



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 12:09 AM EDT

PDB ID : 3V8X  
Title : The crystal structure of transferrin binding protein A (TbpA) from *Neisseria meningitidis* serogroup B in complex with full length human transferrin  
Authors : Noinaj, N.; Easley, N.; Buchanan, S.K.  
Deposited on : 2011-12-23  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

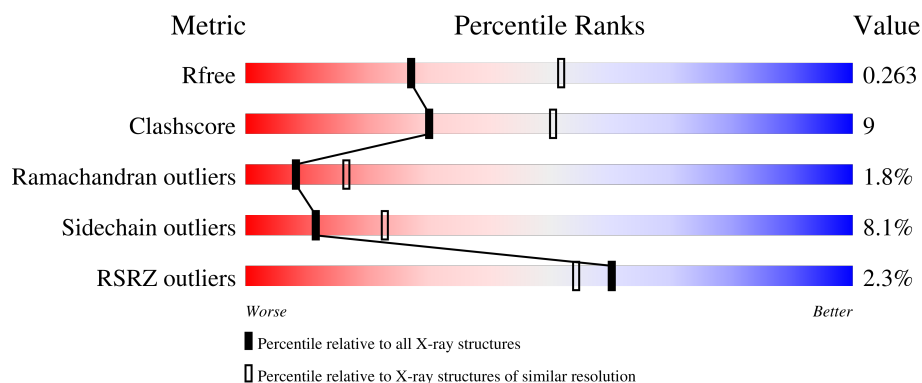
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	904	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>6%</div> </div> </div>
2	B	698	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>
3	C	10	<div> <div>10%</div> <div> <div></div> <div>50%</div> <div>40%</div> </div> </div>
4	D	9	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>22%</div> </div> </div>

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	SIA	C	7	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12233 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 Transferrin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	2	0
			6686	4176	1218	1282	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q9K0U9
A	13	ASP	-	expression tag	UNP Q9K0U9
A	14	ILE	-	expression tag	UNP Q9K0U9
A	15	HIS	-	expression tag	UNP Q9K0U9
A	16	HIS	-	expression tag	UNP Q9K0U9
A	17	HIS	-	expression tag	UNP Q9K0U9
A	18	HIS	-	expression tag	UNP Q9K0U9
A	19	HIS	-	expression tag	UNP Q9K0U9
A	20	HIS	-	expression tag	UNP Q9K0U9
A	21	HIS	-	expression tag	UNP Q9K0U9
A	22	HIS	-	expression tag	UNP Q9K0U9
A	23	HIS	-	expression tag	UNP Q9K0U9
A	24	HIS	-	expression tag	UNP Q9K0U9
A	435	VAL	ILE	variant	UNP Q9K0U9
A	913	TYR	MET	engineered mutation	UNP Q9K0U9

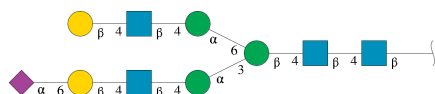
- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	676	Total	C	N	O	S	0	0	0
			5050	3160	868	977	45			

There is a discrepancy between the modelled and reference sequences:

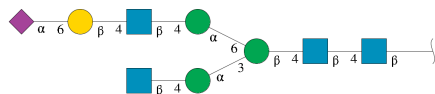
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	variant	UNP P02787

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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.



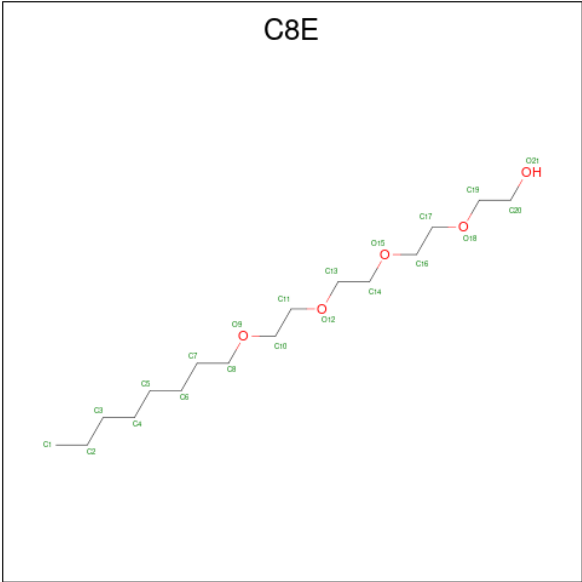
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			131	73	5	53			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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
4	D	9	Total	C	N	O	0	0	0
			120	67	5	48			

- Molecule 5 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).

