



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 PM UTC

PDB ID : 6S82 / pdb_00006s82
Title : Structure Of D80A-Fructofuranosidase From Xanthophyllomyces Dendrorhous
Complexed With Tris-buffer molecule And hydroquinone
Authors : Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on : 2019-07-08
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

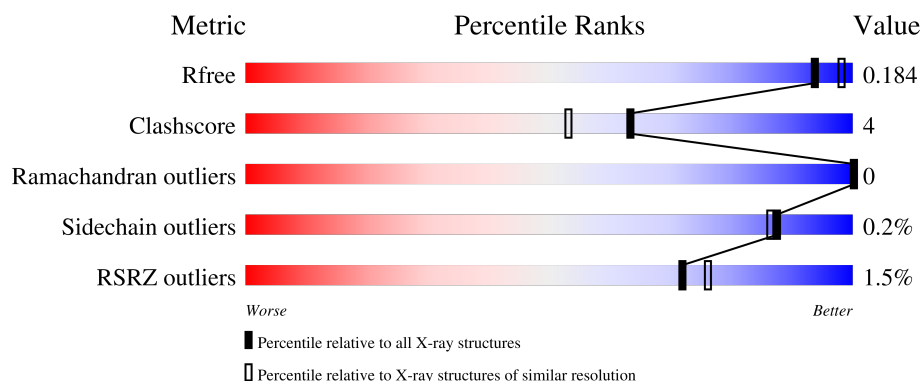
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	665	0% 87% 6% 6%
1	B	665	2% 88% 6% 6%
2	C	7	86% 14%
3	D	10	90% 10%
3	G	10	10% 90%

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	H	2	 100%
5	F	6	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TRS	A	1000	-	-	X	-
6	TRS	B	1000	-	-	X	-
8	EDO	A	1003	-	-	X	-
8	EDO	B	1003	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11911 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.

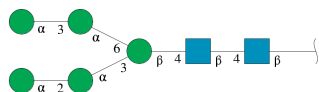
- Molecule 1 is a protein called Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			
1	B	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	ILE	conflict	UNP J7HDY4
A	663	ALA	SER	conflict	UNP J7HDY4
A	665	TYR	ARG	conflict	UNP J7HDY4
B	2	VAL	ILE	conflict	UNP J7HDY4
B	663	ALA	SER	conflict	UNP J7HDY4
B	665	TYR	ARG	conflict	UNP J7HDY4

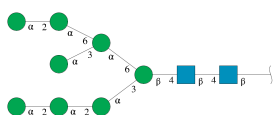
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.

ucopyranose.



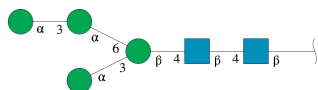
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	0	0	0
			116	64	2	50			
3	G	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 4 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
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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.



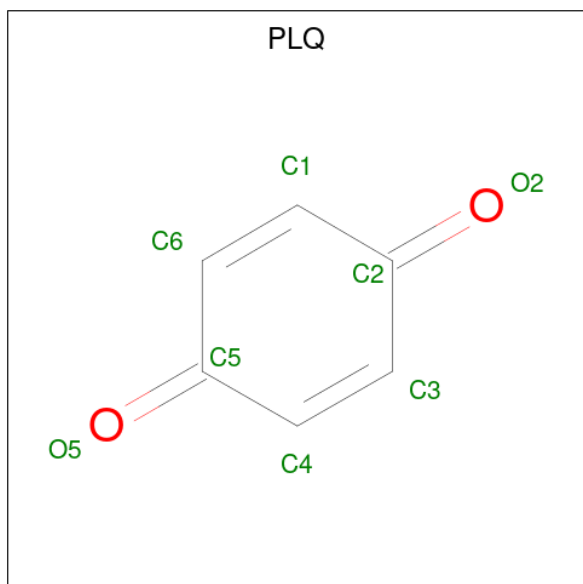
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is 1,4-benzoquinone (CCD ID: PLQ) (formula: C₆H₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

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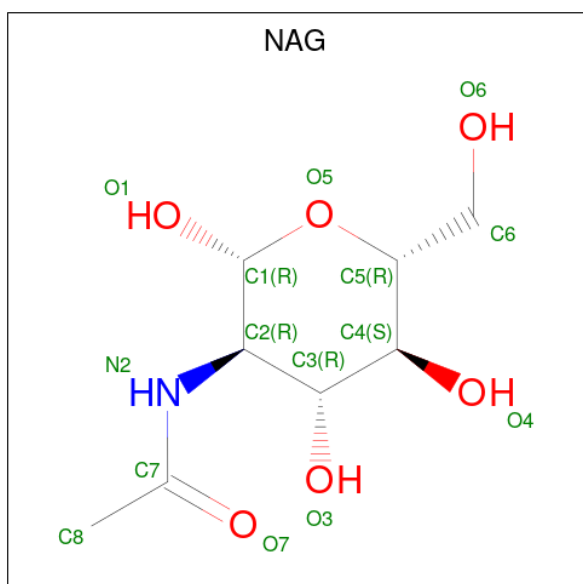
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

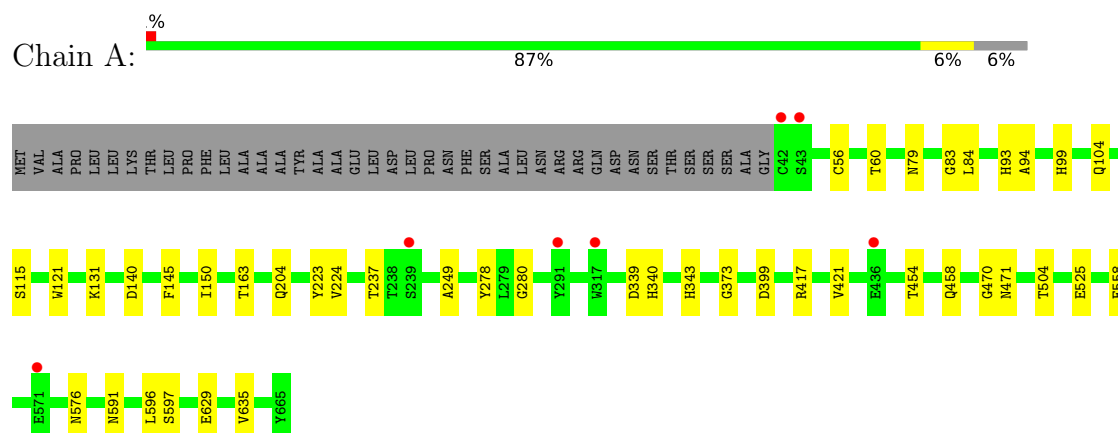
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	728	Total	O	0	0
			728	728		
10	B	620	Total	O	0	0
			620	620		

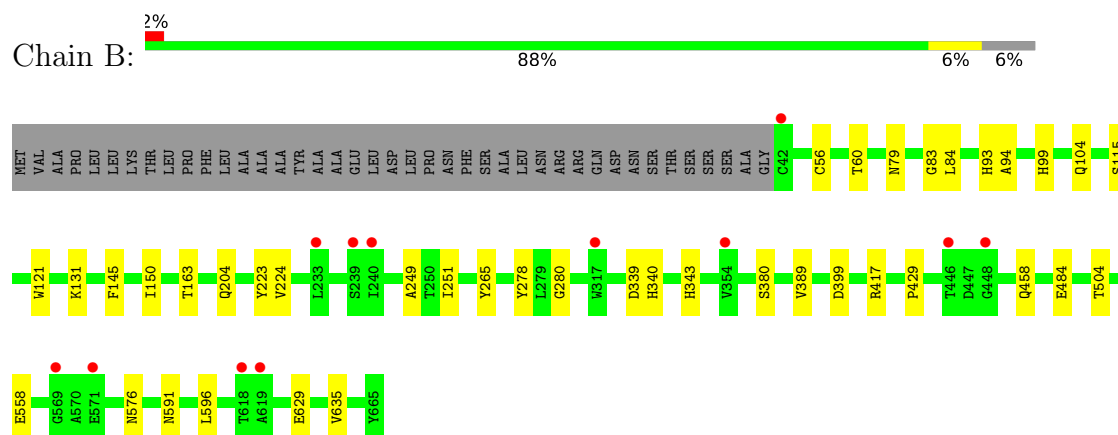
3 Residue-property plots

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.

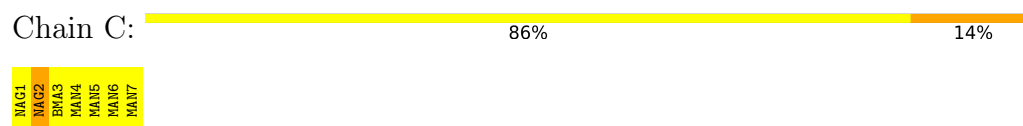
• Molecule 1: Beta-fructofuranosidase



• Molecule 1: Beta-fructofuranosidase



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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

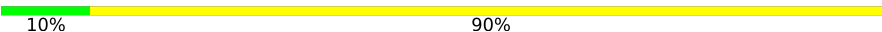


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  90% 10%

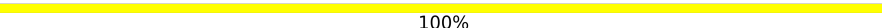
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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:  10% 90%

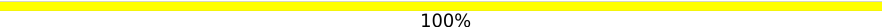
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain E:  100%

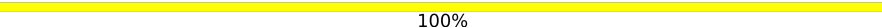
MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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 F:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 205.62Å 145.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.94 – 1.85 83.94 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.94-1.85) 99.9 (83.94-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.154 , 0.175 0.166 , 0.184	Depositor DCC
R_{free} test set	9619 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11911	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.82% 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: PLQ, NAG, EDO, BMA, MAN, TRS

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	1.03	0/4940	1.12	2/6754 (0.0%)
1	B	1.01	0/4940	1.12	1/6754 (0.0%)
All	All	1.02	0/9880	1.12	3/13508 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	79	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	140	ASP	CA-CB-CG	5.04	117.64	112.60

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	4805	0	4498	37	0
1	B	4805	0	4501	30	0
2	C	83	0	70	1	0
3	D	116	0	97	0	1
3	G	116	0	97	0	0
4	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
5	F	72	0	61	0	0
6	A	8	0	12	9	0
6	B	8	0	12	7	0
7	A	72	0	36	2	0
7	B	56	0	28	3	0
8	A	8	0	12	6	0
8	B	8	0	12	6	0
9	A	196	0	182	6	0
9	B	154	0	143	1	0
10	A	728	0	0	7	1
10	B	620	0	0	5	0
All	All	11911	0	9811	81	2

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 (81) 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)
6:B:1000:TRS:H31	8:B:1003:EDO:O1	1.56	1.04
6:A:1000:TRS:H32	8:A:1003:EDO:H21	1.62	0.80
1:A:525:GLU:H	9:A:1606:NAG:H81	1.45	0.79
7:A:1001:PLQ:H6	8:A:1002:EDO:O2	1.83	0.77
1:A:576:ASN:H	1:A:591:ASN:HD21	1.32	0.77
6:A:1000:TRS:H21	8:A:1003:EDO:C2	2.18	0.73
1:A:576:ASN:H	1:A:591:ASN:ND2	1.88	0.72
1:B:576:ASN:H	1:B:591:ASN:HD21	1.37	0.72
1:A:237:THR:HG23	10:A:2220:HOH:O	1.90	0.71
1:B:576:ASN:H	1:B:591:ASN:ND2	1.91	0.69
1:A:204:GLN:HG2	10:A:2571:HOH:O	1.92	0.68
1:B:93:HIS:HE1	10:B:2080:HOH:O	1.77	0.67
1:A:470:GLY:HA3	9:A:1471:NAG:C8	2.25	0.66
1:B:340:HIS:HE1	1:B:558:GLU:OE1	1.80	0.65
1:A:340:HIS:HE1	1:A:558:GLU:OE1	1.81	0.63
1:B:204:GLN:HG2	10:B:2498:HOH:O	1.99	0.63
1:B:417:ARG:HH11	1:B:458:GLN:HE22	1.46	0.63
6:A:1000:TRS:H21	8:A:1003:EDO:H11	1.81	0.62
1:A:145:PHE:CD2	6:A:1000:TRS:H11	2.35	0.62
1:A:343:HIS:HD2	10:A:2088:HOH:O	1.82	0.62
6:A:1000:TRS:H21	8:A:1003:EDO:H21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:PRO:HB3	9:B:1444:NAG:H62	1.80	0.61
1:A:145:PHE:CD2	6:A:1000:TRS:C1	2.83	0.61
1:A:93:HIS:HE1	10:A:2103:HOH:O	1.83	0.60
6:A:1000:TRS:H21	8:A:1003:EDO:C1	2.35	0.57
6:B:1000:TRS:H31	8:B:1003:EDO:C1	2.34	0.57
1:A:417:ARG:HH11	1:A:458:GLN:HE22	1.53	0.57
1:B:343:HIS:HD2	10:B:2126:HOH:O	1.88	0.56
1:B:150:ILE:HG12	1:B:224:VAL:HG11	1.86	0.56
6:B:1000:TRS:H31	8:B:1003:EDO:HO1	1.65	0.55
1:B:145:PHE:CD2	6:B:1000:TRS:H12	2.42	0.54
1:A:131:LYS:HE3	10:A:2292:HOH:O	2.08	0.53
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.90	0.53
1:A:470:GLY:HA3	9:A:1471:NAG:H83	1.90	0.53
1:A:339:ASP:OD1	1:A:340:HIS:HD2	1.92	0.53
7:B:1001:PLQ:H4	8:B:1002:EDO:O1	2.09	0.52
1:B:145:PHE:CD2	6:B:1000:TRS:C1	2.92	0.52
1:B:339:ASP:OD1	1:B:340:HIS:HD2	1.92	0.51
1:A:145:PHE:CD2	6:A:1000:TRS:H12	2.45	0.51
1:B:131:LYS:HE3	10:B:2117:HOH:O	2.11	0.49
1:A:340:HIS:CE1	1:A:558:GLU:OE1	2.65	0.48
10:A:2425:HOH:O	2:C:2:NAG:H83	2.14	0.48
1:B:340:HIS:CE1	1:B:558:GLU:OE1	2.64	0.47
1:B:145:PHE:HB2	1:B:163:THR:HB	1.97	0.46
1:A:421:VAL:CG1	1:A:454:THR:HG23	2.45	0.46
6:B:1000:TRS:C3	8:B:1003:EDO:O1	2.47	0.46
1:A:145:PHE:HB2	1:A:163:THR:HB	1.97	0.46
1:A:470:GLY:HA3	9:A:1471:NAG:H81	1.97	0.45
1:B:484:GLU:O	10:B:2000:HOH:O	2.21	0.45
1:A:399:ASP:HB3	7:A:1004:PLQ:H3	1.99	0.45
1:B:84:LEU:HD23	1:B:94:ALA:HA	1.99	0.45
1:A:83:GLY:O	1:A:93:HIS:HD2	2.00	0.44
1:A:84:LEU:HD23	1:A:94:ALA:HA	2.00	0.44
1:B:380:SER:HA	1:B:389:VAL:O	2.17	0.43
1:B:399:ASP:HB3	7:B:1004:PLQ:H6	2.00	0.43
9:A:1606:NAG:H83	9:A:1606:NAG:H3	1.99	0.43
1:B:115:SER:HB2	1:B:121:TRP:CD2	2.53	0.43
1:B:56:CYS:HB3	1:B:60:THR:OG1	2.19	0.43
1:B:417:ARG:HH11	1:B:458:GLN:NE2	2.13	0.43
1:A:417:ARG:HH11	1:A:458:GLN:NE2	2.14	0.43
1:A:56:CYS:HB3	1:A:60:THR:OG1	2.19	0.42
1:A:145:PHE:CG	6:A:1000:TRS:H11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:O	1:A:249:ALA:HA	2.19	0.42
1:A:596:LEU:C	1:A:596:LEU:HD23	2.45	0.42
1:B:145:PHE:CD2	6:B:1000:TRS:H11	2.54	0.42
1:A:373:GLY:HA3	1:A:597:SER:O	2.20	0.42
7:B:1001:PLQ:H4	8:B:1002:EDO:C1	2.50	0.42
1:A:83:GLY:O	1:A:93:HIS:CD2	2.73	0.41
1:B:278:TYR:CZ	1:B:280:GLY:HA2	2.55	0.41
1:B:596:LEU:C	1:B:596:LEU:HD23	2.45	0.41
1:B:99:HIS:HD2	1:B:104:GLN:O	2.03	0.41
1:A:115:SER:HB2	1:A:121:TRP:CD2	2.55	0.41
1:A:471:ASN:HB3	10:A:2309:HOH:O	2.20	0.41
1:B:251:ILE:HD12	1:B:265:TYR:CE1	2.56	0.41
1:A:525:GLU:H	9:A:1606:NAG:C8	2.25	0.41
1:B:83:GLY:O	1:B:93:HIS:HD2	2.04	0.40
1:B:223:TYR:O	1:B:249:ALA:HA	2.20	0.40
1:B:504:THR:HG22	1:B:629:GLU:HB2	2.02	0.40
1:A:99:HIS:HD2	1:A:104:GLN:O	2.03	0.40
1:A:278:TYR:CZ	1:A:280:GLY:HA2	2.56	0.40
1:A:504:THR:HG22	1:A:629:GLU:HB2	2.01	0.40

All (2) 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)
10:A:2588:HOH:O	10:A:2588:HOH:O[2_555]	1.87	0.33
3:D:8:MAN:O4	3:D:8:MAN:O4[2_555]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	623/665 (94%)	595 (96%)	28 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	623/665 (94%)	595 (96%)	28 (4%)	0	100	100
All	All	1246/1330 (94%)	1190 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/530 (94%)	497 (100%)	1 (0%)	87	86
1	B	498/530 (94%)	497 (100%)	1 (0%)	87	86
All	All	996/1060 (94%)	994 (100%)	2 (0%)	87	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	VAL
1	B	635	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	93	HIS
1	A	183	GLN
1	A	204	GLN
1	A	268	HIS
1	A	340	HIS
1	A	343	HIS
1	A	370	GLN
1	A	388	GLN
1	A	426	ASN
1	A	458	GLN

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Mol	Chain	Res	Type
1	A	591	ASN
1	B	93	HIS
1	B	183	GLN
1	B	268	HIS
1	B	340	HIS
1	B	341	GLN
1	B	343	HIS
1	B	370	GLN
1	B	388	GLN
1	B	426	ASN
1	B	458	GLN
1	B	591	ASN

