	C1-C2-N2	2.39	114.20	110.43
5	B	901	M4D	C9-C10-C7	-2.37	106.89	114.13
5	A	1012	M4D	C1-C-N	-2.35	120.31	122.80
4	A	1010	NAG	O3-C3-C4	-2.31	104.94	110.38
4	A	1006	NAG	C2-N2-C7	-2.23	119.91	122.90
5	C	1011	M4D	C15-C14-C3	-2.18	106.53	114.33
4	A	1006	NAG	O5-C1-C2	-2.13	107.99	111.29
4	A	1011	NAG	C1-O5-C5	2.07	114.96	112.19
4	B	911	NAG	C4-C3-C2	-2.04	108.02	111.02
4	D	907	NAG	O7-C7-N2	2.04	125.59	121.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

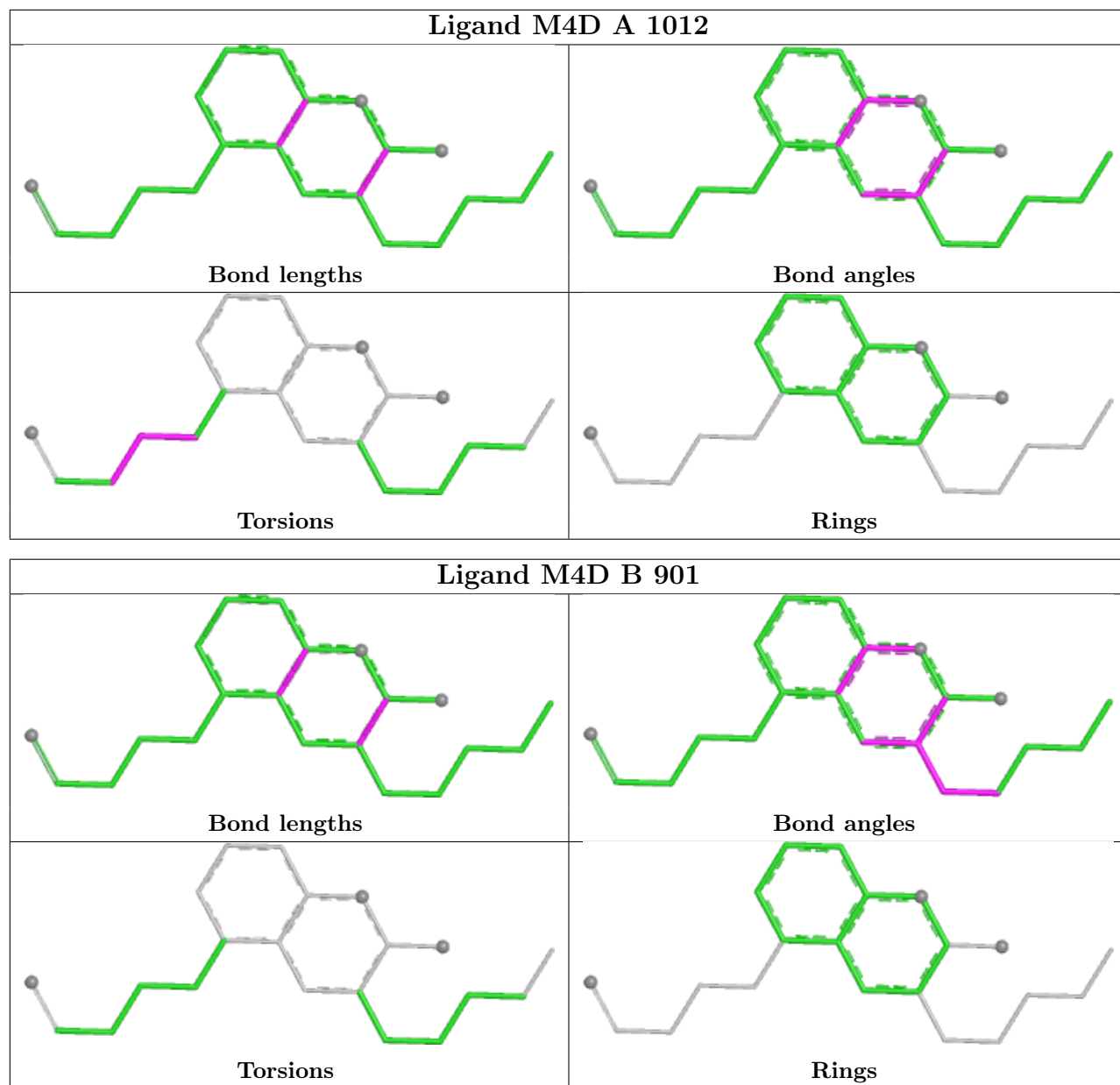
Mol	Chain	Res	Type	Atoms
4	D	911	NAG	O5-C5-C6-O6
4	A	1010	NAG	O5-C5-C6-O6
4	D	907	NAG	O5-C5-C6-O6
4	A	1010	NAG	C4-C5-C6-O6
4	D	911	NAG	C4-C5-C6-O6
4	D	907	NAG	C4-C5-C6-O6
4	B	907	NAG	O5-C5-C6-O6
4	B	907	NAG	C4-C5-C6-O6
4	C	1006	NAG	C8-C7-N2-C2
4	C	1006	NAG	O7-C7-N2-C2
5	C	1011	M4D	C15-C16-C17-N2
5	C	1011	M4D	C14-C15-C16-C17
5	A	1012	M4D	C3-C14-C15-C16
5	A	1012	M4D	C14-C15-C16-C17

