wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 11:45 AM EDT

PDB ID	:	7TPD
Title	:	Integrin alaphIIBbeta3 complex with EF5154
Authors	:	Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2022-01-25
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

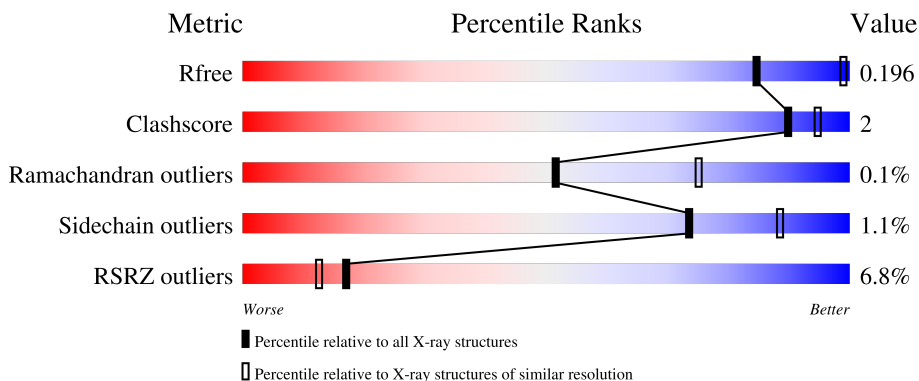|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.196
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		1.1%
RSRZ outliers		6.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	457	% 94% 6%
1	C	457	% 92% 7% ·
2	B	471	8% 94% 5% ·
2	D	471	5% 94% 6%
3	E	216	17% 97% ··

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Mol	Chain	Length	Quality of chain
3	H	216	7% ... 96%
4	F	214	27% ... 96%
4	L	214	2% ... 98%
5	G	5	40% ... 20% ... 40%
6	I	2	50% ... 50%
6	K	2	50% ... 50%
7	J	4	50% ... 50%

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 22205 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total 3542	C 2251	N 611	O 672	S 8	0	7	0
1	C	453	Total 3502	C 2224	N 604	O 666	S 8	0	4	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total 3650	C 2273	N 622	O 721	S 34	4	9	0
2	D	471	Total 3666	C 2285	N 626	O 720	S 35	3	6	0

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total 1631	C 1035	N 264	O 326	S 6	0	0	0
3	H	216	Total 1642	C 1041	N 266	O 329	S 6	0	0	0

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total 1637	C 1019	N 268	O 341	S 9	0	0	0
4	L	214	Total 1637	C 1019	N 268	O 341	S 9	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
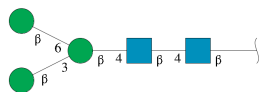
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total 28	C 16	N 2	O 10	0	0	0
6	K	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	Ca 4	0	0
8	B	2	Total 2	Ca 2	0	0
8	C	4	Total 4	Ca 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total Ca 2 2		0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
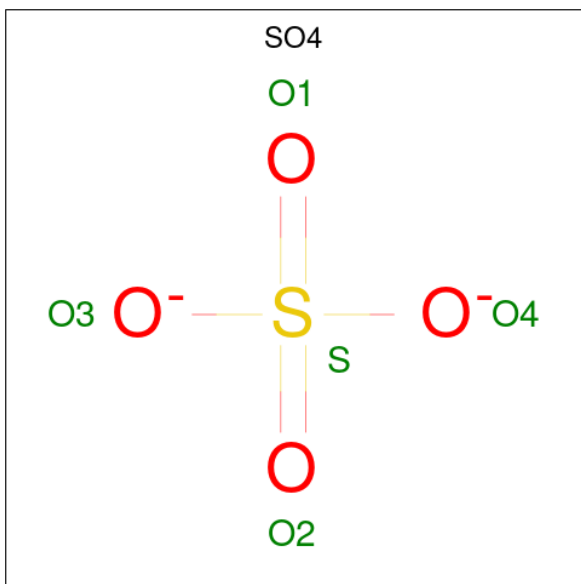
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

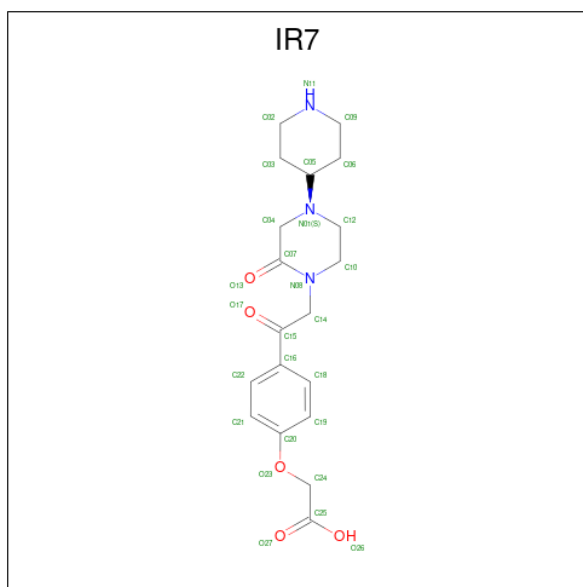| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total Mg 1 1		0	0
10	D	1	Total Mg 1 1		0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: $C_8H_{15}NO_6$).
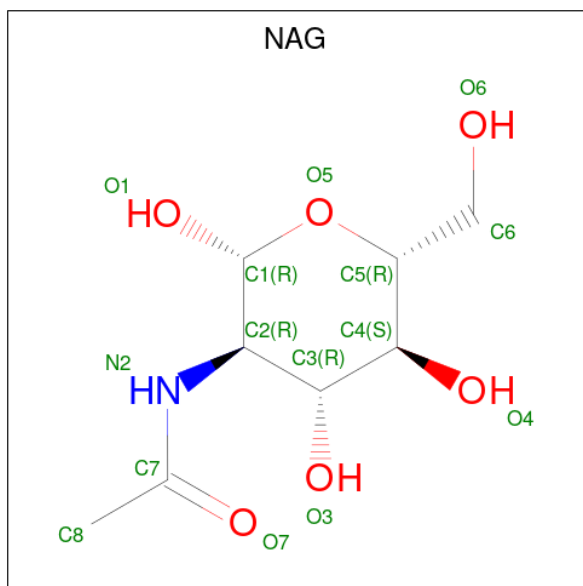
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is (4-{[2-oxo-4-(piperidin-4-yl)piperazin-1-yl]acetyl}phenoxy)acetic acid (three-letter code: IR7) (formula: $C_{19}H_{25}N_3O_5$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total 27	C 19	N 3	O 5	0	0
12	D	1	Total 27	C 19	N 3	O 5	0	0

- Molecule 13 is water.

