



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:28 PM UTC

PDB ID : 5DLV / pdb_00005dlv
Title : Crystal structure of Autotaxin (ENPP2) with tauroursodeoxycholic acid (TUDCA)
Authors : Keune, W.J.; Heidebrecht, T.; von Castelmur, E.; Joosten, R.P.; Perrakis, A.
Deposited on : 2015-09-07
Resolution : 2.00 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

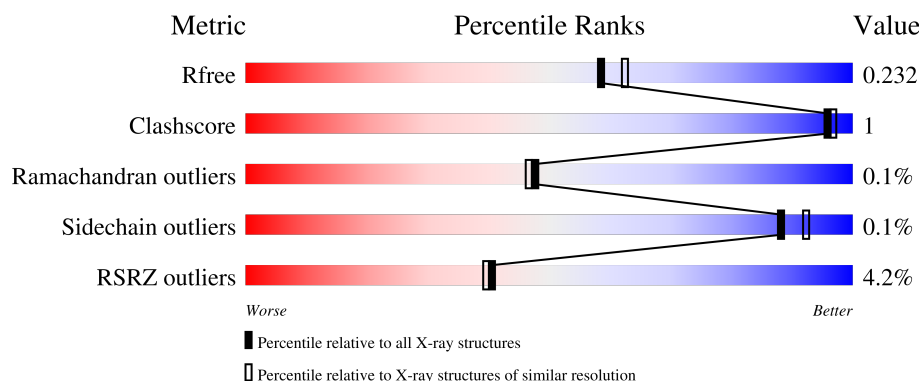
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	827	4% 93% 6%
1	B	827	4% 92% 6%
2	C	9	33% 67%
3	D	7	29% 71%

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	IOD	A	921	-	-	X	-
6	IOD	B	923	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13814 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.

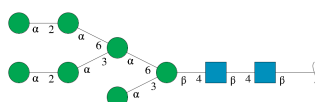
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	5	0
			6354	4035	1095	1175	49			
1	B	781	Total	C	N	O	S	0	5	0
			6354	4035	1095	1175	49			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	cloning artifact	UNP Q64610
A	806	ALA	ASN	engineered mutation	UNP Q64610
B	410	ALA	ASN	engineered mutation	UNP Q64610
B	591	THR	ARG	cloning artifact	UNP Q64610
B	806	ALA	ASN	engineered mutation	UNP Q64610

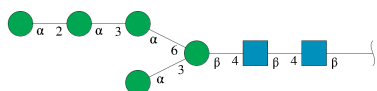
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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-glu

copyranose.



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	I	0	0
			14	14		
6	B	13	Total	I	0	0
			13	13		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

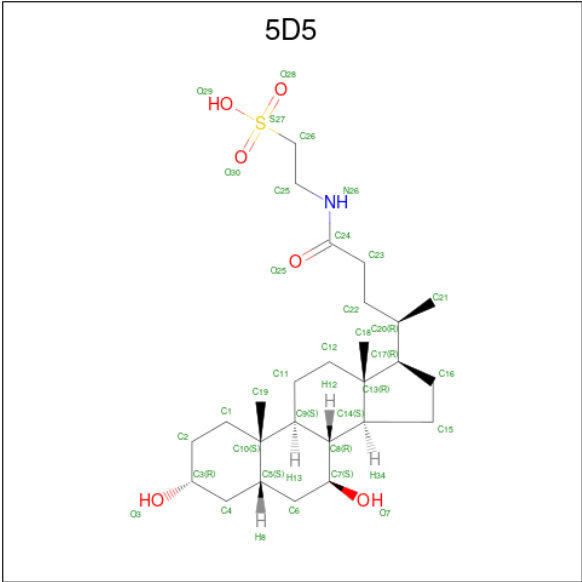


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

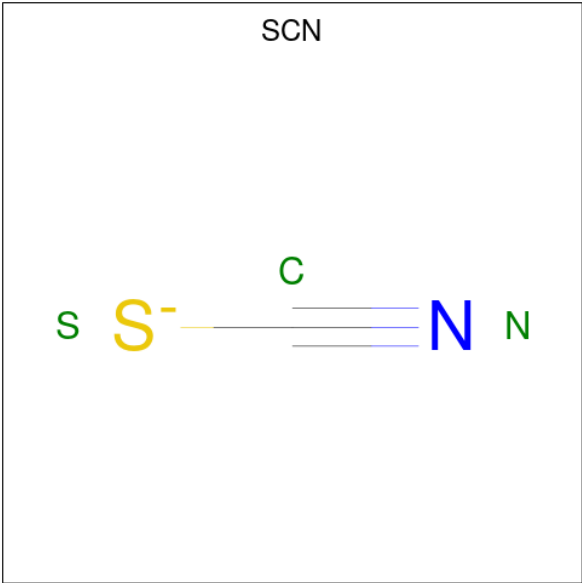
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Na	0	0
			2	2		
8	B	2	Total	Na	0	0
			2	2		

- Molecule 9 is 2-[(3alpha,5beta,7alpha,8alpha,14beta,17alpha)-3,7-dihydroxy-24-oxocholan-24-yl]amino}ethanesulfonic acid (CCD ID: 5D5) (formula: C₂₆H₄₅NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	1
			102	78	3	18	3		
9	B	1	Total	C	N	O	S	0	1
			102	78	3	18	3		

- Molecule 10 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



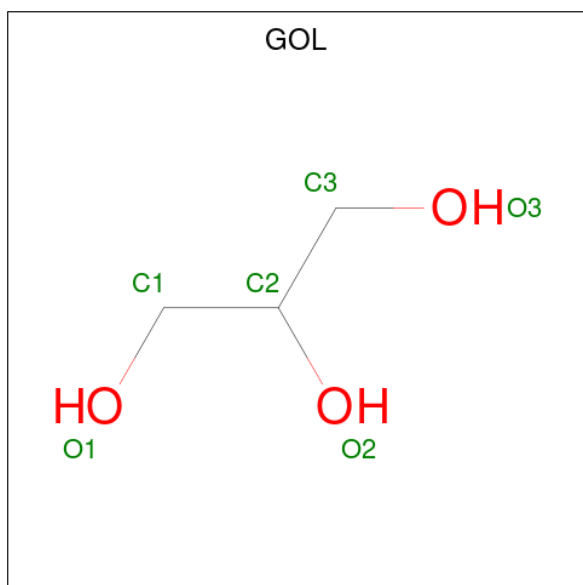
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	S	0	0
			3	1	1	1		
10	A	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	S	0	0
			3	1	1	1		
10	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	299	Total	O	0	1
			300	300		
12	B	288	Total	O	0	1
			289	289		

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

Chain D: 

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.88Å 77.83Å 92.44Å 83.84° 79.29° 77.08°	Depositor
Resolution (Å)	90.61 – 2.00 90.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (90.61-2.00) 95.9 (90.61-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.193 , 0.227 0.200 , 0.232	Depositor DCC
R_{free} test set	5310 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	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	0.95	EDS
Total number of atoms	13814	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: MAN, ZN, PO4, GOL, IOD, BMA, NAG, NA, 5D5, SCN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/6544	0.83	1/8876 (0.0%)
1	B	0.69	0/6544	0.83	1/8876 (0.0%)
All	All	0.69	0/13088	0.83	2/17752 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	PRO	N-CA-C	6.59	118.75	110.70
1	A	70	PRO	N-CA-C	6.57	118.71	110.70

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	6354	0	6112	8	0
1	B	6354	0	6112	12	0
2	C	105	0	88	0	0
3	D	83	0	70	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	14	0	0	3	0
6	B	13	0	0	2	0
7	A	5	0	0	1	0
7	B	5	0	0	1	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	102	0	0	2	0
9	B	102	0	0	4	0
10	A	6	0	0	0	0
10	B	6	0	0	0	0
11	A	36	0	48	0	0
11	B	30	0	40	1	0
12	A	300	0	0	1	0
12	B	289	0	0	1	0
All	All	13814	0	12470	27	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 1.

All (27) 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)
9:A:930[B]:5D5:O25	9:A:930[B]:5D5:C26	2.30	0.80
6:B:923:IOD:I	12:B:1269:HOH:O	2.73	0.76
1:A:197:HIS:CD2	6:A:921:IOD:I	3.16	0.69
6:A:923:IOD:I	12:A:1298:HOH:O	2.86	0.63
1:A:197:HIS:NE2	6:A:921:IOD:I	3.04	0.60
9:A:930[A]:5D5:N26	9:A:930[A]:5D5:O30	2.35	0.59
9:B:927[A]:5D5:O25	9:B:927[A]:5D5:C26	2.50	0.57
1:B:209:THR:OG1	7:B:924:PO4:P	2.67	0.52
1:B:499:LYS:HE2	6:B:923:IOD:I	2.83	0.49
9:B:927[A]:5D5:C12	9:B:927[A]:5D5:C21	2.90	0.49
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.48	0.49
1:B:274:PHE:HA	9:B:927[B]:5D5:O29	2.14	0.48
1:B:222:PRO:HA	1:B:225:HIS:CE1	2.49	0.48
1:B:171:ASP:OD2	1:B:306[B]:TYR:OH	2.20	0.47
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.49	0.47
1:B:371:PHE:CE1	1:B:457:PRO:HA	2.49	0.46
1:A:176:SER:O	1:A:179:LYS:HB2	2.16	0.45
1:B:684:TYR:HE2	11:B:934:GOL:O2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:HIS:CE1	1:A:474:HIS:CE1	3.06	0.44
1:A:209:THR:OG1	7:A:927:PO4:P	2.78	0.42
9:B:927[B]:5D5:C22	9:B:927[B]:5D5:C25	2.95	0.42
1:B:359:HIS:CE1	1:B:474:HIS:CE1	3.08	0.42
1:B:269[B]:ARG:HG2	1:B:300:PRO:HA	2.01	0.41
1:A:201:MET:HE1	1:A:356:VAL:CG2	2.50	0.41
1:B:64:GLU:OE2	1:B:68:VAL:HG21	2.20	0.41
1:B:586:HIS:HB3	1:B:589:GLY:H	1.87	0.40
1:B:711:VAL:HG13	1:B:815:VAL:HG13	2.03	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	781/827 (94%)	756 (97%)	24 (3%)	1 (0%)	48	46
1	B	781/827 (94%)	755 (97%)	25 (3%)	1 (0%)	48	46
All	All	1562/1654 (94%)	1511 (97%)	49 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	B	83	SER