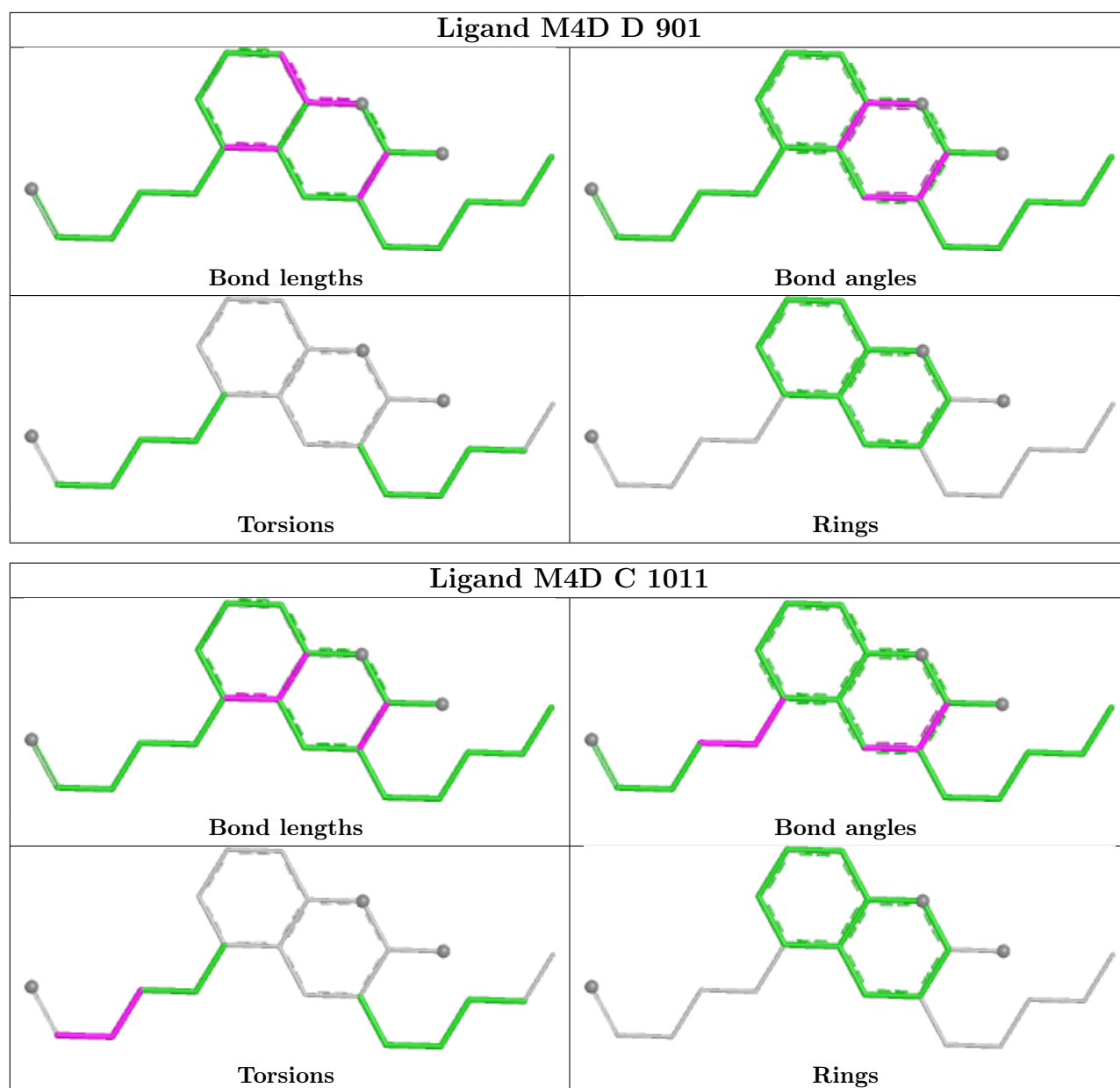
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	M4D	1	0
5	B	901	M4D	1	0
5	C	1011	M4D	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	749/811 (92%)	-0.24	9 (1%) 76 73	31, 46, 82, 114	0
1	B	742/811 (91%)	-0.15	13 (1%) 67 64	30, 50, 88, 118	0
1	C	727/811 (89%)	0.11	19 (2%) 57 52	34, 58, 106, 133	0
1	D	724/811 (89%)	0.51	61 (8%) 17 15	34, 72, 121, 150	0
All	All	2942/3244 (90%)	0.05	102 (3%) 47 42	30, 53, 108, 150	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	VAL	5.6
1	D	100	VAL	5.0
1	D	815	VAL	4.9
1	D	732	LEU	4.6
1	D	678	PHE	4.4
1	D	58	PRO	4.4
1	D	113	GLY	4.3
1	B	100	VAL	4.3
1	D	121	PHE	4.0
1	D	248	LEU	3.9
1	D	122	LEU	3.8
1	B	702	PHE	3.7
1	D	57	VAL	3.7
1	B	678	PHE	3.7
1	D	92	ILE	3.7
1	C	702	PHE	3.6
1	D	495	PHE	3.6
1	D	124	LEU	3.5
1	D	805	SER	3.5
1	D	123	ASN	3.5
1	B	40	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	227	LEU	3.4
1	D	201	THR	3.3
1	D	224	LEU	3.2
1	C	783	PHE	3.2
1	C	64	TYR	3.2
1	C	678	PHE	3.1
1	D	141	PRO	3.1
1	D	166	ILE	3.1
1	C	701	LEU	3.0
1	C	817	LEU	3.0
1	D	47	ALA	2.9
1	D	778	CYS	2.9
1	B	458	ASP	2.9
1	D	702	PHE	2.9
1	C	754	SER	2.8
1	B	817	LEU	2.8
1	A	702	PHE	2.8
1	D	804	ALA	2.7
1	D	242	PHE	2.7
1	B	64	TYR	2.7
1	D	777	THR	2.7
1	D	307	PHE	2.6
1	D	806	PRO	2.6
1	D	283	PHE	2.6
1	B	732	LEU	2.6
1	A	736	SER	2.6
1	D	218	PRO	2.6
1	D	278	ILE	2.6
1	D	89	LEU	2.6
1	D	217	PRO	2.5
1	D	220	LEU	2.5
1	D	140	ILE	2.5
1	D	64	TYR	2.5
1	C	113	GLY	2.5
1	D	114	LEU	2.5
1	D	200	LEU	2.5
1	D	245	LEU	2.5
1	D	306	TRP	2.5
1	D	470	PHE	2.5
1	D	282	ALA	2.5
1	D	79	THR	2.5
1	A	495	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	807	GLY	2.4
1	A	735	VAL	2.4
1	C	763	LYS	2.4
1	C	679	PHE	2.3
1	B	735	VAL	2.3
1	D	653	HIS	2.3
1	D	81	GLU	2.3
1	C	750	THR	2.3
1	C	703	LEU	2.3
1	A	64	TYR	2.3
1	B	127	LEU	2.2
1	D	780	ILE	2.2
1	A	726	HIS	2.2
1	D	311	PRO	2.2
1	C	707	LEU	2.2
1	D	144	LEU	2.2
1	D	192	ILE	2.2
1	C	726	HIS	2.2
1	D	203	LEU	2.2
1	A	762	THR	2.1
1	C	85	GLY	2.1
1	D	161	ILE	2.1
1	B	470	PHE	2.1
1	D	165	GLY	2.1
1	D	169	LEU	2.1
1	C	271	ASP	2.1
1	D	241	ASP	2.1
1	B	736	SER	2.1
1	D	253	LEU	2.1
1	C	601	ASP	2.1
1	A	470	PHE	2.0
1	C	774	PHE	2.0
1	D	735	VAL	2.0
1	B	756	LEU	2.0
1	C	780	ILE	2.0
1	D	731	PHE	2.0
1	D	172	LEU	2.0
1	D	798	LEU	2.0
1	D	115	ASN	2.0

