



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:08 AM UTC

PDB ID : 6EA4 / pdb_00006ea4
Title : ERAP2 bound to Aryl Sulfonamide Uncompetitive Inhibitor
Authors : Maben, Z.; Stern, L.J.
Deposited on : 2018-08-02
Resolution : 2.45 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

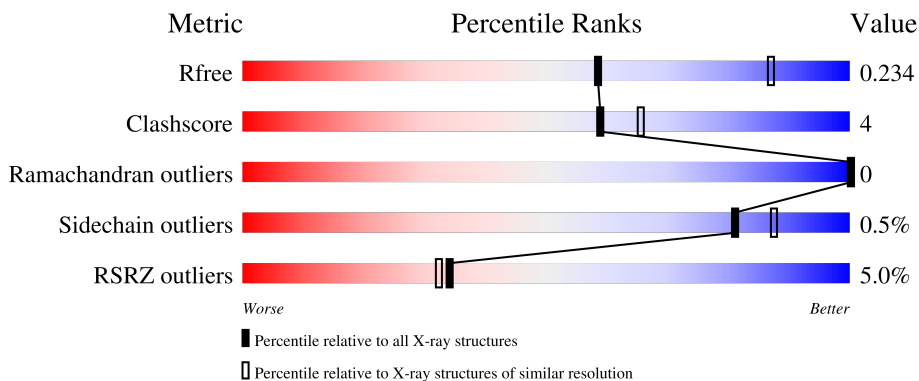
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.




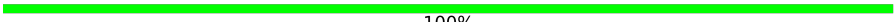
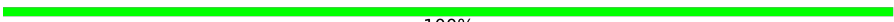


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	911	 88% 9%
1	B	911	 82% 13% 5% 8%
2	C	5	 60% 40%
2	D	5	 60% 40%
2	G	5	 60% 40%

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 100%
3	I	2	 100%
4	H	3	 67%  33%

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 15097 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.

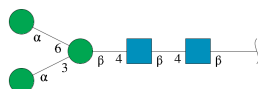
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	883	Total	C	N	O	S	0	7	0
			7212	4653	1201	1328	30			
1	B	869	Total	C	N	O	S	0	2	0
			7054	4550	1169	1306	29			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179

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



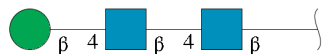
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

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



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

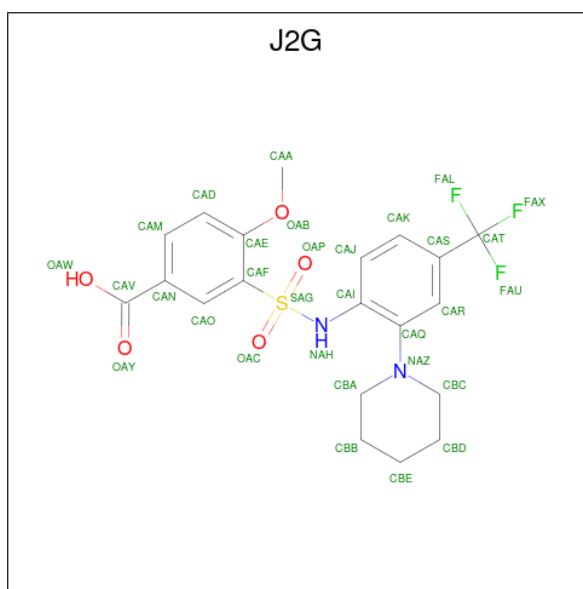
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	12	6	1	4	1	0	0
6	B	1	12	6	1	4	1	0	0

- Molecule 7 is 4-methoxy-3-{{2-(piperidin-1-yl)-4-(trifluoromethyl)phenyl}sulfamoyl}benzoic acid (CCD ID: J2G) (formula: C₂₀H₂₁F₃N₂O₅S) (labeled as "Ligand of Interest" by depositor).



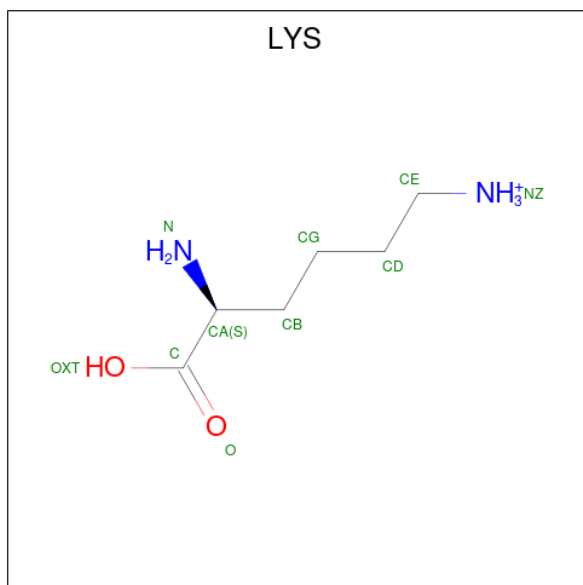
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
7	A	1	62	40	6	4	10	2	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
7	B	1	62	40	6	4	10	2	0	1

- Molecule 8 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂) (labeled as "Ligand of Interest" by depositor).



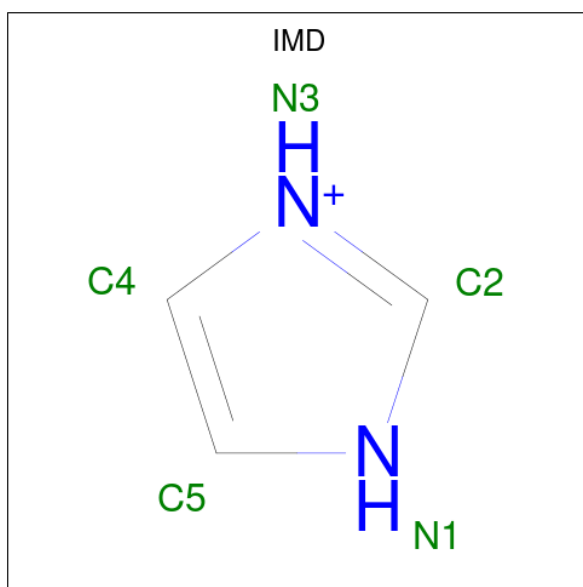
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	10	6	2	2	0	0
8	A	1	10	6	2	2	0	0
8	B	1	10	6	2	2	0	0
8	B	1	10	6	2	2	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



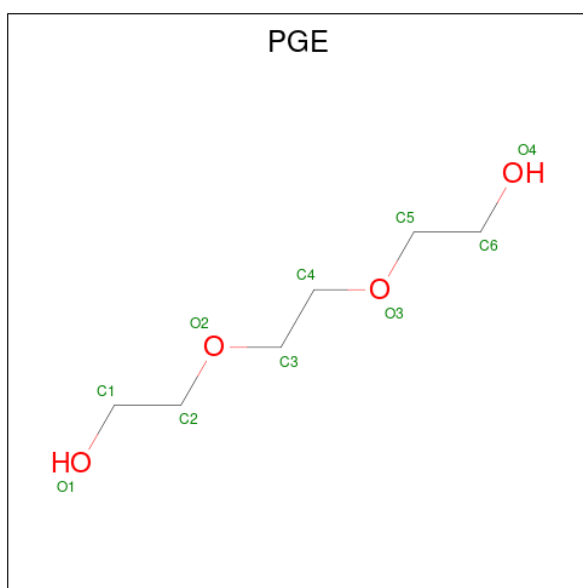
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
9	A	1	14	8	1	5	0	0
9	A	1	14	8	1	5	0	0
9	A	1	14	8	1	5	0	0
9	B	1	14	8	1	5	0	0
9	B	1	14	8	1	5	0	0
9	B	1	14	8	1	5	0	0

- Molecule 10 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



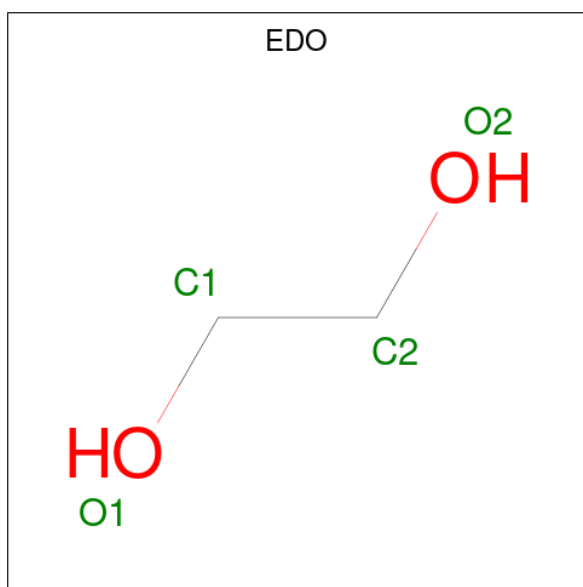
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N 5 3 2	0	0
10	B	1	Total C N 5 3 2	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 10 6 4	0	0

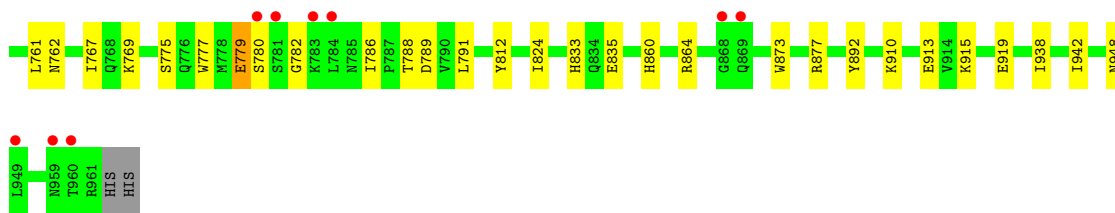
- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 4 2 2	0	0
12	B	1	Total C O 4 2 2	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	175	Total O 175 175	0	0
13	B	34	Total O 34 34	0	0



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

Chain C: 60% 40%



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

Chain D: 60% 40%



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

Chain G: 60% 40%



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

Chain E: 100%



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

Chain F: 100%



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

Chain I:  100%

MAG1
MAG2

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

Chain H:  67% 33%

MAG1
MAG2
BOM3

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.23Å 135.45Å 127.28Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.29 – 2.45 29.29 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.29-2.45) 87.1 (29.29-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.236 0.208 , 0.234	Depositor DCC
R_{free} test set	2027 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15097	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, EDO, BMA, IMD, PGE, J2G, MAN, NAG, ZN

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	0.08	0/7408	0.24	0/10041
1	B	0.07	0/7233	0.23	0/9808
All	All	0.07	0/14641	0.23	0/19849

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	7212	0	7151	51	0
1	B	7054	0	6957	74	0
2	C	61	0	52	0	0
2	D	61	0	52	0	0
2	G	61	0	52	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
4	H	39	0	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	12	3	0
6	B	12	0	12	2	0
7	A	62	0	0	1	0
7	B	62	0	0	0	0
8	A	20	0	24	2	0
8	B	20	0	24	2	0
9	A	56	0	52	0	0
9	B	42	0	39	0	0
10	A	5	0	5	0	0
10	B	5	0	5	2	0
11	A	10	0	14	2	0
12	A	4	0	6	0	0
12	B	4	0	6	0	0
13	A	175	0	0	2	0
13	B	34	0	0	1	0
All	All	15097	0	14572	129	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 4.

All (129) 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:A:777:TRP:HE1	1:A:783:LYS:HD2	1.42	0.83
1:A:383:MET:HE2	1:A:389:ILE:HA	1.63	0.81
1:A:177[B]:GLU:HB3	1:A:203:GLN:HG2	1.67	0.76
1:B:177[B]:GLU:HB3	1:B:203:GLN:HG2	1.72	0.72
1:B:200:GLU:OE1	8:B:1004:LYS:N	2.23	0.71
1:A:177[A]:GLU:HB2	1:A:203:GLN:HG2	1.71	0.71
1:B:565:ARG:H	1:B:581:GLN:HE22	1.37	0.69
1:B:910:LYS:HD3	1:B:913:GLU:OE2	1.95	0.67
1:A:753:ALA:HB2	11:A:1011:PGE:H62	1.76	0.66
1:A:131:MET:HG2	1:A:132:LYS:H	1.65	0.62
1:A:278:THR:HG21	1:A:307:LEU:HD23	1.82	0.61
1:B:383:MET:HE2	1:B:389:ILE:HA	1.80	0.61
1:A:183:THR:HG22	1:A:193:ILE:HD13	1.82	0.61
1:B:650:ASN:HB3	1:B:653:LEU:HD13	1.84	0.60
1:A:915:LYS:HE3	1:A:919:GLU:OE2	2.02	0.59
1:B:177[A]:GLU:HB2	1:B:203:GLN:HG2	1.83	0.59
1:B:374:HIS:HE1	1:B:392:ASN:HB3	1.69	0.58
1:B:183:THR:HG22	1:B:193:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HG	1:A:956:LEU:HD11	1.87	0.55
1:B:339:TRP:CD2	1:B:379:ASN:HB3	2.42	0.55
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.42	0.55
1:A:540:THR:HG21	1:A:587:HIS:H	1.70	0.55
1:A:199:PHE:HA	1:A:203:GLN:HB2	1.89	0.54
1:B:565:ARG:H	1:B:581:GLN:NE2	2.05	0.54
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.89	0.54
1:A:537:MET:O	1:A:540:THR:HG22	2.09	0.53
8:A:1009:LYS:OXT	13:A:1101:HOH:O	2.18	0.53
1:A:362:LEU:HD13	1:A:411:LEU:HB3	1.89	0.53
1:B:915:LYS:HE3	1:B:919:GLU:OE2	2.09	0.53
1:A:72:VAL:HG23	1:A:73:VAL:HG23	1.90	0.52
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.91	0.52
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.91	0.52
1:B:892:TYR:CD2	10:B:1008:IMD:H5	2.45	0.52
1:A:476:LYS:O	1:A:480[A]:GLN:HG2	2.10	0.51
1:B:677:LEU:HD22	1:B:948:ASN:HB3	1.92	0.51
1:A:200:GLU:OE1	8:A:1004:LYS:N	2.43	0.51
1:A:436:ILE:HG22	1:A:542:THR:HA	1.91	0.51
1:B:82:VAL:HG12	1:B:84:PRO:HD3	1.93	0.50
1:B:298:TYR:CZ	1:B:361:LYS:HD2	2.45	0.50
1:B:451:ASP:HA	6:B:1002:MES:H62	1.93	0.50
1:A:82:VAL:HG12	1:A:84:PRO:HD3	1.93	0.50
1:B:455:TYR:OH	8:B:1004:LYS:OXT	2.25	0.49
1:A:122:LEU:HB2	1:A:137:LEU:HD11	1.94	0.49
1:B:684:THR:HA	1:B:687:LEU:HD23	1.93	0.49
1:B:598:ASN:HD22	1:B:598:ASN:N	2.11	0.49
1:A:389:ILE:HG21	1:A:449:MET:HB3	1.93	0.49
1:A:792:LYS:HE3	11:A:1011:PGE:H1	1.95	0.48
1:B:199:PHE:HA	1:B:203:GLN:HB2	1.95	0.47
1:B:477:GLY:HA3	1:B:499:LEU:HD23	1.97	0.47
1:B:122:LEU:HB2	1:B:137:LEU:HD11	1.94	0.47
1:B:236:MET:HG2	1:B:256:THR:HG22	1.96	0.47
1:A:591:THR:O	1:A:624:ASN:N	2.47	0.47
1:A:338:ASN:HB2	1:A:341:LEU:O	2.15	0.46
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.97	0.46
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.81	0.46
1:B:550:LEU:HD22	1:B:590:LEU:HD11	1.98	0.46
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.96	0.46
1:B:892:TYR:HD2	10:B:1008:IMD:H5	1.81	0.46
1:B:333:PRO:O	1:B:345:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MET:HG2	1:A:256:THR:HG22	1.97	0.46
1:B:351:PHE:CZ	1:B:361:LYS:HE3	2.51	0.46
1:A:865:ARG:NE	13:A:1119:HOH:O	2.48	0.46
1:B:723:LYS:HG3	1:B:761:LEU:HB3	1.98	0.46
6:A:1002:MES:H51	6:A:1002:MES:H81	1.71	0.45
1:A:885:LYS:HA	1:A:885:LYS:HE2	1.98	0.45
1:B:73:VAL:HG11	1:B:108:ILE:HG23	1.98	0.45
1:B:591:THR:HG22	1:B:602:ARG:HG2	1.99	0.45
1:B:788:THR:HA	1:B:791:LEU:HB2	1.99	0.45
1:B:833:HIS:HB3	1:B:835:GLU:OE2	2.16	0.45
1:A:339:TRP:CD2	1:A:379:ASN:HB3	2.52	0.45
1:A:591:THR:HG22	1:A:602:ARG:HG2	1.99	0.45
1:B:591:THR:O	1:B:624:ASN:N	2.49	0.45
1:B:640:TRP:HZ3	1:B:662:LEU:HD22	1.82	0.45
1:A:496:TRP:HZ2	1:A:542:THR:HG21	1.82	0.45
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.99	0.44
1:B:436:ILE:HG22	1:B:542:THR:HA	1.98	0.44
1:B:860:HIS:NE2	1:B:864:ARG:HD2	2.32	0.44
1:B:762:ASN:HA	1:B:767:ILE:HD11	2.00	0.44
1:A:540:THR:HG21	1:A:586:TRP:HA	2.00	0.44
1:B:775:SER:O	1:B:779:GLU:HB3	2.16	0.44
1:A:595:SER:HB3	1:A:620:TRP:CE2	2.53	0.44
1:B:95:GLU:OE2	1:B:166:MET:HE3	2.18	0.44
1:B:748:ARG:HE	1:B:789:ASP:CG	2.26	0.44
1:A:664:HIS:O	1:A:668:GLN:HG2	2.18	0.44
1:A:833:HIS:HB3	1:A:835:GLU:OE2	2.17	0.44
1:B:537:MET:HE3	1:B:538:MET:HE2	2.00	0.43
1:B:374:HIS:CE1	1:B:392:ASN:HB3	2.50	0.43
6:B:1002:MES:H51	6:B:1002:MES:H81	1.73	0.43
1:B:110:LEU:HD11	1:B:148:ILE:HD11	2.01	0.43
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.54	0.43
1:B:389:ILE:HG21	1:B:449:MET:HB3	2.01	0.43
1:A:870:GLN:OE1	1:A:910:LYS:NZ	2.50	0.42
1:A:333:PRO:O	1:A:345:ARG:HG3	2.19	0.42
1:B:213:GLU:HB2	1:B:216:PHE:CD1	2.54	0.42
1:B:278:THR:HG21	1:B:307:LEU:HD23	2.01	0.42
1:B:157:THR:HB	1:B:160:LEU:HD12	2.01	0.42
1:B:213:GLU:HB2	1:B:216:PHE:HD1	1.84	0.42
1:A:101:VAL:O	1:A:159:HIS:N	2.47	0.42
1:B:338:ASN:HB2	1:B:341:LEU:O	2.19	0.42
1:B:780:SER:C	1:B:782:GLY:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1002:MES:H72	7:A:1003[B]:J2G:OAP	2.19	0.42
1:B:769:LYS:NZ	13:B:1109:HOH:O	2.52	0.42
1:B:567:LEU:HD13	1:B:567:LEU:HA	1.93	0.42
1:B:629:GLY:HA3	1:B:631:TYR:CE1	2.55	0.42
1:A:733:VAL:O	1:A:737:GLN:HG2	2.19	0.42
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.54	0.41
1:B:647:LEU:HB3	1:B:686:TYR:CG	2.55	0.41
1:B:659:ARG:NE	1:B:690:GLU:OE1	2.53	0.41
1:A:777:TRP:NE1	1:A:783:LYS:HD2	2.22	0.41
1:B:488:ARG:HG2	1:B:489:ASN:H	1.86	0.41
1:B:938:ILE:O	1:B:942:ILE:HG12	2.21	0.41
1:A:79:ASP:O	1:A:95:GLU:HA	2.21	0.41
1:A:196:VAL:HG23	1:A:267:ILE:HG12	2.03	0.41
1:A:428:ASP:O	1:A:546:GLY:HA2	2.21	0.41
1:A:455:TYR:CD2	6:A:1002:MES:H31	2.56	0.41
1:A:780:SER:C	1:A:782:GLY:H	2.29	0.41
1:B:318:TYR:CE2	1:B:320:LEU:HB2	2.55	0.41
1:B:468:PHE:CE2	1:B:537:MET:HE1	2.56	0.41
1:B:571:PHE:N	1:B:574:ASP:OD2	2.39	0.41
1:B:812:TYR:HB2	1:B:824:ILE:HG21	2.03	0.41
1:B:548:PRO:HB3	1:B:586:TRP:CE3	2.56	0.41
1:B:687:LEU:HD12	1:B:696:LEU:HA	2.02	0.41
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.56	0.41
1:A:140:LEU:HB2	1:A:149:ALA:HB3	2.03	0.40
1:B:79:ASP:O	1:B:95:GLU:HA	2.21	0.40
1:B:79:ASP:HB2	1:B:96:LYS:HB3	2.04	0.40
1:B:292:LYS:NZ	1:B:346:GLU:OE1	2.53	0.40
1:B:258:LYS:H	4:H:1:NAG:H62	1.85	0.40
1:B:453:VAL:O	1:B:457:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

