



## Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2025 – 01:12 pm BST

PDB ID : 9I5Q / pdb\_00009i5q  
Title : Recombinant human butyrylcholinesterase in complex with 2-(cyclohexylmethyl)-5-(2,4-difluorophenoxy)-N-(2-(3-(methoxymethyl)piperidin-1-yl)ethyl)-2H-indazole-6-carboxamide  
Authors : Brazzolotto, X.; Ferjancic Benetik, S.; Knez, D.; Proj, M.; Gobec, S.; Nachon, F.  
Deposited on : 2025-01-28  
Resolution : 2.36 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](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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

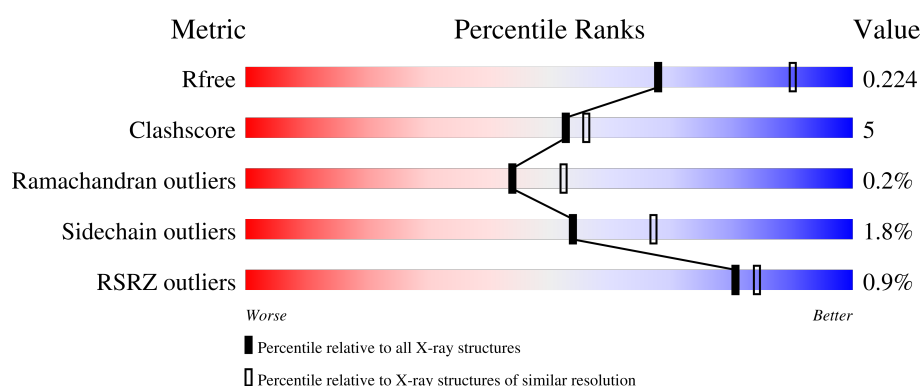
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	529	<div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	B	2	<div> <div>100%</div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>
3	D	3	<div> <div>100%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4571 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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4232	2731	711	774	16	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



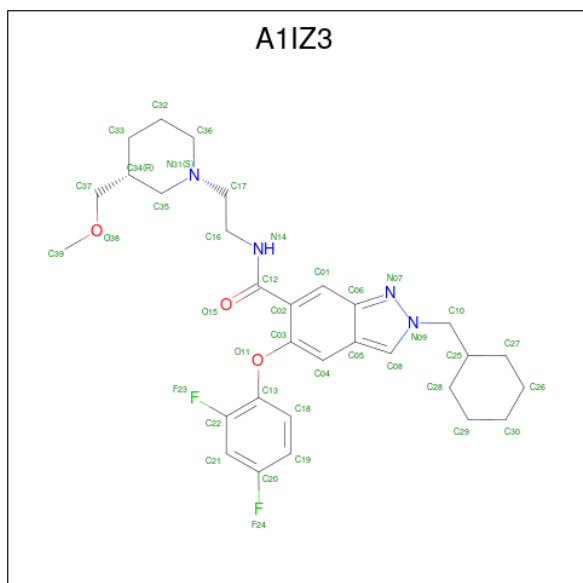
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



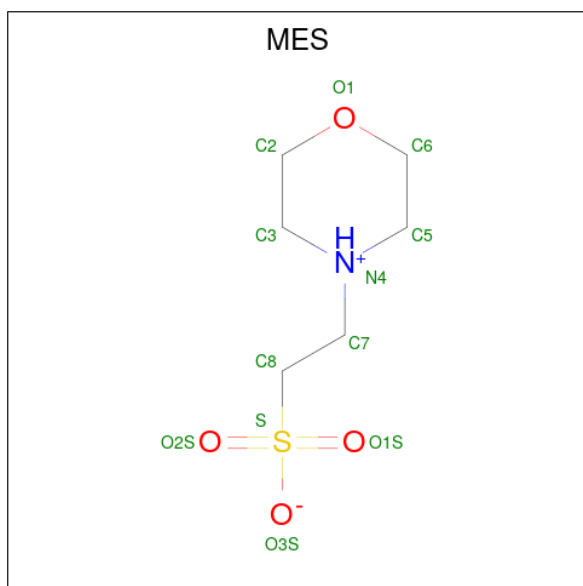
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 5-[2,4-bis(fluoranyl)phenoxy]-2-(cyclohexylmethyl)- {N}-[2-[(3 {R})-3-(methoxymethyl)piperidin-1-yl]ethyl]indazole-6-carboxamide (CCD ID: A1IZ3) (formula:  $C_{30}H_{38}F_2N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).



