



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:37 AM UTC

PDB ID : 4G8A / pdb_00004g8a
Title : Crystal structure of human TLR4 polymorphic variant D299G and T399I in complex with MD-2 and LPS
Authors : Ohto, U.; Shimizu, T.
Deposited on : 2012-07-23
Resolution : 2.40 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:

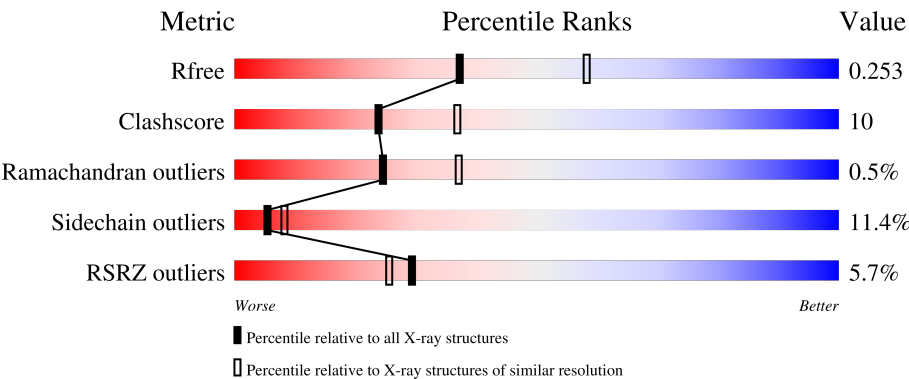
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	635	6% 68% 23% 5% 5%
1	B	635	3% 67% 24% • 5%
2	C	144	9% 70% 24% • •
2	D	144	7% 64% 28% 5% •
3	E	2	100%

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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12381 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4800	3075	790	908	27			
1	B	605	Total	C	N	O	S	0	0	0
			4836	3099	795	915	27			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ARG	-	expression tag	UNP O00206
A	4	SER	-	expression tag	UNP O00206
A	5	PRO	-	expression tag	UNP O00206
A	6	TRP	-	expression tag	UNP O00206
A	7	ASP	-	expression tag	UNP O00206
A	8	TYR	-	expression tag	UNP O00206
A	9	LYS	-	expression tag	UNP O00206
A	10	ASP	-	expression tag	UNP O00206
A	11	ASP	-	expression tag	UNP O00206
A	12	ASP	-	expression tag	UNP O00206
A	13	ASP	-	expression tag	UNP O00206
A	14	LYS	-	expression tag	UNP O00206
A	15	LEU	-	expression tag	UNP O00206
A	16	ALA	-	expression tag	UNP O00206
A	17	ALA	-	expression tag	UNP O00206
A	18	ALA	-	expression tag	UNP O00206
A	19	ASN	-	expression tag	UNP O00206
A	20	SER	-	expression tag	UNP O00206
A	21	SER	-	expression tag	UNP O00206
A	22	ILE	-	expression tag	UNP O00206
A	299	GLY	ASP	engineered mutation	UNP O00206
A	399	ILE	THR	engineered mutation	UNP O00206
A	630	THR	-	expression tag	UNP O00206
A	631	GLY	-	expression tag	UNP O00206
A	632	HIS	-	expression tag	UNP O00206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	expression tag	UNP O00206
A	634	HIS	-	expression tag	UNP O00206
A	635	HIS	-	expression tag	UNP O00206
A	636	HIS	-	expression tag	UNP O00206
A	637	HIS	-	expression tag	UNP O00206
B	3	ARG	-	expression tag	UNP O00206
B	4	SER	-	expression tag	UNP O00206
B	5	PRO	-	expression tag	UNP O00206
B	6	TRP	-	expression tag	UNP O00206
B	7	ASP	-	expression tag	UNP O00206
B	8	TYR	-	expression tag	UNP O00206
B	9	LYS	-	expression tag	UNP O00206
B	10	ASP	-	expression tag	UNP O00206
B	11	ASP	-	expression tag	UNP O00206
B	12	ASP	-	expression tag	UNP O00206
B	13	ASP	-	expression tag	UNP O00206
B	14	LYS	-	expression tag	UNP O00206
B	15	LEU	-	expression tag	UNP O00206
B	16	ALA	-	expression tag	UNP O00206
B	17	ALA	-	expression tag	UNP O00206
B	18	ALA	-	expression tag	UNP O00206
B	19	ASN	-	expression tag	UNP O00206
B	20	SER	-	expression tag	UNP O00206
B	21	SER	-	expression tag	UNP O00206
B	22	ILE	-	expression tag	UNP O00206
B	299	GLY	ASP	engineered mutation	UNP O00206
B	399	ILE	THR	engineered mutation	UNP O00206
B	630	THR	-	expression tag	UNP O00206
B	631	GLY	-	expression tag	UNP O00206
B	632	HIS	-	expression tag	UNP O00206
B	633	HIS	-	expression tag	UNP O00206
B	634	HIS	-	expression tag	UNP O00206
B	635	HIS	-	expression tag	UNP O00206
B	636	HIS	-	expression tag	UNP O00206
B	637	HIS	-	expression tag	UNP O00206

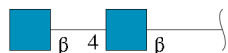
- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			
2	D	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			

There are 2 discrepancies between the modelled and reference sequences:

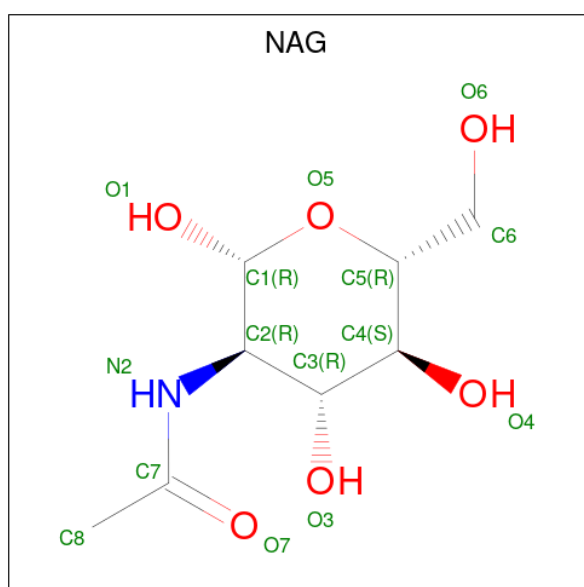
Chain	Residue	Modelled	Actual	Comment	Reference
C	56	GLY	ARG	engineered mutation	UNP Q9Y6Y9
D	56	GLY	ARG	engineered mutation	UNP Q9Y6Y9

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



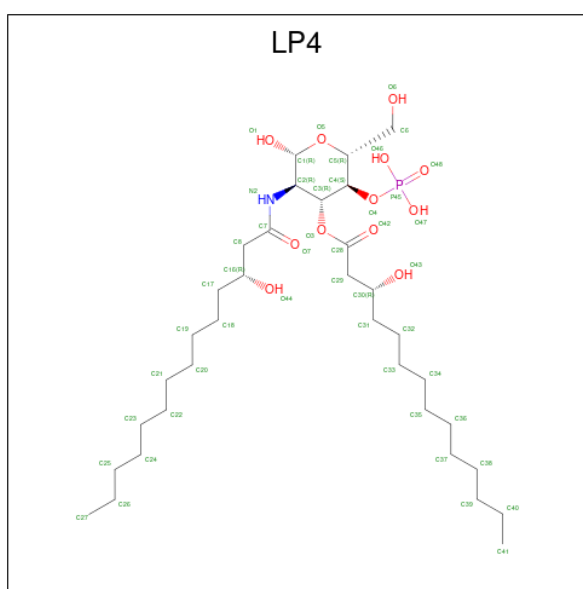
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



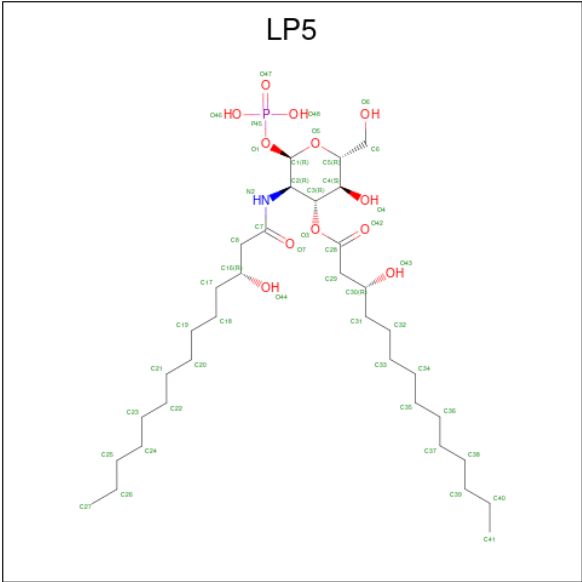
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-deoxy-3-O-[(3R)-3-hydroxytetradecanoyl]-2-[[[(3R)-3-hydroxytetradecanoyl] amino]-4-O-phosphono-beta-D-glucopyranose (CCD ID: LP4) (formula: C₃₄H₆₆NO₁₂P).



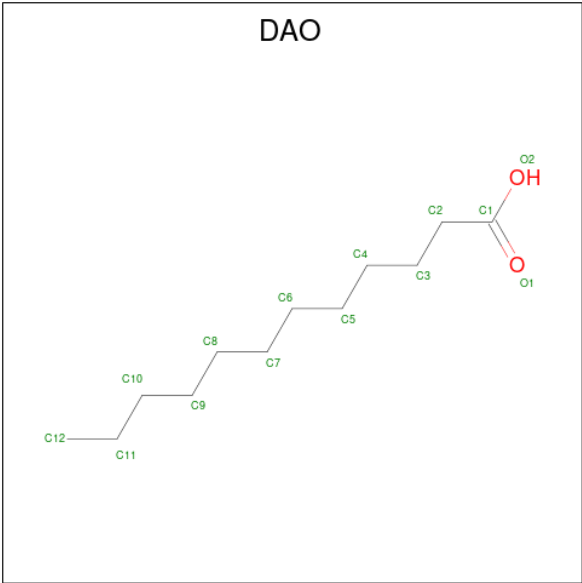
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			45	32	1	11	1		
5	D	1	Total	C	N	O	P	0	0
			45	32	1	11	1		

- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (CCD ID: LP5) (formula: C₃₄H₆₆NO₁₂P).



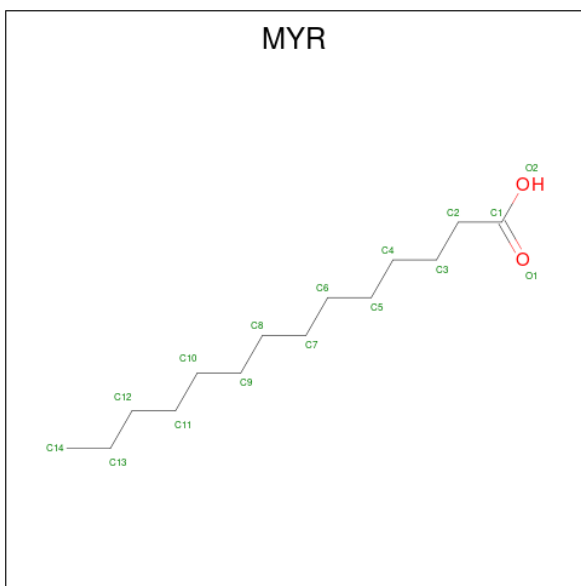
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 48	C 34	N 1	O 12	P 1	0	0
6	D	1	Total 48	C 34	N 1	O 12	P 1	0	0

- Molecule 7 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



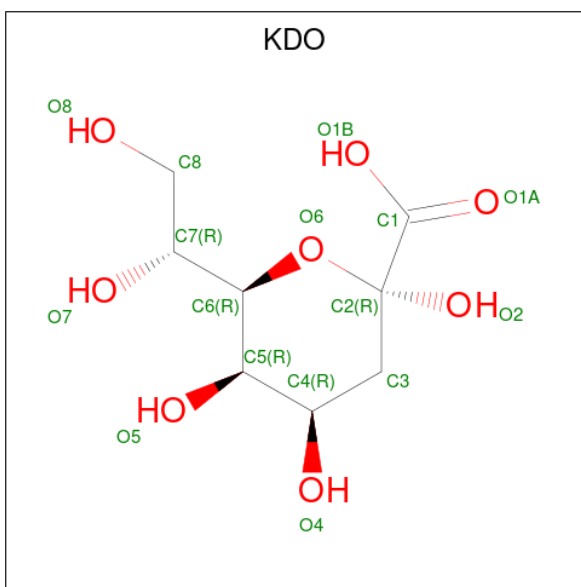
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	C O	0	0
			13	12 1		
7	D	1	Total	C O	0	0
			13	12 1		

- Molecule 8 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			15	14	1		
8	D	1	Total	C	O	0	0
			15	14	1		

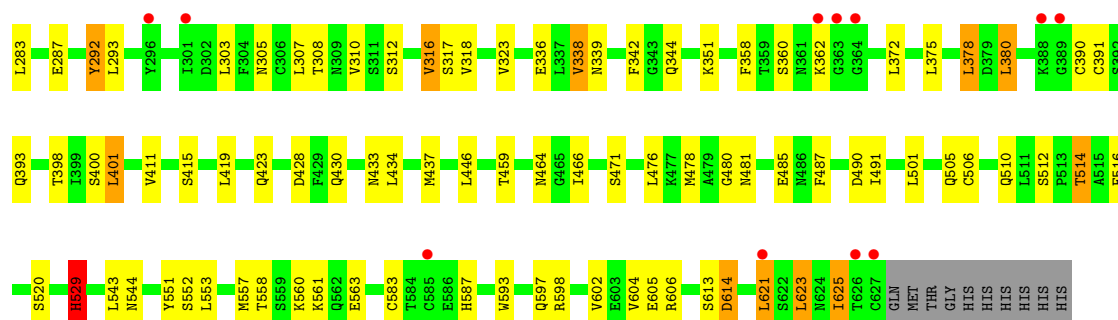
- Molecule 9 is 3-deoxy- α -D-manno-oct-2-ulopyranosonic acid (CCD ID: KDO) (formula: $C_8H_{14}O_8$).