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	886/911 (97%)	859 (97%)	27 (3%)	0	100	100
1	B	863/911 (95%)	835 (97%)	28 (3%)	0	100	100
All	All	1749/1822 (96%)	1694 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	792/819 (97%)	790 (100%)	2 (0%)	86	91
1	B	772/819 (94%)	766 (99%)	6 (1%)	73	83
All	All	1564/1638 (96%)	1556 (100%)	8 (0%)	81	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	650	ASN
1	A	686	TYR
1	B	73	VAL
1	B	567	LEU
1	B	598	ASN
1	B	650	ASN
1	B	755	LEU
1	B	779	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	392	ASN
1	A	544	GLN
1	A	648	ASN
1	A	689	HIS

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Mol	Chain	Res	Type
1	A	869	GLN
1	A	879	ASN
1	B	159	HIS
1	B	338	ASN
1	B	412	GLN
1	B	447	GLN
1	B	544	GLN
1	B	581	GLN
1	B	689	HIS
1	B	869	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 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	C	1	1,2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	C	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	BMA	C	3	2	11,11,12	0.53	0	15,15,17	0.79	0
2	MAN	C	4	2	11,11,12	0.75	0	15,15,17	1.53	2 (13%)
2	MAN	C	5	2	11,11,12	0.56	0	15,15,17	1.00	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.50	0
2	BMA	D	3	2	11,11,12	0.67	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	D	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.56	2 (13%)
2	MAN	D	5	2	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	F	1	1,3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	BMA	G	3	2	11,11,12	0.59	0	15,15,17	0.66	0
2	MAN	G	4	2	11,11,12	0.90	1 (9%)	15,15,17	1.58	2 (13%)
2	MAN	G	5	2	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.17	0	17,19,21	0.42	0
4	NAG	H	2	4	14,14,15	0.25	0	17,19,21	0.46	0
4	BMA	H	3	4	11,11,12	0.61	0	15,15,17	0.65	0
3	NAG	I	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.41	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	C1-C2	2.32	1.57	1.52
2	G	4	MAN	C1-C2	2.31	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	MAN	C1-O5-C5	5.14	119.07	112.19
2	D	4	MAN	C1-O5-C5	4.99	118.88	112.19
2	C	4	MAN	C1-O5-C5	4.85	118.68	112.19
2	G	5	MAN	C1-O5-C5	2.81	115.95	112.19
2	D	5	MAN	C1-O5-C5	2.71	115.82	112.19
2	C	5	MAN	C1-O5-C5	2.69	115.79	112.19
2	D	5	MAN	O2-C2-C3	-2.18	105.63	110.15
2	C	5	MAN	O2-C2-C3	-2.15	105.69	110.15
2	G	5	MAN	O2-C2-C3	-2.14	105.72	110.15
2	C	4	MAN	O2-C2-C3	-2.12	105.75	110.15
2	D	4	MAN	O2-C2-C3	-2.12	105.75	110.15
2	G	4	MAN	O2-C2-C3	-2.10	105.81	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	4	MAN	C4-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6

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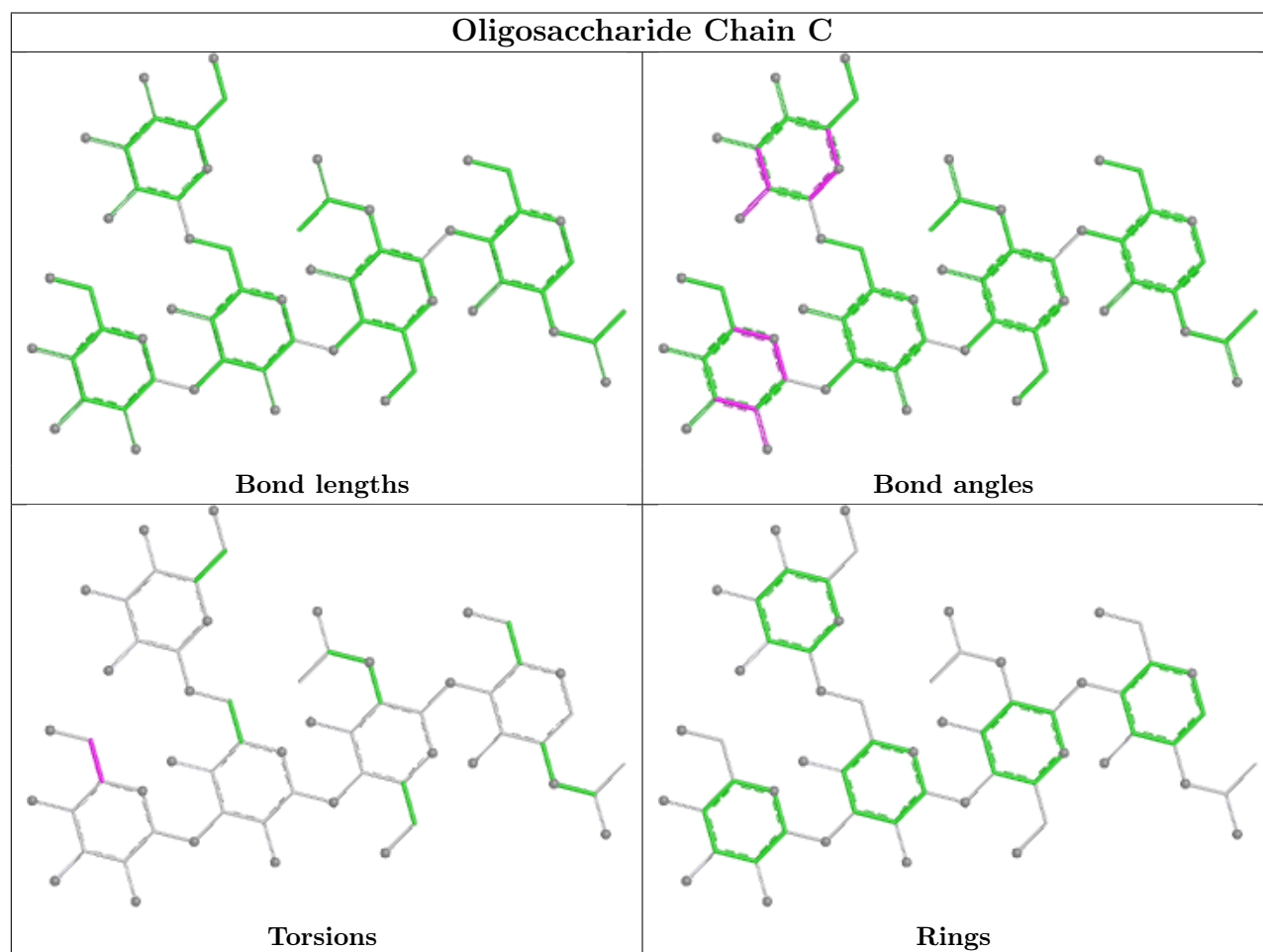
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7

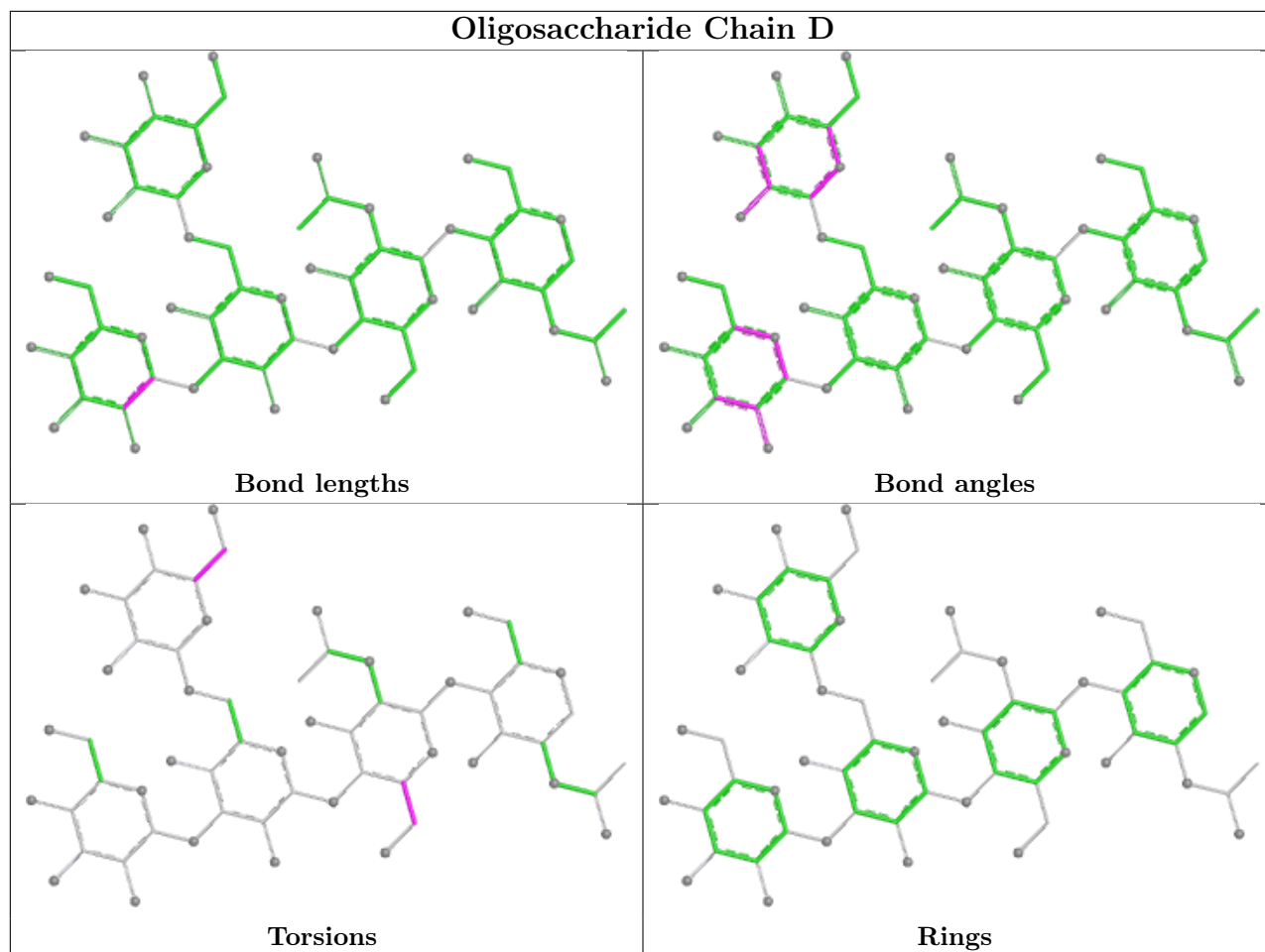
There are no ring outliers.

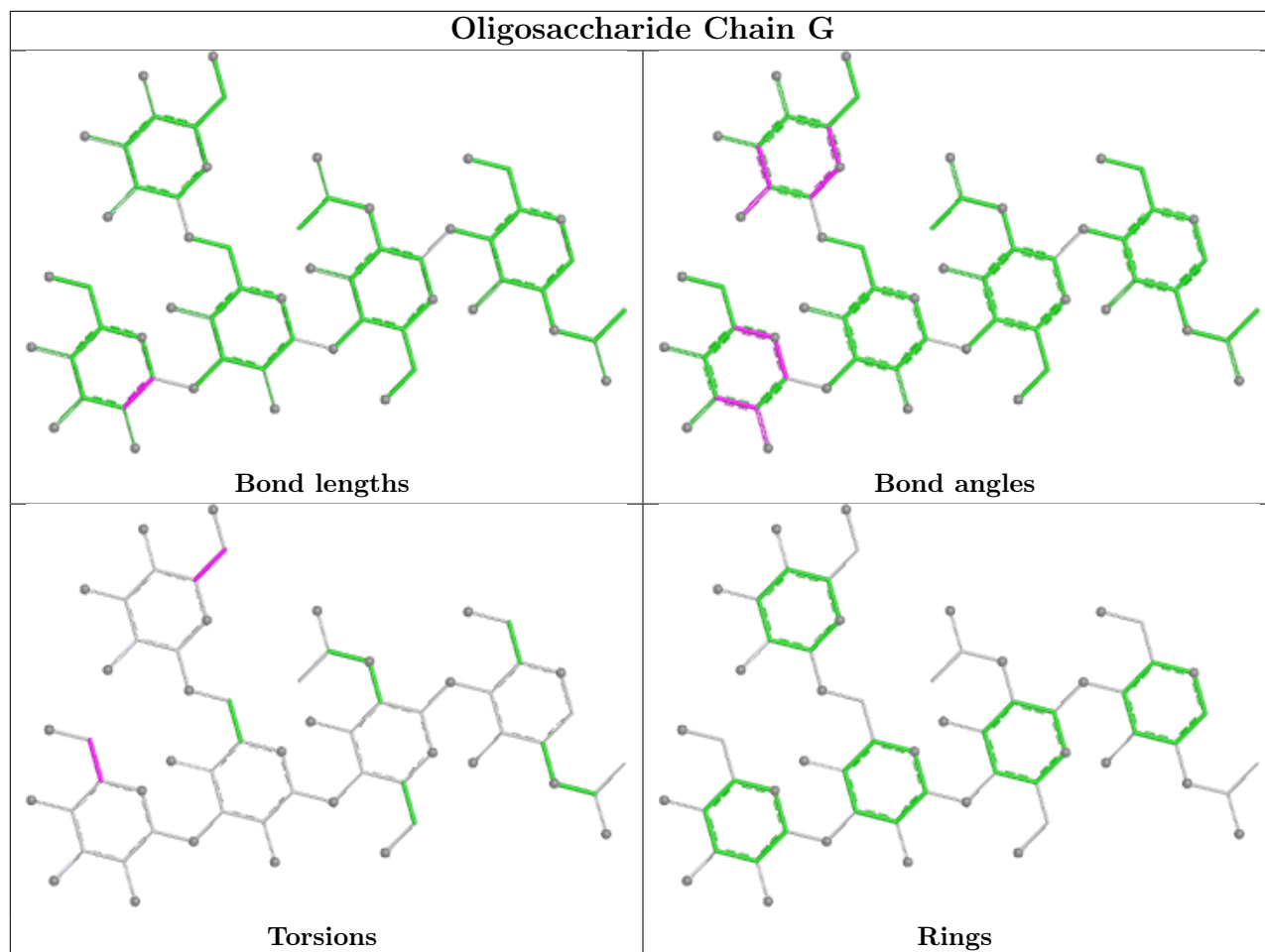
1 monomer is involved in 1 short contact:

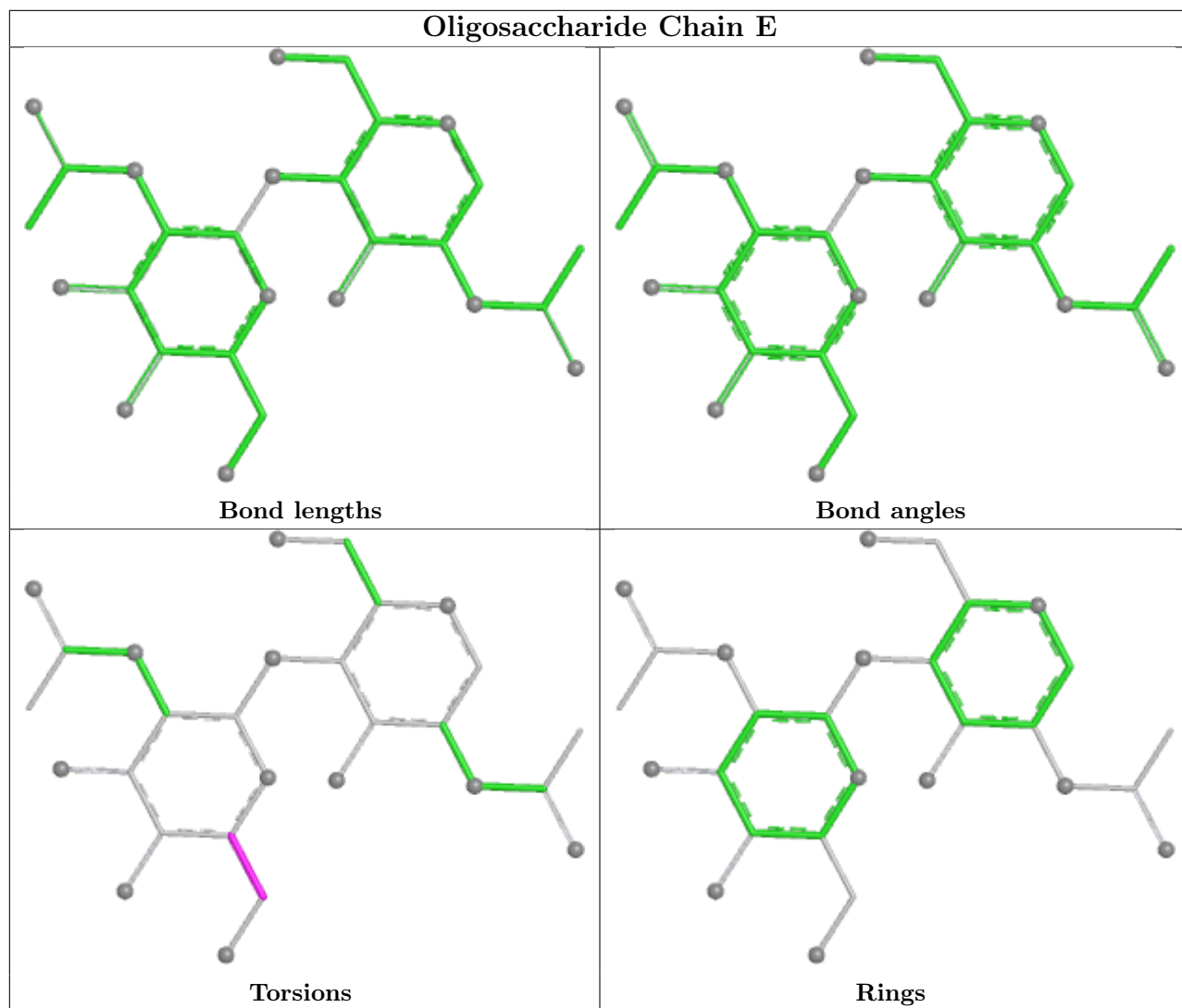
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0

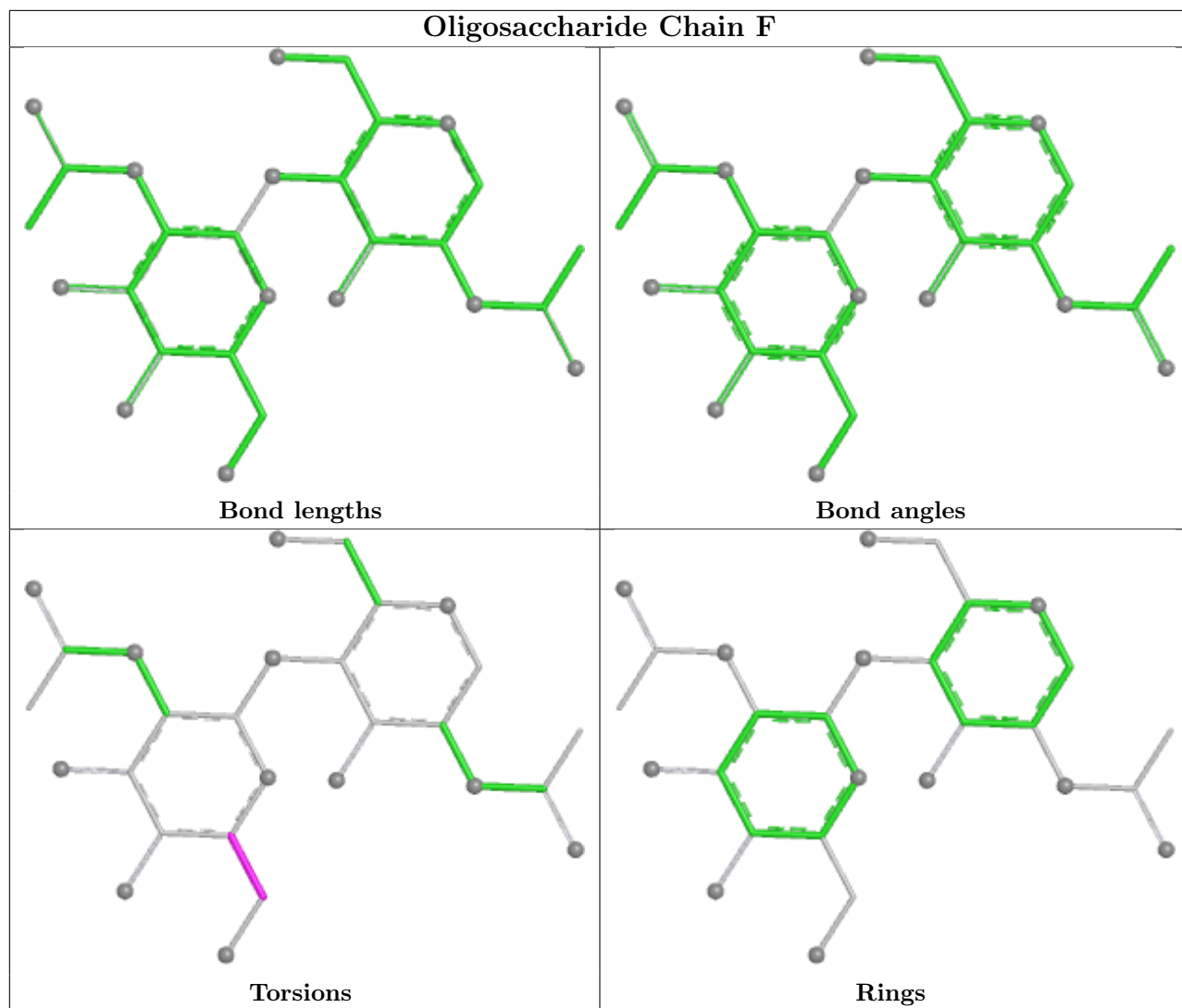
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