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

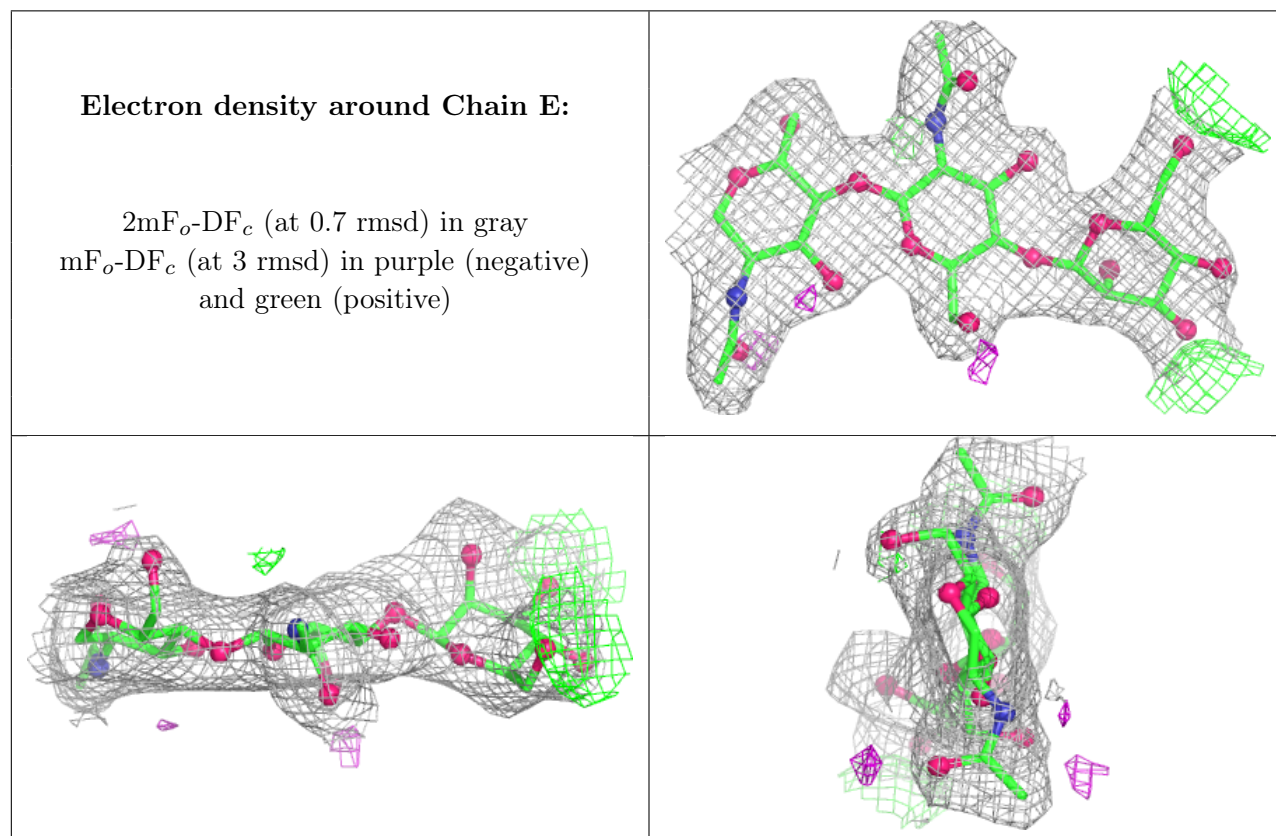
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

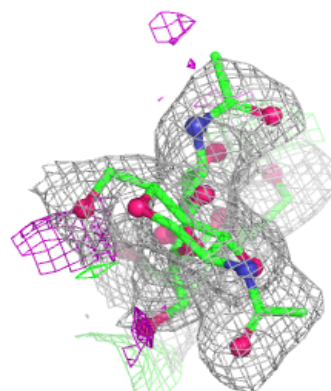
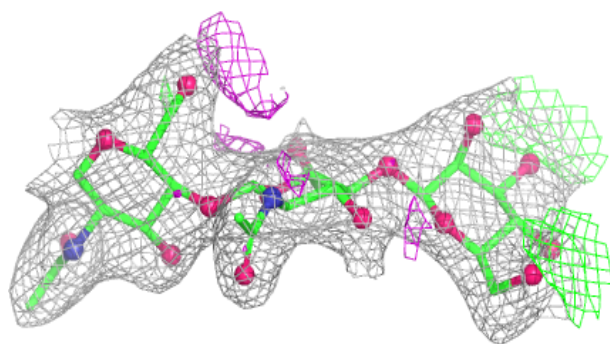
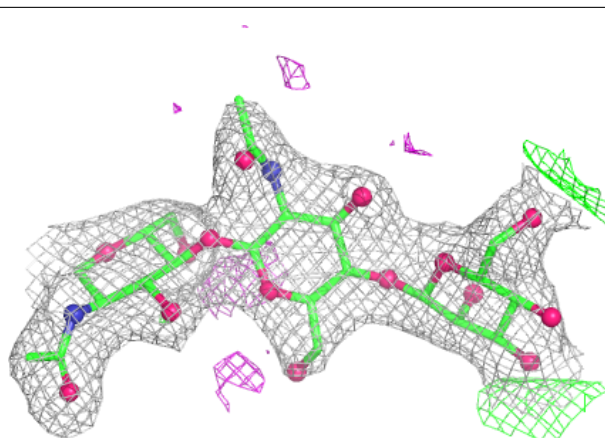
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	N	3	11/12	0.70	0.14	72,79,85,90	0
2	BMA	H	3	11/12	0.81	0.12	44,55,60,61	0
2	BMA	E	3	11/12	0.81	0.10	44,48,54,54	0
2	BMA	K	3	11/12	0.83	0.11	44,54,62,63	0
2	BMA	G	3	11/12	0.83	0.10	52,56,63,70	0
2	BMA	P	3	11/12	0.83	0.13	53,60,77,78	0
2	BMA	M	3	11/12	0.85	0.09	59,66,77,81	0
3	NAG	L	2	14/15	0.86	0.09	47,55,62,65	0
2	BMA	J	3	11/12	0.89	0.08	50,55,60,60	0
3	NAG	I	2	14/15	0.91	0.08	53,60,65,66	0
3	NAG	O	2	14/15	0.91	0.09	58,62,67,70	0
3	NAG	F	2	14/15	0.92	0.08	43,51,57,60	0
2	NAG	N	2	14/15	0.92	0.09	58,66,75,82	0
2	NAG	P	2	14/15	0.93	0.07	37,47,51,55	0
2	NAG	N	1	14/15	0.94	0.08	55,61,69,69	0
2	NAG	K	2	14/15	0.95	0.06	39,45,49,52	0
2	NAG	G	2	14/15	0.95	0.08	39,44,51,53	0
3	NAG	O	1	14/15	0.95	0.07	38,42,44,51	0
2	NAG	K	1	14/15	0.95	0.08	38,41,44,45	0
3	NAG	F	1	14/15	0.96	0.06	32,34,42,42	0
2	NAG	G	1	14/15	0.96	0.05	34,37,38,41	0
2	NAG	H	1	14/15	0.96	0.07	35,40,44,46	0
2	NAG	M	1	14/15	0.96	0.06	45,46,50,50	0
2	NAG	M	2	14/15	0.96	0.07	44,49,53,54	0
2	NAG	H	2	14/15	0.96	0.06	36,45,54,58	0
2	NAG	E	1	14/15	0.97	0.06	30,33,39,50	0
3	NAG	I	1	14/15	0.97	0.06	34,37,41,47	0
2	NAG	P	1	14/15	0.97	0.05	37,44,50,55	0
3	NAG	L	1	14/15	0.97	0.06	38,41,45,48	0
2	NAG	J	1	14/15	0.97	0.05	32,38,40,41	0
2	NAG	J	2	14/15	0.97	0.05	37,39,47,51	0
2	NAG	E	2	14/15	0.97	0.06	30,34,42,44	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.

