



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:19 AM UTC

PDB ID : 3O95 / pdb_00003o95
Title : Crystal Structure of Human DPP4 Bound to TAK-100
Authors : Yano, J.K.; Aertgeerts, K.
Deposited on : 2010-08-03
Resolution : 2.85 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:

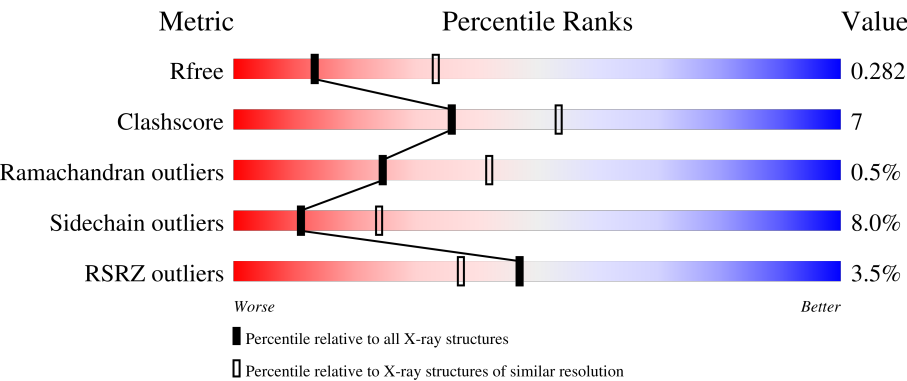
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.85 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.



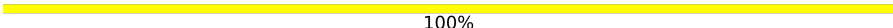
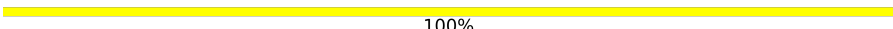
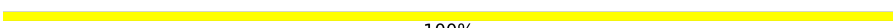
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	740	3% 74% 21% ..
1	B	740	% 75% 22% ..
1	C	740	6% 74% 22% ..
1	D	740	4% 74% 21% ..
2	E	2	50% 50%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	I	1	X	-	-	-
4	NAG	D	5201	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24870 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

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



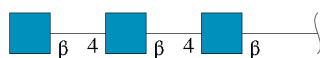
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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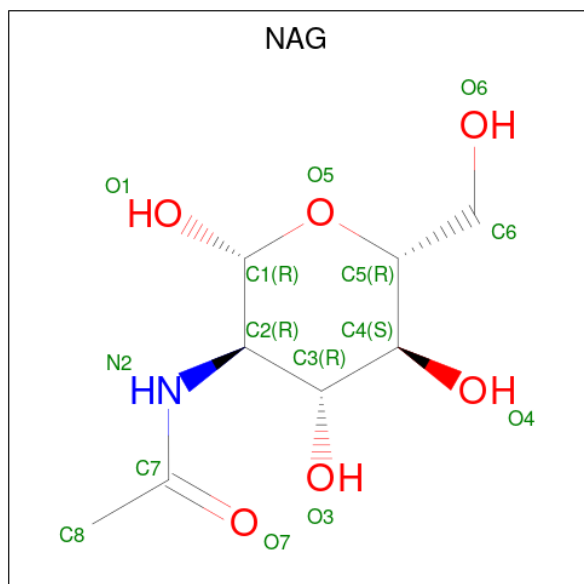
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
3	K	3	Total	C	N	O	0	0	0
			42	24	3	15			

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



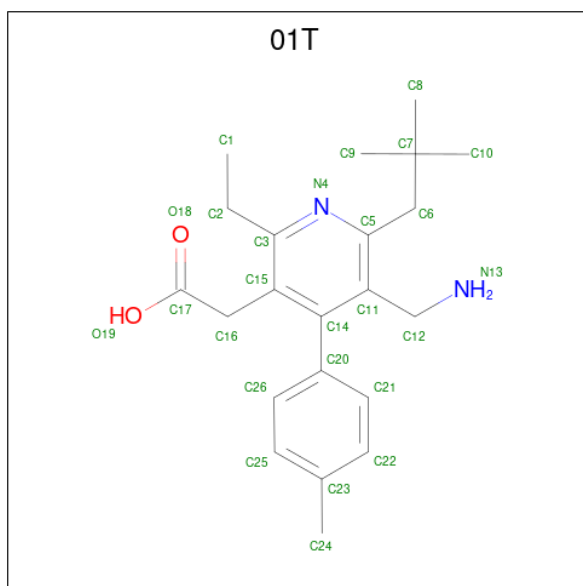
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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	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	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		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

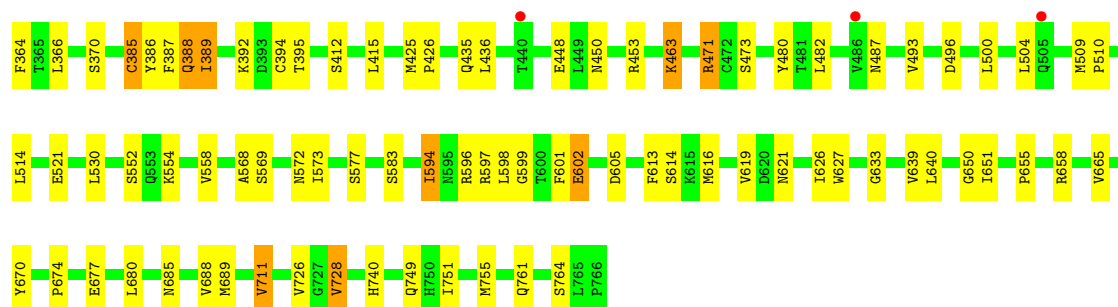
- Molecule 5 is [5-(aminomethyl)-6-(2,2-dimethylpropyl)-2-ethyl-4-(4-methylphenyl)pyridin-3-yl]acetic acid (CCD ID: 01T) (formula: C₂₂H₃₀N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	22	2	2		
5	B	1	Total	C	N	O	0	0
			26	22	2	2		
5	C	1	Total	C	N	O	0	0
			26	22	2	2		
5	D	1	Total	C	N	O	0	0
			26	22	2	2		

- Molecule 6 is water.

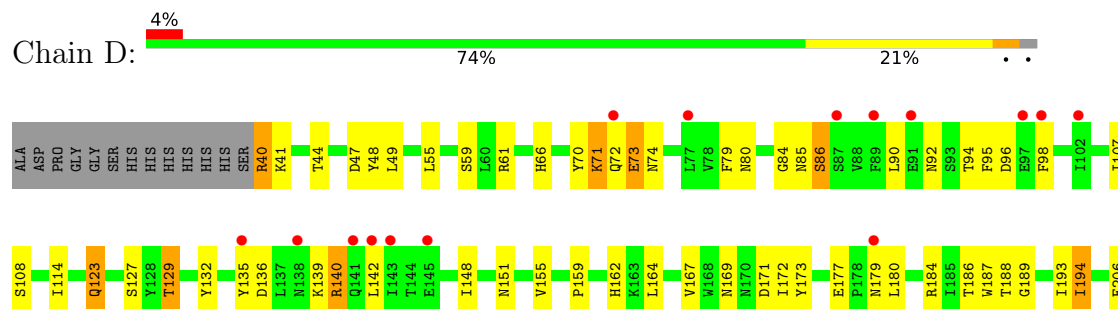
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	B	134	Total	O	0	0
			134	134		
6	C	76	Total	O	0	0
			76	76		
6	D	132	Total	O	0	0
			132	132		

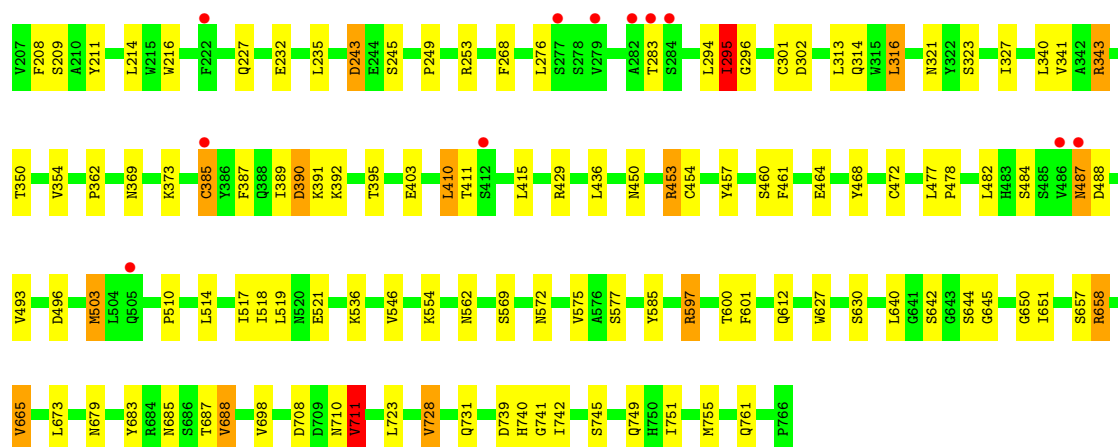


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





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

Chain E: 50% 50%



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 50% 50%



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

Chain I: 100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain K:  67% 33%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.72Å 123.33Å 144.42Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	35.00 – 2.85 35.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.00-2.85) 99.1 (35.00-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.248 0.240 , 0.282	Depositor DCC
R_{free} test set	4489 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24870	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 01T

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	0.66	14/6129 (0.2%)	0.86	8/8336 (0.1%)
1	B	0.62	9/6190 (0.1%)	0.83	5/8419 (0.1%)
1	C	0.60	13/6118 (0.2%)	0.81	9/8322 (0.1%)
1	D	0.64	9/6129 (0.1%)	0.83	2/8336 (0.0%)
All	All	0.63	45/24566 (0.2%)	0.83	24/33413 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	711	VAL	CA-CB	6.22	1.60	1.53
1	A	697	GLN	CD-OE1	6.08	1.35	1.23
1	A	685	ASN	CG-OD1	5.86	1.34	1.23
1	A	572	ASN	CG-OD1	5.45	1.33	1.23
1	A	141	GLN	CD-OE1	5.45	1.33	1.23
1	B	685	ASN	CG-OD1	5.45	1.33	1.23
1	C	74	ASN	CG-OD1	5.43	1.33	1.23
1	B	169	ASN	CG-OD1	5.42	1.33	1.23
1	C	710	ASN	CG-OD1	5.41	1.33	1.23
1	C	533	HIS	ND1-CE1	5.37	1.38	1.32
1	B	487	ASN	CG-OD1	5.35	1.33	1.23
1	B	388	GLN	CD-OE1	5.33	1.33	1.23
1	A	592	HIS	ND1-CE1	5.33	1.37	1.32
1	C	592	HIS	ND1-CE1	5.31	1.37	1.32
1	D	123	GLN	CD-OE1	5.30	1.33	1.23
1	C	455	GLN	CD-OE1	5.29	1.33	1.23
1	B	38	HIS	ND1-CE1	5.29	1.37	1.32
1	D	80	ASN	CG-OD1	5.29	1.33	1.23
1	C	170	ASN	CG-OD1	5.28	1.33	1.23
1	A	100	HIS	ND1-CE1	5.28	1.37	1.32
1	D	685	ASN	CG-OD1	5.27	1.33	1.23
1	A	179	ASN	CG-OD1	5.26	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLN	CD-OE1	5.25	1.33	1.23
1	C	100	HIS	ND1-CE1	5.25	1.37	1.32
1	A	170	ASN	CG-OD1	5.21	1.33	1.23
1	B	344	GLN	CD-OE1	5.21	1.33	1.23
1	C	179	ASN	CG-OD1	5.18	1.33	1.23
1	A	169	ASN	CG-OD1	5.18	1.33	1.23
1	D	487	ASN	CG-OD1	5.18	1.33	1.23
1	D	169	ASN	CG-OD1	5.17	1.33	1.23
1	A	151	ASN	CG-OD1	5.17	1.33	1.23
1	A	153	GLN	CD-OE1	5.17	1.33	1.23
1	C	153	GLN	CD-OE1	5.15	1.33	1.23
1	A	748	HIS	ND1-CE1	5.14	1.37	1.32
1	B	450	ASN	CG-OD1	5.11	1.33	1.23
1	C	75	ASN	CG-OD1	5.10	1.33	1.23
1	D	572	ASN	CG-OD1	5.08	1.33	1.23
1	A	80	ASN	CG-OD1	5.08	1.33	1.23
1	C	430	ASN	CG-OD1	5.08	1.33	1.23
1	D	179	ASN	CG-OD1	5.07	1.33	1.23
1	B	572	ASN	CG-ND2	-5.05	1.22	1.33
1	C	51	ASN	CG-OD1	5.05	1.33	1.23
1	B	435	GLN	CD-OE1	5.02	1.33	1.23
1	C	688	VAL	CA-CB	5.01	1.60	1.54
1	D	710	ASN	CG-ND2	-5.00	1.22	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	630	SER	CB-CA-C	-8.28	107.02	116.54
1	C	94	THR	N-CA-C	-6.71	104.91	113.23
1	A	748	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	38	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	C	533	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	100	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	C	100	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	C	400	GLY	N-CA-C	6.44	118.59	112.08
1	A	592	HIS	CB-CG-CD2	-6.31	123.00	131.20
1	C	592	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	B	530	LEU	CA-C-N	5.75	123.86	119.66
1	B	530	LEU	C-N-CA	5.75	123.86	119.66
1	A	94	THR	N-CA-C	-5.73	106.22	113.43
1	B	38	HIS	CB-CG-ND1	5.65	131.18	122.70
1	A	100	HIS	CB-CG-ND1	5.65	131.18	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	HIS	CB-CG-ND1	5.64	131.17	122.70
1	C	533	HIS	CB-CG-ND1	5.61	131.11	122.70
1	A	748	HIS	CB-CG-ND1	5.59	131.08	122.70
1	C	592	HIS	CB-CG-ND1	5.51	130.97	122.70
1	A	592	HIS	CB-CG-ND1	5.51	130.97	122.70
1	B	335	GLY	N-CA-C	-5.42	107.88	114.92
1	A	391	LYS	N-CA-C	5.33	117.19	108.76
1	D	683	TYR	N-CA-C	-5.20	105.61	111.28
1	C	454	CYS	N-CA-C	5.13	119.22	107.48

There are no chirality outliers.

There are no planarity outliers.

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	5957	0	5673	87	0
1	B	6013	0	5714	85	0
1	C	5946	0	5663	87	0
1	D	5957	0	5674	93	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	L	28	0	25	1	0
3	K	42	0	37	1	0
4	A	28	0	26	0	0
4	B	42	0	39	0	0
4	C	42	0	39	0	0
4	D	56	0	52	1	0
5	A	26	0	29	2	0
5	B	26	0	29	1	0
5	C	26	0	29	0	0
5	D	26	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	145	0	0	1	0
6	B	134	0	0	3	0
6	C	76	0	0	2	0
6	D	132	0	0	6	0
All	All	24870	0	23208	348	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 7.

