



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:05 AM UTC

PDB ID : 7Q1D / pdb_00007q1d
Title : Acetyltransferase(3) type IIIa in complex with 3-N-methyl-nemycin B
Authors : Pontillo, N.; Guskov, A.
Deposited on : 2021-10-18
Resolution : 1.43 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

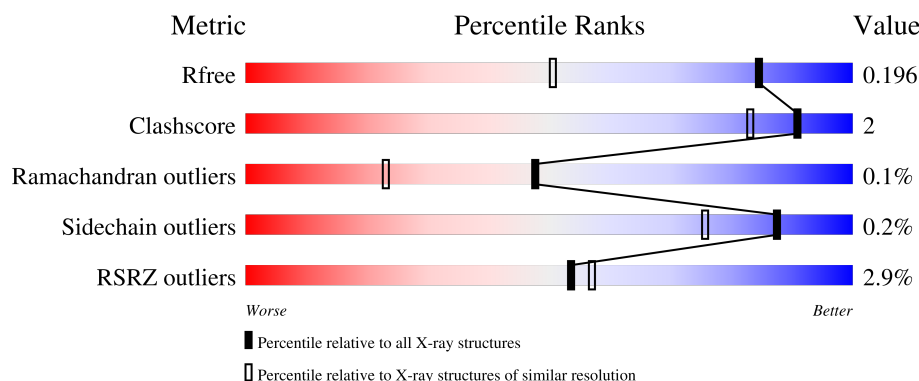
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	287	4% 87% 5% 8%
1	B	287	2% 88% • 9%
1	C	287	• 87% • 9%
1	D	287	5% 92% • 5%

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
3	8I8	A	304	X	-	-	-
3	8I8	B	303	X	-	-	-
3	8I8	C	303	X	-	-	-
3	8I8	D	302	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9888 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 Aminoglycoside N(3)-acetyltransferase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	9	0
			2096	1332	371	382	11			
1	B	261	Total	C	N	O	S	0	5	0
			2051	1307	359	374	11			
1	C	261	Total	C	N	O	S	0	6	0
			2053	1310	356	376	11			
1	D	272	Total	C	N	O	S	0	5	0
			2131	1357	374	388	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	HIS	-	expression tag	UNP P29808
A	6	HIS	-	expression tag	UNP P29808
A	7	HIS	-	expression tag	UNP P29808
A	8	HIS	-	expression tag	UNP P29808
A	9	HIS	-	expression tag	UNP P29808
A	10	HIS	-	expression tag	UNP P29808
A	11	SER	-	expression tag	UNP P29808
A	12	SER	-	expression tag	UNP P29808
A	13	GLY	-	expression tag	UNP P29808
A	14	LEU	-	expression tag	UNP P29808
A	15	VAL	-	expression tag	UNP P29808
A	16	PRO	-	expression tag	UNP P29808
A	17	ARG	-	expression tag	UNP P29808
A	18	GLY	-	expression tag	UNP P29808
A	19	SER	-	expression tag	UNP P29808
A	20	HIS	-	expression tag	UNP P29808
B	5	HIS	-	expression tag	UNP P29808
B	6	HIS	-	expression tag	UNP P29808
B	7	HIS	-	expression tag	UNP P29808
B	8	HIS	-	expression tag	UNP P29808
B	9	HIS	-	expression tag	UNP P29808

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP P29808
B	11	SER	-	expression tag	UNP P29808
B	12	SER	-	expression tag	UNP P29808
B	13	GLY	-	expression tag	UNP P29808
B	14	LEU	-	expression tag	UNP P29808
B	15	VAL	-	expression tag	UNP P29808
B	16	PRO	-	expression tag	UNP P29808
B	17	ARG	-	expression tag	UNP P29808
B	18	GLY	-	expression tag	UNP P29808
B	19	SER	-	expression tag	UNP P29808
B	20	HIS	-	expression tag	UNP P29808
C	5	HIS	-	expression tag	UNP P29808
C	6	HIS	-	expression tag	UNP P29808
C	7	HIS	-	expression tag	UNP P29808
C	8	HIS	-	expression tag	UNP P29808
C	9	HIS	-	expression tag	UNP P29808
C	10	HIS	-	expression tag	UNP P29808
C	11	SER	-	expression tag	UNP P29808
C	12	SER	-	expression tag	UNP P29808
C	13	GLY	-	expression tag	UNP P29808
C	14	LEU	-	expression tag	UNP P29808
C	15	VAL	-	expression tag	UNP P29808
C	16	PRO	-	expression tag	UNP P29808
C	17	ARG	-	expression tag	UNP P29808
C	18	GLY	-	expression tag	UNP P29808
C	19	SER	-	expression tag	UNP P29808
C	20	HIS	-	expression tag	UNP P29808
D	5	HIS	-	expression tag	UNP P29808
D	6	HIS	-	expression tag	UNP P29808
D	7	HIS	-	expression tag	UNP P29808
D	8	HIS	-	expression tag	UNP P29808
D	9	HIS	-	expression tag	UNP P29808
D	10	HIS	-	expression tag	UNP P29808
D	11	SER	-	expression tag	UNP P29808
D	12	SER	-	expression tag	UNP P29808
D	13	GLY	-	expression tag	UNP P29808
D	14	LEU	-	expression tag	UNP P29808
D	15	VAL	-	expression tag	UNP P29808
D	16	PRO	-	expression tag	UNP P29808
D	17	ARG	-	expression tag	UNP P29808
D	18	GLY	-	expression tag	UNP P29808
D	19	SER	-	expression tag	UNP P29808

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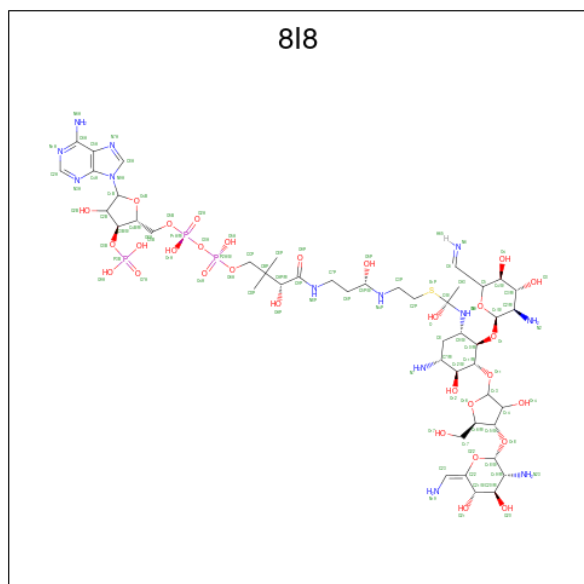
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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P29808

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Na 3 3	0	0

- Molecule 3 is [[(2 {R},3 {S})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl] methoxy-oxidanyl-phosphoryl] [(3 {R})-4-[(3 {S})-3-[2-[(1 {S})-1-[(1 {S},2 {R},3 {R},4 {S} {S},5 {R})-5-azanyl-3-[(4 {S},5 {R})-4-[(2 {S},3 {R},4 {R},5 {S},6 {E})-3-azanyl-6-(azanylm ethylidene)-4,5-bis(oxidanyl)oxan-2-yl]oxy-5-(hydroxymethyl)-3-oxidanyl-oxolan-2-yl]oxy-2-[(2 {S},3 {R},4 {R},5 {S})-3-azanyl-6-(iminomethyl)-4,5-bis(oxidanyl)oxan-2-yl]oxy-4-oxid anyl-cyclohexyl]amino]-1-oxidanyl-ethyl]sulfanylethylamino]-3-oxidanyl-propyl]amino]-2,2 -dimethyl-3-oxidanyl-4-oxidanylidene-butyl] hydrogen phosphate (CCD ID: 8I8) (formula: C₄₆H₈₂N₁₃O₃₀P₃S) (labeled as "Ligand of Interest" by depositor).