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	712/749 (95%)	711 (100%)	1 (0%)	88	92
1	B	712/749 (95%)	711 (100%)	1 (0%)	88	92
All	All	1424/1498 (95%)	1422 (100%)	2 (0%)	88	92

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

Mol	Chain	Res	Type
1	A	66	GLN
1	B	614	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	242	HIS
1	A	481	ASN
1	A	731	ASN
1	B	115	ASN
1	B	242	HIS
1	B	257	GLN
1	B	419	HIS
1	B	647	HIS

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](#)

16 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	2,1	14,14,15	0.37	0	17,19,21	1.24	1 (5%)
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	1.16	2 (11%)
2	BMA	C	3	2	11,11,12	0.47	0	15,15,17	0.84	0
2	MAN	C	4	2	11,11,12	0.41	0	15,15,17	1.07	0
2	MAN	C	5	2	11,11,12	0.46	0	15,15,17	0.67	0
2	MAN	C	6	2	11,11,12	0.48	0	15,15,17	1.17	1 (6%)
2	MAN	C	7	2	11,11,12	0.68	0	15,15,17	1.52	2 (13%)
2	MAN	C	8	2	11,11,12	0.60	0	15,15,17	1.10	1 (6%)
2	MAN	C	9	2	11,11,12	0.66	0	15,15,17	1.45	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	1.34	2 (11%)
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
3	BMA	D	3	3	11,11,12	0.46	0	15,15,17	0.93	0
3	MAN	D	4	3	11,11,12	0.67	0	15,15,17	1.32	1 (6%)
3	MAN	D	5	3	11,11,12	0.72	0	15,15,17	1.17	1 (6%)
3	MAN	D	6	3	11,11,12	0.72	0	15,15,17	0.81	0
3	MAN	D	7	3	11,11,12	0.39	0	15,15,17	1.07	1 (6%)

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	2,1	-	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	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
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-3.73	105.51	111.29
2	C	7	MAN	C6-C5-C4	3.62	121.90	113.02
2	C	9	MAN	C1-O5-C5	3.62	117.03	112.19
3	D	1	NAG	O5-C1-C2	-3.60	105.72	111.29
3	D	4	MAN	C1-C2-C3	3.07	114.12	109.64
2	C	8	MAN	C1-O5-C5	3.06	116.29	112.19
3	D	7	MAN	C1-O5-C5	3.05	116.27	112.19
2	C	2	NAG	O3-C3-C2	-2.74	103.71	109.40
2	C	6	MAN	C1-O5-C5	2.53	115.57	112.19
2	C	9	MAN	C2-C3-C4	2.35	115.00	110.86
3	D	1	NAG	C3-C4-C5	2.33	114.47	110.23
2	C	2	NAG	O5-C5-C4	-2.31	105.20	110.83
3	D	2	NAG	O4-C4-C5	-2.28	103.71	109.32
2	C	7	MAN	O5-C5-C4	-2.15	105.59	110.83
3	D	5	MAN	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

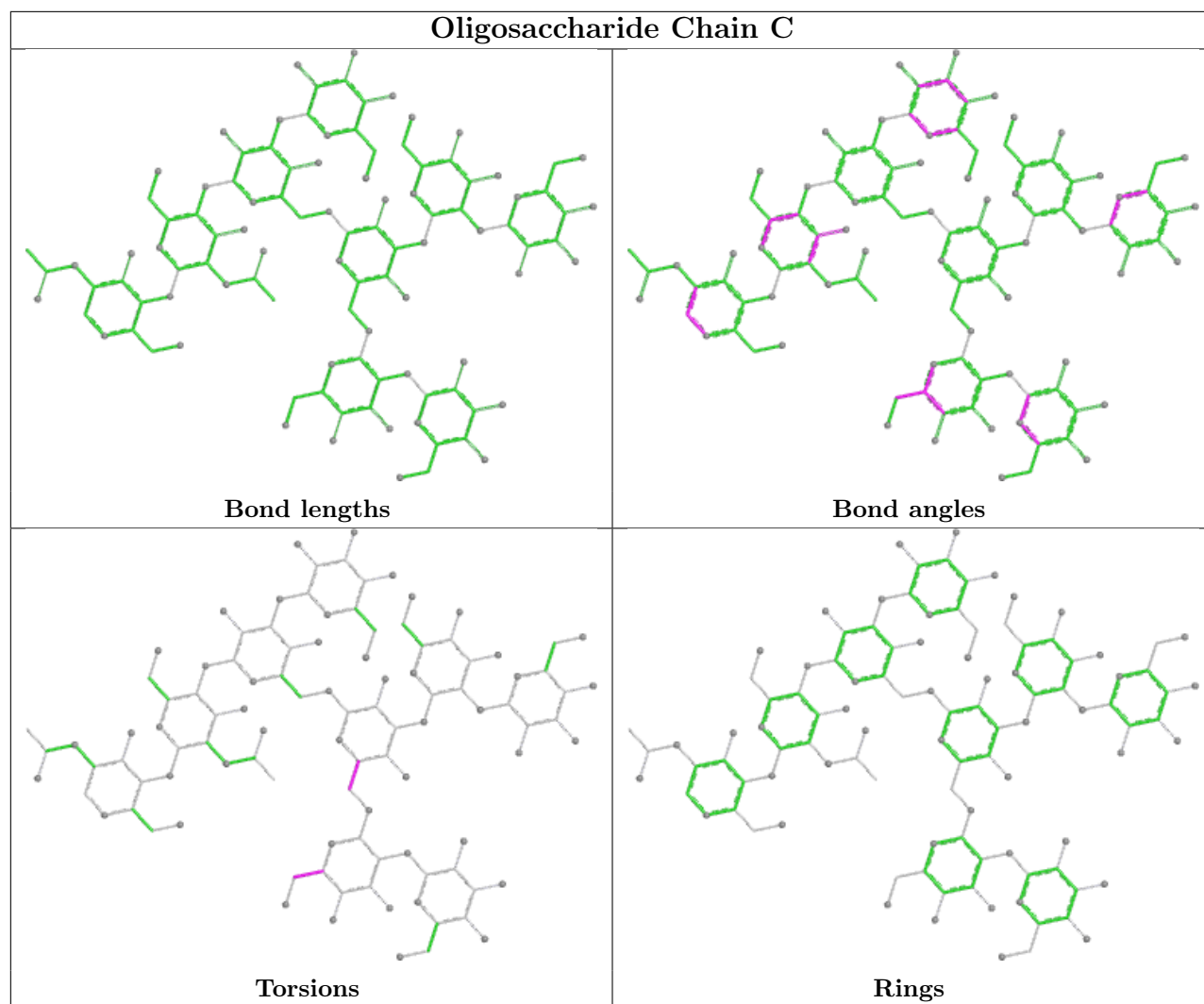
Mol	Chain	Res	Type	Atoms
3	D	7	MAN	C4-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

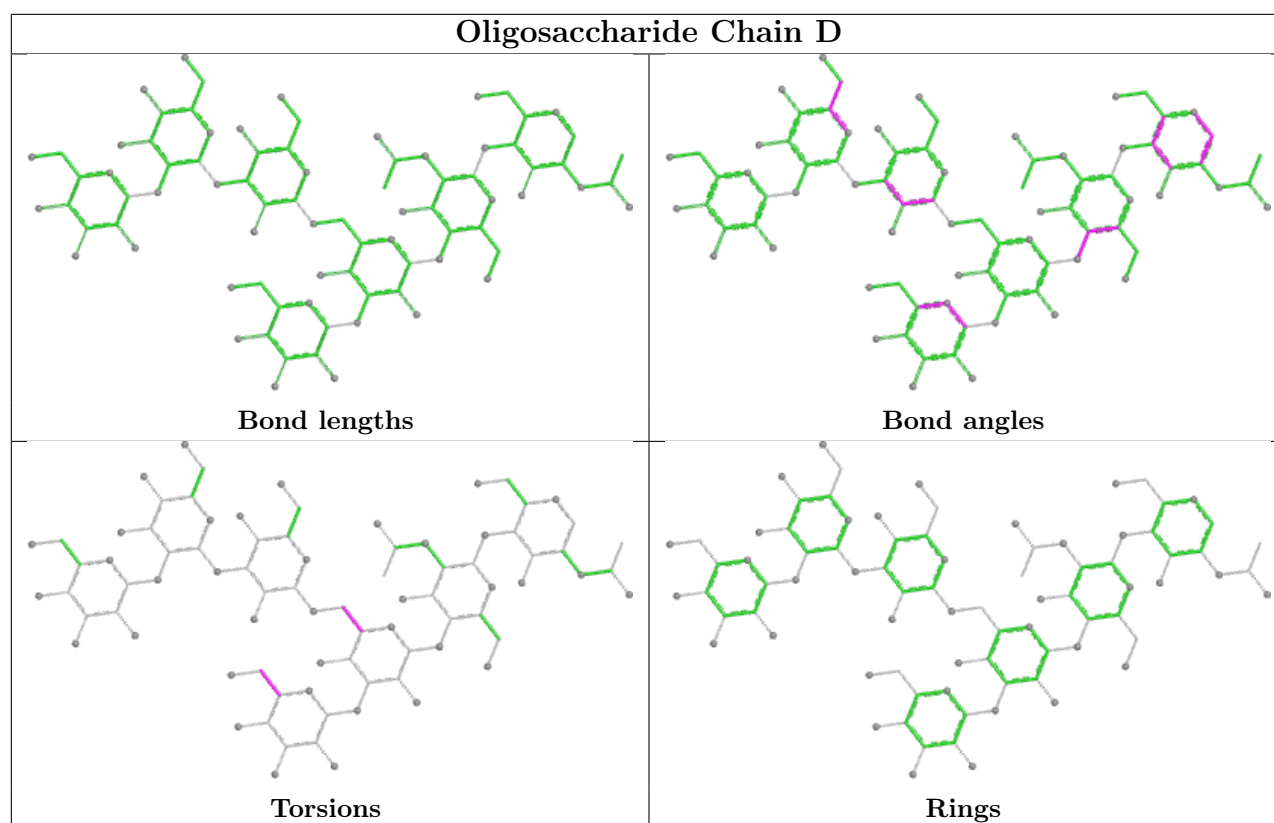
There are no ring outliers.