All (348) 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:193:ILE:HG22	1:D:194:ILE:HD13	1.49	0.94
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.94	0.91
4:D:2811:NAG:H2	6:D:845:HOH:O	1.70	0.89
1:C:511:SER:HB3	6:C:812:HOH:O	1.74	0.88
1:B:73:GLU:HA	6:B:866:HOH:O	1.79	0.82
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.64	0.81
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.63	0.80
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.66	0.78
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.78	0.77
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.20	0.76
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.78	0.76
1:A:91:GLU:O	1:A:94:THR:HG22	1.86	0.75
1:C:72:GLN:O	1:C:73:GLU:HB2	1.86	0.75
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.33	0.73
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.89	0.71
1:B:77:LEU:HD23	1:B:86:SER:HB2	1.72	0.71
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.71	0.71
1:B:614:SER:HA	1:B:619:VAL:HB	1.73	0.70
1:A:343:ARG:HD3	1:A:389:ILE:CG2	2.21	0.69
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.74	0.69
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.74	0.69
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.76	0.68
1:A:343:ARG:HD3	1:A:389:ILE:HG23	1.75	0.67
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.77	0.66
1:D:84:GLY:C	1:D:86:SER:H	2.03	0.66
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.78	0.66
1:C:184:ARG:HD3	1:C:186:THR:O	1.96	0.66
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.78	0.65
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PRO:HG3	1:B:326:ASP:OD1	1.97	0.64
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.28	0.64
1:D:751:ILE:HG12	1:D:755:MET:HE2	1.79	0.63
2:I:1:NAG:H61	2:I:2:NAG:C7	2.29	0.63
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.62	0.63
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.34	0.62
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.80	0.62
1:B:471:ARG:HG2	1:B:480:TYR:CE1	2.34	0.62
1:A:74:ASN:HB2	1:A:92:ASN:HB3	1.80	0.62
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.35	0.62
1:A:751:ILE:O	1:A:755:MET:HG3	2.00	0.61
1:D:72:GLN:C	1:D:74:ASN:H	2.08	0.61
1:D:723:LEU:HD22	1:D:728:VAL:HG11	1.82	0.61
1:B:316:LEU:HD13	1:B:320:GLN:HG2	1.83	0.60
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.37	0.60
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.82	0.60
1:B:184:ARG:HD3	1:B:186:THR:O	2.01	0.59
1:C:614:SER:HA	1:C:619:VAL:HB	1.83	0.59
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.36	0.59
1:C:177:GLU:HB2	1:C:180:LEU:HG	1.83	0.59
1:D:723:LEU:HB3	1:D:728:VAL:HG13	1.84	0.59
1:B:242:SER:OG	1:B:243:ASP:N	2.36	0.59
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.38	0.58
1:B:613:PHE:O	1:B:616:MET:HB2	2.03	0.58
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.85	0.58
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.03	0.58
1:C:167:VAL:HA	1:C:171:ASP:O	2.03	0.58
1:B:73:GLU:O	1:B:74:ASN:HB2	2.04	0.57
1:D:70:TYR:CE2	1:D:71:LYS:HE3	2.40	0.57
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.39	0.57
1:C:72:GLN:O	1:C:73:GLU:CB	2.53	0.57
1:A:72:GLN:O	1:A:73:GLU:HB2	2.05	0.57
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.88	0.56
1:C:657:SER:HA	1:C:688:VAL:CG1	2.36	0.56
1:D:206:GLU:HB3	1:D:665:VAL:CG2	2.35	0.56
1:C:172:ILE:HD13	1:C:214:LEU:HD21	1.88	0.56
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.88	0.56
1:B:127:SER:HB3	1:B:211:TYR:CG	2.41	0.55
1:B:202:VAL:HG22	6:B:799:HOH:O	2.05	0.55
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.36	0.55
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:HE3	6:B:797:HOH:O	2.06	0.55
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.37	0.55
1:A:253:ARG:NH2	1:B:253:ARG:HH21	2.04	0.55
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.41	0.55
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.90	0.54
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.08	0.53
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.90	0.53
1:A:518:ILE:O	1:A:519:LEU:HD13	2.08	0.53
1:B:751:ILE:O	1:B:755:MET:HG3	2.07	0.53
1:A:433:LYS:HD2	1:A:445:LEU:HD21	1.90	0.53
1:C:598:LEU:HG	1:C:631:TYR:OH	2.07	0.53
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.90	0.53
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.90	0.53
1:B:64:SER:O	1:B:463:LYS:HB2	2.09	0.53
1:B:493:VAL:HG11	1:B:496:ASP:HB3	1.91	0.53
1:D:73:GLU:O	1:D:74:ASN:HB2	2.09	0.53
1:A:63:ILE:HD11	1:A:69:LEU:HG	1.92	0.52
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.90	0.52
1:A:242:SER:OG	1:A:243:ASP:N	2.41	0.52
1:C:465:ALA:O	1:C:485:SER:OG	2.24	0.52
1:B:626:ILE:HD13	1:B:639:VAL:HG11	1.91	0.52
1:D:761:GLN:HB3	6:D:880:HOH:O	2.10	0.52
1:A:129:THR:HG23	1:A:151:ASN:HA	1.91	0.52
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.74	0.52
1:A:744:SER:O	1:A:745:SER:C	2.54	0.51
1:B:102:ILE:HD12	1:B:102:ILE:H	1.75	0.51
1:A:598:LEU:HG	1:A:631:TYR:OH	2.11	0.51
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.92	0.51
1:D:184:ARG:HD3	1:D:186:THR:O	2.10	0.51
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.45	0.51
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.44	0.51
1:D:79:PHE:HA	1:D:86:SER:HB3	1.93	0.51
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.93	0.51
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.93	0.51
1:A:550:PRO:HB3	1:A:594:ILE:HD11	1.92	0.51
1:B:415:LEU:C	1:B:415:LEU:HD23	2.35	0.51
1:C:731:GLN:NE2	1:D:731:GLN:OE1	2.44	0.51
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.46	0.50
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.40	0.50
1:A:346:ILE:H	1:A:392:LYS:NZ	2.09	0.50
1:C:75:ASN:HD22	1:C:91:GLU:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:LEU:HD22	1:D:411:THR:O	2.11	0.50
1:B:471:ARG:CG	1:B:480:TYR:CE1	2.94	0.50
1:C:522:THR:HB	1:C:524:PHE:CE2	2.46	0.50
1:D:294:LEU:C	1:D:296:GLY:H	2.19	0.50
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.46	0.50
1:D:107:ILE:HG22	1:D:108:SER:O	2.11	0.50
1:D:389:ILE:HG22	1:D:390:ASP:OD1	2.12	0.50
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.92	0.50
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.47	0.50
1:C:751:ILE:HG12	1:C:755:MET:HE2	1.93	0.50
1:D:189:GLY:HA2	1:D:194:ILE:HG22	1.94	0.50
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.42	0.49
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.42	0.49
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.45	0.49
1:C:756:SER:O	1:C:760:LYS:HG3	2.12	0.49
1:A:42:THR:HB	1:A:569:SER:OG	2.12	0.49
1:D:136:ASP:CG	1:D:139:LYS:HB3	2.37	0.49
1:A:63:ILE:CD1	1:A:69:LEU:HG	2.42	0.49
1:C:586:GLN:HB3	1:C:590:ILE:HD12	1.95	0.49
1:A:154:TRP:CD1	1:A:212:SER:HB2	2.47	0.49
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.49
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.95	0.49
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.93	0.49
1:B:651:ILE:HD13	1:B:755:MET:HB3	1.94	0.49
1:C:343:ARG:HD3	1:C:389:ILE:HG23	1.94	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.48
1:C:195:TYR:N	1:C:195:TYR:CD1	2.81	0.48
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.94	0.48
1:C:91:GLU:HB3	6:C:818:HOH:O	2.12	0.48
1:C:482:LEU:HB2	1:C:494:LEU:HD21	1.94	0.48
1:D:127:SER:HB3	1:D:211:TYR:CG	2.48	0.48
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.28	0.48
1:B:331:ASP:HB3	1:B:334:SER:HB2	1.95	0.48
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.29	0.48
1:B:243:ASP:OD2	1:B:245:SER:HB2	2.13	0.48
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.95	0.48
1:C:221:THR:HG23	1:C:274:ASP:OD2	2.12	0.48
1:D:268:PHE:CD2	1:D:313:LEU:HD11	2.48	0.48
1:B:334:SER:HB3	1:B:336:ARG:H	1.78	0.47
1:C:291:ALA:O	1:C:295:ILE:HG23	2.14	0.47
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.47
1:A:62:TRP:C	1:A:63:ILE:HD12	2.40	0.47
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.95	0.47
1:B:674:PRO:O	1:B:680:LEU:HD13	2.15	0.47
1:C:139:LYS:HB2	1:C:141:GLN:HG2	1.96	0.47
1:C:268:PHE:CE2	1:C:313:LEU:HD11	2.48	0.47
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.95	0.47
1:C:372:TYR:HA	1:C:385:CYS:O	2.15	0.47
1:A:195:TYR:CD1	1:A:195:TYR:N	2.82	0.47
1:D:642:SER:OG	1:D:644:SER:HB3	2.15	0.47
1:A:299:TYR:CE1	1:A:665:VAL:HG22	2.50	0.46
1:B:308:GLN:HA	1:B:308:GLN:OE1	2.14	0.46
1:B:568:ALA:HA	1:B:573:ILE:O	2.15	0.46
1:B:170:ASN:O	1:B:196:ASN:HB2	2.15	0.46
1:C:195:TYR:HB3	1:C:198:ILE:HG13	1.97	0.46
1:D:600:THR:OG1	1:D:601:PHE:N	2.47	0.46
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.97	0.46
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.15	0.46
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.98	0.46
1:B:599:GLY:N	1:B:602:GLU:OE2	2.37	0.46
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.98	0.46
1:B:343:ARG:HD2	1:B:389:ILE:HG23	1.97	0.46
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.97	0.46
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.97	0.46
1:D:708:ASP:OD1	1:D:740:HIS:HA	2.15	0.46
1:D:194:ILE:HG13	2:L:1:NAG:H82	1.98	0.46
1:C:429:ARG:HB2	1:C:457:TYR:H	1.81	0.46
1:C:444:CYS:SG	1:C:445:LEU:N	2.88	0.46
1:D:44:THR:O	1:D:47:ASP:HB2	2.15	0.46
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.15	0.46
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.51	0.45
1:B:109:PRO:HG2	1:B:158:SER:O	2.16	0.45
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.47	0.45
1:C:218:PRO:HD3	1:C:305:TRP:HB3	1.98	0.45
1:C:405:ILE:HG12	1:C:419:SER:HA	1.97	0.45
1:D:450:ASN:O	1:D:454:CYS:HB2	2.16	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:A:253:ARG:HH21	1:B:253:ARG:NH2	2.08	0.45
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.98	0.45
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LYS:O	1:D:139:LYS:HG2	2.15	0.45
1:D:301:CYS:SG	1:D:316:LEU:HB2	2.57	0.45
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.97	0.45
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.98	0.45
1:D:132:TYR:HB2	1:D:148:ILE:HG21	1.98	0.45
1:D:162:HIS:NE2	1:D:177:GLU:OE2	2.45	0.45
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.99	0.45
1:C:464:GLU:HG3	1:C:464:GLU:O	2.16	0.45
1:D:741:GLY:O	1:D:742:ILE:C	2.59	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.17	0.45
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.30	0.45
1:A:171:ASP:OD1	1:A:184:ARG:NH2	2.50	0.45
1:B:71:LYS:HA	1:B:75:ASN:O	2.17	0.45
1:B:156:THR:HG23	1:B:165:ALA:HB3	1.99	0.45
1:D:162:HIS:HE2	1:D:177:GLU:CD	2.25	0.45
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.47	0.45
1:A:139:LYS:O	1:A:140:ARG:HB2	2.17	0.44
1:A:433:LYS:HB3	1:A:445:LEU:HD11	1.99	0.44
1:B:425:MET:HA	1:B:426:PRO:HD3	1.80	0.44
1:B:473:SER:HB3	1:B:558:VAL:HG13	1.99	0.44
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.52	0.44
1:D:484:SER:O	1:D:488:ASP:HA	2.17	0.44
1:D:640:LEU:HB3	1:D:698:VAL:HG21	1.99	0.44
1:A:453:ARG:NH2	1:A:477:LEU:O	2.41	0.44
1:A:293:MET:HG3	1:A:315:TRP:HB2	1.98	0.44
6:A:859:HOH:O	1:D:40:ARG:HG2	2.17	0.44
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.98	0.44
1:C:316:LEU:HD13	1:C:320:GLN:HG2	1.99	0.44
1:C:352:GLY:HA2	1:C:595:ASN:OD1	2.17	0.44
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.52	0.44
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.98	0.44
1:C:312:SER:HB2	1:C:325:MET:HE3	2.00	0.44
1:C:571:GLU:CD	1:C:760:LYS:HD3	2.43	0.44
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.48	0.44
1:D:321:ASN:ND2	6:D:843:HOH:O	2.49	0.44
1:C:199:THR:HA	1:C:228:PHE:CE2	2.53	0.44
1:C:474:GLY:HA2	1:C:476:GLY:O	2.18	0.44
1:D:167:VAL:HA	1:D:171:ASP:O	2.18	0.44
1:D:173:TYR:CE1	1:D:184:ARG:HG3	2.53	0.43
1:D:369:ASN:C	1:D:389:ILE:HD13	2.43	0.43
1:C:232:GLU:HB2	1:C:262:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.43
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.99	0.43
1:A:703:ILE:HG21	1:A:751:ILE:HD12	2.00	0.43
1:C:657:SER:HA	1:C:688:VAL:HG12	1.99	0.43
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.99	0.43
1:C:218:PRO:HD3	1:C:305:TRP:CB	2.49	0.43
1:C:236:ILE:HD12	1:D:249:PRO:HD2	2.00	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HB3	2.01	0.43
1:C:708:ASP:CG	1:C:711:VAL:O	2.62	0.43
1:D:487:ASN:O	1:D:488:ASP:HB2	2.17	0.43
1:D:645:GLY:HA2	6:D:841:HOH:O	2.18	0.43
1:A:215:TRP:HB2	1:A:224:ALA:HB3	1.99	0.43
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.01	0.43
1:B:53:TYR:HB3	1:B:500:LEU:CD1	2.48	0.43
1:B:73:GLU:C	1:B:75:ASN:H	2.27	0.43
1:B:219:ASN:HB3	1:B:308:GLN:NE2	2.33	0.43
1:B:307:THR:OG1	1:B:310:ARG:HB3	2.18	0.43
1:D:385:CYS:HB3	1:D:387:PHE:CE2	2.53	0.43
1:A:636:THR:HG21	1:A:651:ILE:O	2.18	0.43
1:C:720:SER:O	1:C:724:VAL:HG23	2.19	0.43
1:D:657:SER:HA	1:D:688:VAL:HG13	1.99	0.43
1:D:453:ARG:HD2	1:D:477:LEU:O	2.19	0.43
1:A:446:SER:HA	1:A:449:LEU:HG	2.01	0.43
1:B:167:VAL:HA	1:B:171:ASP:O	2.19	0.43
1:B:59:SER:O	1:B:70:TYR:CD1	2.72	0.43
1:B:318:ARG:O	1:B:320:GLN:HG3	2.19	0.43
1:C:153:GLN:HB3	1:C:211:TYR:CE1	2.54	0.43
1:A:431:LEU:HD13	1:A:459:VAL:HG11	2.01	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.52	0.42
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.49	0.42
1:B:658:ARG:HG2	1:B:689:MET:HE1	2.01	0.42
1:D:554:LYS:HB3	1:D:577:SER:HB3	2.02	0.42
1:A:391:LYS:HE2	1:A:391:LYS:HB3	1.85	0.42
1:D:243:ASP:C	1:D:245:SER:N	2.75	0.42
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.84	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.42
1:C:183:TYR:CD2	1:C:276:LEU:HD23	2.55	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.55	0.42
1:A:219:ASN:HB3	1:A:308:GLN:HE22	1.85	0.42
1:A:598:LEU:HD22	1:A:671:MET:HG2	2.01	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:LEU:HD22	1:C:671:MET:HG2	2.01	0.42
1:A:316:LEU:HD13	1:A:320:GLN:HG2	2.02	0.42
1:C:564:ALA:HA	1:C:567:LEU:HD12	2.02	0.42
1:D:142:LEU:HD23	1:D:142:LEU:H	1.84	0.42
1:D:562:ASN:HB2	6:D:869:HOH:O	2.20	0.42
1:A:543:LEU:O	1:A:575:VAL:HA	2.19	0.42
1:B:177:GLU:HB2	1:B:180:LEU:HD22	2.02	0.42
1:A:219:ASN:HB3	1:A:308:GLN:NE2	2.35	0.42
1:C:194:ILE:HD13	3:K:1:NAG:H82	2.01	0.42
1:C:657:SER:HB2	1:C:689:MET:SD	2.60	0.42
5:D:1:01T:C26	5:D:1:01T:H12	2.49	0.42
1:A:49:LEU:HD22	1:A:749:GLN:HA	2.01	0.41
1:A:382:ARG:H	1:A:403:GLU:HG2	1.85	0.41
1:A:597:ARG:HH11	1:A:682:HIS:CB	2.32	0.41
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.41
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.55	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.86	0.41
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.02	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:A:90:LEU:CD2	1:A:114:ILE:HD13	2.50	0.41
1:B:552:SER:O	1:B:583:SER:HB2	2.20	0.41
1:C:114:ILE:HG22	1:C:135:TYR:HB2	2.02	0.41
1:D:84:GLY:C	1:D:86:SER:N	2.73	0.41
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.55	0.41
1:D:651:ILE:HD13	1:D:755:MET:HG2	2.02	0.41
1:D:739:ASP:HB2	6:D:828:HOH:O	2.21	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.41
1:A:720:SER:O	1:A:724:VAL:HG23	2.20	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.41
1:C:73:GLU:HB3	1:C:74:ASN:H	1.65	0.41
1:D:314:GLN:OE1	1:D:362:PRO:HD3	2.19	0.41
1:D:503:MET:H	1:D:503:MET:HG2	1.46	0.41
1:A:285:ILE:HG21	1:A:337:TRP:HD1	1.86	0.41
1:A:493:VAL:HG11	1:A:496:ASP:HB3	2.03	0.41
1:B:633:GLY:HA3	1:B:655:PRO:HB3	2.03	0.41
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.56	0.41
1:D:295:ILE:O	1:D:295:ILE:HG23	2.21	0.41
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.56	0.41
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.02	0.41
5:B:1:01T:H6A	5:B:1:01T:H12A	1.90	0.41
1:A:630:SER:OG	5:A:1:01T:C22	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:HB2	1:B:85:ASN:HB2	2.03	0.41
1:B:258:LYS:O	1:B:259:ALA:C	2.63	0.41
1:B:386:TYR:O	1:B:394:CYS:HB2	2.21	0.41
1:B:601:PHE:O	1:B:605:ASP:N	2.47	0.41
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.56	0.41
1:C:411:THR:C	1:C:413:ASP:H	2.29	0.41
1:D:139:LYS:O	1:D:140:ARG:HB2	2.20	0.41
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.02	0.41
1:A:414:TYR:CD2	1:A:433:LYS:HE2	2.56	0.41
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.02	0.41
5:A:1:01T:H12A	5:A:1:01T:H6A	1.84	0.41
1:B:102:ILE:H	1:B:102:ILE:CD1	2.34	0.41
1:C:154:TRP:CD2	1:C:212:SER:HB3	2.56	0.41
1:A:485:SER:O	1:A:486:VAL:C	2.64	0.40
1:D:208:PHE:O	1:D:209:SER:C	2.63	0.40
1:D:429:ARG:HB2	1:D:457:TYR:H	1.86	0.40
1:D:493:VAL:HG11	1:D:496:ASP:HB3	2.02	0.40
1:B:49:LEU:HB3	1:B:749:GLN:HG2	2.03	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.02	0.40
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.21	0.40
1:C:517:ILE:HD11	1:C:578:PHE:CE1	2.56	0.40
1:C:626:ILE:HG12	1:C:636:THR:HG23	2.03	0.40
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.56	0.40
1:B:594:ILE:HG12	1:B:598:LEU:HD23	2.03	0.40
1:D:129:THR:HG23	1:D:151:ASN:HA	2.04	0.40
1:C:299:TYR:CE1	1:C:665:VAL:HG22	2.56	0.40
1:C:388:GLN:O	1:C:389:ILE:C	2.65	0.40
1:C:658:ARG:CB	1:C:687:THR:HG22	2.50	0.40
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.03	0.40
1:B:208:PHE:O	1:B:209:SER:C	2.63	0.40
1:C:450:ASN:O	1:C:454:CYS:HB2	2.22	0.40
2:J:1:NAG:H62	2:J:2:NAG:N2	2.36	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	725/740 (98%)	674 (93%)	47 (6%)	4 (1%)	21	38
1	B	731/740 (99%)	682 (93%)	47 (6%)	2 (0%)	36	54
1	C	724/740 (98%)	667 (92%)	54 (8%)	3 (0%)	30	48
1	D	725/740 (98%)	675 (93%)	44 (6%)	6 (1%)	16	31
All	All	2905/2960 (98%)	2698 (93%)	192 (7%)	15 (0%)	24	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	85	ASN
1	C	73	GLU
1	D	85	ASN
1	D	140	ARG
1	A	140	ARG
1	D	73	GLU
1	D	86	SER
1	D	521	GLU
1	A	745	SER
1	B	88	VAL
1	C	389	ILE
1	C	109	PRO
1	A	486	VAL
1	D	295	ILE