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 ⓘ

37 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	0.56	0	17,19,21	1.64	3 (17%)
2	NAG	C	2	2	14,14,15	1.37	3 (21%)	17,19,21	1.48	2 (11%)
2	BMA	C	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.71	5 (33%)
2	MAN	C	4	2	11,11,12	0.46	0	15,15,17	1.27	1 (6%)
2	MAN	C	5	2	11,11,12	0.99	1 (9%)	15,15,17	1.81	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	6	2	11,11,12	1.51	2 (18%)	15,15,17	2.06	4 (26%)
2	MAN	C	7	2	11,11,12	1.07	1 (9%)	15,15,17	1.39	2 (13%)
3	NAG	D	1	1,3	14,14,15	1.42	1 (7%)	17,19,21	1.10	0
3	MAN	D	10	3	11,11,12	1.03	0	15,15,17	1.34	1 (6%)
3	NAG	D	2	3	14,14,15	1.26	2 (14%)	17,19,21	1.56	3 (17%)
3	BMA	D	3	3	11,11,12	0.89	0	15,15,17	1.27	1 (6%)
3	MAN	D	4	3	11,11,12	0.63	0	15,15,17	1.70	4 (26%)
3	MAN	D	5	3	11,11,12	0.82	0	15,15,17	1.68	1 (6%)
3	MAN	D	6	3	11,11,12	0.48	0	15,15,17	1.01	1 (6%)
3	MAN	D	7	3	11,11,12	0.81	0	15,15,17	1.39	2 (13%)
3	MAN	D	8	3	11,11,12	1.12	1 (9%)	15,15,17	1.20	3 (20%)
3	MAN	D	9	3	11,11,12	1.06	1 (9%)	15,15,17	1.47	3 (20%)
4	NAG	E	1	4,1	14,14,15	0.53	0	17,19,21	1.34	2 (11%)
4	NAG	E	2	4	14,14,15	0.61	0	17,19,21	1.50	2 (11%)
5	NAG	F	1	1,5	14,14,15	0.50	0	17,19,21	1.61	3 (17%)
5	NAG	F	2	5	14,14,15	1.33	2 (14%)	17,19,21	1.14	2 (11%)
5	BMA	F	3	5	11,11,12	0.69	0	15,15,17	1.47	2 (13%)
5	MAN	F	4	5	11,11,12	1.50	2 (18%)	15,15,17	2.18	4 (26%)
5	MAN	F	5	5	11,11,12	0.83	0	15,15,17	0.99	2 (13%)
5	MAN	F	6	5	11,11,12	0.59	0	15,15,17	1.32	2 (13%)
3	NAG	G	1	1,3	14,14,15	1.38	2 (14%)	17,19,21	1.17	2 (11%)
3	MAN	G	10	3	11,11,12	0.74	0	15,15,17	0.95	0
3	NAG	G	2	3	14,14,15	0.93	0	17,19,21	1.27	3 (17%)
3	BMA	G	3	3	11,11,12	0.85	0	15,15,17	1.05	1 (6%)
3	MAN	G	4	3	11,11,12	0.75	0	15,15,17	1.49	2 (13%)
3	MAN	G	5	3	11,11,12	0.72	0	15,15,17	0.91	1 (6%)
3	MAN	G	6	3	11,11,12	0.68	0	15,15,17	2.25	4 (26%)
3	MAN	G	7	3	11,11,12	0.74	0	15,15,17	1.34	2 (13%)
3	MAN	G	8	3	11,11,12	0.98	1 (9%)	15,15,17	1.20	2 (13%)
3	MAN	G	9	3	11,11,12	1.18	1 (9%)	15,15,17	1.69	4 (26%)
4	NAG	H	1	4,1	14,14,15	0.43	0	17,19,21	1.47	3 (17%)
4	NAG	H	2	4	14,14,15	0.83	0	17,19,21	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	0/2/19/22	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	1/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	MAN	G	10	3	-	0/2/19/22	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1
3	MAN	G	7	3	-	0/2/19/22	0/1/1/1
3	MAN	G	8	3	-	0/2/19/22	0/1/1/1
3	MAN	G	9	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	3.74	1.57	1.52
5	F	2	NAG	O5-C1	-3.58	1.37	1.43
5	F	4	MAN	C2-C3	3.52	1.57	1.52
2	C	2	NAG	C8-C7	-3.10	1.44	1.50
3	G	1	NAG	C1-C2	2.94	1.56	1.52
3	G	1	NAG	O5-C1	-2.93	1.38	1.43
3	D	2	NAG	O5-C1	2.87	1.48	1.43
3	G	9	MAN	C2-C3	2.68	1.56	1.52
2	C	6	MAN	C2-C3	2.50	1.56	1.52
5	F	4	MAN	C1-C2	2.45	1.58	1.52
2	C	6	MAN	C1-C2	2.44	1.58	1.52
3	D	2	NAG	C2-N2	2.44	1.50	1.46
2	C	7	MAN	C2-C3	2.34	1.56	1.52
3	D	8	MAN	O5-C5	2.34	1.48	1.43
3	G	8	MAN	C4-C5	2.32	1.58	1.53
2	C	3	BMA	O5-C5	2.28	1.47	1.43
3	D	9	MAN	C2-C3	2.25	1.55	1.52
2	C	2	NAG	O5-C1	-2.23	1.39	1.43
5	F	2	NAG	C1-C2	2.15	1.55	1.52
2	C	2	NAG	C4-C5	2.06	1.57	1.53
2	C	5	MAN	C1-C2	2.01	1.57	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	4	MAN	C1-C2-C3	6.60	119.26	109.64
3	G	6	MAN	C1-O5-C5	5.87	120.05	112.19
3	D	5	MAN	C1-O5-C5	5.41	119.44	112.19
2	C	5	MAN	C1-C2-C3	4.59	116.33	109.64
3	G	6	MAN	C3-C4-C5	4.52	118.42	110.23
2	C	1	NAG	O5-C1-C2	-4.36	104.55	111.29
2	C	6	MAN	C1-O5-C5	4.10	117.68	112.19
5	F	3	BMA	O5-C5-C6	3.98	115.42	107.66
5	F	1	NAG	C1-O5-C5	3.83	117.32	112.19
2	C	6	MAN	C3-C4-C5	3.81	117.15	110.23
2	C	7	MAN	C1-O5-C5	3.80	117.28	112.19
3	D	4	MAN	C1-O5-C5	3.72	117.17	112.19
2	C	1	NAG	C1-O5-C5	3.71	117.16	112.19
3	D	10	MAN	C1-O5-C5	3.59	117.00	112.19
4	E	2	NAG	C8-C7-N2	3.58	122.05	116.12
2	C	6	MAN	C1-C2-C3	3.57	114.84	109.64
5	F	1	NAG	O5-C1-C2	-3.55	105.79	111.29
3	G	9	MAN	O2-C2-C3	3.50	117.39	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C1-O5-C5	3.49	116.87	112.19
3	D	2	NAG	C1-O5-C5	-3.38	107.66	112.19
2	C	4	MAN	C1-O5-C5	3.32	116.64	112.19
2	C	3	BMA	C6-C5-C4	-3.24	105.07	113.02
2	C	5	MAN	O5-C1-C2	3.18	118.36	110.79
4	H	1	NAG	O7-C7-N2	3.14	127.53	121.98
3	D	9	MAN	O5-C5-C6	3.12	113.75	107.66
5	F	3	BMA	C6-C5-C4	-3.07	105.47	113.02
4	H	1	NAG	C8-C7-N2	-3.00	111.14	116.12
4	E	1	NAG	O5-C5-C4	-2.95	103.64	110.83
2	C	3	BMA	O5-C5-C6	2.95	113.41	107.66
3	G	9	MAN	C2-C3-C4	2.93	116.01	110.86
3	D	4	MAN	O2-C2-C1	-2.90	102.59	109.22
3	G	6	MAN	C2-C3-C4	2.86	115.89	110.86
3	G	4	MAN	C1-O5-C5	2.86	116.02	112.19
5	F	6	MAN	O5-C5-C6	2.84	113.19	107.66
4	E	2	NAG	O7-C7-C8	-2.83	117.02	122.05
3	D	9	MAN	O2-C2-C3	2.80	115.95	110.15
3	D	7	MAN	C3-C4-C5	-2.76	105.22	110.23
3	D	2	NAG	O5-C5-C4	-2.75	104.13	110.83
3	G	4	MAN	O5-C5-C6	2.74	113.00	107.66
2	C	3	BMA	C1-O5-C5	2.73	115.84	112.19
2	C	2	NAG	C2-N2-C7	2.71	126.53	122.90
3	D	3	BMA	O3-C3-C4	-2.63	104.17	110.38
3	G	8	MAN	O2-C2-C3	-2.63	104.70	110.15
3	G	9	MAN	O5-C5-C6	2.62	112.75	107.66
2	C	2	NAG	O7-C7-C8	-2.61	117.41	122.05
2	C	7	MAN	O2-C2-C1	2.57	115.11	109.22
3	G	9	MAN	C3-C4-C5	2.53	114.82	110.23
5	F	6	MAN	C2-C3-C4	2.50	115.25	110.86
4	E	1	NAG	C6-C5-C4	2.46	119.07	113.02
4	H	1	NAG	O5-C5-C4	-2.46	104.85	110.83
3	G	1	NAG	C4-C3-C2	-2.45	107.43	111.02
5	F	4	MAN	O3-C3-C2	2.44	115.03	110.05
3	D	7	MAN	O5-C5-C4	-2.43	104.90	110.83
3	G	2	NAG	O4-C4-C5	-2.43	103.33	109.32
3	G	3	BMA	C6-C5-C4	-2.39	107.15	113.02
3	G	7	MAN	O5-C5-C4	-2.39	105.02	110.83
2	C	3	BMA	C3-C4-C5	2.38	114.54	110.23
3	G	8	MAN	O4-C4-C3	-2.38	104.77	110.38
3	D	8	MAN	O6-C6-C5	-2.37	103.25	111.33
3	G	6	MAN	O5-C5-C4	2.34	116.53	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C4	-2.29	105.26	110.83
3	D	6	MAN	O2-C2-C3	2.28	114.88	110.15
3	D	4	MAN	C1-C2-C3	2.27	112.95	109.64
2	C	5	MAN	C2-C3-C4	2.27	114.85	110.86
5	F	2	NAG	C4-C3-C2	-2.26	107.71	111.02
5	F	1	NAG	C4-C3-C2	-2.25	107.72	111.02
5	F	4	MAN	O4-C4-C5	2.25	114.87	109.32
3	D	2	NAG	O5-C1-C2	-2.18	107.91	111.29
3	D	9	MAN	C1-O5-C5	2.16	115.08	112.19
3	D	8	MAN	O2-C2-C3	-2.14	105.71	110.15
3	D	8	MAN	O5-C5-C6	2.14	111.82	107.66
3	G	2	NAG	O6-C6-C5	-2.13	104.07	111.33
3	G	2	NAG	C2-N2-C7	2.11	125.73	122.90
3	G	1	NAG	C8-C7-N2	-2.10	112.64	116.12
3	D	4	MAN	C6-C5-C4	-2.10	107.87	113.02
2	C	3	BMA	O6-C6-C5	-2.09	104.20	111.33
3	G	5	MAN	O4-C4-C5	2.08	114.45	109.32
2	C	6	MAN	C6-C5-C4	-2.07	107.95	113.02
5	F	5	MAN	C1-C2-C3	2.04	112.61	109.64
5	F	5	MAN	C1-O5-C5	2.03	114.91	112.19
5	F	2	NAG	O6-C6-C5	-2.02	104.44	111.33
3	G	7	MAN	C1-C2-C3	2.02	112.59	109.64
5	F	4	MAN	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	6	MAN	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	E	2	NAG	O7-C7-N2-C2
3	G	6	MAN	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2

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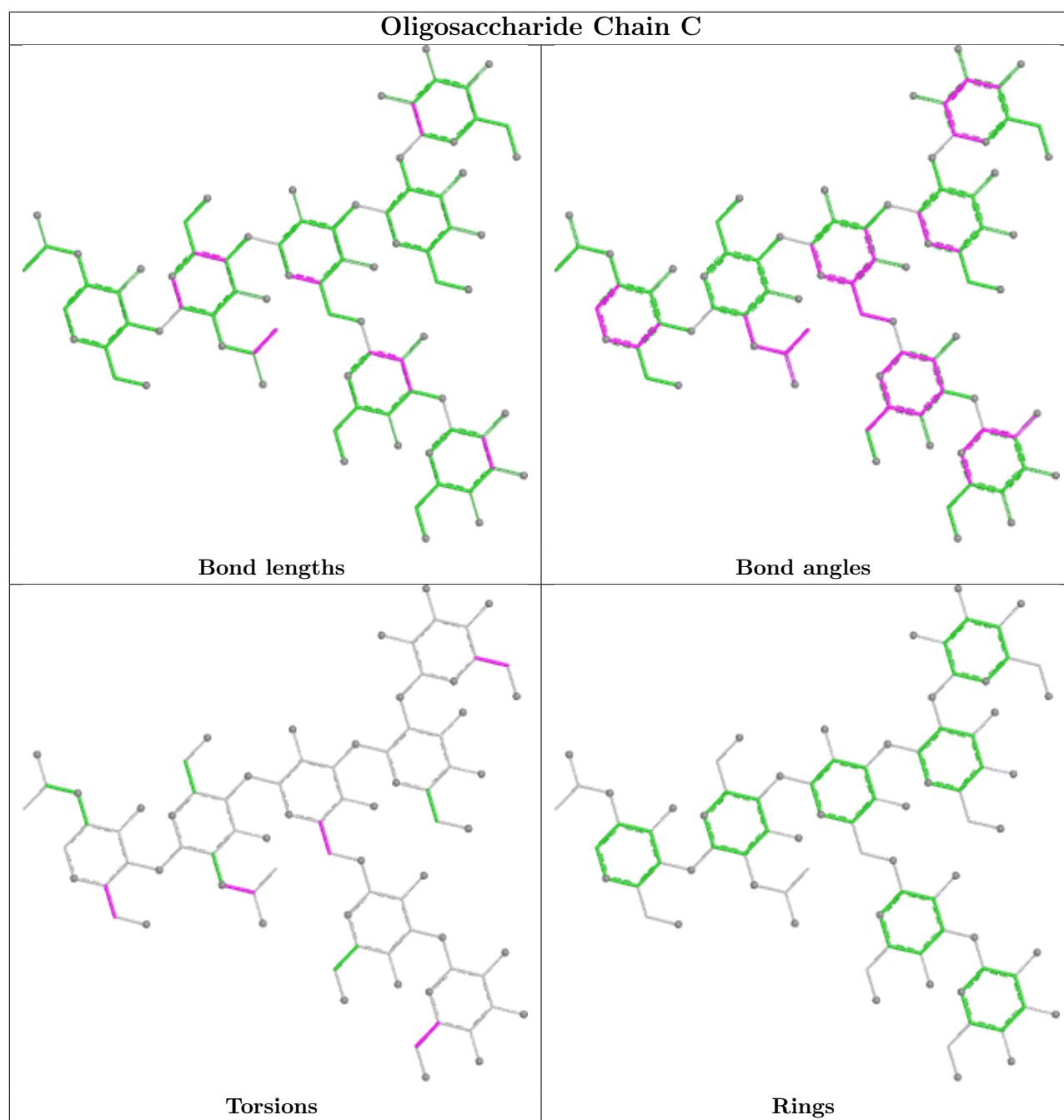
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
3	G	9	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
2	C	7	MAN	C4-C5-C6-O6
5	F	5	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

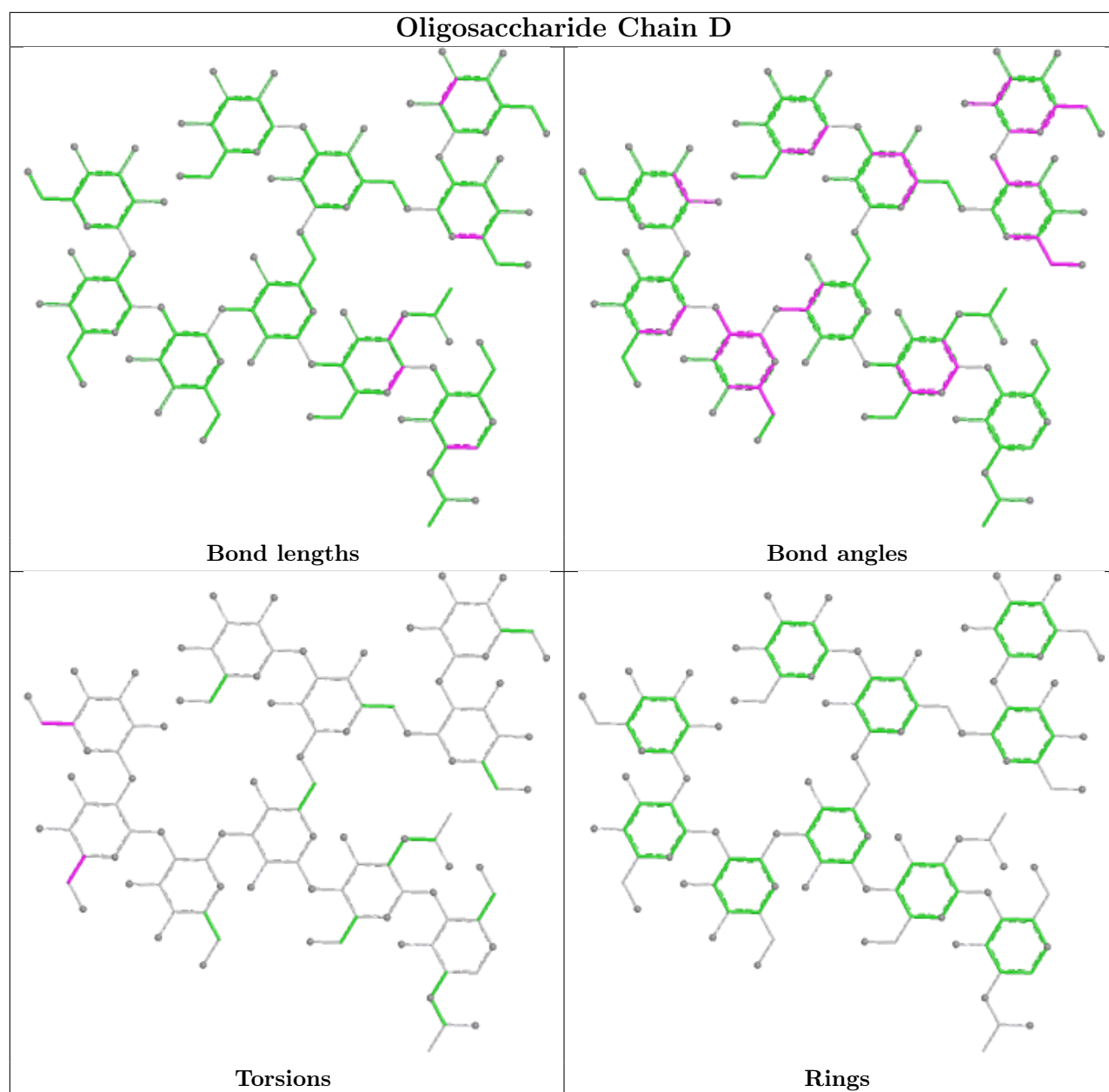
There are no ring outliers.

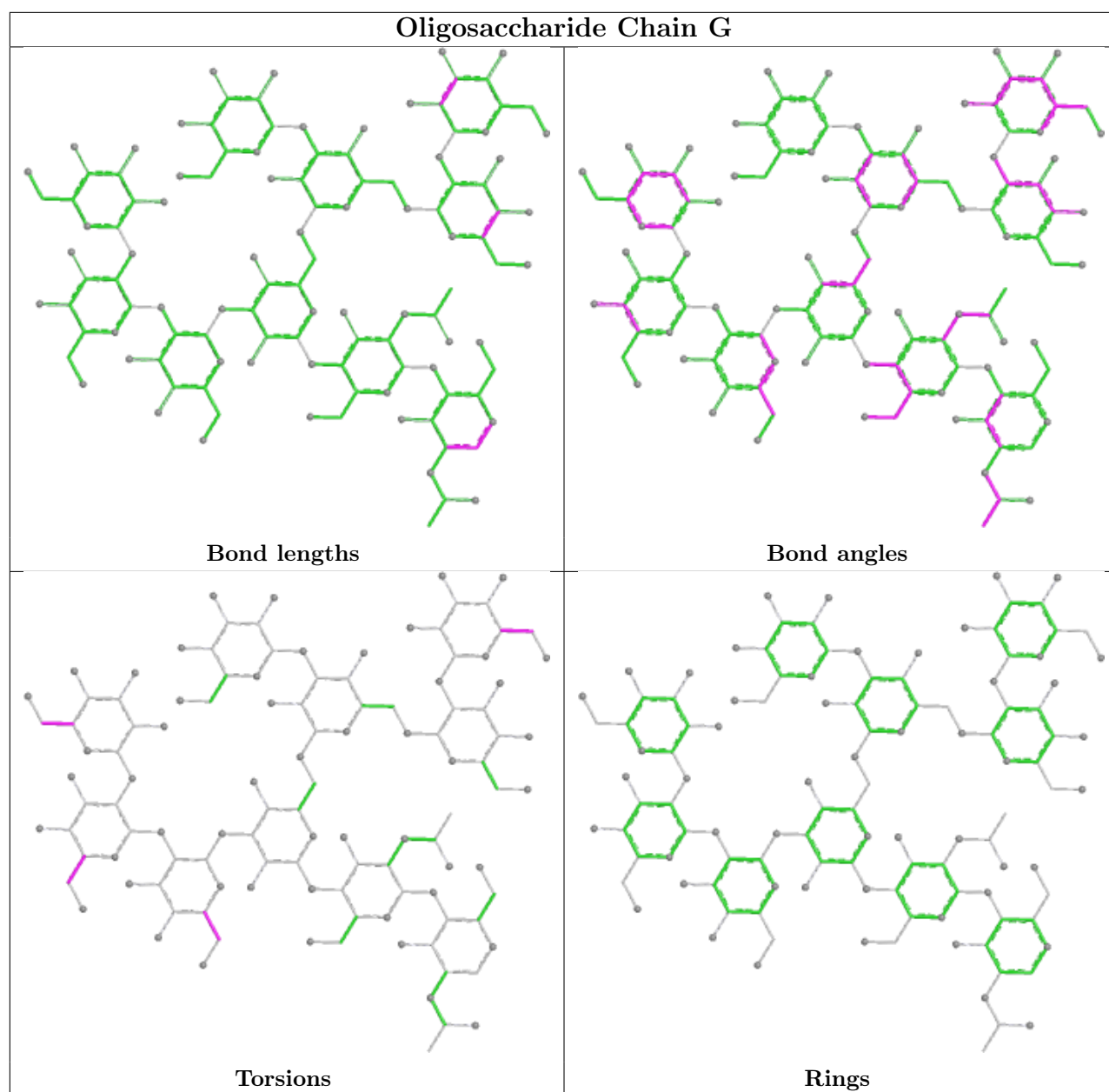
2 monomers are involved in 2 short contacts:

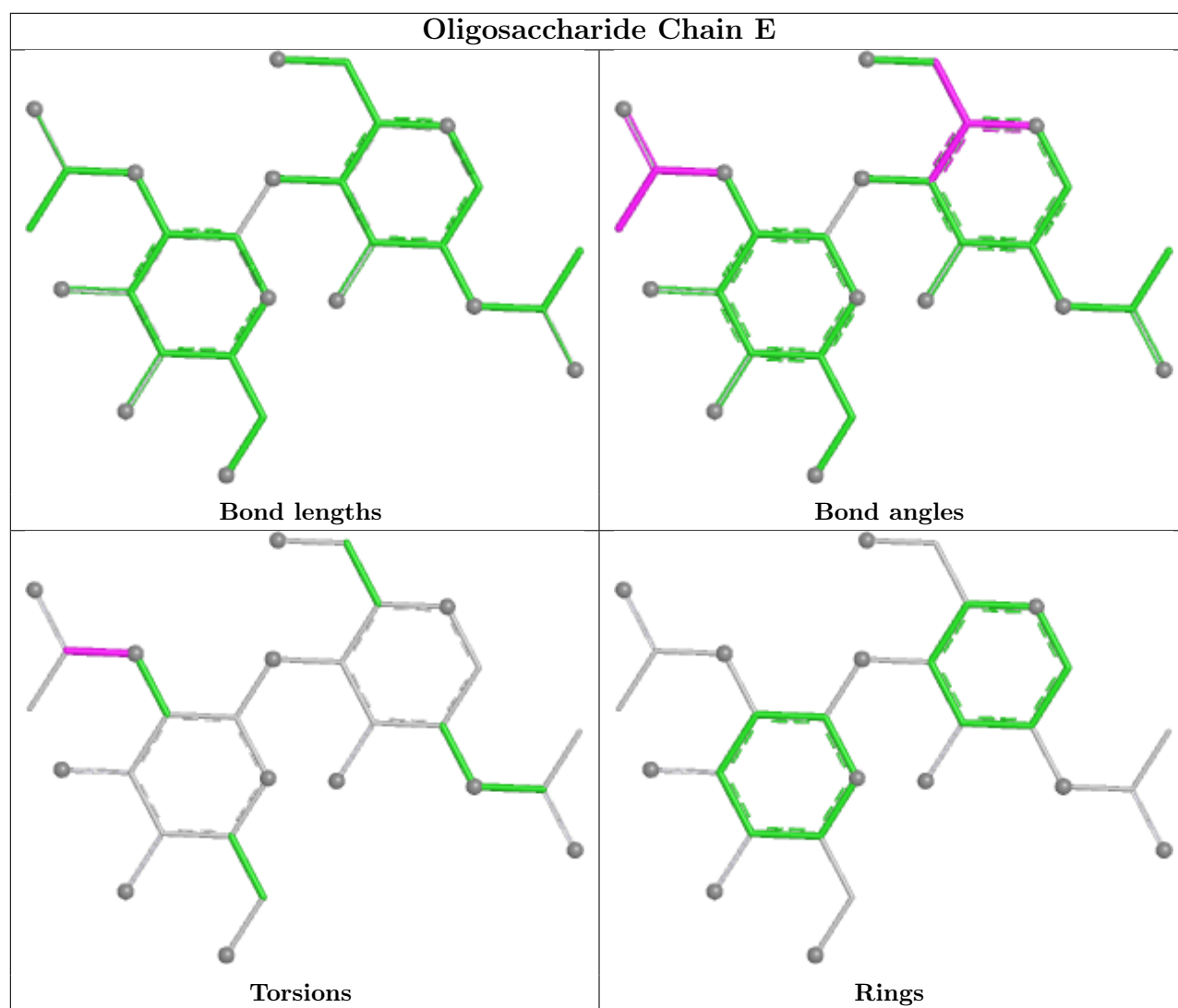
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	MAN	0	1
2	C	2	NAG	1	0

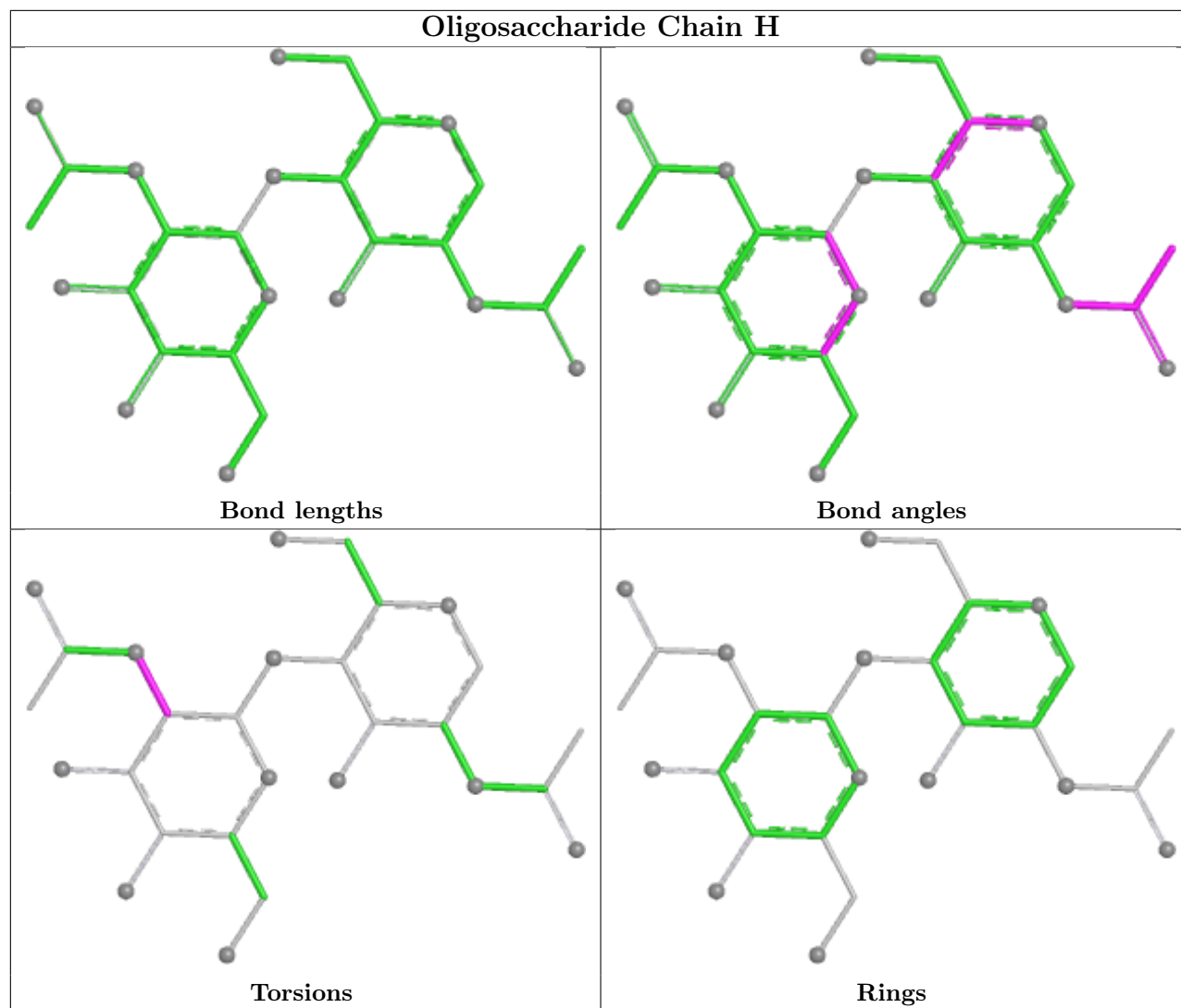
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

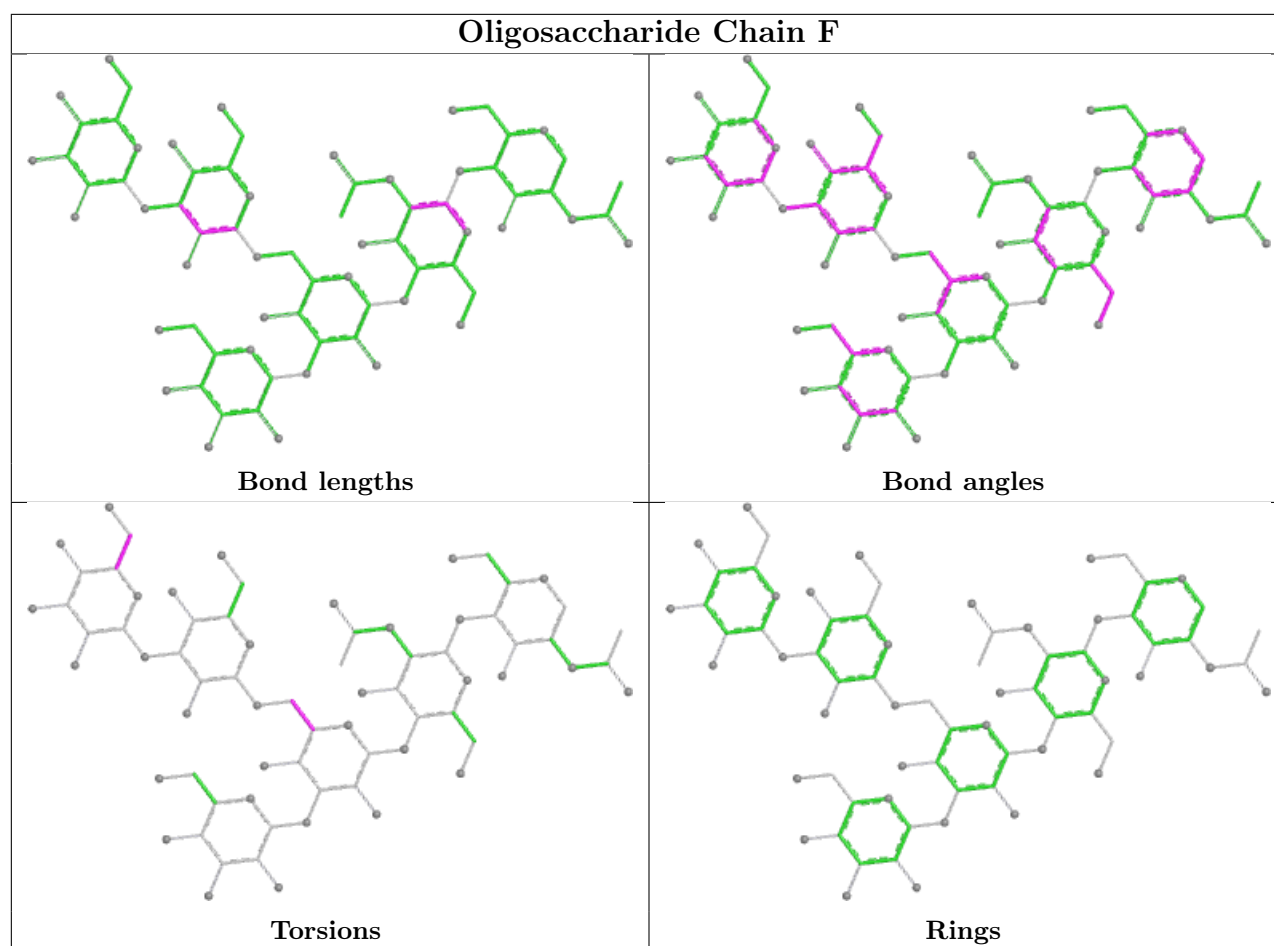












5.6 Ligand geometry [i](#)

47 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	NAG	B	1357	1	14,14,15	0.68	0	17,19,21	1.57	3 (17%)
9	NAG	A	1236	1	14,14,15	1.38	2 (14%)	17,19,21	1.37	3 (17%)
9	NAG	A	1052	1	14,14,15	0.49	0	17,19,21	1.94	5 (29%)
9	NAG	A	1471	1	14,14,15	0.66	0	17,19,21	1.67	2 (11%)
9	NAG	A	1644	1	14,14,15	1.07	1 (7%)	17,19,21	1.35	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	1555	1	14,14,15	0.87	1 (7%)	17,19,21	2.39	10 (58%)
7	PLQ	B	1001	-	8,8,8	0.91	0	10,10,10	0.26	0
9	NAG	A	1242	1	14,14,15	0.43	0	17,19,21	1.60	4 (23%)
9	NAG	A	1215	1	14,14,15	0.89	1 (7%)	17,19,21	2.83	6 (35%)
8	EDO	B	1002	-	3,3,3	0.07	0	2,2,2	0.11	0
9	NAG	A	1539	1	14,14,15	1.03	2 (14%)	17,19,21	1.63	2 (11%)
7	PLQ	A	1011	-	8,8,8	0.91	0	10,10,10	0.26	0
8	EDO	A	1002	-	3,3,3	0.06	0	2,2,2	0.29	0
7	PLQ	B	1005	-	8,8,8	0.93	0	10,10,10	0.27	0
7	PLQ	A	1010	-	8,8,8	0.93	0	10,10,10	0.28	0
7	PLQ	B	1004	-	8,8,8	0.92	0	10,10,10	0.26	0
7	PLQ	B	1009	-	8,8,8	0.92	0	10,10,10	0.27	0
9	NAG	B	1319	1	14,14,15	0.51	0	17,19,21	2.00	2 (11%)
9	NAG	B	1539	1	14,14,15	1.26	2 (14%)	17,19,21	2.03	5 (29%)
7	PLQ	A	1009	-	8,8,8	0.92	0	10,10,10	0.27	0
7	PLQ	A	1001	-	8,8,8	0.92	0	10,10,10	0.27	0
8	EDO	B	1003	-	3,3,3	0.06	0	2,2,2	0.22	0
9	NAG	B	1483	1	14,14,15	0.50	0	17,19,21	1.79	3 (17%)
9	NAG	B	1471	1	14,14,15	0.90	0	17,19,21	1.36	2 (11%)
6	TRS	B	1000	-	7,7,7	0.79	0	9,9,9	1.47	2 (22%)
7	PLQ	B	1006	-	8,8,8	0.92	0	10,10,10	0.26	0
9	NAG	B	1242	1	14,14,15	0.82	0	17,19,21	2.40	6 (35%)
9	NAG	B	1052	1	14,14,15	0.30	0	17,19,21	1.01	0
9	NAG	A	1357	1	14,14,15	0.87	0	17,19,21	1.71	4 (23%)
9	NAG	A	1606	1	14,14,15	0.67	0	17,19,21	2.14	5 (29%)
9	NAG	A	1512	1	14,14,15	0.49	0	17,19,21	2.43	5 (29%)
8	EDO	A	1003	-	3,3,3	0.13	0	2,2,2	0.37	0
7	PLQ	A	1004	-	8,8,8	0.91	0	10,10,10	0.27	0
9	NAG	A	1483	1	14,14,15	0.57	0	17,19,21	1.33	4 (23%)
7	PLQ	A	1005	-	8,8,8	0.91	0	10,10,10	0.27	0
7	PLQ	A	1008	-	8,8,8	0.92	0	10,10,10	0.27	0
6	TRS	A	1000	-	7,7,7	1.03	0	9,9,9	1.82	3 (33%)
7	PLQ	B	1008	-	8,8,8	0.91	0	10,10,10	0.26	0
9	NAG	B	1215	1	14,14,15	0.60	0	17,19,21	1.88	4 (23%)
9	NAG	B	1444	1	14,14,15	0.94	1 (7%)	17,19,21	1.61	2 (11%)
9	NAG	B	1644	1	14,14,15	1.07	2 (14%)	17,19,21	1.45	2 (11%)
7	PLQ	B	1007	-	8,8,8	0.92	0	10,10,10	0.28	0
7	PLQ	A	1006	-	8,8,8	0.92	0	10,10,10	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	1319	1	14,14,15	0.72	0	17,19,21	1.24	3 (17%)
9	NAG	A	1444	1	14,14,15	0.89	0	17,19,21	1.11	2 (11%)
7	PLQ	A	1007	-	8,8,8	0.92	0	10,10,10	0.27	0
9	NAG	B	1555	1	14,14,15	1.04	1 (7%)	17,19,21	1.24	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1357	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1052	1	-	3/6/23/26	0/1/1/1
9	NAG	A	1471	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1555	1	-	3/6/23/26	0/1/1/1
7	PLQ	B	1001	-	-	-	0/1/1/1
9	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1215	1	-	1/6/23/26	0/1/1/1
8	EDO	B	1002	-	-	1/1/1/1	-
9	NAG	A	1539	1	-	2/6/23/26	0/1/1/1
7	PLQ	A	1011	-	-	-	0/1/1/1
8	EDO	A	1002	-	-	1/1/1/1	-
7	PLQ	B	1005	-	-	-	0/1/1/1
7	PLQ	A	1010	-	-	-	0/1/1/1
7	PLQ	B	1004	-	-	-	0/1/1/1
7	PLQ	B	1009	-	-	-	0/1/1/1
9	NAG	B	1319	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1539	1	-	2/6/23/26	0/1/1/1
8	EDO	B	1003	-	-	1/1/1/1	-
9	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
7	PLQ	A	1001	-	-	-	0/1/1/1
7	PLQ	A	1009	-	-	-	0/1/1/1
9	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
6	TRS	B	1000	-	-	3/9/9/9	-
9	NAG	B	1242	1	-	2/6/23/26	0/1/1/1
7	PLQ	B	1006	-	-	-	0/1/1/1
9	NAG	B	1052	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1357	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1606	1	-	4/6/23/26	0/1/1/1
9	NAG	A	1512	1	-	4/6/23/26	0/1/1/1
8	EDO	A	1003	-	-	1/1/1/1	-
9	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
7	PLQ	A	1004	-	-	-	0/1/1/1
7	PLQ	A	1005	-	-	-	0/1/1/1
7	PLQ	A	1008	-	-	-	0/1/1/1
6	TRS	A	1000	-	-	3/9/9/9	-
7	PLQ	B	1008	-	-	-	0/1/1/1
9	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1444	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1644	1	-	0/6/23/26	0/1/1/1
7	PLQ	B	1007	-	-	-	0/1/1/1
9	NAG	A	1319	1	-	2/6/23/26	0/1/1/1
7	PLQ	A	1006	-	-	-	0/1/1/1
9	NAG	A	1444	1	-	2/6/23/26	0/1/1/1
7	PLQ	A	1007	-	-	-	0/1/1/1
9	NAG	B	1555	1	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1539	NAG	C1-C2	3.30	1.56	1.52
9	A	1644	NAG	C1-C2	2.94	1.56	1.52
9	B	1644	NAG	C1-C2	2.83	1.56	1.52
9	A	1539	NAG	C1-C2	2.57	1.55	1.52
9	B	1555	NAG	C1-C2	2.45	1.55	1.52
9	B	1539	NAG	O5-C1	2.45	1.47	1.43
9	A	1236	NAG	O5-C1	2.29	1.47	1.43
9	A	1236	NAG	C2-N2	2.19	1.49	1.46
9	A	1539	NAG	O5-C1	2.18	1.47	1.43
9	A	1555	NAG	C1-C2	2.15	1.55	1.52
9	B	1644	NAG	C4-C5	2.11	1.57	1.53
9	B	1444	NAG	O5-C1	-2.03	1.40	1.43
9	A	1215	NAG	O5-C5	2.00	1.47	1.43