No monomer is involved in short contacts.

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 60 ligands modelled in this entry, 37 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	5D5	B	927[A]	-	37,37,37	1.58	2 (5%)	57,58,58	1.42	10 (17%)
7	PO4	A	927	4	4,4,4	0.85	0	6,6,6	0.77	0
11	GOL	A	934	-	5,5,5	0.51	0	5,5,5	0.75	0
11	GOL	A	936	-	5,5,5	0.35	0	5,5,5	0.13	0
11	GOL	B	930	-	5,5,5	0.27	0	5,5,5	0.16	0
11	GOL	B	932	-	5,5,5	0.23	0	5,5,5	0.43	0
9	5D5	A	930[A]	-	37,37,37	1.54	1 (2%)	57,58,58	1.23	6 (10%)
10	SCN	B	928	-	1,2,2	0.14	0	0,1,1	-	-
11	GOL	B	934	-	5,5,5	0.25	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	B	924	4	4,4,4	0.58	0	6,6,6	1.22	0
9	5D5	B	927[C]	-	37,37,37	1.50	1 (2%)	57,58,58	1.62	13 (22%)
10	SCN	B	929	-	1,2,2	0.19	0	0,1,1	-	-
11	GOL	A	937	-	5,5,5	0.27	0	5,5,5	0.18	0
9	5D5	B	927[B]	-	37,37,37	1.62	1 (2%)	57,58,58	1.36	11 (19%)
11	GOL	B	931	-	5,5,5	0.53	0	5,5,5	0.64	0
11	GOL	A	935	-	5,5,5	0.24	0	5,5,5	0.28	0
10	SCN	A	931	-	1,2,2	0.17	0	0,1,1	-	-
10	SCN	A	932	-	1,2,2	0.34	0	0,1,1	-	-
9	5D5	A	930[C]	-	37,37,37	1.49	1 (2%)	57,58,58	1.55	13 (22%)
9	5D5	A	930[B]	-	37,37,37	1.55	2 (5%)	57,58,58	1.18	5 (8%)
11	GOL	B	933	-	5,5,5	0.34	0	5,5,5	0.40	0
11	GOL	A	933	-	5,5,5	0.28	0	5,5,5	0.19	0
11	GOL	A	938	-	5,5,5	0.17	0	5,5,5	0.48	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
11	GOL	A	936	-	-	2/4/4/4	-
9	5D5	B	927[A]	-	-	6/16/77/77	0/4/4/4
9	5D5	B	927[C]	-	-	9/16/77/77	0/4/4/4
11	GOL	A	937	-	-	0/4/4/4	-
9	5D5	B	927[B]	-	-	8/16/77/77	0/4/4/4
9	5D5	A	930[C]	-	-	10/16/77/77	0/4/4/4
9	5D5	A	930[A]	-	-	10/16/77/77	0/4/4/4
11	GOL	B	930	-	-	0/4/4/4	-
11	GOL	B	932	-	-	0/4/4/4	-
9	5D5	A	930[B]	-	-	9/16/77/77	0/4/4/4
11	GOL	A	934	-	-	0/4/4/4	-
11	GOL	B	933	-	-	0/4/4/4	-
11	GOL	B	931	-	-	2/4/4/4	-
11	GOL	A	935	-	-	0/4/4/4	-
11	GOL	B	934	-	-	4/4/4/4	-
11	GOL	A	933	-	-	0/4/4/4	-
11	GOL	A	938	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	927[B]	5D5	C26-S27	-8.83	1.65	1.77
9	B	927[A]	5D5	C26-S27	-8.22	1.66	1.77
9	A	930[A]	5D5	C26-S27	-8.16	1.66	1.77
9	A	930[B]	5D5	C26-S27	-8.08	1.66	1.77
9	B	927[C]	5D5	C26-S27	-8.00	1.66	1.77
9	A	930[C]	5D5	C26-S27	-7.63	1.66	1.77
9	B	927[A]	5D5	C10-C9	-2.02	1.52	1.56
9	A	930[B]	5D5	C10-C9	-2.01	1.52	1.56

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	930[C]	5D5	C13-C17-C20	-5.07	111.66	119.50
9	B	927[C]	5D5	C13-C17-C20	-4.57	112.44	119.50
9	B	927[C]	5D5	C14-C13-C17	3.48	104.09	100.10
9	B	927[A]	5D5	C11-C9-C10	-3.46	110.01	113.91
9	A	930[A]	5D5	C13-C17-C20	-3.34	114.34	119.50
9	A	930[C]	5D5	C14-C13-C17	3.28	103.87	100.10
9	B	927[B]	5D5	O30-S27-C26	3.18	111.53	106.73
9	B	927[B]	5D5	C25-N26-C24	-3.15	116.96	122.82
9	B	927[C]	5D5	C13-C14-C8	-2.97	110.17	113.93
9	B	927[A]	5D5	C13-C17-C20	-2.94	114.96	119.50
9	B	927[B]	5D5	C6-C7-C8	2.87	114.64	111.50
9	B	927[C]	5D5	C1-C10-C5	2.87	111.86	107.75
9	B	927[C]	5D5	C9-C8-C7	-2.86	108.26	111.86
9	B	927[A]	5D5	C4-C3-C2	-2.86	107.13	110.62
9	B	927[C]	5D5	C10-C9-C8	-2.82	108.70	111.84
9	A	930[C]	5D5	C13-C14-C8	-2.80	110.38	113.93
9	B	927[B]	5D5	C4-C3-C2	-2.78	107.22	110.62
9	B	927[A]	5D5	C5-C4-C3	-2.73	108.59	112.71
9	B	927[C]	5D5	C21-C20-C17	-2.72	108.81	112.88
9	B	927[B]	5D5	O29-S27-C26	2.69	111.28	106.00
9	B	927[B]	5D5	C4-C5-C10	-2.67	109.82	112.66
9	A	930[C]	5D5	C21-C20-C17	-2.61	108.97	112.88
9	B	927[C]	5D5	C11-C9-C10	-2.61	110.97	113.91
9	B	927[C]	5D5	C11-C12-C13	-2.60	108.35	112.74
9	A	930[C]	5D5	C5-C4-C3	-2.58	108.82	112.71
9	B	927[A]	5D5	C19-C10-C9	-2.55	107.75	111.18
9	B	927[A]	5D5	C13-C14-C8	-2.52	110.74	113.93
9	B	927[C]	5D5	C4-C3-C2	-2.52	107.55	110.62
9	A	930[C]	5D5	C14-C8-C9	-2.49	106.27	109.75
9	B	927[A]	5D5	C11-C12-C13	-2.45	108.61	112.74
9	B	927[A]	5D5	C5-C6-C7	-2.44	111.50	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	930[C]	5D5	C11-C9-C10	-2.44	111.17	113.91
9	A	930[B]	5D5	C11-C12-C13	-2.41	108.67	112.74
9	A	930[C]	5D5	O29-S27-C26	2.39	110.69	106.00
9	A	930[B]	5D5	C13-C17-C20	-2.36	115.85	119.50
9	A	930[B]	5D5	C5-C4-C3	-2.36	109.15	112.71
9	B	927[A]	5D5	C1-C10-C5	2.33	111.09	107.75
9	A	930[C]	5D5	C1-C10-C5	2.32	111.07	107.75
9	A	930[C]	5D5	C11-C12-C13	-2.29	108.87	112.74
9	B	927[B]	5D5	C1-C10-C5	2.26	111.00	107.75
9	B	927[B]	5D5	C5-C4-C3	-2.26	109.30	112.71
9	B	927[C]	5D5	O29-S27-C26	2.24	110.39	106.00
9	A	930[A]	5D5	C11-C12-C13	-2.23	108.98	112.74
9	B	927[C]	5D5	C5-C4-C3	-2.18	109.42	112.71
9	A	930[B]	5D5	O30-S27-C26	2.18	110.02	106.73
9	B	927[B]	5D5	C23-C24-N26	-2.17	112.39	116.34
9	A	930[A]	5D5	C1-C10-C5	2.16	110.85	107.75
9	B	927[A]	5D5	O29-S27-C26	2.14	110.20	106.00
9	A	930[A]	5D5	C21-C20-C17	-2.14	109.67	112.88
9	A	930[C]	5D5	C19-C10-C9	-2.14	108.30	111.18
9	A	930[C]	5D5	C5-C6-C7	-2.12	111.88	114.40
9	A	930[A]	5D5	O29-S27-C26	2.12	110.15	106.00
9	B	927[C]	5D5	C19-C10-C9	-2.11	108.34	111.18
9	A	930[B]	5D5	C4-C5-C10	-2.07	110.46	112.66
9	B	927[B]	5D5	C11-C12-C13	-2.06	109.26	112.74
9	A	930[A]	5D5	C5-C4-C3	-2.03	109.64	112.71
9	B	927[B]	5D5	C23-C22-C20	-2.03	110.68	114.46
9	A	930[C]	5D5	C16-C17-C13	2.02	106.22	103.84