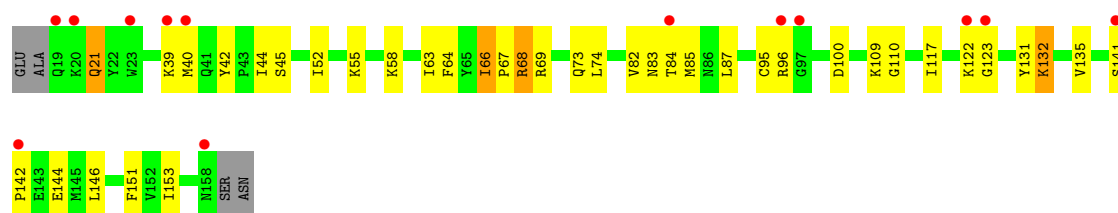
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			15	8	7		
9	D	1	Total	C	O	0	0
			15	8	7		

- Molecule 10 is water.

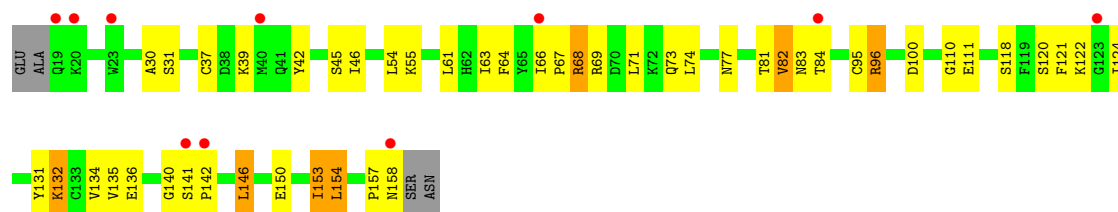
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	15	Total	O	0	0
			15	15		
10	B	21	Total	O	0	0
			21	21		
10	D	3	Total	O	0	0
			3	3		



• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96



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



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

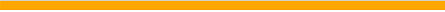


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

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

Chain H:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.04Å 124.68Å 109.14Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	39.18 – 2.40 39.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.18-2.40) 88.8 (39.18-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.249 (Not available) , 0.253	Depositor DCC
R_{free} test set	3769 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12381	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: LP5, DAO, MYR, KDO, NAG, LP4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	0/4900	0.88	4/6634 (0.1%)
1	B	0.70	3/4939 (0.1%)	0.86	3/6688 (0.0%)
2	C	0.68	0/1159	0.93	0/1562
2	D	0.67	0/1159	0.91	1/1562 (0.1%)
All	All	0.69	3/12157 (0.0%)	0.88	8/16446 (0.0%)

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
2	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	VAL	CA-CB	6.46	1.59	1.54
1	B	32	VAL	CA-CB	-5.48	1.47	1.54
1	B	529	HIS	CG-CD2	5.19	1.41	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	THR	CA-C-N	-7.25	109.80	120.46
1	A	611	THR	C-N-CA	-7.25	109.80	120.46
1	A	362	LYS	N-CA-C	5.87	117.95	110.61
1	B	201	MET	N-CA-C	5.81	118.05	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	GLU	N-CA-C	5.61	118.61	108.69
1	A	46	TYR	N-CA-C	-5.60	106.29	113.23
2	D	82	VAL	CB-CA-C	-5.57	102.87	110.77
1	B	33	VAL	CB-CA-C	-5.03	105.08	110.16