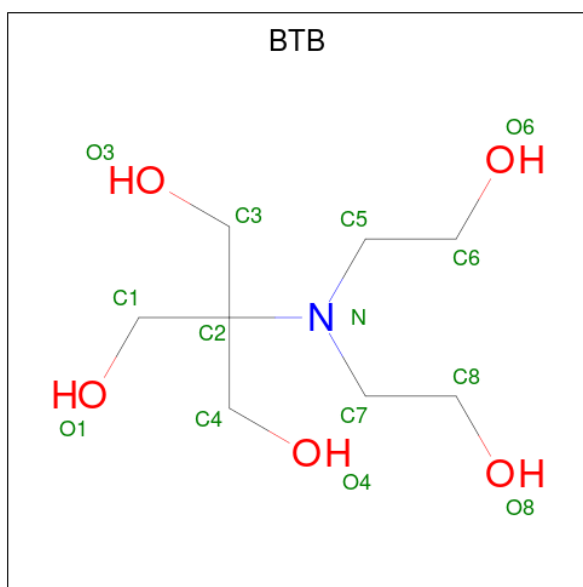
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			93	46	13	30	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			93	46	13	30	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			93	46	13	30	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			93	46	13	30	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



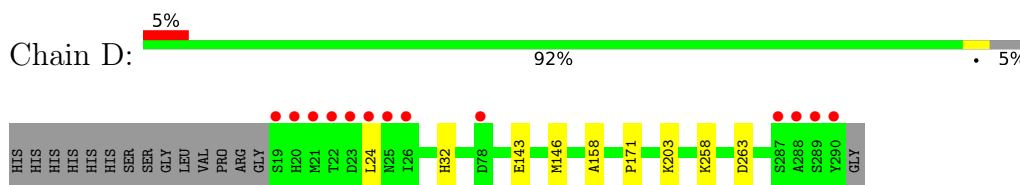
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	287	Total	O	0	0
			287	287		
7	B	283	Total	O	0	1
			283	283		
7	C	289	Total	O	0	2
			289	289		
7	D	284	Total	O	0	1
			284	284		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	90.96Å 100.49Å 131.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.15 – 1.43 47.15 – 1.43	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.15-1.43) 98.6 (47.15-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.200 0.172 , 0.196	Depositor DCC
R_{free} test set	10954 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2580e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BTB, NA, CL, 8I8, GOL

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	0.25	0/2163	0.45	0/2945
1	B	0.27	0/2113	0.47	0/2880
1	C	0.26	0/2118	0.47	0/2888
1	D	0.24	0/2200	0.46	0/2997
All	All	0.26	0/8594	0.46	0/11710

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2096	0	2061	9	0
1	B	2051	0	2009	5	0
1	C	2053	0	2011	8	0
1	D	2131	0	2100	6	0
2	A	3	0	0	0	0
3	A	93	0	0	1	0
3	B	93	0	0	1	0
3	C	93	0	0	2	0
3	D	93	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	12	0	16	0	0
5	B	14	0	19	0	0
6	D	1	0	0	0	0
7	A	287	0	0	1	0
7	B	283	0	0	1	0
7	C	289	0	0	2	0
7	D	284	0	0	1	0
All	All	9888	0	8232	28	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 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95[B]:ASP:HA	1:A:102:LYS:HE3	1.65	0.79
1:A:95[A]:ASP:HA	1:A:102:LYS:HE3	1.69	0.72
1:A:207:LYS:NZ	7:A:401:HOH:O	2.26	0.66
1:C:205:ARG:NH1	7:C:401:HOH:O	2.31	0.63
1:B:207:LYS:NZ	7:B:401:HOH:O	2.33	0.62
1:C:205:ARG:NH2	1:C:237:ASP:OD2	2.34	0.60
1:C:196:HIS:NE2	3:C:303:8I8:N9	2.55	0.53
1:C:143:GLU:OE2	3:C:303:8I8:N7	2.42	0.53
1:A:118[B]:ARG:CZ	1:A:128:GLU:OE2	2.63	0.47
1:B:168:VAL:HG13	1:B:200:TYR:CE1	2.50	0.47
1:D:143:GLU:OE2	3:D:302:8I8:N7	2.49	0.46
1:A:177:ALA:HB1	1:D:158:ALA:HB1	2.00	0.44
1:B:143:GLU:OE2	3:B:303:8I8:N7	2.51	0.44
1:C:48:LEU:HD11	1:C:183:LEU:HB2	2.00	0.44
1:A:87:TRP:CD1	1:A:117:ALA:HB1	2.53	0.43
3:D:302:8I8:O16	3:D:302:8I8:N2	2.52	0.43
1:A:143:GLU:OE2	3:A:304:8I8:N7	2.52	0.42
1:D:32:HIS:HD2	7:D:600:HOH:O	2.02	0.42
1:B:26:ILE:HA	1:B:27:PRO:HD3	1.91	0.42
1:A:168:VAL:HG13	1:A:169:GLU:HG2	2.01	0.41
1:D:146:MET:HG3	1:D:171:PRO:HG2	2.02	0.41
1:A:48:LEU:HD11	1:A:183:LEU:HB2	2.02	0.41
1:D:203:LYS:HA	1:D:203:LYS:HD3	1.80	0.41
1:B:87:TRP:CD1	1:B:117:ALA:HB1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TRP:CD1	1:C:134:PRO:HD2	2.57	0.40
1:C:32[A]:HIS:HD2	7:C:605:HOH:O	2.05	0.40
1:D:258:LYS:HE2	1:D:263:ASP:OD1	2.21	0.40
1:C:87:TRP:CD1	1:C:117:ALA:HB1	2.57	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	270/287 (94%)	264 (98%)	5 (2%)	1 (0%)	30	11
1	B	264/287 (92%)	257 (97%)	7 (3%)	0	100	100
1	C	265/287 (92%)	258 (97%)	7 (3%)	0	100	100
1	D	275/287 (96%)	269 (98%)	6 (2%)	0	100	100
All	All	1074/1148 (94%)	1048 (98%)	25 (2%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	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	215/227 (95%)	215 (100%)	0	100	100
1	B	210/227 (92%)	208 (99%)	2 (1%)	68	39
1	C	211/227 (93%)	211 (100%)	0	100	100
1	D	220/227 (97%)	219 (100%)	1 (0%)	81	63
All	All	856/908 (94%)	853 (100%)	3 (0%)	87	69

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151[A]	ARG
1	B	151[B]	ARG
1	D	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	B	270	GLN
1	C	28	HIS
1	C	152	GLN
1	D	32	HIS
1	D	159	ASN
1	D	270	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	8I8	B	303	-	90,99,99	1.75	13 (14%)	119,150,150	2.84	32 (26%)
3	8I8	D	302	-	90,99,99	1.73	14 (15%)	119,150,150	2.80	27 (22%)
4	GOL	B	301	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	A	305	-	5,5,5	0.85	0	5,5,5	1.08	0
5	BTB	B	302	-	13,13,13	0.44	0	7,16,16	0.61	0
3	8I8	A	304	-	90,99,99	1.71	12 (13%)	119,150,150	2.76	27 (22%)
4	GOL	C	301	-	5,5,5	0.98	0	5,5,5	1.04	0
4	GOL	C	302	-	5,5,5	1.00	0	5,5,5	1.08	0
3	8I8	C	303	-	90,99,99	1.75	12 (13%)	119,150,150	2.73	27 (22%)