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	930[A]	5D5	N26-C25-C26-S27
9	A	930[B]	5D5	C26-C25-N26-C24
9	A	930[B]	5D5	C25-C26-S27-O30
9	B	927[A]	5D5	C26-C25-N26-C24
9	B	927[B]	5D5	C25-C26-S27-O30
9	B	927[B]	5D5	C25-C26-S27-O29
9	B	927[C]	5D5	N26-C25-C26-S27
9	B	927[C]	5D5	C25-C26-S27-O28
9	B	927[C]	5D5	C25-C26-S27-O29
11	A	936	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
11	B	934	GOL	O1-C1-C2-C3
9	A	930[A]	5D5	C13-C17-C20-C21
9	B	927[C]	5D5	C21-C20-C22-C23
9	A	930[A]	5D5	C16-C17-C20-C21
9	A	930[A]	5D5	C13-C17-C20-C22
9	A	930[C]	5D5	C23-C24-N26-C25
9	B	927[B]	5D5	C23-C24-N26-C25
9	B	927[C]	5D5	C23-C24-N26-C25
9	A	930[A]	5D5	C21-C20-C22-C23
9	A	930[C]	5D5	C21-C20-C22-C23
9	A	930[A]	5D5	C16-C17-C20-C22
9	B	927[A]	5D5	C13-C17-C20-C21
9	A	930[C]	5D5	O25-C24-N26-C25
9	B	927[B]	5D5	O25-C24-N26-C25
9	B	927[C]	5D5	O25-C24-N26-C25
9	B	927[A]	5D5	C16-C17-C20-C22
9	A	930[C]	5D5	C17-C20-C22-C23
9	A	930[A]	5D5	C17-C20-C22-C23
9	B	927[C]	5D5	C17-C20-C22-C23
9	A	930[C]	5D5	C25-C26-S27-O29
9	A	930[B]	5D5	C17-C20-C22-C23
9	A	930[B]	5D5	C21-C20-C22-C23
11	A	936	GOL	C1-C2-C3-O3
11	B	931	GOL	C1-C2-C3-O3
11	B	934	GOL	C1-C2-C3-O3
11	B	934	GOL	O1-C1-C2-O2
9	A	930[B]	5D5	C22-C23-C24-O25
9	A	930[A]	5D5	C22-C23-C24-N26
9	A	930[B]	5D5	C22-C23-C24-N26
9	B	927[B]	5D5	C20-C22-C23-C24
9	A	930[A]	5D5	C22-C23-C24-O25
9	A	930[B]	5D5	C25-C26-S27-O29
9	A	930[A]	5D5	C20-C22-C23-C24
9	A	930[B]	5D5	C20-C22-C23-C24
9	B	927[A]	5D5	C16-C17-C20-C21
11	B	931	GOL	O2-C2-C3-O3
11	B	934	GOL	O2-C2-C3-O3
9	A	930[C]	5D5	C20-C22-C23-C24
9	B	927[C]	5D5	C20-C22-C23-C24
9	A	930[B]	5D5	C25-C26-S27-O28
9	A	930[C]	5D5	C25-C26-S27-O30
9	A	930[C]	5D5	C25-C26-S27-O28

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Mol	Chain	Res	Type	Atoms
9	B	927[B]	5D5	C25-C26-S27-O28
9	B	927[C]	5D5	C25-C26-S27-O30
9	B	927[A]	5D5	C13-C17-C20-C22
9	A	930[C]	5D5	C13-C17-C20-C21
9	A	930[C]	5D5	C13-C17-C20-C22
9	B	927[B]	5D5	C22-C23-C24-O25
11	A	938	GOL	O1-C1-C2-C3
9	B	927[A]	5D5	N26-C25-C26-S27
9	B	927[B]	5D5	C22-C23-C24-N26

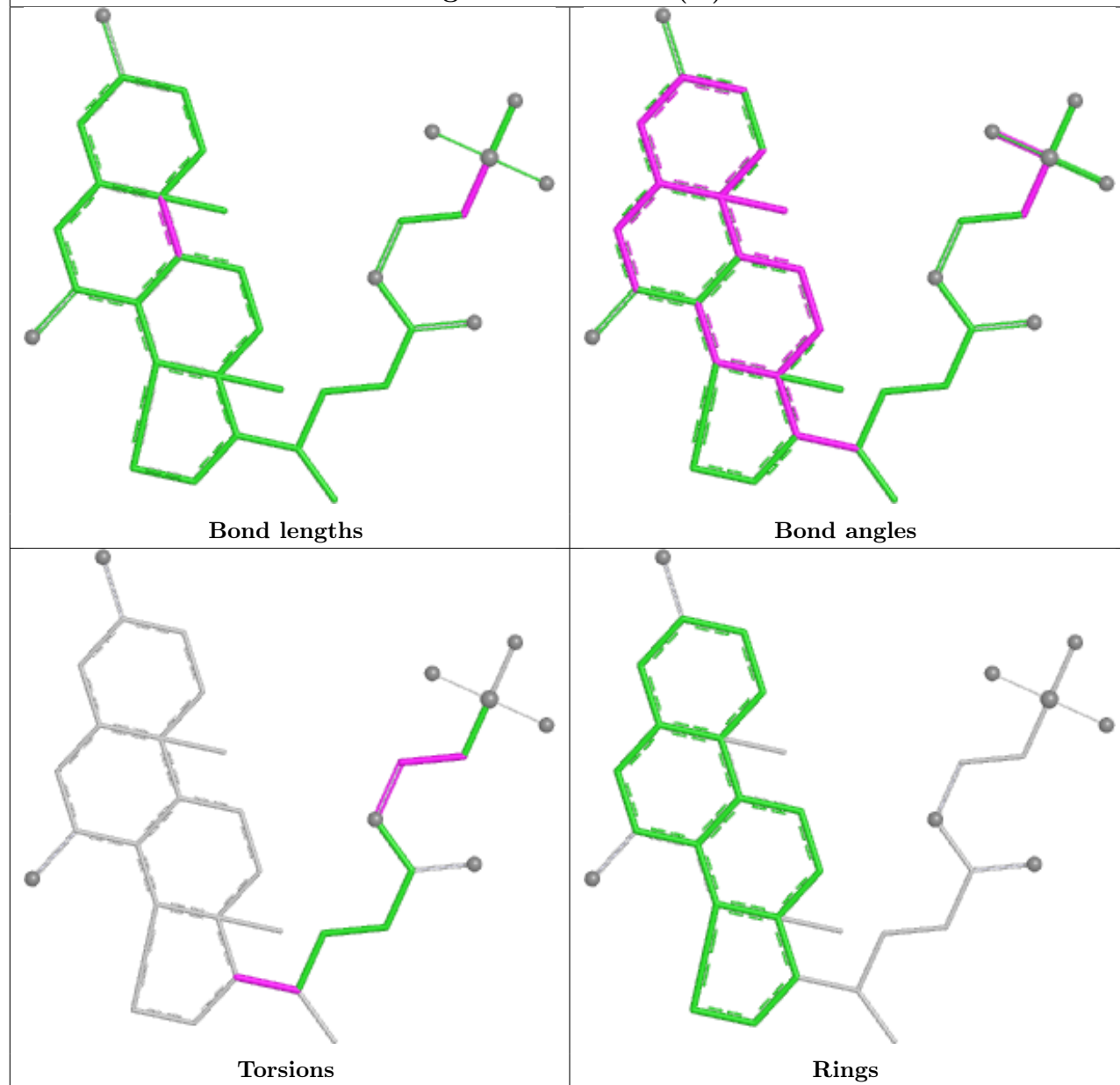
There are no ring outliers.

7 monomers are involved in 9 short contacts:

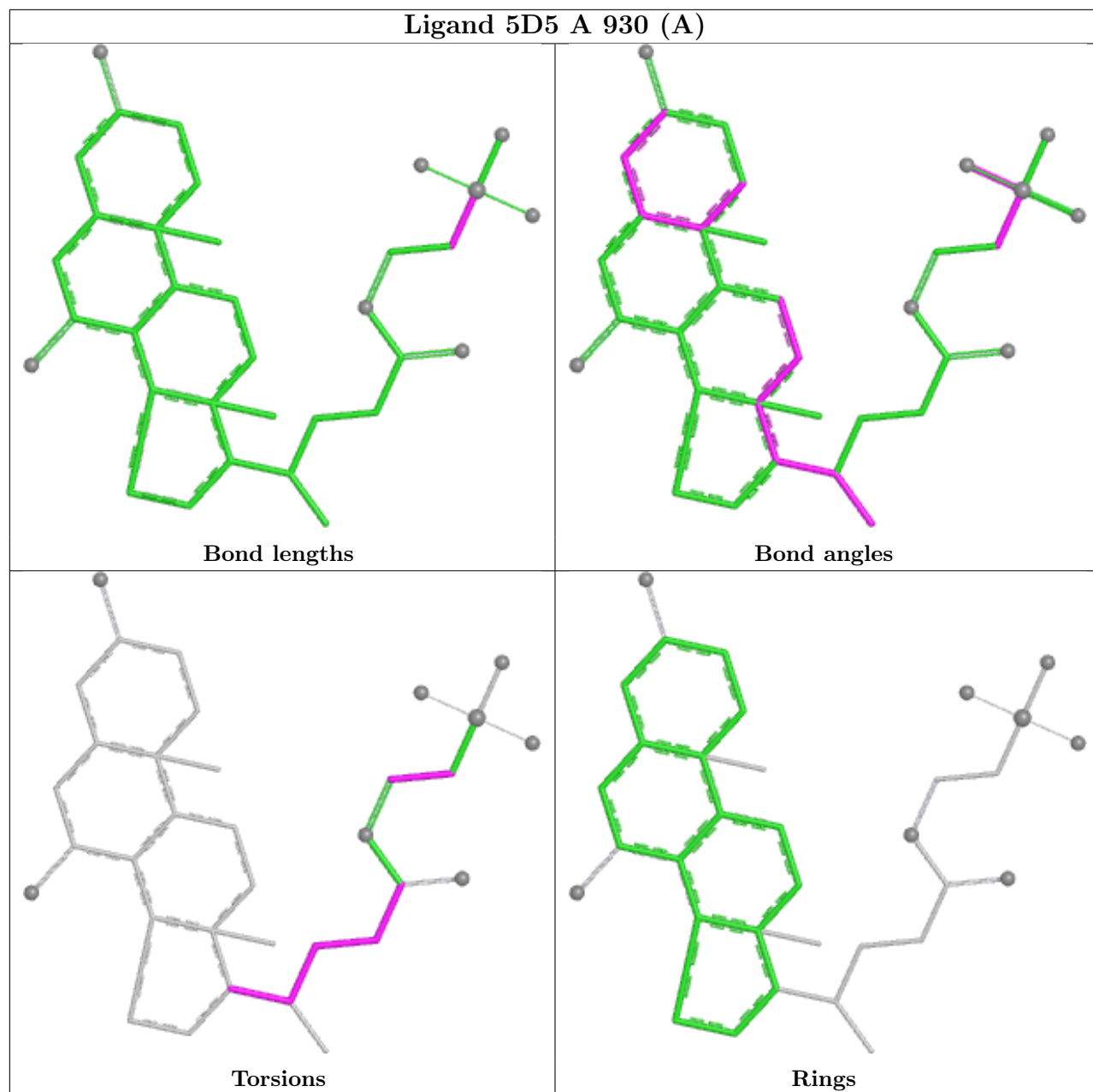
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	927[A]	5D5	2	0
7	A	927	PO4	1	0
9	A	930[A]	5D5	1	0
11	B	934	GOL	1	0
7	B	924	PO4	1	0
9	B	927[B]	5D5	2	0
9	A	930[B]	5D5	1	0