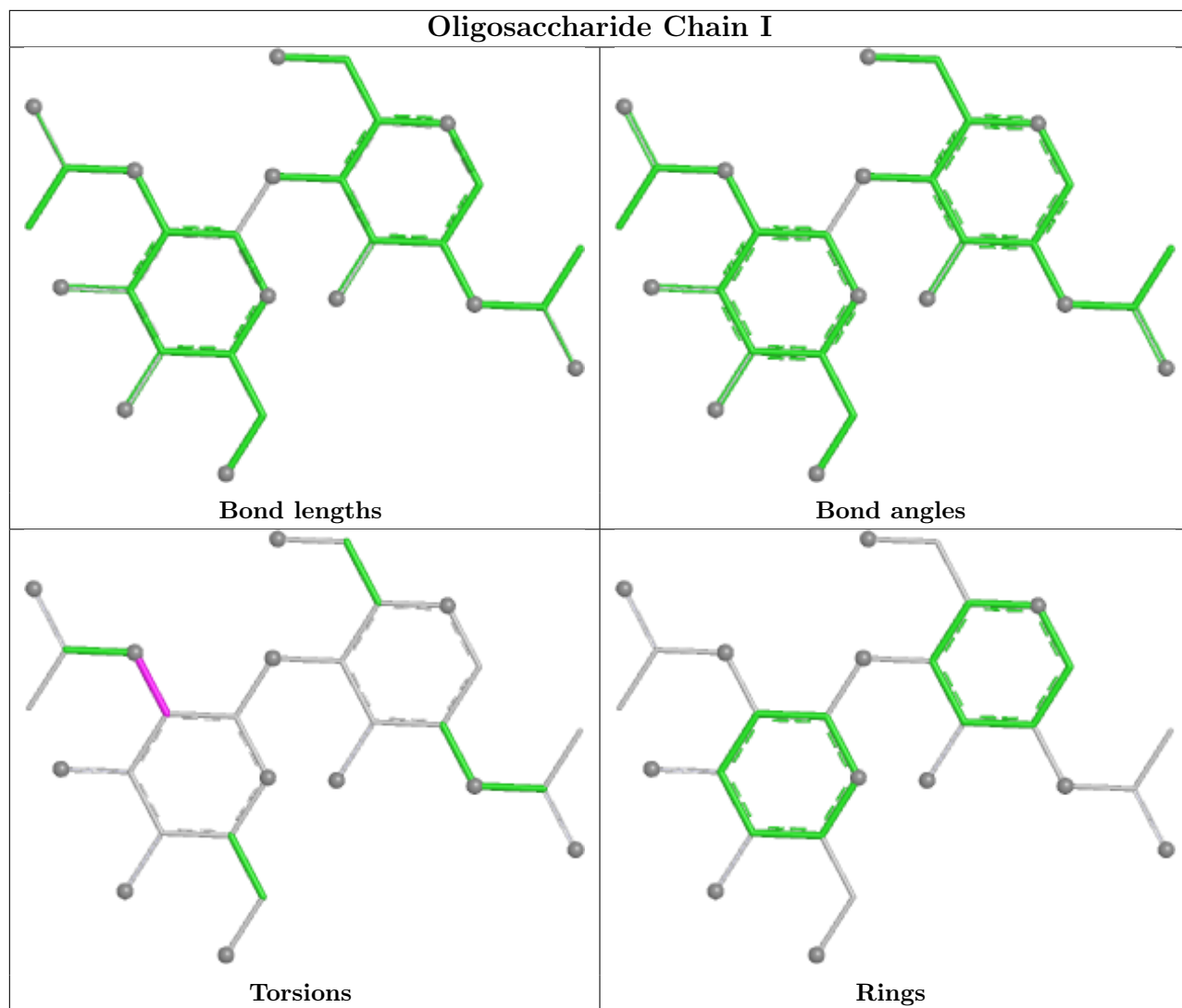


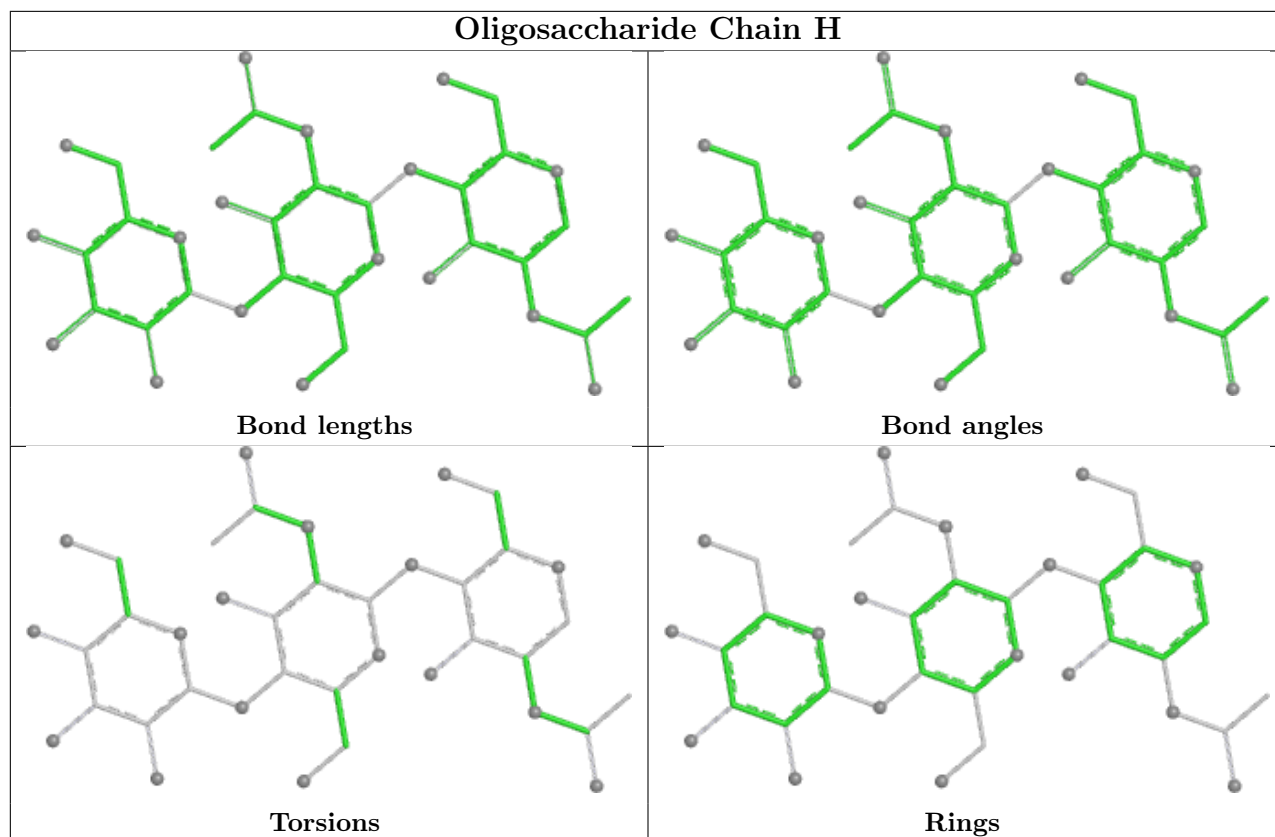












5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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
6	MES	B	1002	-	12,12,12	2.31	1 (8%)	15,16,16	1.87	3 (20%)
8	LYS	B	1010	-	8,9,9	0.85	1 (12%)	7,10,10	0.94	1 (14%)
12	EDO	B	1009	-	3,3,3	0.43	0	2,2,2	0.37	0
12	EDO	A	1012	-	3,3,3	0.43	0	2,2,2	0.38	0
9	NAG	A	1007	1	14,14,15	0.31	0	17,19,21	0.47	0
9	NAG	A	1008	1	14,14,15	0.33	0	17,19,21	0.47	0
11	PGE	A	1011	-	9,9,9	0.31	0	8,8,8	0.28	0
9	NAG	B	1007	1	14,14,15	0.25	0	17,19,21	0.48	0
9	NAG	B	1005	1	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LYS	A	1004	5	8,9,9	0.85	1 (12%)	7,10,10	1.07	1 (14%)
9	NAG	A	1006	1	14,14,15	0.24	0	17,19,21	0.46	0
10	IMD	B	1008	-	5,5,5	0.63	0	5,5,5	0.44	0
8	LYS	B	1004	5	8,9,9	0.85	1 (12%)	7,10,10	1.08	1 (14%)
9	NAG	A	1005	1	14,14,15	0.24	0	17,19,21	0.44	0
7	J2G	A	1003[A]	-	33,33,33	0.94	2 (6%)	48,49,49	1.26	7 (14%)
8	LYS	A	1009	-	8,9,9	0.87	1 (12%)	7,10,10	0.95	1 (14%)
7	J2G	A	1003[B]	-	33,33,33	0.94	2 (6%)	48,49,49	1.26	4 (8%)
6	MES	A	1002	-	12,12,12	2.37	1 (8%)	15,16,16	1.73	5 (33%)
9	NAG	B	1006	1	14,14,15	0.24	0	17,19,21	0.44	0
7	J2G	B	1003[A]	-	33,33,33	0.93	2 (6%)	48,49,49	1.25	7 (14%)
10	IMD	A	1010	-	5,5,5	0.64	0	5,5,5	0.43	0
7	J2G	B	1003[B]	-	33,33,33	0.93	1 (3%)	48,49,49	1.26	4 (8%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MES	B	1002	-	-	0/6/14/14	0/1/1/1
8	LYS	B	1010	-	-	2/9/9/9	-
12	EDO	B	1009	-	-	0/1/1/1	-
12	EDO	A	1012	-	-	0/1/1/1	-
9	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
11	PGE	A	1011	-	-	3/7/7/7	-
9	NAG	B	1007	1	-	4/6/23/26	0/1/1/1
9	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
8	LYS	A	1004	5	-	4/9/9/9	-
9	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
10	IMD	B	1008	-	-	-	0/1/1/1
8	LYS	B	1004	5	-	4/9/9/9	-
9	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
7	J2G	A	1003[A]	-	-	18/27/35/35	0/3/3/3
8	LYS	A	1009	-	-	2/9/9/9	-
7	J2G	A	1003[B]	-	-	13/27/35/35	0/3/3/3
6	MES	A	1002	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1006	1	-	1/6/23/26	0/1/1/1
7	J2G	B	1003[A]	-	-	17/27/35/35	0/3/3/3
10	IMD	A	1010	-	-	-	0/1/1/1
7	J2G	B	1003[B]	-	-	13/27/35/35	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	MES	C8-S	-7.92	1.66	1.77
6	B	1002	MES	C8-S	-7.71	1.66	1.77
7	A	1003[A]	J2G	SAG-NAH	2.61	1.67	1.63
7	B	1003[A]	J2G	SAG-NAH	2.55	1.67	1.63
7	B	1003[B]	J2G	OAB-CAE	-2.37	1.33	1.37
8	A	1009	LYS	OXT-C	-2.28	1.23	1.30
8	A	1004	LYS	OXT-C	-2.27	1.23	1.30
7	A	1003[B]	J2G	OAB-CAE	-2.26	1.33	1.37
8	B	1010	LYS	OXT-C	-2.24	1.23	1.30
8	B	1004	LYS	OXT-C	-2.23	1.23	1.30
7	B	1003[A]	J2G	OAB-CAE	-2.22	1.33	1.37
7	A	1003[A]	J2G	OAB-CAE	-2.14	1.33	1.37
7	A	1003[B]	J2G	CAI-CAQ	2.09	1.42	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1002	MES	C5-N4-C3	4.09	117.66	108.84
7	A	1003[B]	J2G	CAF-SAG-NAH	-3.86	102.76	107.30
7	B	1003[B]	J2G	CBC-NAZ-CBA	3.63	119.73	111.57
7	B	1003[B]	J2G	OAC-SAG-CAF	3.57	113.58	107.68
6	A	1002	MES	C5-N4-C3	3.49	116.37	108.84
7	A	1003[B]	J2G	OAC-SAG-CAF	3.46	113.39	107.68
7	B	1003[B]	J2G	CAF-SAG-NAH	-3.44	103.24	107.30
7	B	1003[A]	J2G	CBC-NAZ-CBA	3.20	118.77	111.57
6	B	1002	MES	C6-C5-N4	-3.09	105.43	110.12
7	A	1003[A]	J2G	CBC-NAZ-CBA	3.01	118.33	111.57
7	B	1003[A]	J2G	OAC-SAG-CAF	3.01	112.64	107.68
7	A	1003[B]	J2G	CBC-NAZ-CBA	2.89	118.07	111.57
7	A	1003[A]	J2G	OAC-SAG-CAF	2.87	112.43	107.68
6	A	1002	MES	C6-C5-N4	-2.82	105.84	110.12
7	A	1003[A]	J2G	CBB-CBA-NAZ	2.74	116.24	111.06
8	A	1004	LYS	OXT-C-O	-2.74	117.86	124.08
7	A	1003[A]	J2G	OAB-CAE-CAF	2.73	118.58	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1004	LYS	OXT-C-O	-2.72	117.90	124.08
7	B	1003[A]	J2G	OAB-CAE-CAF	2.44	118.36	116.49
8	B	1010	LYS	OXT-C-O	-2.38	118.68	124.08
8	A	1009	LYS	OXT-C-O	-2.33	118.80	124.08
7	B	1003[A]	J2G	CBB-CBA-NAZ	2.30	115.41	111.06
7	B	1003[B]	J2G	CBD-CBC-NAZ	2.26	115.33	111.06
7	B	1003[A]	J2G	CBD-CBE-CBB	-2.25	104.49	111.19
6	A	1002	MES	O1S-S-C8	2.18	110.02	106.73
6	A	1002	MES	C7-N4-C5	2.14	116.95	111.24
7	B	1003[A]	J2G	OAY-CAV-CAN	-2.13	115.87	121.46
7	A	1003[A]	J2G	CBD-CBE-CBB	-2.12	104.91	111.19
7	B	1003[A]	J2G	OAP-SAG-CAF	-2.10	104.21	107.68
6	B	1002	MES	O2S-S-C8	2.08	109.87	106.73
6	A	1002	MES	O3S-S-C8	2.08	110.07	106.00
7	A	1003[A]	J2G	OAP-SAG-CAF	-2.05	104.29	107.68
7	A	1003[B]	J2G	CBB-CBA-NAZ	2.05	114.94	111.06
7	A	1003[A]	J2G	OAY-CAV-CAN	-2.03	116.12	121.46

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	MES	C7-C8-S-O2S
6	A	1002	MES	C7-C8-S-O3S
7	A	1003[A]	J2G	CAE-CAF-SAG-NAH
7	A	1003[A]	J2G	CAE-CAF-SAG-OAC
7	A	1003[A]	J2G	CAE-CAF-SAG-OAP
7	A	1003[B]	J2G	CAF-CAE-OAB-CAA
7	A	1003[B]	J2G	CAE-CAF-SAG-NAH
7	A	1003[B]	J2G	CAE-CAF-SAG-OAP
7	A	1003[B]	J2G	CAM-CAN-CAV-OAW
7	A	1003[B]	J2G	CAI-NAH-SAG-CAF
7	B	1003[A]	J2G	CAE-CAF-SAG-NAH
7	B	1003[A]	J2G	CAE-CAF-SAG-OAC
7	B	1003[A]	J2G	CAE-CAF-SAG-OAP
7	B	1003[B]	J2G	CAF-CAE-OAB-CAA
7	B	1003[B]	J2G	CAE-CAF-SAG-NAH
7	B	1003[B]	J2G	CAE-CAF-SAG-OAP
7	B	1003[B]	J2G	CAM-CAN-CAV-OAW
7	A	1003[B]	J2G	CAO-CAN-CAV-OAY
7	B	1003[B]	J2G	CAO-CAN-CAV-OAY
7	A	1003[A]	J2G	CAO-CAN-CAV-OAW

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Mol	Chain	Res	Type	Atoms
7	A	1003[B]	J2G	CAO-CAN-CAV-OAW
7	B	1003[A]	J2G	CAO-CAN-CAV-OAW
7	B	1003[B]	J2G	CAO-CAN-CAV-OAW
7	A	1003[A]	J2G	CAM-CAN-CAV-OAY
7	A	1003[A]	J2G	CAO-CAN-CAV-OAY
7	A	1003[B]	J2G	CAM-CAN-CAV-OAY
7	B	1003[A]	J2G	CAM-CAN-CAV-OAY
7	B	1003[A]	J2G	CAO-CAN-CAV-OAY
7	B	1003[B]	J2G	CAM-CAN-CAV-OAY
7	B	1003[A]	J2G	CAM-CAN-CAV-OAW
7	A	1003[A]	J2G	CAM-CAN-CAV-OAW
7	A	1003[A]	J2G	CAI-NAH-SAG-OAC
7	A	1003[B]	J2G	CAI-NAH-SAG-OAP
7	B	1003[A]	J2G	CAI-NAH-SAG-OAC
7	B	1003[B]	J2G	CAI-NAH-SAG-OAP
7	A	1003[A]	J2G	CAI-NAH-SAG-CAF
7	B	1003[A]	J2G	CAI-NAH-SAG-CAF
7	B	1003[B]	J2G	CAI-NAH-SAG-CAF
9	A	1006	NAG	O5-C5-C6-O6
9	A	1005	NAG	O5-C5-C6-O6
9	A	1006	NAG	C4-C5-C6-O6
11	A	1011	PGE	O2-C3-C4-O3
7	A	1003[B]	J2G	CAO-CAF-SAG-OAP
7	B	1003[B]	J2G	CAO-CAF-SAG-OAP
9	B	1007	NAG	C8-C7-N2-C2
9	B	1007	NAG	O7-C7-N2-C2
8	A	1004	LYS	OXT-C-CA-N
8	B	1004	LYS	OXT-C-CA-N
9	B	1006	NAG	O5-C5-C6-O6
7	A	1003[B]	J2G	CAD-CAE-OAB-CAA
9	B	1005	NAG	C4-C5-C6-O6
7	B	1003[B]	J2G	CAD-CAE-OAB-CAA
7	A	1003[B]	J2G	CAO-CAF-SAG-NAH
7	B	1003[B]	J2G	CAO-CAF-SAG-NAH
9	A	1005	NAG	C4-C5-C6-O6
7	B	1003[A]	J2G	CAF-CAE-OAB-CAA
9	B	1005	NAG	O5-C5-C6-O6
7	A	1003[A]	J2G	CAF-CAE-OAB-CAA
7	A	1003[B]	J2G	CAE-CAF-SAG-OAC
7	B	1003[B]	J2G	CAE-CAF-SAG-OAC
7	A	1003[A]	J2G	CAO-CAF-SAG-OAP
7	B	1003[A]	J2G	CAO-CAF-SAG-OAC

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Mol	Chain	Res	Type	Atoms
7	B	1003[A]	J2G	CAO-CAF-SAG-OAP
7	A	1003[A]	J2G	CAR-CAQ-NAZ-CBC
7	B	1003[A]	J2G	CAR-CAQ-NAZ-CBC
9	B	1007	NAG	C4-C5-C6-O6
8	A	1004	LYS	O-C-CA-CB
8	A	1004	LYS	OXT-C-CA-CB
8	B	1004	LYS	O-C-CA-CB
8	B	1004	LYS	OXT-C-CA-CB
7	A	1003[A]	J2G	CAO-CAF-SAG-OAC
7	A	1003[A]	J2G	CAR-CAQ-NAZ-CBA
7	B	1003[A]	J2G	CAR-CAQ-NAZ-CBA
8	A	1004	LYS	O-C-CA-N
8	B	1004	LYS	O-C-CA-N
6	A	1002	MES	C7-C8-S-O1S
11	A	1011	PGE	C1-C2-O2-C3
8	A	1009	LYS	OXT-C-CA-CB
7	B	1003[A]	J2G	CAD-CAE-OAB-CAA
7	A	1003[A]	J2G	CAD-CAE-OAB-CAA
8	B	1010	LYS	O-C-CA-CB
8	B	1010	LYS	OXT-C-CA-CB
7	B	1003[A]	J2G	CAO-CAF-SAG-NAH
7	A	1003[A]	J2G	CAO-CAF-SAG-NAH
9	A	1007	NAG	C4-C5-C6-O6
9	B	1007	NAG	O5-C5-C6-O6
8	A	1009	LYS	O-C-CA-CB
7	A	1003[A]	J2G	CAI-CAQ-NAZ-CBC
7	B	1003[A]	J2G	CAI-CAQ-NAZ-CBC
7	A	1003[A]	J2G	CAI-CAQ-NAZ-CBA
9	A	1007	NAG	O5-C5-C6-O6
11	A	1011	PGE	C3-C4-O3-C5

There are no ring outliers.

8 monomers are involved in 13 short contacts:

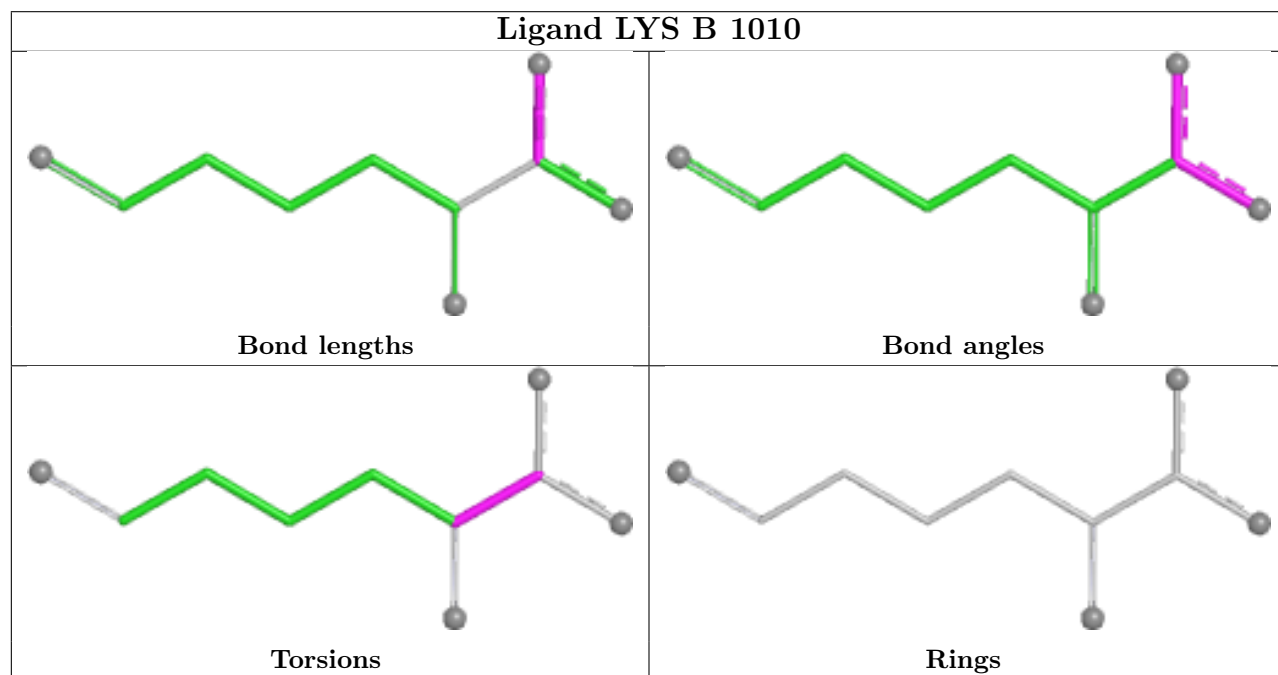
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1002	MES	2	0
11	A	1011	PGE	2	0
8	A	1004	LYS	1	0
10	B	1008	IMD	2	0
8	B	1004	LYS	2	0
8	A	1009	LYS	1	0
7	A	1003[B]	J2G	1	0