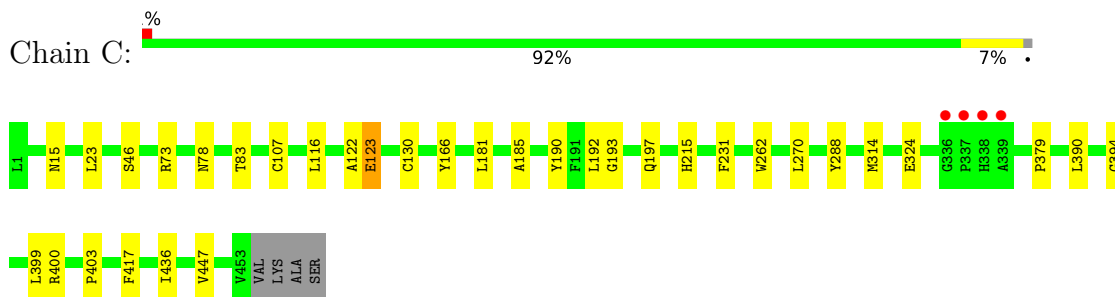| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	374	Total 374	O 374	0	0
13	B	190	Total 190	O 190	0	0
13	C	233	Total 233	O 233	0	0
13	D	132	Total 132	O 132	0	0
13	E	13	Total 13	O 13	0	0
13	F	6	Total 6	O 6	0	0
13	H	21	Total 21	O 21	0	0
13	L	41	Total 41	O 41	0	0

3 Residue-property plots ⓘ

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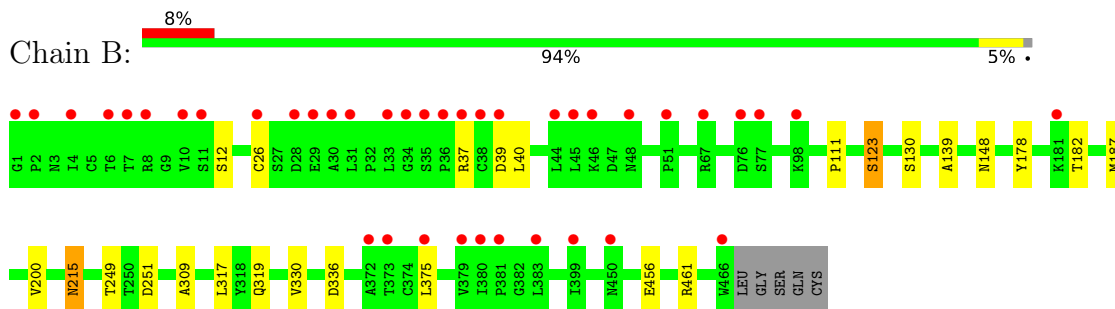
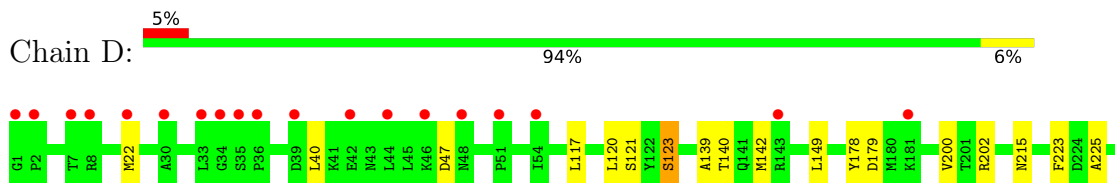- Molecule 1: Integrin alpha-IIb heavy chain
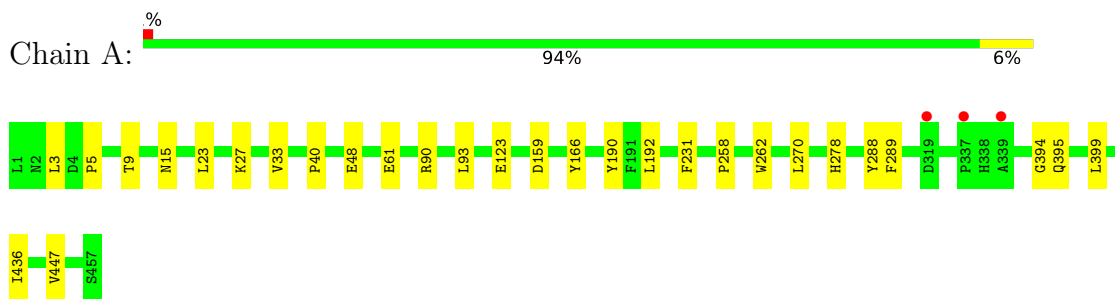
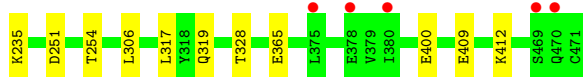- Molecule 1: Integrin alpha-IIb heavy chain

- Molecule 2: Integrin beta-3

- Molecule 2: Integrin beta-3
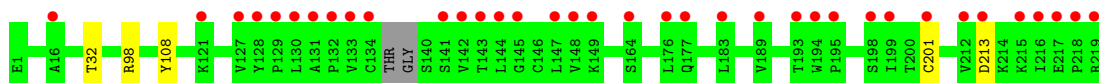
K235 D251 T254 L306 L317 Y318 Q319 T328 E365 L375 E378 V379 I380 E400 E409 K412 S469 Q470 C471

• Molecule 3: Fab heavy chain

Chain E:

17%

97%

E1 A16 T32 R98 Y108 K121 V127 Y128 P129 L130 A131 P132 V133 C134 THR GLY S140 S141 V142 T143 L144 G145 C146 L147 V148 K149 S164 L176 Q177 L183 V189 T193 W194 P195 S198 I199 T200 C201 V212 D213 K214 K215 I216 E217 P218 R219

• Molecule 3: Fab heavy chain

Chain H:

7%

96%

E1 V12 L86 T87 R98 Y108 P125 V133 C134 T138 V142 T143 L144 Y151 W160 G163 T188 V189 I199 T200 C201 A207 S208 K211 V212 D213 K214 K215 I216 E217 P218 R219

• Molecule 4: Fab light chain

Chain F:

27%

96%

D1 M4 V13 S14 V19 N32 Q90 V115 S116 I117 F118 P119 S122 E123 Q124 L125 T126 S127 G128 G129 A130 S131 V132 V133 C134 F135 L136 I144 N145 V146 K147 W148 K149 I150 D151 G152 S153 E154 R155 Q156 N157 G158 V159 L160 M175 S176 S177 T178 L179 L180 L181

T182 K183 D184 E185 Y186 N190 S191 Y192 T193 C194 E195 I205 V206 K207 S208 F209 N210 R211 N212 E213 C214

• Molecule 4: Fab light chain

Chain L:

2%

98%

D1 L54 S60 I106 E185 R211 N212 E213 C214

• Molecule 5: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

40%
20%
40%

NAG1 NAG2 BMA3 BMA4 BMA5

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

50%
50%

NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

50%   50%

NAG1 NAG2

• Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

50%   50%

NAG1 NAG2 BMA3 BMA4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	260.18Å 144.34Å 104.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.60 48.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.32-2.60) 99.9 (48.32-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.165 , 0.194 0.166 , 0.196	Depositor DCC
R_{free} test set	1022 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22205	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, SO4, MG, BMA, IR7

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	0.27	0/3657	0.55	0/4982
1	C	0.26	0/3605	0.53	0/4912
2	B	0.25	0/3729	0.49	0/5055
2	D	0.25	0/3748	0.49	0/5082
3	E	0.24	0/1673	0.47	0/2290
3	H	0.24	0/1684	0.48	0/2305
4	F	0.25	0/1673	0.46	0/2269
4	L	0.25	0/1673	0.49	0/2269
All	All	0.25	0/21442	0.50	0/29164