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
3	8I8	B	303	-	5/5/31/36	11/64/167/167	0/7/7/7
3	8I8	D	302	-	5/5/31/36	9/64/167/167	0/7/7/7
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	A	305	-	-	1/4/4/4	-
5	BTB	B	302	-	-	2/21/21/21	-
3	8I8	A	304	-	5/5/31/36	12/64/167/167	0/7/7/7
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
3	8I8	C	303	-	5/5/31/36	7/64/167/167	0/7/7/7

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	8I8	C23-C22	8.93	1.53	1.34
3	D	302	8I8	C23-C22	8.93	1.53	1.34
3	B	303	8I8	C23-C22	8.86	1.53	1.34
3	A	304	8I8	C23-C22	8.79	1.52	1.34
3	B	303	8I8	C2B-C1B	-6.58	1.32	1.53
3	A	304	8I8	C2B-C1B	-6.45	1.33	1.53
3	D	302	8I8	C2B-C1B	-6.45	1.33	1.53
3	C	303	8I8	C2B-C1B	-6.30	1.33	1.53
3	C	303	8I8	C9-N9	4.88	1.50	1.47
3	B	303	8I8	O2B-C2B	-4.10	1.32	1.43
3	C	303	8I8	O2B-C2B	-4.08	1.32	1.43
3	D	302	8I8	O2B-C2B	-4.08	1.32	1.43
3	A	304	8I8	O2B-C2B	-4.06	1.32	1.43
3	B	303	8I8	C9-N9	4.02	1.50	1.47
3	C	303	8I8	O14-C14	-3.84	1.33	1.43
3	B	303	8I8	O14-C14	-3.83	1.33	1.43
3	A	304	8I8	O14-C14	-3.81	1.33	1.43
3	D	302	8I8	O14-C14	-3.79	1.33	1.43
3	C	303	8I8	O22-C22	3.58	1.46	1.38
3	A	304	8I8	O22-C22	3.54	1.46	1.38
3	D	302	8I8	O22-C22	3.43	1.46	1.38
3	B	303	8I8	O22-C22	3.35	1.46	1.38
3	D	302	8I8	C1B-N9A	-3.34	1.37	1.46
3	B	303	8I8	C1B-N9A	-3.24	1.37	1.46
3	A	304	8I8	C1B-N9A	-3.16	1.37	1.46
3	C	303	8I8	C1B-N9A	-3.00	1.38	1.46
3	B	303	8I8	C13-C14	-2.95	1.49	1.52
3	A	304	8I8	C9-N9	2.84	1.49	1.47
3	D	302	8I8	C9-N9	2.71	1.49	1.47
3	B	303	8I8	C4A-N9A	-2.68	1.32	1.37
3	A	304	8I8	C13-C14	-2.68	1.49	1.52
3	B	303	8I8	C8A-N7A	2.67	1.36	1.31
3	D	302	8I8	C8A-N7A	2.65	1.36	1.31
3	D	302	8I8	C8A-N9A	-2.64	1.33	1.37
3	A	304	8I8	C8A-N7A	2.59	1.36	1.31
3	D	302	8I8	C2P-S1P	-2.58	1.76	1.81
3	C	303	8I8	C8A-N7A	2.55	1.36	1.31
3	D	302	8I8	C13-C14	-2.48	1.49	1.52
3	A	304	8I8	C4A-N9A	-2.44	1.32	1.37
3	B	303	8I8	C8A-N9A	-2.38	1.33	1.37
3	A	304	8I8	C8A-N9A	-2.37	1.33	1.37
3	A	304	8I8	C2P-S1P	-2.36	1.76	1.81
3	C	303	8I8	C13-C14	-2.34	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	8I8	C4A-N9A	-2.30	1.32	1.37
3	C	303	8I8	C4A-N9A	-2.28	1.33	1.37
3	C	303	8I8	P1A-O3A	2.26	1.61	1.59
3	B	303	8I8	C2P-S1P	-2.16	1.77	1.81
3	C	303	8I8	C2P-S1P	-2.08	1.77	1.81
3	D	302	8I8	O16-C13	2.07	1.45	1.41
3	B	303	8I8	C14-C15	-2.05	1.48	1.53
3	D	302	8I8	O5-C5	2.01	1.47	1.43