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	ALA	Peptide
2	C	122	LYS	Peptide
2	C	141	SER	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	4800	0	4750	97	0
1	B	4836	0	4779	102	0
2	C	1133	0	1129	23	0
2	D	1133	0	1129	29	0
3	E	28	0	25	2	0
3	F	28	0	25	2	0
3	G	28	0	25	0	0
3	H	28	0	25	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	C	45	0	52	5	0
5	D	45	0	52	3	0
6	C	48	0	63	4	0
6	D	48	0	63	4	0
7	C	13	0	23	1	0
7	D	13	0	23	0	0
8	C	15	0	27	0	0
8	D	15	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	15	0	12	0	0
9	D	15	0	12	0	0
10	A	15	0	0	1	0
10	B	21	0	0	0	0
10	D	3	0	0	0	0
All	All	12381	0	12293	249	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 10.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:VAL:HG11	1:B:621:LEU:HG	1.50	0.94
2:D:81:THR:HB	2:D:132:LYS:HG3	1.49	0.93
2:C:42:TYR:CE1	2:C:68:ARG:HG3	2.04	0.93
2:D:96:ARG:HG2	2:D:96:ARG:HH21	1.38	0.84
1:B:287:GLU:HG2	1:B:312:SER:HB3	1.62	0.82
1:B:202:PRO:O	1:B:204:LEU:HD23	1.81	0.81
2:D:124:ILE:HD12	6:D:203:LP5:H30	1.65	0.78
1:B:598:ARG:HG2	1:B:621:LEU:HD11	1.66	0.78
1:A:195:LEU:HD23	1:A:198:LEU:HD12	1.65	0.77
1:B:400:SER:HA	1:B:423:GLN:NE2	2.00	0.77
1:A:604:VAL:HG13	1:A:621:LEU:HD13	1.68	0.76
1:A:60:ASP:OD1	1:A:62:SER:OG	2.03	0.76
1:B:375:LEU:HD21	1:B:378:LEU:HG	1.70	0.74
1:B:162:ILE:H	1:B:185:ASN:HD22	1.36	0.73
1:A:561:LYS:HD2	1:A:563:GLU:HB2	1.69	0.72
1:B:51:ASN:H	1:B:51:ASN:HD22	1.39	0.71
1:A:375:LEU:HD21	1:A:378:LEU:HG	1.73	0.71
1:A:415:SER:HB2	6:D:203:LP5:H82	1.72	0.71
2:D:69:ARG:NH1	2:D:140:GLY:HA3	2.05	0.70
1:B:598:ARG:CG	1:B:621:LEU:HD11	2.20	0.70
2:D:42:TYR:CZ	2:D:68:ARG:HG3	2.27	0.70
2:D:81:THR:OG1	2:D:132:LYS:HE2	1.90	0.70
1:A:160:ASN:HB2	1:A:185:ASN:HD21	1.57	0.69
1:B:77:PHE:HB3	1:B:80:LEU:HG	1.75	0.68
2:D:42:TYR:CE1	2:D:68:ARG:HG3	2.28	0.68
2:C:82:VAL:HG13	2:C:131:TYR:CE2	2.29	0.68
1:A:277:LEU:HG	1:A:280:LEU:HD22	1.76	0.67
1:A:323:VAL:HG12	1:A:326:PHE:HE2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:HG3	1:B:38:TYR:CE2	2.29	0.67
1:A:51:ASN:HD22	1:A:51:ASN:H	1.42	0.67
1:B:160:ASN:HB2	1:B:185:ASN:HD21	1.59	0.67
1:A:270:GLU:HG3	10:A:805:HOH:O	1.95	0.66
1:A:228:LEU:HD22	1:A:253:LEU:HD11	1.78	0.65
1:B:48:ILE:HD12	1:B:48:ILE:H	1.60	0.65
1:A:324:LYS:HE2	1:A:344:GLN:HE22	1.62	0.65
2:C:42:TYR:CZ	2:C:68:ARG:HG3	2.32	0.65
1:B:583:CYS:HB3	1:B:623:LEU:HD11	1.78	0.64
1:A:135:GLU:HA	1:A:159:HIS:O	1.98	0.64
2:C:67:PRO:O	2:C:109:LYS:O	2.16	0.64
1:A:537:THR:OG1	1:A:563:GLU:O	2.16	0.63
1:A:323:VAL:HG12	1:A:326:PHE:CE2	2.33	0.63
1:B:593:TRP:O	1:B:597:GLN:HG2	1.99	0.63
2:D:71:LEU:CD2	2:D:146:LEU:HD11	2.29	0.62
1:A:87:ARG:HG2	2:C:66:ILE:HD11	1.83	0.61
1:A:583:CYS:HA	1:A:591:LEU:HD11	1.81	0.61
1:B:604:VAL:HG11	1:B:621:LEU:CG	2.29	0.61
2:D:134:VAL:HG22	2:D:150:GLU:HG3	1.83	0.61
2:C:96:ARG:HG2	2:C:100:ASP:OD1	2.01	0.60
1:B:623:LEU:HD13	1:B:625:ILE:HG12	1.81	0.60
1:A:326:PHE:HB3	1:A:348:LEU:HD23	1.84	0.60
1:B:437:MET:HE3	1:B:466:ILE:HD11	1.84	0.60
1:A:604:VAL:CG1	1:A:621:LEU:HD13	2.32	0.60
1:B:464:ASN:HA	1:B:491:ILE:HG22	1.84	0.59
2:C:117:ILE:HD13	5:C:202:LP4:H35	1.82	0.59
1:B:378:LEU:HB2	1:B:401:LEU:HD21	1.84	0.59
1:A:561:LYS:C	1:A:563:GLU:H	2.10	0.59
2:D:96:ARG:HG2	2:D:96:ARG:NH2	2.14	0.59
1:A:538:PHE:HB2	1:A:563:GLU:HG2	1.85	0.59
2:D:73:GLN:HA	2:D:95:CYS:O	2.02	0.58
1:A:62:SER:HB2	1:A:63:PHE:HD1	1.68	0.58
2:C:40:MET:HB3	2:C:42:TYR:CZ	2.39	0.58
1:A:448:ASN:O	1:A:450:ILE:HD12	2.03	0.58
1:B:218:ILE:HD12	1:B:246:CYS:HB3	1.85	0.57
1:B:156:ASN:C	1:B:156:ASN:HD22	2.12	0.57
1:B:419:LEU:HD12	2:C:123:GLY:HA2	1.87	0.57
1:B:552:SER:OG	3:H:1:NAG:H82	2.05	0.57
1:A:612:PRO:HG2	1:A:615:LYS:HB2	1.87	0.56
1:B:529:HIS:HA	1:B:553:LEU:O	2.06	0.56
1:B:48:ILE:HD12	1:B:48:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:HE1	1:B:272:PHE:CE2	2.42	0.55
1:A:323:VAL:HG11	1:A:342:PHE:CD2	2.41	0.55
1:B:280:LEU:HD23	1:B:307:LEU:HD21	1.89	0.54
1:B:602:VAL:HG11	3:H:1:NAG:H61	1.90	0.54
1:A:195:LEU:HD13	1:A:222:ALA:O	2.08	0.54
1:A:358:PHE:HB3	1:A:380:LEU:HD12	1.90	0.53
1:B:48:ILE:H	1:B:48:ILE:CD1	2.22	0.53
1:B:372:LEU:O	1:B:398:THR:HB	2.09	0.53
1:B:358:PHE:HB3	1:B:380:LEU:HD12	1.91	0.53
1:A:339:ASN:HA	1:A:360:SER:O	2.09	0.53
1:B:92:THR:HA	1:B:116:SER:O	2.09	0.53
1:B:560:LYS:HB2	1:B:563:GLU:HG2	1.92	0.52
1:B:166:LYS:HD2	1:B:194:ASP:HA	1.91	0.52
1:B:481:ASN:O	1:B:506:CYS:HA	2.10	0.51
1:B:598:ARG:HD3	1:B:598:ARG:C	2.36	0.51
2:C:82:VAL:O	2:C:83:ASN:C	2.53	0.51
1:B:212:LEU:HD21	1:B:266:GLU:CG	2.41	0.51
2:D:82:VAL:O	2:D:83:ASN:C	2.54	0.51
1:B:305:ASN:O	1:B:308:THR:HG23	2.11	0.51
1:B:316:VAL:HB	1:B:338:VAL:HG22	1.93	0.50
1:A:31:GLU:HG3	1:A:38:TYR:CE2	2.45	0.50
2:D:63:ILE:HD13	5:D:202:LP4:H38A	1.93	0.50
1:B:323:VAL:HG11	1:B:342:PHE:HB3	1.93	0.50
1:B:400:SER:HA	1:B:423:GLN:HE21	1.72	0.50
1:B:459:THR:O	1:B:481:ASN:HB3	2.11	0.50
1:A:336:GLU:HG2	1:A:338:VAL:HG12	1.94	0.50
2:D:141:SER:OG	2:D:142:PRO:CD	2.59	0.50
3:E:2:NAG:O6	3:F:1:NAG:H82	2.11	0.50
1:B:476:LEU:HD11	1:B:478:MET:SD	2.52	0.50
1:A:614:ASP:OD2	1:A:615:LYS:HE2	2.11	0.49
2:C:73:GLN:HA	2:C:95:CYS:O	2.12	0.49
2:D:141:SER:OG	2:D:142:PRO:HD3	2.12	0.49
1:A:366:ALA:HA	1:A:386:SER:HB3	1.94	0.49
2:D:30:ALA:HB1	2:D:153:ILE:HD12	1.93	0.49
1:A:156:ASN:ND2	1:A:158:ALA:H	2.11	0.49
1:B:490:ASP:OD1	1:B:514:THR:HG22	2.13	0.49
1:A:286:GLU:O	1:A:310:VAL:HG22	2.12	0.49
1:A:563:GLU:C	1:A:565:GLN:H	2.20	0.49
1:B:197:VAL:HA	1:B:200:GLN:NE2	2.27	0.49
1:B:317:SER:HA	1:B:339:ASN:O	2.13	0.49
1:A:372:LEU:O	1:A:398:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HG	1:A:280:LEU:CD2	2.43	0.48
1:B:156:ASN:HD22	1:B:157:VAL:N	2.11	0.48
1:B:201:MET:HA	1:B:202:PRO:HD3	1.68	0.48
1:B:476:LEU:HD12	1:B:501:LEU:CD1	2.43	0.48
1:A:272:PHE:CE1	1:A:303:LEU:HD21	2.48	0.48
1:B:87:ARG:HD3	2:D:110:GLY:O	2.14	0.48
1:B:428:ASP:OD1	1:B:430:GLN:HB2	2.13	0.48
1:B:604:VAL:CG1	1:B:621:LEU:HG	2.33	0.48
1:B:212:LEU:HD21	1:B:266:GLU:HG2	1.95	0.47
2:D:67:PRO:HD2	2:D:111:GLU:O	2.15	0.47
2:D:81:THR:O	2:D:131:TYR:HA	2.13	0.47
1:B:130:LYS:HG3	1:B:154:GLU:HG3	1.96	0.47
1:B:520:SER:HB2	1:B:544:ASN:HD22	1.79	0.47
1:A:66:LEU:C	1:A:68:HIS:H	2.22	0.47
1:B:339:ASN:HA	1:B:360:SER:O	2.14	0.47
1:B:476:LEU:HD13	1:B:476:LEU:C	2.39	0.47
1:A:51:ASN:HD22	1:A:51:ASN:N	2.08	0.47
1:A:256:HIS:O	1:A:286:GLU:HB3	2.14	0.47
1:A:479:ALA:HA	1:A:504:SER:O	2.14	0.47
1:B:598:ARG:HD3	1:B:598:ARG:O	2.15	0.47
1:A:156:ASN:C	1:A:156:ASN:HD22	2.22	0.47
1:A:470:LEU:HB2	1:A:495:LEU:CD2	2.45	0.47
2:D:69:ARG:HH12	2:D:140:GLY:HA3	1.79	0.47
1:A:437:MET:HE3	1:A:466:ILE:HD11	1.97	0.46
1:A:77:PHE:HB3	1:A:80:LEU:HG	1.98	0.46
1:B:247:ILE:HA	1:B:250:LEU:HD22	1.96	0.46
5:D:202:LP4:H22A	6:D:203:LP5:H371	1.97	0.46
2:D:96:ARG:HG2	2:D:100:ASP:OD1	2.15	0.46
1:B:415:SER:HB2	6:C:203:LP5:H81	1.96	0.46
1:A:323:VAL:HG21	1:A:344:GLN:O	2.15	0.46
1:A:564:LEU:HD22	1:A:593:TRP:CD2	2.50	0.46
1:B:262:GLU:O	1:B:292:TYR:HB3	2.16	0.46
1:B:434:LEU:HD13	1:B:437:MET:SD	2.56	0.46
1:A:191:TYR:O	1:A:194:ASP:HB2	2.15	0.46
2:C:69:ARG:CZ	2:C:144:GLU:HB2	2.46	0.46
1:B:433:ASN:C	1:B:433:ASN:HD22	2.24	0.46
1:A:125:LEU:HB3	1:A:128:LEU:HB2	1.98	0.46
1:A:360:SER:HA	1:A:382:ARG:O	2.15	0.46
1:A:496:ARG:HH11	1:A:518:SER:HB2	1.80	0.46
1:B:516:PHE:HB3	1:B:543:LEU:HD21	1.97	0.46
1:A:293:LEU:HD13	1:A:295:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLU:C	1:A:565:GLN:N	2.74	0.45
1:B:63:PHE:HA	1:B:87:ARG:O	2.16	0.45
1:B:112:ASN:O	1:B:136:THR:HA	2.16	0.45
1:A:51:ASN:H	1:A:51:ASN:ND2	2.13	0.45
1:A:338:VAL:HA	1:A:359:THR:O	2.16	0.45
1:B:195:LEU:HD23	1:B:198:LEU:HD12	1.99	0.45
1:A:169:GLU:HG2	1:A:196:ARG:HH22	1.81	0.45
1:B:336:GLU:HG2	1:B:338:VAL:HG13	1.99	0.45
2:C:63:ILE:CD1	5:C:202:LP4:H38A	2.47	0.45
2:D:31:SER:HB3	2:D:154:LEU:HB2	1.99	0.45
1:B:156:ASN:ND2	1:B:158:ALA:H	2.15	0.45
1:B:263:PHE:HB2	1:B:266:GLU:HB2	1.98	0.45
1:A:149:LEU:O	1:A:152:LEU:HB2	2.17	0.45
1:A:320:ILE:O	1:A:342:PHE:HA	2.18	0.44
1:A:154:GLU:HB3	1:A:179:HIS:HB2	1.99	0.44
1:A:317:SER:HA	1:A:339:ASN:O	2.17	0.44
1:B:74:PHE:HB2	1:B:101:LEU:HD11	2.00	0.44
1:B:233:LEU:HD23	1:B:236:ASN:ND2	2.32	0.44
1:A:167:LEU:HD12	1:A:198:LEU:HG	2.00	0.44
1:B:66:LEU:O	1:B:68:HIS:N	2.47	0.44
1:A:110:THR:HA	1:A:134:VAL:O	2.16	0.43
2:C:52:ILE:HG21	6:C:203:LP5:H362	2.00	0.43
1:A:104:LEU:HB3	1:A:125:LEU:HD12	1.99	0.43
1:B:93:ILE:HB	1:B:117:LEU:HD12	2.01	0.43
1:B:44:ASN:HD22	1:B:44:ASN:HA	1.64	0.43
1:B:243:MET:CE	1:B:276:ALA:HB1	2.48	0.43
1:A:563:GLU:O	1:A:565:GLN:N	2.51	0.43
1:B:135:GLU:HA	1:B:159:HIS:O	2.19	0.43
1:B:220:PRO:HA	1:B:249:GLY:HA2	2.00	0.43
1:B:598:ARG:HG3	1:B:621:LEU:HD11	1.97	0.43
2:D:77:ASN:HB2	2:D:136:GLU:HB3	2.01	0.43
1:A:81:GLN:C	1:A:104:LEU:HD12	2.43	0.43
2:C:117:ILE:HG21	5:C:202:LP4:H33	2.01	0.43
1:A:189:SER:HA	1:A:217:PHE:O	2.18	0.43
1:A:39:GLN:NE2	1:A:60:ASP:OD2	2.52	0.43
1:A:378:LEU:HB2	1:A:401:LEU:HD21	2.01	0.43
1:B:400:SER:HA	1:B:423:GLN:HE22	1.78	0.43
2:D:118:SER:OG	5:D:202:LP4:O47	2.30	0.43
1:A:66:LEU:O	1:A:68:HIS:N	2.49	0.42
1:B:487:PHE:HD2	1:B:510:GLN:HB2	1.84	0.42
1:A:583:CYS:H	1:A:612:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HA	1:B:134:VAL:O	2.19	0.42
1:A:447:ARG:HE	1:A:447:ARG:HB2	1.61	0.42
1:A:561:LYS:C	1:A:563:GLU:N	2.77	0.42
1:B:156:ASN:C	1:B:156:ASN:ND2	2.77	0.42
2:C:63:ILE:HD13	5:C:202:LP4:H38A	2.00	0.42
1:A:87:ARG:HD3	2:C:110:GLY:O	2.19	0.42
1:A:464:ASN:HA	1:A:491:ILE:HG22	2.01	0.42
1:B:191:TYR:O	1:B:194:ASP:HB2	2.20	0.42
1:A:87:ARG:HG2	2:C:66:ILE:CD1	2.48	0.42
1:B:92:THR:HB	1:B:116:SER:HB3	2.02	0.42
1:B:133:ALA:HB3	1:B:157:VAL:HG12	2.01	0.42
1:B:170:TYR:CD1	1:B:170:TYR:C	2.98	0.42
1:B:512:SER:C	1:B:514:THR:H	2.27	0.42
2:C:132:LYS:HA	2:C:151:PHE:O	2.20	0.42
2:D:82:VAL:HG13	2:D:131:TYR:CE2	2.55	0.42
1:B:188:GLN:HA	1:B:214:PRO:O	2.20	0.42
1:B:202:PRO:HB2	1:B:203:LEU:H	1.66	0.42
1:A:477:LYS:HA	1:A:502:ASP:HB3	2.01	0.42
2:C:45:SER:HB3	2:C:64:PHE:HB3	2.01	0.42
3:E:1:NAG:HO3	3:F:2:NAG:HO6	1.64	0.42
1:A:410:GLY:HA2	1:B:411:VAL:HG21	2.01	0.42
1:A:618:MET:HE3	1:A:618:MET:HB2	1.97	0.42
1:A:301:ILE:O	1:A:302:ASP:HB2	2.20	0.42
6:C:203:LP5:H381	7:C:204:DAO:H91	2.01	0.42
1:A:247:ILE:HA	1:A:250:LEU:HD22	2.01	0.41
1:B:230:LYS:HA	1:B:257:ARG:O	2.20	0.41
1:B:253:LEU:HG	1:B:255:VAL:HG22	2.01	0.41
1:B:31:GLU:CD	1:B:34:PRO:HA	2.45	0.41
1:A:67:ARG:HA	1:A:89:GLU:O	2.20	0.41
1:B:28:PRO:HG2	1:B:43:LEU:HD13	2.01	0.41
2:C:87:LEU:HD11	6:C:203:LP5:H273	2.01	0.41
2:D:45:SER:HB3	2:D:64:PHE:HB3	2.01	0.41
2:D:121:PHE:HA	6:D:203:LP5:O4	2.21	0.41
1:A:590:PHE:O	1:A:594:ILE:HG12	2.21	0.41
1:A:156:ASN:HD22	1:A:158:ALA:H	1.65	0.41
1:A:162:ILE:H	1:A:185:ASN:HD22	1.69	0.41
1:B:247:ILE:O	1:B:250:LEU:HB2	2.21	0.41
2:C:96:ARG:N	2:C:100:ASP:OD1	2.48	0.41
1:B:480:GLY:HA2	1:B:505:GLN:O	2.19	0.41
1:A:264:ARG:NH2	5:C:202:LP4:H29A	2.36	0.41
1:B:505:GLN:HA	1:B:529:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:THR:CG2	1:B:587:HIS:CD2	3.04	0.41
2:C:21:GLN:HE21	2:C:21:GLN:HB3	1.65	0.41
2:D:46:ILE:HG23	2:D:61:LEU:HD11	2.02	0.41
2:D:157:PRO:O	2:D:158:ASN:HB3	2.21	0.41
1:B:162:ILE:H	1:B:185:ASN:ND2	2.12	0.40
1:A:36:ILE:HG23	1:A:57:LYS:HG3	2.03	0.40
1:A:257:ARG:NH1	1:A:287:GLU:OE1	2.52	0.40
1:A:300:ILE:HG13	1:A:325:ASP:HB2	2.02	0.40
1:A:138:LEU:O	1:A:160:ASN:HB3	2.21	0.40
1:A:169:GLU:CG	1:A:196:ARG:HH22	2.34	0.40
1:A:221:GLY:HA2	1:A:224:LYS:HG3	2.03	0.40
1:A:390:CYS:HA	1:A:391:CYS:HA	1.94	0.40
1:A:429:PHE:O	1:A:430:GLN:C	2.65	0.40
1:B:614:ASP:OD2	1:B:614:ASP:N	2.54	0.40
1:A:460:ARG:HD3	1:A:482:SER:OG	2.20	0.40
1:A:563:GLU:O	1:A:563:GLU:HG3	2.21	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	599/635 (94%)	559 (93%)	37 (6%)	3 (0%)	24	37
1	B	603/635 (95%)	562 (93%)	37 (6%)	4 (1%)	18	28
2	C	138/144 (96%)	131 (95%)	6 (4%)	1 (1%)	18	28
2	D	138/144 (96%)	133 (96%)	5 (4%)	0	100	100
All	All	1478/1558 (95%)	1385 (94%)	85 (6%)	8 (0%)	24	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	142	PRO
1	A	564	LEU
1	B	202	PRO
1	B	292	TYR
1	A	292	TYR
1	A	562	GLN
1	B	203	LEU
1	B	67	ARG

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	558/588 (95%)	494 (88%)	64 (12%)	5	8
1	B	562/588 (96%)	499 (89%)	63 (11%)	6	9
2	C	130/133 (98%)	116 (89%)	14 (11%)	6	9
2	D	130/133 (98%)	114 (88%)	16 (12%)	4	6
All	All	1380/1442 (96%)	1223 (89%)	157 (11%)	5	8

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	51	ASN
1	A	57	LYS
1	A	62	SER
1	A	69	LEU
1	A	80	LEU
1	A	95	ASP
1	A	125	LEU
1	A	126	SER
1	A	138	LEU
1	A	141	LEU
1	A	150	LYS
1	A	154	GLU
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	169	GLU
1	A	195	LEU
1	A	204	LEU
1	A	206	LEU
1	A	228	LEU
1	A	231	LEU
1	A	235	ASN
1	A	239	SER
1	A	240	LEU
1	A	250	LEU
1	A	255	VAL
1	A	266	GLU
1	A	270	GLU
1	A	271	LYS
1	A	280	LEU
1	A	283	LEU
1	A	293	LEU
1	A	303	LEU
1	A	307	LEU
1	A	308	THR
1	A	309	ASN
1	A	310	VAL
1	A	316	VAL
1	A	323	VAL
1	A	338	VAL
1	A	378	LEU
1	A	380	LEU
1	A	388	LYS
1	A	393	GLN
1	A	401	LEU
1	A	446	LEU
1	A	447	ARG
1	A	450	ILE
1	A	476	LEU
1	A	485	GLU
1	A	517	ASN
1	A	529	HIS
1	A	544	ASN
1	A	561	LYS
1	A	562	GLN
1	A	566	HIS
1	A	591	LEU