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1215	NAG	C1-O5-C5	7.19	121.82	112.19
9	A	1512	NAG	C1-O5-C5	6.89	121.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1242	NAG	C1-O5-C5	6.76	121.25	112.19
9	B	1539	NAG	C1-O5-C5	5.97	120.19	112.19
9	A	1215	NAG	C1-C2-N2	5.84	119.63	110.43
9	B	1319	NAG	C1-O5-C5	5.79	119.95	112.19
9	A	1539	NAG	C1-O5-C5	5.32	119.31	112.19
9	B	1444	NAG	C1-O5-C5	5.31	119.30	112.19
9	B	1215	NAG	C1-O5-C5	4.88	118.73	112.19
9	A	1606	NAG	C8-C7-N2	4.75	124.00	116.12
9	A	1471	NAG	C1-O5-C5	4.63	118.39	112.19
9	B	1483	NAG	C1-O5-C5	4.44	118.13	112.19
9	A	1215	NAG	C4-C3-C2	-4.42	104.54	111.02
9	A	1512	NAG	C4-C3-C2	-4.30	104.71	111.02
9	A	1555	NAG	C2-N2-C7	4.29	128.65	122.90
9	B	1319	NAG	O5-C1-C2	4.29	117.93	111.29
9	B	1483	NAG	O5-C1-C2	-4.21	104.78	111.29
9	A	1242	NAG	C1-O5-C5	4.14	117.73	112.19
9	A	1052	NAG	O5-C1-C2	-4.10	104.95	111.29
9	A	1357	NAG	C2-N2-C7	4.00	128.26	122.90
9	B	1242	NAG	C4-C3-C2	-3.65	105.67	111.02
9	A	1644	NAG	C1-C2-N2	-3.63	104.71	110.43
9	A	1606	NAG	C2-N2-C7	3.62	127.75	122.90
9	A	1555	NAG	O6-C6-C5	-3.59	99.11	111.33
9	A	1606	NAG	O7-C7-C8	-3.50	115.81	122.05
9	A	1555	NAG	C1-O5-C5	3.49	116.86	112.19
9	A	1555	NAG	C8-C7-N2	3.29	121.58	116.12
9	A	1512	NAG	C8-C7-N2	3.19	121.40	116.12
9	B	1471	NAG	C1-O5-C5	3.14	116.40	112.19
9	B	1357	NAG	C1-O5-C5	3.07	116.30	112.19
9	A	1052	NAG	C3-C4-C5	-3.07	104.67	110.23
9	B	1555	NAG	O5-C1-C2	-3.06	106.56	111.29
9	B	1242	NAG	C8-C7-N2	3.03	121.14	116.12
9	A	1052	NAG	C8-C7-N2	3.00	121.09	116.12
9	A	1236	NAG	O5-C1-C2	-2.96	106.71	111.29
9	B	1471	NAG	C6-C5-C4	2.96	120.28	113.02
9	B	1215	NAG	O5-C1-C2	2.90	115.78	111.29
9	B	1242	NAG	C6-C5-C4	-2.90	105.90	113.02
6	A	1000	TRS	O3-C3-C	2.90	118.95	110.88
9	A	1606	NAG	O5-C1-C2	2.88	115.75	111.29
9	B	1539	NAG	C1-C2-N2	2.84	114.91	110.43
9	A	1555	NAG	C6-C5-C4	-2.80	106.15	113.02
9	A	1052	NAG	C6-C5-C4	2.78	119.85	113.02
9	A	1215	NAG	O5-C1-C2	-2.78	106.99	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1555	NAG	O5-C1-C2	-2.76	107.02	111.29
9	A	1606	NAG	C1-O5-C5	2.73	115.84	112.19
9	B	1644	NAG	C8-C7-N2	2.71	120.61	116.12
6	B	1000	TRS	O2-C2-C	2.71	118.42	110.88
9	A	1242	NAG	O6-C6-C5	-2.68	102.22	111.33
9	A	1471	NAG	C2-N2-C7	2.67	126.48	122.90
9	A	1512	NAG	O5-C5-C4	2.64	117.26	110.83
6	A	1000	TRS	O2-C2-C	2.64	118.23	110.88
9	A	1555	NAG	O5-C5-C4	2.63	117.24	110.83
6	A	1000	TRS	C3-C-C2	2.62	117.63	110.66
9	A	1444	NAG	C3-C4-C5	2.61	114.96	110.23
9	A	1215	NAG	C6-C5-C4	-2.61	106.62	113.02
9	A	1483	NAG	C2-N2-C7	-2.60	119.42	122.90
9	A	1357	NAG	O5-C1-C2	-2.59	107.28	111.29
9	B	1357	NAG	C2-N2-C7	-2.57	119.45	122.90
9	B	1242	NAG	O7-C7-N2	-2.54	117.48	121.98
9	A	1555	NAG	O7-C7-N2	-2.48	117.60	121.98
9	A	1539	NAG	C1-C2-N2	2.48	114.33	110.43
9	A	1242	NAG	C1-C2-N2	2.43	114.26	110.43
9	B	1539	NAG	C4-C3-C2	2.40	114.53	111.02
9	A	1357	NAG	O6-C6-C5	-2.39	103.20	111.33
9	B	1539	NAG	O3-C3-C2	-2.38	104.45	109.40
9	B	1644	NAG	O5-C5-C6	2.38	112.30	107.66
9	A	1236	NAG	C1-C2-N2	2.37	114.17	110.43
9	A	1319	NAG	O5-C5-C4	-2.35	105.10	110.83
9	A	1483	NAG	C1-O5-C5	2.35	115.34	112.19
9	A	1357	NAG	C1-C2-N2	-2.35	106.73	110.43
9	A	1512	NAG	C1-C2-N2	2.34	114.12	110.43
9	A	1215	NAG	O5-C5-C4	2.34	116.52	110.83
9	A	1319	NAG	O5-C5-C6	2.31	112.16	107.66
9	A	1483	NAG	O5-C5-C4	-2.24	105.38	110.83
9	B	1357	NAG	C1-C2-N2	-2.22	106.94	110.43
9	A	1555	NAG	C1-C2-N2	2.22	113.93	110.43
9	A	1052	NAG	C4-C3-C2	-2.22	107.77	111.02
6	B	1000	TRS	O3-C3-C	2.19	116.97	110.88
9	A	1555	NAG	C3-C4-C5	2.18	114.18	110.23
9	A	1483	NAG	O3-C3-C2	-2.18	104.88	109.40
9	A	1242	NAG	C6-C5-C4	-2.17	107.69	113.02
9	A	1319	NAG	O5-C1-C2	2.16	114.63	111.29
9	A	1236	NAG	C3-C4-C5	2.15	114.13	110.23
9	A	1444	NAG	C1-O5-C5	2.12	115.03	112.19
9	B	1242	NAG	O5-C5-C4	2.12	115.98	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1483	NAG	C3-C4-C5	2.12	114.07	110.23
9	B	1539	NAG	C3-C4-C5	2.10	114.04	110.23
9	B	1444	NAG	C3-C4-C5	2.09	114.02	110.23
9	B	1215	NAG	C6-C5-C4	-2.09	107.89	113.02
9	A	1644	NAG	C8-C7-N2	2.08	119.57	116.12
9	B	1215	NAG	C2-N2-C7	2.07	125.67	122.90

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1000	TRS	N-C-C1-O1
9	A	1215	NAG	C1-C2-N2-C7
9	A	1512	NAG	O5-C5-C6-O6
9	A	1512	NAG	C4-C5-C6-O6
9	B	1539	NAG	C4-C5-C6-O6
9	A	1319	NAG	O5-C5-C6-O6
9	A	1052	NAG	C8-C7-N2-C2
9	A	1052	NAG	O7-C7-N2-C2
9	A	1357	NAG	C8-C7-N2-C2
9	A	1357	NAG	O7-C7-N2-C2
9	A	1471	NAG	C8-C7-N2-C2
9	A	1471	NAG	O7-C7-N2-C2
9	A	1512	NAG	C8-C7-N2-C2
9	A	1512	NAG	O7-C7-N2-C2
9	A	1555	NAG	C8-C7-N2-C2
9	A	1555	NAG	O7-C7-N2-C2
9	A	1606	NAG	C8-C7-N2-C2
9	A	1606	NAG	O7-C7-N2-C2
9	B	1242	NAG	C8-C7-N2-C2
9	B	1242	NAG	O7-C7-N2-C2
9	A	1319	NAG	C4-C5-C6-O6
9	B	1539	NAG	O5-C5-C6-O6
9	B	1357	NAG	C4-C5-C6-O6
9	A	1539	NAG	C4-C5-C6-O6
8	B	1003	EDO	O1-C1-C2-O2
9	B	1444	NAG	C4-C5-C6-O6
9	B	1357	NAG	O5-C5-C6-O6
9	B	1444	NAG	O5-C5-C6-O6
6	B	1000	TRS	C3-C-C1-O1
6	B	1000	TRS	N-C-C1-O1
9	A	1555	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	1319	NAG	C4-C5-C6-O6
9	A	1539	NAG	O5-C5-C6-O6
6	A	1000	TRS	C3-C-C1-O1
9	A	1606	NAG	C3-C2-N2-C7
9	A	1052	NAG	C4-C5-C6-O6
9	B	1052	NAG	C4-C5-C6-O6
6	B	1000	TRS	C2-C-C1-O1
9	A	1606	NAG	O5-C5-C6-O6
8	A	1003	EDO	O1-C1-C2-O2
9	A	1444	NAG	O5-C5-C6-O6
6	A	1000	TRS	C2-C-C1-O1
8	A	1002	EDO	O1-C1-C2-O2
8	B	1002	EDO	O1-C1-C2-O2
9	A	1444	NAG	C4-C5-C6-O6

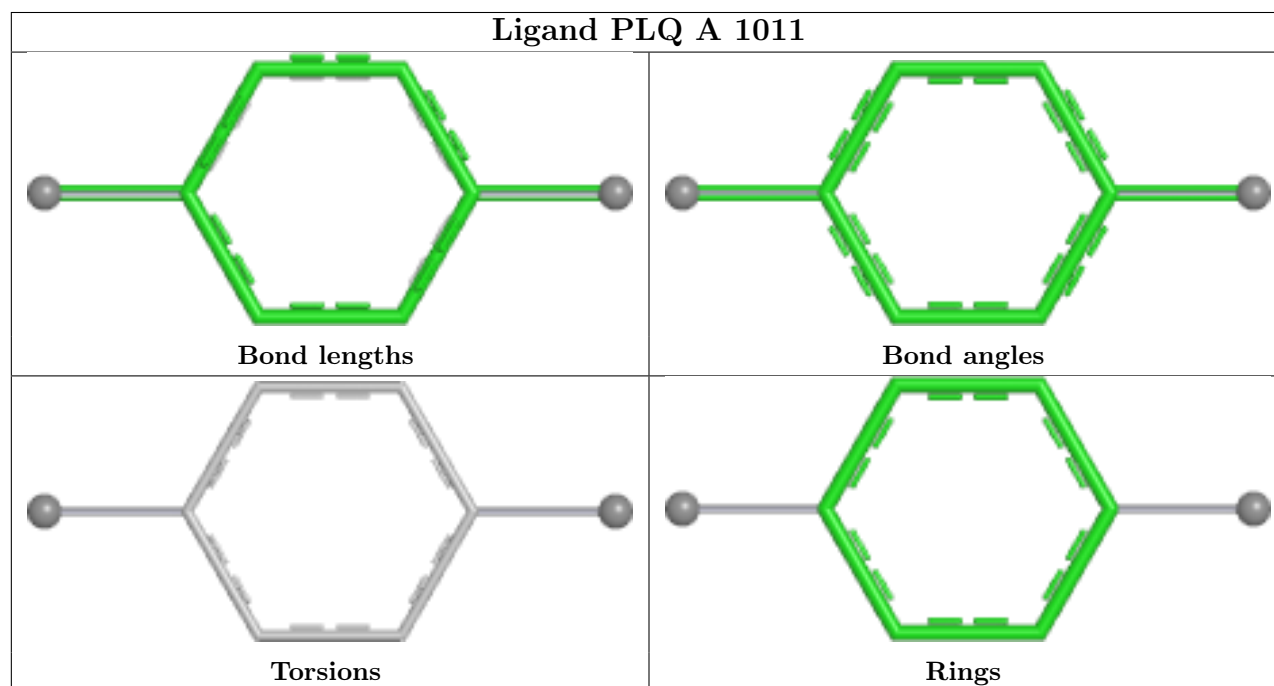
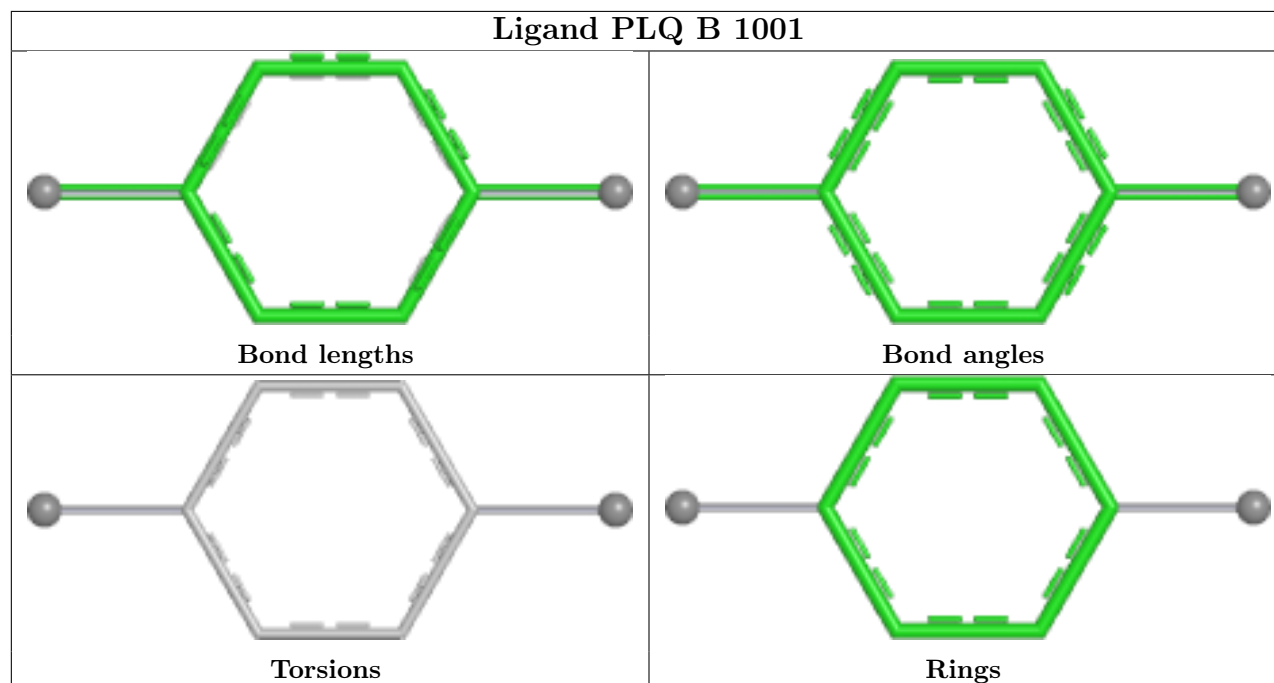
There are no ring outliers.

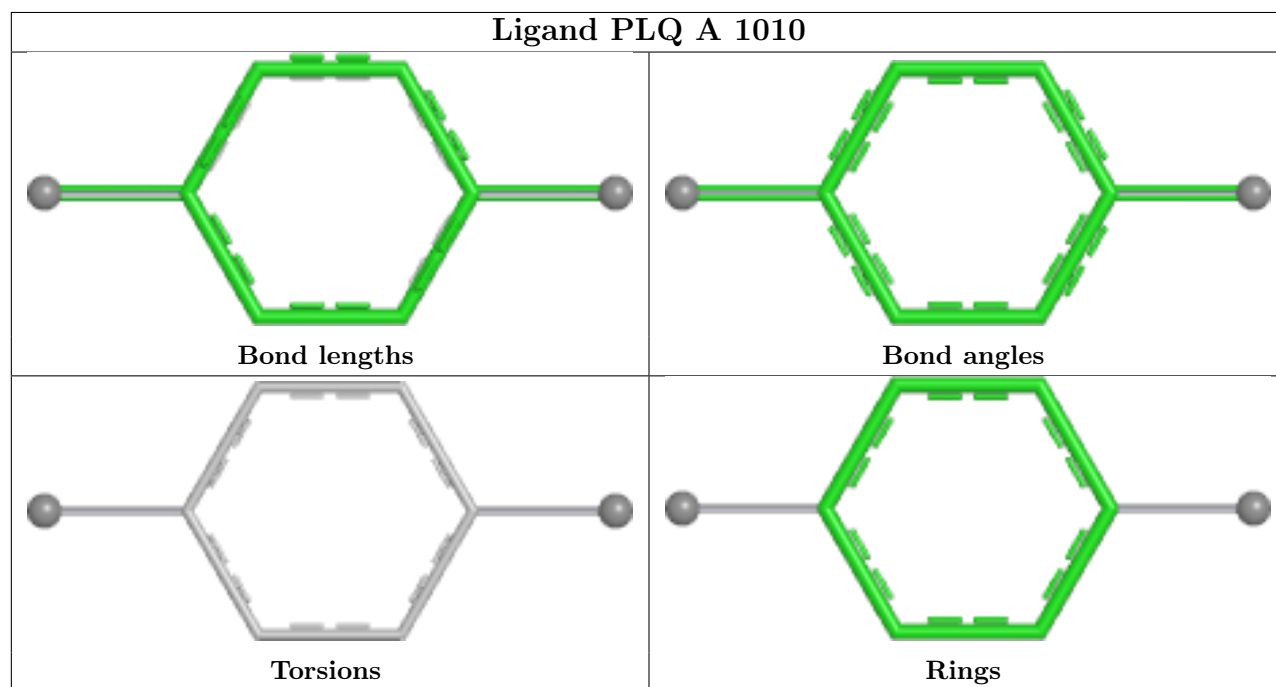
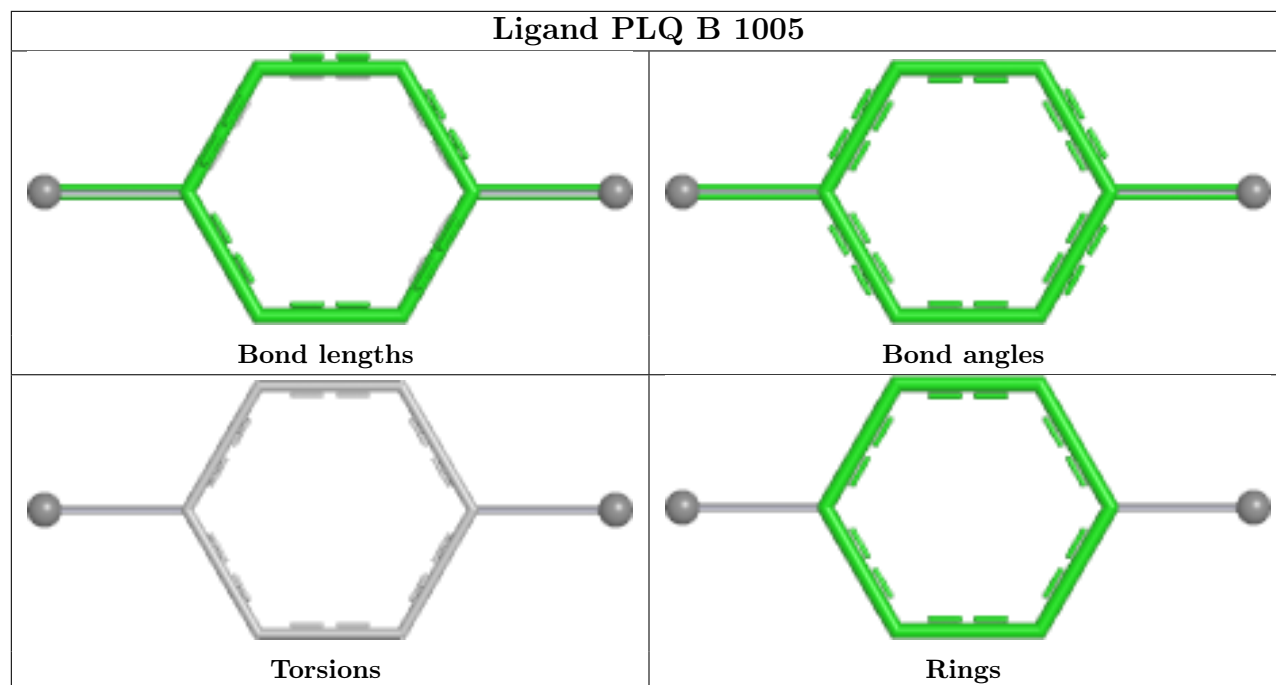
13 monomers are involved in 28 short contacts:

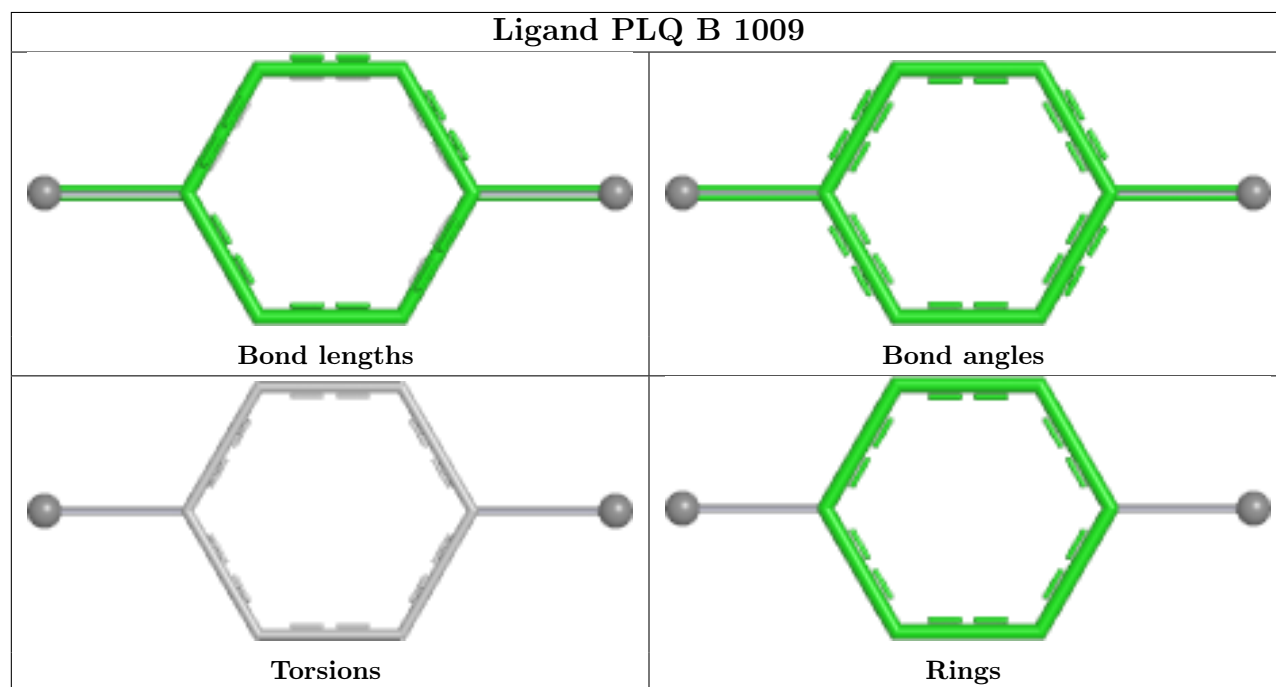
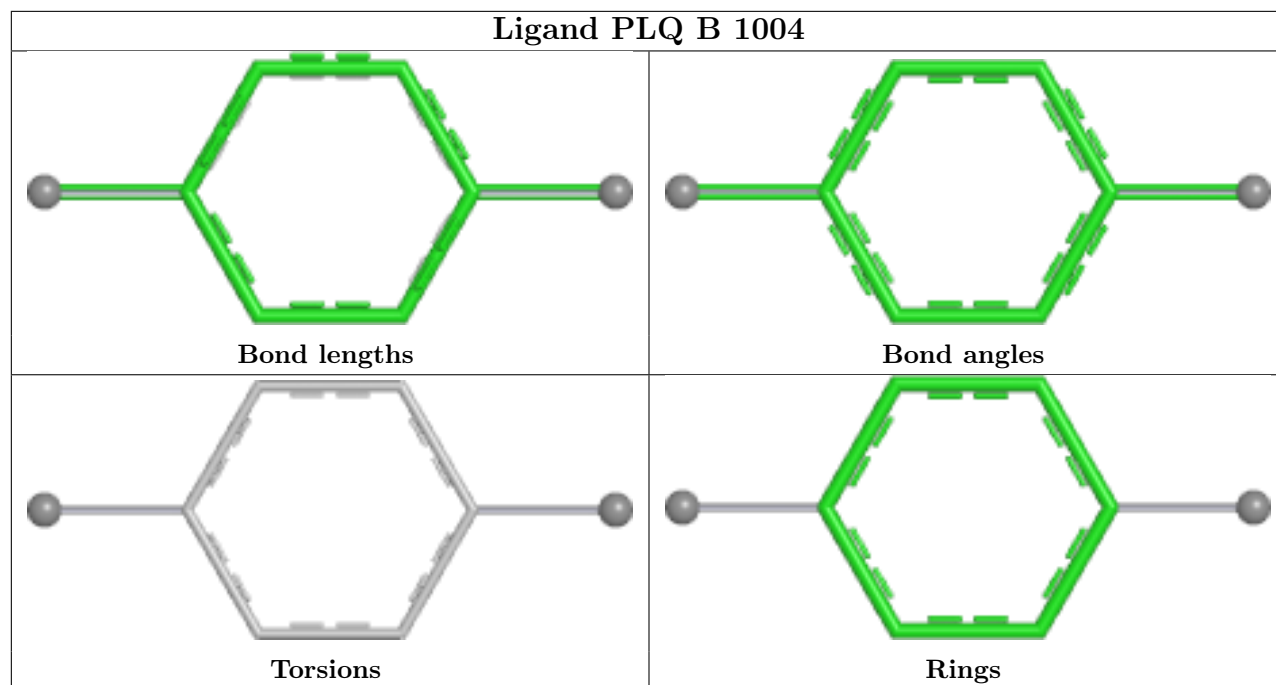
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1471	NAG	3	0
7	B	1001	PLQ	2	0
8	B	1002	EDO	2	0
8	A	1002	EDO	1	0
7	B	1004	PLQ	1	0
7	A	1001	PLQ	1	0
8	B	1003	EDO	4	0
6	B	1000	TRS	7	0
9	A	1606	NAG	3	0
8	A	1003	EDO	5	0
7	A	1004	PLQ	1	0
6	A	1000	TRS	9	0
9	B	1444	NAG	1	0