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	8I8	O11-C13-O16	16.74	128.46	111.37
3	D	302	8I8	O11-C13-O16	16.73	128.45	111.37
3	C	303	8I8	O11-C13-O16	16.53	128.25	111.37
3	A	304	8I8	O11-C13-O16	16.03	127.74	111.37
3	C	303	8I8	O4B-C1B-N9A	8.51	124.42	108.09
3	B	303	8I8	O4B-C1B-N9A	8.47	124.35	108.09
3	B	303	8I8	C4A-N9A-C8A	8.31	114.46	105.74
3	D	302	8I8	O4B-C1B-N9A	8.30	124.03	108.09
3	A	304	8I8	C4A-N9A-C8A	8.18	114.32	105.74
3	D	302	8I8	C4A-N9A-C8A	7.94	114.07	105.74
3	A	304	8I8	O4B-C1B-N9A	7.67	122.82	108.09
3	A	304	8I8	N9A-C8A-N7A	-7.52	103.27	113.94
3	C	303	8I8	C4A-N9A-C8A	7.34	113.45	105.74
3	D	302	8I8	N9A-C8A-N7A	-7.32	103.54	113.94
3	B	303	8I8	N9A-C8A-N7A	-7.32	103.55	113.94
3	A	304	8I8	O14-C14-C15	6.85	130.35	111.19
3	C	303	8I8	N9A-C8A-N7A	-6.83	104.24	113.94
3	B	303	8I8	O14-C14-C13	6.69	130.66	111.82
3	B	303	8I8	O14-C14-C15	6.67	129.85	111.19
3	C	303	8I8	O14-C14-C15	6.63	129.74	111.19
3	A	304	8I8	O14-C14-C13	6.58	130.37	111.82
3	D	302	8I8	O14-C14-C15	6.56	129.55	111.19
3	C	303	8I8	O14-C14-C13	6.22	129.34	111.82
3	D	302	8I8	O14-C14-C13	6.18	129.23	111.82
3	D	302	8I8	C8-C9-N9	-6.03	107.23	112.23
3	A	304	8I8	C2B-C1B-N9A	5.97	128.15	113.30
3	C	303	8I8	C2B-C1B-N9A	5.81	127.74	113.30
3	A	304	8I8	O2B-C2B-C1B	5.66	129.59	110.10
3	C	303	8I8	O2B-C2B-C1B	5.52	129.12	110.10
3	D	302	8I8	C2B-C1B-N9A	5.48	126.92	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	8I8	O2B-C2B-C1B	5.44	128.84	110.10
3	B	303	8I8	C2B-C1B-N9A	5.37	126.65	113.30
3	B	303	8I8	O2B-C2B-C1B	5.30	128.35	110.10
3	D	302	8I8	N3A-C2A-N1A	-5.25	120.63	128.58
3	A	304	8I8	N3A-C2A-N1A	-5.24	120.64	128.58
3	B	303	8I8	N3A-C2A-N1A	-5.24	120.65	128.58
3	C	303	8I8	N3A-C2A-N1A	-5.16	120.77	128.58
3	B	303	8I8	C8-C9-N9	-5.15	107.95	112.23
3	D	302	8I8	C2B-C3B-C4B	-5.04	94.42	103.24
3	B	303	8I8	O2B-C2B-C3B	4.91	124.93	111.19
3	D	302	8I8	O2B-C2B-C3B	4.90	124.91	111.19
3	A	304	8I8	C18-O18-C15	-4.83	106.53	117.98
3	C	303	8I8	C2B-C3B-C4B	-4.80	94.84	103.24
3	A	304	8I8	C2B-C3B-C4B	-4.73	94.97	103.24
3	A	304	8I8	O2B-C2B-C3B	4.64	124.17	111.19
3	B	303	8I8	C2B-C3B-C4B	-4.56	95.25	103.24
3	B	303	8I8	C18-O18-C15	-4.45	107.43	117.98
3	C	303	8I8	O2B-C2B-C3B	4.41	123.53	111.19
3	D	302	8I8	C18-O18-C15	-4.41	107.53	117.98
3	A	304	8I8	C8-C9-N9	-4.24	108.71	112.23
3	C	303	8I8	C18-O18-C15	-4.11	108.23	117.98
3	C	303	8I8	C8-C9-N9	-4.03	108.89	112.23
3	A	304	8I8	C5A-N7A-C8A	3.96	109.67	103.45
3	D	302	8I8	C5A-C4A-N3A	-3.94	121.30	126.72
3	D	302	8I8	C5A-N7A-C8A	3.91	109.60	103.45
3	B	303	8I8	C4A-N9A-C1B	-3.89	117.53	126.63
3	D	302	8I8	O5-C5-C6	3.87	119.45	108.30
3	C	303	8I8	C5A-C4A-N3A	-3.87	121.39	126.72
3	A	304	8I8	C4A-N9A-C1B	-3.84	117.65	126.63
3	A	304	8I8	O5-C5-C6	3.84	119.37	108.30
3	B	303	8I8	C5A-N7A-C8A	3.69	109.26	103.45
3	B	303	8I8	C2P-C3P-N4P	-3.69	101.78	112.05
3	A	304	8I8	C2P-C3P-N4P	-3.67	101.81	112.05
3	C	303	8I8	C5A-N7A-C8A	3.65	109.18	103.45
3	A	304	8I8	C5A-C4A-N3A	-3.61	121.75	126.72
3	D	302	8I8	C4A-N9A-C1B	-3.60	118.22	126.63
3	D	302	8I8	N3A-C4A-N9A	3.54	133.19	127.17
3	B	303	8I8	C5A-C4A-N3A	-3.48	121.93	126.72
3	C	303	8I8	O5-C5-C6	3.46	118.27	108.30
3	B	303	8I8	C13-O11-C11	3.46	126.17	117.98
3	B	303	8I8	O5-C5-C6	3.41	118.14	108.30
3	C	303	8I8	N3A-C4A-N9A	3.40	132.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	8I8	C3B-C2B-C1B	3.29	107.13	99.89
3	A	304	8I8	N3A-C4A-N9A	3.27	132.74	127.17
3	C	303	8I8	C4A-N9A-C1B	-3.27	118.99	126.63
3	B	303	8I8	N3A-C4A-N9A	3.26	132.72	127.17
3	D	302	8I8	C2P-C3P-N4P	-3.23	103.03	112.05
3	B	303	8I8	C3B-C2B-C1B	3.04	106.57	99.89
3	D	302	8I8	C2A-N3A-C4A	2.97	119.09	111.83
3	A	304	8I8	C4A-C5A-N7A	-2.94	107.23	110.58
3	B	303	8I8	C14-C15-C16	-2.91	98.14	103.24
3	D	302	8I8	C4A-C5A-N7A	-2.89	107.28	110.58
3	C	303	8I8	C2A-N3A-C4A	2.82	118.72	111.83
3	D	302	8I8	C3B-C2B-C1B	2.80	106.06	99.89
3	B	303	8I8	C4A-C5A-N7A	-2.80	107.38	110.58
3	A	304	8I8	C2A-N3A-C4A	2.80	118.66	111.83
3	B	303	8I8	O5A-P2A-O3A	2.78	114.79	107.27
3	A	304	8I8	C3B-C2B-C1B	2.78	106.00	99.89
3	B	303	8I8	C2A-N3A-C4A	2.76	118.58	111.83
3	C	303	8I8	C4A-C5A-N7A	-2.72	107.47	110.58
3	D	302	8I8	C4B-O4B-C1B	-2.58	103.78	109.47
3	A	304	8I8	C13-O11-C11	2.52	123.94	117.98
3	A	304	8I8	C4B-O4B-C1B	-2.47	104.00	109.47
3	B	303	8I8	C1-O5-C5	2.46	115.91	113.08
3	C	303	8I8	O18-C18-C19	2.45	112.08	108.08
3	B	303	8I8	O1A-P1A-O3A	2.44	113.86	107.27
3	A	304	8I8	C13-C14-C15	-2.42	99.19	102.10
3	C	303	8I8	CEP-CBP-CAP	2.41	112.87	108.77
3	C	303	8I8	C13-O11-C11	2.41	123.68	117.98
3	C	303	8I8	C2P-C3P-N4P	-2.41	105.34	112.05
3	B	303	8I8	C13-C14-C15	-2.38	99.23	102.10
3	B	303	8I8	C4B-O4B-C1B	-2.34	104.29	109.47
3	D	302	8I8	O18-C18-C19	2.26	111.78	108.08
3	D	302	8I8	O6A-CCP-CBP	-2.24	106.94	110.55
3	D	302	8I8	O1A-P1A-O3A	2.21	113.26	107.27
3	C	303	8I8	O16-C16-C15	2.20	109.56	104.92
3	B	303	8I8	O18-C18-C19	2.16	111.62	108.08
3	A	304	8I8	C1-O5-C5	2.15	115.55	113.08
3	A	304	8I8	O5A-P2A-O3A	2.13	113.04	107.27
3	D	302	8I8	C1-O5-C5	2.11	115.50	113.08
3	C	303	8I8	C1-O5-C5	2.10	115.49	113.08
3	B	303	8I8	CEP-CBP-CAP	2.02	112.22	108.77
3	B	303	8I8	O3-C3-C4	-2.00	105.66	110.38

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	304	8I8	C13
3	A	304	8I8	C5
3	A	304	8I8	C2B
3	A	304	8I8	C1B
3	A	304	8I8	C14
3	B	303	8I8	C13
3	B	303	8I8	C5
3	B	303	8I8	C2B
3	B	303	8I8	C1B
3	B	303	8I8	C14
3	C	303	8I8	C13
3	C	303	8I8	C5
3	C	303	8I8	C2B
3	C	303	8I8	C1B
3	C	303	8I8	C14
3	D	302	8I8	C13
3	D	302	8I8	C5
3	D	302	8I8	C2B
3	D	302	8I8	C1B
3	D	302	8I8	C14

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	8I8	C14-C13-O11-C11
3	A	304	8I8	S1P-C2P-C3P-N4P
3	A	304	8I8	C8-C9-N9-C
3	A	304	8I8	C10-C9-N9-C
3	B	303	8I8	C14-C13-O11-C11
3	B	303	8I8	S1P-C2P-C3P-N4P
3	B	303	8I8	C8-C9-N9-C
3	B	303	8I8	C10-C9-N9-C
3	C	303	8I8	C14-C13-O11-C11
3	C	303	8I8	C8-C9-N9-C
3	C	303	8I8	C10-C9-N9-C
3	D	302	8I8	C14-C13-O11-C11
3	D	302	8I8	C8-C9-N9-C
3	D	302	8I8	C10-C9-N9-C
4	B	301	GOL	O1-C1-C2-C3
4	C	301	GOL	C1-C2-C3-O3
4	C	302	GOL	O1-C1-C2-C3
5	B	302	BTB	N-C2-C3-O3
3	C	303	8I8	O22-C18-O18-C15