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Mol	Chain	Res	Type
1	A	597	GLN
1	A	598	ARG
1	A	602	VAL
1	A	613	SER
1	A	615	LYS
1	A	621	LEU
1	A	623	LEU
1	A	625	ILE
1	B	24	GLU
1	B	44	ASN
1	B	48	ILE
1	B	51	ASN
1	B	57	LYS
1	B	69	LEU
1	B	79	GLU
1	B	92	THR
1	B	116	SER
1	B	125	LEU
1	B	126	SER
1	B	138	LEU
1	B	141	LEU
1	B	151	THR
1	B	155	LEU
1	B	172	SER
1	B	175	THR
1	B	203	LEU
1	B	204	LEU
1	B	206	LEU
1	B	216	ASN
1	B	228	LEU
1	B	231	LEU
1	B	235	ASN
1	B	240	LEU
1	B	250	LEU
1	B	255	VAL
1	B	266	GLU
1	B	271	LYS
1	B	274	LYS
1	B	277	LEU
1	B	280	LEU
1	B	283	LEU
1	B	293	LEU

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Mol	Chain	Res	Type
1	B	303	LEU
1	B	310	VAL
1	B	316	VAL
1	B	318	VAL
1	B	338	VAL
1	B	344	GLN
1	B	351	LYS
1	B	362	LYS
1	B	378	LEU
1	B	380	LEU
1	B	390	CYS
1	B	391	CYS
1	B	393	GLN
1	B	401	LEU
1	B	446	LEU
1	B	471	SER
1	B	485	GLU
1	B	514	THR
1	B	529	HIS
1	B	551	TYR
1	B	557	MET
1	B	561	LYS
1	B	605	GLU
1	B	606	ARG
1	B	613	SER
1	B	614	ASP
1	B	621	LEU
1	B	623	LEU
1	B	625	ILE
2	C	21	GLN
2	C	39	LYS
2	C	44	ILE
2	C	55	LYS
2	C	58	LYS
2	C	66	ILE
2	C	68	ARG
2	C	74	LEU
2	C	84	THR
2	C	85	MET
2	C	132	LYS
2	C	135	VAL
2	C	146	LEU

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Mol	Chain	Res	Type
2	C	153	ILE
2	D	37	CYS
2	D	39	LYS
2	D	54	LEU
2	D	55	LYS
2	D	66	ILE
2	D	68	ARG
2	D	74	LEU
2	D	84	THR
2	D	96	ARG
2	D	120	SER
2	D	122	LYS
2	D	132	LYS
2	D	135	VAL
2	D	146	LEU
2	D	153	ILE
2	D	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	51	ASN
1	A	156	ASN
1	A	185	ASN
1	A	199	HIS
1	A	200	GLN
1	A	229	HIS
1	A	236	ASN
1	A	282	ASN
1	A	339	ASN
1	A	344	GLN
1	A	430	GLN
1	A	433	ASN
1	A	458	HIS
1	A	486	ASN
1	A	497	ASN
1	A	505	GLN
1	A	517	ASN
1	A	562	GLN
1	A	578	GLN
1	A	592	GLN

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Mol	Chain	Res	Type
1	B	44	ASN
1	B	51	ASN
1	B	129	GLN
1	B	156	ASN
1	B	185	ASN
1	B	229	HIS
1	B	236	ASN
1	B	268	ASN
1	B	282	ASN
1	B	309	ASN
1	B	333	GLN
1	B	344	GLN
1	B	423	GLN
1	B	426	HIS
1	B	430	GLN
1	B	431	HIS
1	B	433	ASN
1	B	458	HIS
1	B	486	ASN
1	B	510	GLN
1	B	517	ASN
1	B	544	ASN
1	B	597	GLN
1	B	616	GLN
2	C	21	GLN
2	C	26	ASN
2	C	41	GLN
2	D	21	GLN
2	D	26	ASN
2	D	156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.78	4 (23%)
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	1.54	3 (17%)
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	1.90	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.65	0	17,19,21	1.23	1 (5%)
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	2.10	5 (29%)
3	NAG	H	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	2.12	2 (11%)
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.13	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	6.75	121.23	112.19
3	G	2	NAG	C1-O5-C5	6.32	120.65	112.19
3	F	2	NAG	C1-O5-C5	5.73	119.87	112.19
3	E	2	NAG	C1-O5-C5	4.75	118.55	112.19
3	F	1	NAG	C2-N2-C7	3.93	128.17	122.90
3	E	2	NAG	C2-N2-C7	-3.48	118.23	122.90
3	F	1	NAG	C8-C7-N2	3.07	121.21	116.12
3	F	2	NAG	C6-C5-C4	-3.01	105.63	113.02
3	G	2	NAG	C4-C3-C2	-3.01	106.61	111.02
3	H	1	NAG	C6-C5-C4	-2.89	105.92	113.02
3	G	2	NAG	C8-C7-N2	2.81	120.78	116.12
3	G	1	NAG	C2-N2-C7	-2.79	119.16	122.90
3	E	1	NAG	C1-O5-C5	2.51	115.55	112.19
3	E	2	NAG	C3-C4-C5	-2.51	105.68	110.23
3	F	1	NAG	C4-C3-C2	2.39	114.52	111.02
3	G	2	NAG	C2-N2-C7	2.38	126.09	122.90
3	F	2	NAG	O3-C3-C4	-2.12	105.37	110.38
3	H	2	NAG	C1-C2-N2	2.10	113.75	110.43
3	G	2	NAG	O7-C7-C8	-2.08	118.36	122.05
3	E	2	NAG	O4-C4-C5	2.07	114.43	109.32
3	H	2	NAG	O4-C4-C5	2.06	114.40	109.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

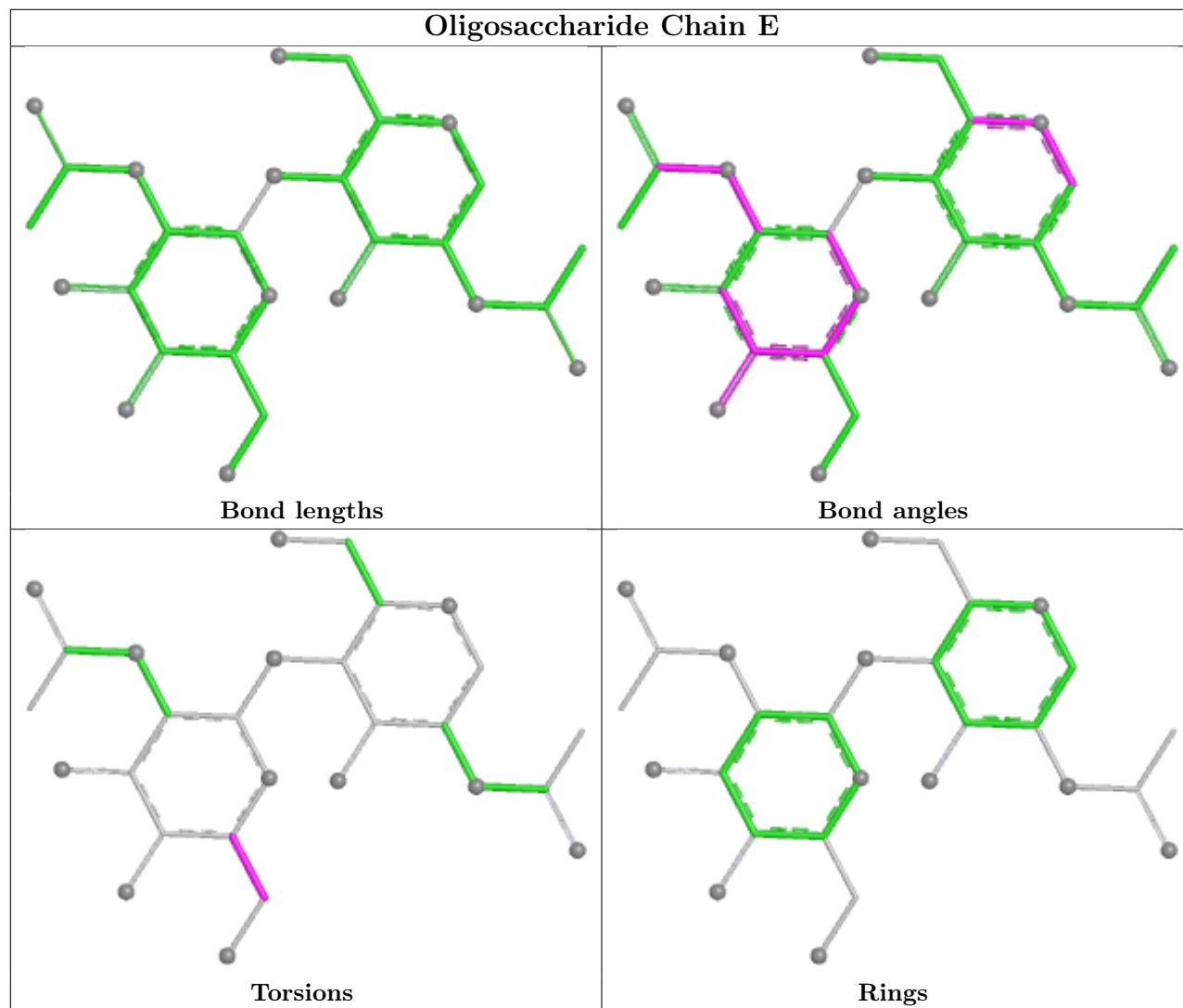
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

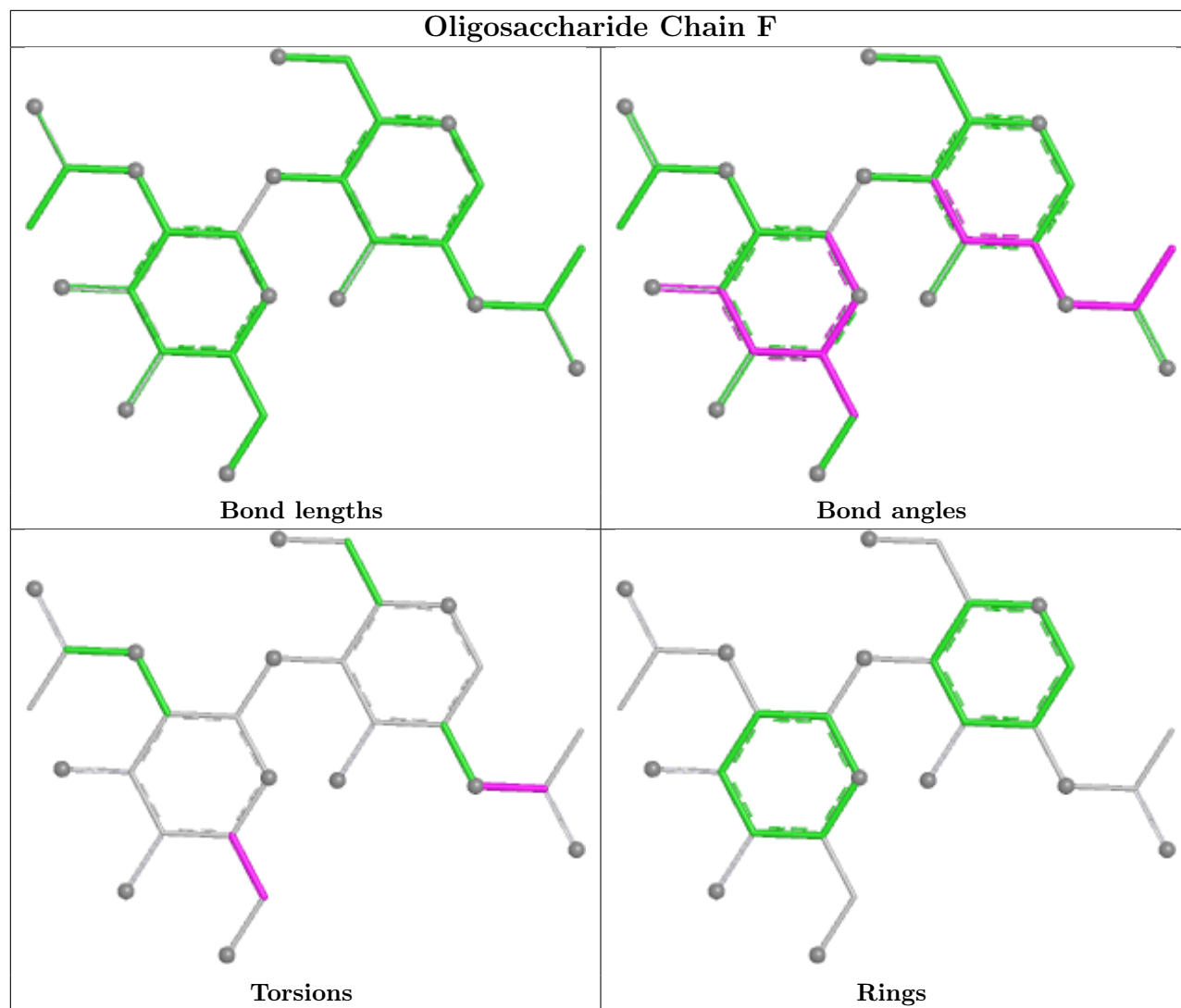
There are no ring outliers.