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	652/662 (98%)	599 (92%)	53 (8%)	11	23
1	B	658/662 (99%)	602 (92%)	56 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	651/662 (98%)	610 (94%)	41 (6%)	16	34
1	D	652/662 (98%)	592 (91%)	60 (9%)	8	19
All	All	2613/2648 (99%)	2403 (92%)	210 (8%)	11	24

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	50	LYS
1	A	51	ASN
1	A	57	LEU
1	A	74	ASN
1	A	77	LEU
1	A	78	VAL
1	A	129	THR
1	A	155	VAL
1	A	156	THR
1	A	164	LEU
1	A	195	TYR
1	A	212	SER
1	A	235	LEU
1	A	236	ILE
1	A	246	LEU
1	A	276	LEU
1	A	316	LEU
1	A	327	ILE
1	A	340	LEU
1	A	341	VAL
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	391	LYS
1	A	392	LYS
1	A	395	THR
1	A	399	LYS
1	A	410	LEU
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	443	THR

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Mol	Chain	Res	Type
1	A	448	GLU
1	A	453	ARG
1	A	463	LYS
1	A	464	GLU
1	A	482	LEU
1	A	504	LEU
1	A	505	GLN
1	A	507	VAL
1	A	512	LYS
1	A	514	LEU
1	A	517	ILE
1	A	519	LEU
1	A	538	LYS
1	A	575	VAL
1	A	598	LEU
1	A	615	LYS
1	A	673	LEU
1	A	684	ARG
1	A	688	VAL
1	B	55	LEU
1	B	56	LYS
1	B	57	LEU
1	B	60	LEU
1	B	66	HIS
1	B	71	LYS
1	B	96	ASP
1	B	102	ILE
1	B	107	ILE
1	B	129	THR
1	B	137	LEU
1	B	143	ILE
1	B	145	GLU
1	B	156	THR
1	B	164	LEU
1	B	180	LEU
1	B	184	ARG
1	B	190	LYS
1	B	202	VAL
1	B	227	GLN
1	B	262	VAL
1	B	276	LEU
1	B	313	LEU

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Mol	Chain	Res	Type
1	B	316	LEU
1	B	339	CYS
1	B	341	VAL
1	B	343	ARG
1	B	351	THR
1	B	354	VAL
1	B	366	LEU
1	B	370	SER
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	392	LYS
1	B	395	THR
1	B	412	SER
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	471	ARG
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	521	GLU
1	B	594	ILE
1	B	597	ARG
1	B	602	GLU
1	B	627	TRP
1	B	665	VAL
1	B	677	GLU
1	B	688	VAL
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	B	764	SER
1	C	61	ARG
1	C	63	ILE
1	C	77	LEU
1	C	129	THR
1	C	137	LEU
1	C	140	ARG
1	C	144	THR
1	C	164	LEU
1	C	184	ARG

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Mol	Chain	Res	Type
1	C	193	ILE
1	C	202	VAL
1	C	239	SER
1	C	246	LEU
1	C	278	SER
1	C	308	GLN
1	C	316	LEU
1	C	323	SER
1	C	339	CYS
1	C	370	SER
1	C	378	GLU
1	C	379	GLU
1	C	385	CYS
1	C	398	THR
1	C	413	ASP
1	C	444	CYS
1	C	447	CYS
1	C	452	GLU
1	C	463	LYS
1	C	482	LEU
1	C	492	ARG
1	C	504	LEU
1	C	511	SER
1	C	519	LEU
1	C	538	LYS
1	C	565	THR
1	C	594	ILE
1	C	597	ARG
1	C	598	LEU
1	C	677	GLU
1	C	688	VAL
1	C	759	ILE
1	D	40	ARG
1	D	41	LYS
1	D	55	LEU
1	D	59	SER
1	D	61	ARG
1	D	66	HIS
1	D	71	LYS
1	D	92	ASN
1	D	94	THR
1	D	96	ASP

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Mol	Chain	Res	Type
1	D	98	PHE
1	D	123	GLN
1	D	129	THR
1	D	155	VAL
1	D	164	LEU
1	D	180	LEU
1	D	188	THR
1	D	194	ILE
1	D	227	GLN
1	D	232	GLU
1	D	235	LEU
1	D	243	ASP
1	D	276	LEU
1	D	283	THR
1	D	295	ILE
1	D	316	LEU
1	D	323	SER
1	D	327	ILE
1	D	341	VAL
1	D	343	ARG
1	D	350	THR
1	D	354	VAL
1	D	373	LYS
1	D	385	CYS
1	D	390	ASP
1	D	391	LYS
1	D	392	LYS
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	453	ARG
1	D	460	SER
1	D	464	GLU
1	D	482	LEU
1	D	503	MET
1	D	514	LEU
1	D	518	ILE
1	D	519	LEU
1	D	536	LYS
1	D	546	VAL
1	D	575	VAL

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Mol	Chain	Res	Type
1	D	597	ARG
1	D	658	ARG
1	D	665	VAL
1	D	673	LEU
1	D	688	VAL
1	D	711	VAL
1	D	728	VAL
1	D	745	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	369	ASN
1	A	435	GLN
1	A	505	GLN
1	B	112	GLN
1	B	430	ASN
1	C	72	GLN
1	C	227	GLN
1	C	606	GLN
1	C	697	GLN
1	C	748	HIS
1	D	85	ASN
1	D	112	GLN
1	D	344	GLN
1	D	430	ASN
1	D	435	GLN
1	D	505	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 ⓘ

17 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	1,2	14,14,15	0.67	0	17,19,21	2.10	4 (23%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	0.86	0
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	1.51	2 (11%)
2	NAG	F	2	2	14,14,15	0.70	0	17,19,21	1.45	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.60	0	17,19,21	1.14	2 (11%)
2	NAG	G	2	2	14,14,15	0.64	0	17,19,21	1.32	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.77	0	17,19,21	1.64	3 (17%)
2	NAG	H	2	2	14,14,15	0.56	0	17,19,21	0.76	0
2	NAG	I	1	1,2	14,14,15	0.58	0	17,19,21	1.28	0
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	0.85	0
2	NAG	J	1	1,2	14,14,15	0.60	0	17,19,21	1.31	1 (5%)
2	NAG	J	2	2	14,14,15	0.67	0	17,19,21	1.61	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.43	0	17,19,21	1.31	2 (11%)
3	NAG	K	2	3	14,14,15	0.54	0	17,19,21	2.90	6 (35%)
3	NAG	K	3	3	14,14,15	0.37	0	17,19,21	1.15	3 (17%)
2	NAG	L	1	1,2	14,14,15	0.57	0	17,19,21	1.45	3 (17%)
2	NAG	L	2	2	14,14,15	0.51	0	17,19,21	0.89	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
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	3	3	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	NAG	C1-O5-C5	7.29	121.95	112.19
3	K	2	NAG	O4-C4-C5	5.68	123.32	109.32
3	K	2	NAG	C4-C3-C2	-5.49	102.97	111.02
2	E	1	NAG	C1-O5-C5	5.33	119.33	112.19
2	F	1	NAG	C2-N2-C7	4.59	129.06	122.90
2	H	1	NAG	C4-C3-C2	4.52	117.64	111.02
2	F	2	NAG	C4-C3-C2	4.02	116.91	111.02
2	J	2	NAG	C3-C4-C5	3.94	117.37	110.23
2	E	1	NAG	C4-C3-C2	-3.59	105.75	111.02
2	J	2	NAG	C4-C3-C2	3.59	116.28	111.02
2	J	1	NAG	C1-O5-C5	3.55	116.94	112.19
2	E	1	NAG	C2-N2-C7	3.45	127.53	122.90
2	H	1	NAG	C1-O5-C5	3.32	116.63	112.19
3	K	2	NAG	C8-C7-N2	3.17	121.37	116.12
2	E	1	NAG	C1-C2-N2	3.13	115.36	110.43
3	K	1	NAG	C1-O5-C5	2.98	116.19	112.19
2	L	1	NAG	C1-O5-C5	2.96	116.16	112.19
3	K	3	NAG	C1-O5-C5	2.90	116.07	112.19
2	G	2	NAG	C1-O5-C5	2.89	116.05	112.19
2	G	1	NAG	O5-C1-C2	-2.79	106.97	111.29
2	H	1	NAG	C3-C4-C5	2.71	115.14	110.23
2	L	1	NAG	C4-C3-C2	2.70	114.97	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C3-C4-C5	2.44	114.65	110.23
2	F	2	NAG	C3-C4-C5	2.44	114.65	110.23
3	K	3	NAG	O5-C1-C2	-2.36	107.64	111.29
3	K	2	NAG	C3-C4-C5	-2.22	106.20	110.23
3	K	1	NAG	O5-C1-C2	-2.10	108.04	111.29
3	K	2	NAG	O7-C7-C8	-2.08	118.35	122.05
2	G	1	NAG	C4-C3-C2	2.07	114.05	111.02
2	F	1	NAG	C1-C2-N2	2.07	113.69	110.43
2	G	2	NAG	O7-C7-C8	-2.05	118.39	122.05
2	J	2	NAG	O5-C1-C2	-2.05	108.12	111.29
3	K	3	NAG	O5-C5-C6	2.02	111.60	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	1	NAG	C1

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	L	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O7-C7-N2-C2

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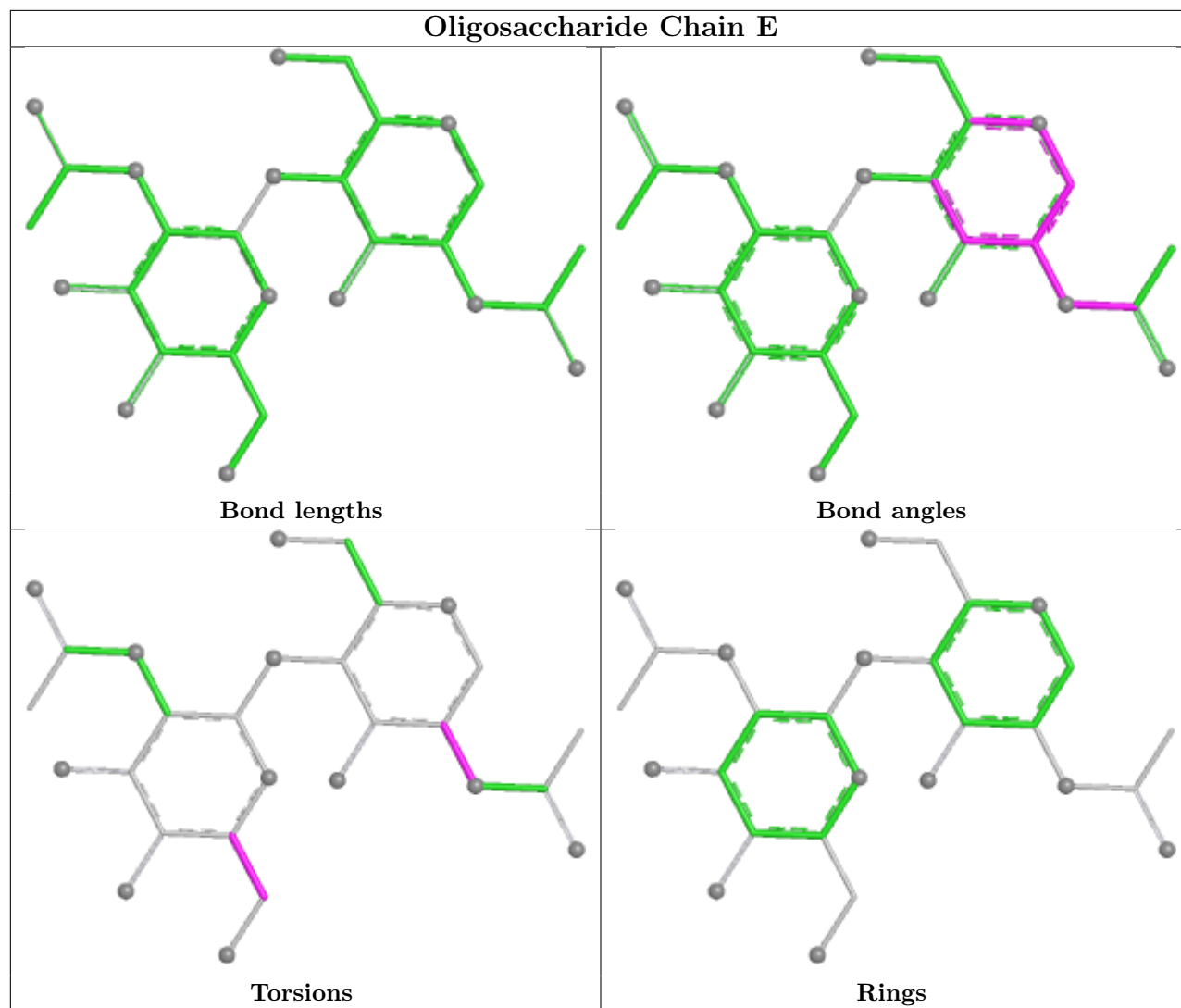
Mol	Chain	Res	Type	Atoms
2	H	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C3-C2-N2-C7
3	K	3	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7