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Mol	Chain	Res	Type	Atoms
3	D	302	8I8	O22-C18-O18-C15
3	A	304	8I8	N4P-C5P-C6P-C7P
3	B	303	8I8	N4P-C5P-C6P-C7P
3	C	303	8I8	N4P-C5P-C6P-C7P
3	D	302	8I8	N4P-C5P-C6P-C7P
4	B	301	GOL	O1-C1-C2-O2
4	C	302	GOL	O1-C1-C2-O2
3	C	303	8I8	S1P-C2P-C3P-N4P
4	C	301	GOL	O2-C2-C3-O3
3	B	303	8I8	O22-C18-O18-C15
4	A	305	GOL	O2-C2-C3-O3
3	A	304	8I8	O5P-C5P-C6P-C7P
3	B	303	8I8	O5P-C5P-C6P-C7P
3	D	302	8I8	O5P-C5P-C6P-C7P
3	A	304	8I8	O22-C18-O18-C15
3	D	302	8I8	O4B-C1B-N9A-C8A
3	B	303	8I8	P1A-O3A-P2A-O4A
5	B	302	BTB	N-C5-C6-O6
3	A	304	8I8	O4B-C1B-N9A-C8A
3	B	303	8I8	O4B-C1B-N9A-C8A
3	A	304	8I8	P1A-O3A-P2A-O5A
3	B	303	8I8	P1A-O3A-P2A-O5A
3	C	303	8I8	O4B-C1B-N9A-C8A
3	A	304	8I8	C3B-O3B-P3B-O8A
3	B	303	8I8	C3B-O3B-P3B-O8A
3	D	302	8I8	C3B-O3B-P3B-O8A
3	A	304	8I8	C16-C15-O18-C18
3	A	304	8I8	N8P-C9P-CAP-OAP
3	D	302	8I8	N8P-C9P-CAP-OAP

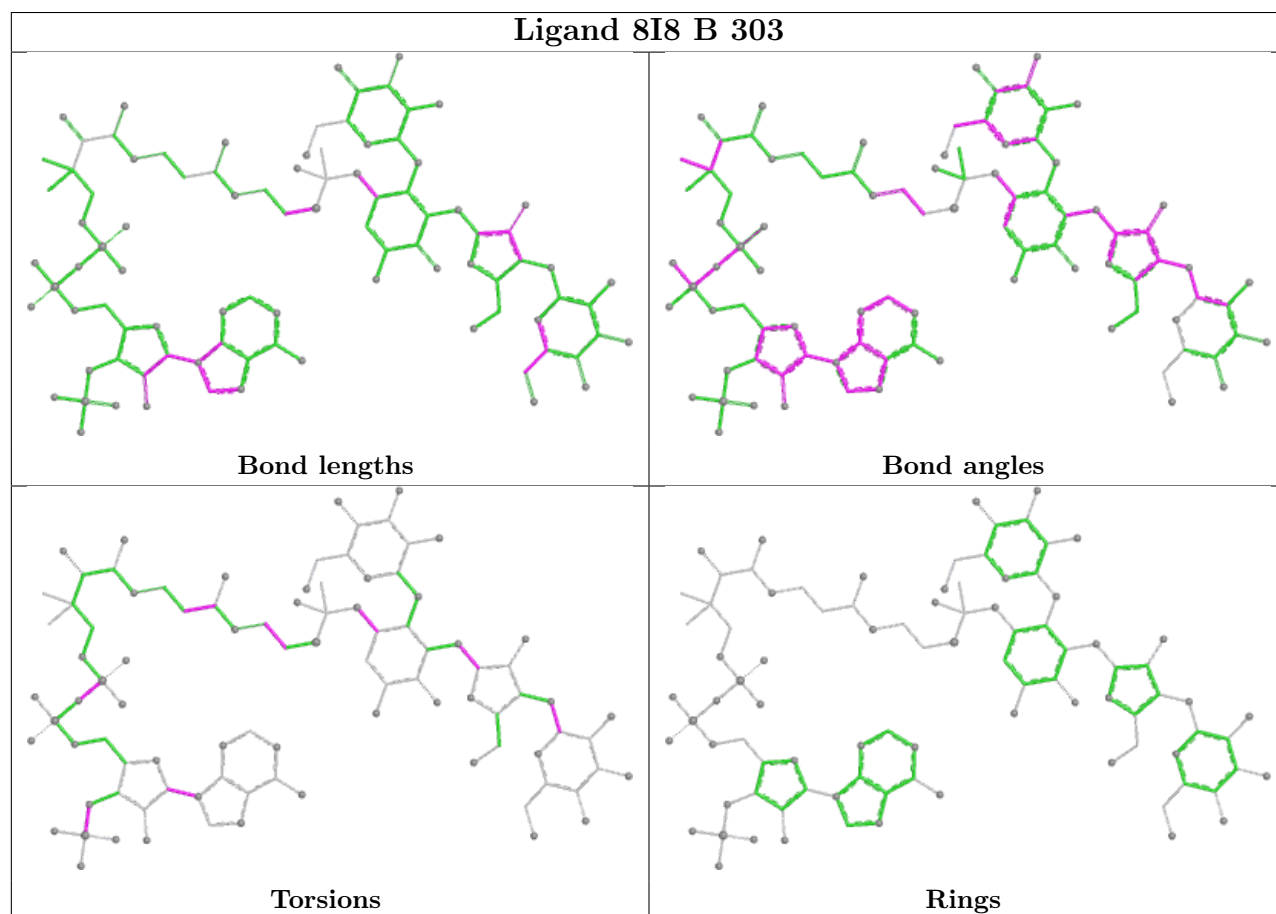
There are no ring outliers.

4 monomers are involved in 6 short contacts:

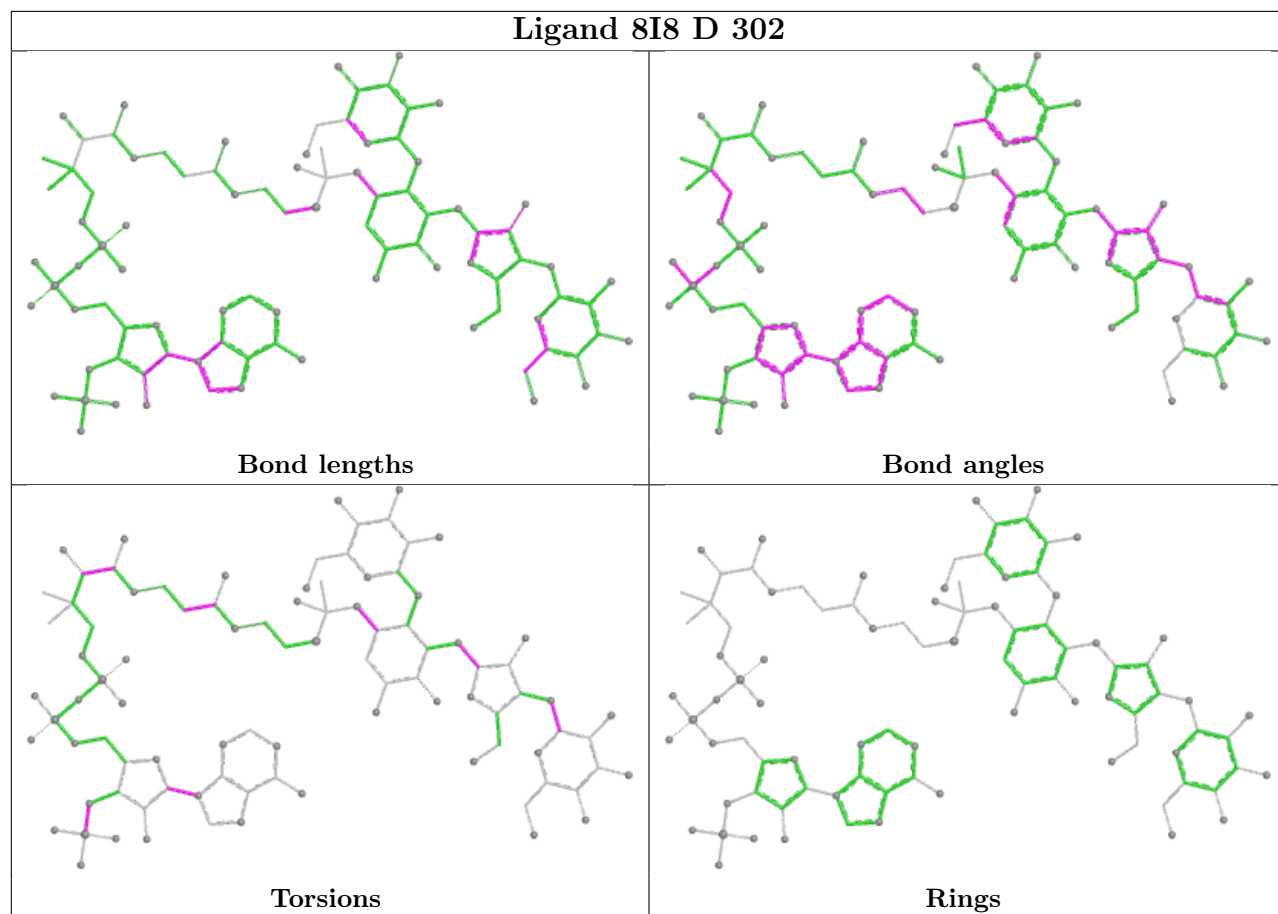
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	8I8	1	0
3	D	302	8I8	2	0
3	A	304	8I8	1	0
3	C	303	8I8	2	0

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

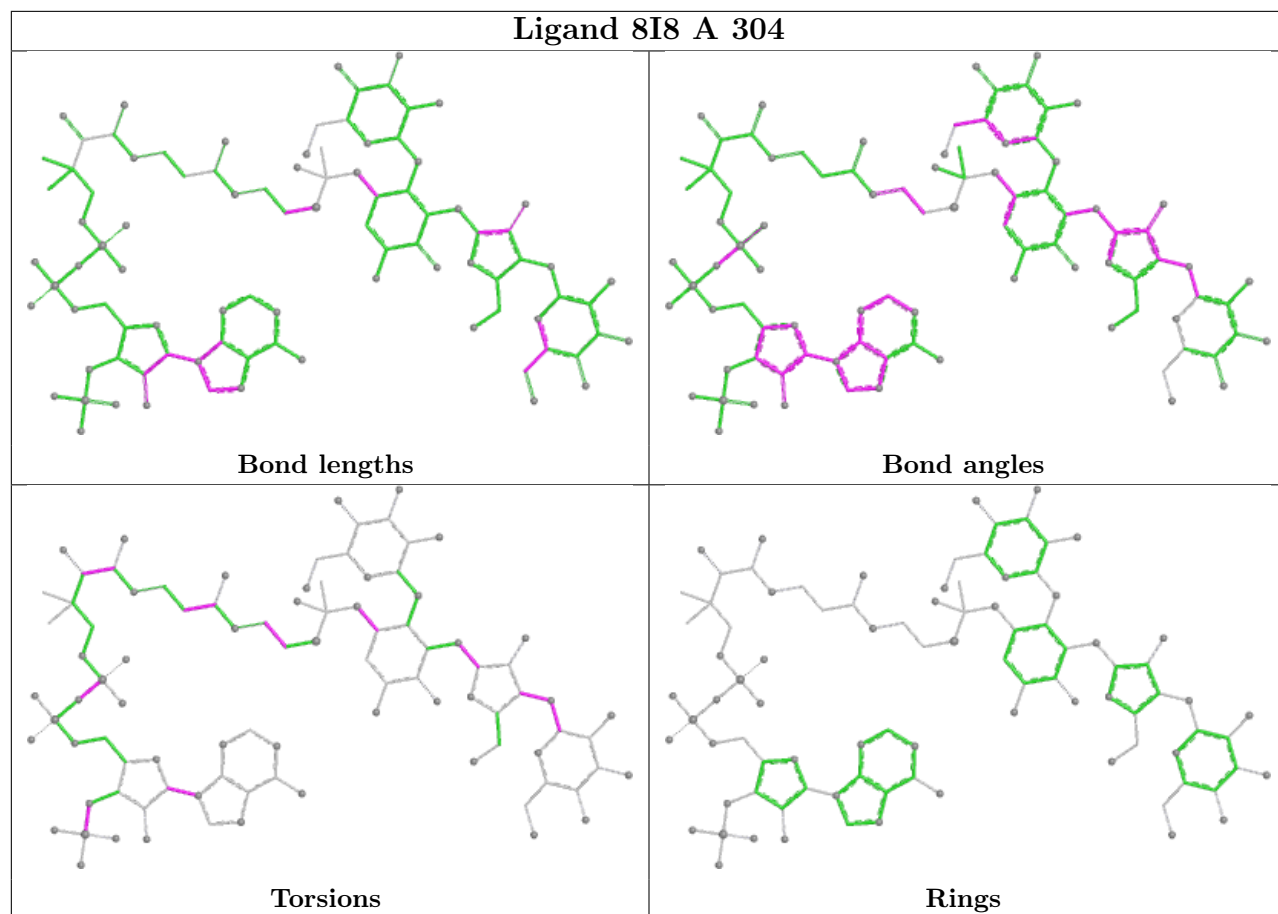
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