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3542	0	3391	15	0
1	C	3502	0	3334	18	0
2	B	3650	0	3572	13	0
2	D	3666	0	3584	16	0
3	E	1631	0	1590	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	4	0
4	F	1637	0	1553	4	0
4	L	1637	0	1553	3	0
5	G	61	0	52	1	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	50	0	43	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	15	0	0	1	0
9	C	10	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	27	0	0	0	0
12	D	27	0	0	1	0
13	A	374	0	0	5	1
13	B	190	0	0	0	0
13	C	233	0	0	3	1
13	D	132	0	0	3	0
13	E	13	0	0	0	0
13	F	6	0	0	0	0
13	H	21	0	0	1	0
13	L	41	0	0	1	0
All	All	22205	0	20348	74	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 74 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)
2:B:123[B]:SER:OG	2:B:251:ASP:OD2	2.07	0.71
1:A:15[B]:ASN:ND2	13:A:605:HOH:O	2.26	0.69
1:A:159[A]:ASP:OD2	13:A:602:HOH:O	2.11	0.67
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.31	0.63
1:C:73:ARG:NH1	13:C:604:HOH:O	2.30	0.63

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:923:HOH:O	13:C:788:HOH:O[1_554]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/457 (101%)	450 (97%)	11 (2%)	1 (0%)	47	71
1	C	455/457 (100%)	442 (97%)	12 (3%)	1 (0%)	47	71
2	B	473/471 (100%)	455 (96%)	17 (4%)	1 (0%)	47	71
2	D	475/471 (101%)	461 (97%)	14 (3%)	0	100	100
3	E	210/216 (97%)	199 (95%)	11 (5%)	0	100	100
3	H	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2711/2716 (100%)	2619 (97%)	89 (3%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
1	C	123	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/364 (102%)	364 (98%)	7 (2%)	57	79
1	C	365/364 (100%)	359 (98%)	6 (2%)	62	82
2	B	421/416 (101%)	416 (99%)	5 (1%)	71	87
2	D	422/416 (101%)	416 (99%)	6 (1%)	67	85
3	E	186/187 (100%)	185 (100%)	1 (0%)	88	96
3	H	187/187 (100%)	185 (99%)	2 (1%)	73	88
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	96
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2328/2310 (101%)	2300 (99%)	28 (1%)	73	87

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	TYR
3	H	213	ASP
1	C	288	TYR
3	E	201	CYS
1	C	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	438	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   ⓘ

13 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
5	NAG	G	1	5,2	14,14,15	0.35	0	17,19,21	0.57	0
5	NAG	G	2	5	14,14,15	0.37	0	17,19,21	0.52	0
5	BMA	G	3	5	11,11,12	1.72	4 (36%)	15,15,17	2.31	3 (20%)
5	BMA	G	4	5	11,11,12	0.93	0	15,15,17	1.43	3 (20%)
5	BMA	G	5	5	11,11,12	1.17	1 (9%)	15,15,17	1.47	3 (20%)
6	NAG	I	1	2,6	14,14,15	0.90	1 (7%)	17,19,21	0.76	0
6	NAG	I	2	6	14,14,15	0.48	0	17,19,21	0.46	0
7	NAG	J	1	2,7	14,14,15	0.35	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.41	0	17,19,21	0.41	0
7	BMA	J	3	7	11,11,12	1.06	1 (9%)	15,15,17	1.28	1 (6%)
7	BMA	J	4	7	11,11,12	1.07	2 (18%)	15,15,17	1.85	3 (20%)
6	NAG	K	1	2,6	14,14,15	0.59	0	17,19,21	0.57	0
6	NAG	K	2	6	14,14,15	0.48	0	17,19,21	0.46	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	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	BMA	G	4	5	-	2/2/19/22	0/1/1/1
5	BMA	G	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	BMA	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	2/6/23/26	0/1/1/1

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	C2-C3	3.58	1.57	1.52
5	G	5	BMA	C1-C2	3.10	1.59	1.52
6	I	1	NAG	O5-C1	-2.80	1.39	1.43
7	J	3	BMA	C2-C3	2.77	1.56	1.52
5	G	3	BMA	O5-C1	2.49	1.47	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O3-C3-C2	5.70	120.91	109.99
5	G	3	BMA	O5-C5-C6	5.13	115.25	107.20
7	J	4	BMA	C1-C2-C3	-4.82	103.74	109.67
7	J	3	BMA	O3-C3-C2	3.67	117.03	109.99
5	G	3	BMA	C1-C2-C3	-3.42	105.46	109.67

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	BMA	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	4	BMA	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3	BMA	1	0
6	K	1	NAG	1	0
5	G	5	BMA	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.