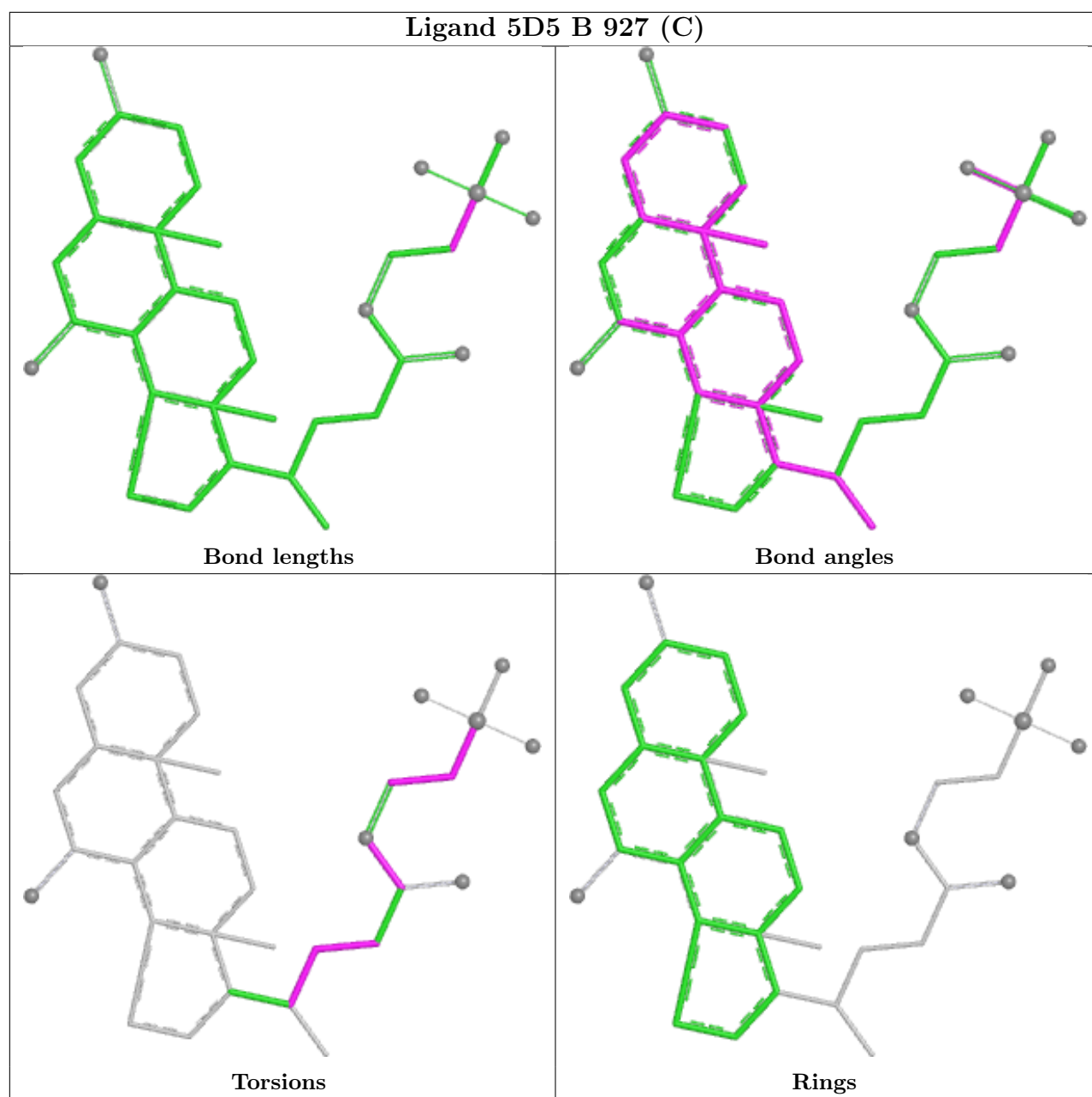
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 5D5 B 927 (A)