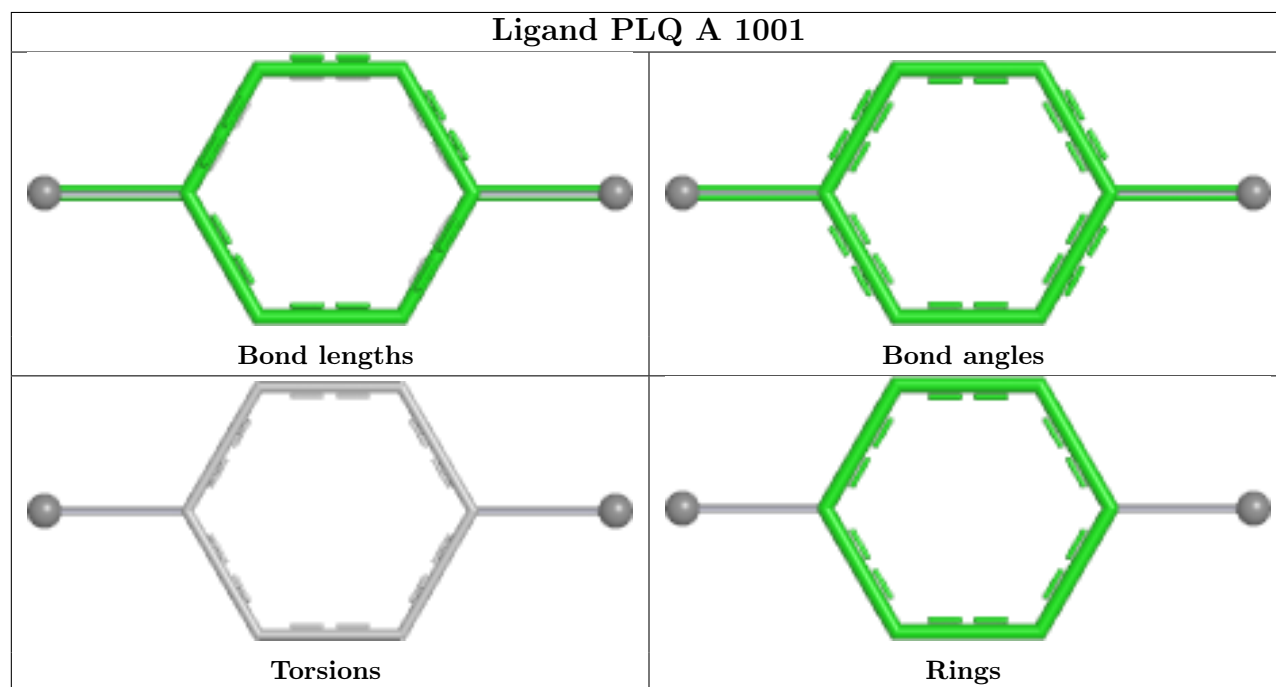
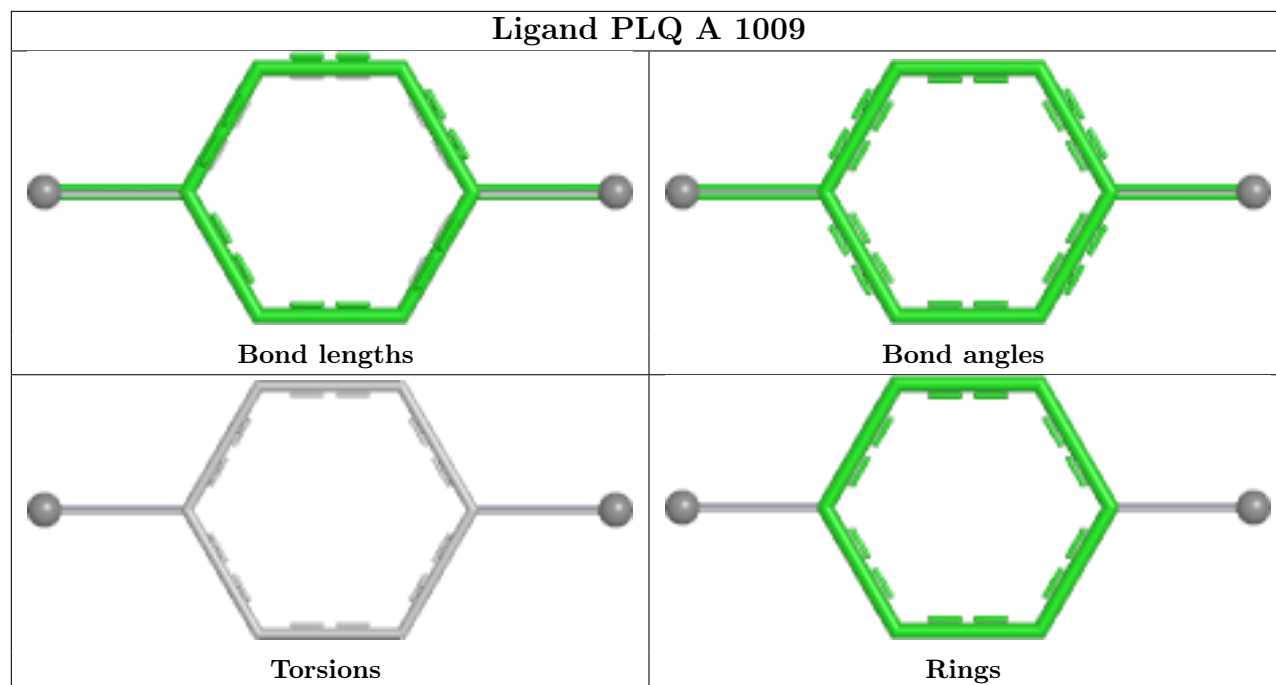
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

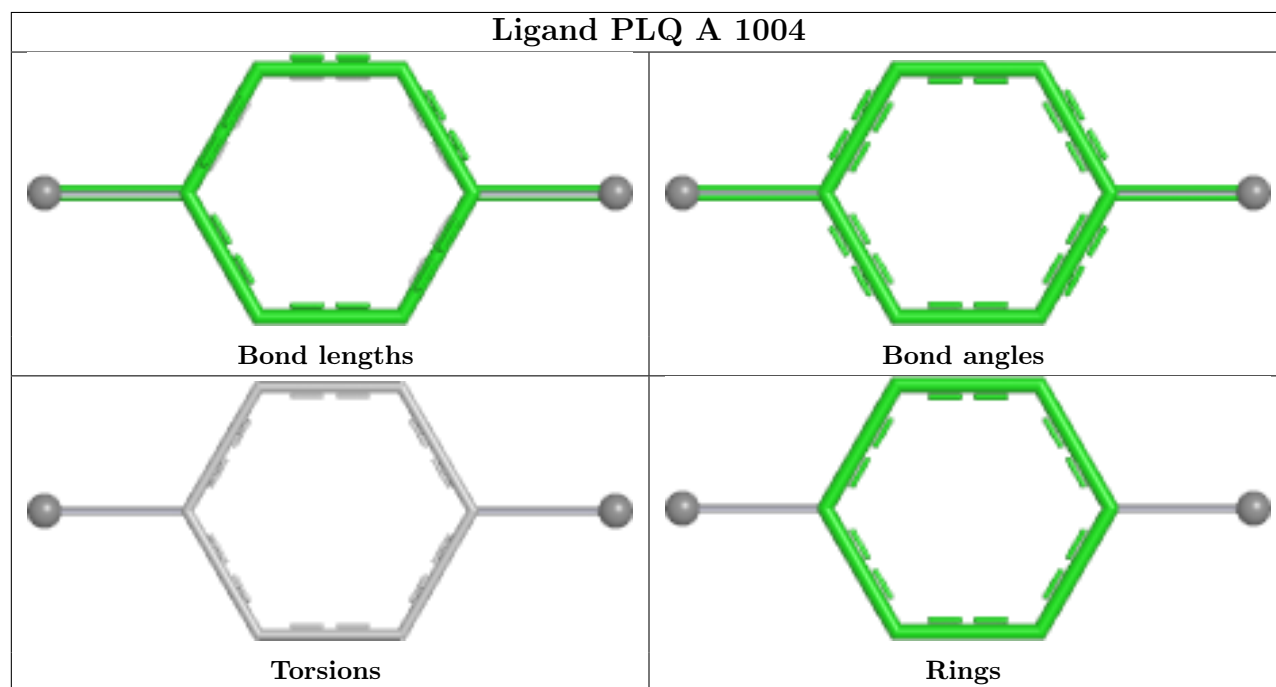
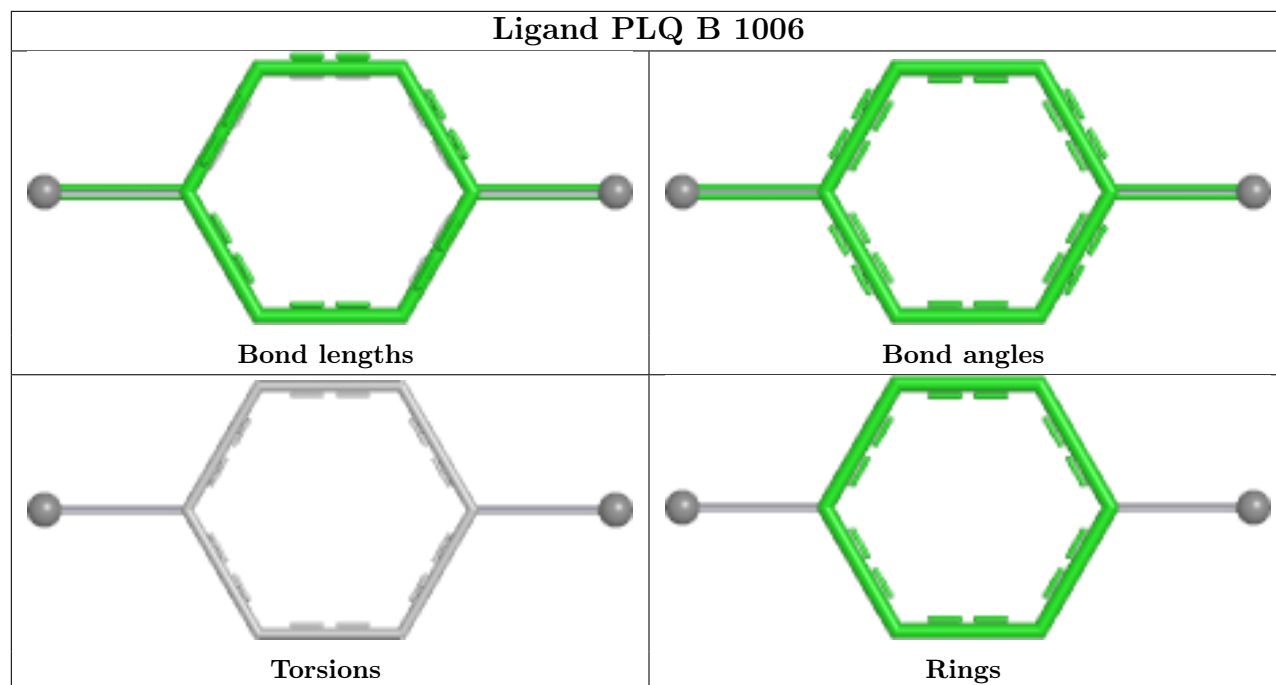
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

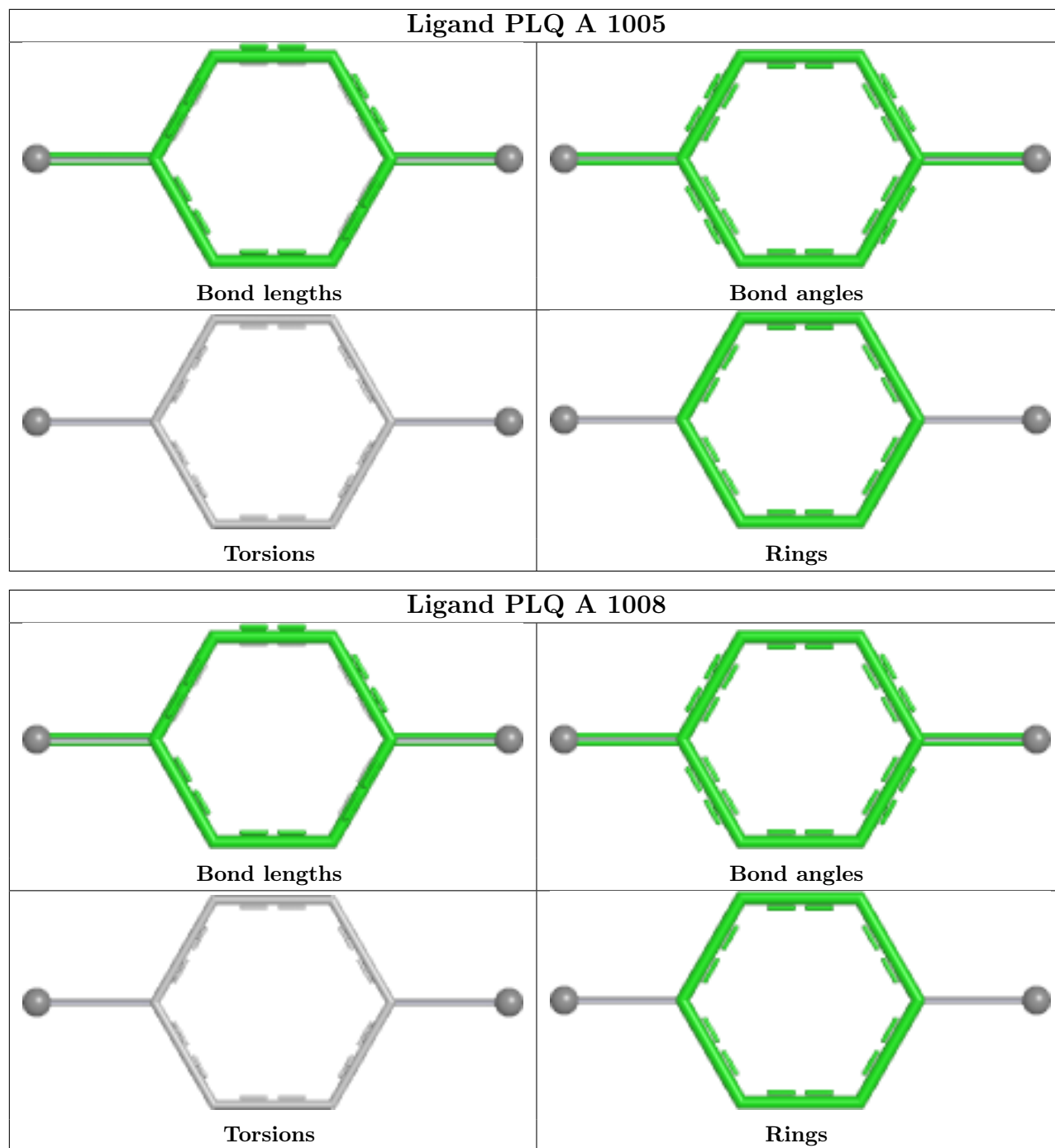


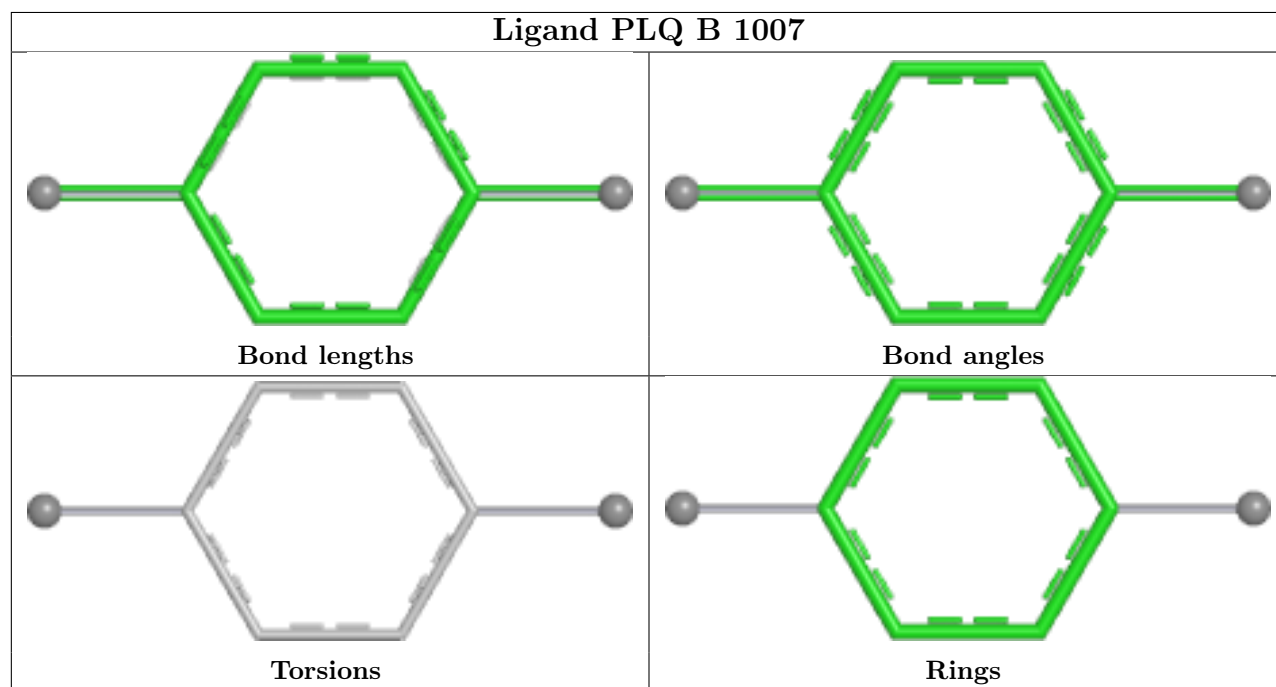
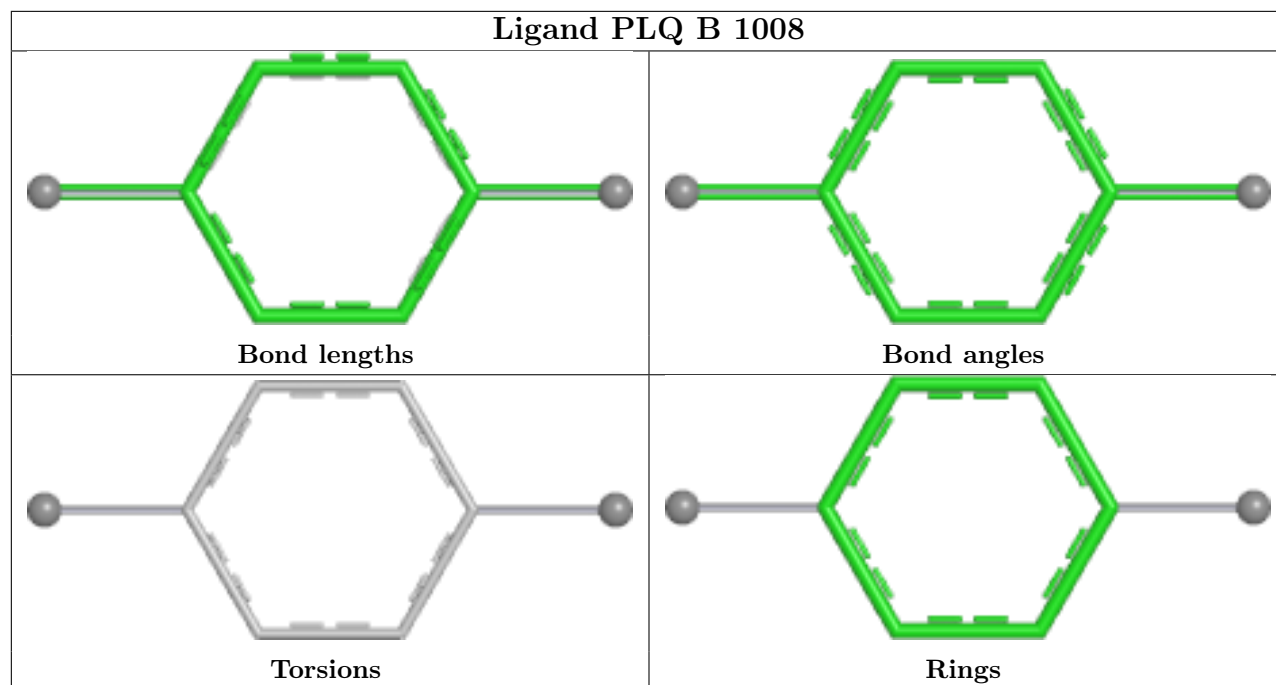