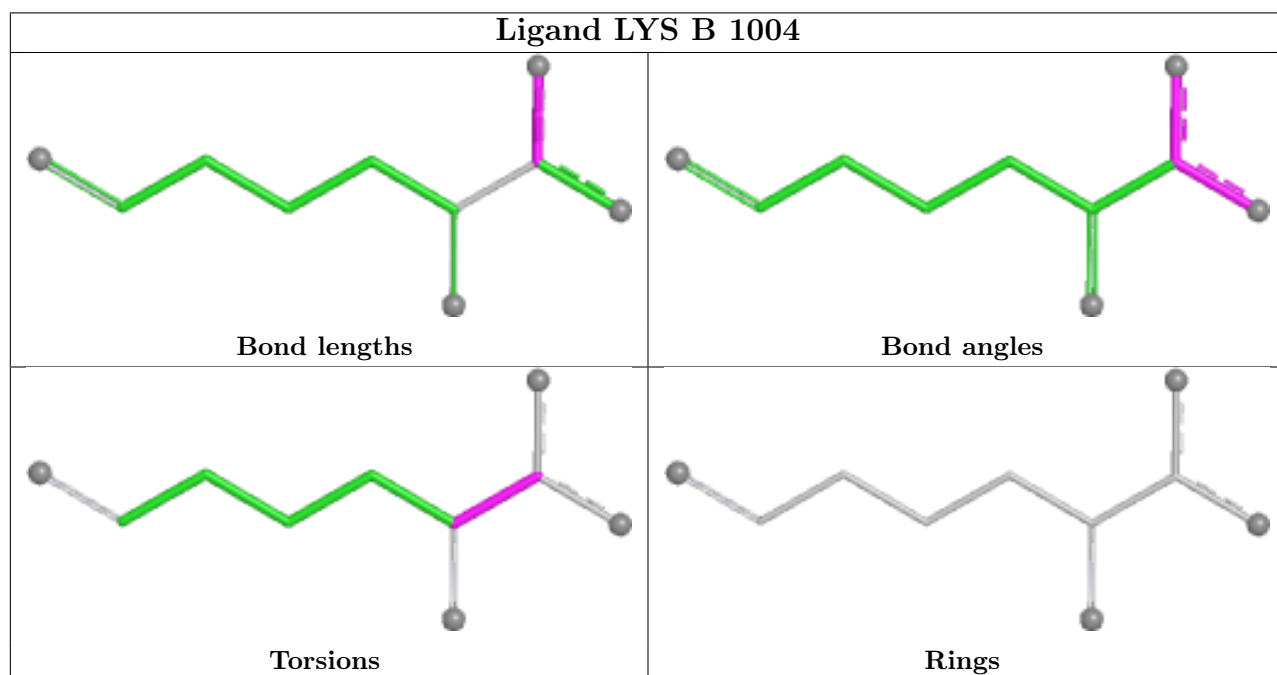
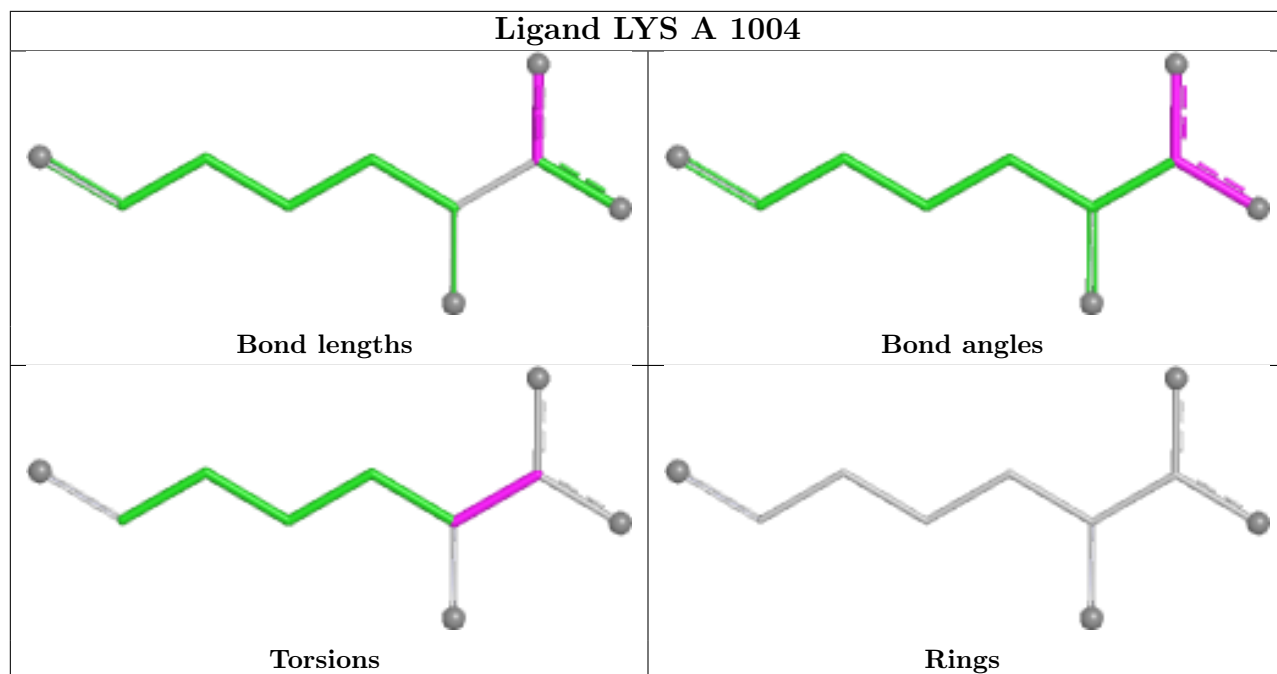
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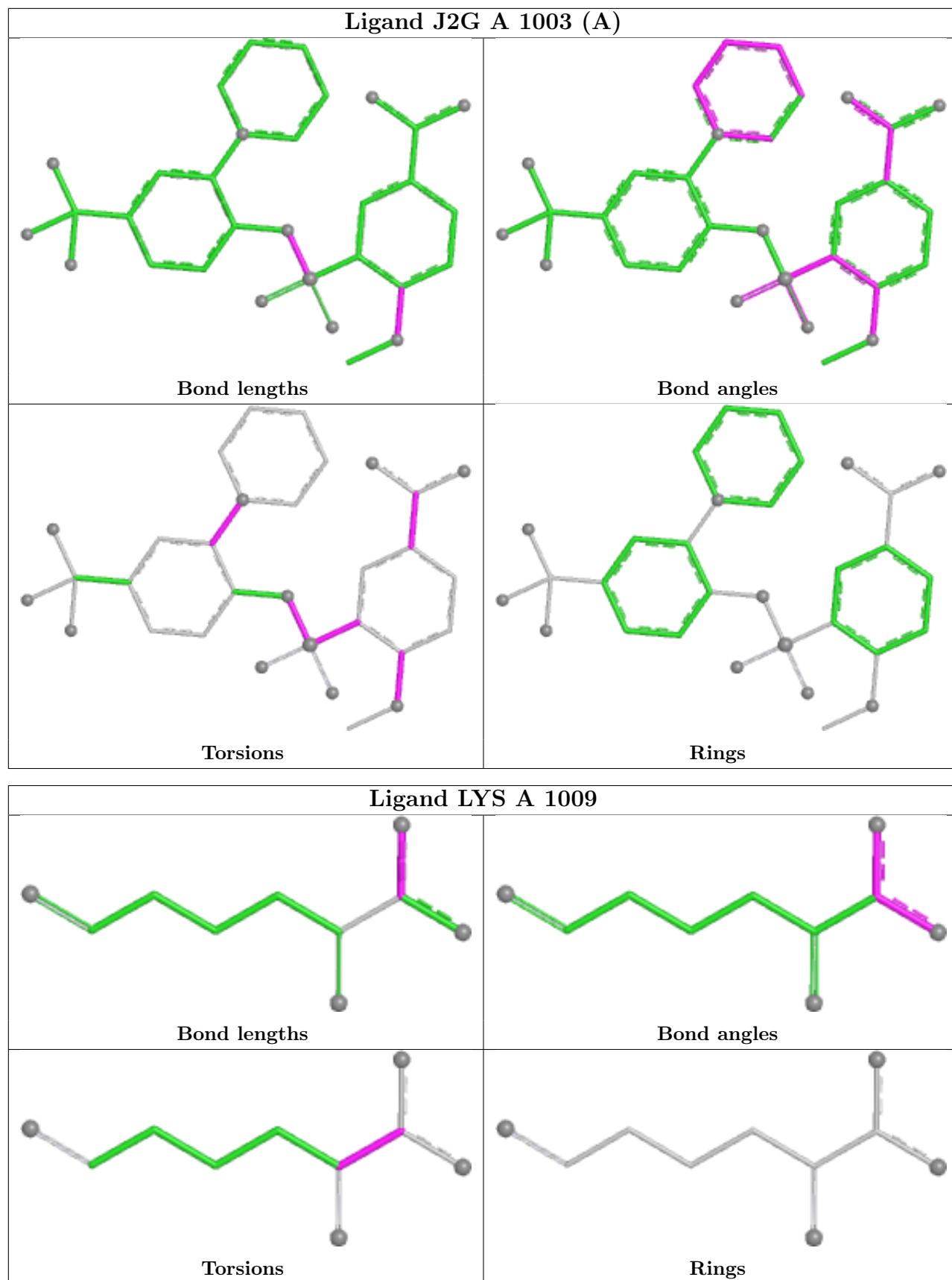
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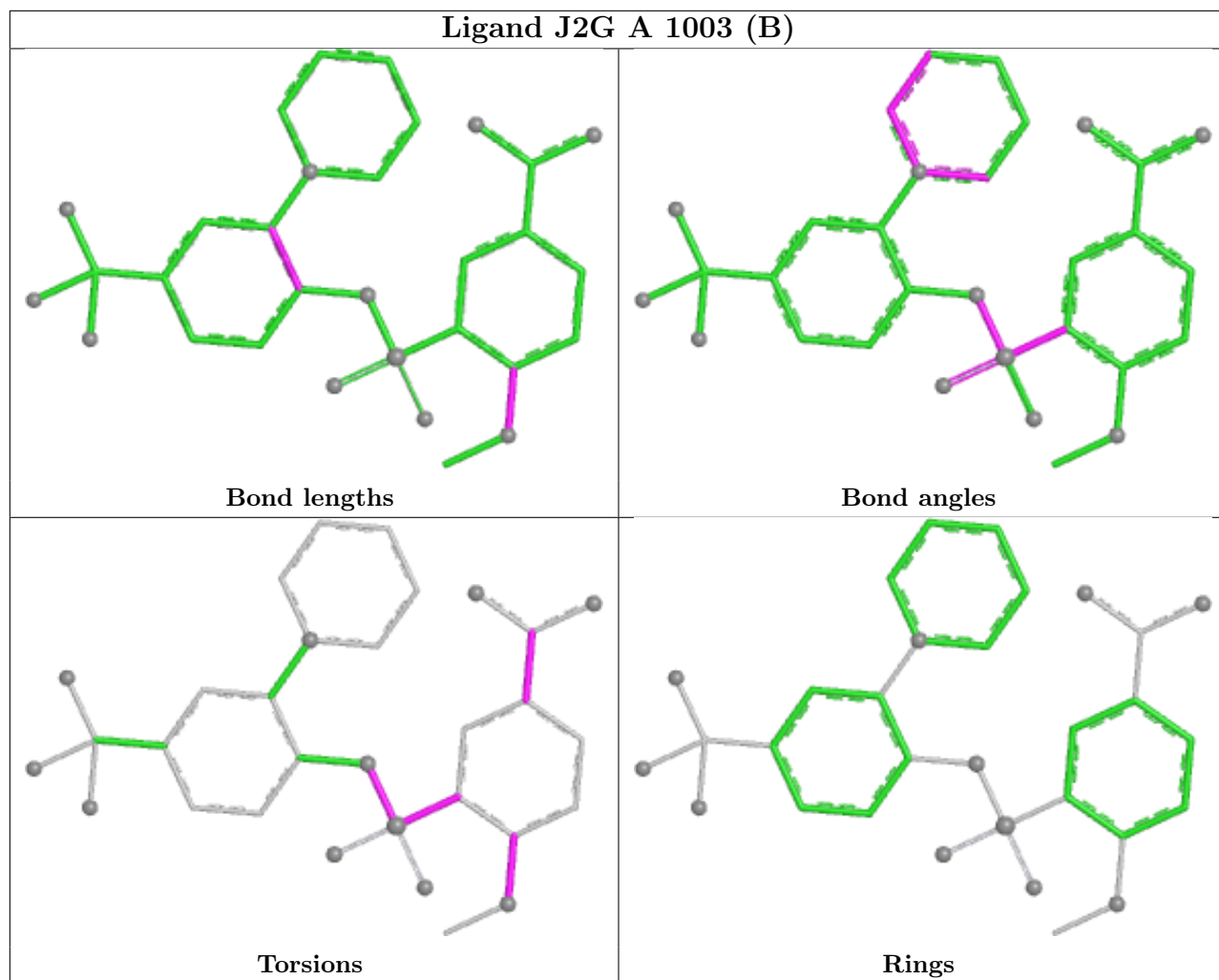
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	MES	3	0

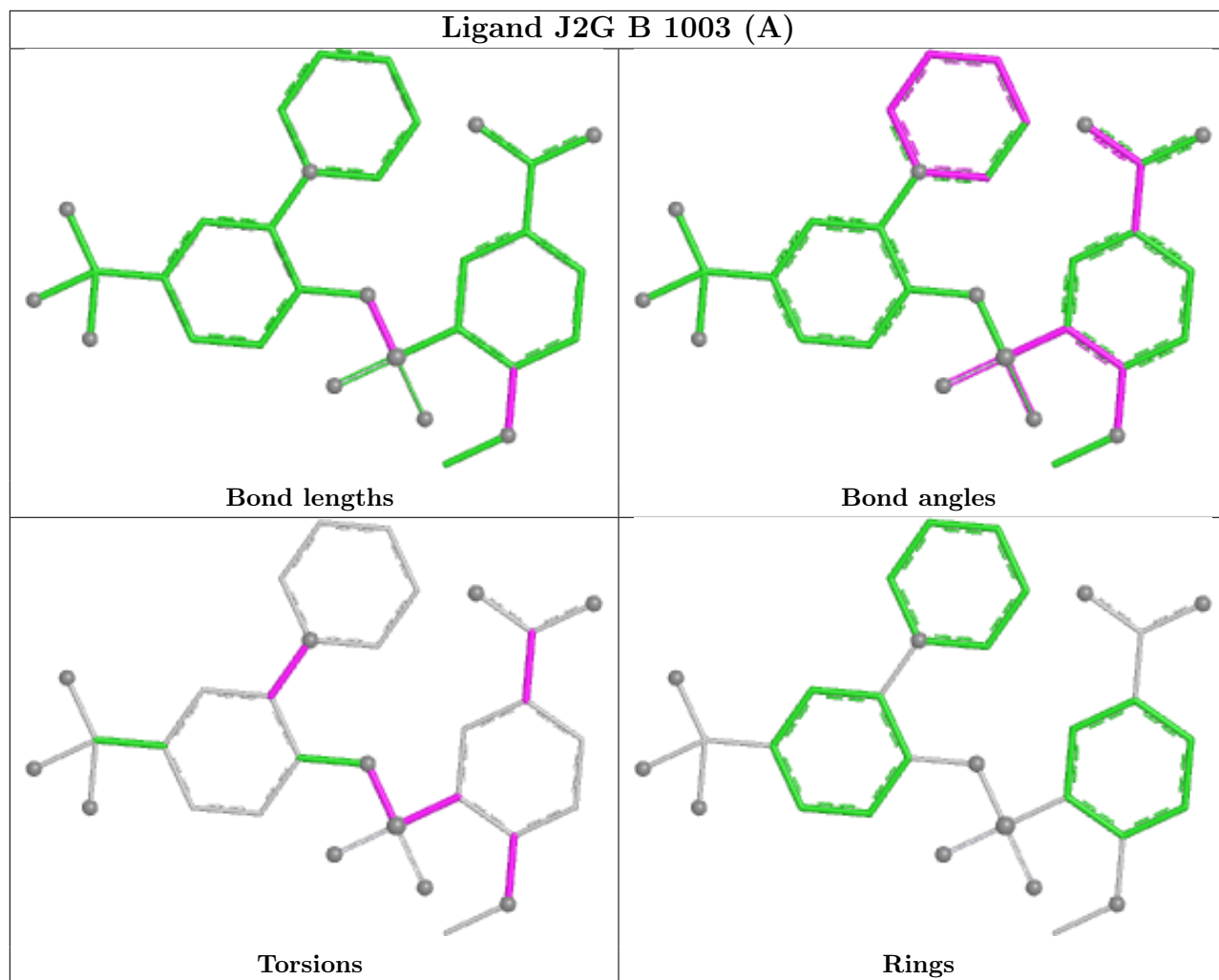
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