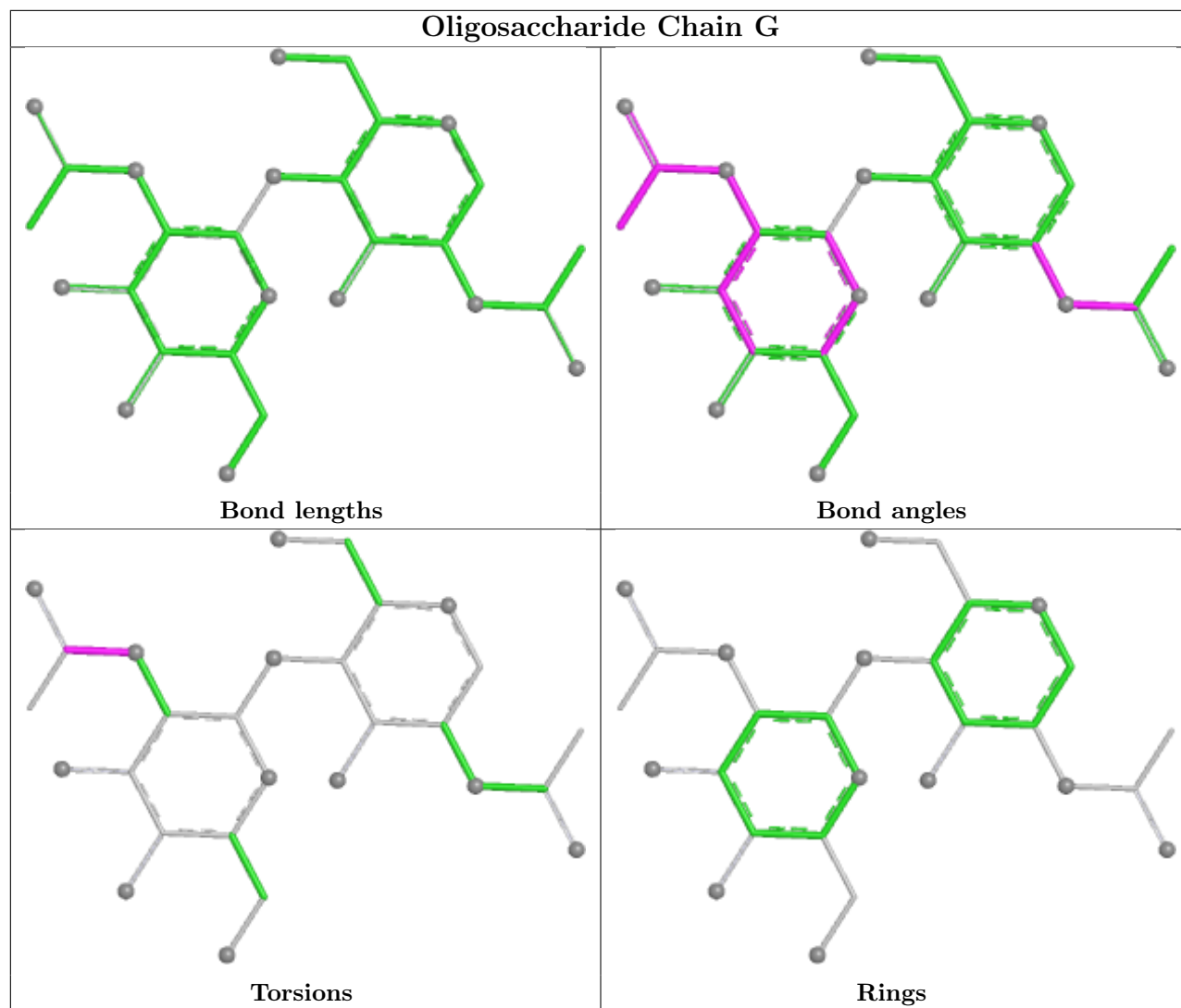
5 monomers are involved in 4 short contacts:

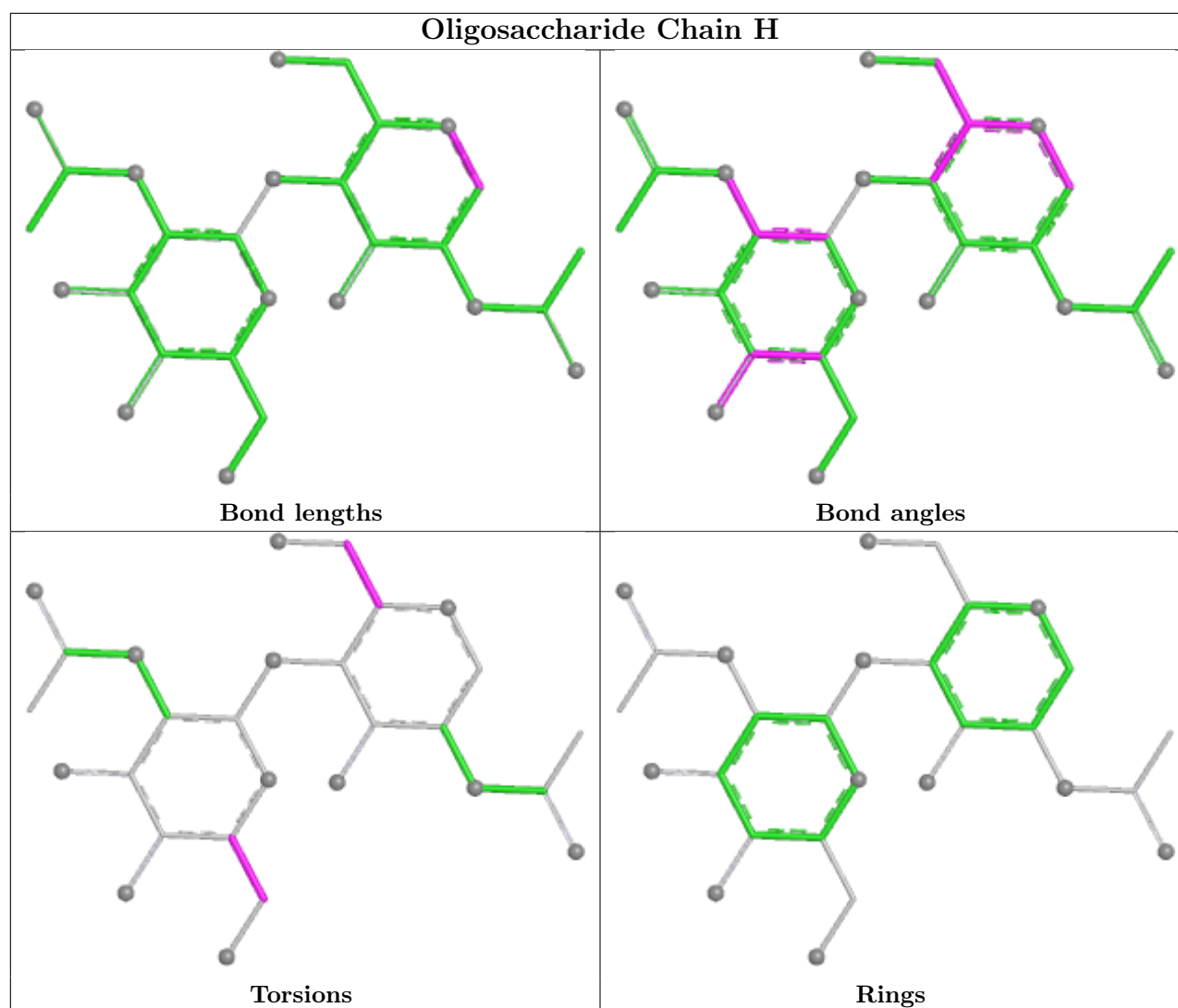
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
3	H	1	NAG	2	0
3	F	1	NAG	1	0
3	F	2	NAG	1	0
3	E	2	NAG	1	0

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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LP4	C	202	7,6,8,9	45,45,48	0.66	0	54,56,60	1.15	3 (5%)
6	LP5	C	203	5	47,48,48	1.02	2 (4%)	58,60,60	1.26	6 (10%)
7	DAO	C	204	5	12,12,13	0.96	1 (8%)	11,11,13	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	KDO	C	206	5	15,15,16	0.67	0	17,21,24	1.09	1 (5%)
9	KDO	D	206	5	15,15,16	0.84	0	17,21,24	1.36	2 (11%)
4	NAG	C	201	2	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
4	NAG	B	701	1	14,14,15	0.66	0	17,19,21	1.93	3 (17%)
4	NAG	A	701	1	14,14,15	0.51	0	17,19,21	0.98	0
5	LP4	D	202	7,6,8,9	45,45,48	0.80	2 (4%)	54,56,60	1.42	8 (14%)
4	NAG	D	201	2	14,14,15	0.52	0	17,19,21	1.33	1 (5%)
8	MYR	C	205	5	14,14,15	0.89	1 (7%)	13,13,15	0.87	0
6	LP5	D	203	5	47,48,48	0.86	2 (4%)	58,60,60	1.31	6 (10%)
7	DAO	D	204	5	12,12,13	0.99	1 (8%)	11,11,13	0.77	0
8	MYR	D	205	5	14,14,15	0.86	1 (7%)	13,13,15	0.81	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
5	LP4	C	202	7,6,8,9	-	11/43/60/65	0/1/1/1
6	LP5	C	203	5	-	14/44/65/65	0/1/1/1
7	DAO	C	204	5	-	5/10/10/11	-
9	KDO	C	206	5	-	6/10/26/30	0/1/1/1
9	KDO	D	206	5	-	2/10/26/30	0/1/1/1
4	NAG	C	201	2	-	0/6/23/26	0/1/1/1
4	NAG	B	701	1	-	3/6/23/26	0/1/1/1
4	NAG	A	701	1	-	1/6/23/26	0/1/1/1
5	LP4	D	202	7,6,8,9	-	17/43/60/65	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
8	MYR	C	205	5	-	10/12/12/13	-
6	LP5	D	203	5	-	16/44/65/65	0/1/1/1
7	DAO	D	204	5	-	8/10/10/11	-
8	MYR	D	205	5	-	11/12/12/13	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	203	LP5	P45-O47	4.70	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	204	DAO	O2-C1	-3.38	1.24	1.42
6	D	203	LP5	P45-O47	3.38	1.61	1.50
7	C	204	DAO	O2-C1	-3.29	1.25	1.42
8	C	205	MYR	O2-C1	-3.24	1.25	1.42
8	D	205	MYR	O2-C1	-3.19	1.25	1.42
6	C	203	LP5	P45-O1	2.51	1.63	1.59
5	D	202	LP4	O3-C3	-2.44	1.41	1.44
6	D	203	LP5	O3-C3	-2.13	1.41	1.44
5	D	202	LP4	P45-O46	-2.12	1.46	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	LP4	C1-O5-C5	-5.08	105.38	112.19
4	B	701	NAG	C2-N2-C7	4.82	129.36	122.90
4	C	201	NAG	C1-O5-C5	4.11	117.70	112.19
4	D	201	NAG	C1-O5-C5	4.06	117.62	112.19
6	D	203	LP5	O5-C1-O1	-3.85	106.33	111.36
5	C	202	LP4	C1-O5-C5	-3.72	107.20	112.19
4	B	701	NAG	C4-C3-C2	3.50	116.15	111.02
4	B	701	NAG	C1-C2-N2	-3.45	105.00	110.43
5	D	202	LP4	C8-C7-N2	-3.40	111.62	116.25
6	D	203	LP5	O5-C5-C6	-3.09	98.77	106.44
9	D	206	KDO	O1B-C1-C2	3.00	120.51	112.71
6	C	203	LP5	C3-C2-N2	-2.99	106.14	110.91
5	D	202	LP4	C1-C2-N2	-2.99	105.73	110.43
6	D	203	LP5	C8-C7-N2	-2.96	112.21	116.25
9	C	206	KDO	O1B-C1-C2	2.68	119.68	112.71
6	D	203	LP5	C1-C2-N2	-2.57	106.61	110.92
6	C	203	LP5	C3-O3-C28	2.52	121.69	117.59
9	D	206	KDO	O6-C6-C7	2.51	111.48	106.60
6	C	203	LP5	C8-C7-N2	-2.36	113.03	116.25
5	D	202	LP4	C32-C31-C30	-2.32	108.29	114.68
6	C	203	LP5	C17-C16-C8	-2.31	105.11	112.88
6	C	203	LP5	O5-C1-C2	-2.30	106.24	110.59
5	D	202	LP4	C3-O3-C28	-2.28	113.88	117.59
6	C	203	LP5	O5-C5-C6	-2.25	100.87	106.44
5	C	202	LP4	O47-P45-O4	-2.17	97.40	105.85
6	D	203	LP5	C3-O3-C28	2.16	121.10	117.59
5	D	202	LP4	C3-C2-N2	-2.15	107.07	110.57
5	C	202	LP4	C32-C31-C30	-2.13	108.80	114.68
5	D	202	LP4	O47-P45-O4	-2.09	97.71	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	LP4	O44-C16-C8	-2.06	104.30	109.64
6	D	203	LP5	C17-C16-C8	-2.05	105.99	112.88