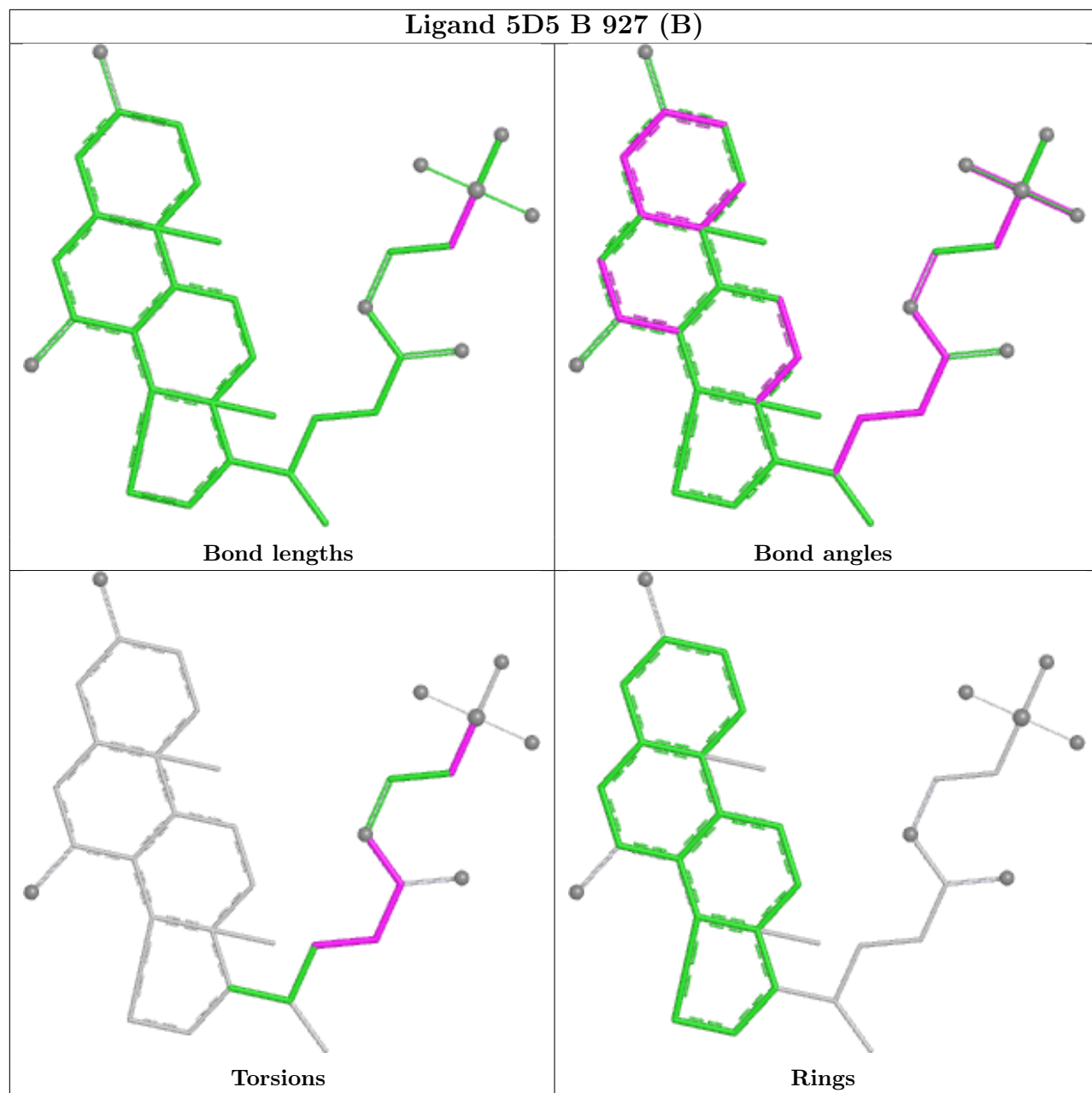


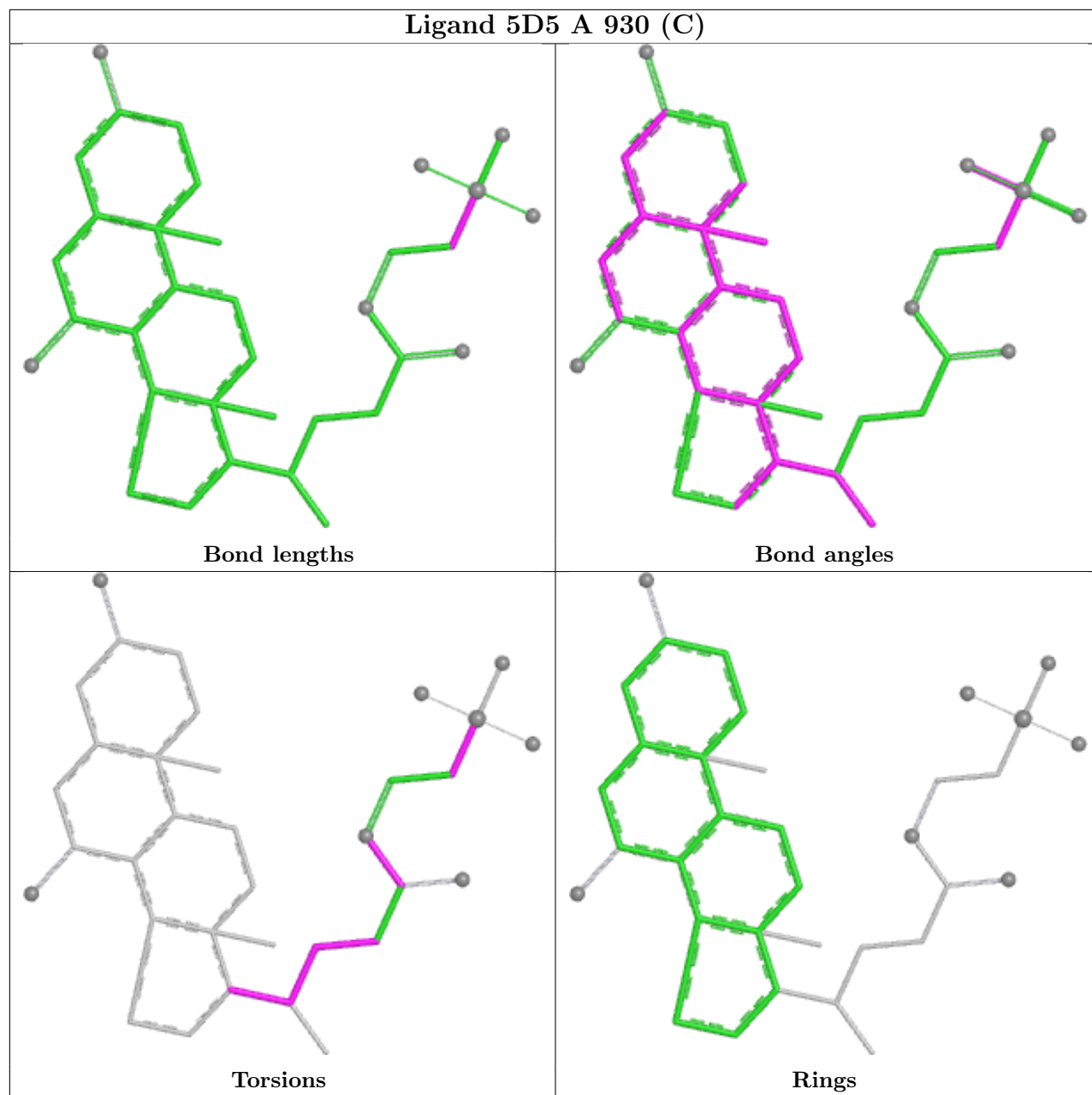
Ligand 5D5 A 930 (A)

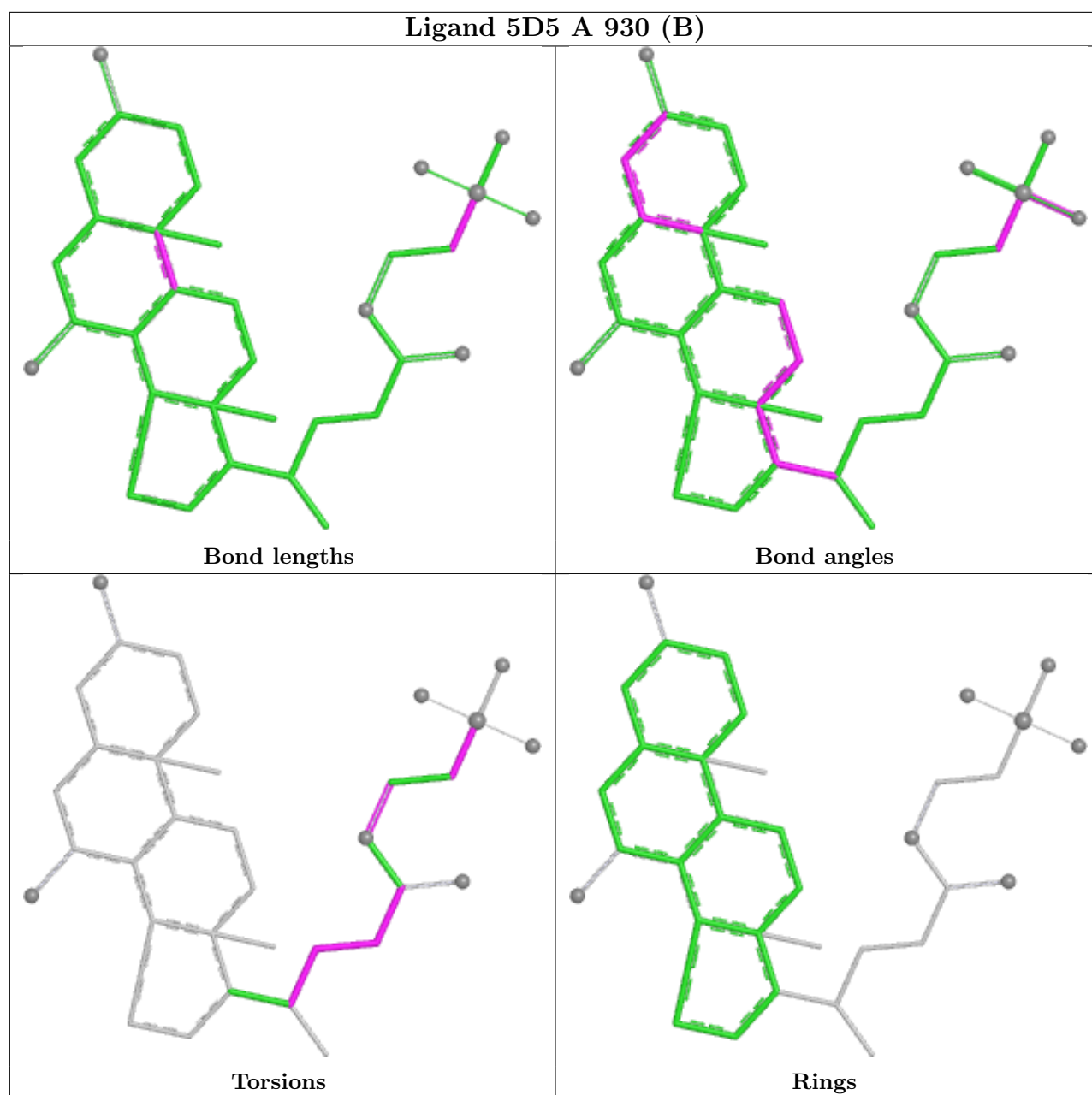




Ligand 5D5 B 927 (B)







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	781/827 (94%)	0.03	31 (3%)	42 41	8, 32, 66, 107	5 (0%)
1	B	781/827 (94%)	0.06	34 (4%)	39 38	7, 33, 66, 110	5 (0%)
All	All	1562/1654 (94%)	0.05	65 (4%)	40 39	7, 33, 66, 110	10 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	ILE	5.2
1	B	469	PHE	4.7
1	A	306[A]	TYR	4.7
1	A	469	PHE	4.5
1	B	586	HIS	4.3
1	A	587	THR	4.2
1	B	460	VAL	4.1
1	A	558	LEU	4.0
1	B	68	VAL	3.9
1	B	71	PRO	3.8
1	B	306[A]	TYR	3.8
1	B	643	SER	3.8
1	A	398	ASN	3.7
1	A	460	VAL	3.7
1	B	587	THR	3.6
1	B	70	PRO	3.6
1	A	586	HIS	3.4
1	B	69	GLY	3.3
1	B	589	GLY	3.3
1	A	397	ILE	3.3
1	A	71	PRO	3.2
1	A	69	GLY	3.1
1	A	68	VAL	3.1
1	B	569	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	70	PRO	3.0
1	B	82	TYR	2.9
1	A	82	TYR	2.8
1	A	644	ILE	2.8
1	B	556	MET	2.7
1	B	83	SER	2.7
1	A	589	GLY	2.7
1	B	179	LYS	2.5
1	B	398	ASN	2.5
1	B	378	ASN	2.5
1	A	65	LEU	2.4
1	B	644	ILE	2.4
1	B	401	LYS	2.4
1	A	648	LEU	2.4
1	A	87	HIS	2.4
1	A	649	THR	2.4
1	B	639	ALA	2.3
1	A	538	THR	2.3
1	A	783	LYS	2.3
1	A	555	ILE	2.3
1	A	569	ASP	2.3
1	B	588	LYS	2.2
1	B	417	ASP	2.2
1	B	468	CYS	2.2
1	B	243	LEU	2.2
1	B	66	GLN	2.2
1	A	556	MET	2.2
1	A	859	GLU	2.1
1	B	555	ILE	2.1
1	B	558	LEU	2.1
1	B	648	LEU	2.1
1	A	416	PRO	2.1
1	A	643	SER	2.1
1	B	183	LYS	2.1
1	B	646	GLU	2.1
1	A	645	PRO	2.1
1	B	470	PHE	2.1
1	A	417	ASP	2.0
1	A	641	VAL	2.0
1	A	243	LEU	2.0
1	B	567	THR	2.0

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

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

6.3 Carbohydrates ⓘ

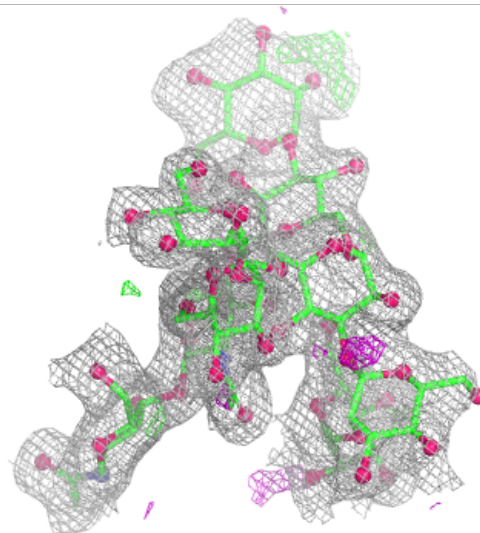
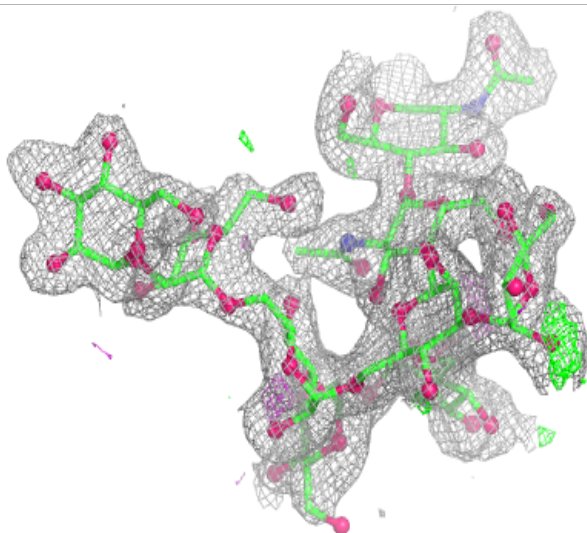
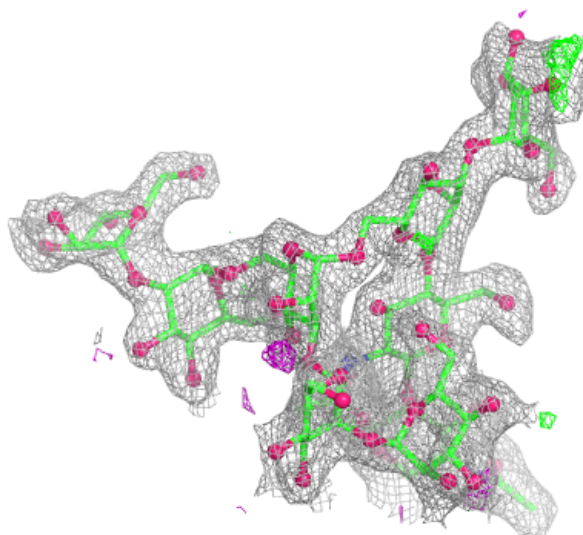
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