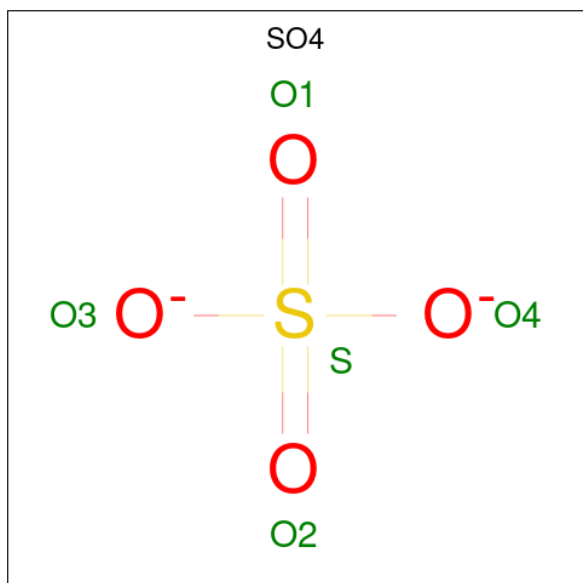
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			39	30	2	4	3		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	Cl	0	0
			3	3		

- Molecule 10 is water.

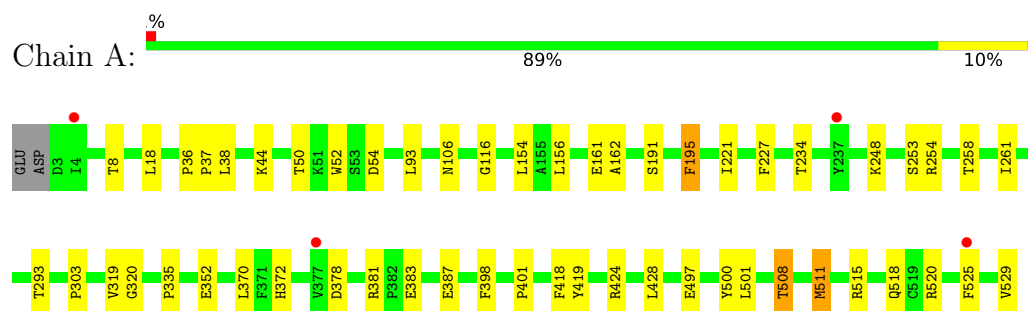
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	105	Total	O	0	0
			105	105		



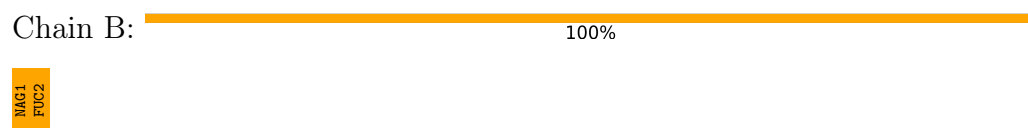
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

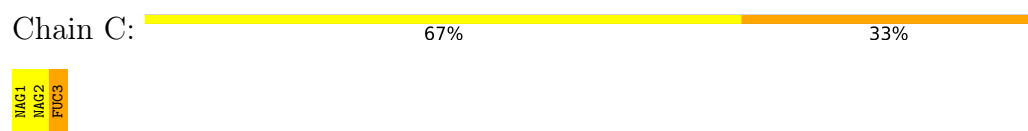
- Molecule 1: Cholinesterase



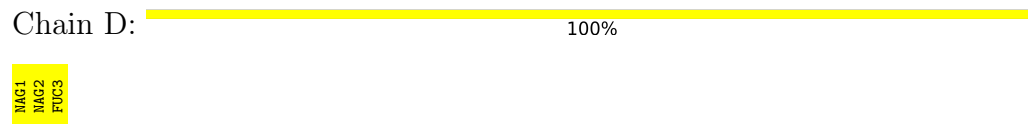
- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.39Å 155.39Å 126.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.51 – 2.36 41.51 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.9 (41.51-2.36) 97.9 (41.51-2.36)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.182 , 0.222 0.185 , 0.224	Depositor DCC
$R_{free}$ test set	1577 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, A1IZ3, NAG, FUC, MES, SO4, CL

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	0.33	0/4355	0.50	0/5911

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

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	4232	0	4130	41	0
2	B	24	0	22	2	0
3	C	38	0	34	1	0
3	D	38	0	34	0	0
4	A	42	0	39	0	0
5	A	18	0	24	2	0
6	A	39	0	0	0	0
7	A	12	0	13	4	0
8	A	20	0	0	0	0
9	A	3	0	0	1	0
10	A	105	0	0	3	0
All	All	4571	0	4296	43	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 5.