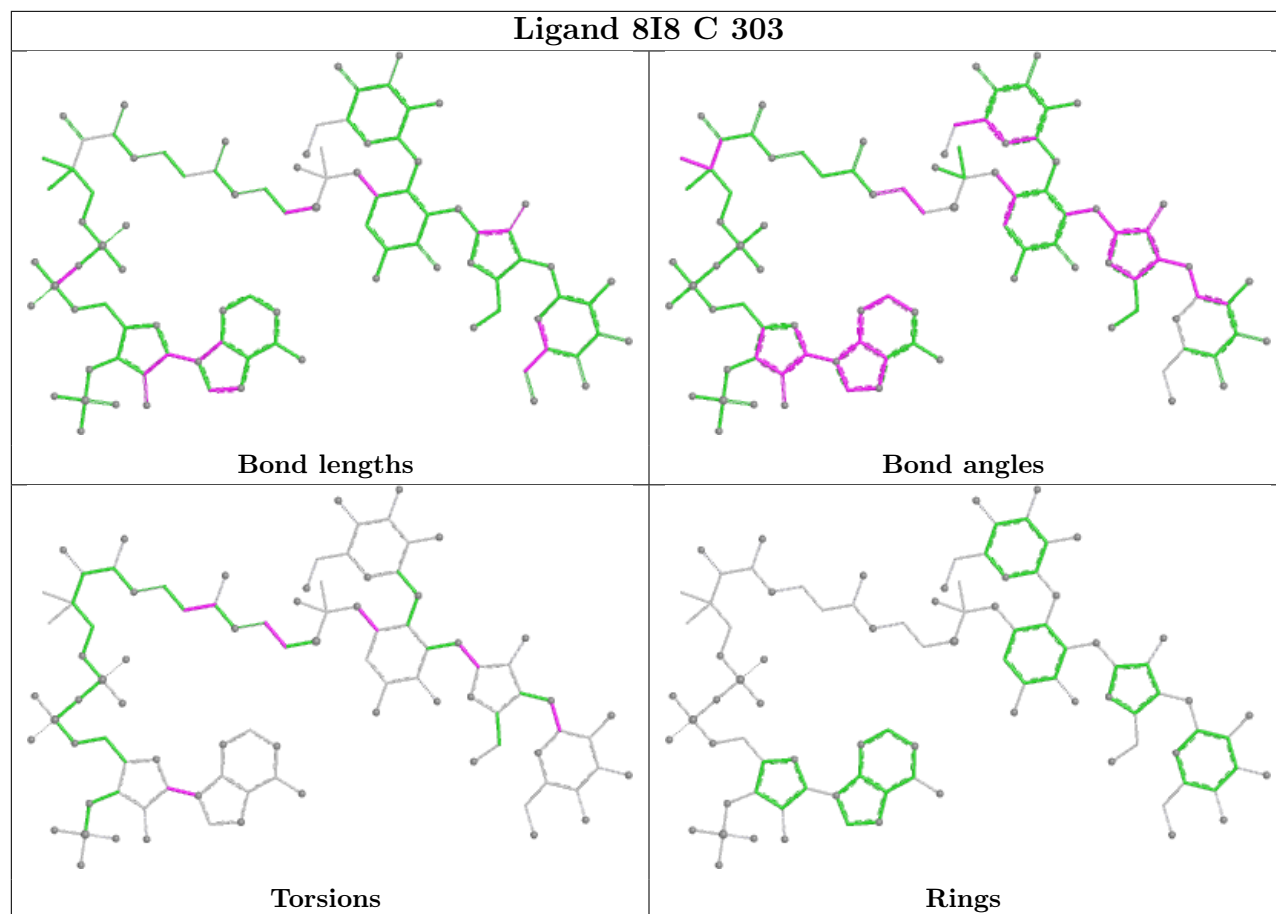


Ligand 8I8 D 302



Ligand 8I8 A 304





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	263/287 (91%)	-0.03	11 (4%) 40 44	10, 21, 39, 58	9 (3%)
1	B	261/287 (90%)	-0.09	5 (1%) 66 70	12, 20, 36, 59	5 (1%)
1	C	261/287 (90%)	-0.17	2 (0%) 82 86	9, 20, 34, 48	6 (2%)
1	D	272/287 (94%)	0.06	13 (4%) 35 38	12, 22, 41, 79	5 (1%)
All	All	1057/1148 (92%)	-0.06	31 (2%) 53 57	9, 21, 38, 79	25 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	290	TYR	4.7
1	D	24	LEU	4.6
1	A	26	ILE	4.1
1	D	20	HIS	4.1
1	D	288	ALA	4.0
1	D	287	SER	3.7
1	A	101	LEU	3.5
1	D	19	SER	3.3
1	A	288	ALA	3.2
1	A	100	ALA	3.1
1	D	21	MET	3.1
1	D	25	ASN	3.0
1	B	26	ILE	3.0
1	D	22	THR	2.8
1	A	99	ASP	2.6
1	B	100	ALA	2.6
1	D	289	SER	2.6
1	D	23	ASP	2.5
1	C	286	ASP	2.5
1	A	97	LEU	2.4
1	D	26	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	96	SER	2.4
1	A	287	SER	2.3
1	B	101	LEU	2.3
1	A	95[A]	ASP	2.2
1	C	205	ARG	2.2
1	A	93	PHE	2.1
1	D	78	ASP	2.1
1	B	256	ARG	2.0
1	B	32[A]	HIS	2.0
1	A	122	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

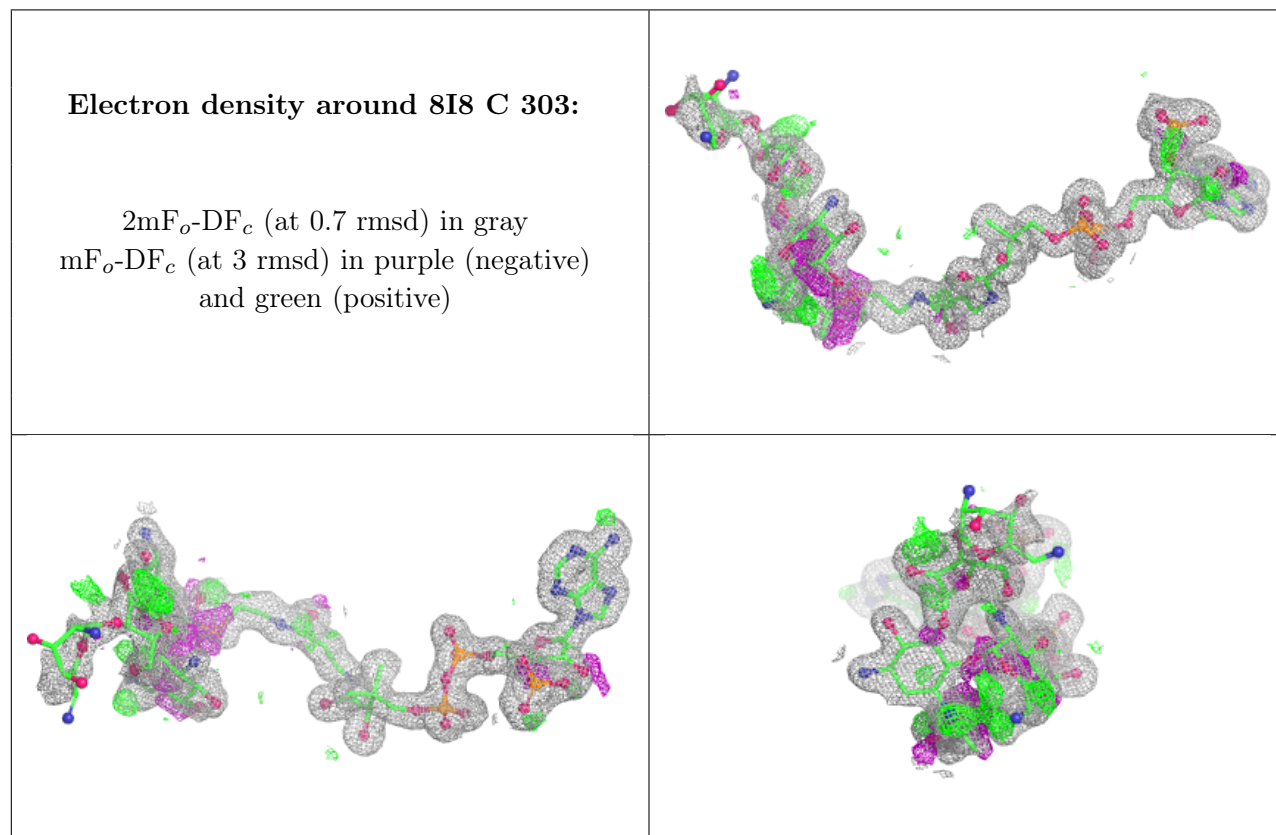
There are no oligosaccharides in this entry.