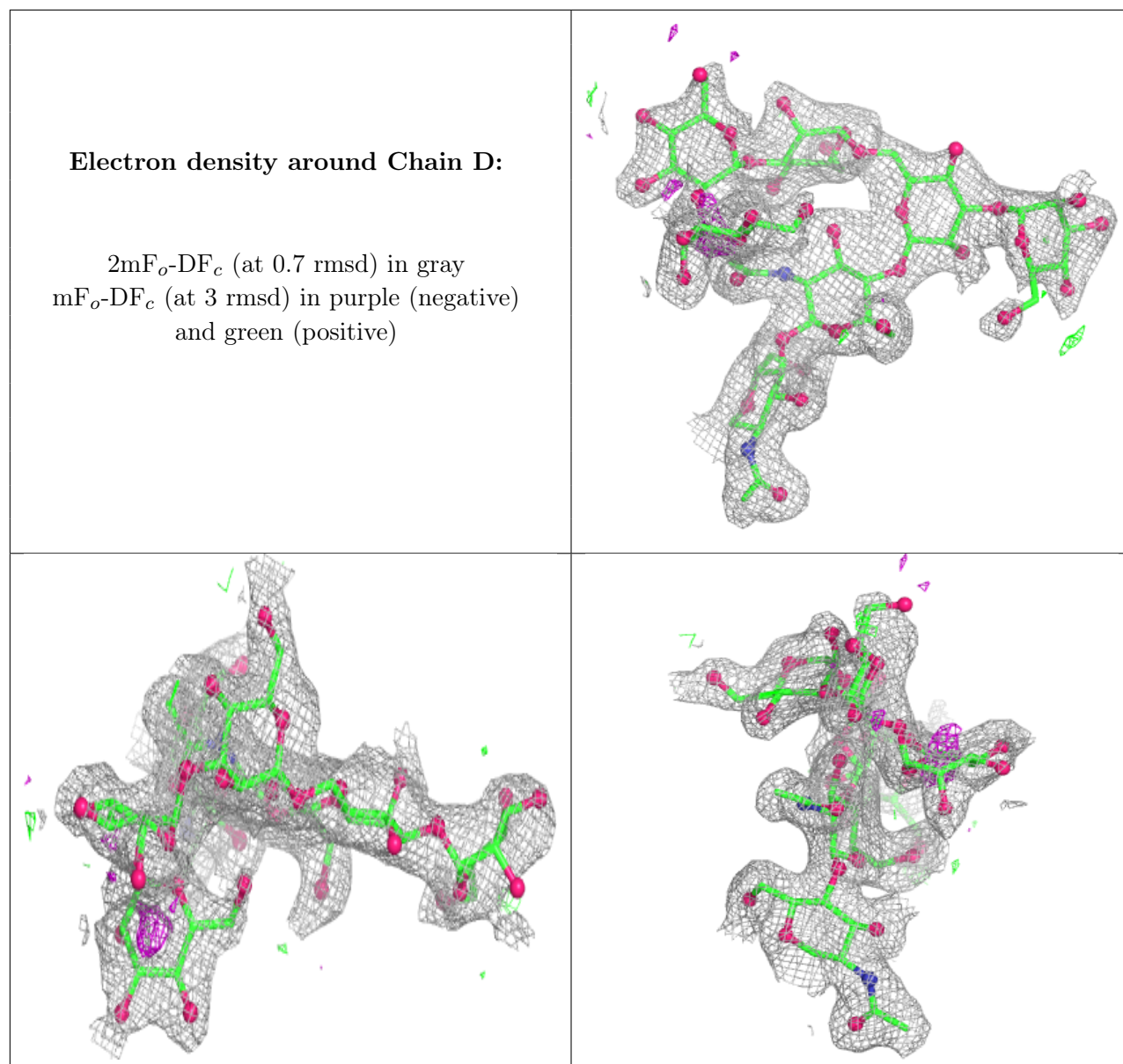
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	7	11/12	0.60	0.14	70,78,83,90	0
3	MAN	D	5	11/12	0.80	0.15	50,59,63,66	0
2	MAN	C	9	11/12	0.81	0.13	43,49,51,53	0
3	MAN	D	6	11/12	0.85	0.14	36,49,52,53	0
3	BMA	D	3	11/12	0.85	0.10	51,59,66,66	0
3	MAN	D	4	11/12	0.86	0.10	49,51,53,59	0
2	MAN	C	8	11/12	0.86	0.10	45,47,49,50	0
2	MAN	C	7	11/12	0.87	0.11	33,44,47,48	0
2	MAN	C	5	11/12	0.87	0.12	39,47,55,64	0
2	MAN	C	4	11/12	0.89	0.10	36,39,44,45	0
2	MAN	C	6	11/12	0.89	0.10	26,33,40,45	0
3	NAG	D	2	14/15	0.93	0.08	28,33,39,45	0
2	BMA	C	3	11/12	0.93	0.07	32,37,42,43	0
2	NAG	C	2	14/15	0.96	0.06	22,24,26,28	0
2	NAG	C	1	14/15	0.96	0.06	17,18,20,21	0
3	NAG	D	1	14/15	0.98	0.04	18,19,22,24	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 C:

$2mF_o-DF_c$ (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	5D5	A	930[A]	34/34	0.62	0.23	41,58,59,60	34
9	5D5	A	930[B]	34/34	0.62	0.23	30,31,35,37	34
9	5D5	A	930[C]	34/34	0.62	0.23	32,55,57,57	34
9	5D5	B	927[A]	34/34	0.75	0.16	26,27,28,29	34
9	5D5	B	927[B]	34/34	0.75	0.16	13,15,16,16	34

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	5D5	B	927[C]	34/34	0.75	0.16	32,53,56,57	34
10	SCN	A	931	3/3	0.76	0.18	53,53,60,86	0
11	GOL	B	932	6/6	0.76	0.22	49,58,59,70	0
11	GOL	B	933	6/6	0.77	0.18	46,51,57,57	0
11	GOL	B	931	6/6	0.78	0.20	31,46,48,51	0
11	GOL	B	930	6/6	0.82	0.18	56,61,63,66	0
7	PO4	A	927	5/5	0.82	0.15	38,44,58,82	0
7	PO4	B	924	5/5	0.83	0.16	35,38,53,71	0
11	GOL	A	935	6/6	0.84	0.15	41,50,57,62	0
11	GOL	A	938	6/6	0.84	0.17	38,41,47,65	0
11	GOL	A	933	6/6	0.84	0.18	58,63,63,70	0
10	SCN	B	928	3/3	0.85	0.12	39,39,40,63	0
11	GOL	A	934	6/6	0.85	0.18	27,43,46,51	0
11	GOL	B	934	6/6	0.86	0.16	36,40,45,60	0
11	GOL	A	936	6/6	0.87	0.12	43,45,52,54	0
10	SCN	A	932	3/3	0.90	0.13	29,29,40,44	0
10	SCN	B	929	3/3	0.90	0.12	41,41,46,54	0
11	GOL	A	937	6/6	0.90	0.12	33,39,42,45	0
8	NA	B	926	1/1	0.92	0.07	44,44,44,44	0
8	NA	B	925	1/1	0.92	0.07	39,39,39,39	0
8	NA	A	928	1/1	0.93	0.06	37,37,37,37	0
8	NA	A	929	1/1	0.94	0.08	39,39,39,39	0
4	ZN	A	911	1/1	0.96	0.12	71,71,71,71	0
6	IOD	B	919	1/1	0.97	0.09	67,67,67,67	1
4	ZN	B	909	1/1	0.97	0.12	63,63,63,63	0
6	IOD	B	921	1/1	0.98	0.05	48,48,48,48	1
6	IOD	A	923	1/1	0.98	0.04	58,58,58,58	1
6	IOD	A	926	1/1	0.98	0.05	61,61,61,61	1
6	IOD	A	921	1/1	0.98	0.05	59,59,59,59	1
6	IOD	A	917	1/1	0.99	0.05	43,43,43,43	1
6	IOD	B	915	1/1	0.99	0.03	40,40,40,40	1
6	IOD	B	917	1/1	0.99	0.02	55,55,55,55	1
6	IOD	B	918	1/1	0.99	0.03	57,57,57,57	1
6	IOD	A	920	1/1	0.99	0.04	48,48,48,48	1
6	IOD	B	920	1/1	0.99	0.04	53,53,53,53	1
6	IOD	A	915	1/1	0.99	0.03	68,68,68,68	1
6	IOD	B	922	1/1	0.99	0.03	60,60,60,60	1
6	IOD	B	923	1/1	0.99	0.08	67,67,67,67	1
6	IOD	A	922	1/1	0.99	0.03	48,48,48,48	1
6	IOD	A	916	1/1	0.99	0.04	37,37,37,37	1
6	IOD	A	925	1/1	0.99	0.04	52,52,52,52	1
4	ZN	A	910	1/1	1.00	0.02	29,29,29,29	0