All (43) 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:518:GLN:HE22	7:A:606:MES:H22	1.58	0.69
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.34	0.61
1:A:500:TYR:CZ	1:A:511[B]:MET:HB2	2.37	0.59
1:A:54:ASP:OD1	1:A:54:ASP:N	2.34	0.58
1:A:378:ASP:HB3	1:A:381:ARG:HG3	1.86	0.57
1:A:515:ARG:NH1	7:A:606:MES:H71	2.20	0.57
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.88	0.56
1:A:253:SER:O	1:A:254:ARG:HD3	2.05	0.56
1:A:161:GLU:HB3	1:A:261:ILE:HG21	1.89	0.54
1:A:319:VAL:O	1:A:418:PHE:HA	2.08	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.44	0.53
1:A:525:PHE:C	1:A:525:PHE:CD1	2.86	0.53
1:A:335:PRO:HG3	1:A:352:GLU:HB3	1.92	0.51
1:A:515:ARG:HH12	7:A:606:MES:H71	1.75	0.51
1:A:18:LEU:HD13	5:A:604:GOL:H11	1.94	0.49
1:A:191:SER:HB2	2:B:2:FUC:H3	1.95	0.49
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.95	0.49
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.44	0.48
1:A:227:PHE:CD1	1:A:227:PHE:C	2.90	0.48
1:A:525:PHE:C	1:A:525:PHE:HD1	2.21	0.47
1:A:234:THR:HB	1:A:293:THR:HG22	1.97	0.47
1:A:270:GLN:H	1:A:270:GLN:CD	2.23	0.47
1:A:195:PHE:HB3	1:A:221:ILE:HB	1.97	0.47
1:A:106:ASN:ND2	2:B:1:NAG:H83	2.31	0.45
1:A:248:LYS:HD2	1:A:253:SER:OG	2.16	0.45
1:A:383:GLU:O	1:A:387:GLU:HG3	2.18	0.44
1:A:520:ARG:NH1	9:A:613:CL:CL	2.88	0.43
1:A:278:PHE:O	3:C:3:FUC:O4	2.34	0.43
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.95	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.54	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.54	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.75	0.42
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.74	0.42
1:A:398:PHE:C	1:A:401:PRO:HD2	2.44	0.42
1:A:52:TRP:HB2	1:A:54:ASP:OD1	2.20	0.41
5:A:607:GOL:O3	5:A:607:GOL:O1	2.37	0.41
1:A:424:ARG:NH1	1:A:428:LEU:HD23	2.36	0.41
1:A:501:LEU:HD11	1:A:508:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:606:MES:H82	7:A:606:MES:H31	1.89	0.41
1:A:44:LYS:NZ	10:A:709:HOH:O	2.52	0.41
1:A:372:HIS:HB3	10:A:799:HOH:O	2.21	0.40
1:A:383:GLU:CD	1:A:383:GLU:H	2.30	0.40
1:A:497:GLU:HG3	10:A:754:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	529/529 (100%)	507 (96%)	21 (4%)	1 (0%)	44 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY

### 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	456/454 (100%)	447 (98%)	9 (2%)	50 63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	38	LEU
1	A	50	THR
1	A	195	PHE
1	A	370	LEU
1	A	508	THR
1	A	511[A]	MET
1	A	511[B]	MET
1	A	529	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	176	GLN
1	A	289	ASN
1	A	311	GLN
1	A	372	HIS
1	A	486	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

8 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	B	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	1.84	5 (29%)
2	FUC	B	2	2	10,10,11	1.08	1 (10%)	14,14,16	1.72	3 (21%)
3	NAG	C	1	1,3	14,14,15	0.73	0	17,19,21	1.31	3 (17%)
3	NAG	C	2	3	14,14,15	0.79	1 (7%)	17,19,21	1.31	1 (5%)
3	FUC	C	3	3	10,10,11	0.72	0	14,14,16	2.02	3 (21%)
3	NAG	D	1	1,3	14,14,15	0.76	0	17,19,21	1.42	4 (23%)
3	NAG	D	2	3	14,14,15	0.73	0	17,19,21	1.29	3 (17%)
3	FUC	D	3	3	10,10,11	0.79	0	14,14,16	1.62	4 (28%)