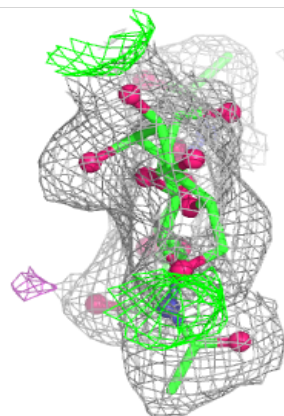
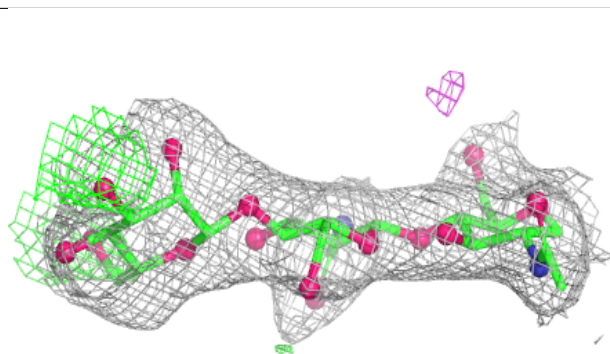
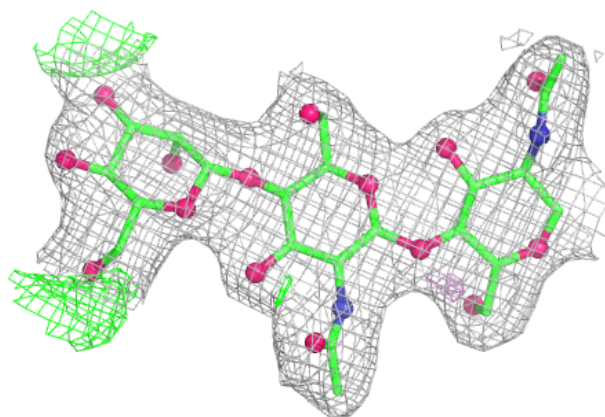


Electron density around Chain G:

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

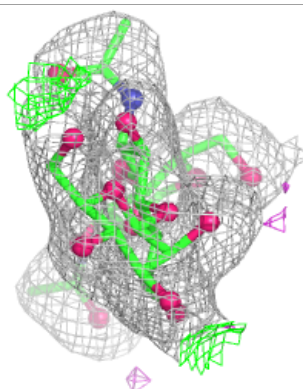
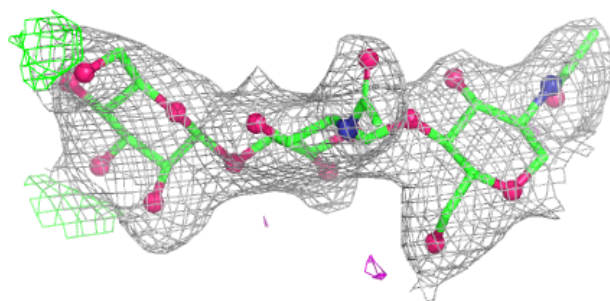
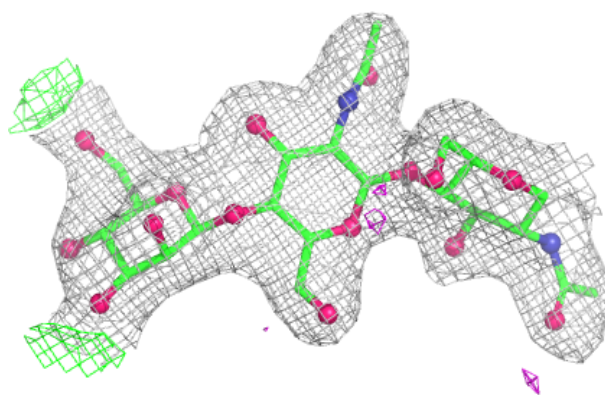
**Electron density around Chain H:**