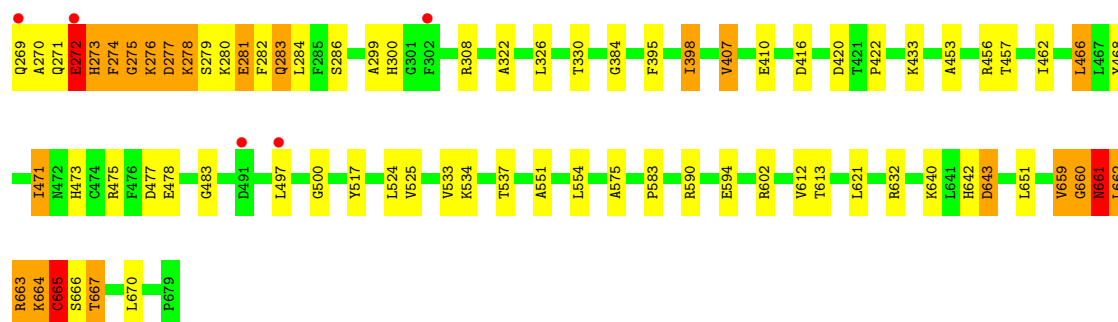


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	16	5		
5	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	62	Total	O	0	0
			62	62		





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 10% 50% 40%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 D: 11% 67% 22%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.01Å 129.36Å 198.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.60 49.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.92-2.60) 98.0 (49.47-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.208 , 0.267 0.208 , 0.263	Depositor DCC
$R_{free}$ test set	3603 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, MAN, C8E, GAL, NAG, SIA

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	0.29	0/6834	0.47	1/9244 (0.0%)
2	B	0.29	0/5166	0.44	1/7025 (0.0%)
All	All	0.29	0/12000	0.45	2/16269 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	GLY	N-CA-C	-5.57	99.18	113.10
1	A	448	ALA	N-CA-C	-5.07	97.30	111.00

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	6686	0	6396	91	0
2	B	5050	0	4646	120	0
3	C	131	0	110	7	0
4	D	120	0	101	2	0
5	A	42	0	68	6	0
6	A	142	0	0	2	0
6	B	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12233	0	11321	217	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 9.

The worst 5 of 217 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:PHE:O	2:B:283:GLN:HG2	1.46	1.15
2:B:275:GLY:HA2	2:B:281:GLU:O	1.48	1.12
2:B:659:VAL:HG23	2:B:660:GLY:H	0.91	1.05
2:B:269:GLN:HA	2:B:272:GLU:HG3	1.39	1.02
2:B:659:VAL:CG2	2:B:660:GLY:H	1.69	1.00

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	849/904 (94%)	807 (95%)	39 (5%)	3 (0%)	34	57
2	B	674/698 (97%)	593 (88%)	57 (8%)	24 (4%)	3	4
All	All	1523/1602 (95%)	1400 (92%)	96 (6%)	27 (2%)	8	16

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	780	SER
2	B	31	PRO
2	B	272	GLU
2	B	281	GLU

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Mol	Chain	Res	Type
2	B	283	GLN

### 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	685/741 (92%)	616 (90%)	69 (10%)	7	14
2	B	520/585 (89%)	490 (94%)	30 (6%)	20	40
All	All	1205/1326 (91%)	1106 (92%)	99 (8%)	11	22

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	782	LEU
2	B	49	ILE
1	A	828	LEU
1	A	888	VAL
2	B	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	779	GLN
2	B	283	GLN
2	B	469	ASN
2	B	661	ASN