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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	FUC	C	3	3	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	FUC	C1-C2	2.34	1.57	1.52
2	B	1	NAG	C1-C2	2.12	1.55	1.52
3	C	2	NAG	C1-C2	2.01	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	FUC	C1-C2-C3	4.54	115.25	109.67
2	B	1	NAG	C2-N2-C7	4.54	129.36	122.90
3	C	3	FUC	C1-C2-C3	4.34	115.00	109.67
3	C	3	FUC	C1-O5-C5	3.90	121.62	112.78
3	C	2	NAG	C1-O5-C5	3.61	117.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	FUC	C1-O5-C5	3.30	120.26	112.78
3	D	2	NAG	O5-C5-C6	3.05	111.99	107.20
3	C	1	NAG	C1-O5-C5	2.80	115.98	112.19
3	C	1	NAG	C3-C4-C5	-2.78	105.28	110.24
2	B	1	NAG	C1-O5-C5	2.73	115.89	112.19
2	B	1	NAG	O4-C4-C5	2.70	116.00	109.30
2	B	2	FUC	O4-C4-C5	2.59	115.41	109.67
3	D	1	NAG	O4-C4-C3	-2.57	104.42	110.35
3	D	2	NAG	C3-C4-C5	-2.54	105.70	110.24
3	D	3	FUC	O4-C4-C5	2.53	115.28	109.67
3	D	1	NAG	O4-C4-C5	2.36	115.15	109.30
3	D	1	NAG	C2-N2-C7	2.33	126.22	122.90
3	D	1	NAG	C1-O5-C5	2.31	115.33	112.19
3	D	3	FUC	C3-C4-C5	-2.26	106.25	109.77
2	B	2	FUC	C1-O5-C5	2.23	117.84	112.78
3	D	3	FUC	C1-C2-C3	2.22	112.39	109.67
2	B	1	NAG	C6-C5-C4	2.19	118.14	113.00
3	C	3	FUC	O3-C3-C2	-2.15	105.89	109.99
3	D	2	NAG	O4-C4-C5	2.14	114.62	109.30
2	B	1	NAG	C3-C4-C5	-2.05	106.58	110.24
3	C	1	NAG	O5-C1-C2	-2.04	108.07	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	FUC	1	0
2	B	2	FUC	1	0