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

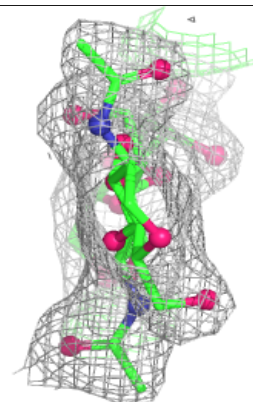
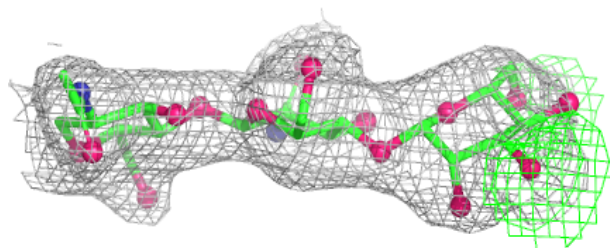
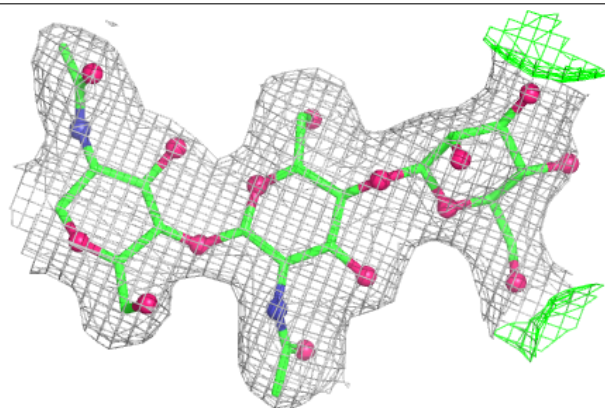


Electron density around Chain J:

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

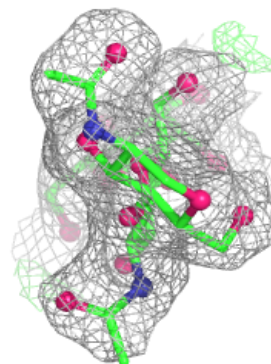
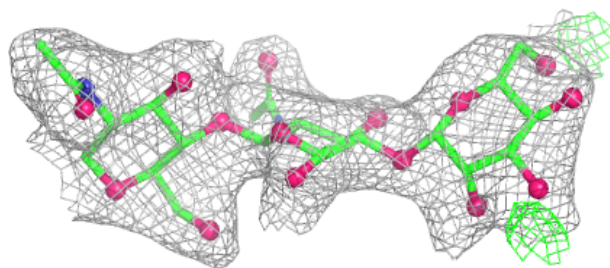
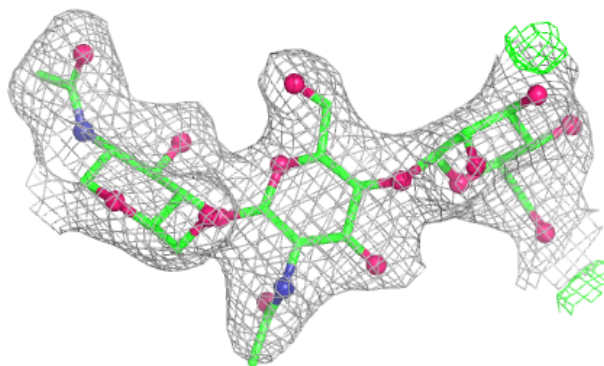
**Electron density around Chain K:**

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

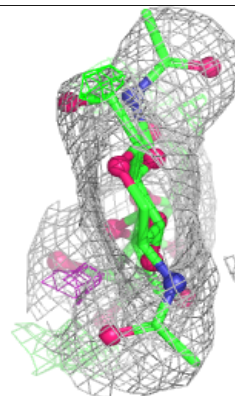
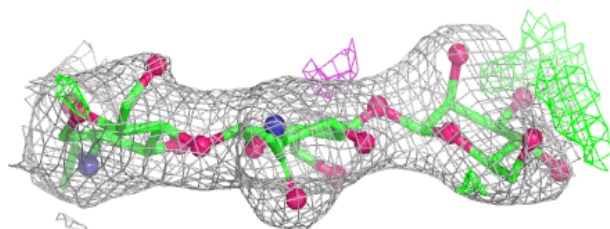
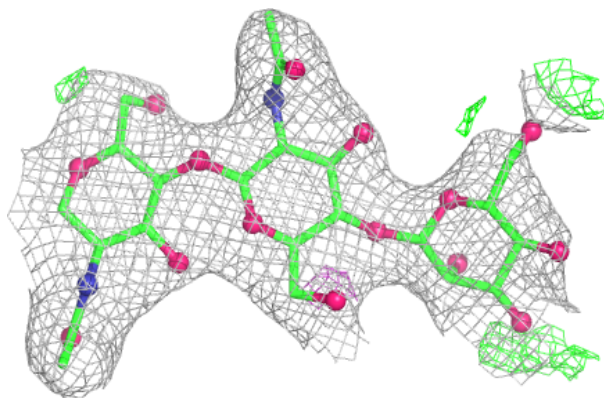


Electron density around Chain M:

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

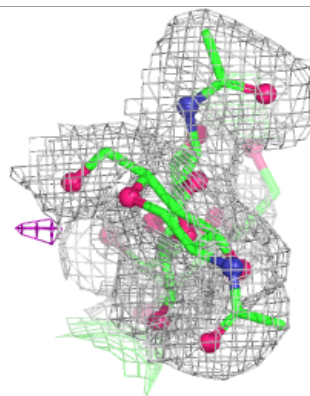
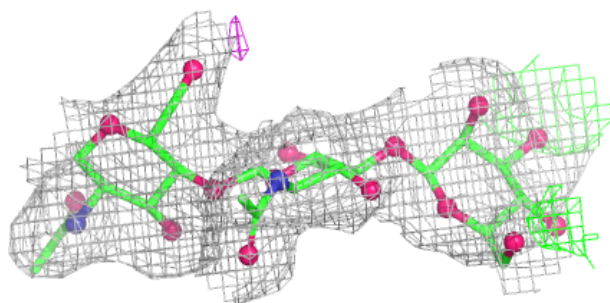
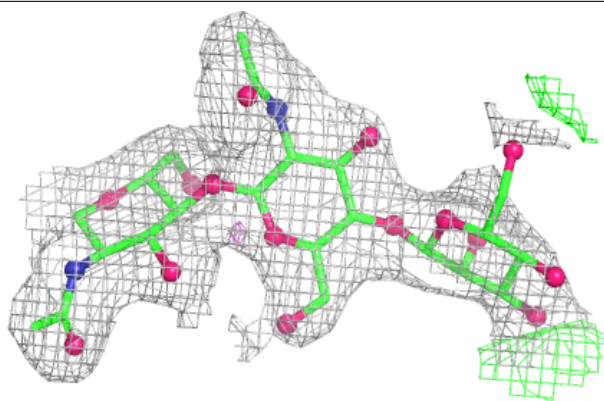
**Electron density around Chain N:**