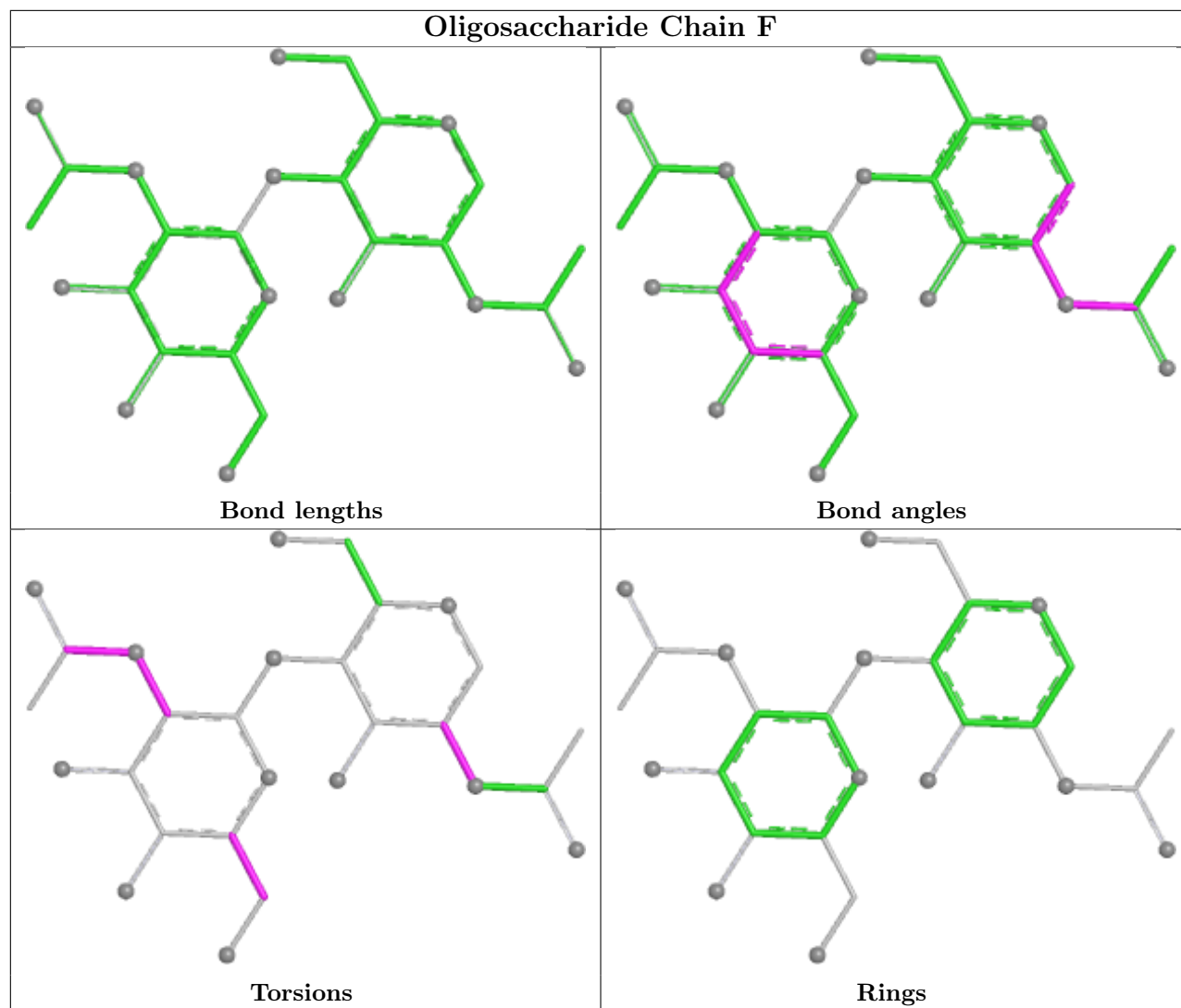
There are no ring outliers.

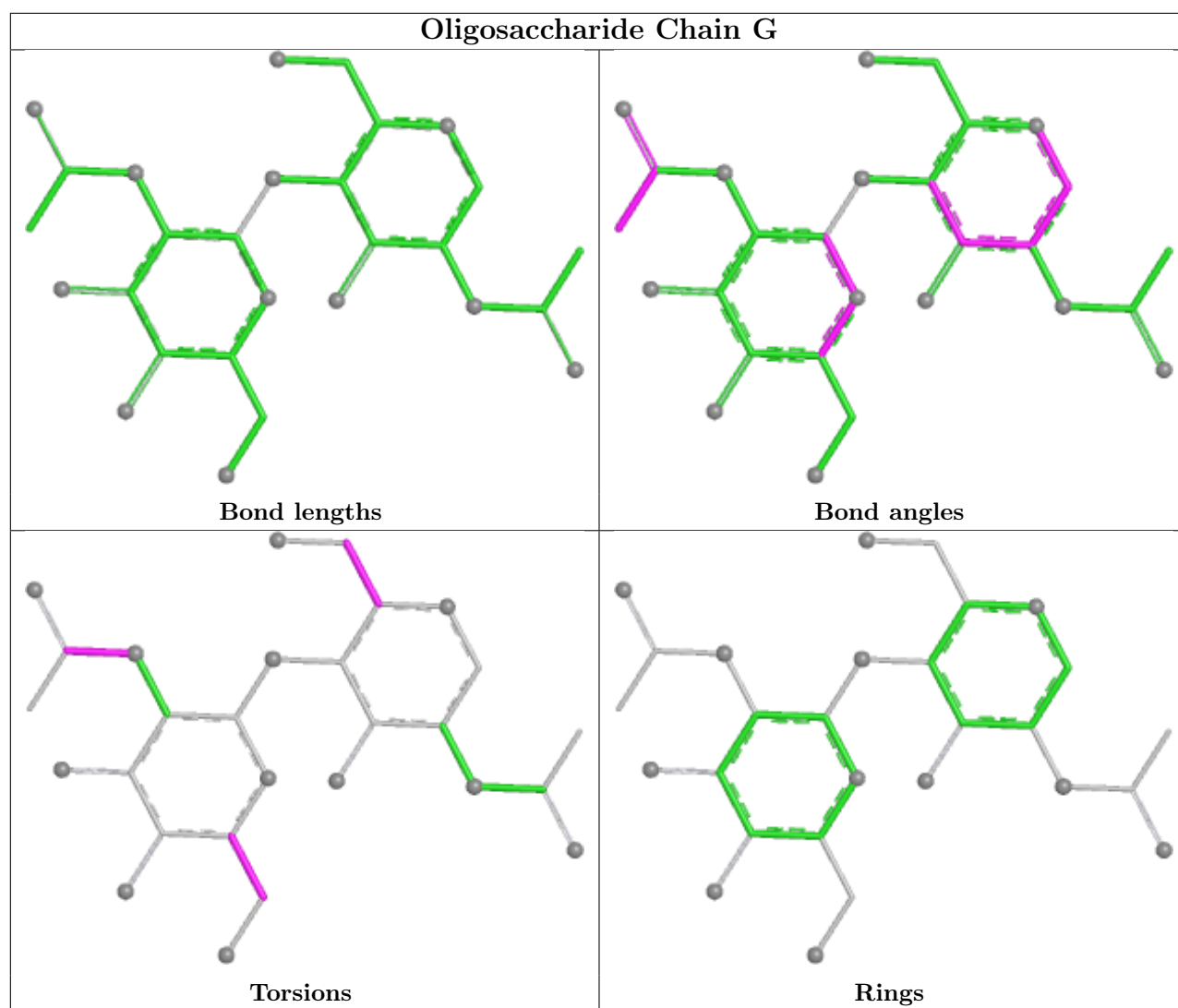
6 monomers are involved in 4 short contacts:

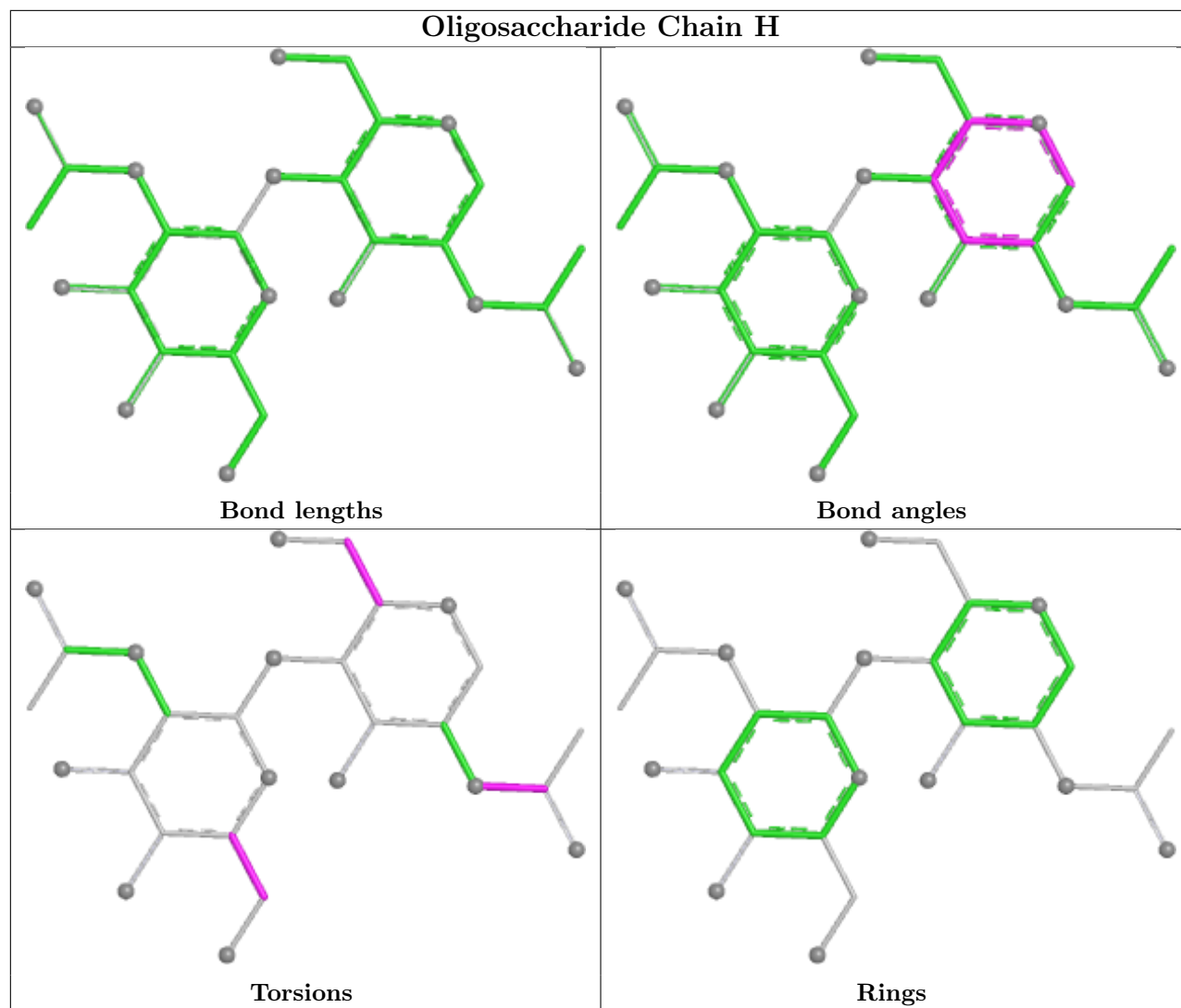
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	1	0
2	L	1	NAG	1	0
2	I	2	NAG	1	0
2	I	1	NAG	1	0
3	K	1	NAG	1	0
2	J	1	NAG	1	0

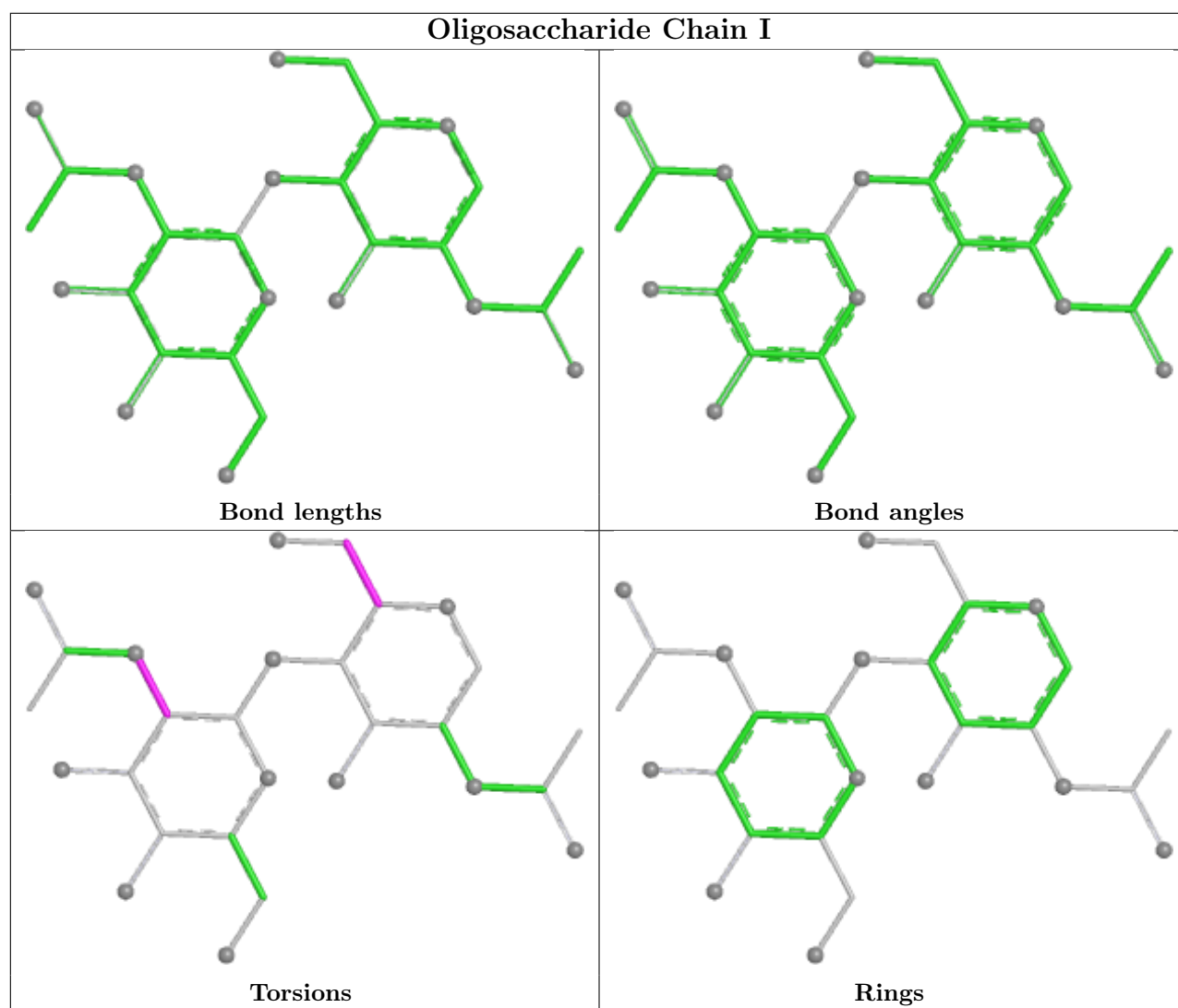
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