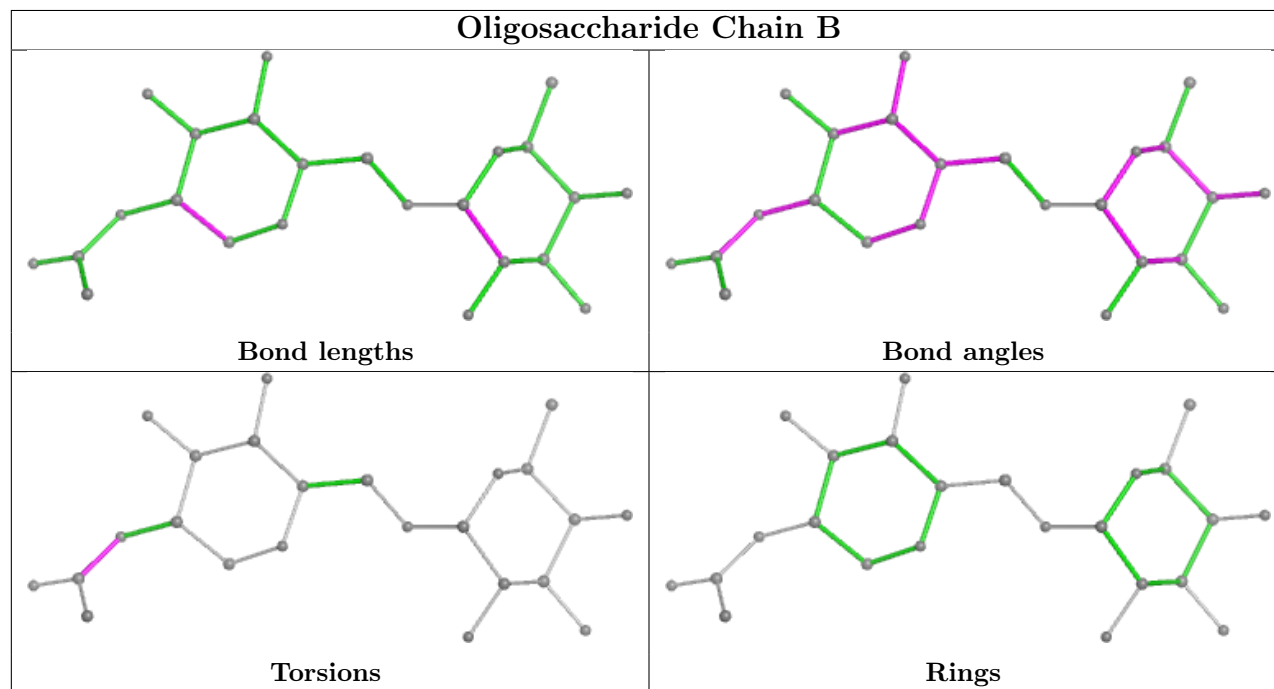
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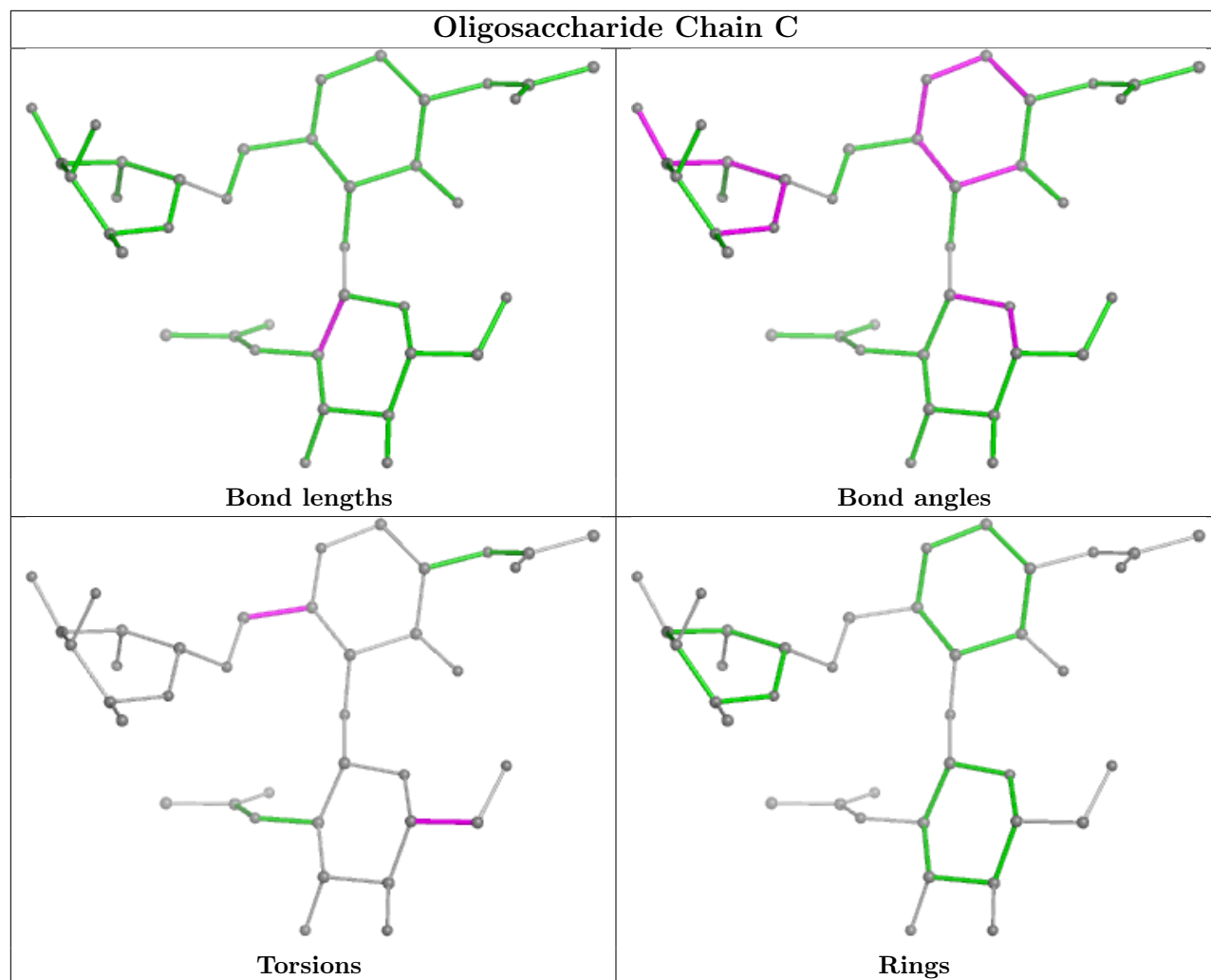