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings
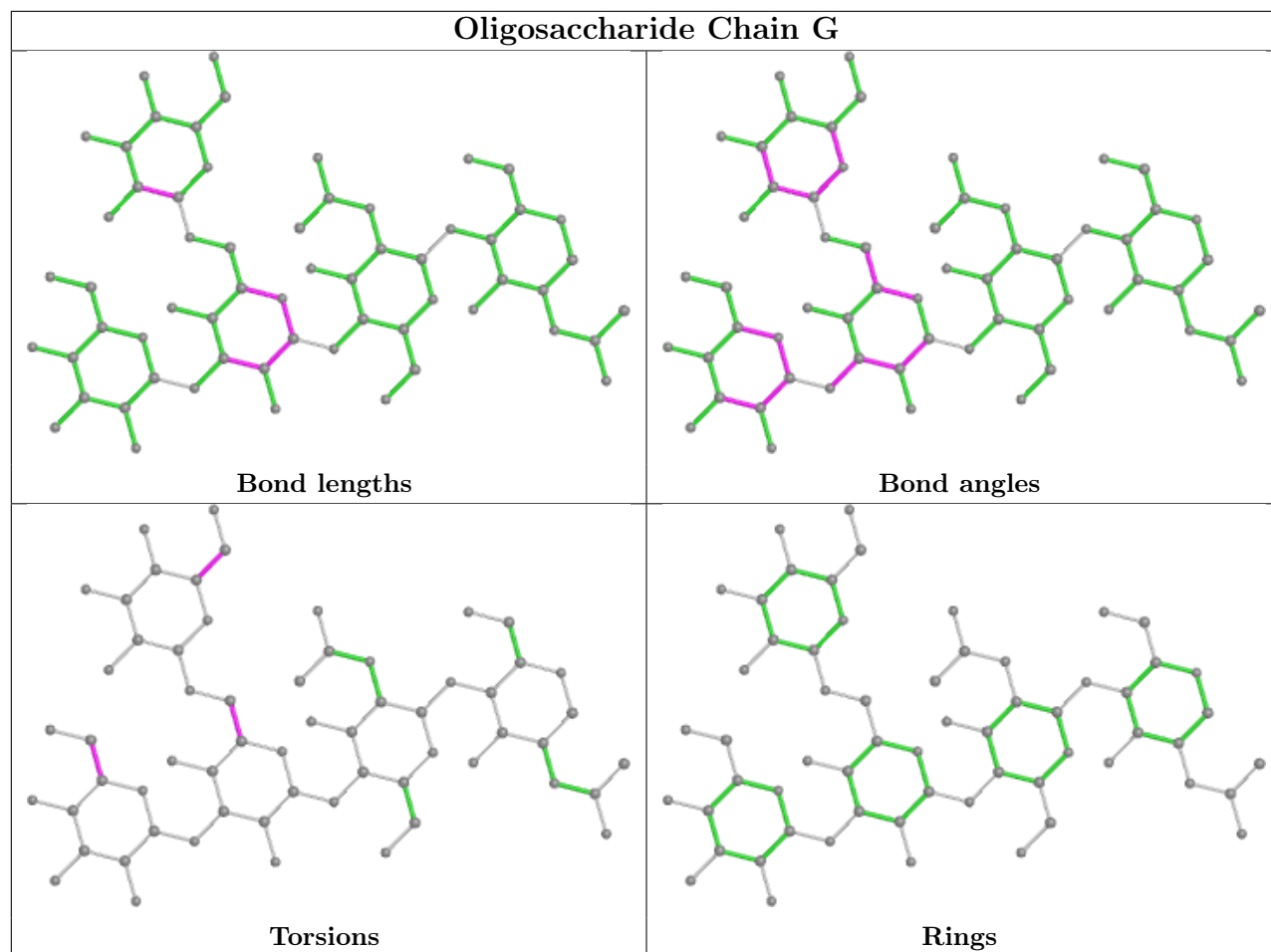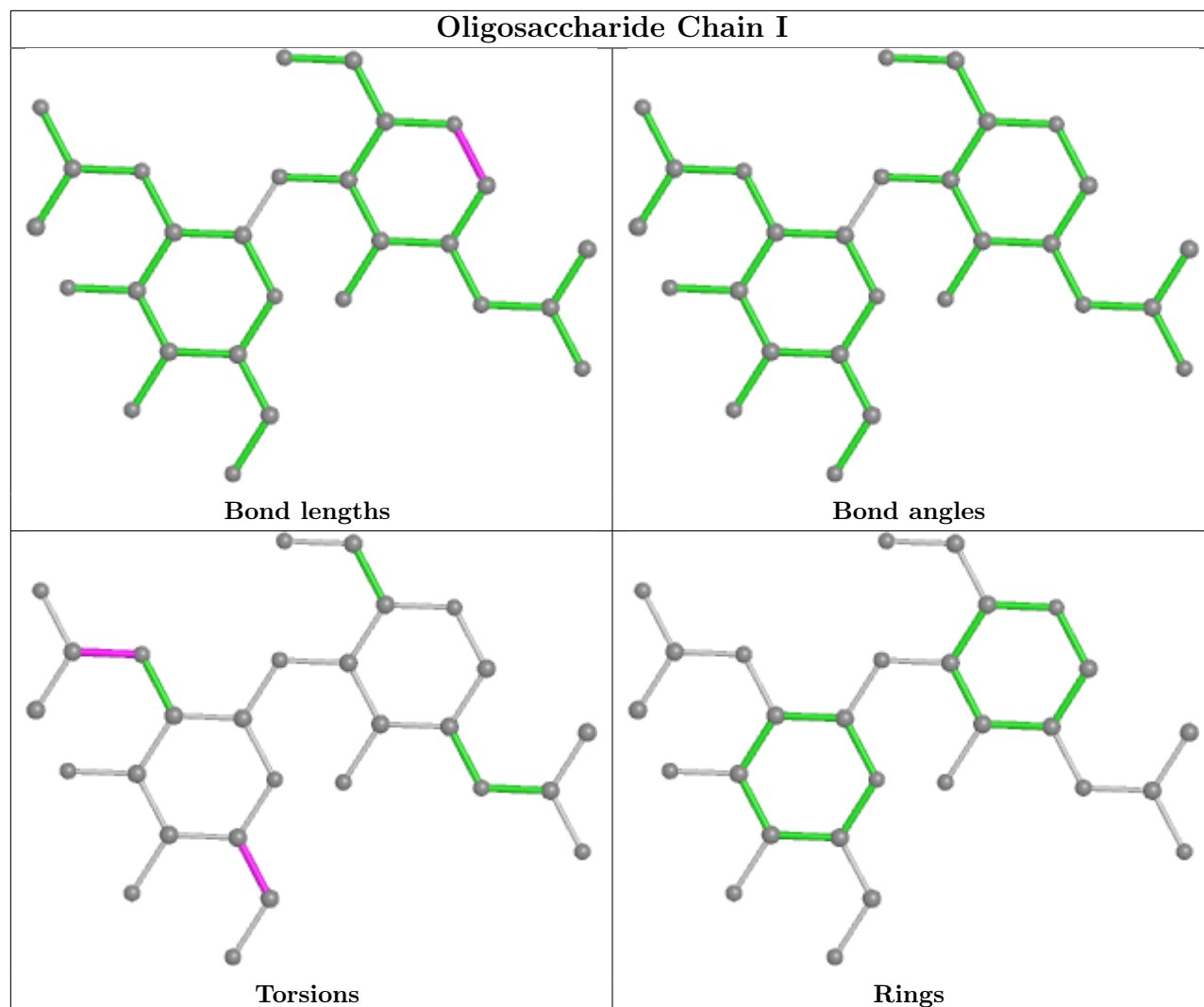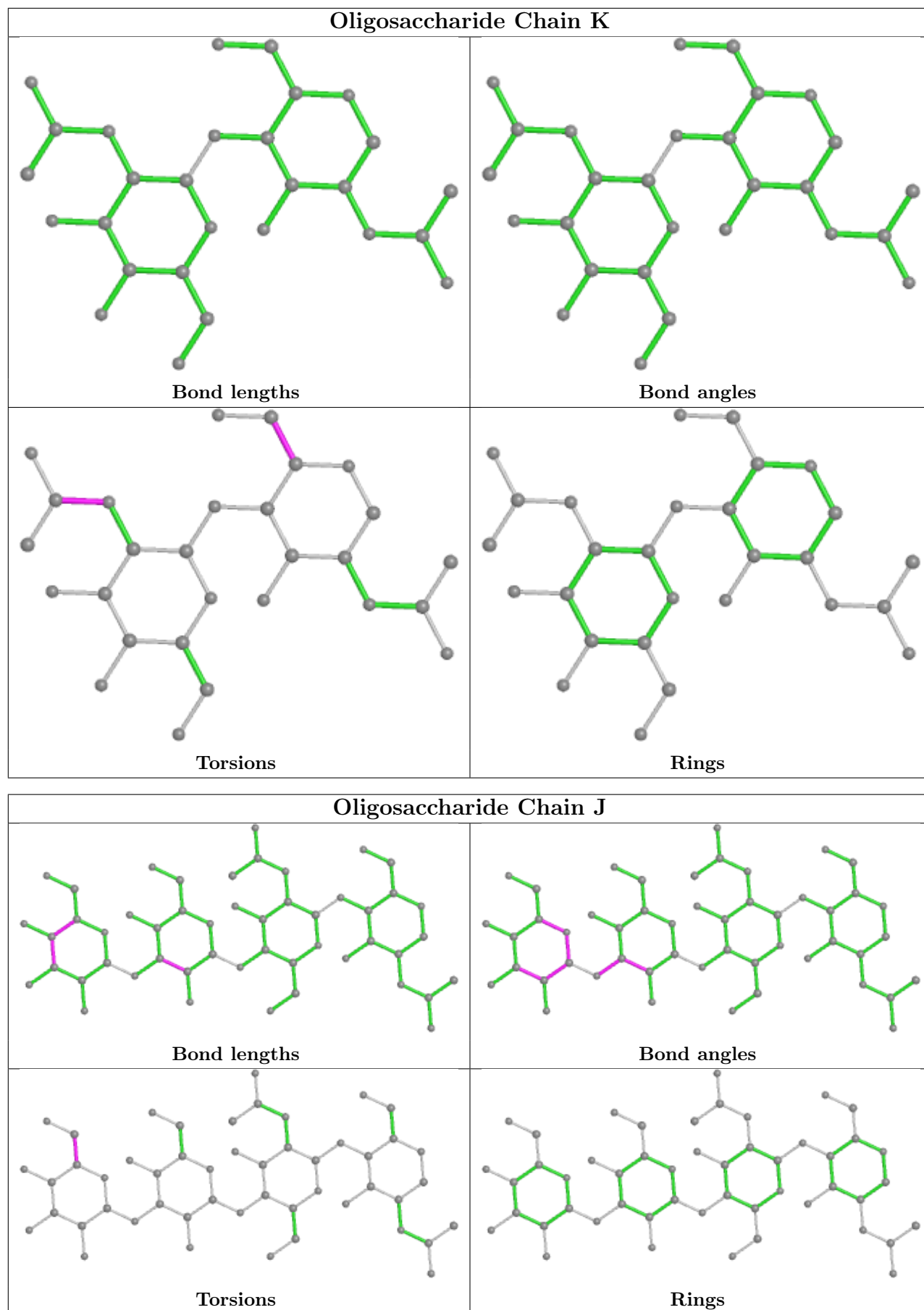
5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 14 are monoatomic - leaving 9 for Mogul analysis.