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.

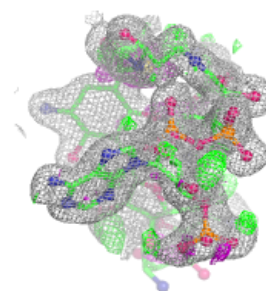
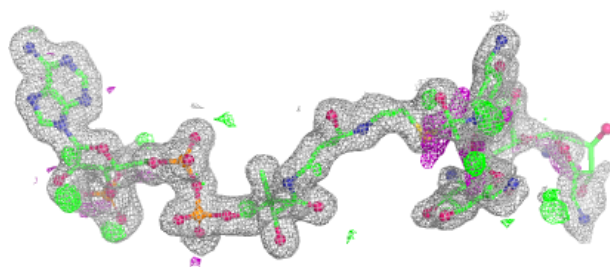
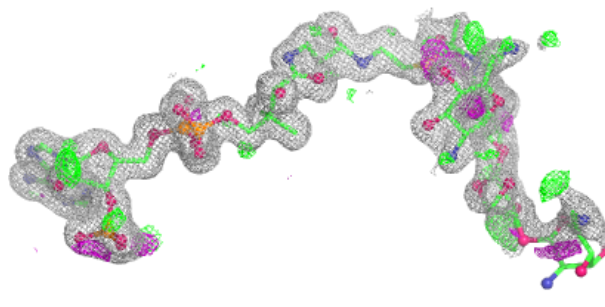
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	302	6/6	0.70	0.16	35,41,45,50	0
4	GOL	B	301	6/6	0.78	0.14	33,36,42,52	0
2	NA	A	301	1/1	0.79	0.19	49,49,49,49	0
4	GOL	C	301	6/6	0.83	0.16	45,47,49,53	0
5	BTB	B	302	14/14	0.83	0.15	21,26,30,36	14
4	GOL	A	305	6/6	0.84	0.14	37,43,46,49	0
6	CL	D	301	1/1	0.87	0.12	58,58,58,58	0
2	NA	A	302	1/1	0.88	0.19	45,45,45,45	0
3	8I8	C	303	93/93	0.94	0.12	16,29,70,79	0
3	8I8	D	302	93/93	0.94	0.11	18,28,70,77	0
3	8I8	A	304	93/93	0.94	0.10	18,26,56,64	0
3	8I8	B	303	93/93	0.94	0.10	15,24,51,58	0
2	NA	A	303	1/1	0.96	0.09	39,39,39,39	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.

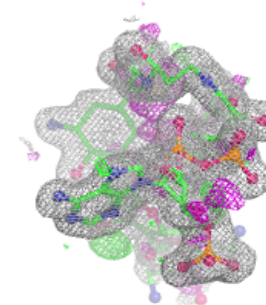
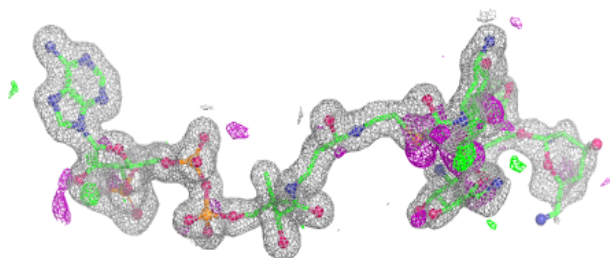
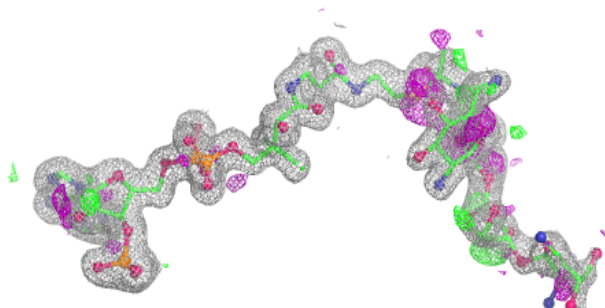


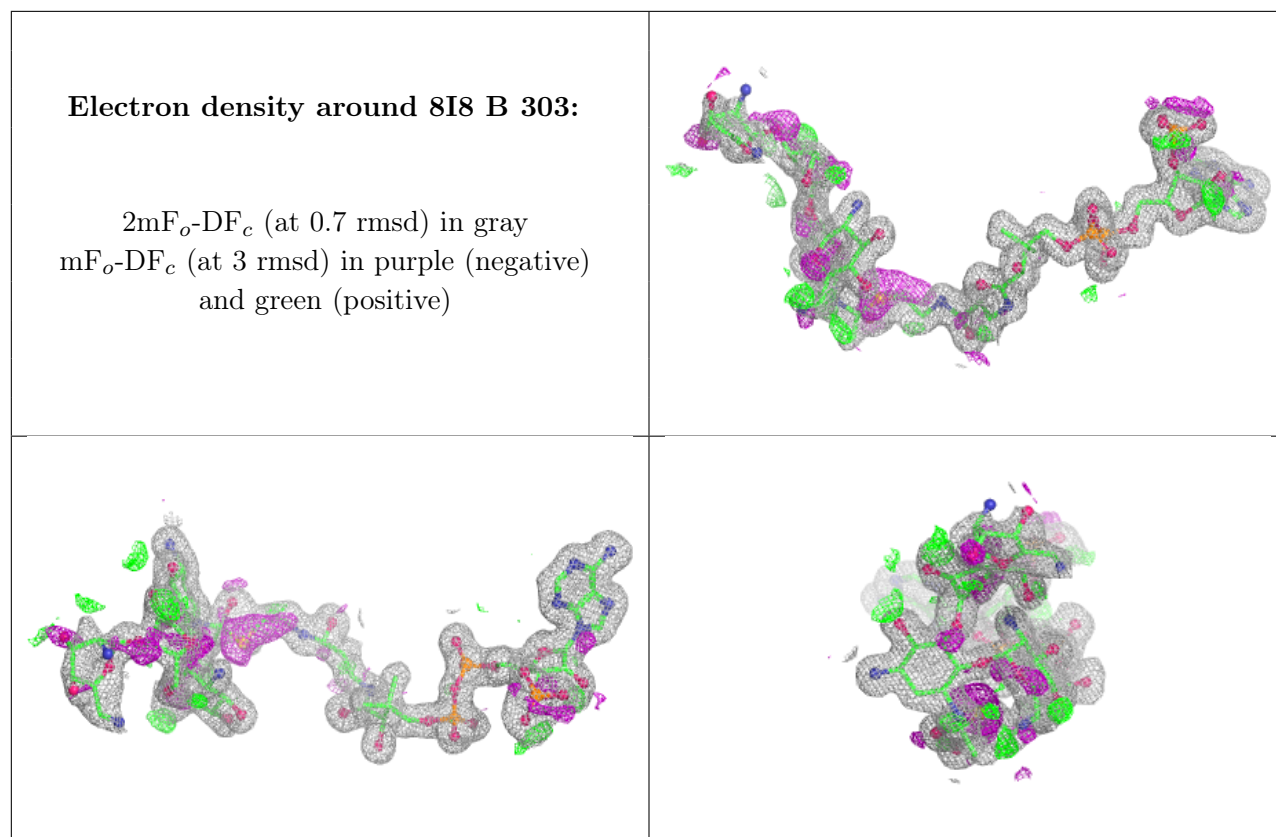
Electron density around 8I8 D 302:

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

**Electron density around 8I8 A 304:**

$2mF_o-DF_c$ (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.