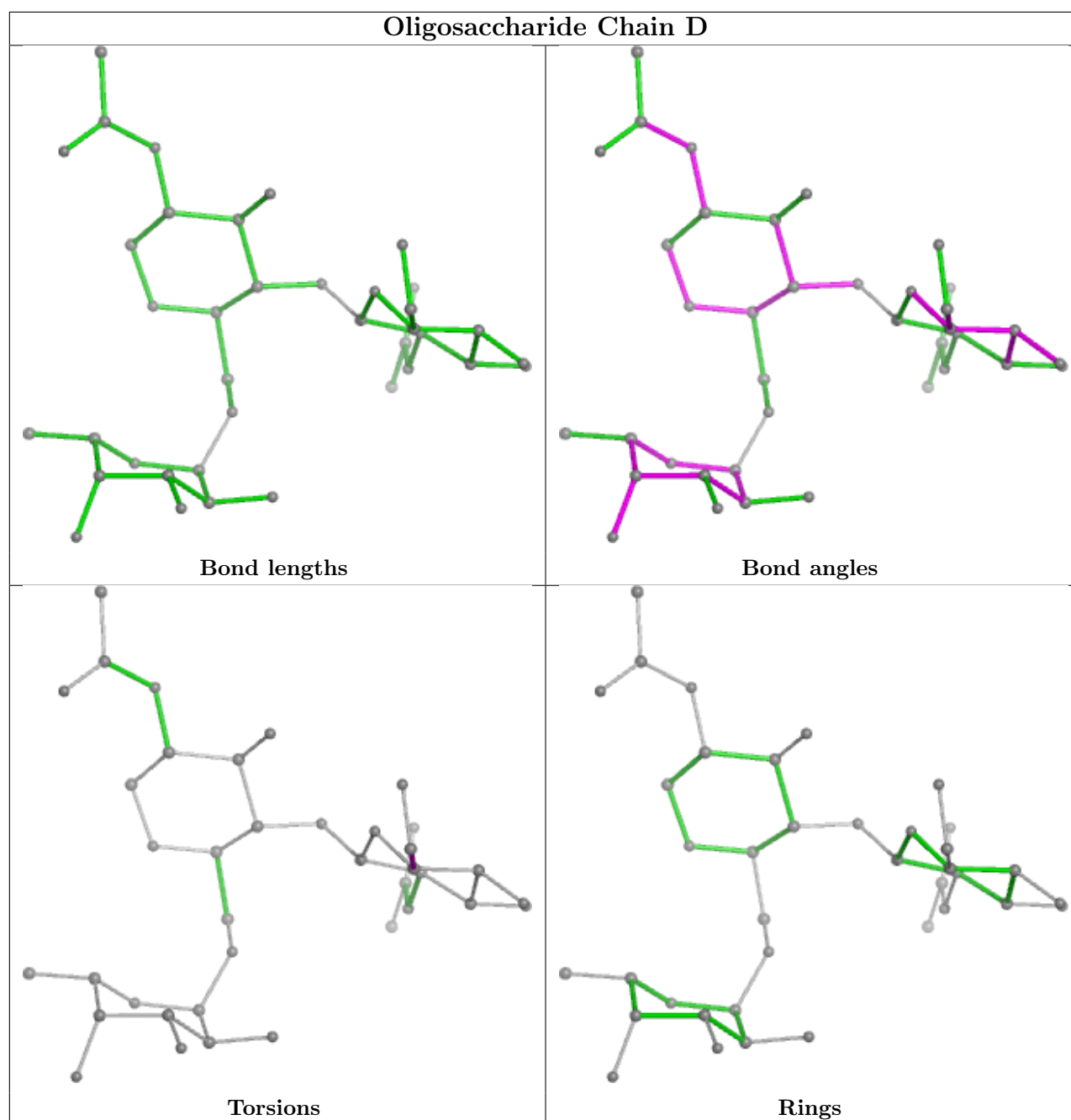
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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
8	SO4	A	610	-	4,4,4	0.76	0	6,6,6	0.41	0
4	NAG	A	602	1	14,14,15	0.66	0	17,19,21	1.16	2 (11%)
4	NAG	A	603	1	14,14,15	0.65	0	17,19,21	1.67	2 (11%)
5	GOL	A	607	-	5,5,5	0.27	0	5,5,5	0.42	0
8	SO4	A	609	-	4,4,4	0.70	0	6,6,6	0.23	0
5	GOL	A	604	-	5,5,5	0.26	0	5,5,5	1.14	0
8	SO4	A	612	-	4,4,4	0.66	0	6,6,6	0.09	0
5	GOL	A	608	-	5,5,5	0.54	0	5,5,5	0.73	0
7	MES	A	606	-	12,12,12	1.33	1 (8%)	14,16,16	0.98	0
4	NAG	A	601	1	14,14,15	0.62	0	17,19,21	1.65	3 (17%)
6	A1IZ3	A	605	-	41,43,43	1.79	10 (24%)	51,59,59	2.34	16 (31%)
8	SO4	A	611	-	4,4,4	0.71	0	6,6,6	0.33	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
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	1/6/23/26	0/1/1/1
5	GOL	A	607	-	-	2/4/4/4	-
5	GOL	A	604	-	-	1/4/4/4	-
5	GOL	A	608	-	-	4/4/4/4	-
7	MES	A	606	-	-	0/6/14/14	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
6	A1IZ3	A	605	-	-	3/21/39/39	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	A1IZ3	C08-N09	5.58	1.41	1.35
6	A	605	A1IZ3	C02-C03	4.05	1.48	1.40
6	A	605	A1IZ3	C12-N14	3.65	1.41	1.33
7	A	606	MES	C8-S	3.57	1.82	1.77
6	A	605	A1IZ3	C10-N09	2.90	1.55	1.47
6	A	605	A1IZ3	C01-C06	2.71	1.46	1.41
6	A	605	A1IZ3	C16-N14	2.43	1.51	1.46
6	A	605	A1IZ3	C21-C20	2.17	1.41	1.37