### 5.3.3 RNA [i](#)

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 ⓘ

19 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	$\# Z  > 2$
3	NAG	C	1	3,2	14,14,15	0.68	0	17,19,21	1.02	2 (11%)
3	GAL	C	10	3	11,11,12	0.67	0	15,15,17	1.48	1 (6%)
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
3	BMA	C	3	3	11,11,12	1.07	1 (9%)	15,15,17	1.61	4 (26%)
3	MAN	C	4	3	11,11,12	0.82	0	15,15,17	1.73	3 (20%)
3	NAG	C	5	3	14,14,15	0.58	0	17,19,21	1.52	2 (11%)
3	GAL	C	6	3	11,11,12	0.65	0	15,15,17	0.53	0
3	SIA	C	7	3	20,20,21	0.73	0	21,28,31	1.87	5 (23%)
3	MAN	C	8	3	11,11,12	0.64	0	15,15,17	1.34	1 (6%)
3	NAG	C	9	3	14,14,15	0.61	0	17,19,21	0.97	1 (5%)
4	NAG	D	1	2,4	14,14,15	0.70	0	17,19,21	1.25	1 (5%)
4	NAG	D	2	4	14,14,15	0.51	0	17,19,21	1.71	3 (17%)
4	BMA	D	3	4	11,11,12	1.94	3 (27%)	15,15,17	1.95	6 (40%)
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	0.66	0
4	NAG	D	5	4	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
4	GAL	D	6	4	11,11,12	0.56	0	15,15,17	2.06	4 (26%)
4	SIA	D	7	4	20,20,21	0.68	0	21,28,31	1.04	3 (14%)
4	MAN	D	8	4	11,11,12	0.65	0	15,15,17	1.29	1 (6%)
4	NAG	D	9	4	14,14,15	0.53	0	17,19,21	0.58	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	GAL	C	10	3	-	1/2/19/22	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	GAL	C	6	3	-	2/2/19/22	0/1/1/1
3	SIA	C	7	3	-	5/18/34/38	0/1/1/1
3	MAN	C	8	3	-	2/2/19/22	1/1/1/1
3	NAG	C	9	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	NAG	D	5	4	-	0/6/23/26	0/1/1/1
4	GAL	D	6	4	-	1/2/19/22	0/1/1/1
4	SIA	D	7	4	-	3/18/34/38	0/1/1/1
4	MAN	D	8	4	-	1/2/19/22	0/1/1/1
4	NAG	D	9	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C1-C2	4.85	1.63	1.52
4	D	3	BMA	C2-C3	2.26	1.56	1.52
3	C	3	BMA	C2-C3	2.07	1.55	1.52
4	D	3	BMA	O5-C1	2.07	1.47	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	SIA	O6-C2-C3	5.11	117.43	110.56
4	D	6	GAL	O2-C2-C3	4.93	120.37	110.15
4	D	2	NAG	C1-O5-C5	4.78	118.59	112.19
3	C	7	SIA	C6-C5-N5	4.54	118.14	110.91
4	D	6	GAL	O2-C2-C1	4.44	119.39	109.22

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	9	NAG	C3-C2-N2-C7
3	C	9	NAG	C8-C7-N2-C2
3	C	9	NAG	O7-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6