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	202	LP4	C17-C16-C8-C7
5	C	202	LP4	O44-C16-C8-C7
5	C	202	LP4	C8-C16-C17-C18
5	D	202	LP4	C17-C16-C8-C7
5	D	202	LP4	O44-C16-C8-C7
6	C	203	LP5	O44-C16-C8-C7
6	C	203	LP5	C17-C16-C8-C7
6	D	203	LP5	O44-C16-C8-C7
6	D	203	LP5	C17-C16-C8-C7
9	C	206	KDO	C5-C6-C7-O7
9	C	206	KDO	C5-C6-C7-C8
9	C	206	KDO	O6-C6-C7-O7
9	C	206	KDO	O6-C6-C7-C8
9	C	206	KDO	C6-C7-C8-O8
9	C	206	KDO	O7-C7-C8-O8
9	D	206	KDO	C6-C7-C8-O8
7	D	204	DAO	C1-C2-C3-C4
4	B	701	NAG	C4-C5-C6-O6
4	B	701	NAG	O5-C5-C6-O6
5	C	202	LP4	O44-C16-C17-C18
9	D	206	KDO	O7-C7-C8-O8
7	C	204	DAO	C5-C6-C7-C8
8	C	205	MYR	C10-C11-C12-C13
8	D	205	MYR	O2-C1-C2-C3
5	D	202	LP4	C19-C20-C21-C22
8	C	205	MYR	C9-C10-C11-C12
5	D	202	LP4	C8-C16-C17-C18
6	C	203	LP5	C18-C19-C20-C21
8	C	205	MYR	C6-C7-C8-C9
7	C	204	DAO	C11-C10-C9-C8
7	D	204	DAO	C5-C6-C7-C8
6	D	203	LP5	C18-C19-C20-C21
6	D	203	LP5	C19-C20-C21-C22
8	D	205	MYR	C6-C7-C8-C9
7	D	204	DAO	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	C	205	MYR	C7-C8-C9-C10
6	C	203	LP5	C35-C36-C37-C38
6	C	203	LP5	O5-C5-C6-O6
5	D	202	LP4	C17-C18-C19-C20
6	D	203	LP5	C32-C33-C34-C35
8	D	205	MYR	C1-C2-C3-C4
5	D	202	LP4	C21-C22-C23-C24
8	D	205	MYR	C2-C3-C4-C5
7	D	204	DAO	C11-C10-C9-C8
8	D	205	MYR	C9-C10-C11-C12
6	C	203	LP5	C19-C20-C21-C22
6	C	203	LP5	C20-C21-C22-C23
6	C	203	LP5	C31-C32-C33-C34
5	D	202	LP4	C18-C19-C20-C21
5	D	202	LP4	C35-C36-C37-C38
8	D	205	MYR	C7-C8-C9-C10
8	C	205	MYR	C1-C2-C3-C4
6	D	203	LP5	C20-C21-C22-C23
7	D	204	DAO	O2-C1-C2-C3
8	C	205	MYR	O2-C1-C2-C3
8	D	205	MYR	C5-C6-C7-C8
4	B	701	NAG	C3-C2-N2-C7
6	C	203	LP5	C34-C35-C36-C37
6	D	203	LP5	C37-C38-C39-C40
6	C	203	LP5	C32-C33-C34-C35
6	D	203	LP5	C31-C32-C33-C34
6	D	203	LP5	C24-C25-C26-C27
5	D	202	LP4	C32-C33-C34-C35
5	D	202	LP4	C34-C35-C36-C37
7	C	204	DAO	C3-C4-C5-C6
8	C	205	MYR	C11-C12-C13-C14
7	D	204	DAO	C3-C4-C5-C6
8	D	205	MYR	C11-C12-C13-C14
8	C	205	MYR	C2-C3-C4-C5
5	C	202	LP4	C38-C39-C40-C41
6	D	203	LP5	C34-C35-C36-C37
7	C	204	DAO	C6-C7-C8-C9
8	C	205	MYR	C11-C10-C9-C8
4	A	701	NAG	O5-C5-C6-O6
8	C	205	MYR	C5-C6-C7-C8
6	D	203	LP5	C23-C24-C25-C26
5	D	202	LP4	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	D	204	DAO	C6-C7-C8-C9
6	C	203	LP5	C4-C5-C6-O6
7	D	204	DAO	C9-C10-C11-C12
5	D	202	LP4	C37-C38-C39-C40
5	D	202	LP4	O44-C16-C17-C18
5	D	202	LP4	C22-C23-C24-C25
5	C	202	LP4	C18-C19-C20-C21
5	C	202	LP4	C37-C38-C39-C40
6	D	203	LP5	C21-C22-C23-C24
6	C	203	LP5	O43-C30-C31-C32
5	D	202	LP4	C38-C39-C40-C41
6	D	203	LP5	C33-C34-C35-C36
5	D	202	LP4	C29-C28-O3-C3
6	C	203	LP5	C30-C31-C32-C33
6	C	203	LP5	C24-C25-C26-C27
6	D	203	LP5	O5-C5-C6-O6
5	C	202	LP4	C21-C22-C23-C24
8	D	205	MYR	C4-C5-C6-C7
5	D	202	LP4	O42-C28-O3-C3
8	D	205	MYR	C3-C4-C5-C6
5	C	202	LP4	C16-C17-C18-C19
6	D	203	LP5	C1-C2-N2-C7
5	C	202	LP4	C29-C28-O3-C3
6	D	203	LP5	C1-O1-P45-O46
7	C	204	DAO	C7-C8-C9-C10
8	D	205	MYR	C10-C11-C12-C13
5	C	202	LP4	O42-C28-O3-C3

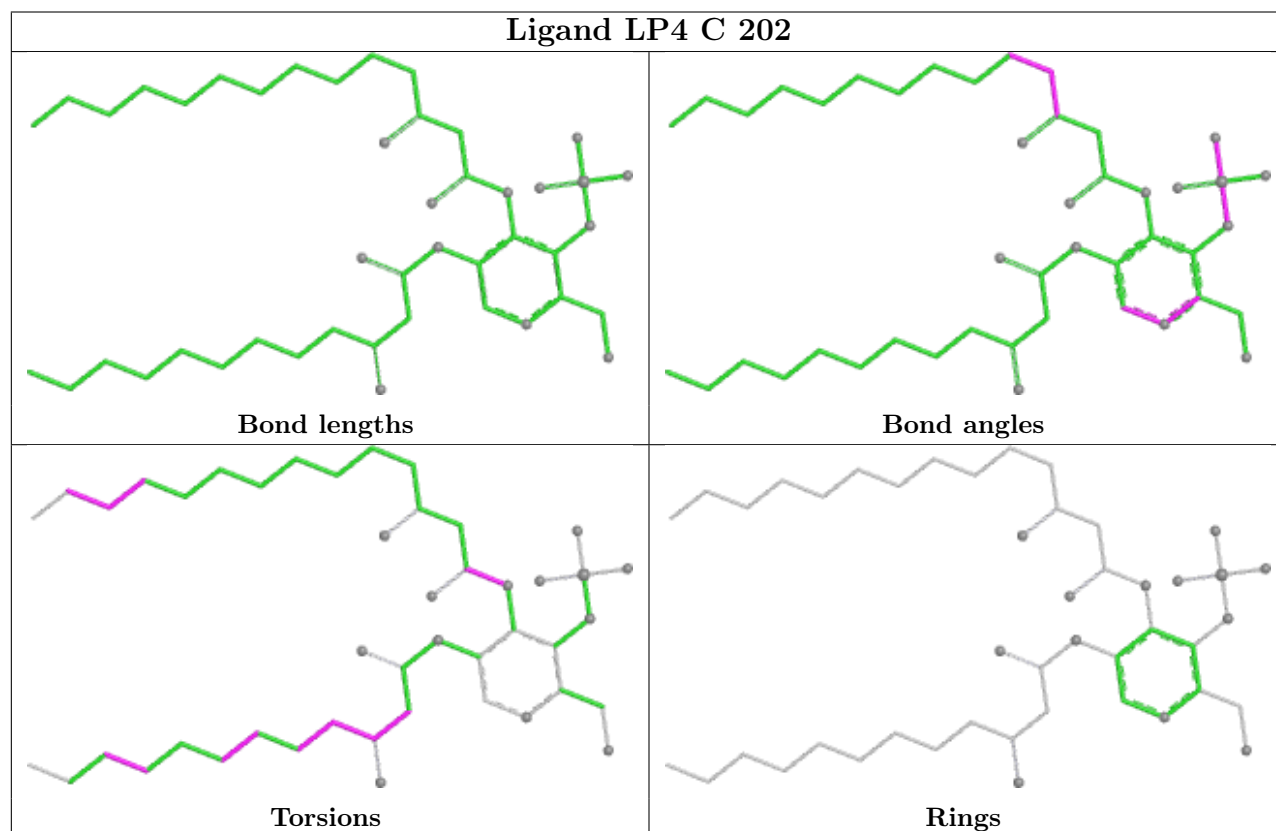
There are no ring outliers.

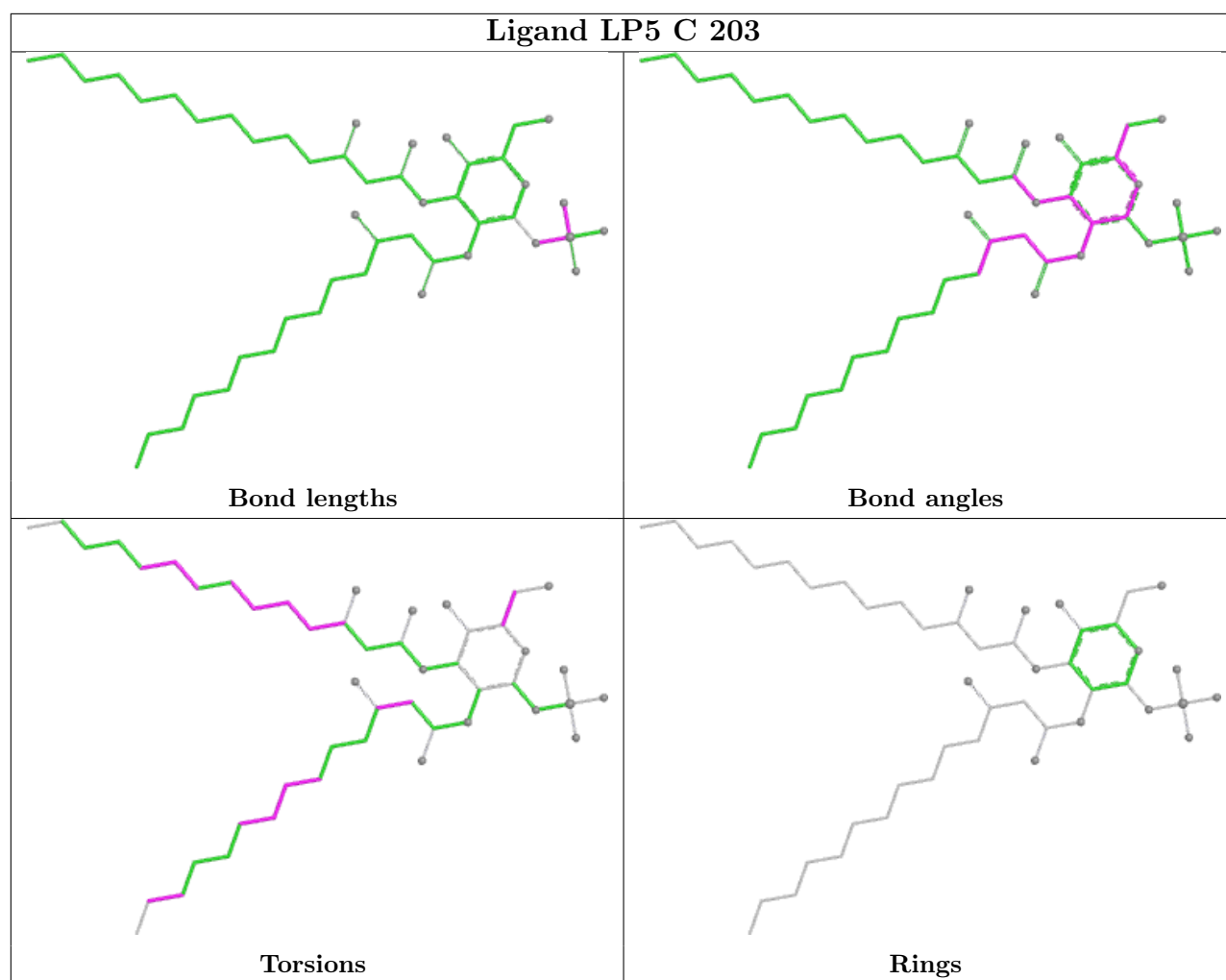
5 monomers are involved in 15 short contacts:

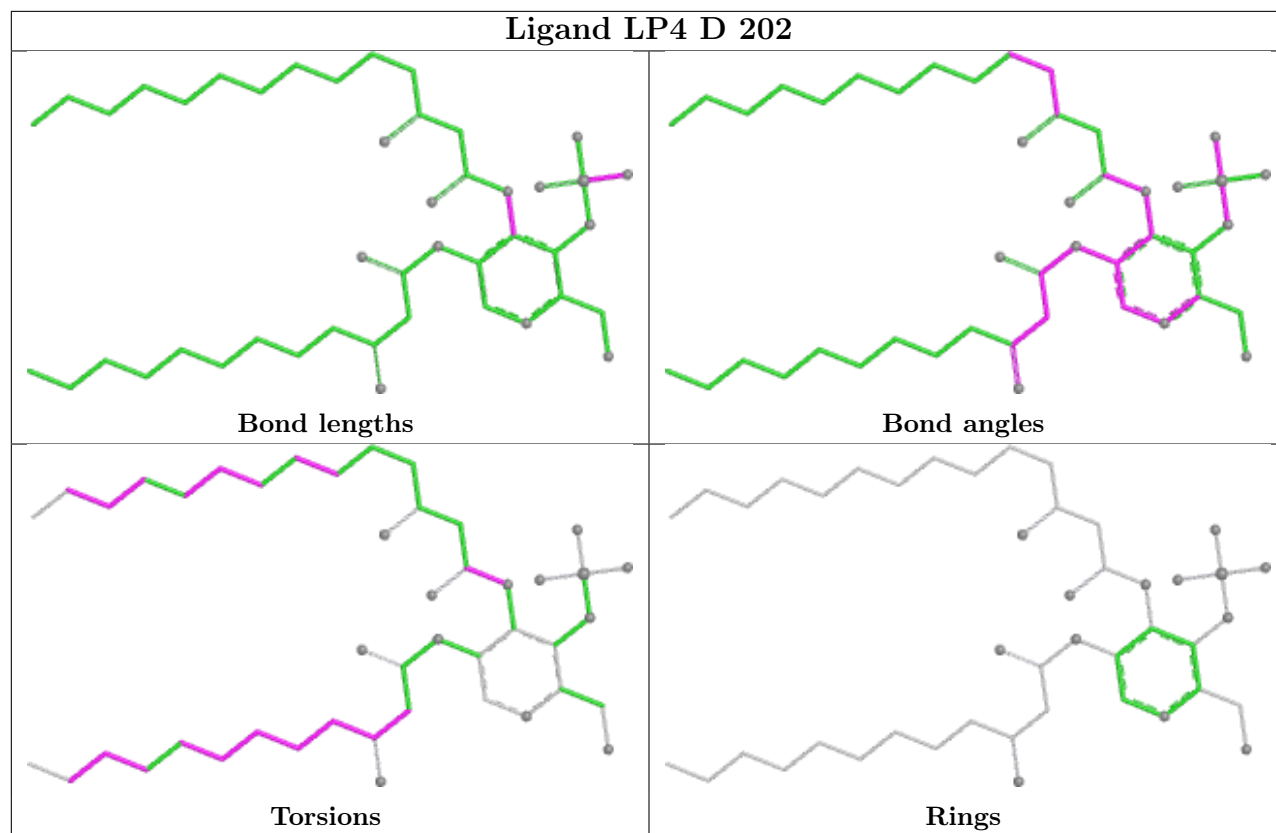
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	LP4	5	0
6	C	203	LP5	4	0
7	C	204	DAO	1	0
5	D	202	LP4	3	0
6	D	203	LP5	4	0