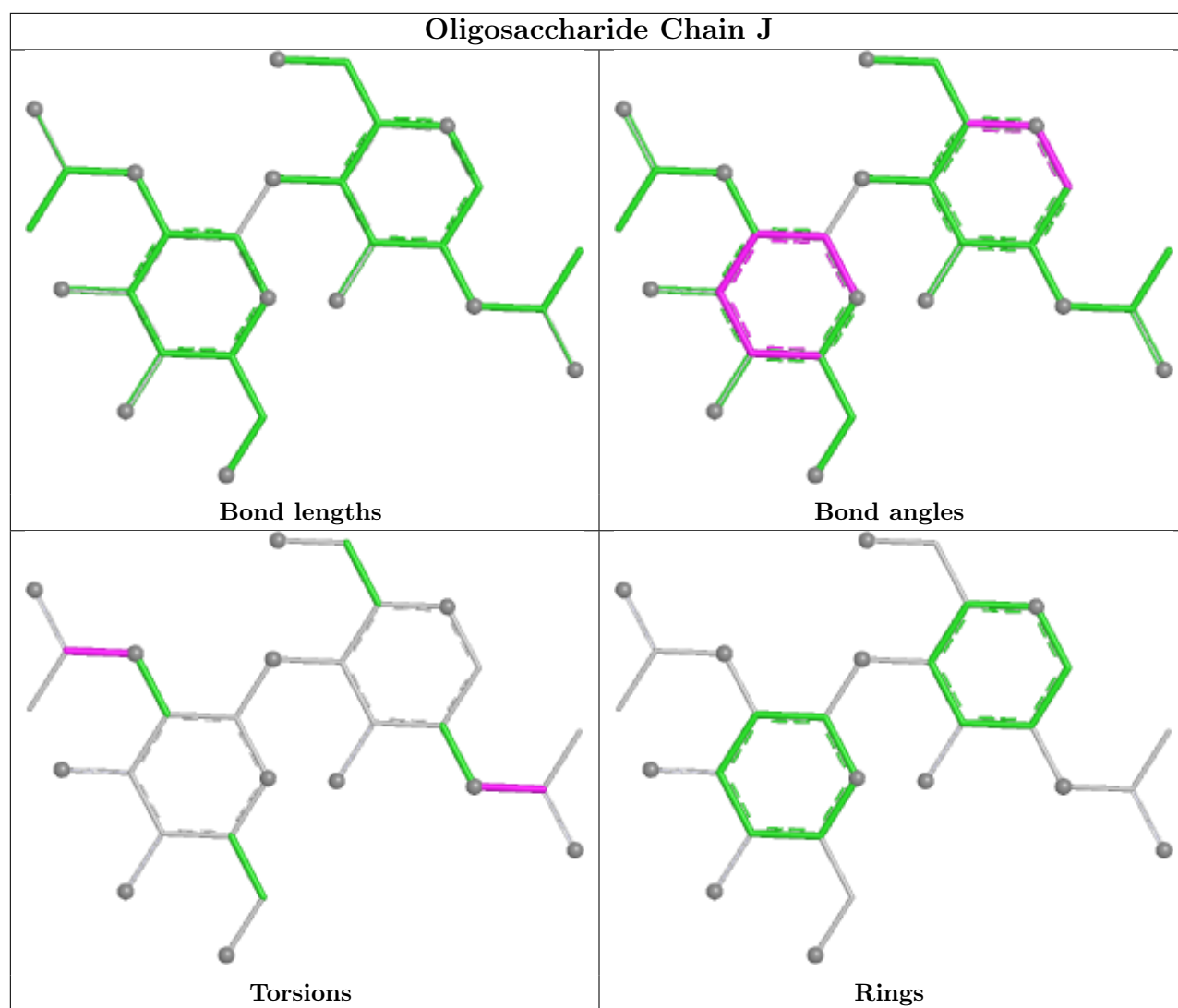


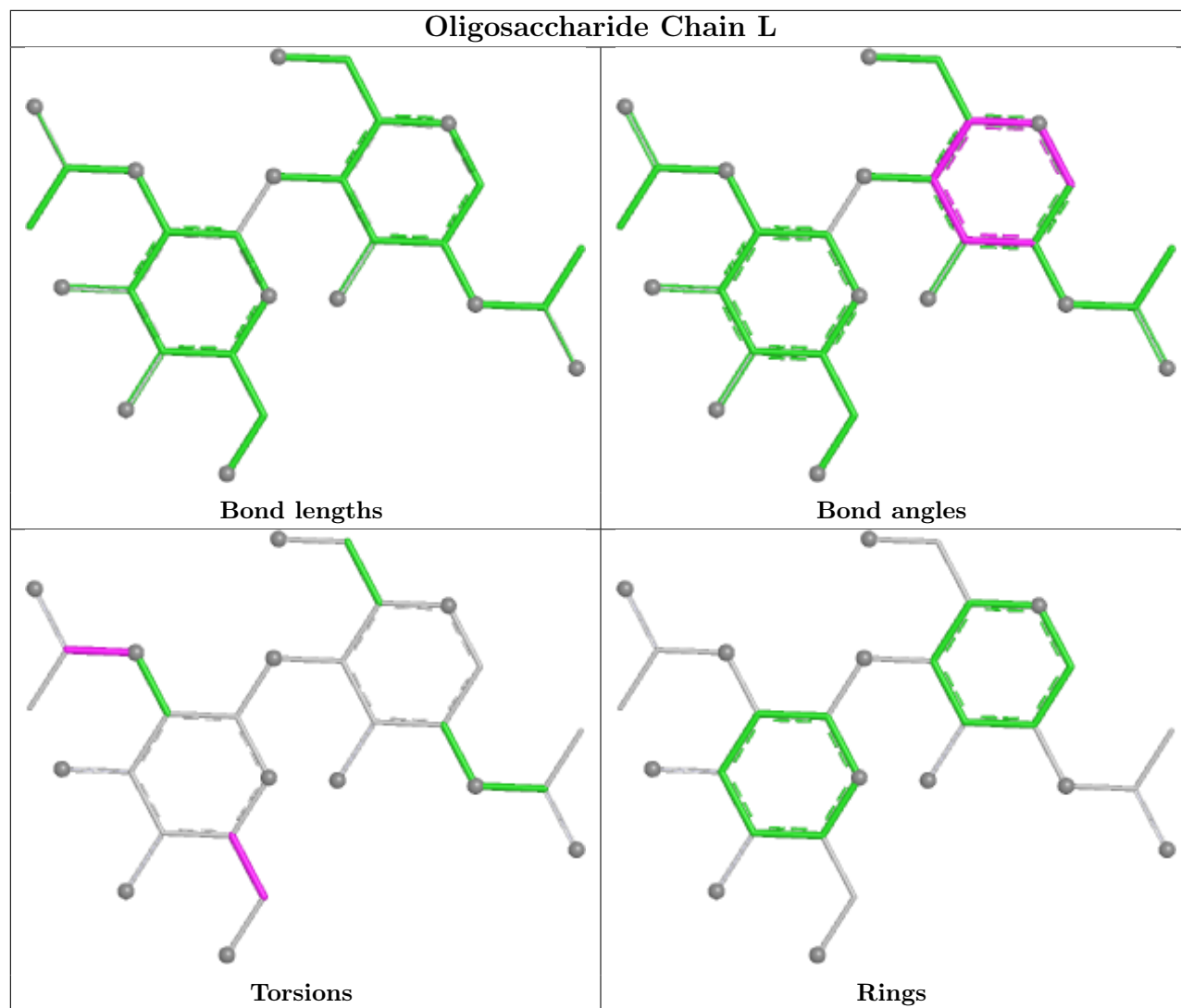


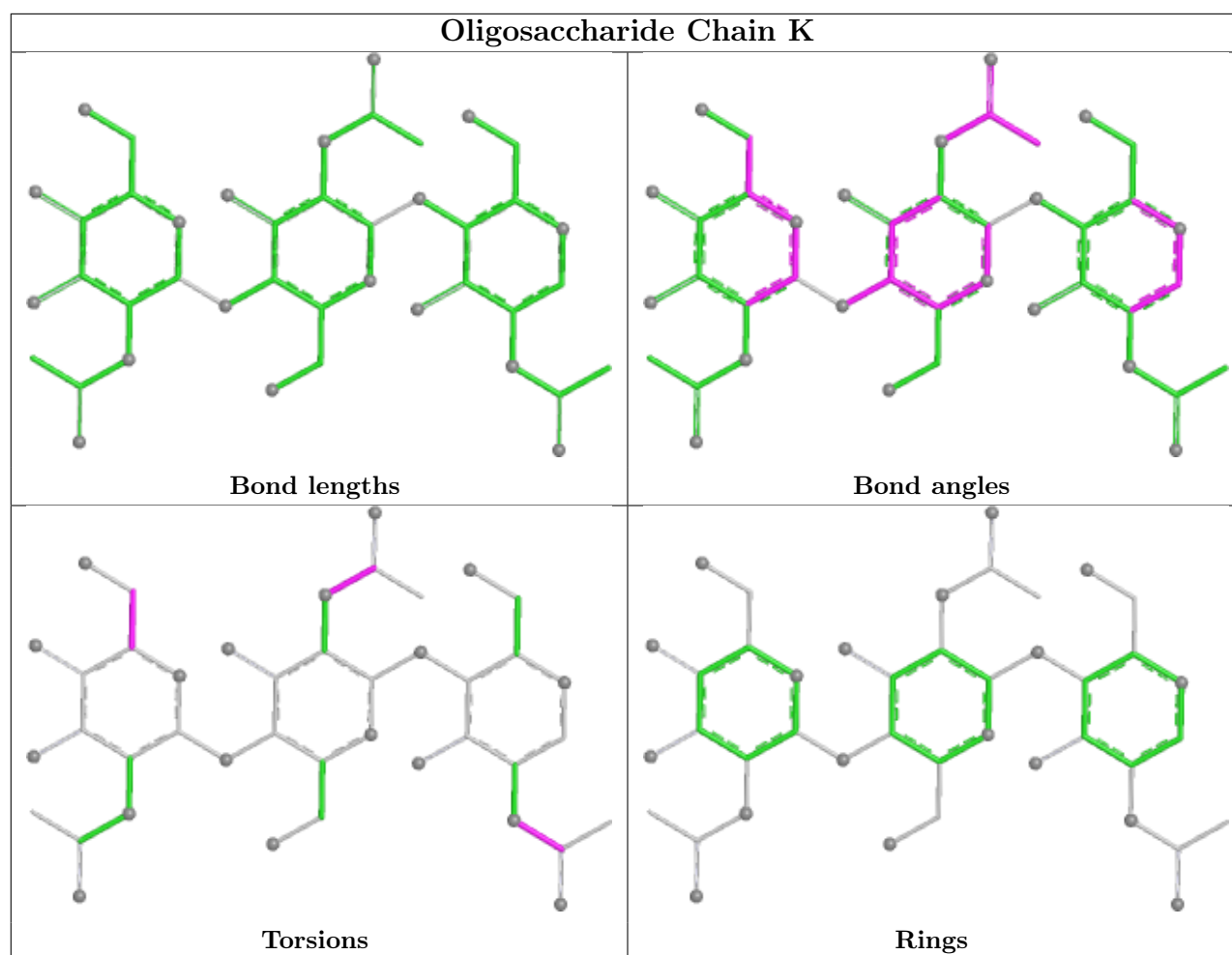












5.6 Ligand geometry [i](#)

16 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	B	3211	1	14,14,15	0.69	0	17,19,21	1.58	4 (23%)
4	NAG	C	2811	1	14,14,15	0.68	1 (7%)	17,19,21	1.39	2 (11%)
4	NAG	D	1501	1	14,14,15	0.71	0	17,19,21	1.96	3 (17%)
5	01T	A	1	-	26,27,27	0.57	0	33,39,39	1.93	9 (27%)
4	NAG	D	2191	1	14,14,15	0.65	0	17,19,21	1.56	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	01T	C	1	-	26,27,27	0.71	0	33,39,39	1.86	7 (21%)
4	NAG	C	3211	1	14,14,15	0.77	0	17,19,21	1.33	3 (17%)
4	NAG	D	2811	1	14,14,15	0.84	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	B	1501	1	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
4	NAG	D	5201	1	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
5	01T	D	1	-	26,27,27	0.74	1 (3%)	33,39,39	1.84	5 (15%)
4	NAG	A	2191	1	14,14,15	0.60	0	17,19,21	1.41	2 (11%)
4	NAG	C	1501	1	14,14,15	0.62	0	17,19,21	1.92	4 (23%)
5	01T	B	1	-	26,27,27	0.65	0	33,39,39	1.67	6 (18%)
4	NAG	A	3211	1	14,14,15	0.60	0	17,19,21	1.48	1 (5%)
4	NAG	B	2811	1	14,14,15	0.57	0	17,19,21	1.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
5	01T	A	1	-	-	4/16/17/17	0/2/2/2
4	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
5	01T	C	1	-	-	4/16/17/17	0/2/2/2
4	NAG	D	5201	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	C	3211	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	2811	1	-	4/6/23/26	0/1/1/1
5	01T	D	1	-	-	3/16/17/17	0/2/2/2
4	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
5	01T	B	1	-	-	1/16/17/17	0/2/2/2
4	NAG	A	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2811	NAG	C1-C2	2.26	1.55	1.52
4	C	2811	NAG	C1-C2	2.10	1.55	1.52
5	D	1	01T	C3-N4	2.08	1.37	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	01T	C15-C3-N4	-6.36	118.58	123.48
4	C	1501	NAG	C1-O5-C5	6.15	120.42	112.19
5	D	1	01T	C11-C5-N4	-5.75	119.05	123.48
4	D	1501	NAG	C1-O5-C5	5.65	119.75	112.19
4	B	2811	NAG	C1-O5-C5	5.61	119.70	112.19
5	A	1	01T	C11-C5-N4	-5.43	119.30	123.48
5	A	1	01T	C15-C3-N4	-5.22	119.46	123.48
5	D	1	01T	C15-C3-N4	-5.12	119.54	123.48
5	B	1	01T	C11-C5-N4	-5.10	119.56	123.48
4	A	3211	NAG	C1-O5-C5	5.04	118.94	112.19
4	C	2811	NAG	C1-O5-C5	4.42	118.11	112.19
5	B	1	01T	C15-C3-N4	-4.41	120.08	123.48
4	B	3211	NAG	C4-C3-C2	4.19	117.15	111.02
5	C	1	01T	C11-C5-N4	-4.04	120.37	123.48
4	A	2191	NAG	C1-O5-C5	4.04	117.60	112.19
4	B	1501	NAG	C1-O5-C5	3.58	116.99	112.19
4	D	2191	NAG	C4-C3-C2	3.55	116.22	111.02
4	D	1501	NAG	C2-N2-C7	3.46	127.54	122.90
5	A	1	01T	C15-C16-C17	3.41	118.15	114.20
4	D	2811	NAG	C4-C3-C2	3.40	116.00	111.02
4	D	2811	NAG	C1-O5-C5	3.15	116.41	112.19
4	D	2191	NAG	C1-O5-C5	3.13	116.38	112.19
4	D	5201	NAG	C1-O5-C5	3.08	116.31	112.19
4	C	3211	NAG	C1-O5-C5	2.83	115.97	112.19
5	A	1	01T	C3-N4-C5	2.77	123.01	118.14
4	B	3211	NAG	C1-O5-C5	2.75	115.88	112.19
5	C	1	01T	C3-N4-C5	2.65	122.81	118.14
5	D	1	01T	C14-C11-C5	2.64	119.85	117.88
4	C	2811	NAG	O5-C5-C6	2.64	112.79	107.66
4	C	1501	NAG	C3-C4-C5	2.63	115.00	110.23
4	C	3211	NAG	C4-C3-C2	2.58	114.80	111.02
5	C	1	01T	C7-C6-C5	-2.54	111.63	117.95
4	A	2191	NAG	C2-N2-C7	-2.54	119.50	122.90
5	C	1	01T	C15-C16-C17	-2.53	111.27	114.20
4	C	1501	NAG	O5-C5-C6	2.48	112.50	107.66
5	A	1	01T	O18-C17-C16	-2.43	115.61	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	01T	C3-N4-C5	2.42	122.39	118.14
5	D	1	01T	C3-N4-C5	2.41	122.38	118.14
5	D	1	01T	C16-C15-C14	-2.31	119.78	122.75
4	C	1501	NAG	C4-C3-C2	2.29	114.38	111.02
5	A	1	01T	C14-C11-C5	2.24	119.55	117.88
4	D	2191	NAG	C3-C4-C5	2.23	114.28	110.23
4	D	1501	NAG	O3-C3-C2	2.18	113.93	109.40
4	C	3211	NAG	C2-N2-C7	2.17	125.80	122.90
5	B	1	01T	C14-C11-C5	2.16	119.48	117.88
5	A	1	01T	O19-C17-C16	2.14	122.12	113.98
4	B	3211	NAG	C2-N2-C7	-2.12	120.06	122.90
4	B	3211	NAG	C3-C4-C5	2.11	114.06	110.23
5	C	1	01T	C21-C22-C23	-2.11	118.94	121.37
5	A	1	01T	C26-C25-C23	-2.07	118.98	121.37
5	C	1	01T	C26-C20-C21	2.06	121.37	117.68
5	A	1	01T	C7-C6-C5	-2.03	112.90	117.95
5	B	1	01T	O18-C17-C16	-2.02	116.85	122.94
5	B	1	01T	O19-C17-C16	2.01	121.65	113.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	5201	NAG	C1

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	01T	C1-C2-C3-C15
5	C	1	01T	C1-C2-C3-C15
4	C	2811	NAG	O5-C5-C6-O6
4	D	2811	NAG	O7-C7-N2-C2
4	B	2811	NAG	O5-C5-C6-O6
4	C	2811	NAG	C4-C5-C6-O6
4	C	1501	NAG	C4-C5-C6-O6
4	B	2811	NAG	C4-C5-C6-O6
4	D	2811	NAG	C8-C7-N2-C2
4	C	1501	NAG	O5-C5-C6-O6
4	D	5201	NAG	O5-C5-C6-O6
4	D	5201	NAG	C4-C5-C6-O6
4	B	2811	NAG	C8-C7-N2-C2
4	D	2811	NAG	O5-C5-C6-O6
4	D	2811	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2811	NAG	O7-C7-N2-C2
4	D	5201	NAG	C8-C7-N2-C2
4	D	1501	NAG	C3-C2-N2-C7
4	D	1501	NAG	C8-C7-N2-C2
4	D	5201	NAG	O7-C7-N2-C2
4	D	1501	NAG	C4-C5-C6-O6
4	D	1501	NAG	O7-C7-N2-C2
4	A	3211	NAG	C8-C7-N2-C2
5	A	1	01T	C14-C11-C12-N13
5	B	1	01T	C1-C2-C3-C15
5	A	1	01T	C15-C16-C17-O19
5	C	1	01T	C15-C16-C17-O18
5	A	1	01T	C15-C16-C17-O18
5	C	1	01T	C15-C16-C17-O19
4	A	3211	NAG	O7-C7-N2-C2
5	C	1	01T	C1-C2-C3-N4
5	D	1	01T	C15-C16-C17-O19
5	D	1	01T	C15-C16-C17-O18
4	B	3211	NAG	C4-C5-C6-O6
5	D	1	01T	C1-C2-C3-N4
4	B	3211	NAG	O5-C5-C6-O6