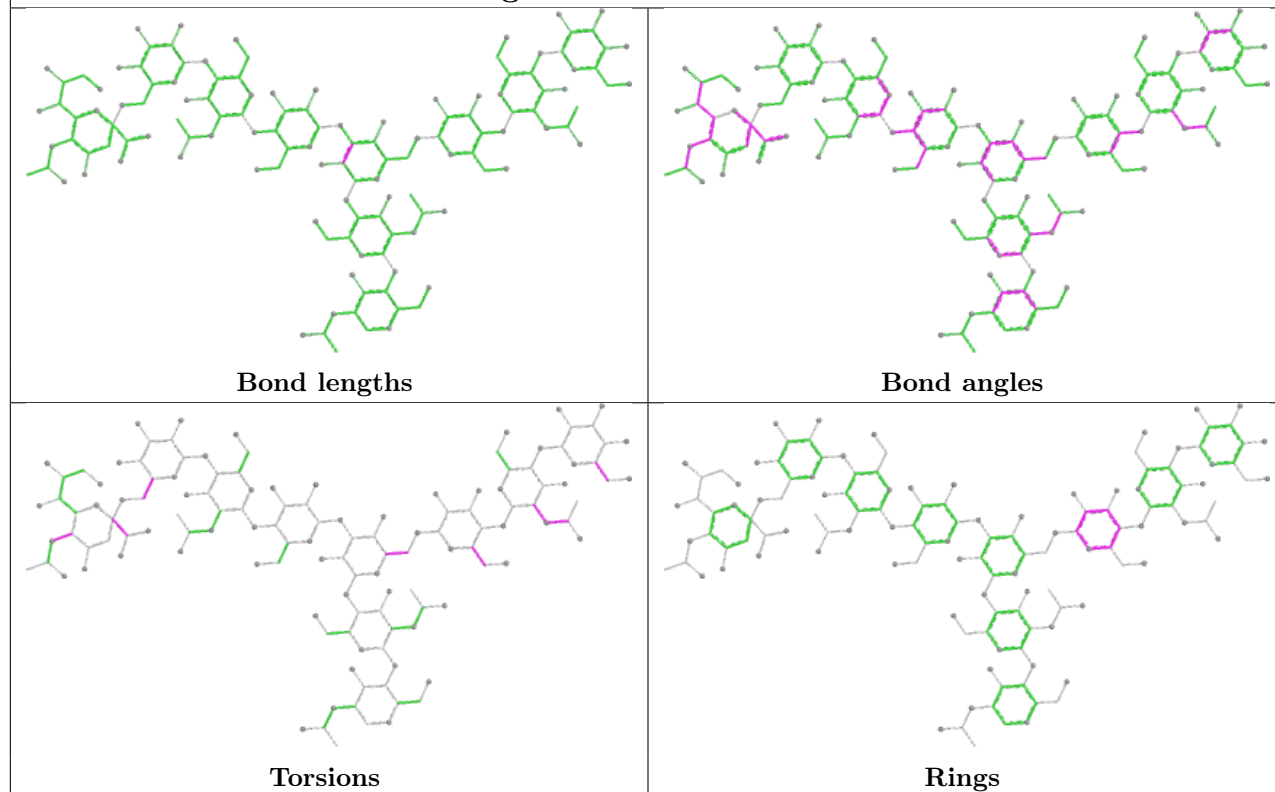
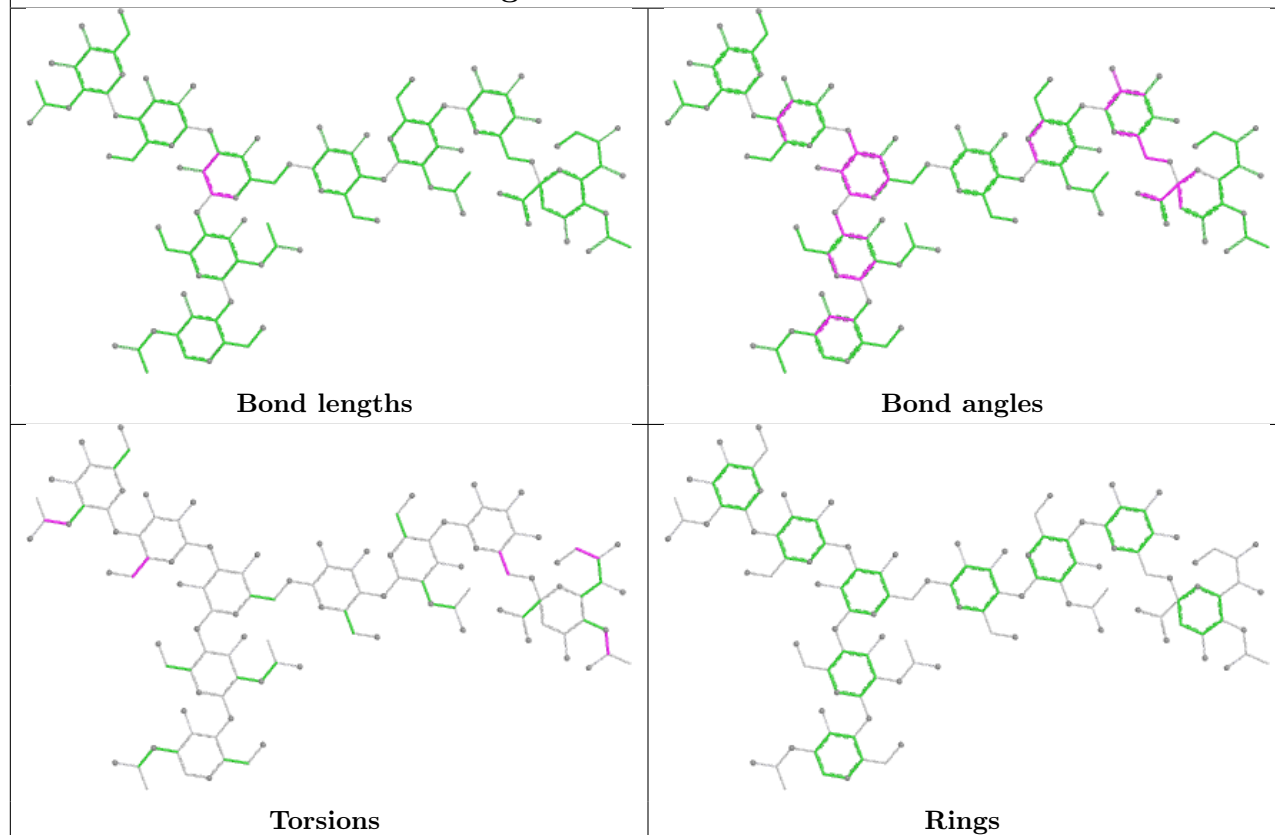
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	8	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	4	0
3	C	3	BMA	1	0
4	D	5	NAG	1	0
4	D	4	MAN	2	0
4	D	3	BMA	1	0
3	C	5	NAG	1	0
3	C	7	SIA	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 oligosaccharide.