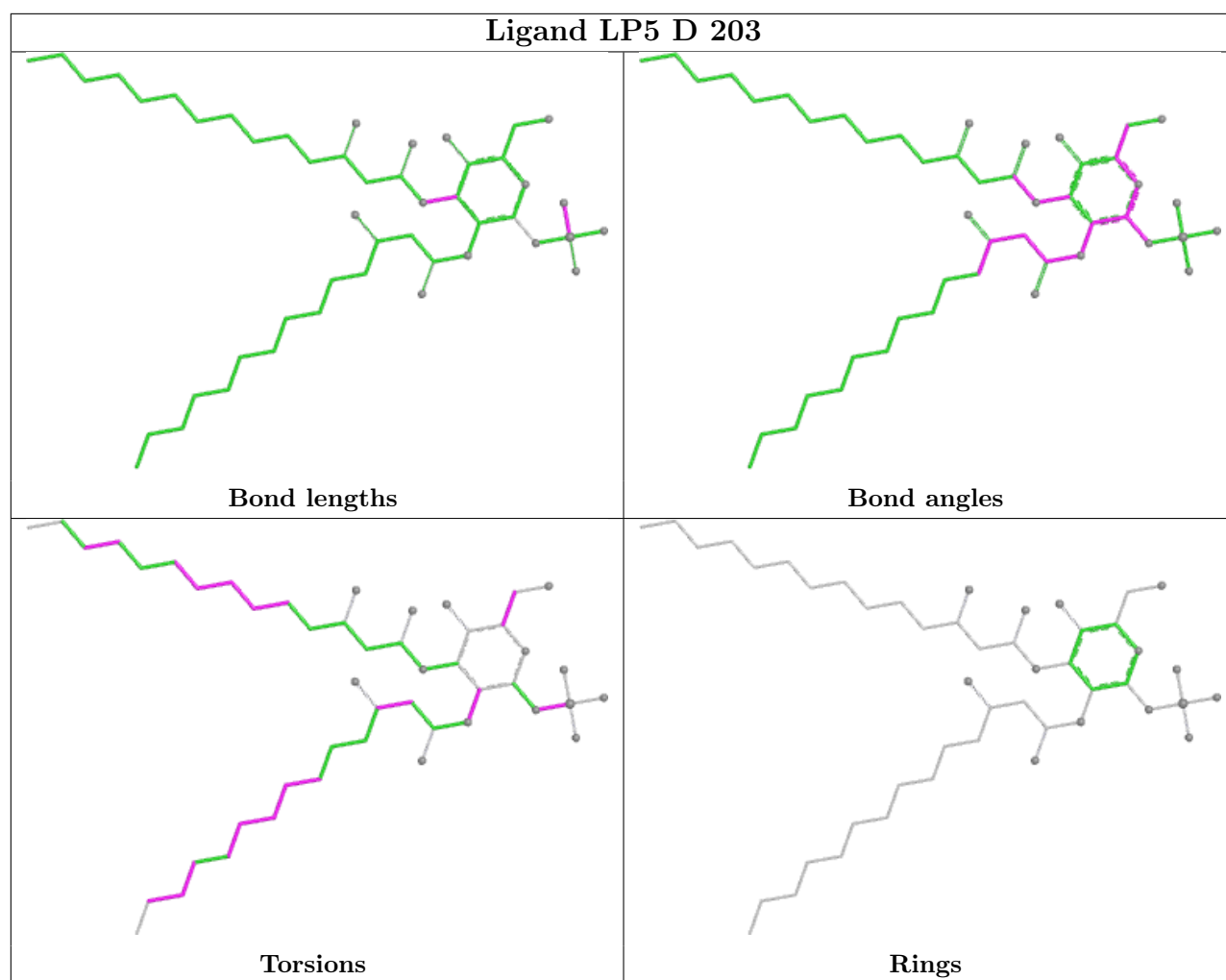
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	601/635 (94%)	0.29	40 (6%)	24 20	26, 44, 79, 120	0
1	B	605/635 (95%)	0.17	22 (3%)	46 42	27, 44, 69, 106	0
2	C	140/144 (97%)	0.45	13 (9%)	14 11	32, 49, 83, 103	0
2	D	140/144 (97%)	0.28	10 (7%)	22 18	33, 44, 76, 102	0
All	All	1486/1558 (95%)	0.25	85 (5%)	29 25	26, 44, 74, 120	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	7.3
1	B	202	PRO	5.8
2	C	123	GLY	4.7
1	A	561	LYS	4.5
1	A	119	LEU	4.5
1	A	54	PHE	4.4
1	A	625	ILE	4.1
1	A	611	THR	4.1
1	A	626	THR	4.1
1	A	75	PHE	4.1
2	C	142	PRO	4.0
1	A	563	GLU	4.0
2	C	20	LYS	4.0
1	A	270	GLU	3.7
1	B	204	LEU	3.7
1	A	564	LEU	3.6
2	C	23	TRP	3.6
1	B	54	PHE	3.4
1	A	301	ILE	3.4
1	A	326	PHE	3.3
1	B	301	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	627	CYS	3.2
2	D	141	SER	3.2
1	B	296	TYR	3.2
1	A	562	GLN	3.2
1	A	624	ASN	3.1
1	A	328	TYR	3.1
1	A	566	HIS	3.1
2	D	142	PRO	3.1
1	B	627	CYS	3.0
2	D	19	GLN	3.0
2	C	141	SER	2.9
1	B	363	GLY	2.9
2	C	39	LYS	2.8
2	C	122	LYS	2.8
1	A	309	ASN	2.7
1	A	583	CYS	2.7
1	B	23	PRO	2.7
1	A	559	SER	2.7
2	C	40	MET	2.7
1	B	362	LYS	2.6
1	B	389	GLY	2.6
2	C	96	ARG	2.6
1	A	364	GLY	2.6
2	D	123	GLY	2.6
1	A	116	SER	2.6
2	C	158	ASN	2.5
1	A	558	THR	2.5
1	A	46	TYR	2.5
2	D	23	TRP	2.5
1	A	363	GLY	2.5
2	D	40	MET	2.5
2	C	19	GLN	2.5
2	D	66	ILE	2.4
2	D	158	ASN	2.4
1	B	626	THR	2.4
1	B	143	ASN	2.4
1	A	327	SER	2.4
1	A	612	PRO	2.4
1	A	117	LEU	2.4
1	A	604	VAL	2.4
1	B	75	PHE	2.3
1	A	143	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	585	CYS	2.2
1	A	271	LYS	2.2
1	A	617	GLY	2.2
1	B	364	GLY	2.2
1	A	93	ILE	2.2
1	B	48	ILE	2.2
1	A	175	THR	2.2
1	A	298	ASP	2.2
2	D	20	LYS	2.2
1	A	606	ARG	2.2
1	A	347	THR	2.1
1	B	621	LEU	2.1
2	C	84	THR	2.1
1	B	137	ASN	2.1
2	C	97	GLY	2.1
1	A	613	SER	2.1
1	B	201	MET	2.1
1	B	270	GLU	2.1
1	A	150	LYS	2.1
2	D	84	THR	2.0
1	A	34	PRO	2.0
1	B	388	LYS	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.

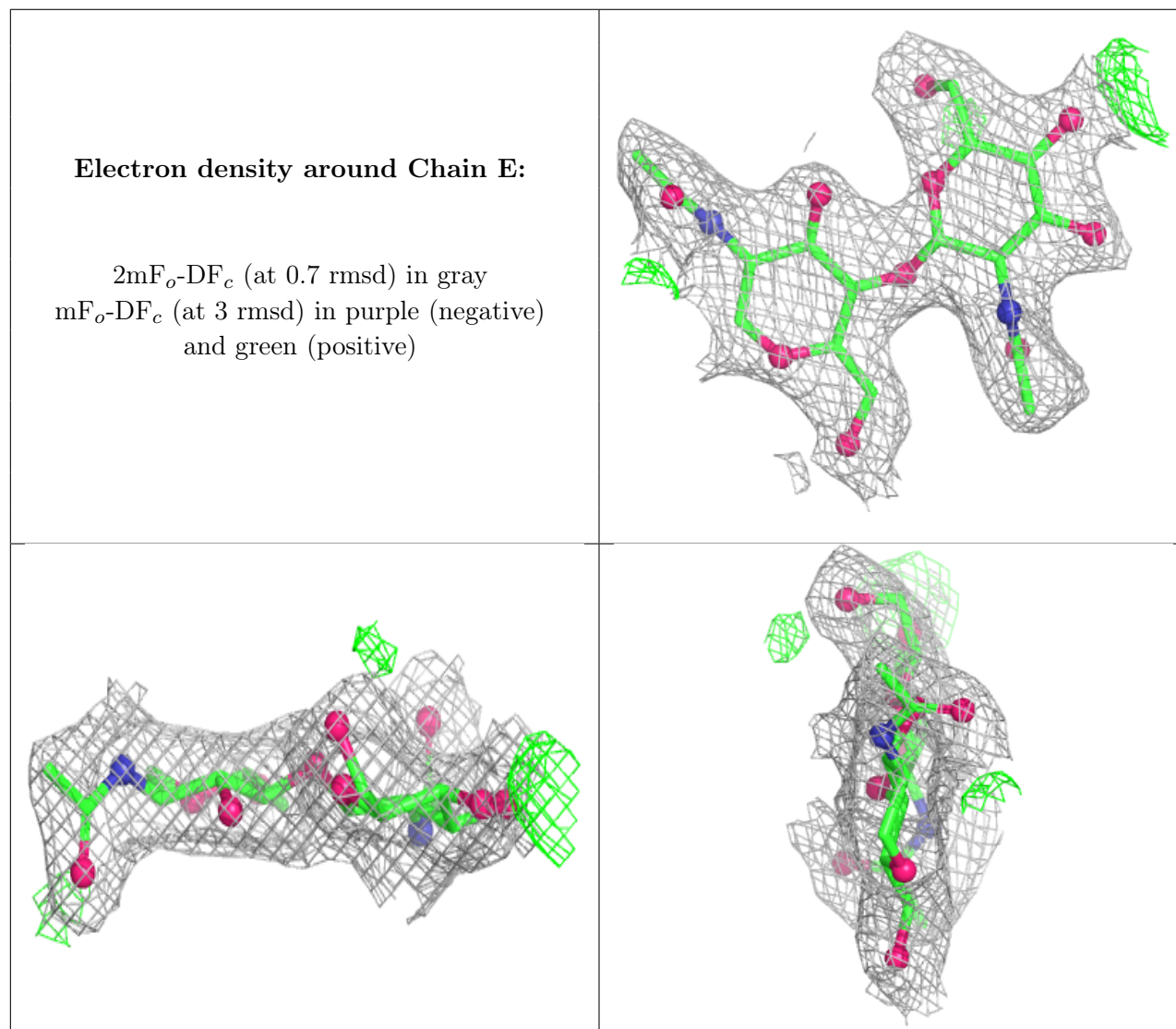
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.78	0.16	53,59,64,66	0
3	NAG	G	2	14/15	0.83	0.16	51,55,59,64	0
3	NAG	H	2	14/15	0.88	0.11	41,49,59,60	0
3	NAG	F	2	14/15	0.89	0.12	57,58,61,63	0
3	NAG	F	1	14/15	0.93	0.10	46,49,50,55	0
3	NAG	H	1	14/15	0.94	0.09	35,36,44,51	0

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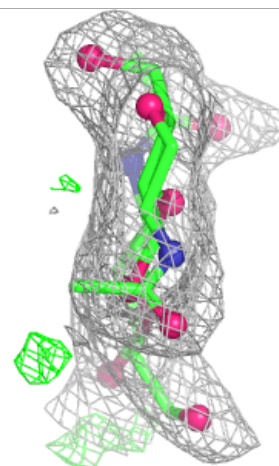
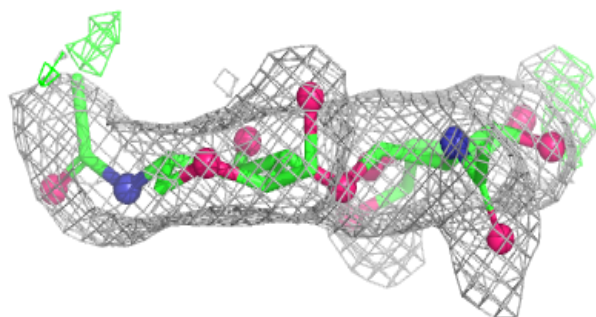
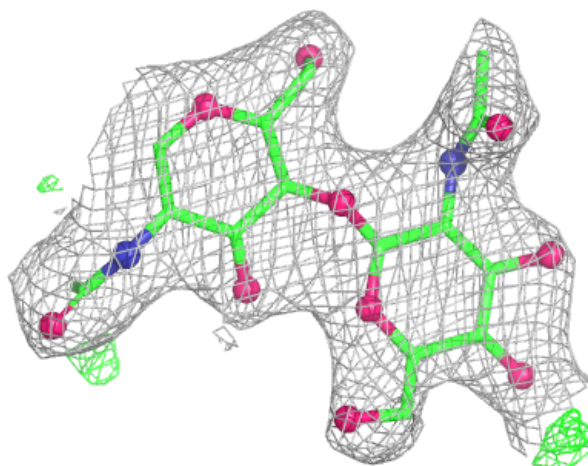
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	1	14/15	0.94	0.08	37,43,47,51	0
3	NAG	G	1	14/15	0.95	0.09	34,37,45,47	0

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.