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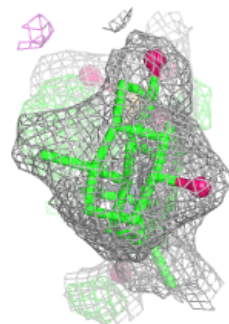
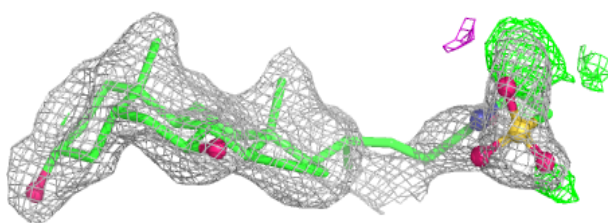
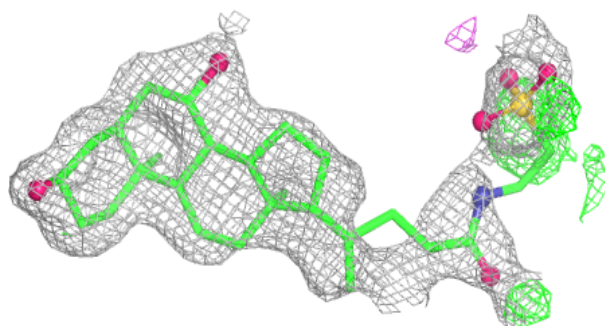
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	912	1/1	1.00	0.01	23,23,23,23	0
6	IOD	B	911	1/1	1.00	0.01	25,25,25,25	0
6	IOD	B	912	1/1	1.00	0.02	56,56,56,56	1
6	IOD	B	913	1/1	1.00	0.04	67,67,67,67	1
6	IOD	B	914	1/1	1.00	0.03	40,40,40,40	1
6	IOD	A	918	1/1	1.00	0.04	39,39,39,39	1
6	IOD	B	916	1/1	1.00	0.03	40,40,40,40	1
6	IOD	A	919	1/1	1.00	0.03	58,58,58,58	1
5	CA	B	910	1/1	1.00	0.01	20,20,20,20	0
6	IOD	A	913	1/1	1.00	0.01	26,26,26,26	0
6	IOD	A	914	1/1	1.00	0.02	50,50,50,50	1
4	ZN	B	908	1/1	1.00	0.02	29,29,29,29	0
6	IOD	A	924	1/1	1.00	0.02	51,51,51,51	1

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.

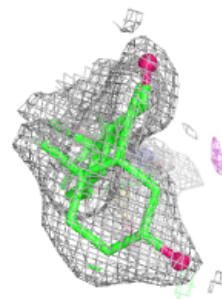
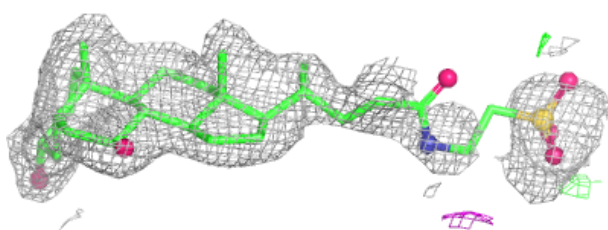
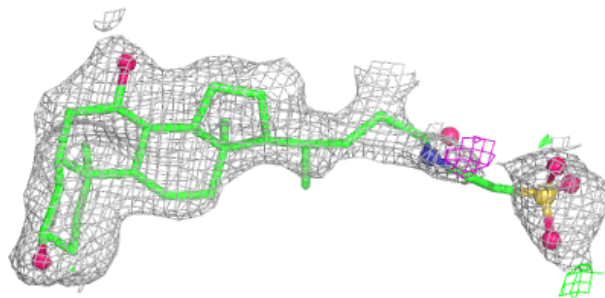
Electron density around 5D5 A 930 (A):

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

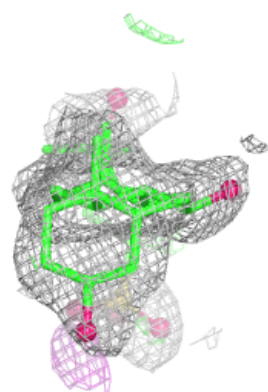
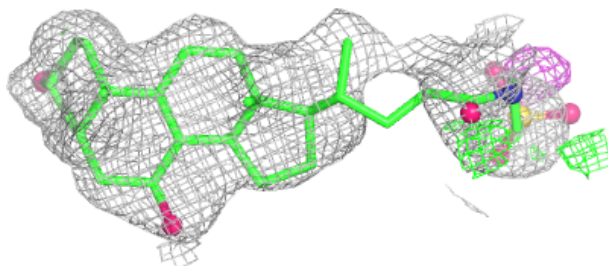
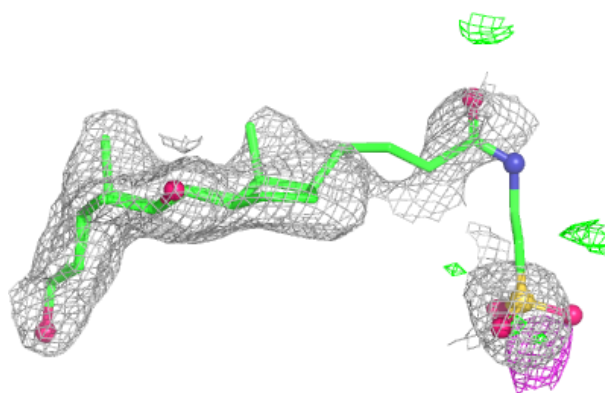


Electron density around 5D5 A 930 (B):

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

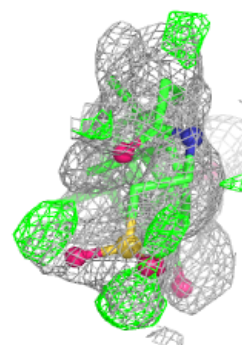
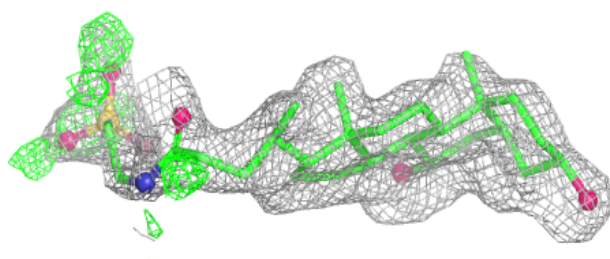
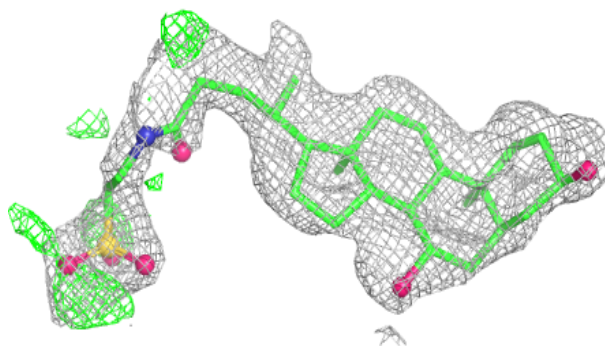
**Electron density around 5D5 A 930 (C):**

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

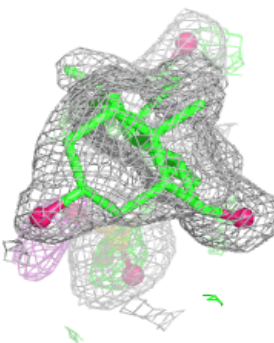
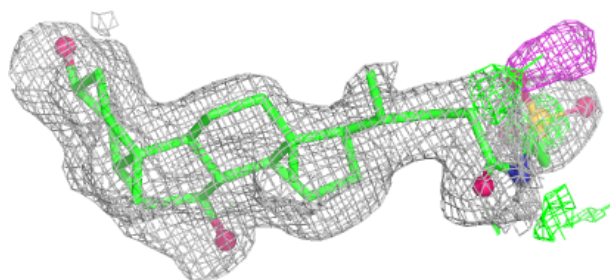
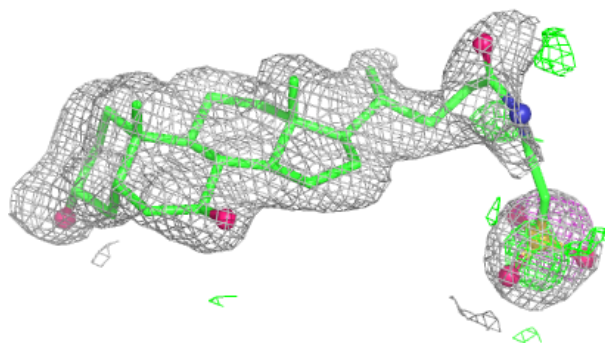


Electron density around 5D5 B 927 (A):

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and green (positive)

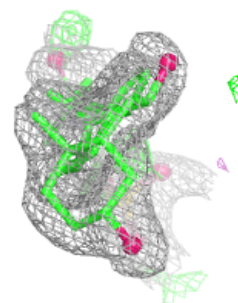
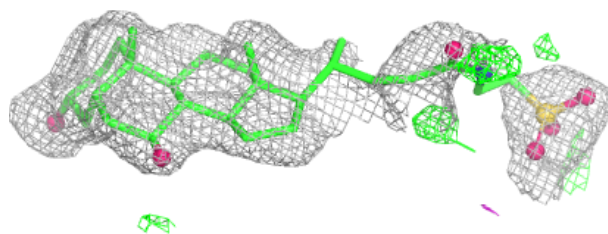
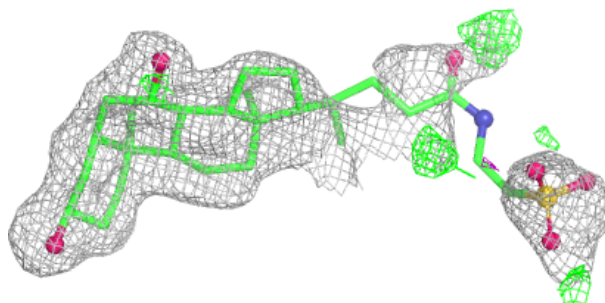
**Electron density around 5D5 B 927 (B):**

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



Electron density around 5D5 B 927 (C):

$2mF_o-DF_c$ (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.