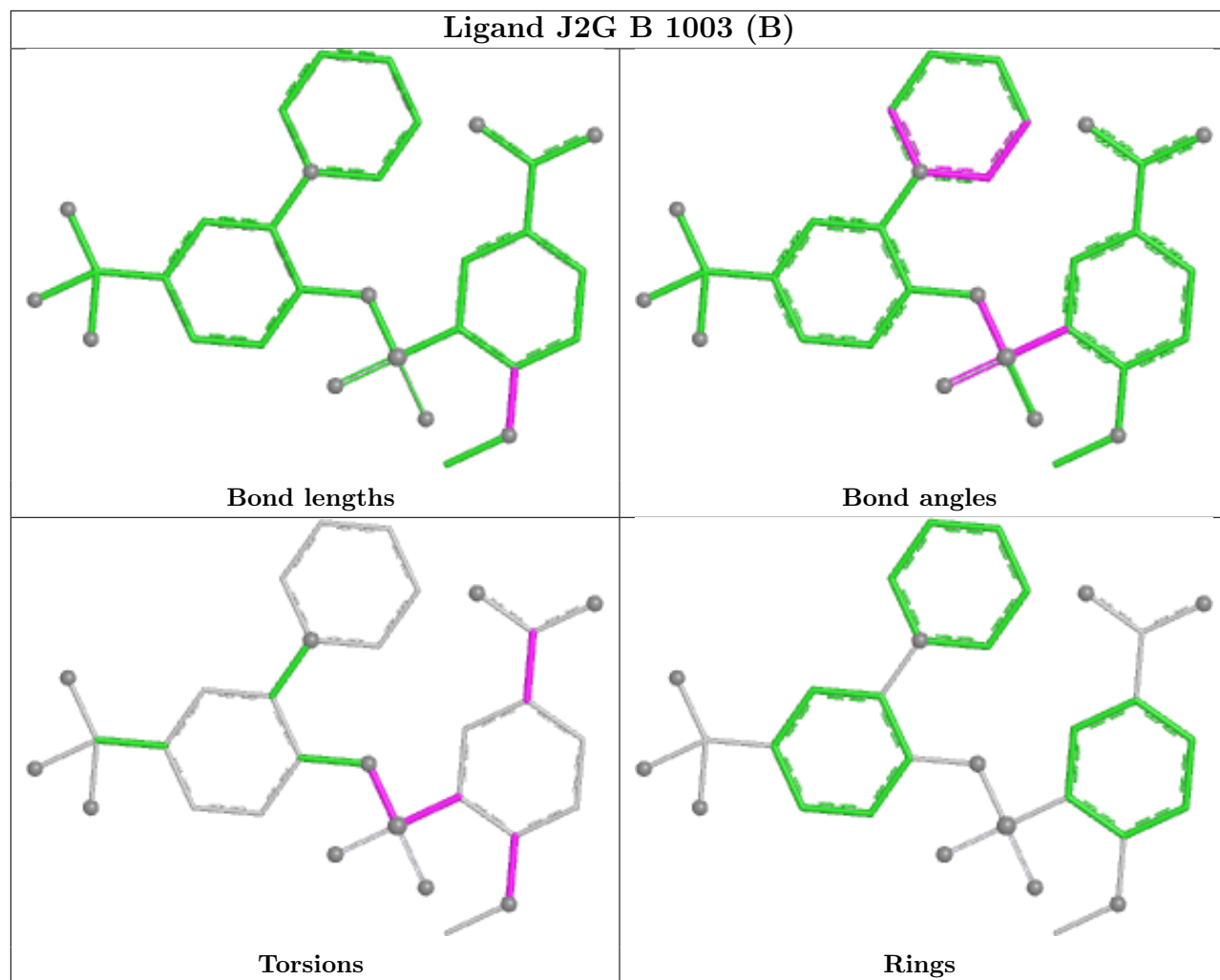












5.7 Other polymers [i](#)

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	883/911 (96%)	0.06	12 (1%) 73 75	28, 59, 95, 142	7 (0%)
1	B	869/911 (95%)	0.81	75 (8%) 16 14	42, 98, 158, 198	2 (0%)
All	All	1752/1822 (96%)	0.43	87 (4%) 34 32	28, 73, 144, 198	9 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	783	LYS	5.8
1	A	531	ASN	4.5
1	B	578	ARG	4.4
1	A	963	HIS	4.4
1	A	784	LEU	3.9
1	A	530	GLU	3.8
1	B	594	THR	3.7
1	B	401	LEU	3.6
1	B	534	VAL	3.4
1	B	647	LEU	3.4
1	B	600	ILE	3.3
1	B	279	SER	3.3
1	B	54	PRO	3.3
1	B	745	VAL	3.2
1	B	638	HIS	3.1
1	B	215	LEU	3.1
1	B	584	TYR	3.1
1	B	313	TYR	3.0
1	B	869	GLN	3.0
1	B	396	ALA	3.0
1	B	579	ALA	3.0
1	B	609	THR	2.9
1	B	430	LEU	2.9
1	B	633	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	580	LEU	2.9
1	A	53	PHE	2.9
1	B	635	TYR	2.9
1	A	596	SER	2.8
1	B	604	ILE	2.8
1	B	576	GLU	2.8
1	B	55	VAL	2.7
1	B	784	LEU	2.7
1	B	613	ASP	2.7
1	B	128	SER	2.7
1	B	436	ILE	2.6
1	B	575	PRO	2.6
1	B	868	GLY	2.6
1	B	162	TYR	2.6
1	A	782	GLY	2.6
1	B	960	THR	2.5
1	A	333	PRO	2.5
1	B	577	TRP	2.5
1	B	473	LYS	2.5
1	B	398	TYR	2.5
1	B	621	VAL	2.4
1	A	332	ALA	2.4
1	B	619	SER	2.4
1	B	439	PRO	2.3
1	B	570	VAL	2.3
1	B	552	VAL	2.3
1	B	598	ASN	2.3
1	B	625	VAL	2.3
1	B	392	ASN	2.2
1	B	557	CYS	2.3
1	B	589	PRO	2.3
1	B	562	GLN	2.2
1	B	618	THR	2.2
1	B	652	THR	2.2
1	B	543	LEU	2.2
1	B	620	TRP	2.2
1	B	501	ASN	2.2
1	B	106	GLN	2.2
1	B	949	LEU	2.2
1	B	781	SER	2.1
1	B	959	ASN	2.1
1	B	391	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	550	LEU	2.1
1	B	663	ILE	2.1
1	B	245	GLU	2.1
1	A	783	LYS	2.1
1	B	742	LYS	2.1
1	B	69	LEU	2.1
1	B	461	ILE	2.1
1	B	62	PHE	2.1
1	B	309	PHE	2.1
1	B	485	PHE	2.1
1	B	640	TRP	2.1
1	B	588	ILE	2.1
1	B	702	TYR	2.1
1	B	623	PHE	2.0
1	A	785	ASN	2.0
1	B	612	LEU	2.0
1	B	780	SER	2.0
1	A	962	HIS	2.0
1	B	602	ARG	2.0
1	B	490	ALA	2.0
1	B	648	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

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

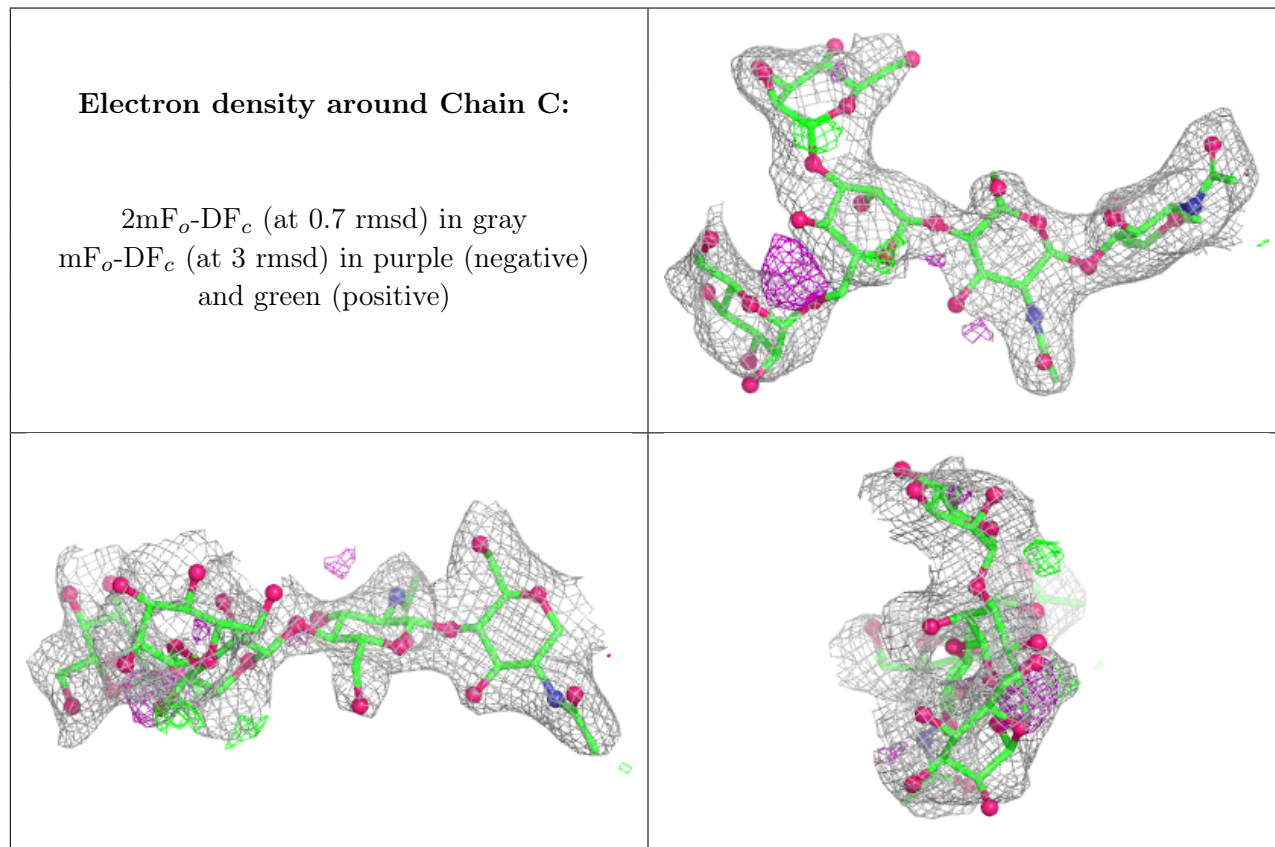
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	D	4	11/12	0.43	0.16	141,143,147,148	0
2	BMA	D	3	11/12	0.47	0.15	114,120,135,140	0
2	BMA	G	3	11/12	0.52	0.16	104,109,118,123	0
4	BMA	H	3	11/12	0.52	0.14	136,139,143,143	0
2	MAN	G	5	11/12	0.53	0.18	72,96,106,108	0
2	MAN	C	4	11/12	0.54	0.12	124,128,132,134	0
2	MAN	C	5	11/12	0.55	0.14	98,112,119,121	0

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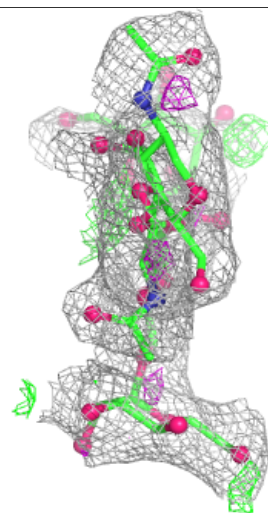
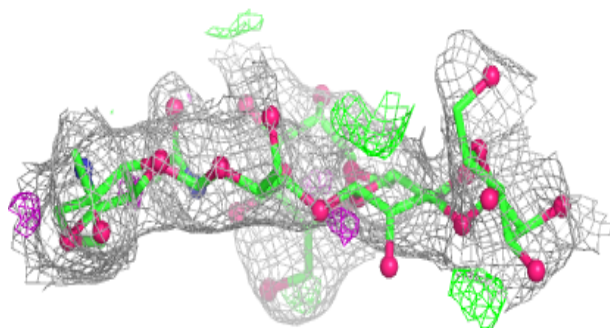
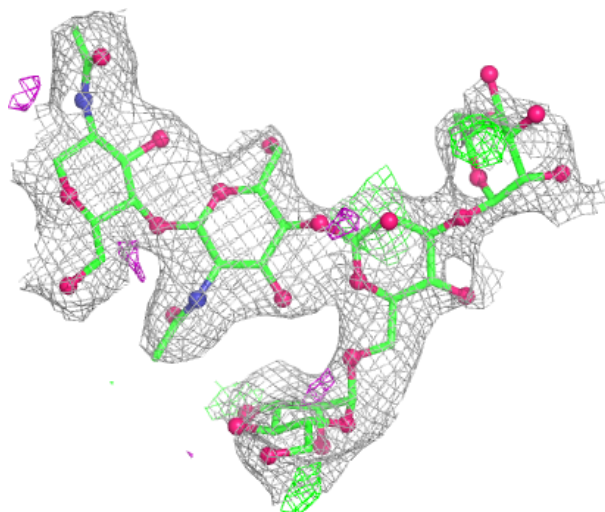
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	G	4	11/12	0.57	0.11	129,132,135,136	0
2	MAN	D	5	11/12	0.60	0.16	91,103,112,112	0
2	BMA	C	3	11/12	0.61	0.14	114,117,123,128	0
3	NAG	I	2	14/15	0.66	0.15	135,142,143,143	0
3	NAG	F	2	14/15	0.66	0.12	122,136,140,141	0
3	NAG	E	2	14/15	0.68	0.15	106,117,121,121	0
4	NAG	H	2	14/15	0.69	0.13	113,121,126,132	0
3	NAG	I	1	14/15	0.70	0.17	112,125,134,139	0
4	NAG	H	1	14/15	0.71	0.15	89,100,111,114	0
3	NAG	F	1	14/15	0.72	0.14	96,105,123,130	0
2	NAG	C	2	14/15	0.83	0.13	68,86,99,102	0
3	NAG	E	1	14/15	0.83	0.11	71,87,102,111	0
2	NAG	G	2	14/15	0.84	0.12	63,80,93,100	0
2	NAG	D	2	14/15	0.88	0.11	65,76,89,108	0
2	NAG	G	1	14/15	0.91	0.09	52,63,73,83	0
2	NAG	C	1	14/15	0.92	0.08	53,64,76,78	0
2	NAG	D	1	14/15	0.94	0.07	40,57,62,62	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.



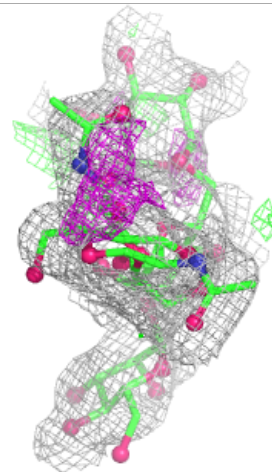
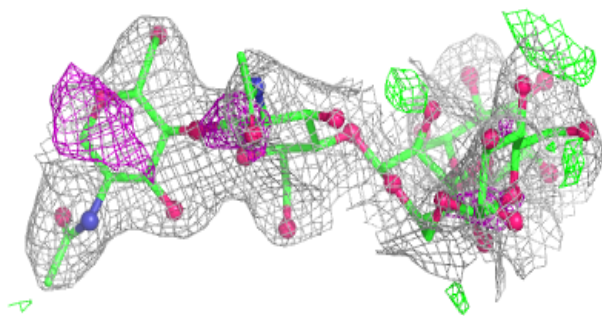
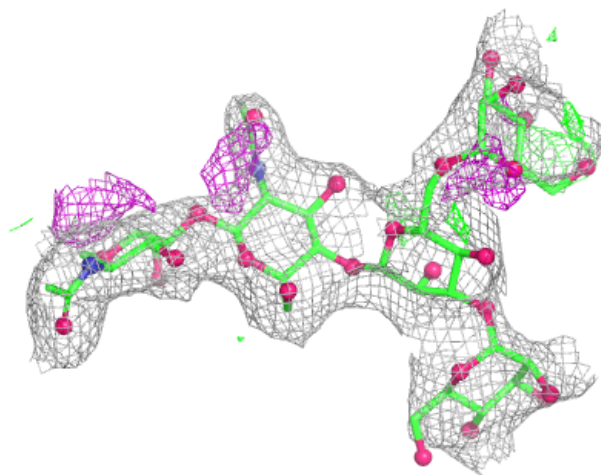
Electron density around Chain D:

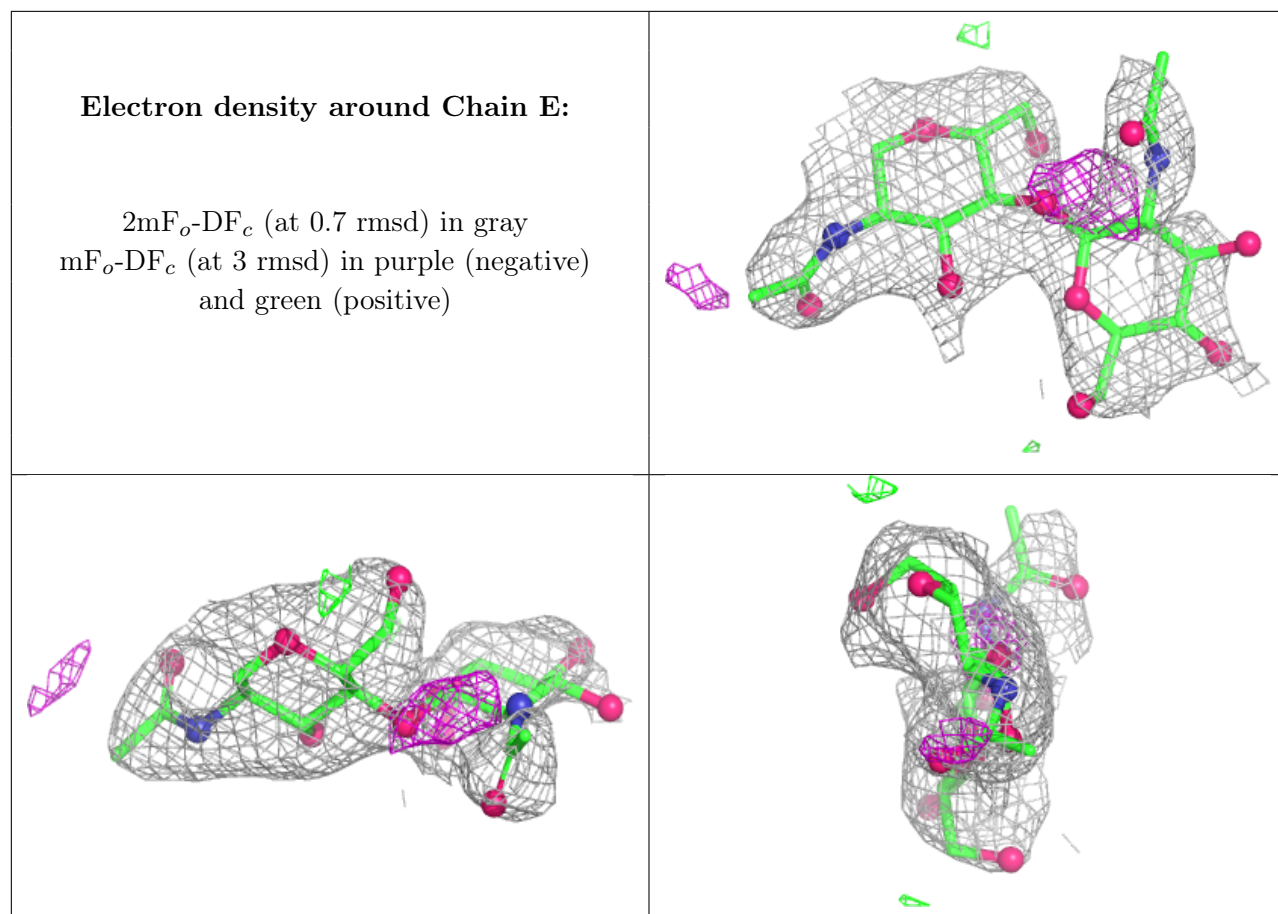
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