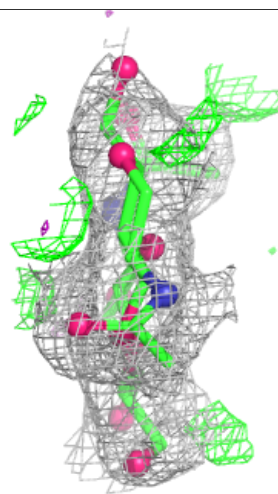
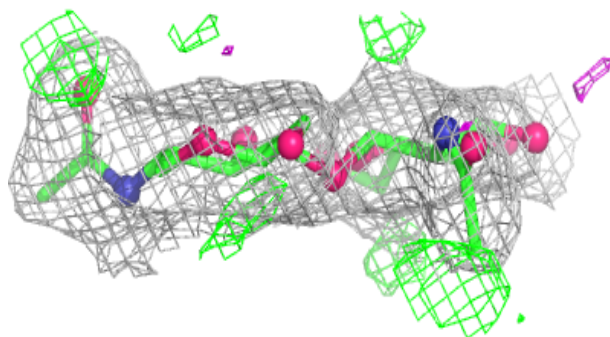
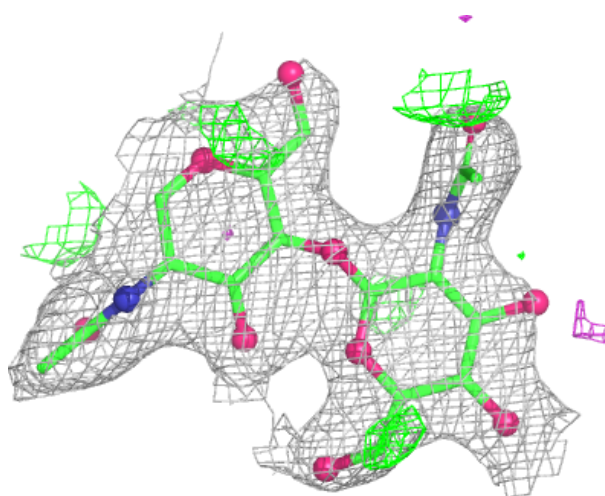
Electron density around Chain F:

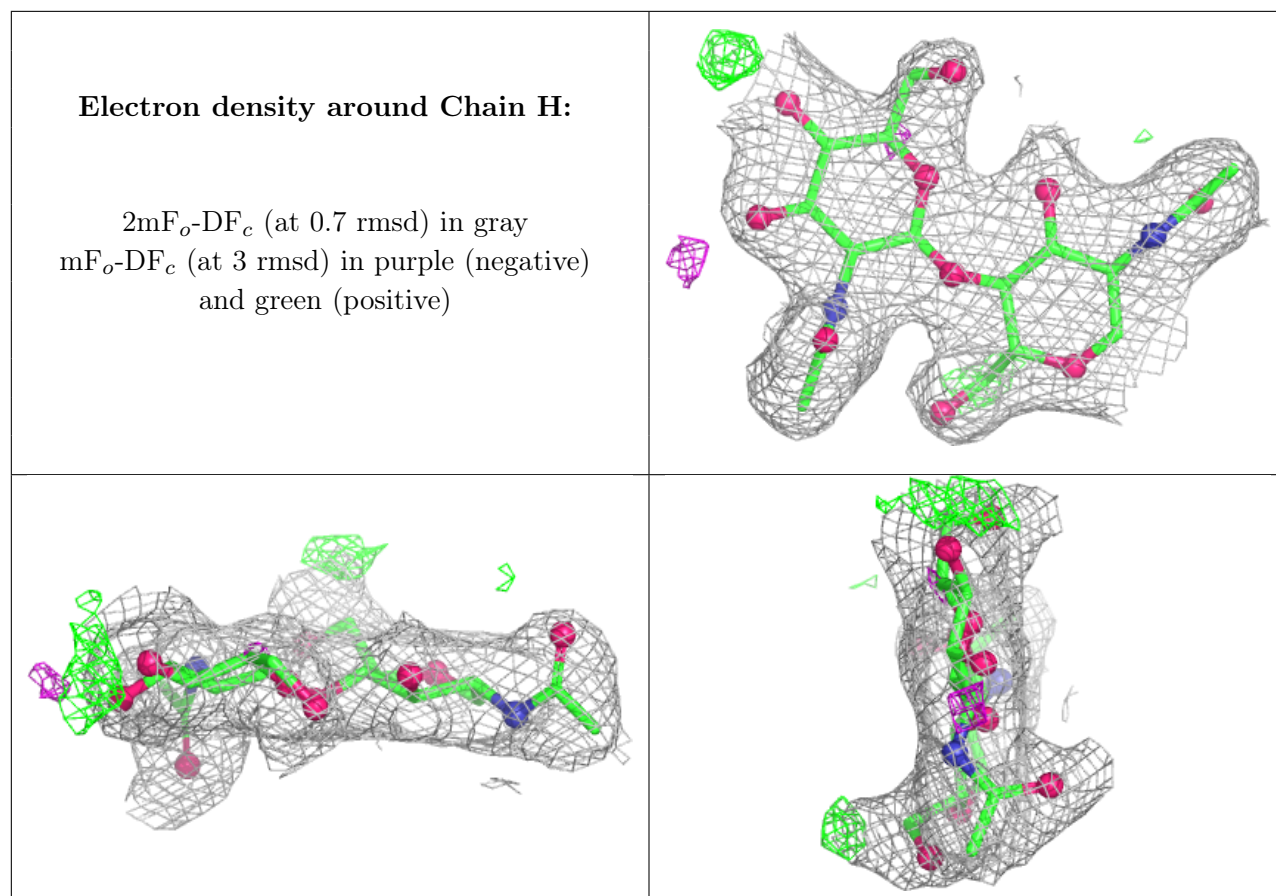
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands ⓘ

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	A	701	14/15	0.68	0.22	90,101,105,108	0
4	NAG	B	701	14/15	0.68	0.18	95,105,111,112	0
9	KDO	D	206	15/16	0.71	0.20	62,66,78,82	0
9	KDO	C	206	15/16	0.80	0.13	62,67,71,73	0
4	NAG	C	201	14/15	0.84	0.14	66,73,81,81	0
4	NAG	D	201	14/15	0.84	0.13	61,69,72,73	0
7	DAO	D	204	13/14	0.91	0.14	48,51,53,56	0
5	LP4	D	202	45/48	0.93	0.12	37,45,52,57	0
6	LP5	C	203	48/48	0.93	0.12	49,54,64,70	0
6	LP5	D	203	48/48	0.93	0.12	40,52,58,65	0
5	LP4	C	202	45/48	0.94	0.09	36,45,53,56	0
8	MYR	C	205	15/16	0.94	0.15	51,54,60,66	0
7	DAO	C	204	13/14	0.95	0.12	50,52,54,58	0

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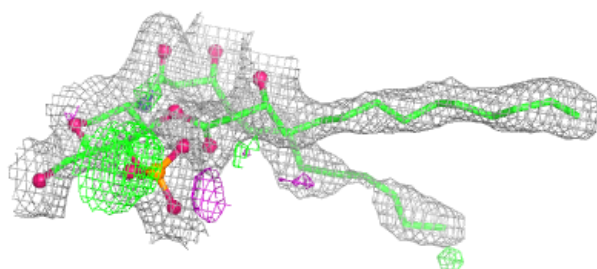
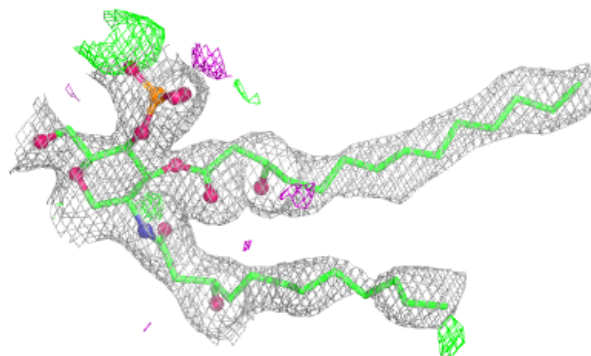
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MYR	D	205	15/16	0.95	0.11	41,50,55,55	0

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.

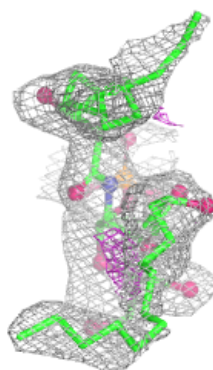
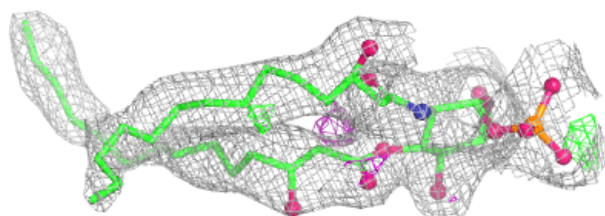
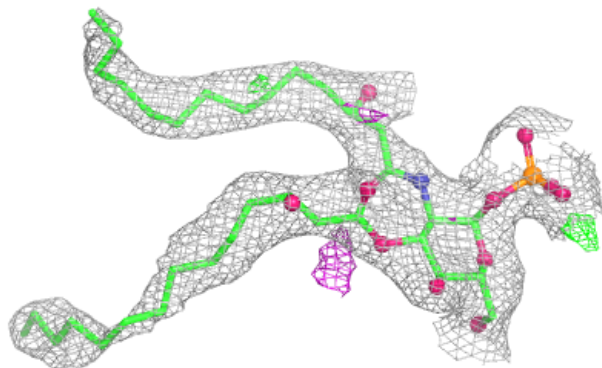
Electron density around LP4 D 202:

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

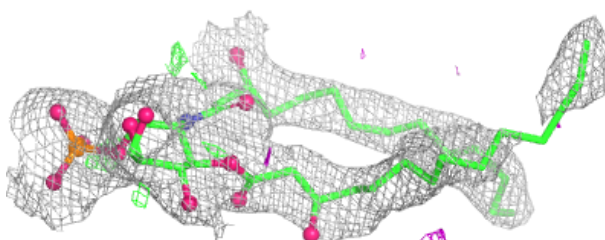
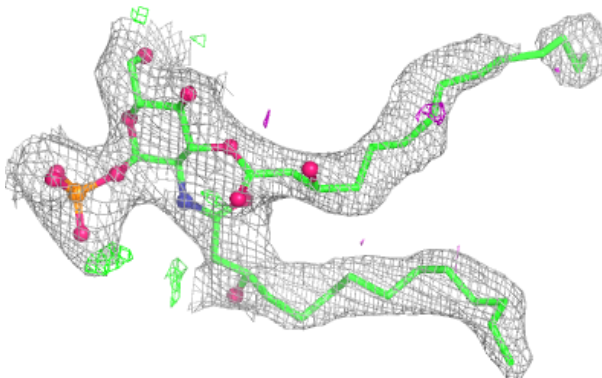


Electron density around LP5 C 203:

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

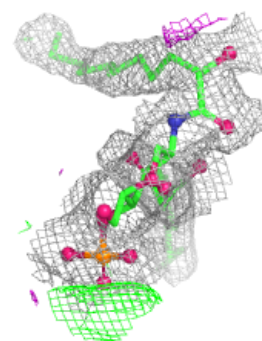
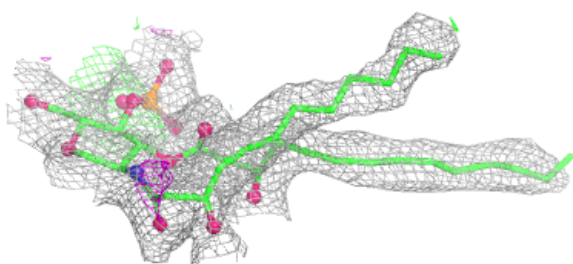
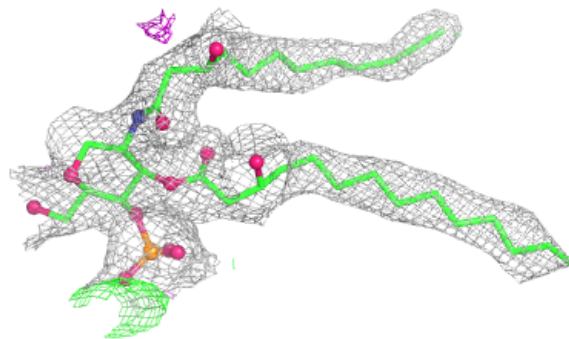
**Electron density around LP5 D 203:**

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



Electron density around LP4 C 202:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.