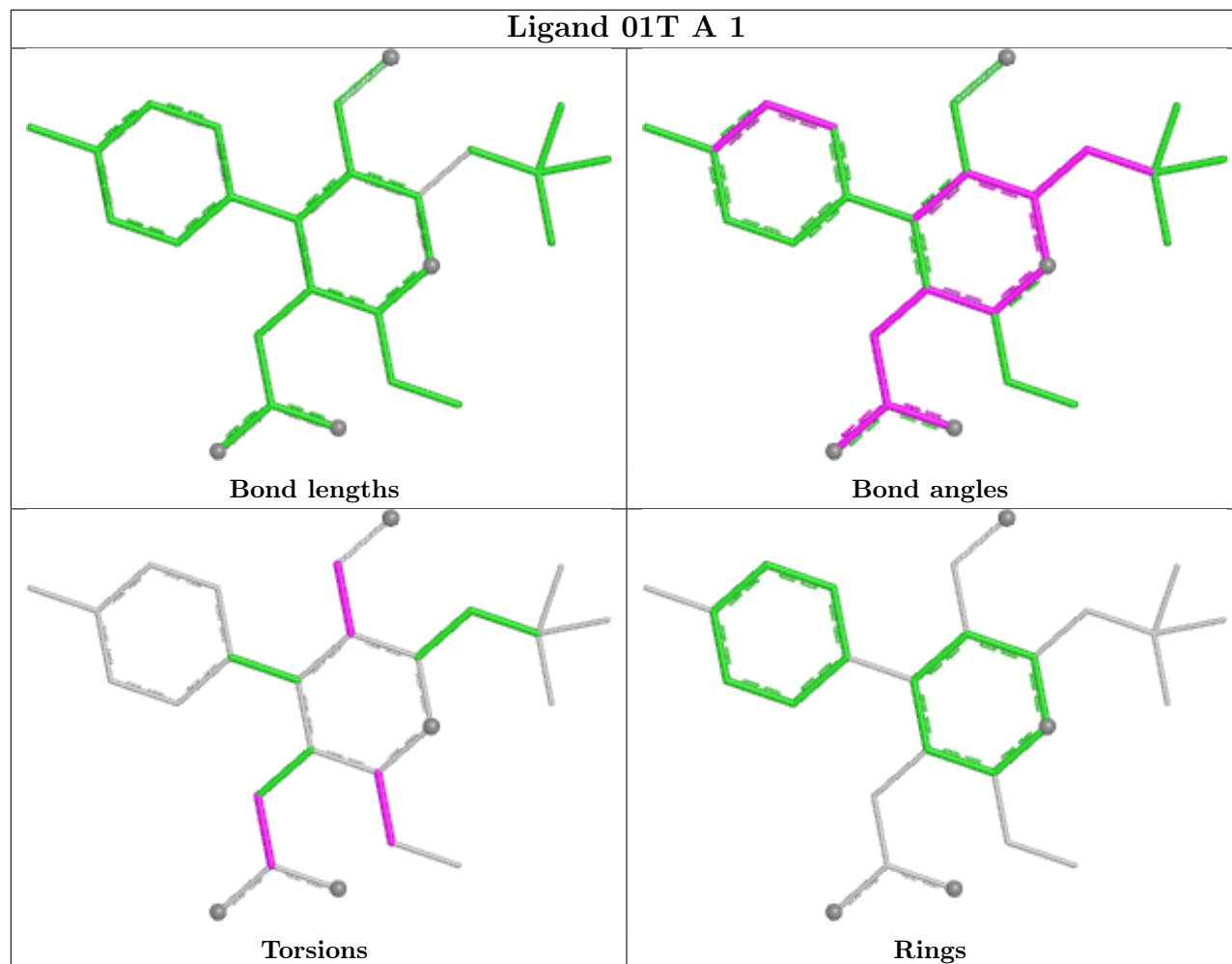
There are no ring outliers.

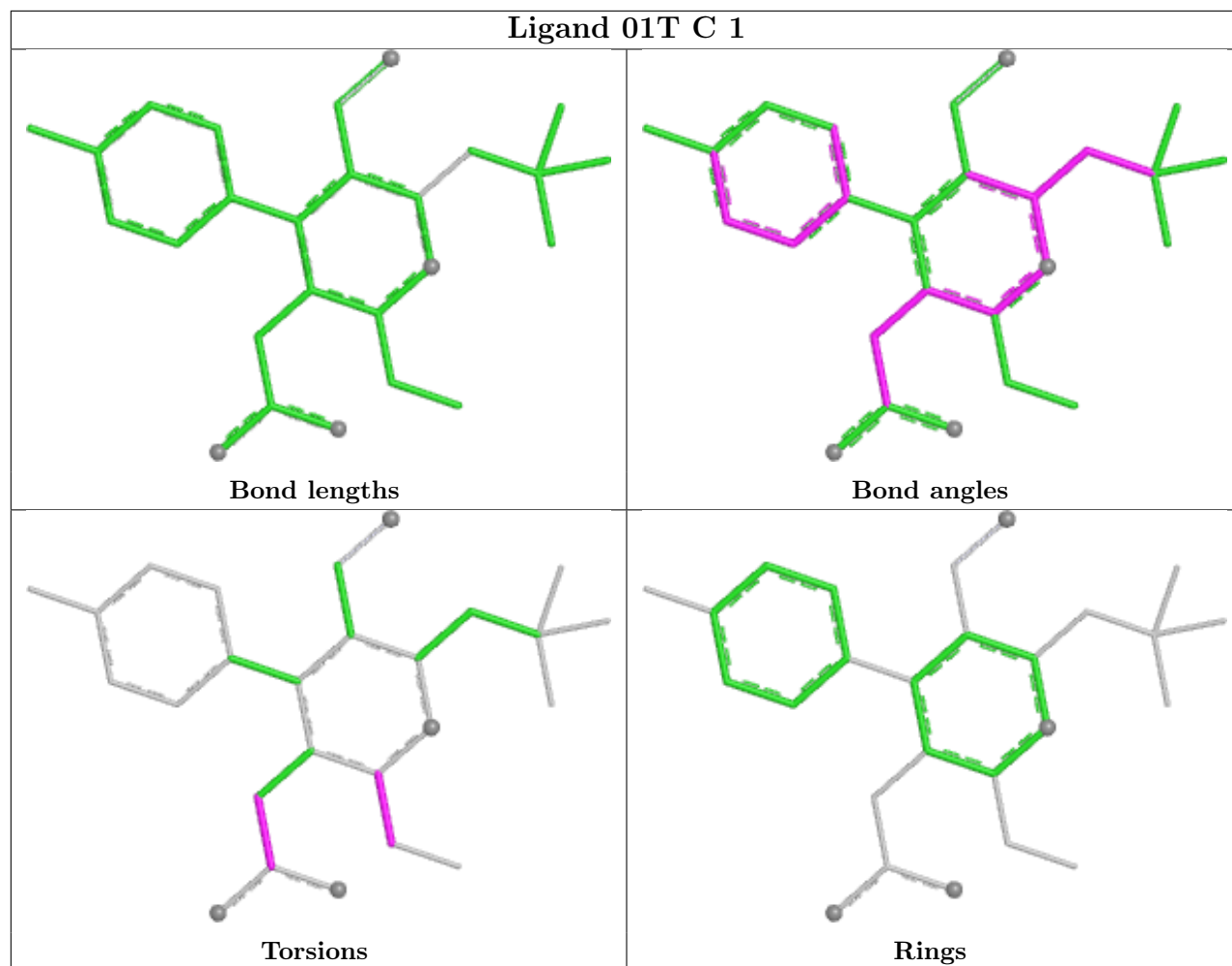
4 monomers are involved in 5 short contacts:

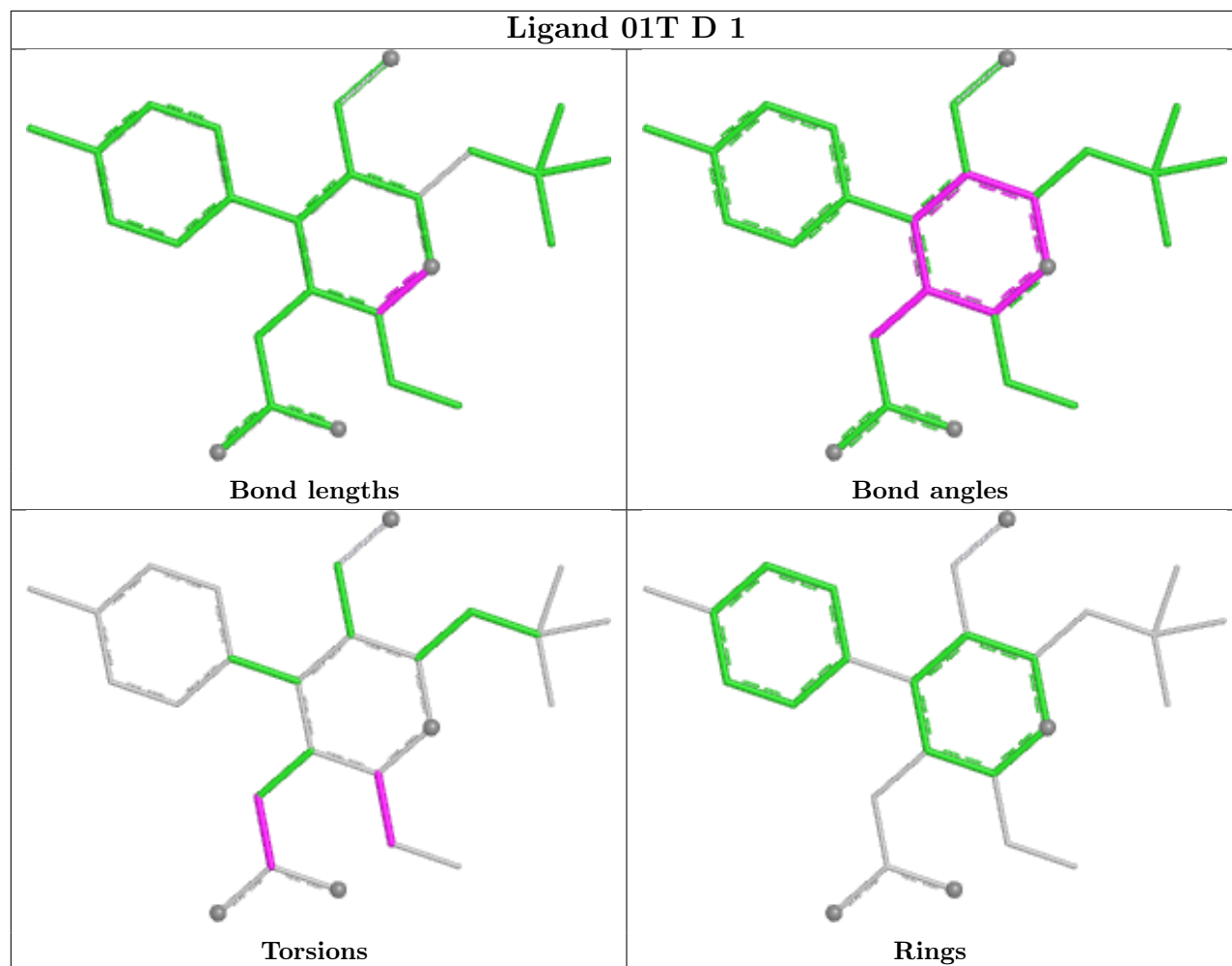
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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4	D	2811	NAG	1	0
5	D	1	01T	1	0
5	B	1	01T	1	0

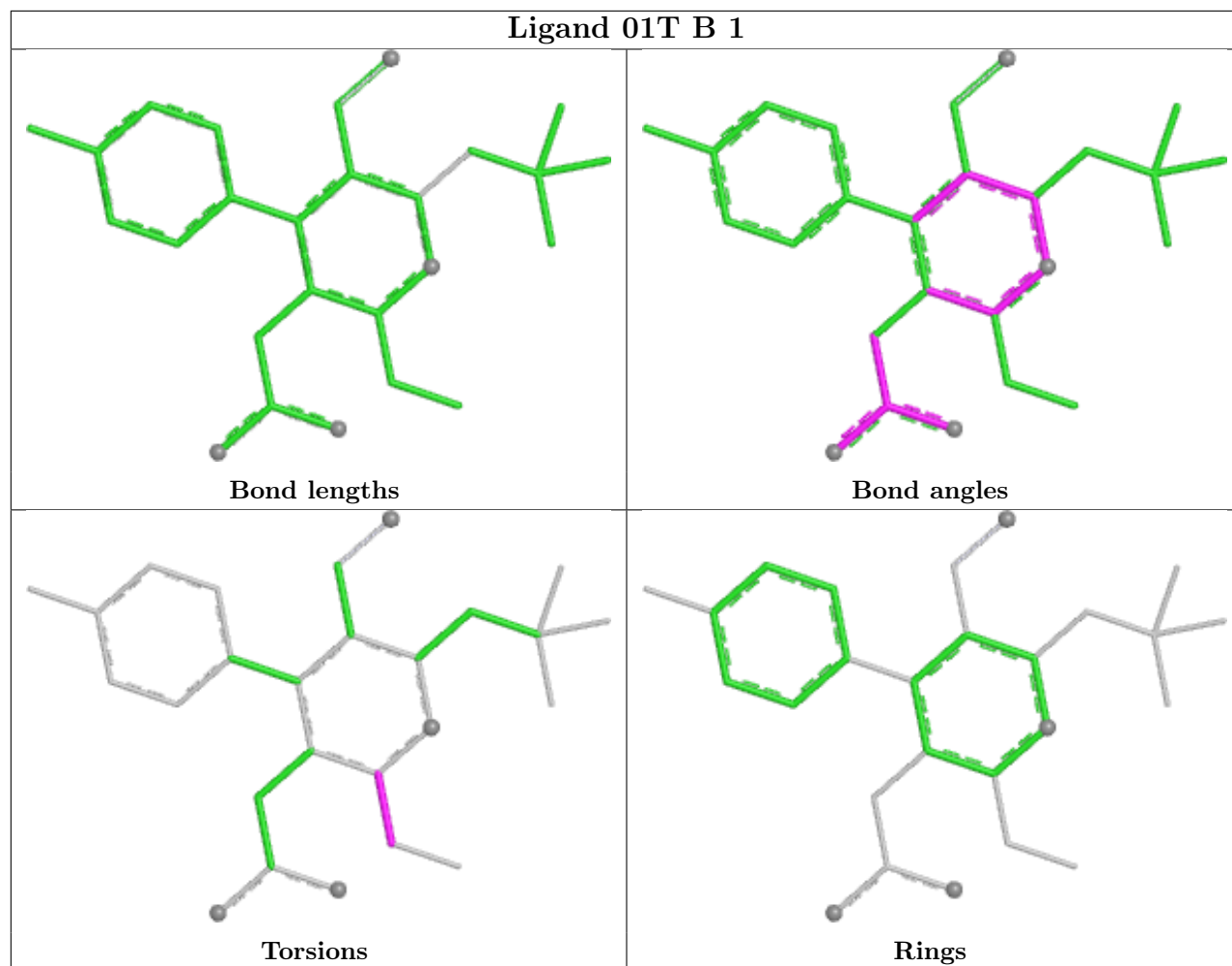
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	727/740 (98%)	0.54	21 (2%) 53 45	37, 47, 63, 78	0
1	B	733/740 (99%)	0.38	9 (1%) 76 71	35, 47, 61, 80	0
1	C	726/740 (98%)	0.69	45 (6%) 26 19	39, 48, 67, 80	0
1	D	727/740 (98%)	0.55	26 (3%) 46 36	37, 47, 62, 71	0
All	All	2913/2960 (98%)	0.54	101 (3%) 47 37	35, 47, 64, 80	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	ASN	4.2
1	C	83	TYR	4.1
1	C	348	MET	3.4
1	C	81	ALA	3.4
1	C	414	TYR	3.3
1	C	412	SER	3.3
1	D	89	PHE	3.1
1	D	91	GLU	3.1
1	C	467	TYR	3.1
1	C	488	ASP	3.1
1	A	88	VAL	3.1
1	C	339	CYS	3.0
1	C	483	HIS	2.9
1	C	322	TYR	2.9
1	D	279	VAL	2.9
1	C	436	LEU	2.9
1	D	135	TYR	2.8
1	C	135	TYR	2.8
1	C	88	VAL	2.8
1	A	72	GLN	2.8
1	C	487	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	333	SER	2.7
1	A	98	PHE	2.7
1	A	78	VAL	2.7
1	C	63	ILE	2.7
1	B	505	GLN	2.7
1	A	135	TYR	2.6
1	D	141	GLN	2.6
1	C	178	PRO	2.6
1	A	140	ARG	2.6
1	A	506	ASN	2.6
1	C	80	ASN	2.6
1	C	468	TYR	2.5
1	D	97	GLU	2.5
1	A	138	ASN	2.5
1	C	338	ASN	2.5
1	A	93	SER	2.5
1	D	142	LEU	2.5
1	C	78	VAL	2.5
1	D	102	ILE	2.5
1	D	412	SER	2.5
1	C	285	ILE	2.5
1	A	95	PHE	2.5
1	A	433	LYS	2.4
1	C	280	THR	2.4
1	B	328	CYS	2.4
1	A	399	LYS	2.4
1	C	438	ASP	2.4
1	A	89	PHE	2.4
1	C	372	TYR	2.4
1	C	416	TYR	2.4
1	B	34	HIS	2.4
1	C	87	SER	2.3
1	D	222	PHE	2.3
1	C	432	TYR	2.3
1	B	81	ALA	2.3
1	B	486	VAL	2.3
1	C	484	SER	2.3
1	C	439	TYR	2.3
1	A	73	GLU	2.2
1	C	141	GLN	2.2
1	C	386	TYR	2.2
1	D	87	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	84	GLY	2.2
1	C	89	PHE	2.2
1	C	375	ILE	2.2
1	C	417	TYR	2.2
1	D	284	SER	2.2
1	D	282	ALA	2.2
1	A	76	ILE	2.2
1	C	66	HIS	2.1
1	C	335	GLY	2.1
1	D	385	CYS	2.1
1	D	179	ASN	2.1
1	C	99	GLY	2.1
1	C	440	THR	2.1
1	D	77	LEU	2.1
1	D	98	PHE	2.1
1	A	105	TYR	2.1
1	A	547	TYR	2.1
1	D	143	ILE	2.1
1	B	440	THR	2.1
1	B	83	TYR	2.1
1	D	277	SER	2.1
1	D	505	GLN	2.0
1	A	279	VAL	2.0
1	A	656	VAL	2.0
1	C	98	PHE	2.0
1	C	395	THR	2.0
1	A	379	GLU	2.0
1	D	145	GLU	2.0
1	B	86	SER	2.0
1	C	370	SER	2.0
1	D	72	GLN	2.0
1	C	482	LEU	2.0
1	D	487	ASN	2.0
1	C	411	THR	2.0
1	D	283	THR	2.0
1	A	97	GLU	2.0
1	B	70	TYR	2.0
1	D	486	VAL	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