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	$\#|Z| > 2$
9	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.07	0
9	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.09	0
9	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.08	0
11	NAG	D	2004	2	14,14,15	0.37	0	17,19,21	0.53	0
12	IR7	B	2005	10	29,29,29	2.05	9 (31%)	35,39,39	1.57	7 (20%)
9	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.06	0
12	IR7	D	2005	10	29,29,29	1.96	8 (27%)	35,39,39	1.60	6 (17%)
9	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.06	0
11	NAG	B	2004	2	14,14,15	0.41	0	17,19,21	0.52	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
12	IR7	B	2005	10	-	1/17/38/38	0/3/3/3
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	IR7	D	2005	10	-	1/17/38/38	0/3/3/3
11	NAG	D	2004	2	-	1/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	IR7	C07-N08	6.96	1.43	1.34
12	D	2005	IR7	C07-N08	6.52	1.43	1.34
12	B	2005	IR7	C16-C15	3.77	1.55	1.49
12	D	2005	IR7	C16-C15	3.22	1.54	1.49
12	D	2005	IR7	C12-N01	-3.13	1.41	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	2005	IR7	C07-C04-N01	-4.87	101.41	112.78
12	B	2005	IR7	C07-C04-N01	-4.13	103.15	112.78
12	D	2005	IR7	O26-C25-O27	4.11	133.55	123.30
12	B	2005	IR7	O26-C25-O27	4.06	133.42	123.30
12	B	2005	IR7	O13-C07-N08	-3.99	118.68	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	IR7	C15-C14-N08-C10
11	D	2004	NAG	O5-C5-C6-O6
12	D	2005	IR7	C15-C14-N08-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	505	SO4	1	0
12	D	2005	IR7	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 then 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.

Ligand IR7 B 2005

Bond lengths

Bond angles

Torsions

Rings

Ligand IR7 D 2005

Bond lengths

Bond angles

Torsions

Rings
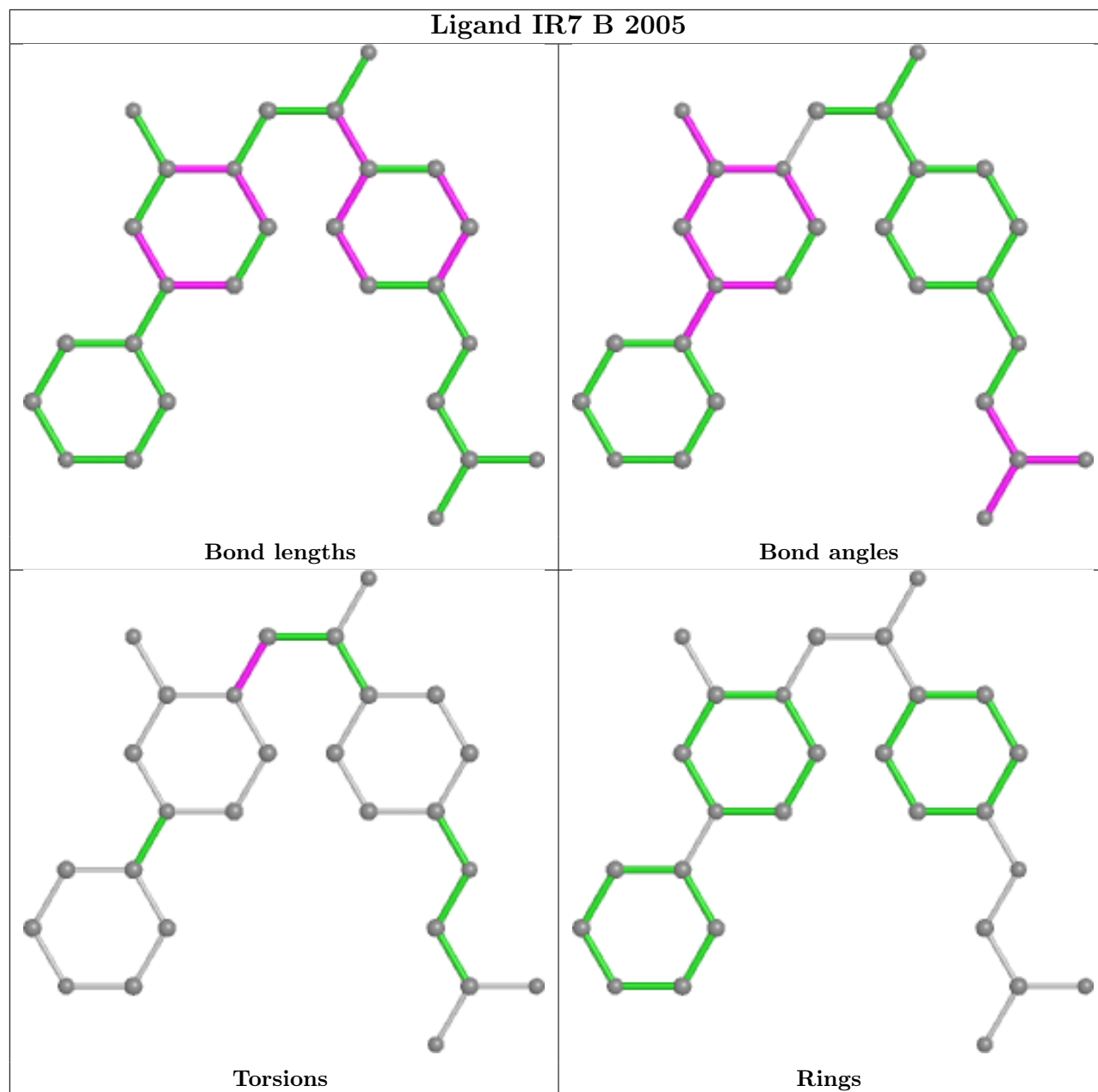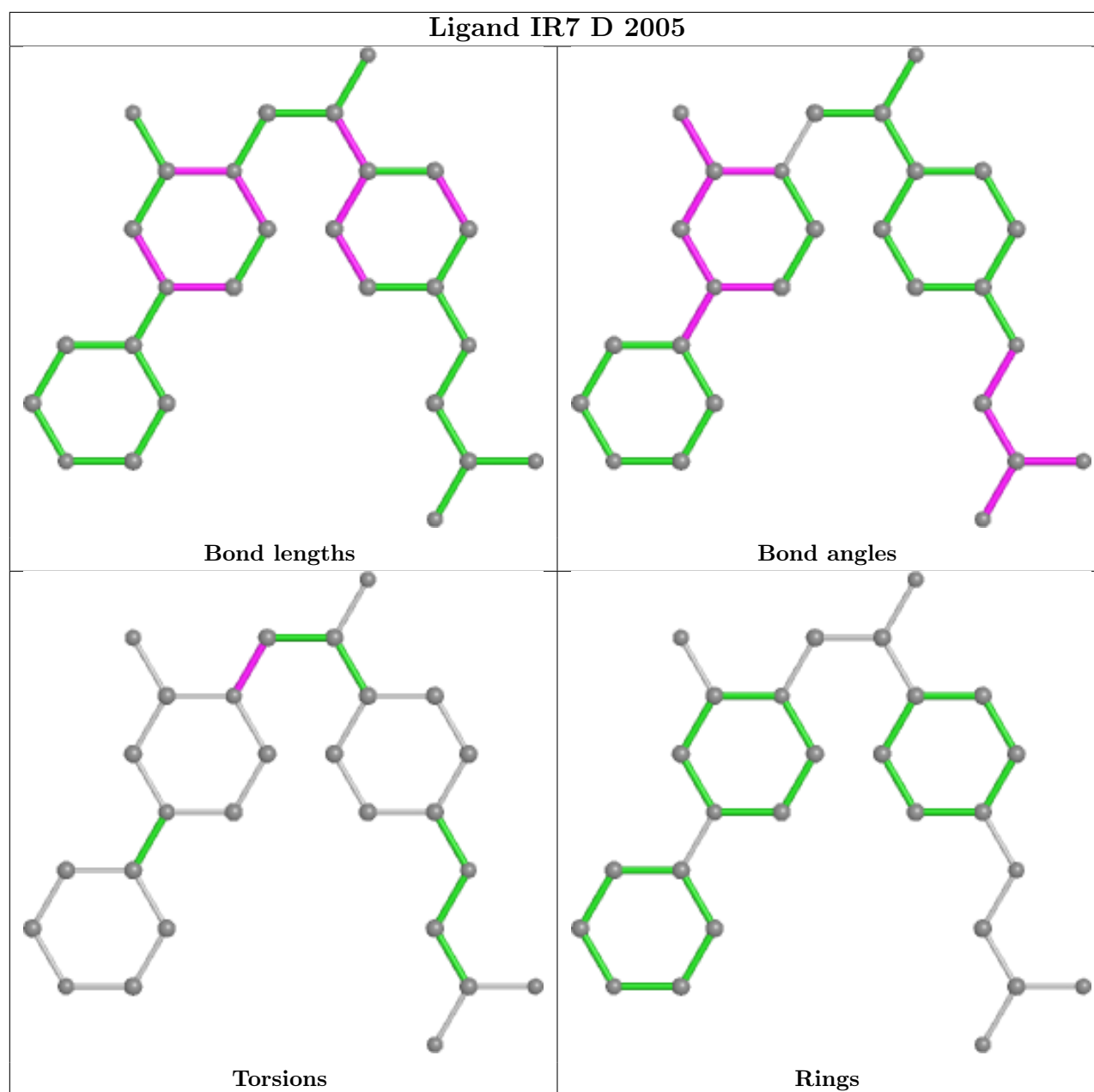
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	6.87