6	A	605	A1IZ3	C36-N31	2.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	A1IZ3	C04-C05	2.04	1.46	1.42
6	A	605	A1IZ3	C33-C34	-2.00	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605	A1IZ3	C34-C35-N31	-7.69	99.23	111.28
4	A	603	NAG	C1-O5-C5	4.95	118.90	112.19
6	A	605	A1IZ3	C36-N31-C35	4.70	116.70	109.52
4	A	601	NAG	C1-O5-C5	4.49	118.28	112.19
6	A	605	A1IZ3	C02-C12-N14	3.99	125.20	117.36
6	A	605	A1IZ3	C33-C32-C36	3.94	116.37	110.85
6	A	605	A1IZ3	C22-C21-C20	-3.91	112.52	116.62
6	A	605	A1IZ3	C32-C33-C34	-3.83	104.91	112.15
6	A	605	A1IZ3	O15-C12-N14	-3.80	115.04	122.61
6	A	605	A1IZ3	C21-C22-C13	3.18	127.48	122.81
6	A	605	A1IZ3	C33-C34-C35	-2.99	105.30	108.68
6	A	605	A1IZ3	C03-C02-C12	-2.87	120.92	126.16
6	A	605	A1IZ3	C33-C34-C37	2.85	118.44	111.28
6	A	605	A1IZ3	C17-N31-C35	-2.79	105.09	111.66
4	A	603	NAG	C2-N2-C7	2.76	126.83	122.90
6	A	605	A1IZ3	O11-C13-C22	2.76	124.94	119.26
4	A	601	NAG	O5-C5-C6	2.74	111.51	107.20
6	A	605	A1IZ3	C32-C36-N31	2.74	115.73	111.33
6	A	605	A1IZ3	C35-C34-C37	2.56	114.84	110.61
4	A	602	NAG	C2-N2-C7	2.45	126.39	122.90
6	A	605	A1IZ3	C30-C29-C28	2.45	116.41	111.42
4	A	601	NAG	C2-N2-C7	2.25	126.11	122.90
4	A	602	NAG	C1-O5-C5	2.16	115.12	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	GOL	O1-C1-C2-C3
5	A	608	GOL	C1-C2-C3-O3
6	A	605	A1IZ3	C33-C34-C37-O38
6	A	605	A1IZ3	C34-C37-O38-C39
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
6	A	605	A1IZ3	C35-C34-C37-O38
5	A	607	GOL	O1-C1-C2-C3