**Oligosaccharide Chain C****Oligosaccharide Chain D**



## 5.6 Ligand geometry

2 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	$\# Z  > 2$
5	C8E	A	1002	-	20,20,20	0.43	0	19,19,19	0.65	0
5	C8E	A	1001	-	20,20,20	0.39	0	19,19,19	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	C8E	A	1002	-	-	12/18/18/18	-
5	C8E	A	1001	-	-	9/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	C8E	C17-C16-O15-C14
5	A	1001	C8E	O12-C13-C14-O15
5	A	1002	C8E	O15-C16-C17-O18
5	A	1002	C8E	C16-C17-O18-C19
5	A	1001	C8E	O18-C19-C20-O21

There are no ring outliers.

2 monomers are involved in 6 short contacts:

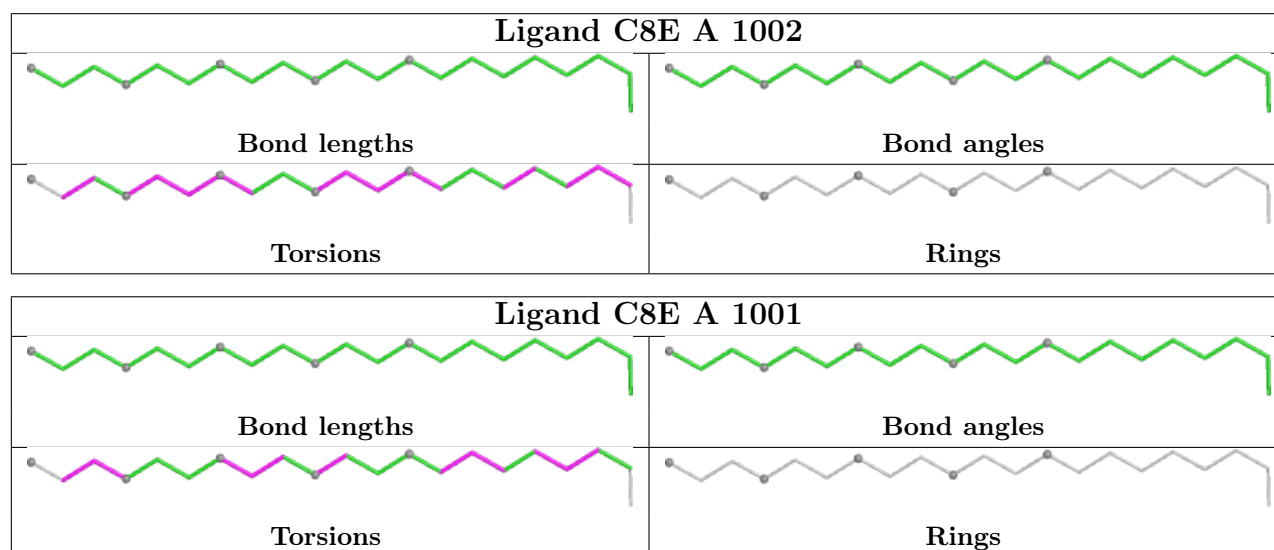
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	C8E	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	C8E	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	853/904 (94%)	-0.13	12 (1%) 75 71	37, 69, 111, 155	0
2	B	676/698 (96%)	-0.08	23 (3%) 45 38	43, 82, 152, 212	0
All	All	1529/1602 (95%)	-0.11	35 (2%) 60 54	37, 74, 136, 212	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	267	LEU	4.9
2	B	256	MET	4.6
2	B	37	VAL	4.2
2	B	24	ASP	4.1
2	B	302	PHE	3.9