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

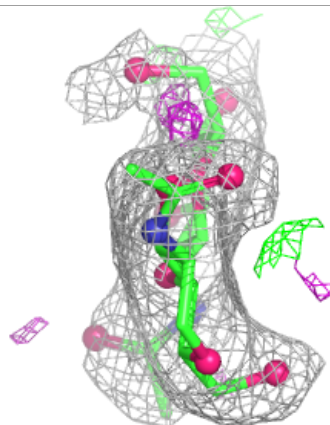
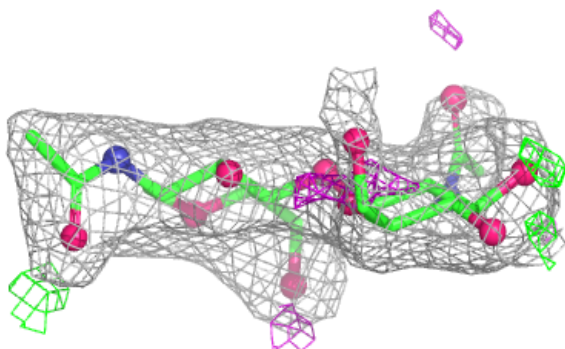
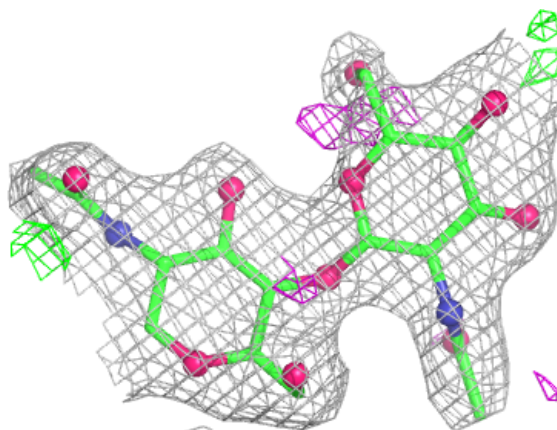


Electron density around Chain P:

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

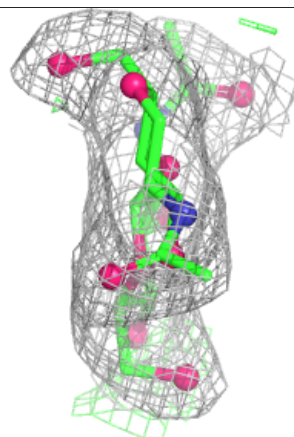
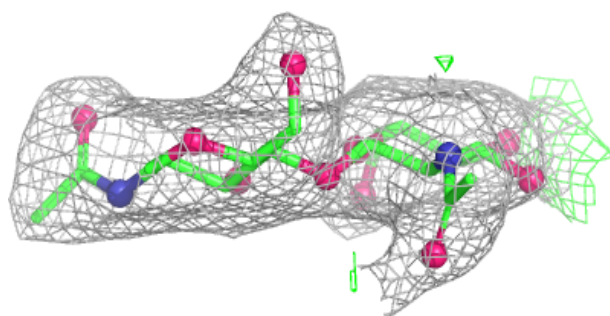
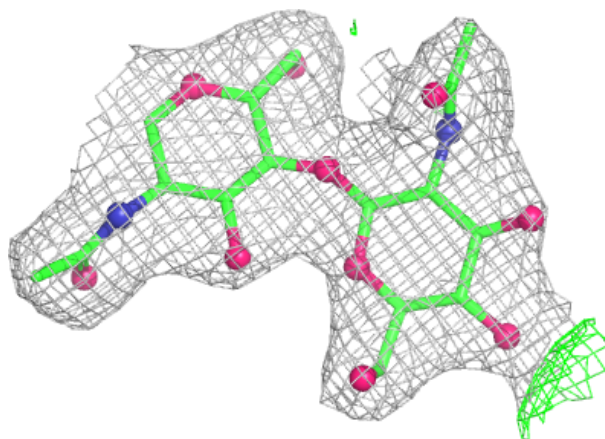
**Electron density around Chain F:**

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



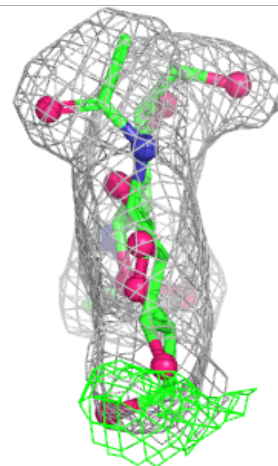
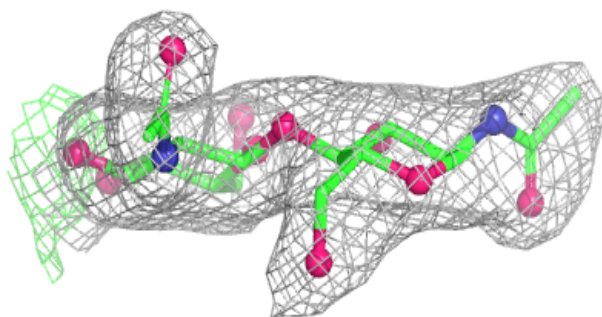
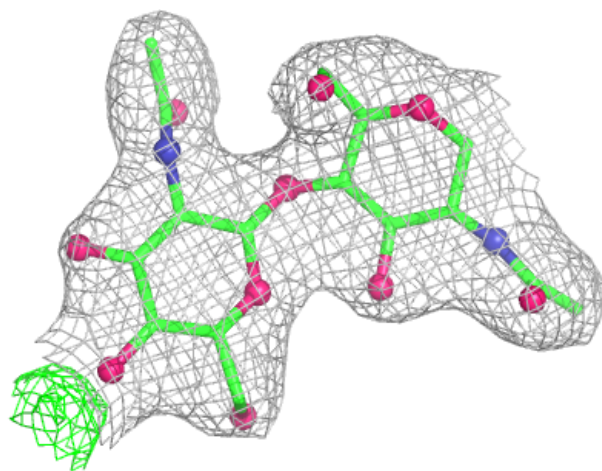
Electron density around Chain I:

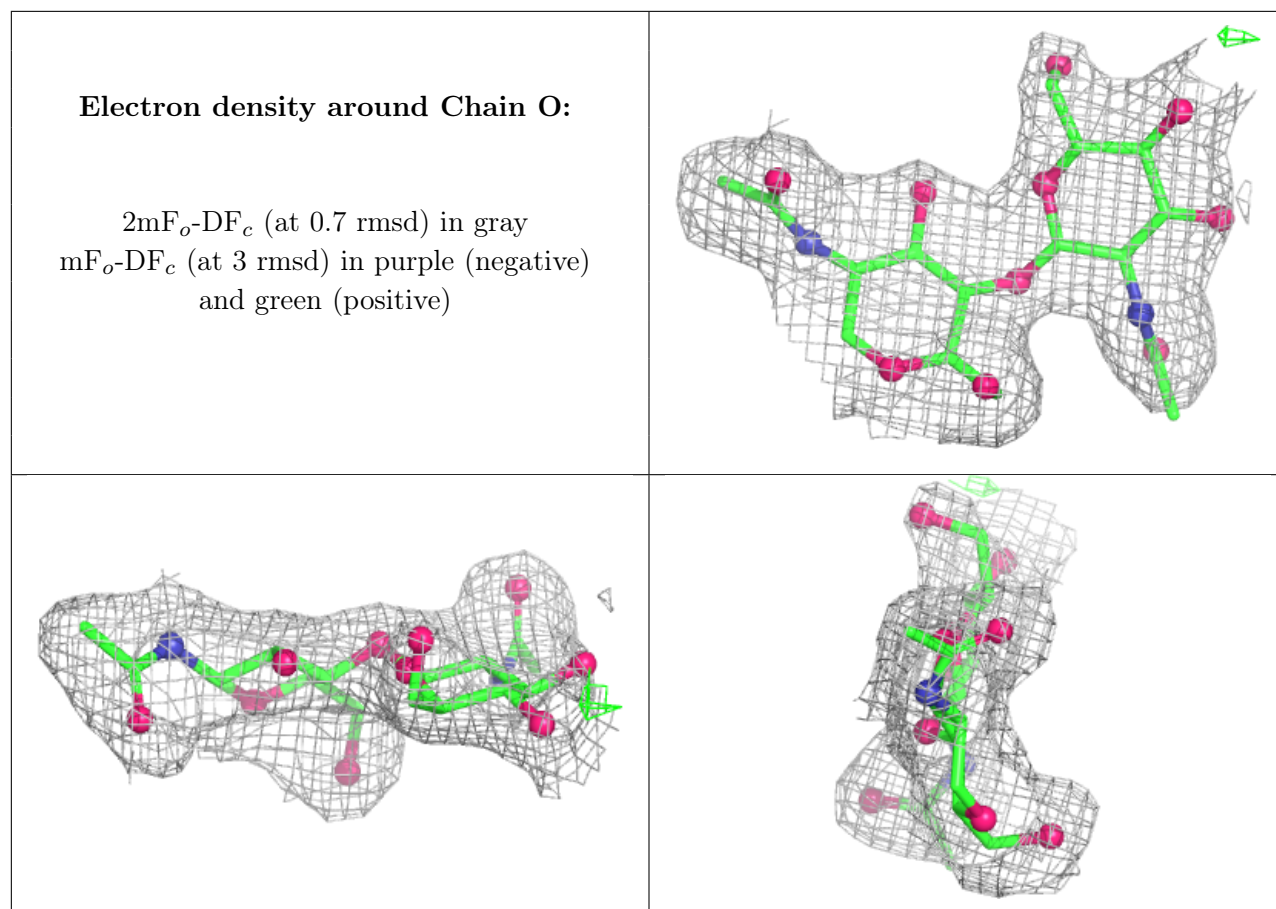
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

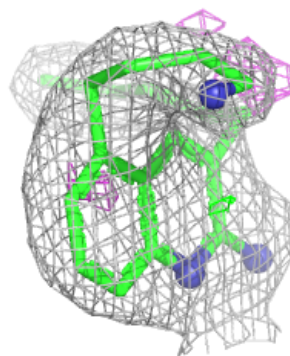
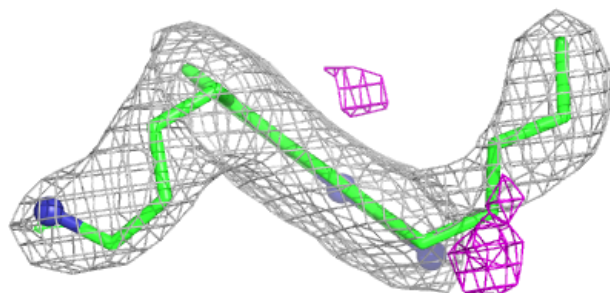
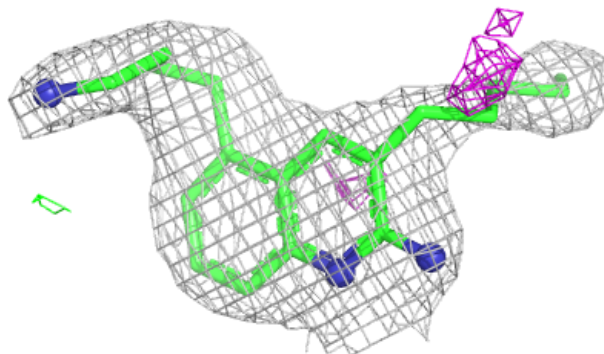
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NAG	C	1006	14/15	0.80	0.14	74,83,107,117	0
4	NAG	D	907	14/15	0.88	0.11	56,69,82,87	0
4	NAG	C	1010	14/15	0.89	0.09	78,82,87,88	0
4	NAG	B	907	14/15	0.89	0.12	55,62,70,72	0
4	NAG	B	911	14/15	0.91	0.07	56,59,67,70	0
4	NAG	A	1011	14/15	0.91	0.08	59,64,69,69	0
4	NAG	D	911	14/15	0.91	0.10	58,67,74,74	0
5	M4D	C	1011	21/21	0.91	0.13	48,52,61,63	0
4	NAG	A	1006	14/15	0.92	0.09	56,64,71,73	0
4	NAG	A	1010	14/15	0.92	0.09	60,70,81,85	0
5	M4D	B	901	21/21	0.95	0.09	39,42,46,47	0
5	M4D	A	1012	21/21	0.96	0.07	32,37,47,49	0
5	M4D	D	901	21/21	0.96	0.08	35,37,41,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