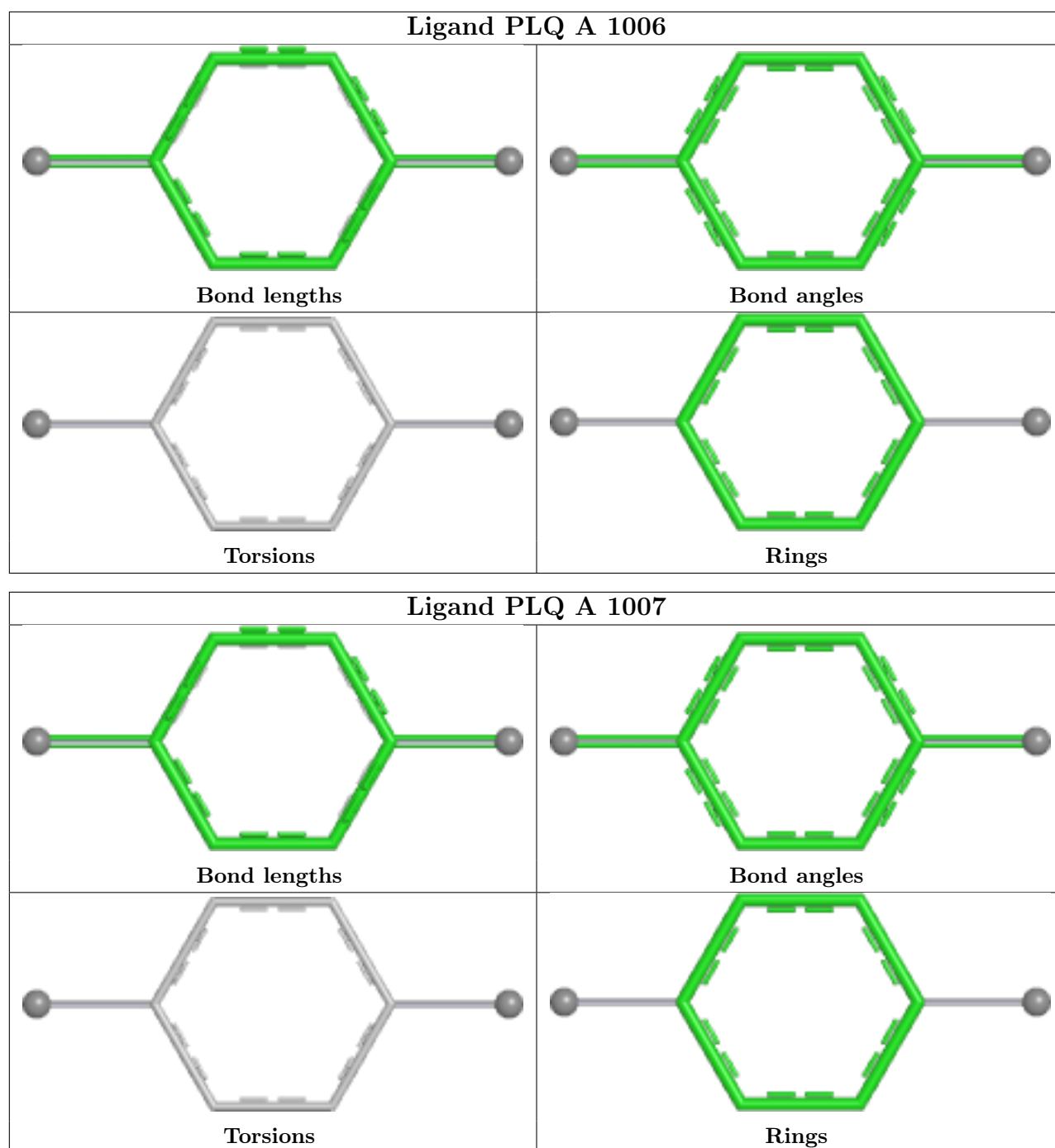












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	624/665 (93%)	-0.18	7 (1%) 78 81	12, 23, 36, 54	1 (0%)
1	B	624/665 (93%)	0.03	12 (1%) 66 70	14, 27, 42, 67	1 (0%)
All	All	1248/1330 (93%)	-0.07	19 (1%) 72 76	12, 25, 40, 67	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	TRP	5.7
1	A	317	TRP	4.3
1	B	42	CYS	3.8
1	B	240	ILE	3.5
1	A	291	TYR	3.1
1	A	43	SER	3.0
1	B	446	THR	2.8
1	B	619	ALA	2.7
1	A	436	GLU	2.5
1	A	571	GLU	2.3
1	B	569	GLY	2.3
1	B	239	SER	2.3
1	A	239	SER	2.2
1	A	42	CYS	2.2
1	B	354	VAL	2.2
1	B	233	LEU	2.2
1	B	571	GLU	2.0
1	B	448	GLY	2.0
1	B	618	THR	2.0

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

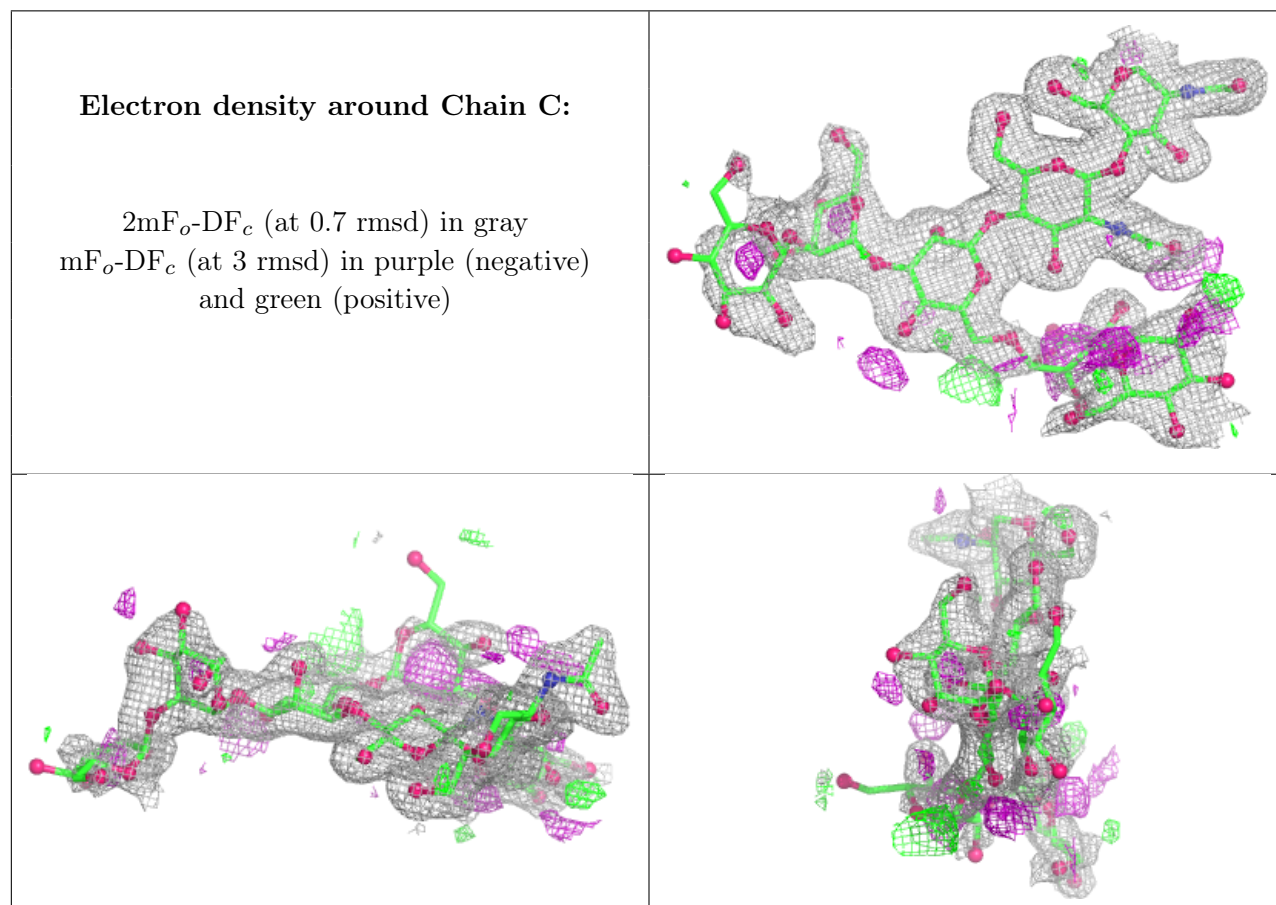
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.

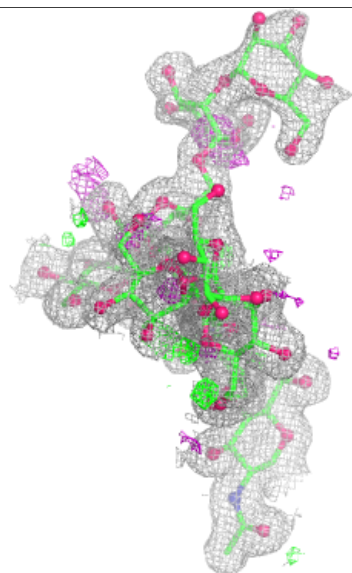
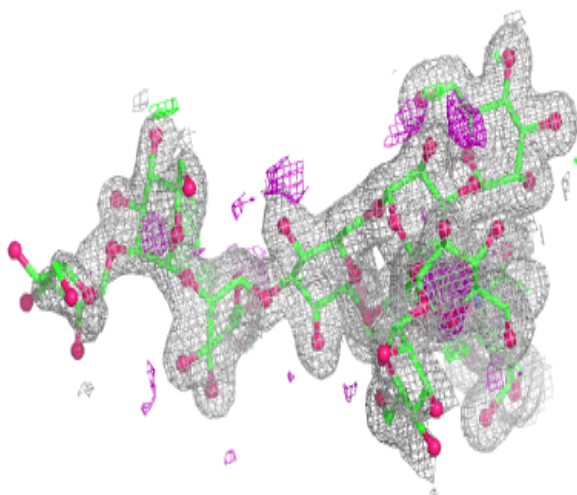
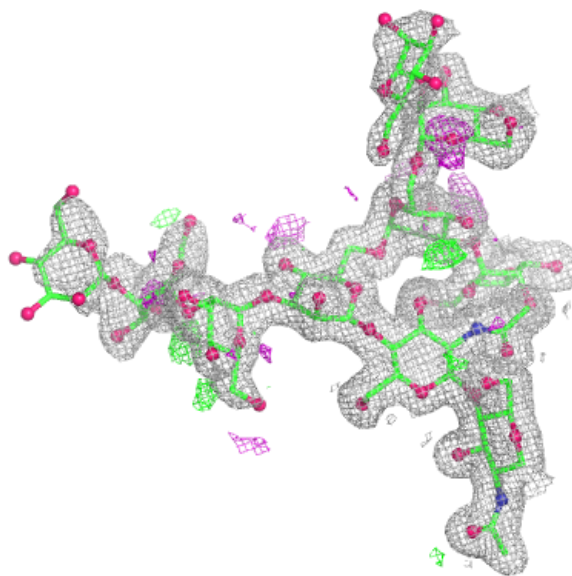
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	5	11/12	0.49	0.18	80,92,98,102	0
3	MAN	G	6	11/12	0.51	0.17	83,95,102,103	0
3	MAN	D	6	11/12	0.55	0.16	93,100,108,112	0
4	NAG	E	2	14/15	0.57	0.19	70,86,93,99	0
2	MAN	C	6	11/12	0.61	0.23	62,81,87,93	0
4	NAG	H	2	14/15	0.62	0.17	66,85,94,96	0
5	MAN	F	4	11/12	0.62	0.20	76,90,94,96	0
5	MAN	F	6	11/12	0.63	0.15	75,81,85,93	0
3	MAN	D	9	11/12	0.66	0.18	64,76,83,83	0
3	MAN	G	9	11/12	0.67	0.18	60,71,78,81	0
2	MAN	C	4	11/12	0.80	0.13	61,72,74,76	0
2	MAN	C	7	11/12	0.83	0.18	57,61,70,71	0
3	MAN	D	5	11/12	0.83	0.14	55,61,67,75	0
4	NAG	E	1	14/15	0.88	0.12	43,49,57,76	0
3	MAN	G	4	11/12	0.88	0.12	36,45,53,64	0
4	NAG	H	1	14/15	0.88	0.12	43,52,63,73	0
3	MAN	G	5	11/12	0.88	0.12	52,59,66,75	0
3	MAN	D	8	11/12	0.88	0.13	36,43,52,56	0
5	MAN	F	5	11/12	0.88	0.16	72,80,86,88	0
3	MAN	D	4	11/12	0.88	0.13	35,44,54,64	0
5	BMA	F	3	11/12	0.89	0.12	37,48,62,69	0
3	MAN	G	8	11/12	0.91	0.12	41,44,50,54	0
2	BMA	C	3	11/12	0.91	0.11	33,40,48,64	0
5	NAG	F	2	14/15	0.95	0.08	28,30,35,36	0
3	BMA	G	3	11/12	0.96	0.06	22,23,26,31	0
3	MAN	G	7	11/12	0.97	0.07	19,20,27,32	0
5	NAG	F	1	14/15	0.97	0.07	22,26,37,39	0
2	NAG	C	2	14/15	0.97	0.07	23,27,31,45	0
2	NAG	C	1	14/15	0.97	0.07	19,22,31,34	0
3	NAG	D	2	14/15	0.97	0.06	17,18,20,21	0
3	MAN	D	7	11/12	0.97	0.06	18,20,26,31	0
3	BMA	D	3	11/12	0.97	0.05	21,22,24,29	0
3	MAN	D	10	11/12	0.98	0.05	16,17,17,18	0
3	NAG	G	1	14/15	0.98	0.04	17,19,22,22	0
3	NAG	G	2	14/15	0.98	0.05	19,20,21,22	0
3	NAG	D	1	14/15	0.98	0.04	15,16,17,19	0
3	MAN	G	10	11/12	0.99	0.04	17,19,19,20	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.



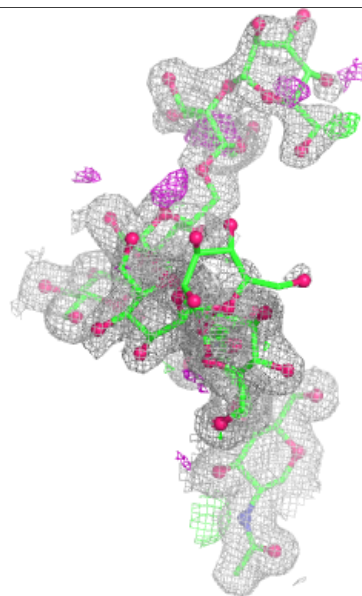
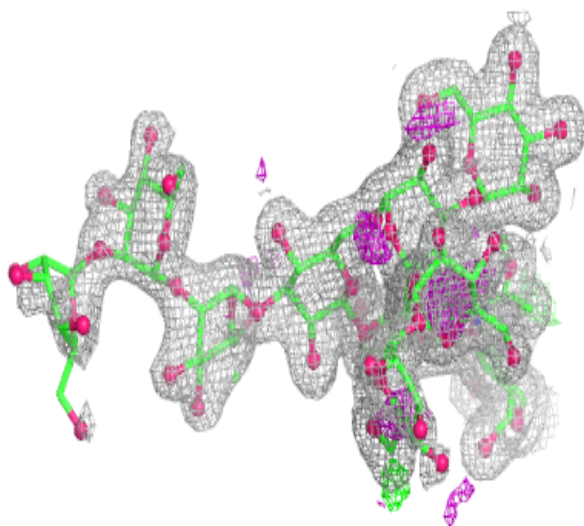
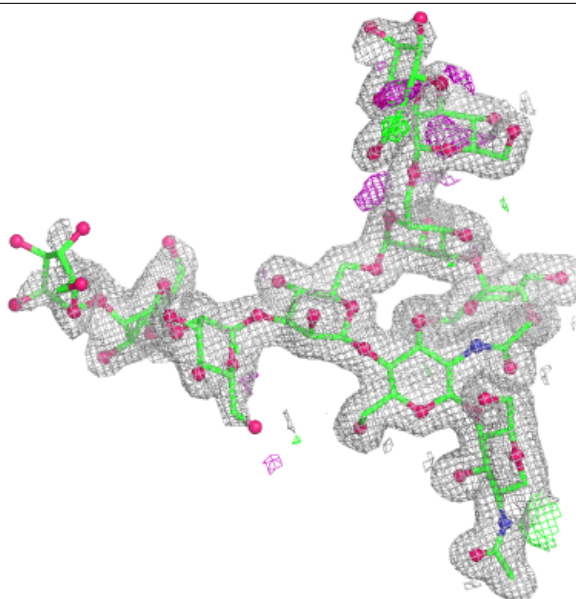
Electron density around Chain D:

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



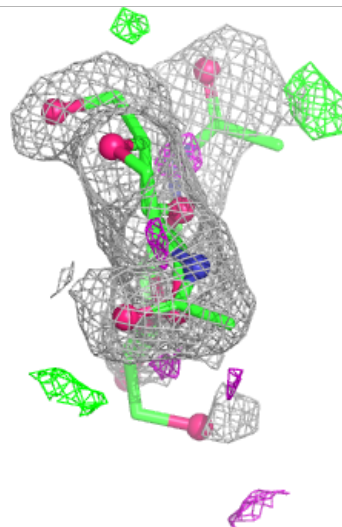
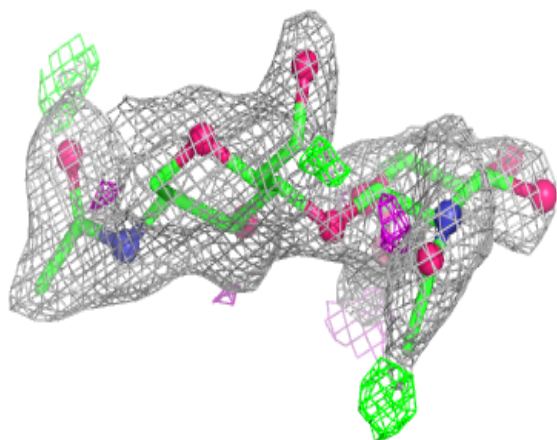
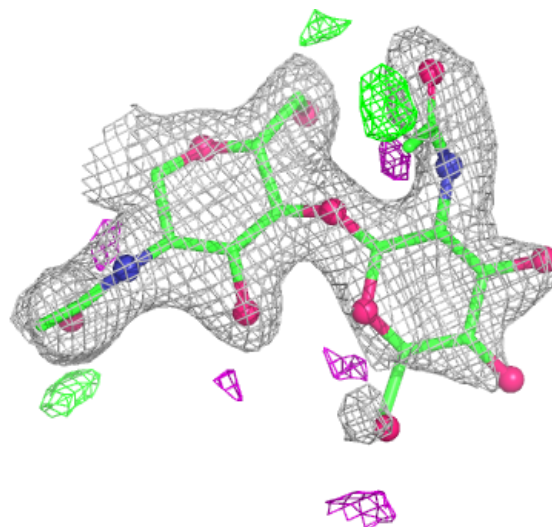
Electron density around Chain G:

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



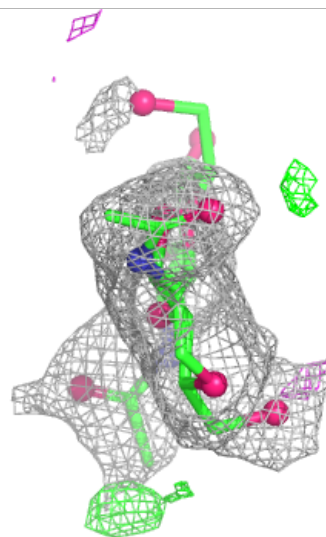
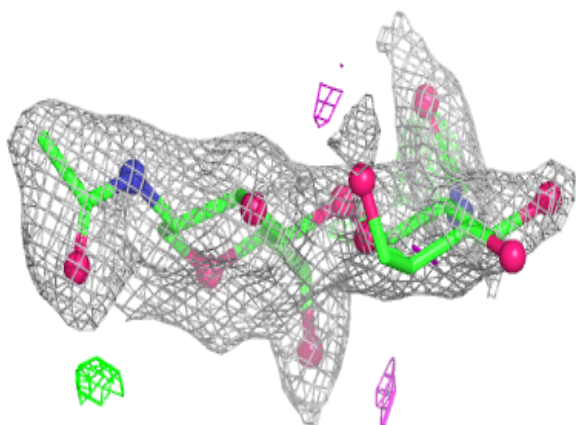
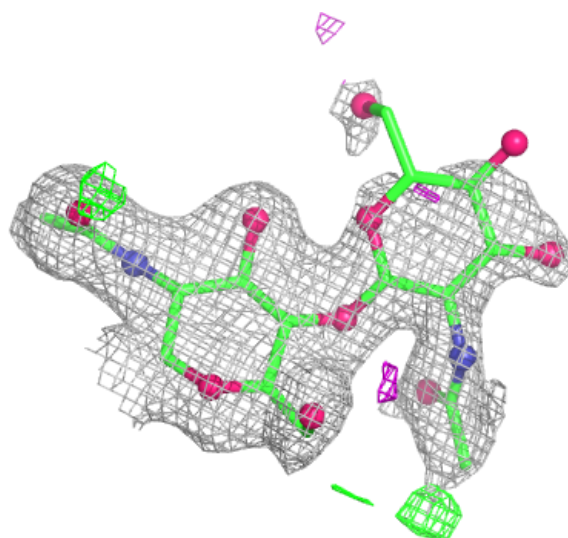
Electron density around Chain E:

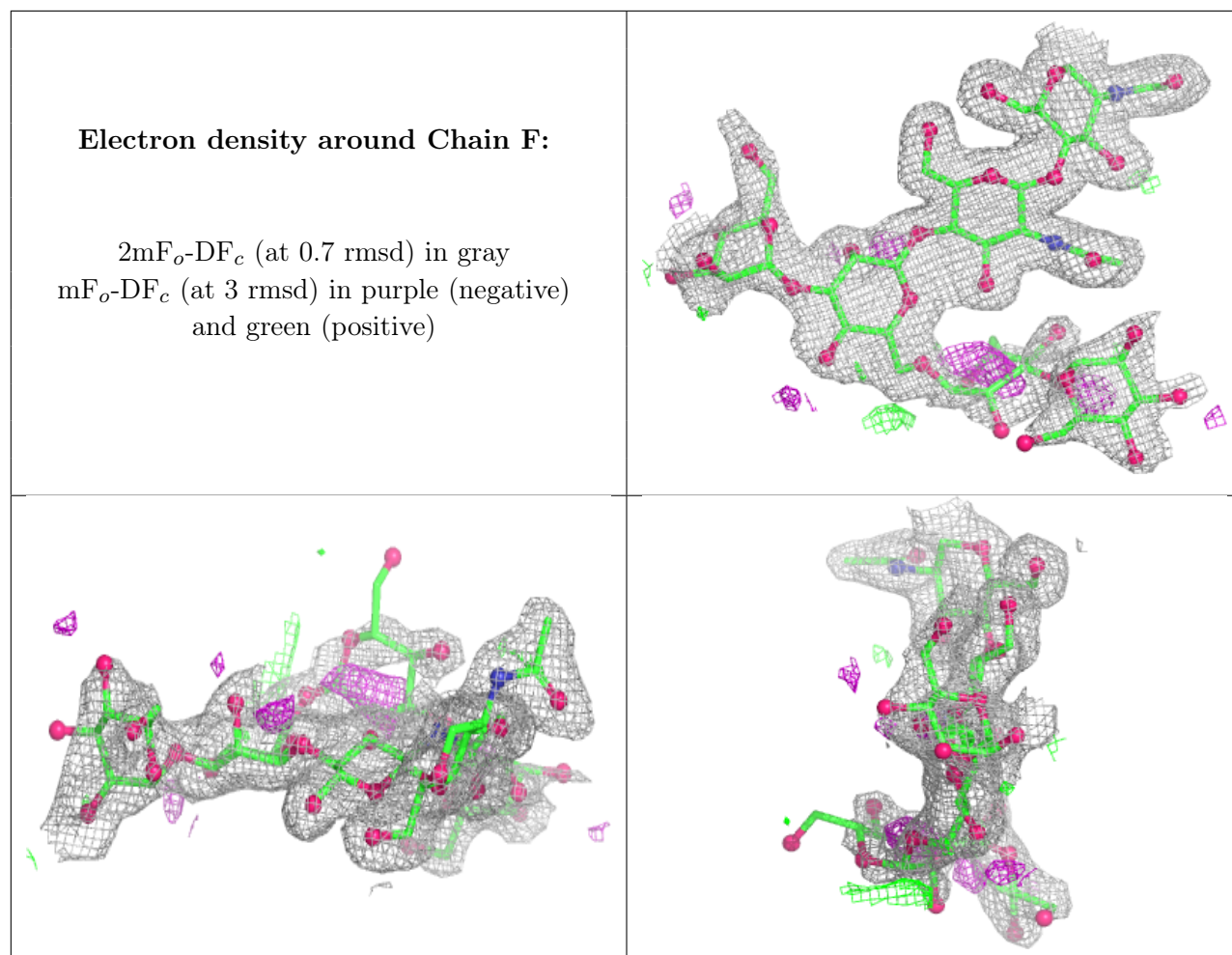
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	B	1242	14/15	0.52	0.18	77,86,95,105	0
9	NAG	B	1319	14/15	0.55	0.20	76,85,90,94	0
9	NAG	A	1512	14/15	0.72	0.17	56,80,93,105	0
7	PLQ	A	1001	8/8	0.73	0.27	59,64,69,70	0
9	NAG	B	1215	14/15	0.73	0.16	62,70,77,83	0
9	NAG	A	1215	14/15	0.74	0.17	60,68,77,85	0
7	PLQ	B	1001	8/8	0.74	0.30	65,73,81,82	0
9	NAG	A	1555	14/15	0.74	0.17	38,45,52,57	0
9	NAG	A	1319	14/15	0.75	0.16	65,68,78,83	0
7	PLQ	A	1006	8/8	0.76	0.25	50,58,67,68	0

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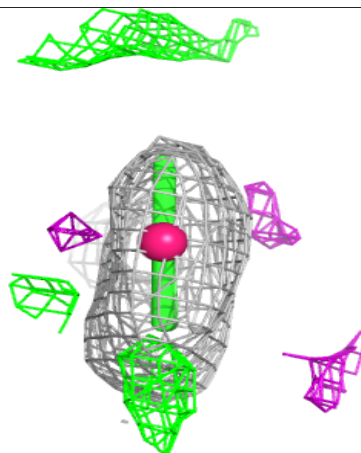
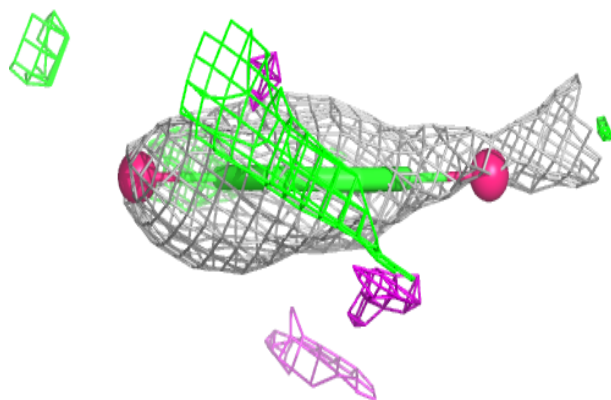
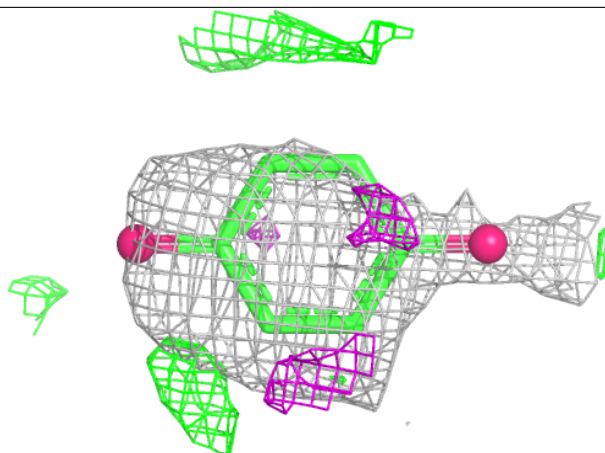
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	A	1242	14/15	0.76	0.16	59,66,73,77	0
9	NAG	A	1606	14/15	0.77	0.15	43,52,57,63	0
9	NAG	A	1052	14/15	0.77	0.17	50,59,64,65	0
7	PLQ	A	1010	8/8	0.78	0.18	48,54,60,63	0
9	NAG	A	1539	14/15	0.79	0.17	52,63,71,76	0
8	EDO	A	1002	4/4	0.79	0.23	56,60,61,62	0
7	PLQ	B	1008	8/8	0.80	0.20	50,52,61,62	0
7	PLQ	B	1009	8/8	0.80	0.19	55,65,70,72	0
9	NAG	B	1052	14/15	0.81	0.15	54,62,70,74	0
7	PLQ	A	1007	8/8	0.83	0.15	34,36,41,42	0
8	EDO	B	1003	4/4	0.83	0.20	42,49,50,54	0
7	PLQ	A	1005	8/8	0.84	0.17	38,48,50,53	0
7	PLQ	B	1005	8/8	0.84	0.17	44,55,58,65	0
8	EDO	B	1002	4/4	0.84	0.21	59,61,65,66	0
7	PLQ	A	1004	8/8	0.84	0.20	31,58,63,63	0
9	NAG	B	1483	14/15	0.84	0.15	50,60,67,67	0
9	NAG	B	1539	14/15	0.84	0.16	51,63,67,68	0
7	PLQ	A	1009	8/8	0.85	0.16	44,49,50,53	0
8	EDO	A	1003	4/4	0.85	0.20	35,43,47,54	0
7	PLQ	A	1011	8/8	0.85	0.21	55,60,67,72	0
7	PLQ	A	1008	8/8	0.86	0.18	35,48,58,69	0
7	PLQ	B	1006	8/8	0.86	0.16	35,40,43,45	0
7	PLQ	B	1004	8/8	0.87	0.17	33,57,62,65	0
9	NAG	A	1483	14/15	0.87	0.13	42,51,56,64	0
6	TRS	A	1000	8/8	0.88	0.19	24,44,53,55	0
9	NAG	A	1236	14/15	0.88	0.12	29,35,42,43	0
6	TRS	B	1000	8/8	0.88	0.20	32,52,64,66	0
7	PLQ	B	1007	8/8	0.90	0.15	33,56,62,80	0
9	NAG	B	1555	14/15	0.90	0.10	35,38,41,42	0
9	NAG	B	1471	14/15	0.93	0.09	33,36,46,47	0
9	NAG	A	1357	14/15	0.93	0.10	32,35,40,47	0
9	NAG	B	1357	14/15	0.93	0.10	38,40,49,50	0
9	NAG	B	1444	14/15	0.93	0.09	32,35,40,41	0
9	NAG	A	1471	14/15	0.94	0.09	31,35,39,49	0
9	NAG	A	1644	14/15	0.94	0.08	23,28,39,40	0
9	NAG	B	1644	14/15	0.94	0.08	27,29,41,45	0
9	NAG	A	1444	14/15	0.96	0.07	26,29,32,36	0

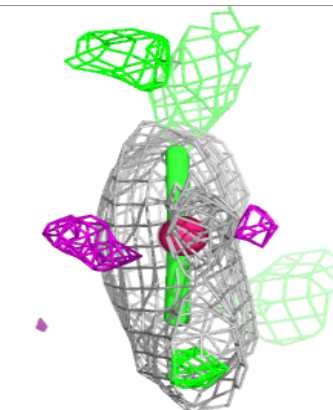
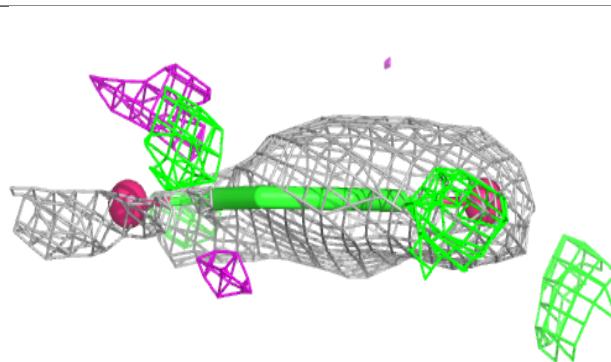
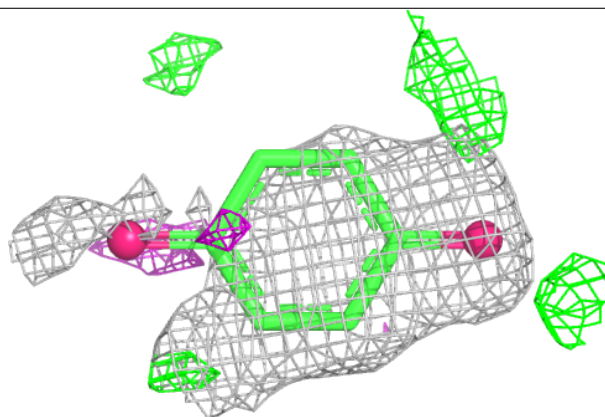
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLQ A 1001:

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

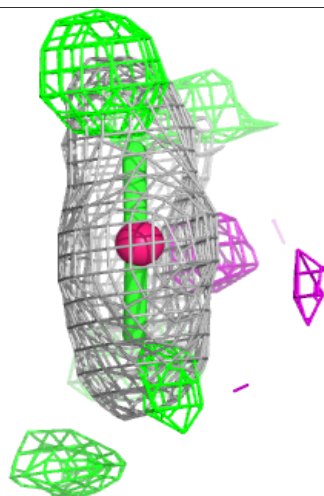
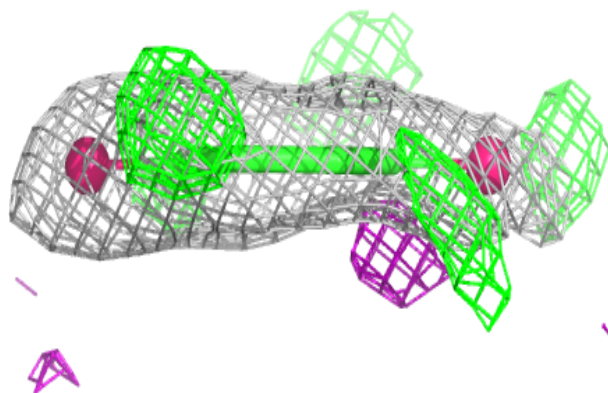
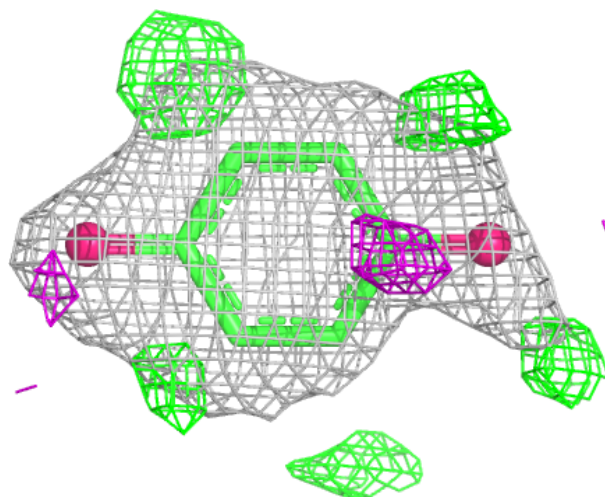
**Electron density around PLQ B 1001:**

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



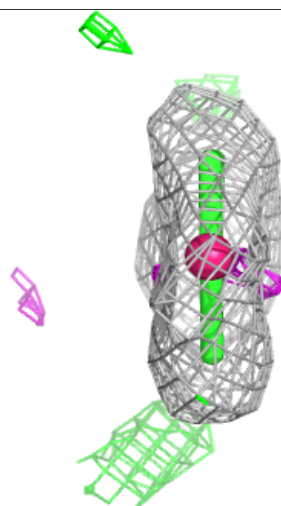
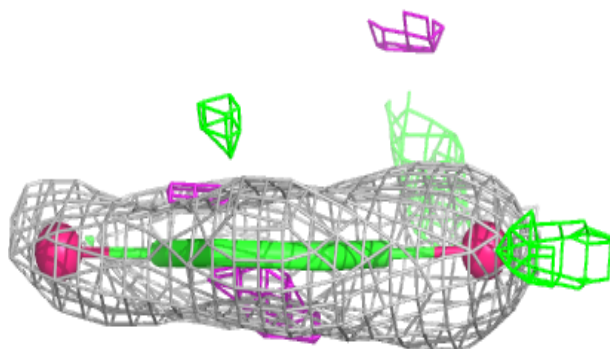
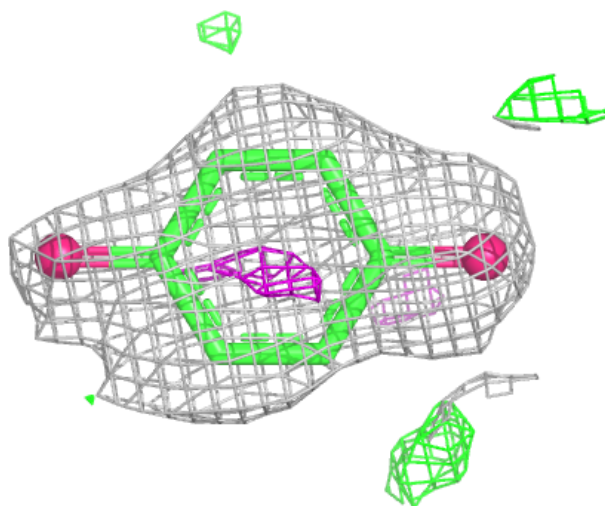
Electron density around PLQ A 1006:

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



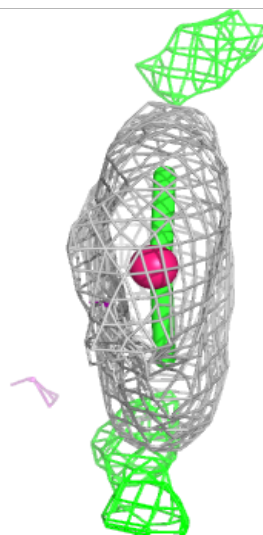
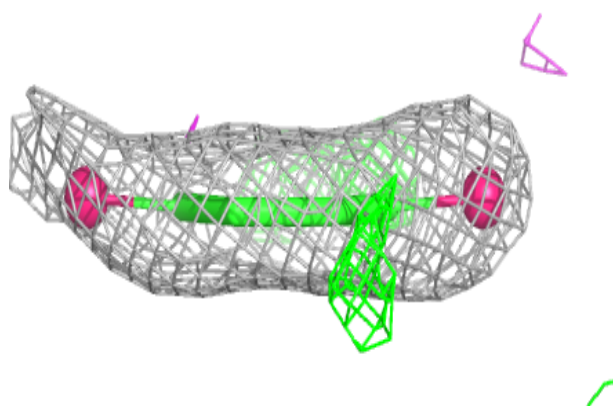
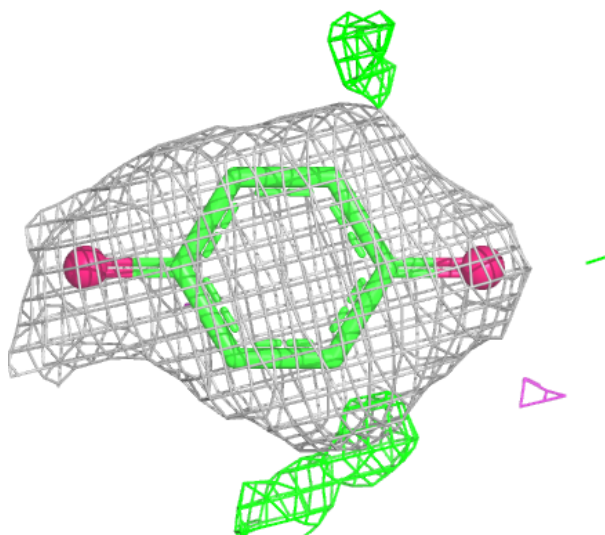
Electron density around PLQ A 1010:

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



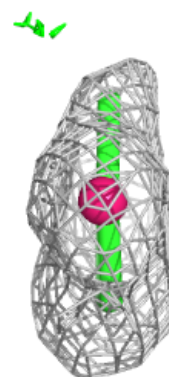
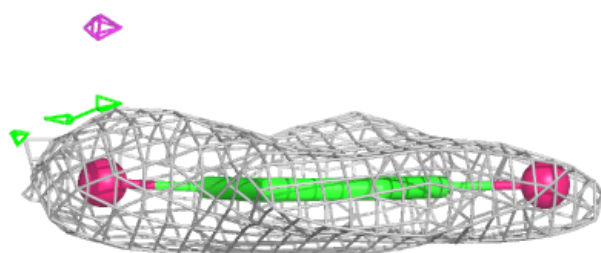
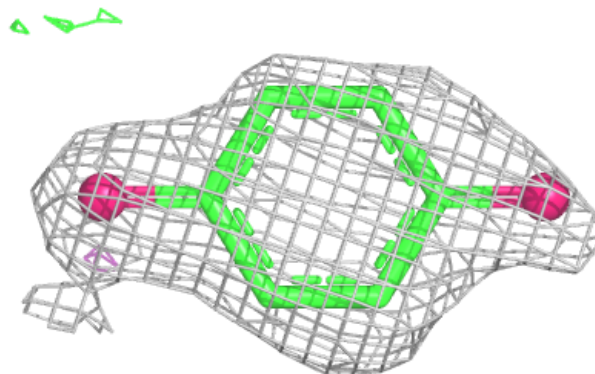
Electron density around PLQ B 1008:

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

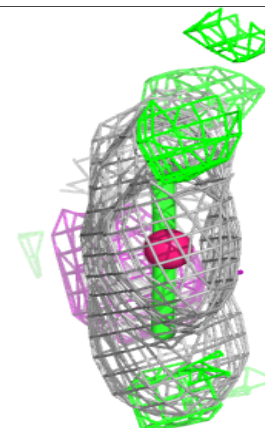
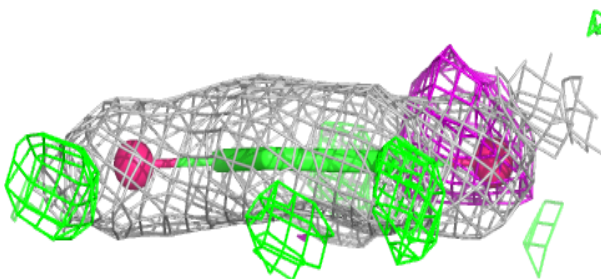
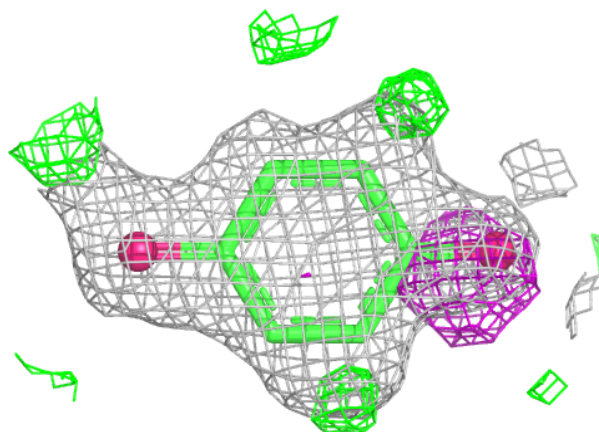


Electron density around PLQ B 1009:

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

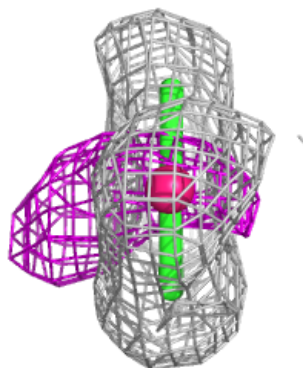
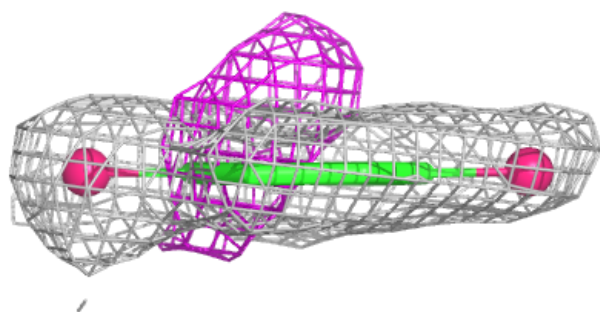
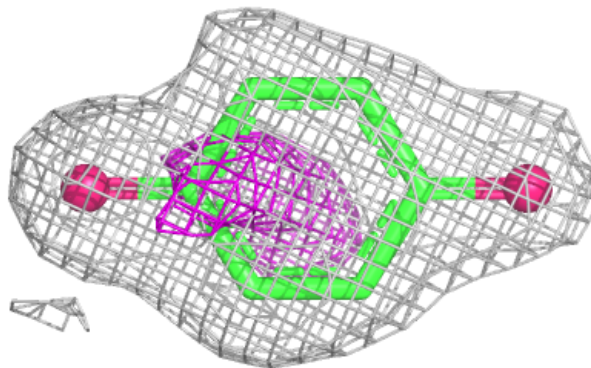
**Electron density around PLQ A 1007:**

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

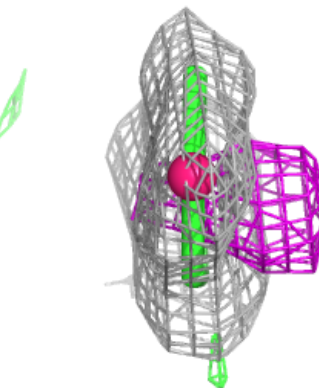
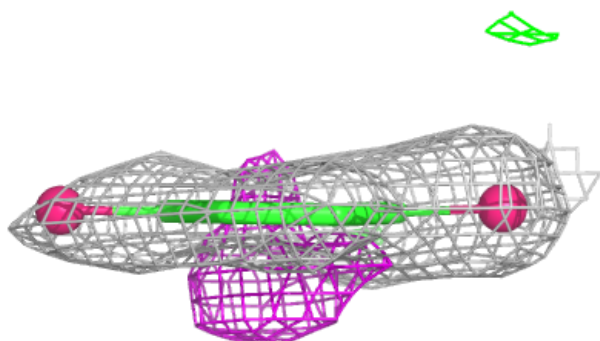
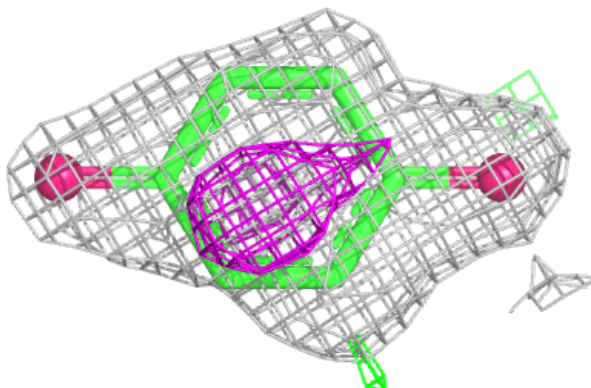


Electron density around PLQ A 1005:

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

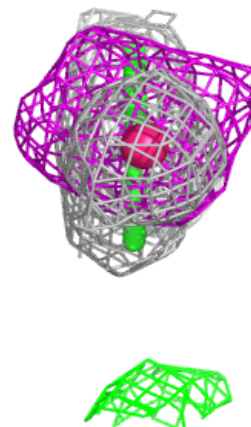
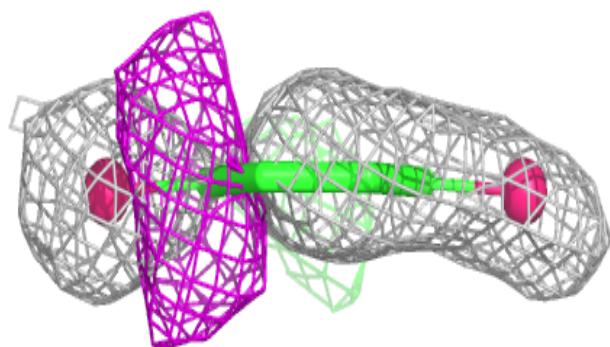
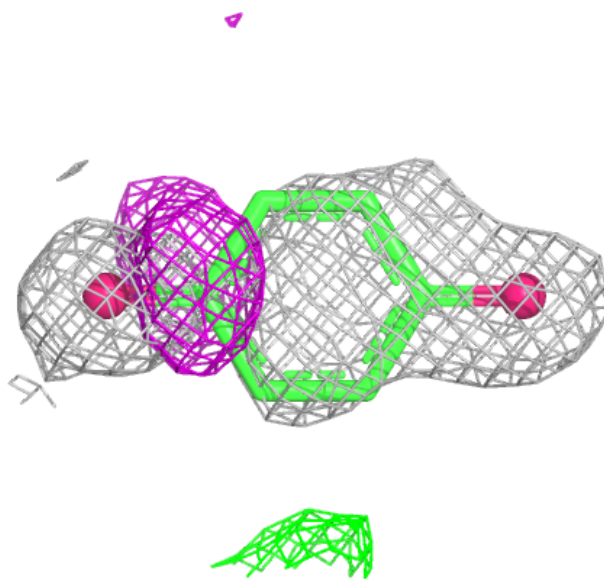
**Electron density around PLQ B 1005:**

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



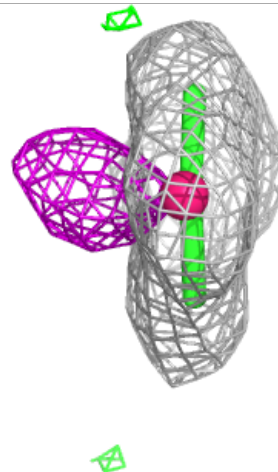
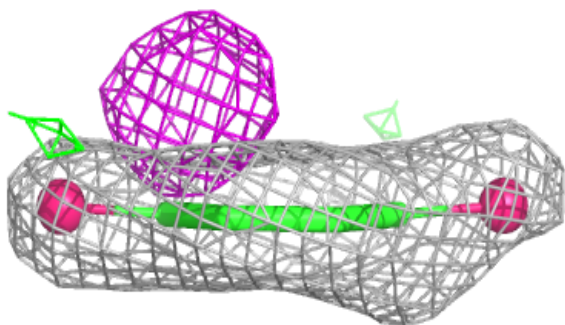
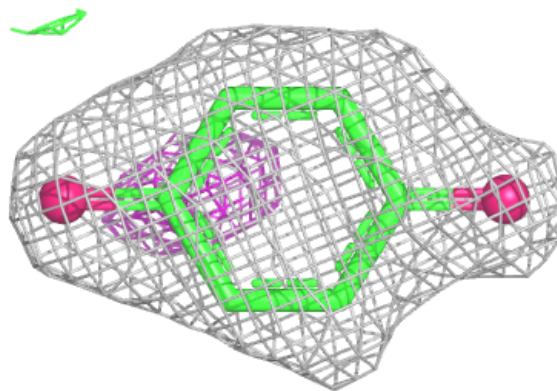
Electron density around PLQ A 1004:

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



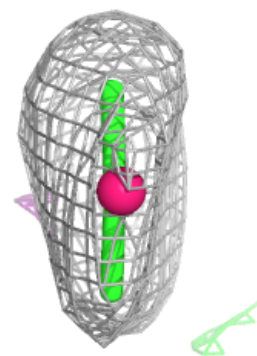
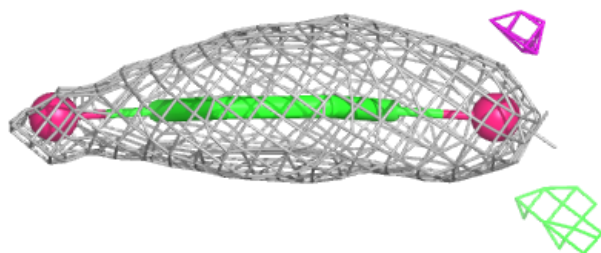
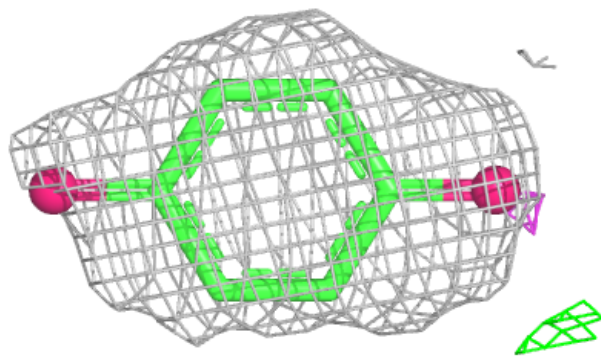
Electron density around PLQ A 1009:

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



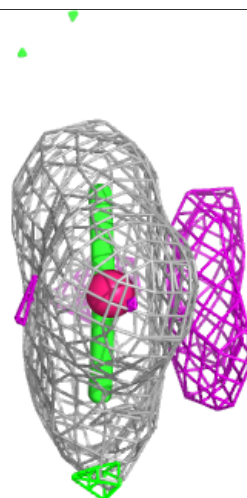
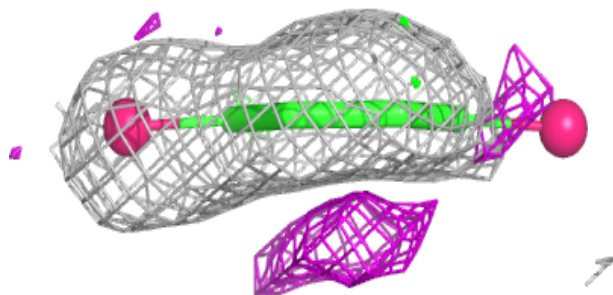
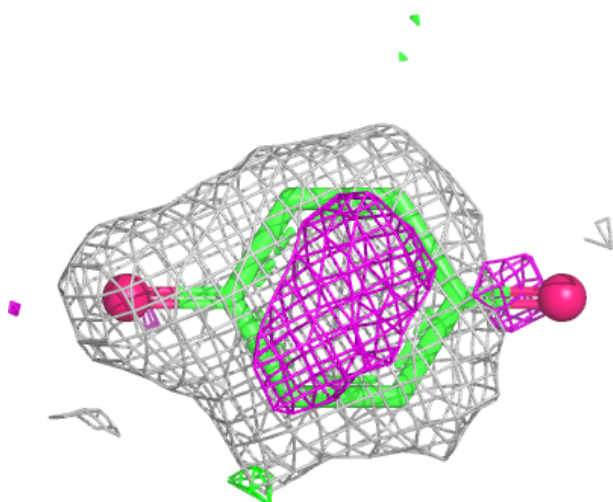
Electron density around PLQ A 1011:

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



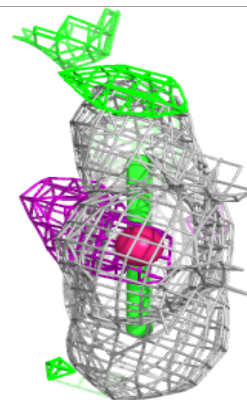
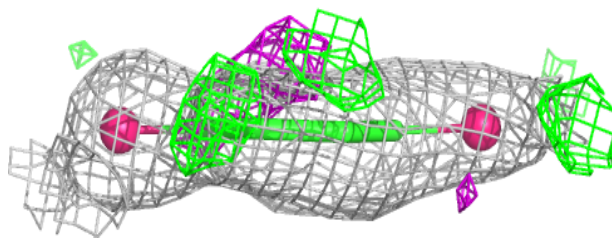
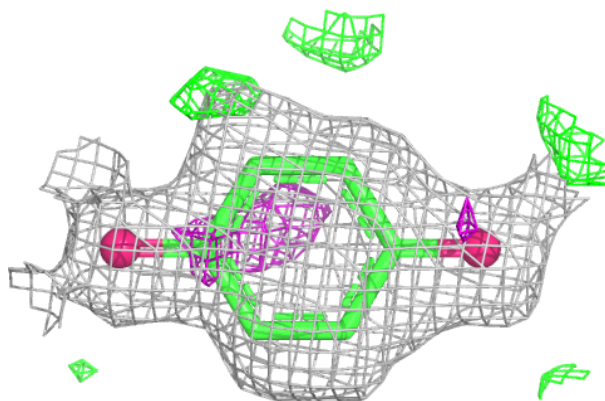
Electron density around PLQ A 1008:

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



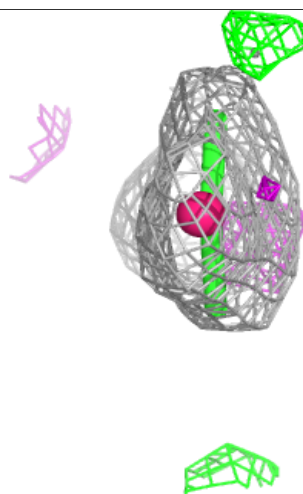
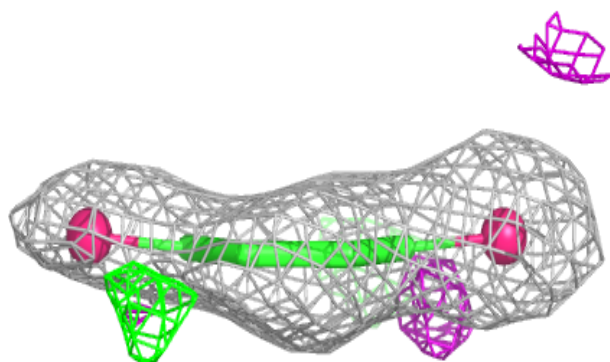
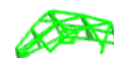
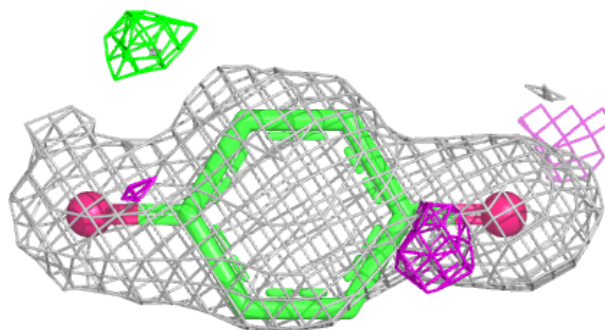
Electron density around PLQ B 1006:

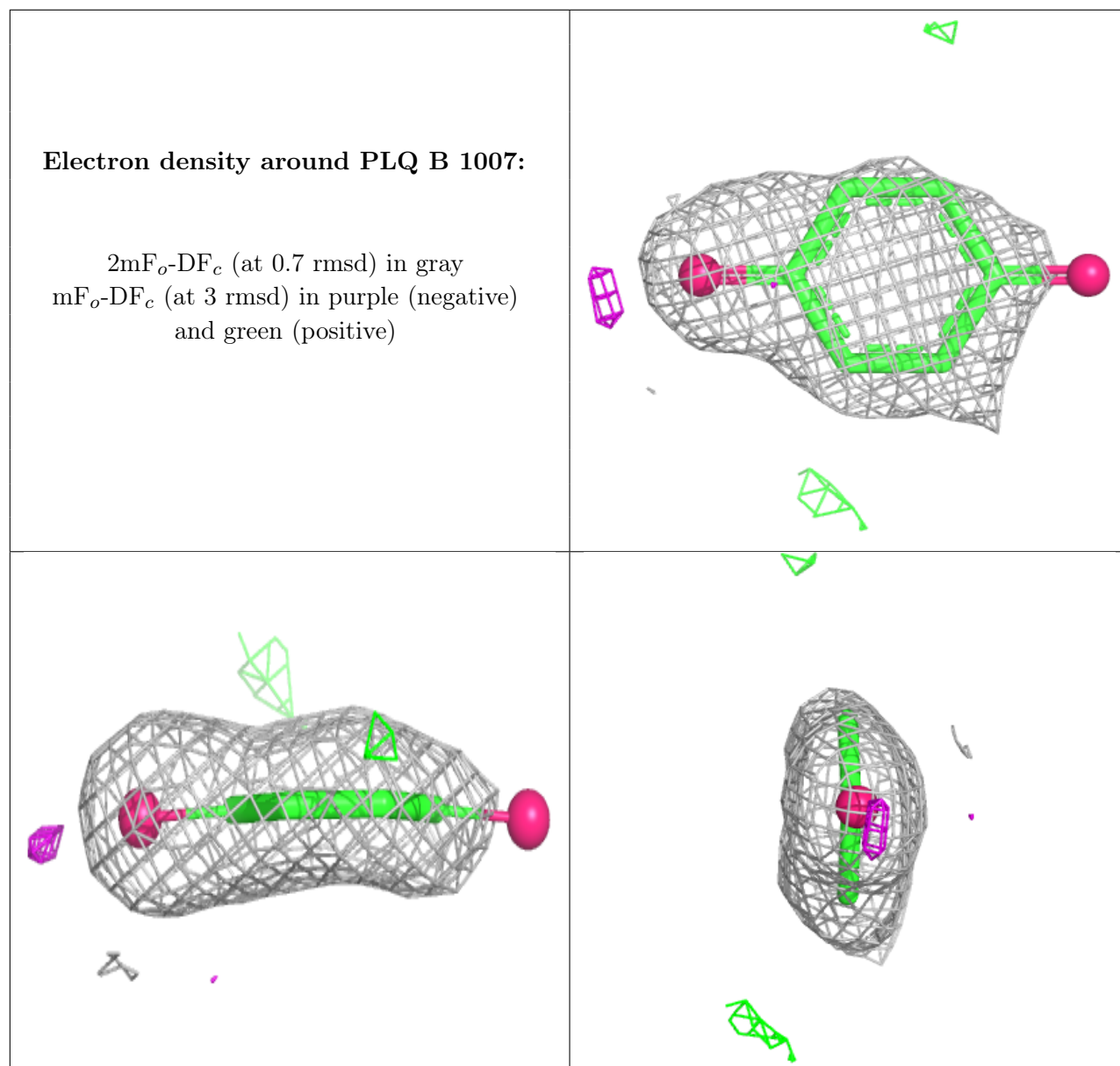
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLQ B 1004:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.