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GAL	D	6	11/12	0.50	0.40	30,133,150,153	0
3	GAL	C	6	11/12	0.59	0.28	30,142,156,165	0
4	MAN	D	8	11/12	0.62	0.21	167,175,185,187	0
4	NAG	D	9	14/15	0.62	0.35	157,178,187,187	0
4	BMA	D	3	11/12	0.63	0.19	150,169,201,202	0

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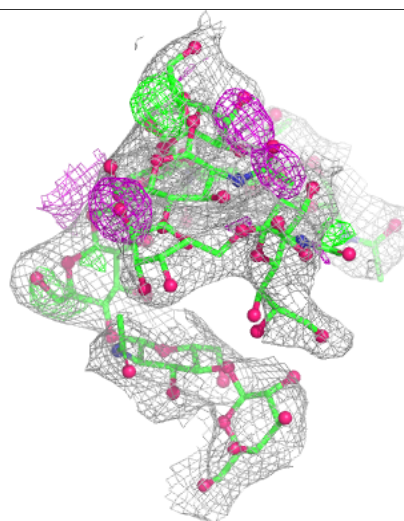
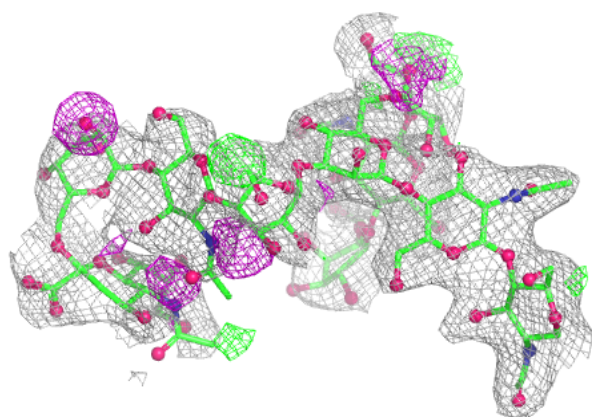
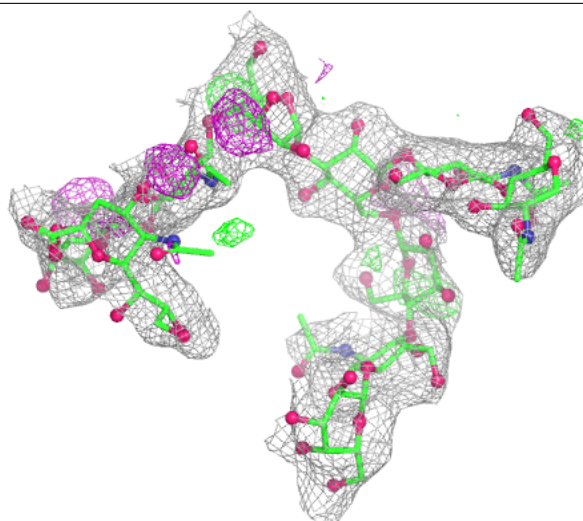
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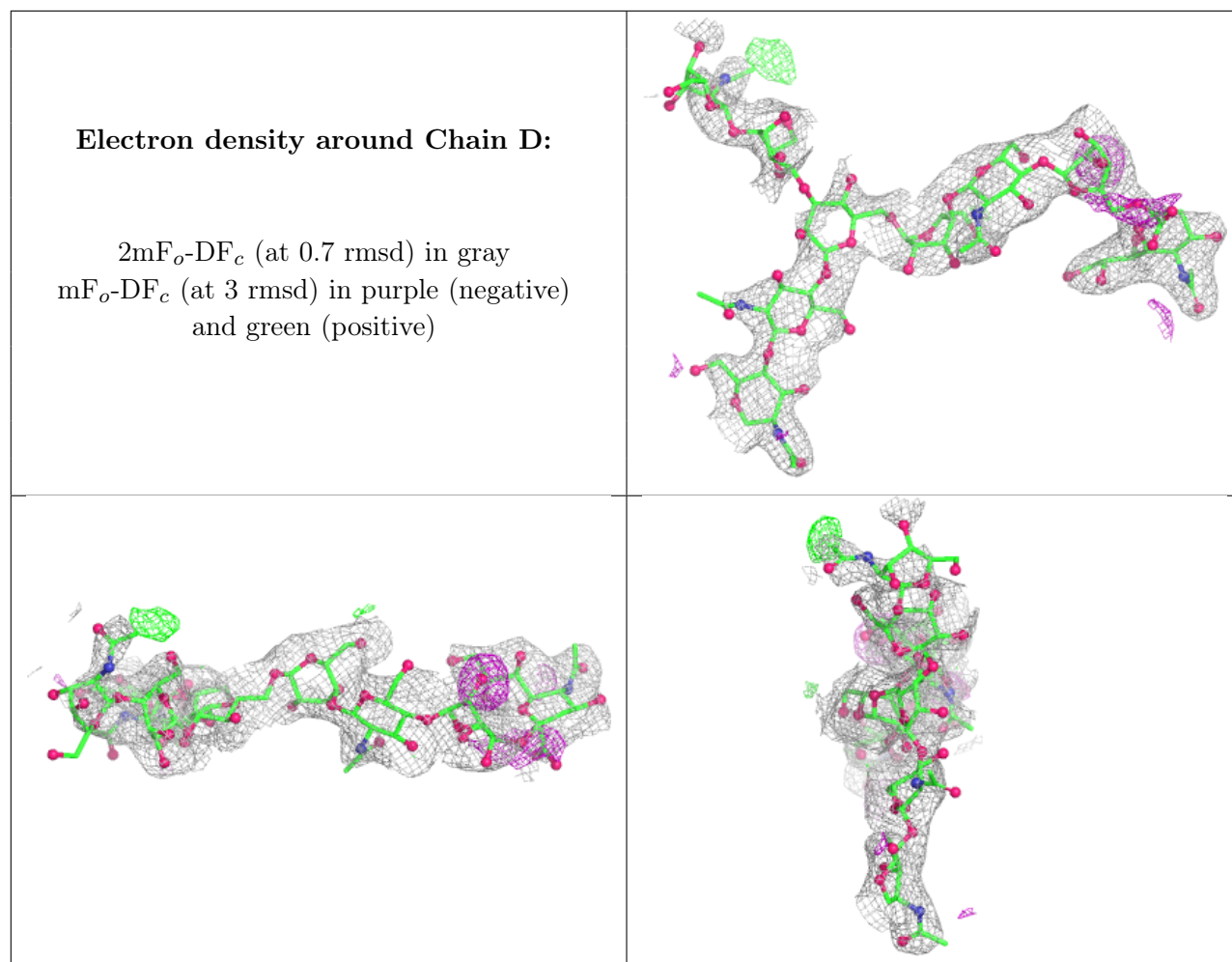
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SIA	C	7	20/21	0.63	0.41	149,166,174,174	0
3	GAL	C	10	11/12	0.78	0.16	139,154,157,160	0
3	MAN	C	8	11/12	0.79	0.25	85,118,141,153	0
3	MAN	C	4	11/12	0.83	0.28	79,95,116,128	0
4	MAN	D	4	11/12	0.84	0.17	137,153,155,157	0
4	NAG	D	2	14/15	0.85	0.21	111,144,158,162	0
4	NAG	D	5	14/15	0.87	0.23	113,135,143,144	0
4	SIA	D	7	20/21	0.88	0.32	73,91,144,146	0
3	NAG	C	9	14/15	0.90	0.14	118,125,145,150	0
3	NAG	C	5	14/15	0.91	0.25	81,103,113,123	0
4	NAG	D	1	14/15	0.91	0.18	67,113,122,131	0
3	NAG	C	1	14/15	0.95	0.14	54,67,82,86	0
3	BMA	C	3	11/12	0.95	0.13	54,64,85,108	0
3	NAG	C	2	14/15	0.97	0.10	55,66,71,80	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, 95<sup>th</sup> 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.