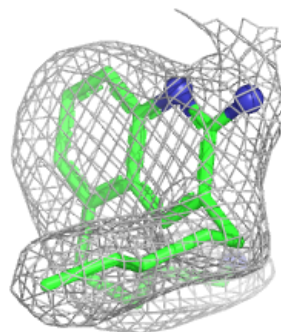
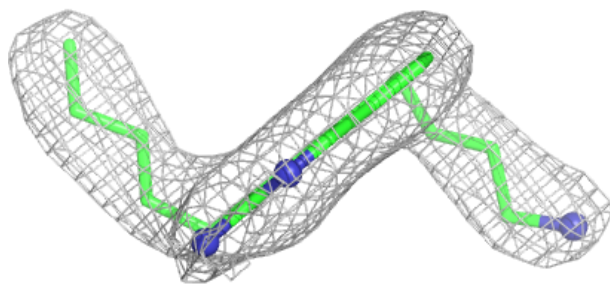
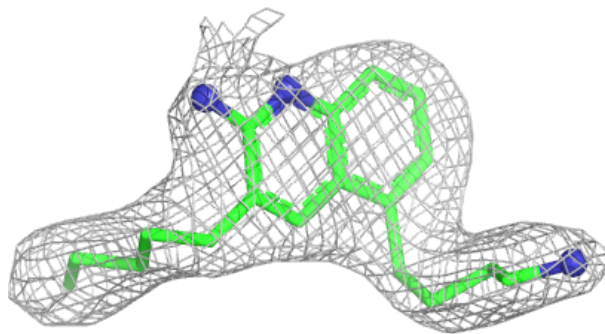
Electron density around M4D C 1011:

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

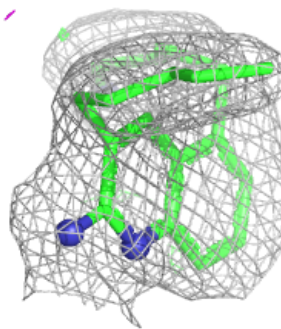
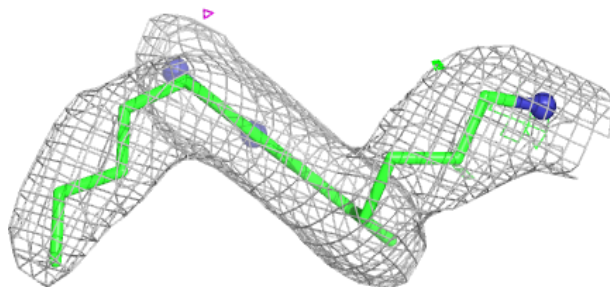
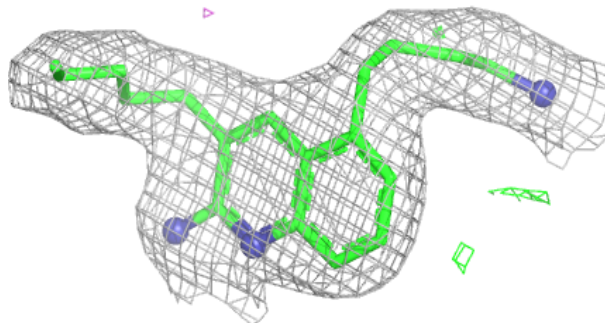


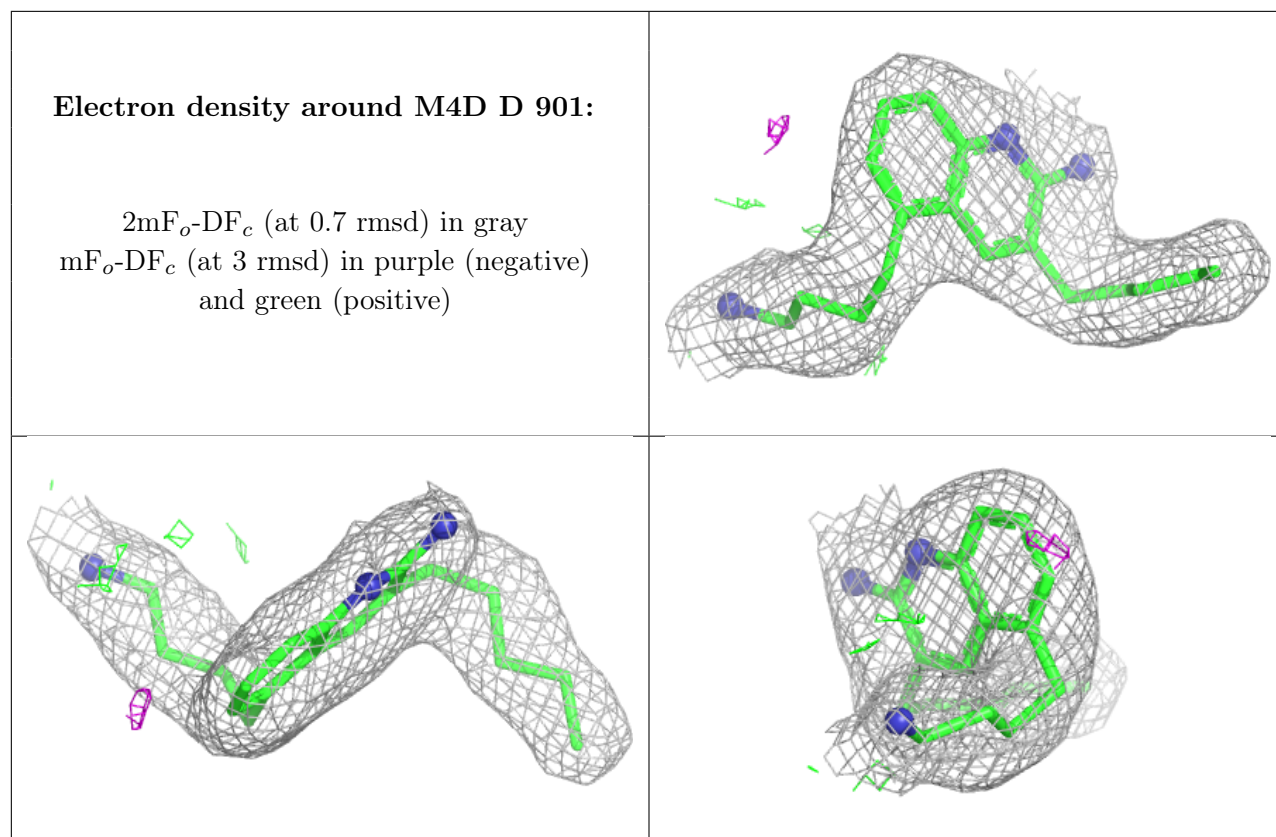
Electron density around M4D B 901:

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

**Electron density around M4D A 1012:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.