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	457/457 (100%)	-0.23	3 (0%)	87	86	19, 28, 53, 113	3 (0%)
1	C	453/457 (99%)	-0.24	4 (0%)	84	82	22, 44, 74, 115	0
2	B	466/471 (98%)	0.36	40 (8%)	10	7	17, 55, 142, 187	1 (0%)
2	D	471/471 (100%)	0.07	24 (5%)	28	22	25, 60, 120, 166	2 (0%)
3	E	214/216 (99%)	0.81	36 (16%)	1	1	52, 100, 151, 179	0
3	H	216/216 (100%)	0.22	16 (7%)	14	10	34, 82, 136, 153	0
4	F	214/214 (100%)	1.34	58 (27%)	0	0	56, 100, 180, 208	0
4	L	214/214 (100%)	0.00	4 (1%)	66	62	40, 71, 97, 161	0
All	All	2705/2716 (99%)	0.18	185 (6%)	17	12	17, 58, 139, 208	6 (0%)

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	214	CYS	9.6
4	F	193	THR	9.0
2	B	10	VAL	6.9
3	E	134	CYS	6.8
2	D	469	SER	6.7

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

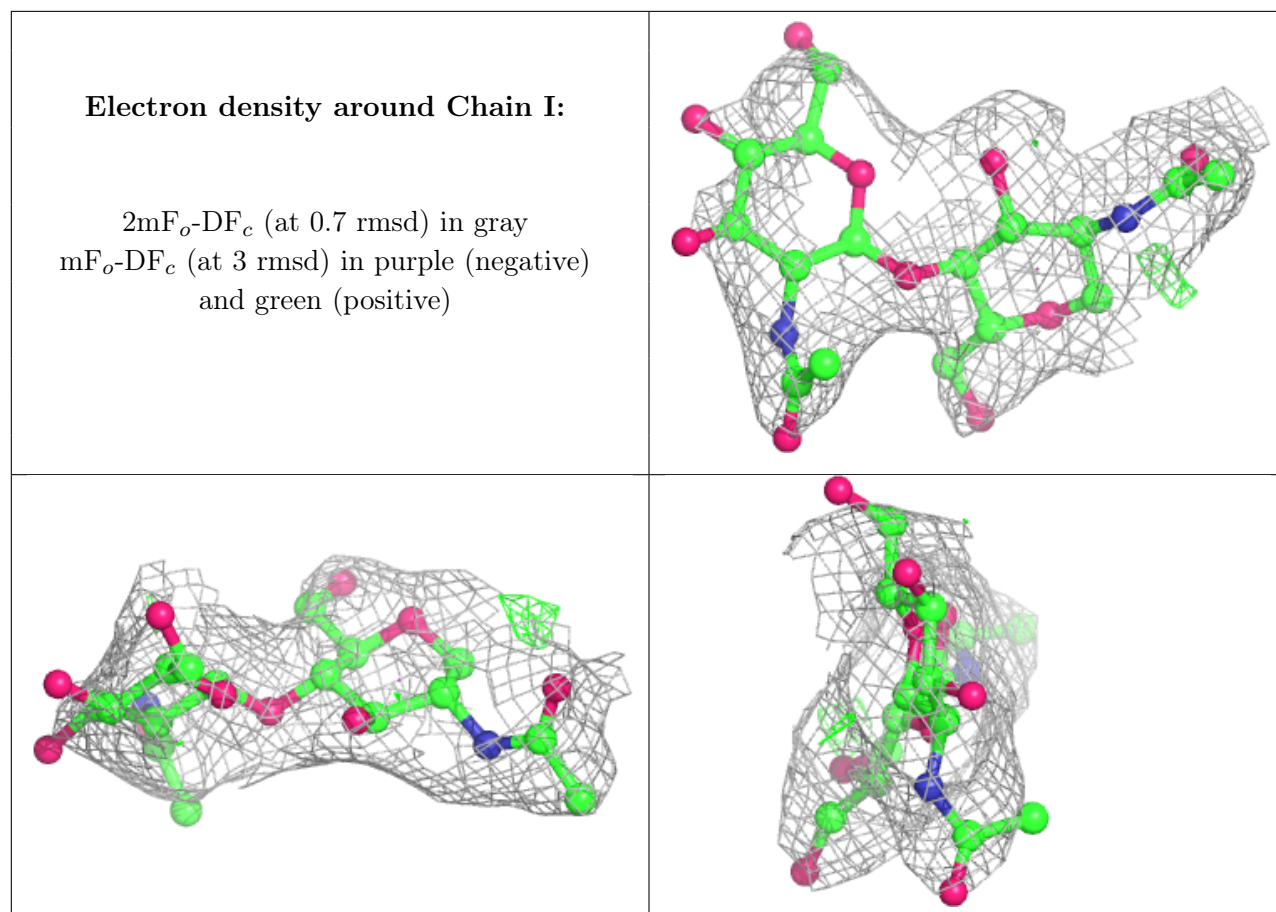There are no non-standard protein/DNA/RNA residues in this entry.