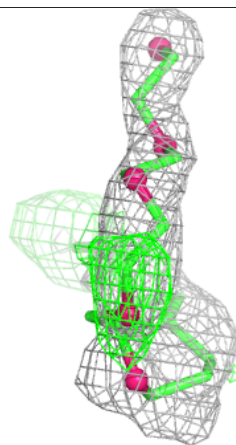
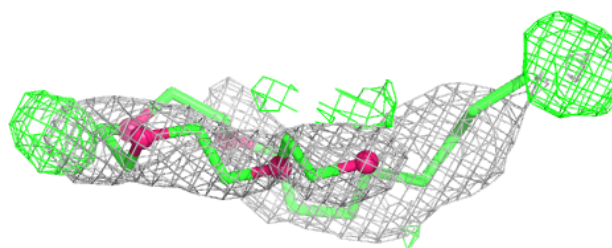
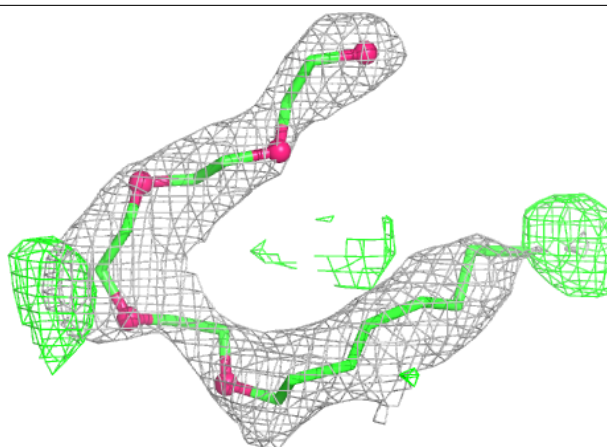
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	C8E	A	1001	21/21	0.79	0.24	70,101,117,118	0
5	C8E	A	1002	21/21	0.83	0.26	48,77,98,106	0

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.

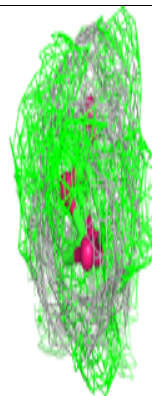
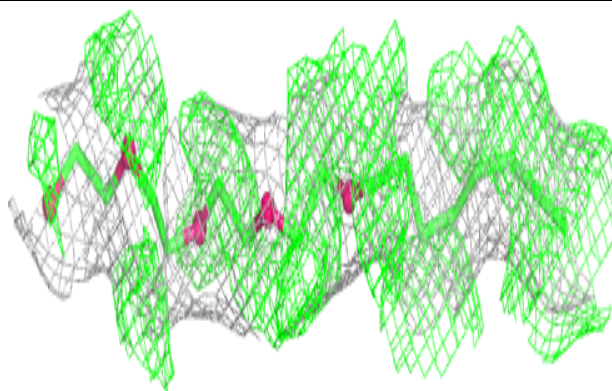
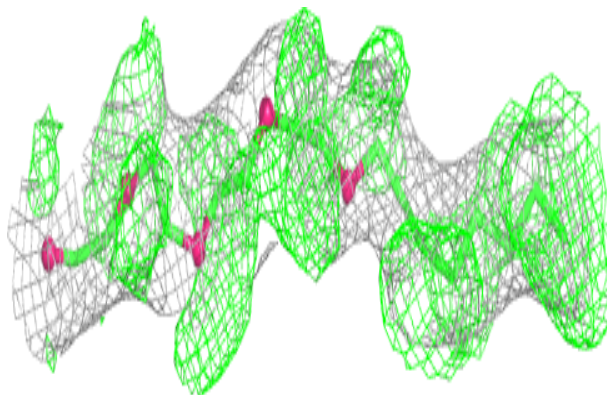


**Electron density around C8E A 1001:**

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

**Electron density around C8E A 1002:**

$2mF_o-DF_c$  (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.