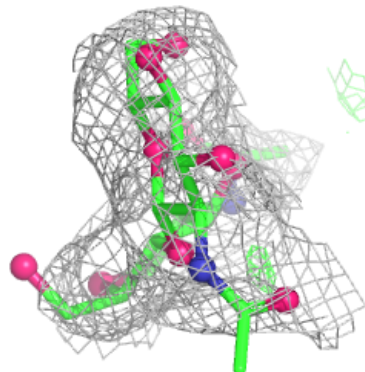
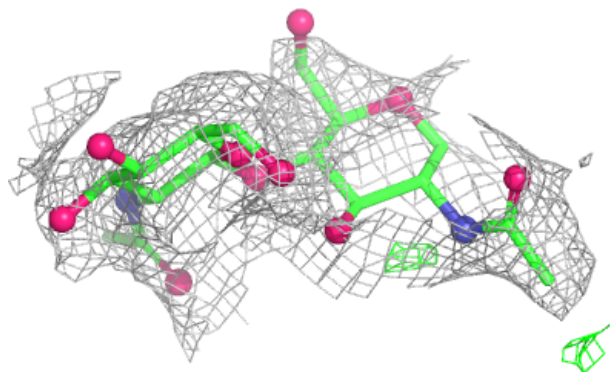
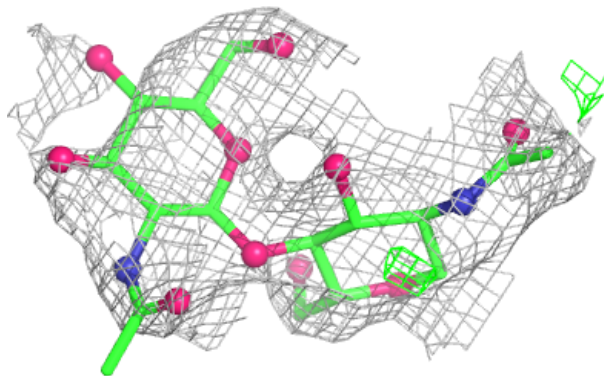
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



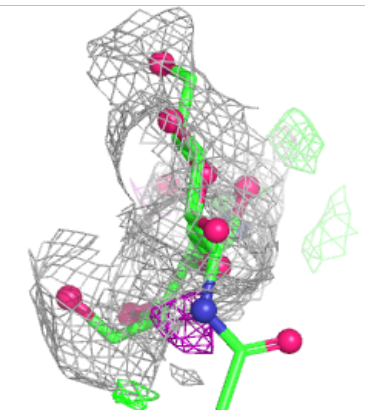
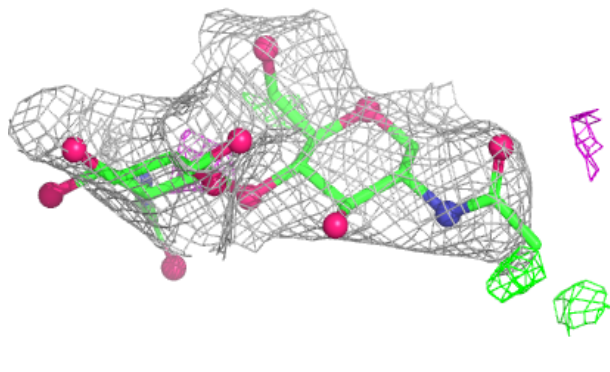
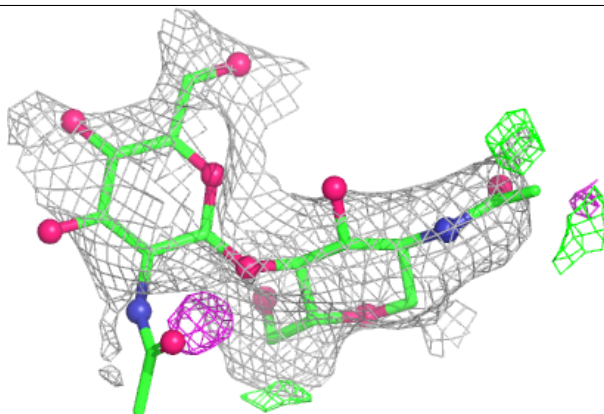


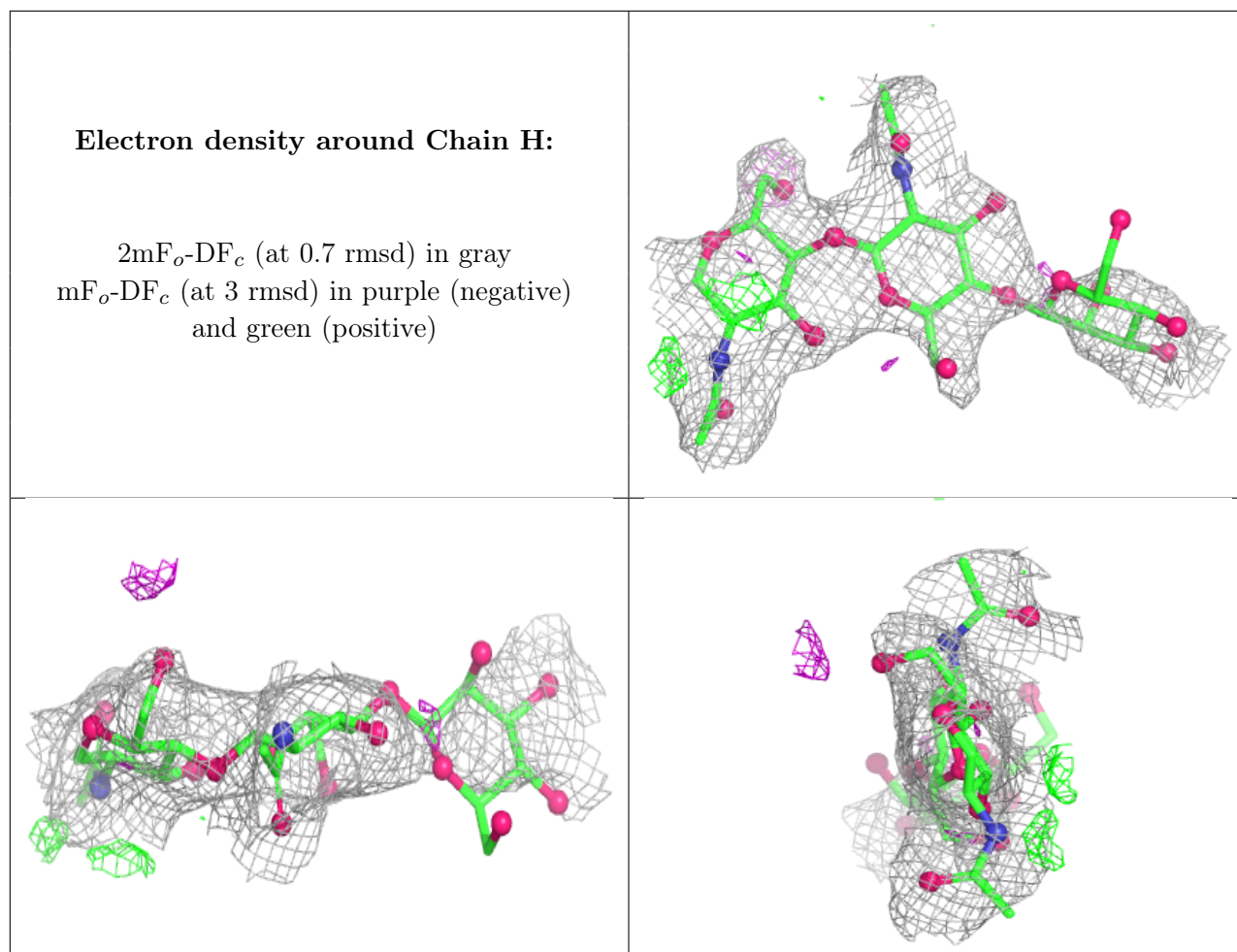
Electron density around Chain F:

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

**Electron density around Chain I:**

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





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.

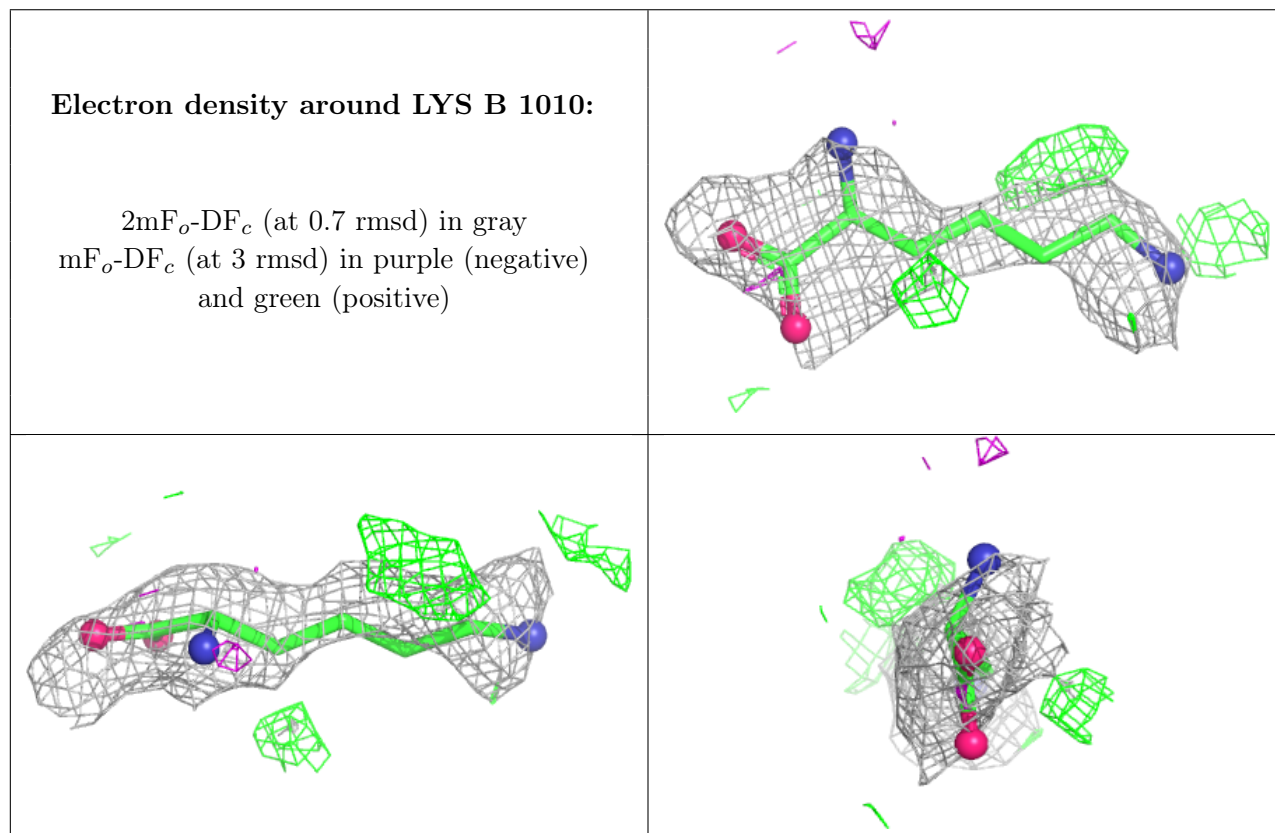
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	B	1006	14/15	0.54	0.15	169,174,181,182	0
9	NAG	B	1005	14/15	0.59	0.16	143,153,157,157	0
9	NAG	A	1008	14/15	0.61	0.15	107,127,134,144	0
9	NAG	B	1007	14/15	0.68	0.20	188,196,199,200	0
8	LYS	B	1010	10/10	0.69	0.25	83,90,93,93	10
9	NAG	A	1005	14/15	0.69	0.16	119,128,137,141	0
11	PGE	A	1011	10/10	0.69	0.18	55,66,72,82	10
9	NAG	A	1006	14/15	0.70	0.12	89,106,117,118	0
10	IMD	B	1008	5/5	0.72	0.27	95,97,103,111	5
9	NAG	A	1007	14/15	0.73	0.18	118,121,127,131	0
10	IMD	A	1010	5/5	0.74	0.25	54,59,62,64	5

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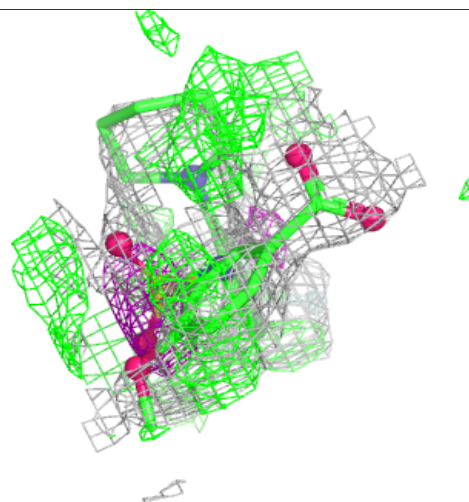
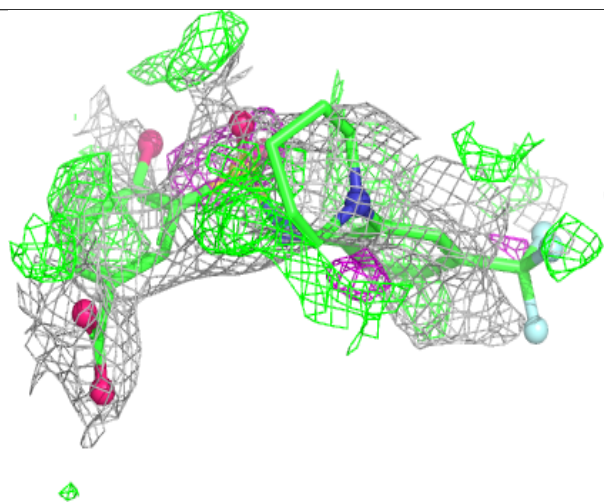
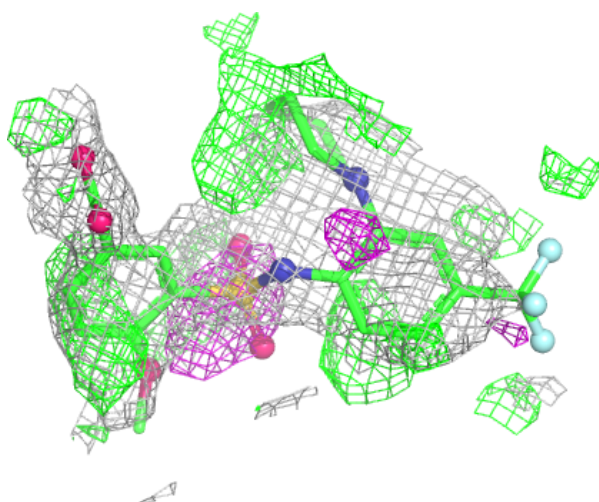
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	J2G	A	1003[B]	31/31	0.75	0.23	50,58,62,63	31
7	J2G	A	1003[A]	31/31	0.75	0.23	50,59,63,64	31
8	LYS	A	1009	10/10	0.76	0.18	63,68,71,72	10
7	J2G	B	1003[A]	31/31	0.79	0.23	81,86,89,89	31
7	J2G	B	1003[B]	31/31	0.79	0.23	81,85,88,90	31
8	LYS	B	1004	10/10	0.81	0.17	82,85,88,90	0
12	EDO	B	1009	4/4	0.85	0.26	98,103,108,112	0
6	MES	B	1002	12/12	0.86	0.18	82,87,88,100	12
6	MES	A	1002	12/12	0.89	0.16	51,58,71,81	12
12	EDO	A	1012	4/4	0.91	0.15	64,67,68,77	0
8	LYS	A	1004	10/10	0.93	0.13	49,51,61,65	0
5	ZN	B	1001	1/1	0.98	0.05	73,73,73,73	0
5	ZN	A	1001	1/1	1.00	0.04	41,41,41,41	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.