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
5	BMA	G	5	11/12	0.62	0.29	120,123,125,125	0
6	NAG	K	2	14/15	0.76	0.33	115,119,123,123	0
7	BMA	J	3	11/12	0.76	0.25	110,115,120,122	0
6	NAG	K	1	14/15	0.81	0.31	79,92,103,110	0
7	BMA	J	4	11/12	0.83	0.26	118,123,135,135	0
5	BMA	G	4	11/12	0.84	0.27	103,107,111,112	0
5	BMA	G	3	11/12	0.85	0.23	92,114,121,123	0
6	NAG	I	1	14/15	0.86	0.27	77,87,98,106	0
6	NAG	I	2	14/15	0.88	0.34	109,115,121,122	0
5	NAG	G	2	14/15	0.91	0.15	56,63,77,90	0
7	NAG	J	2	14/15	0.92	0.23	74,87,95,104	0
7	NAG	J	1	14/15	0.98	0.14	47,53,62,72	0
5	NAG	G	1	14/15	0.98	0.12	25,33,44,46	0

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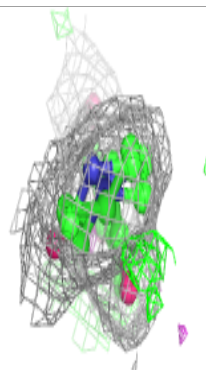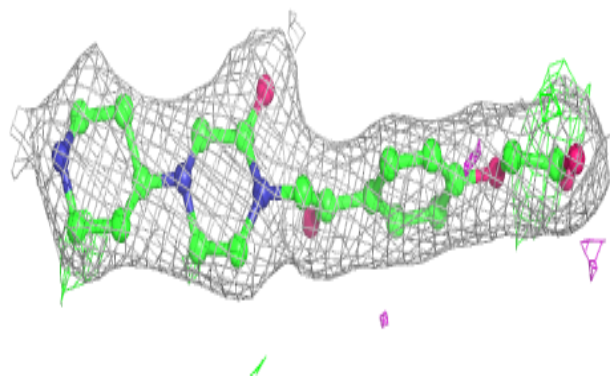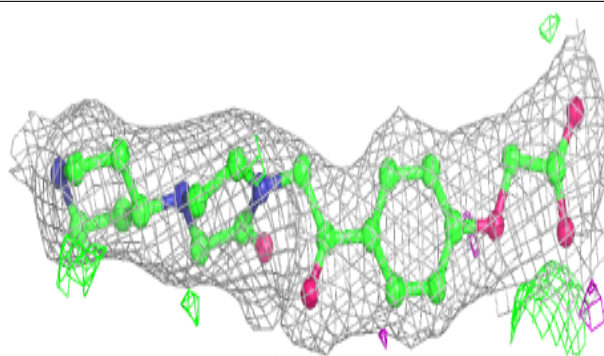

Electron density around Chain G:

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

Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
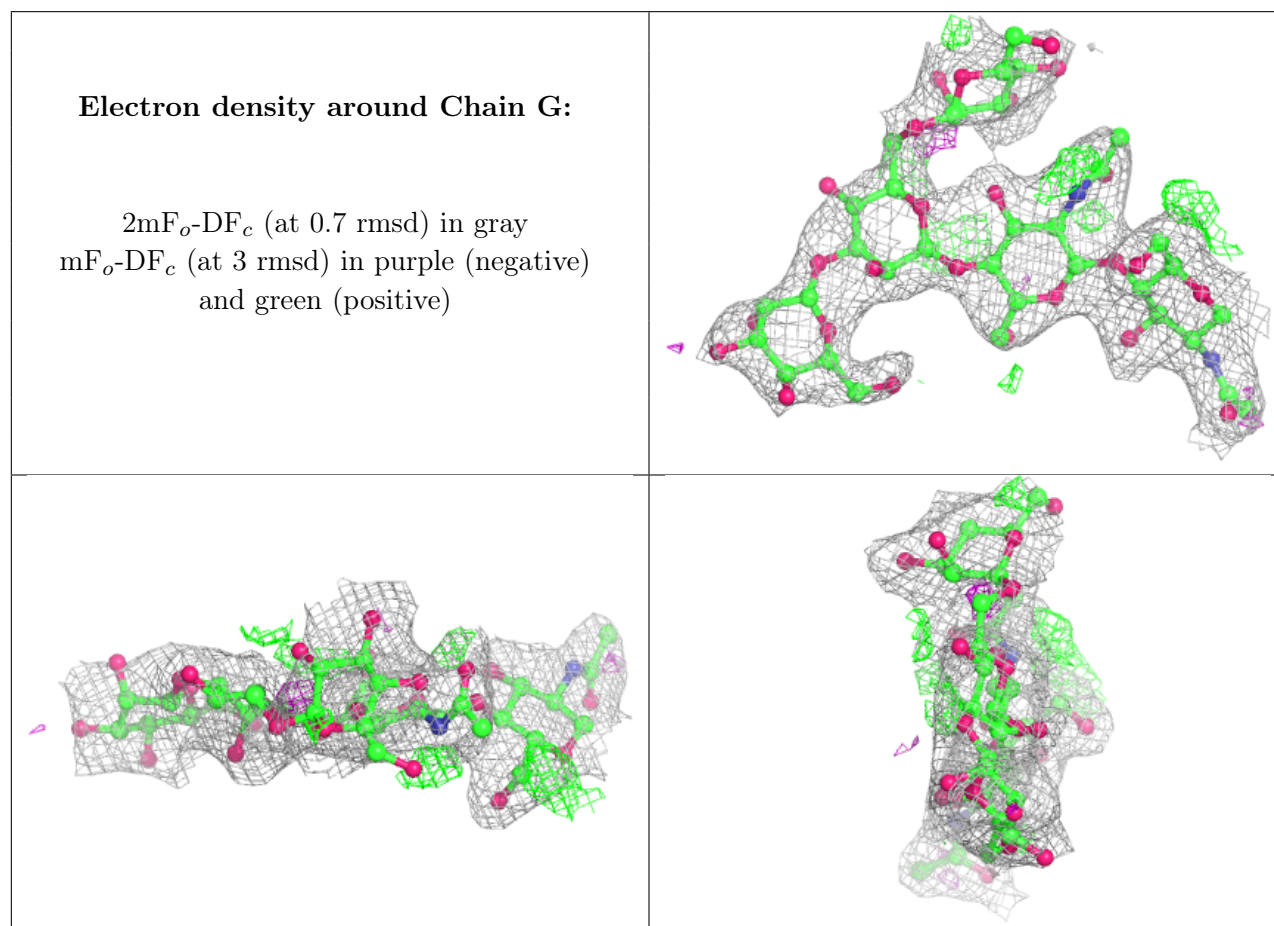
Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
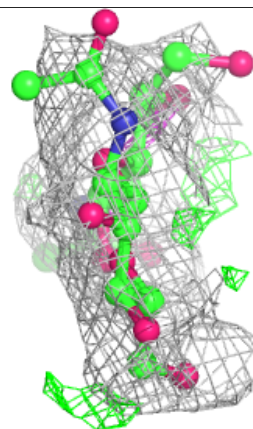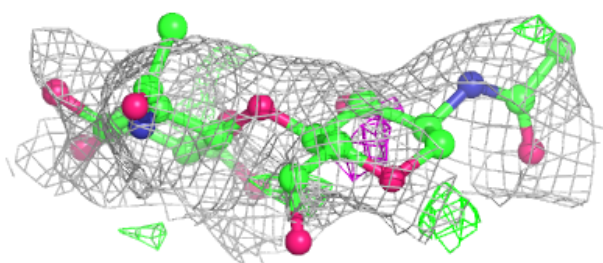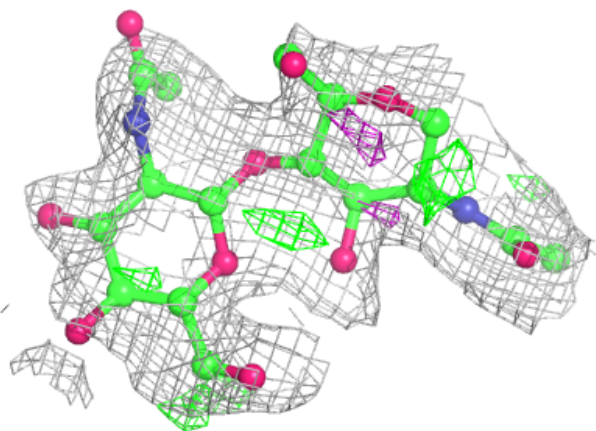
Electron density around Chain J:

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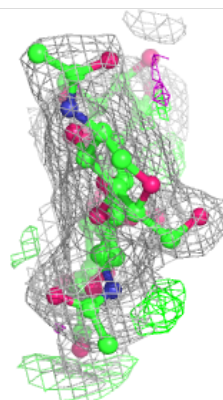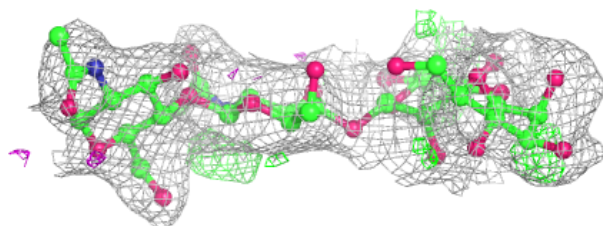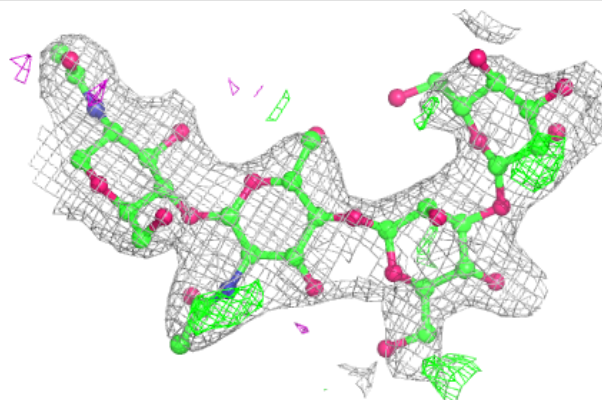
6.4 Ligands ⓘ

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.

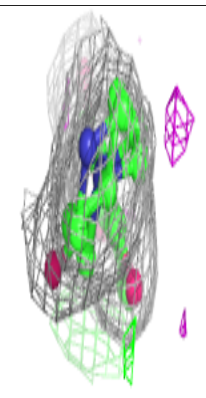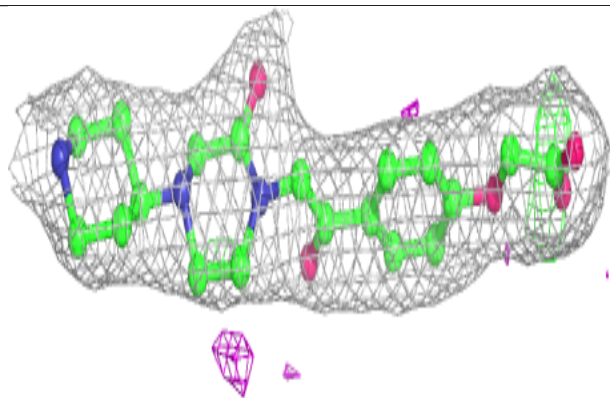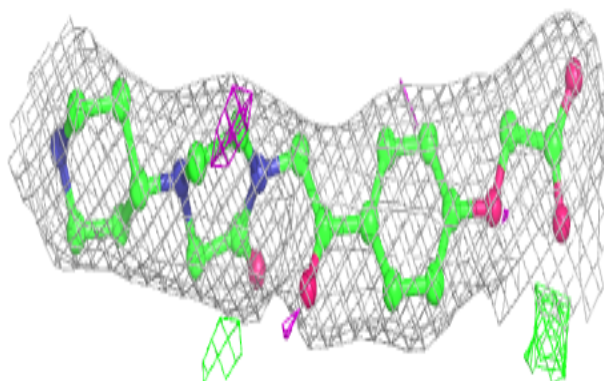| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	C	506	5/5	0.78	0.21	126,127,128,128	0
9	SO4	A	505	5/5	0.79	0.28	113,114,115,117	0
11	NAG	D	2004	14/15	0.81	0.37	85,95,102,104	0
9	SO4	C	505	5/5	0.82	0.26	111,114,116,118	0
11	NAG	B	2004	14/15	0.90	0.41	89,100,104,105	0
8	CA	C	501	1/1	0.92	0.04	70,70,70,70	0
9	SO4	A	506	5/5	0.93	0.20	93,98,100,101	0
9	SO4	A	507	5/5	0.94	0.13	89,91,95,96	0
8	CA	B	2002	1/1	0.95	0.06	70,70,70,70	0
10	MG	D	2001	1/1	0.95	0.22	33,33,33,33	0
10	MG	B	2001	1/1	0.97	0.26	21,21,21,21	0
12	IR7	B	2005	27/27	0.97	0.14	19,30,42,46	0
12	IR7	D	2005	27/27	0.97	0.16	23,42,50,52	0
8	CA	D	2002	1/1	0.98	0.08	57,57,57,57	0
8	CA	C	503	1/1	0.98	0.09	44,44,44,44	0
8	CA	C	504	1/1	0.99	0.09	51,51,51,51	0
8	CA	A	501	1/1	0.99	0.05	37,37,37,37	0
8	CA	D	2003	1/1	0.99	0.16	34,34,34,34	0
8	CA	B	2003	1/1	0.99	0.15	19,19,19,19	0
8	CA	A	502	1/1	0.99	0.11	29,29,29,29	0
8	CA	C	502	1/1	0.99	0.04	54,54,54,54	0
8	CA	A	504	1/1	0.99	0.13	24,24,24,24	0
8	CA	A	503	1/1	1.00	0.17	24,24,24,24	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 IR7 B 2005:

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

Electron density around IR7 D 2005:

$2mF_o$-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.