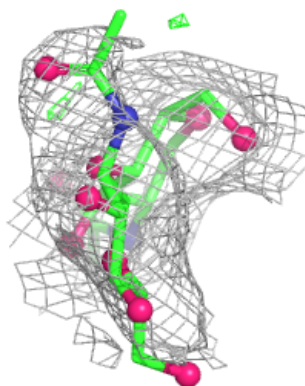
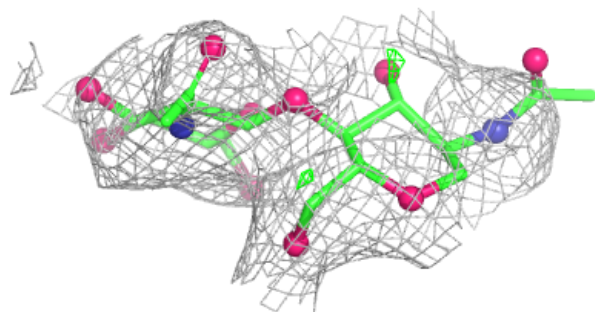
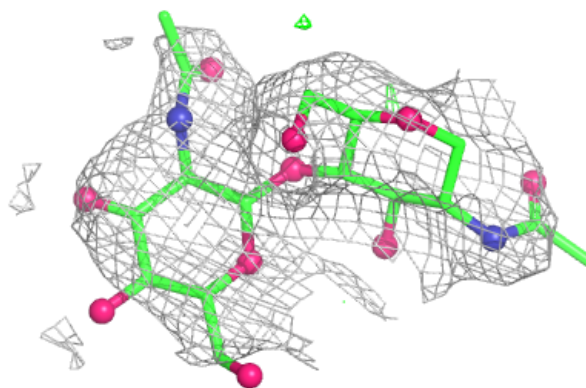
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	F	1	14/15	0.54	0.17	86,88,90,92	0
2	NAG	F	2	14/15	0.60	0.18	94,94,96,96	0
2	NAG	E	2	14/15	0.61	0.13	86,88,89,89	0
2	NAG	H	1	14/15	0.61	0.16	64,68,70,73	0
2	NAG	E	1	14/15	0.65	0.15	73,78,80,84	0
2	NAG	I	1	14/15	0.66	0.13	87,89,91,93	0
3	NAG	K	3	14/15	0.66	0.17	83,85,87,88	0
2	NAG	I	2	14/15	0.69	0.15	95,97,97,97	0
3	NAG	K	2	14/15	0.70	0.13	70,73,76,80	0
2	NAG	G	2	14/15	0.76	0.12	61,63,65,66	0
2	NAG	H	2	14/15	0.78	0.13	76,78,78,78	0
2	NAG	L	2	14/15	0.78	0.12	74,76,79,80	0
2	NAG	J	2	14/15	0.82	0.10	71,72,73,73	0
2	NAG	L	1	14/15	0.86	0.11	60,63,67,71	0
2	NAG	J	1	14/15	0.86	0.11	58,61,63,67	0
3	NAG	K	1	14/15	0.89	0.11	60,63,65,68	0
2	NAG	G	1	14/15	0.91	0.10	55,57,59,61	0

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

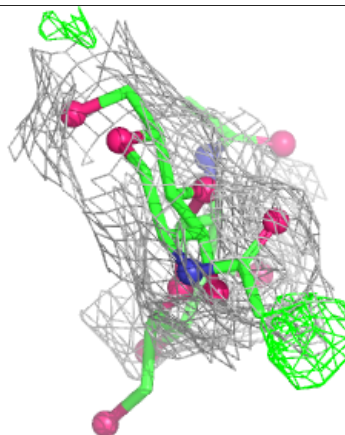
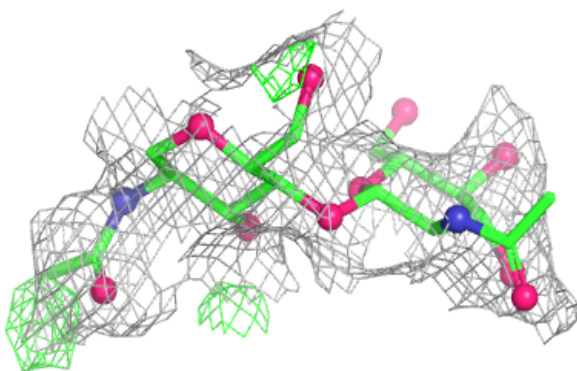
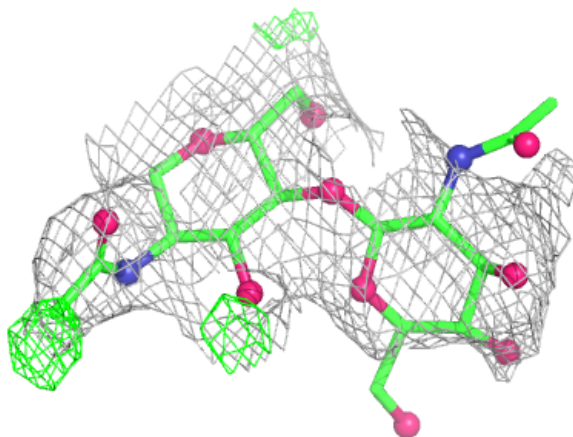
Electron density around Chain E:

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

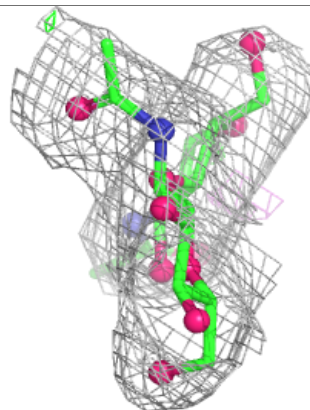
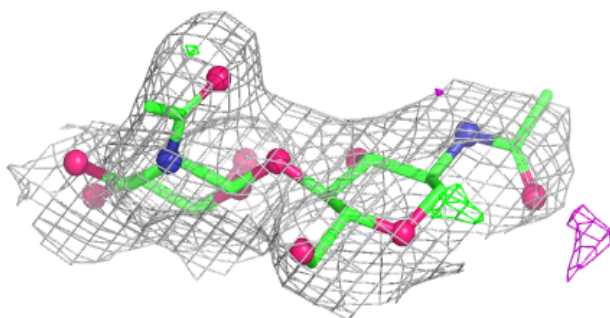
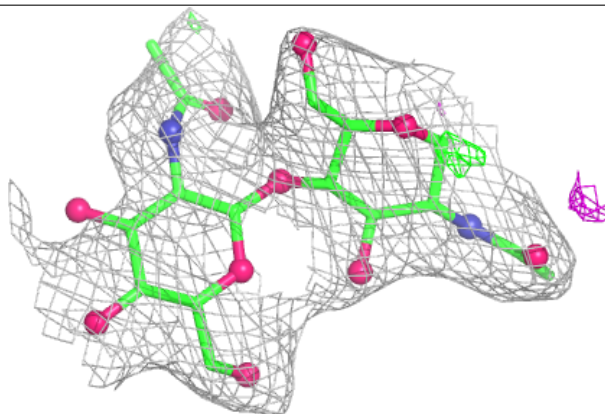


Electron density around Chain F:

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

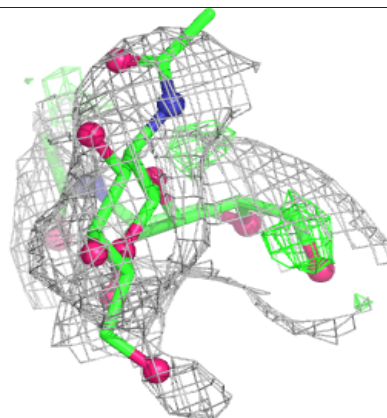
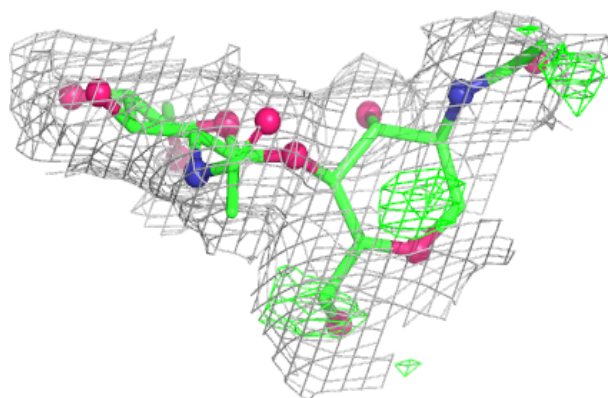
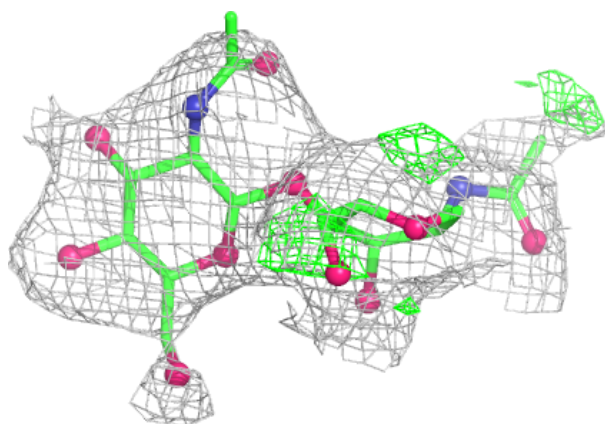
**Electron density around Chain G:**

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



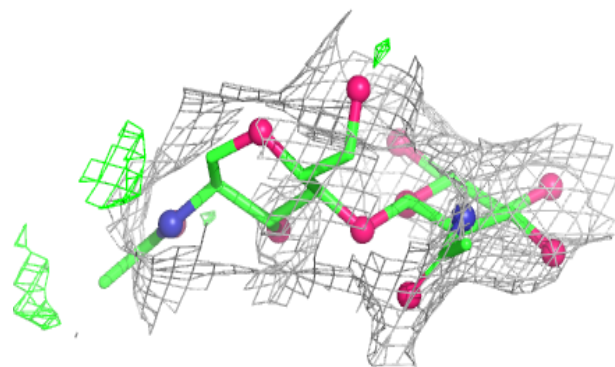
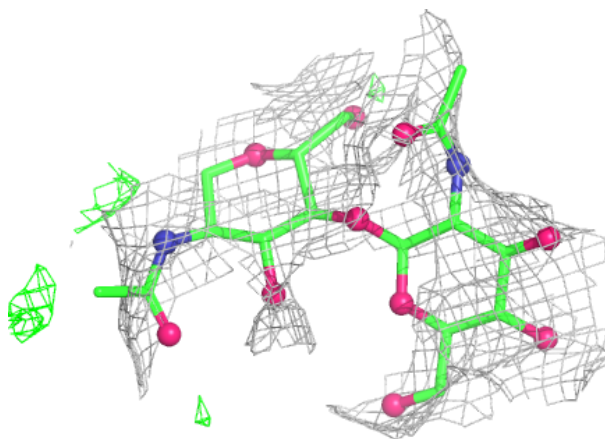
Electron density around Chain H:

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



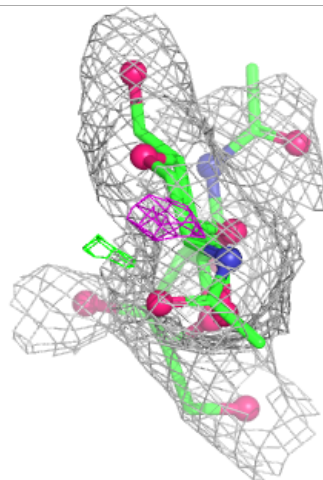
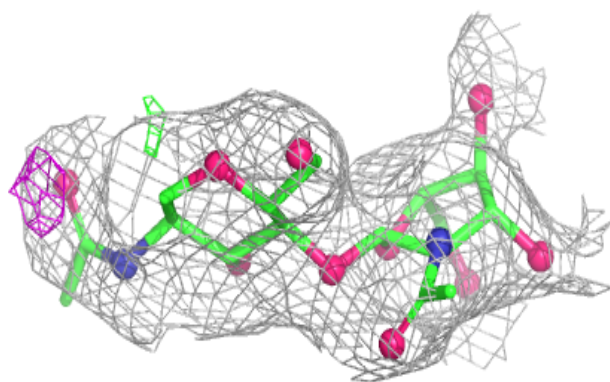
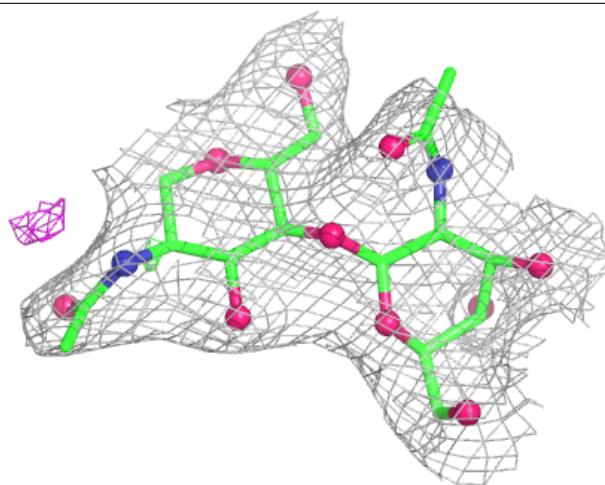
Electron density around Chain I:

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



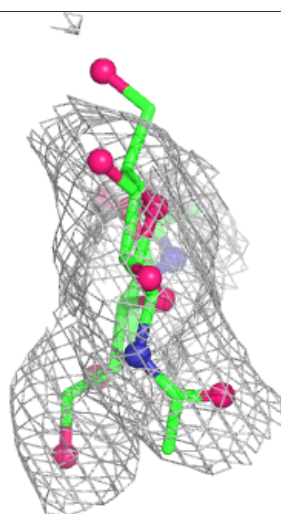
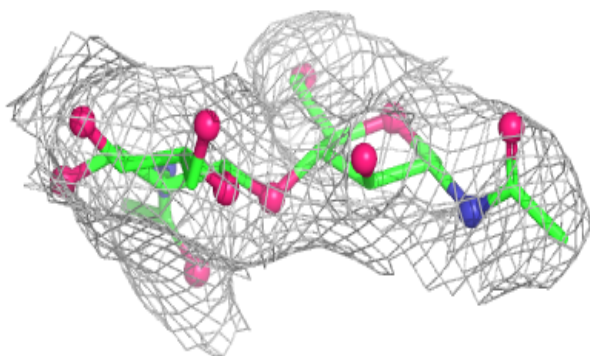
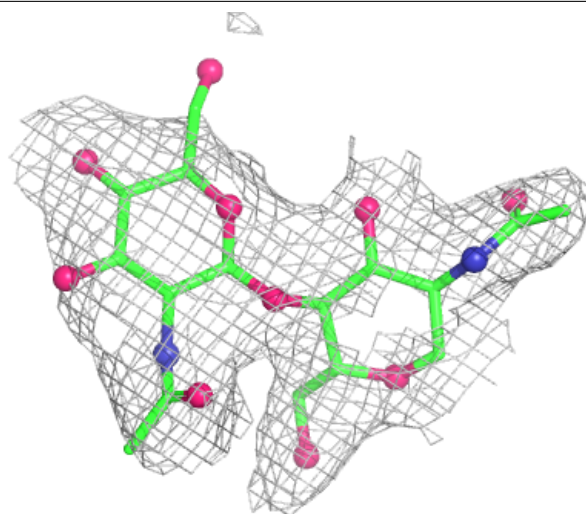
Electron density around Chain J:

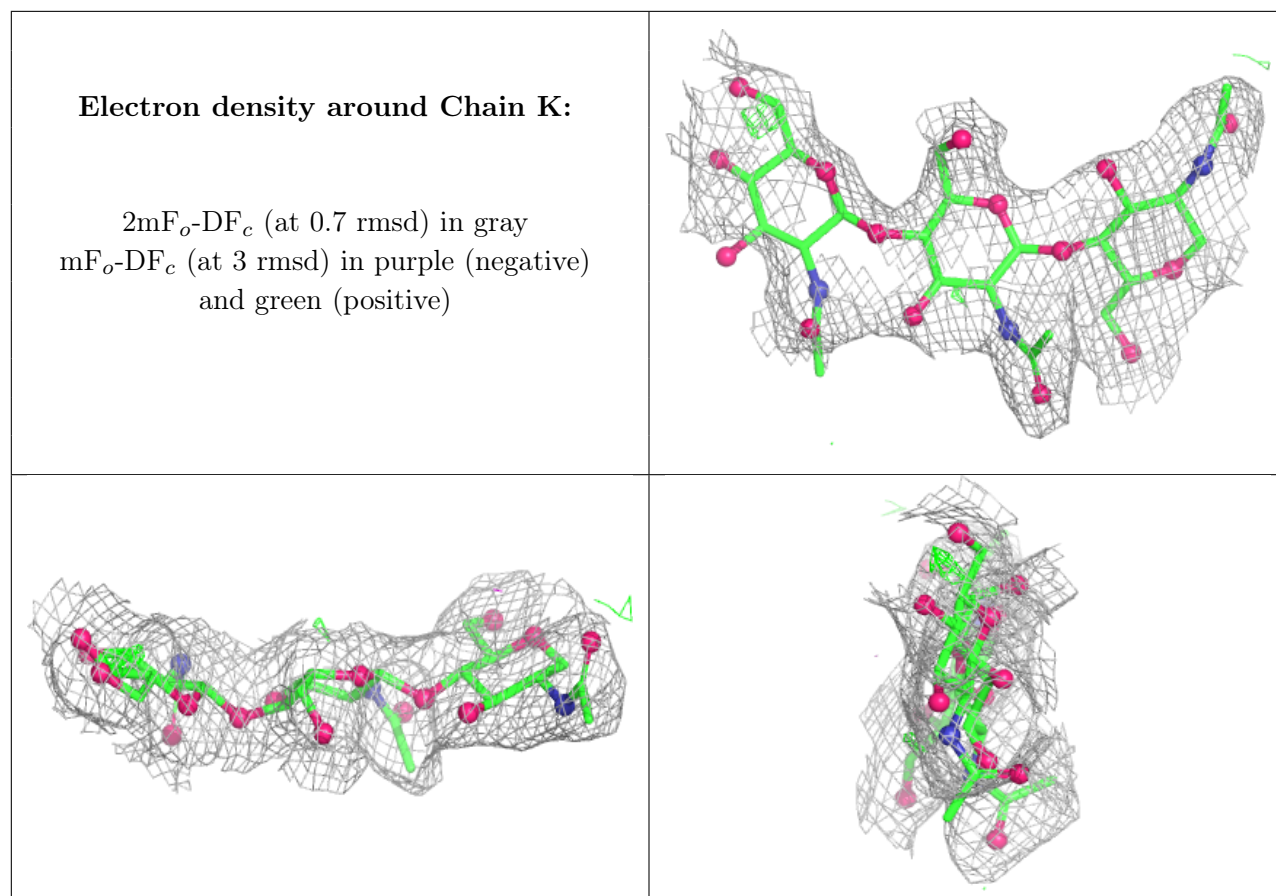
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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.

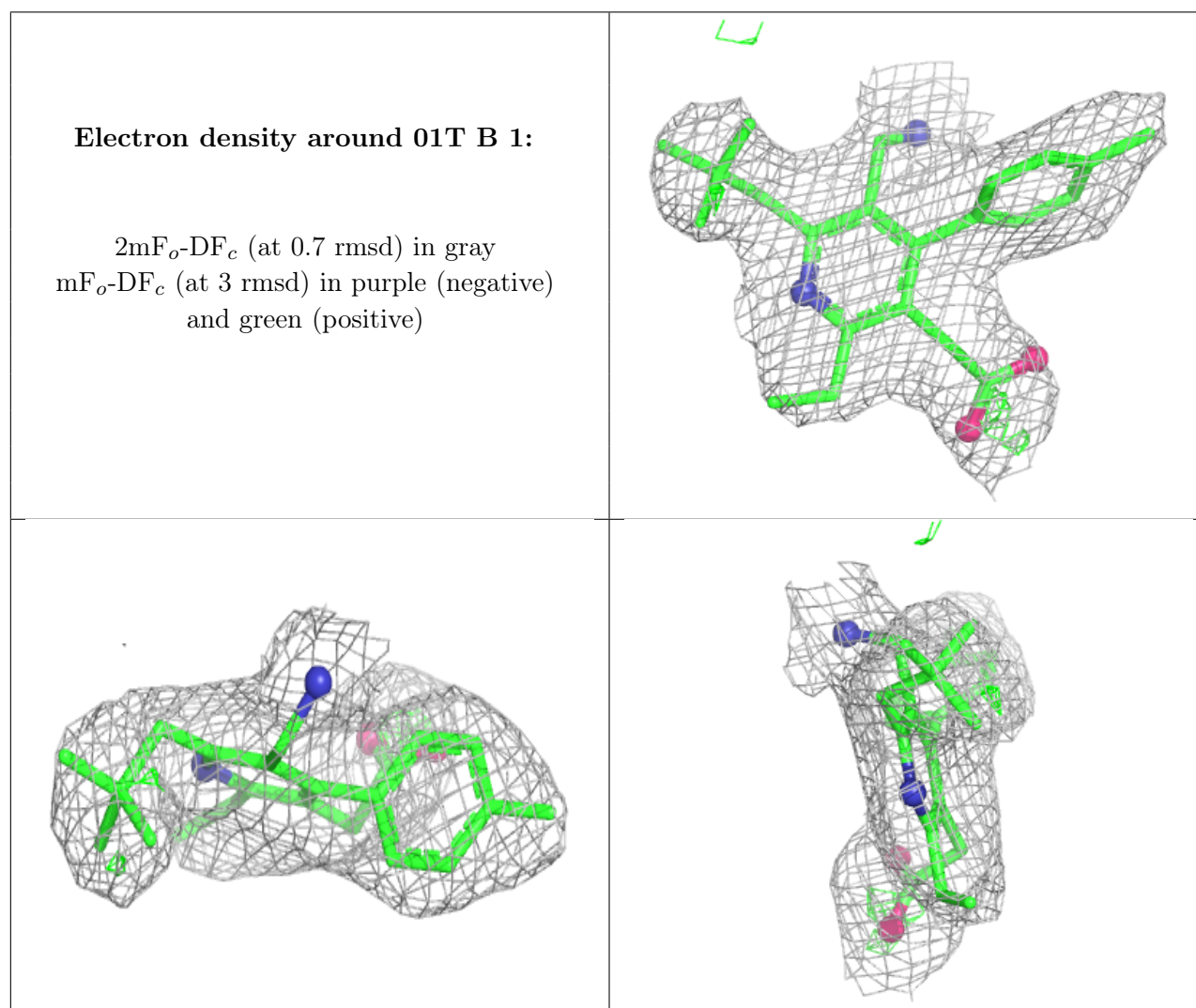
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	1501	14/15	0.61	0.15	63,66,66,66	0
4	NAG	D	5201	14/15	0.63	0.19	75,78,81,82	0
4	NAG	D	2811	14/15	0.64	0.16	63,65,67,67	0
4	NAG	A	2191	14/15	0.66	0.14	61,65,70,70	0
4	NAG	C	3211	14/15	0.68	0.17	66,69,75,76	0
4	NAG	B	3211	14/15	0.71	0.14	59,62,63,63	0
4	NAG	C	1501	14/15	0.72	0.12	64,66,67,67	0
4	NAG	A	3211	14/15	0.74	0.14	55,57,62,62	0
4	NAG	D	2191	14/15	0.79	0.12	60,64,67,68	0
4	NAG	B	1501	14/15	0.80	0.11	61,62,63,64	0
4	NAG	C	2811	14/15	0.82	0.10	63,65,67,67	0
4	NAG	B	2811	14/15	0.88	0.09	57,59,60,61	0
5	01T	B	1	26/26	0.93	0.15	45,48,51,55	0

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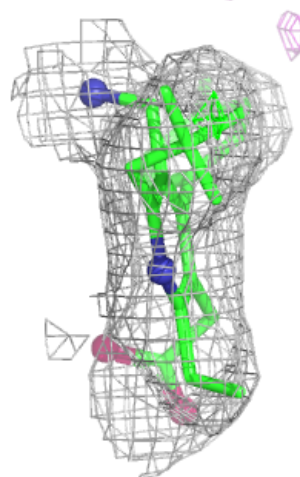
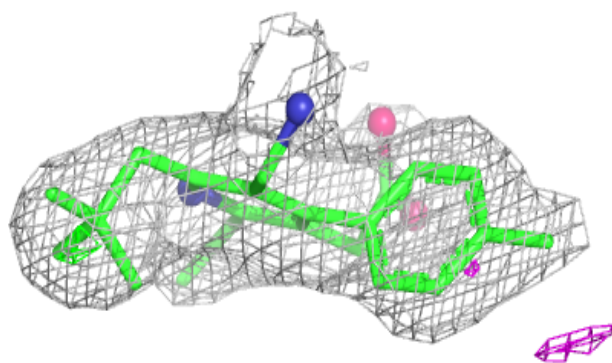
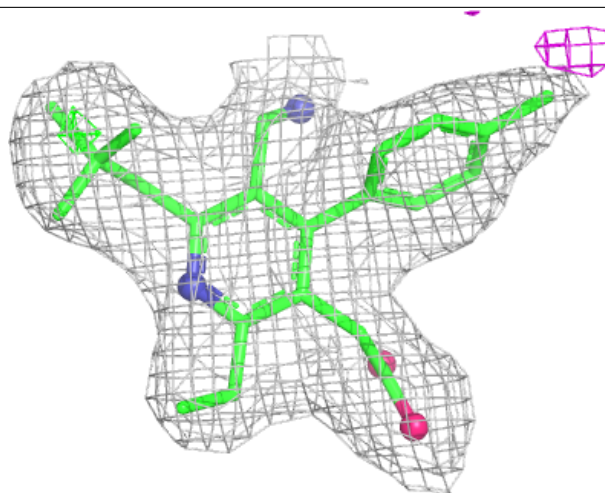
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	01T	D	1	26/26	0.93	0.15	45,48,55,58	0
5	01T	C	1	26/26	0.95	0.10	44,47,50,51	0
5	01T	A	1	26/26	0.95	0.15	46,49,56,59	0

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.



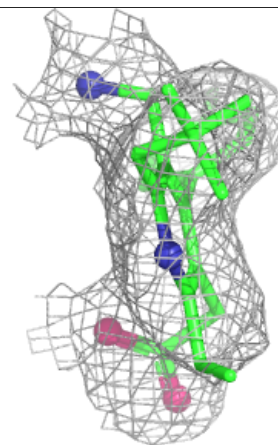
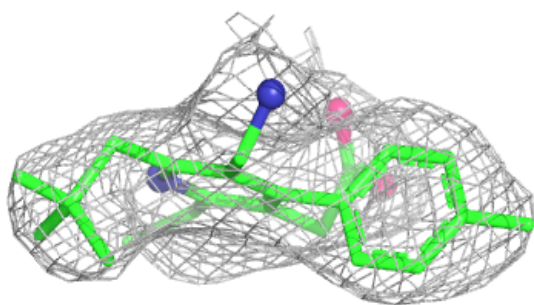
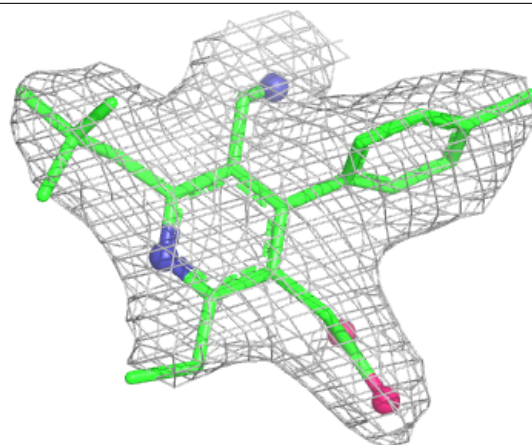
Electron density around 01T D 1:

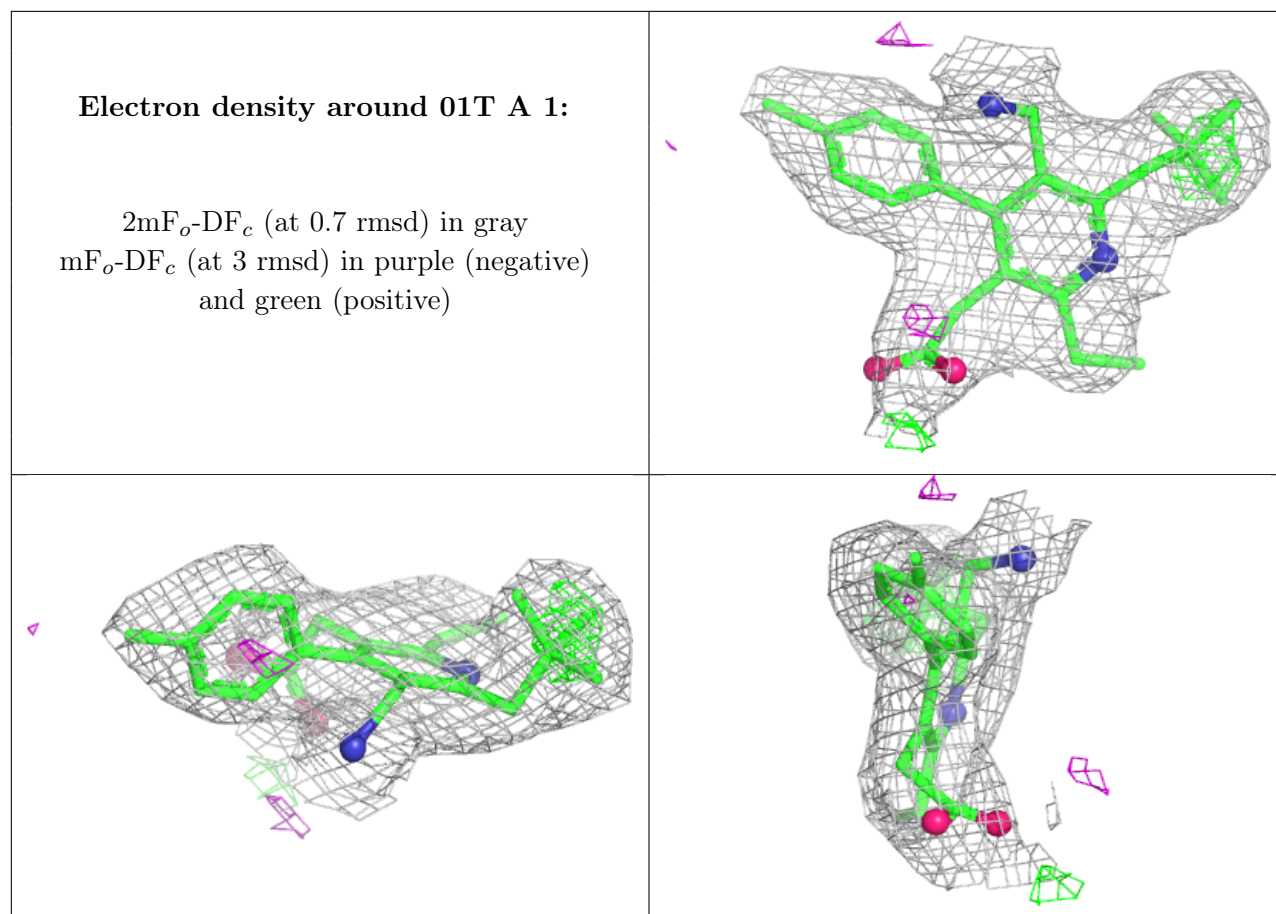
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 01T C 1:

$2mF_o-DF_c$ (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.