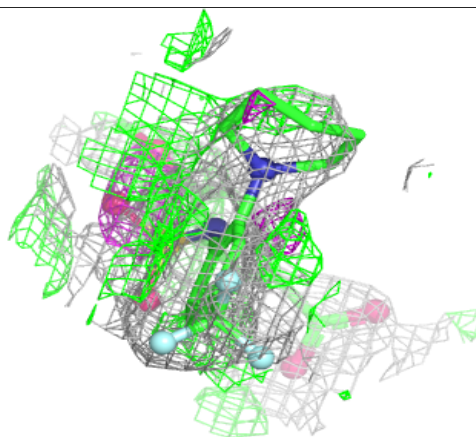
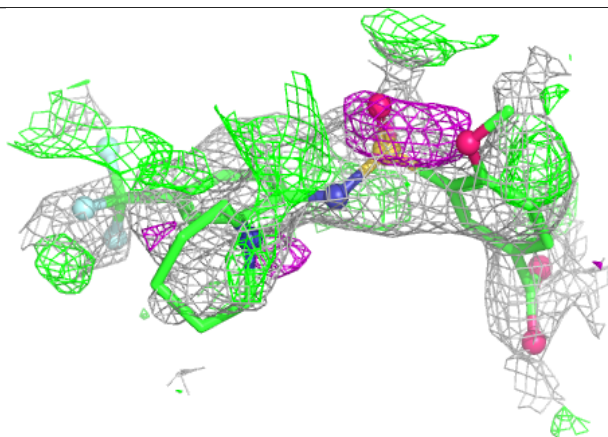
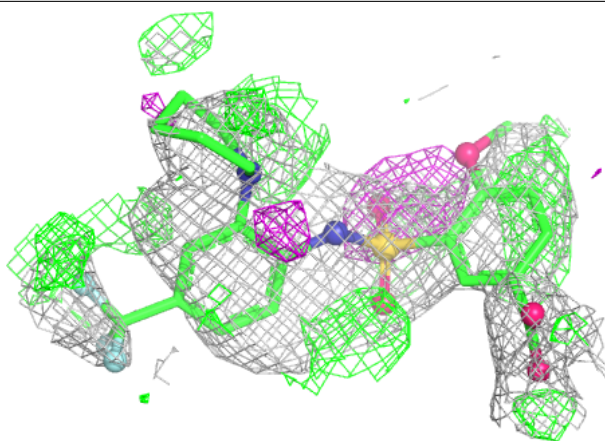
Electron density around J2G A 1003 (B):

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

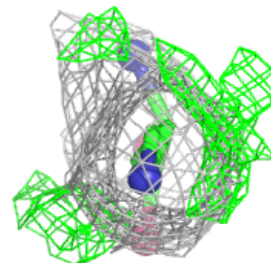
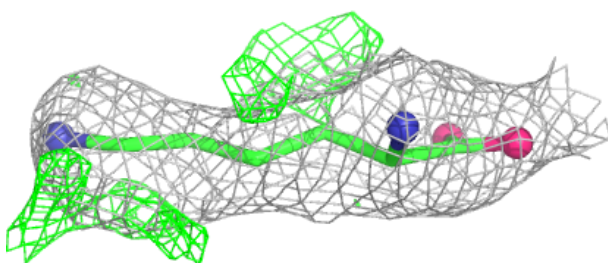
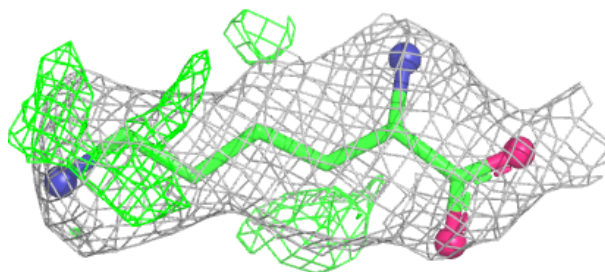


Electron density around J2G A 1003 (A):

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

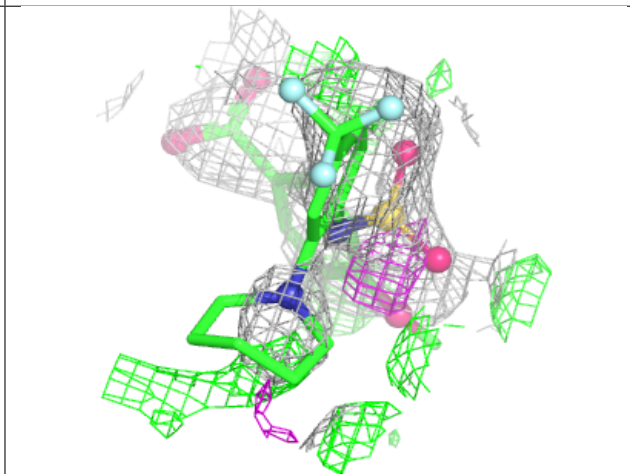
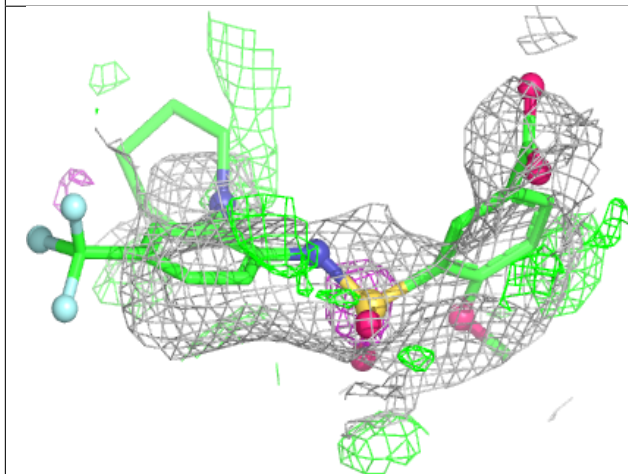
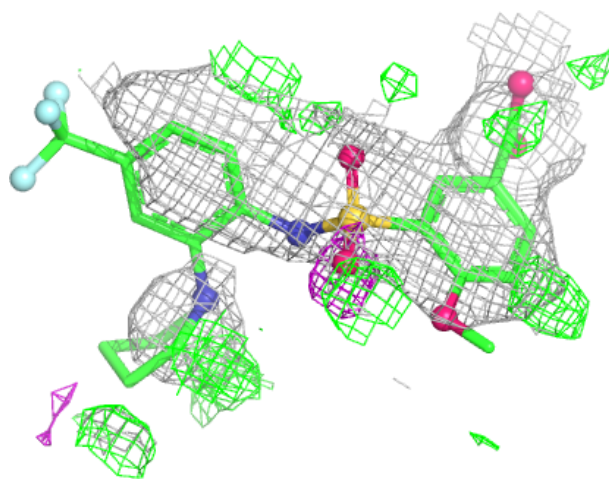
**Electron density around LYS A 1009:**

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



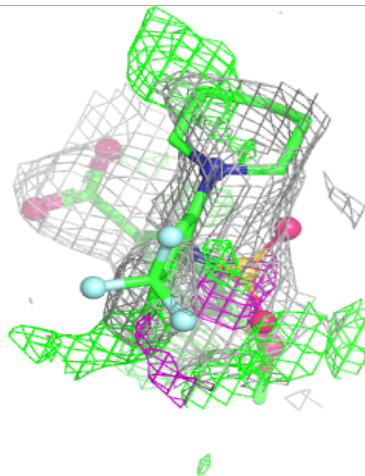
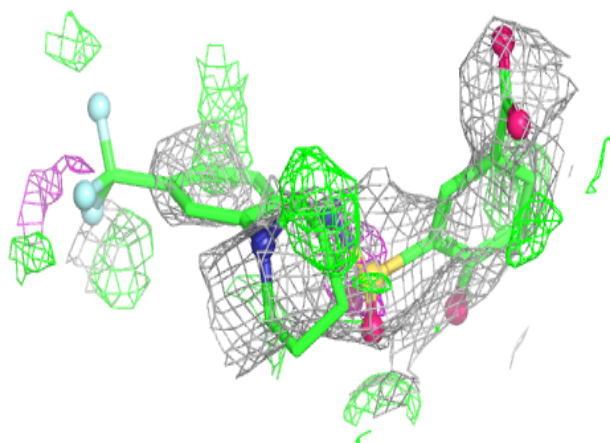
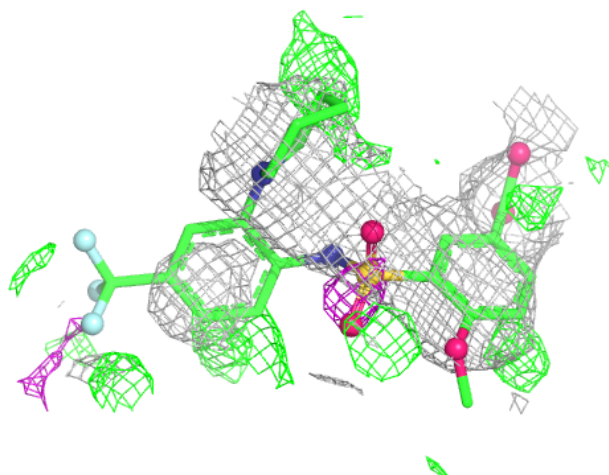
Electron density around J2G B 1003 (A):

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



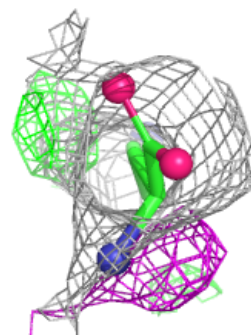
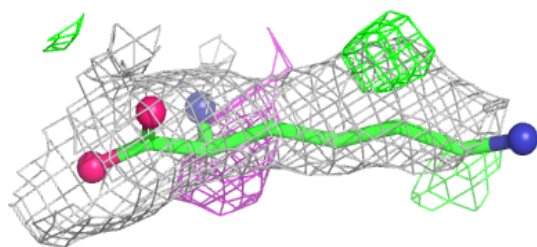
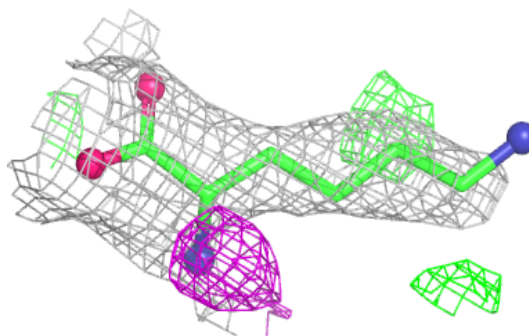
Electron density around J2G B 1003 (B):

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

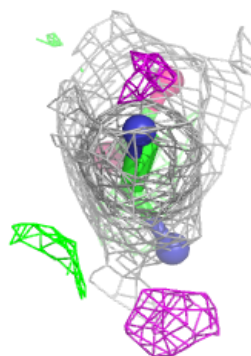
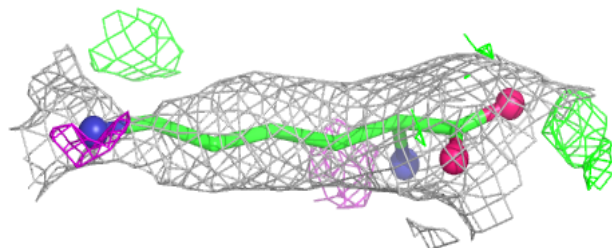
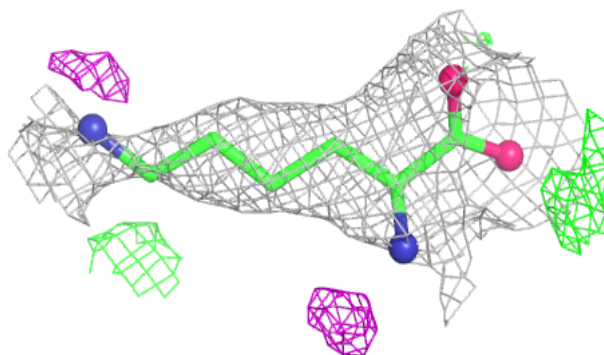


Electron density around LYS B 1004:

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

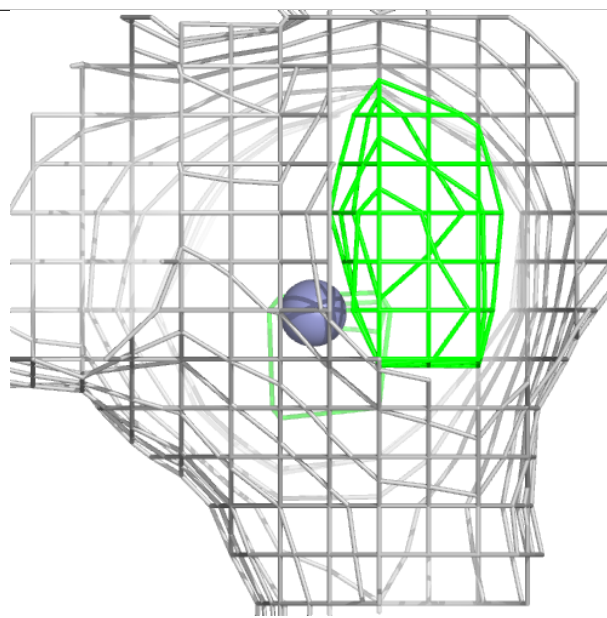
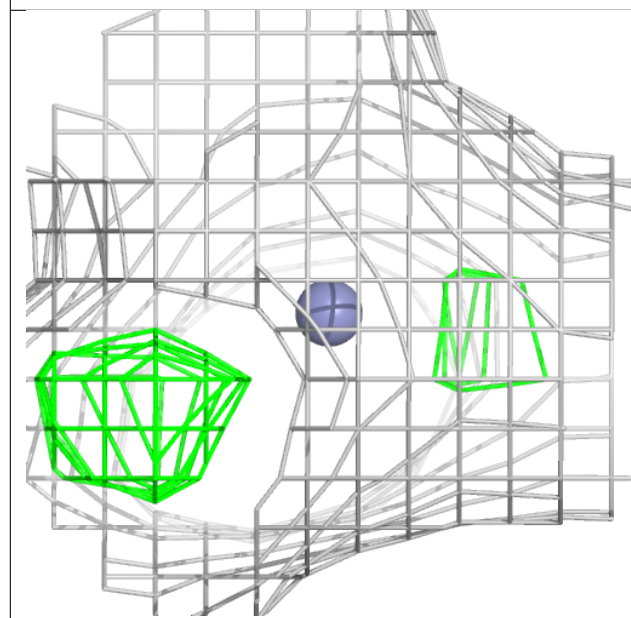
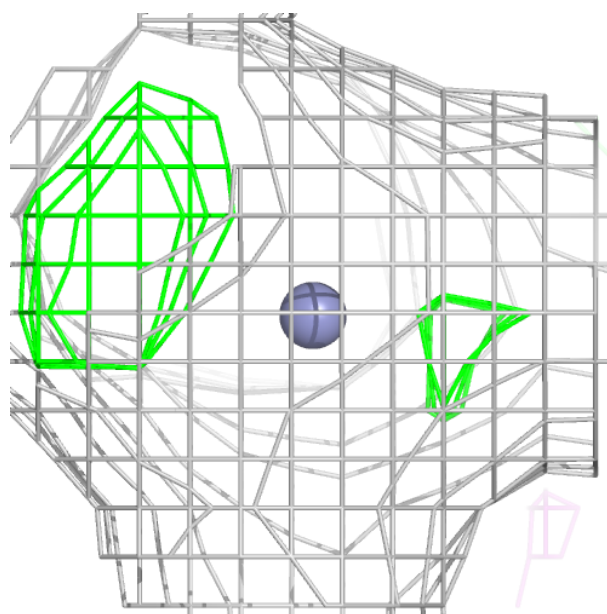
**Electron density around LYS A 1004:**

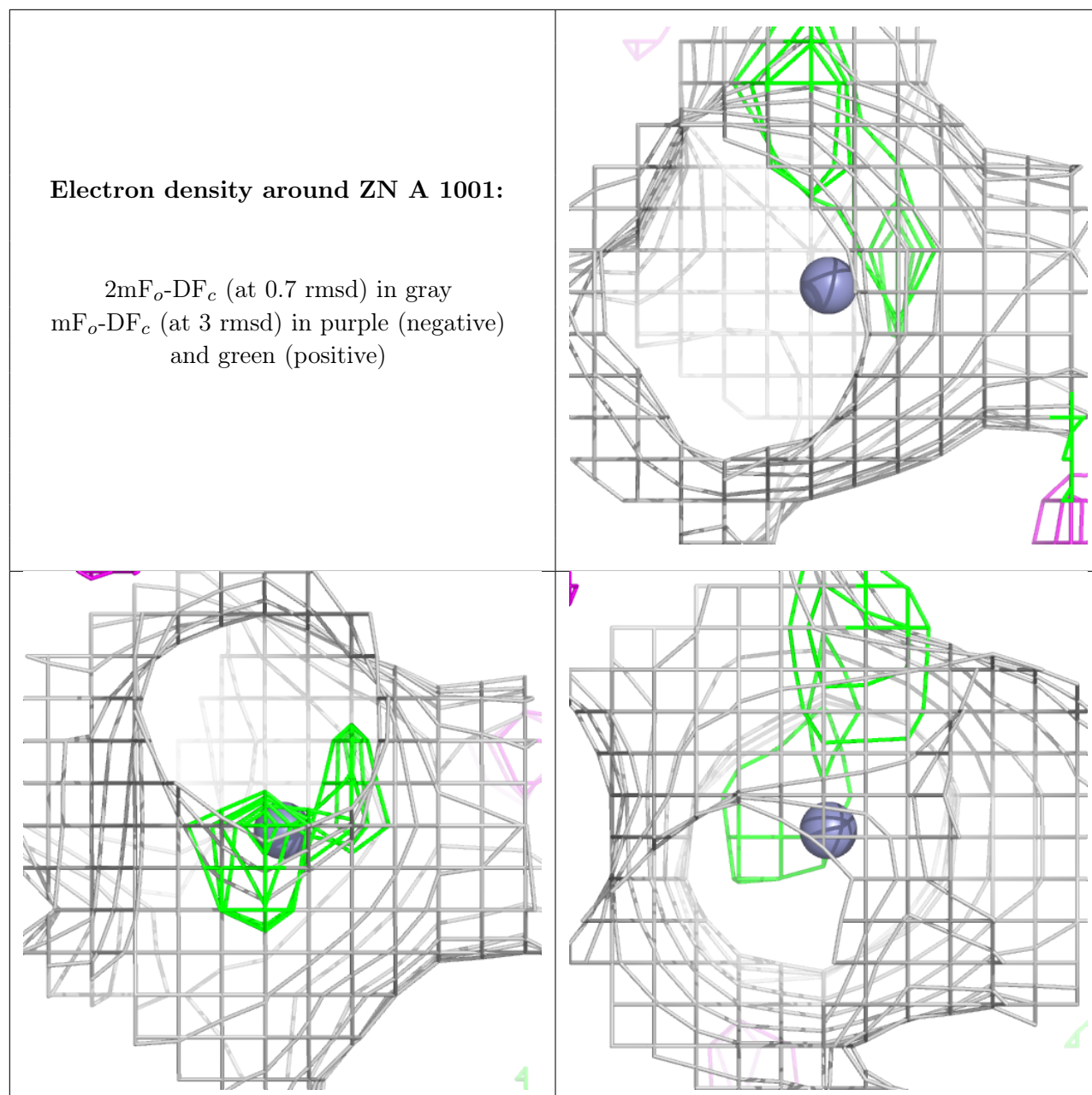
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 1001:

$2mF_o-DF_c$ (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.