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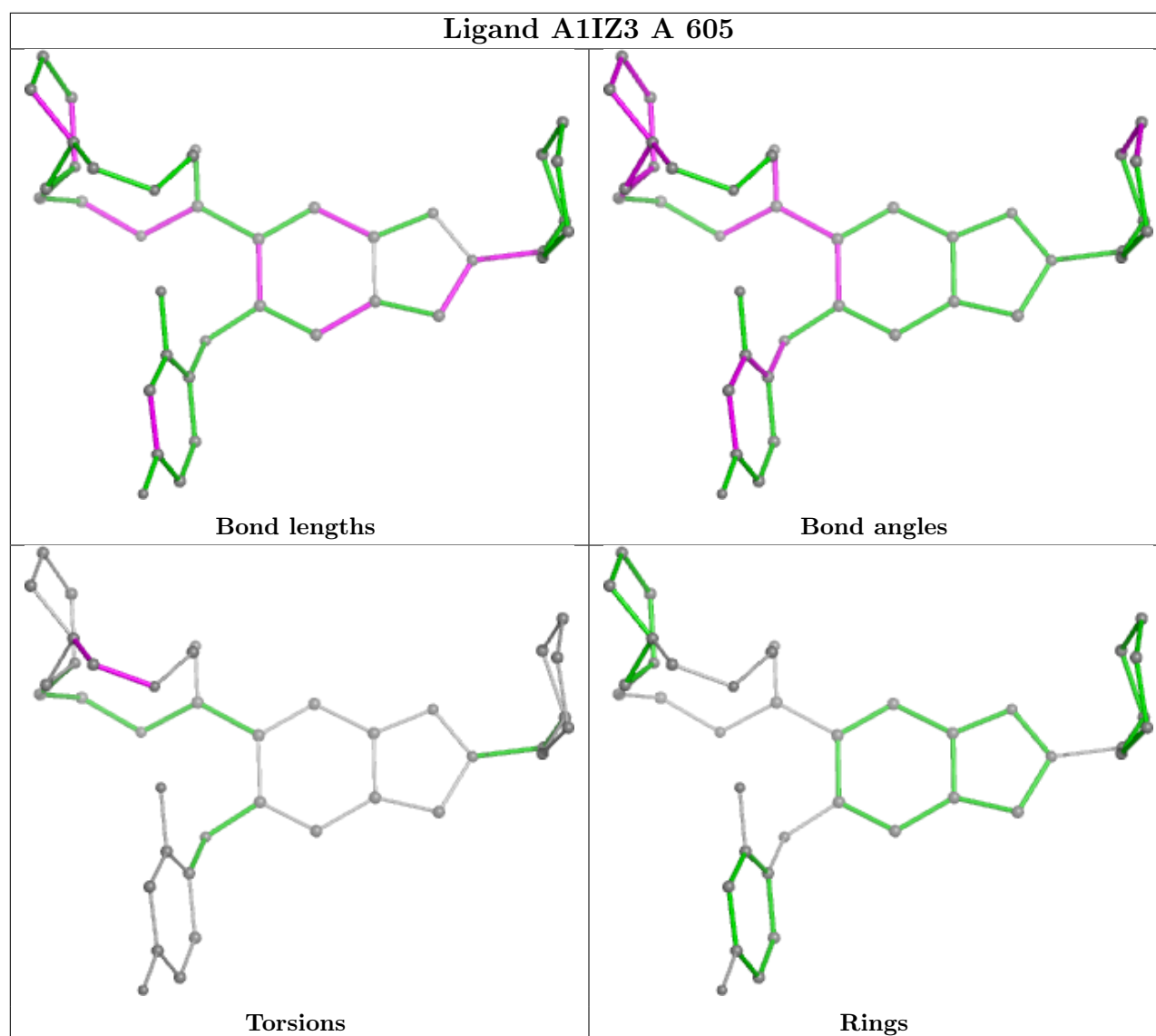
Mol	Chain	Res	Type	Atoms
5	A	607	GOL	O1-C1-C2-O2
5	A	608	GOL	O1-C1-C2-O2
5	A	608	GOL	O2-C2-C3-O3
5	A	604	GOL	C1-C2-C3-O3
4	A	603	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	607	GOL	1	0
5	A	604	GOL	1	0
7	A	606	MES	4	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	527/529 (99%)	-0.14	5 (0%) 81 84	25, 57, 90, 127	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	4.4
1	A	237	TYR	3.3
1	A	282	TYR	3.1
1	A	4	ILE	2.1
1	A	525	PHE	2.1

### 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
3	NAG	C	2	14/15	0.64	0.14	102,113,123,126	0
2	NAG	B	1	14/15	0.73	0.14	75,81,85,86	0
3	FUC	D	3	10/11	0.77	0.16	75,86,88,92	0
3	NAG	D	2	14/15	0.79	0.14	90,93,102,106	0
3	NAG	C	1	14/15	0.79	0.10	99,106,111,111	0
3	FUC	C	3	10/11	0.81	0.14	88,95,100,104	0
2	FUC	B	2	10/11	0.83	0.15	72,85,87,90	0

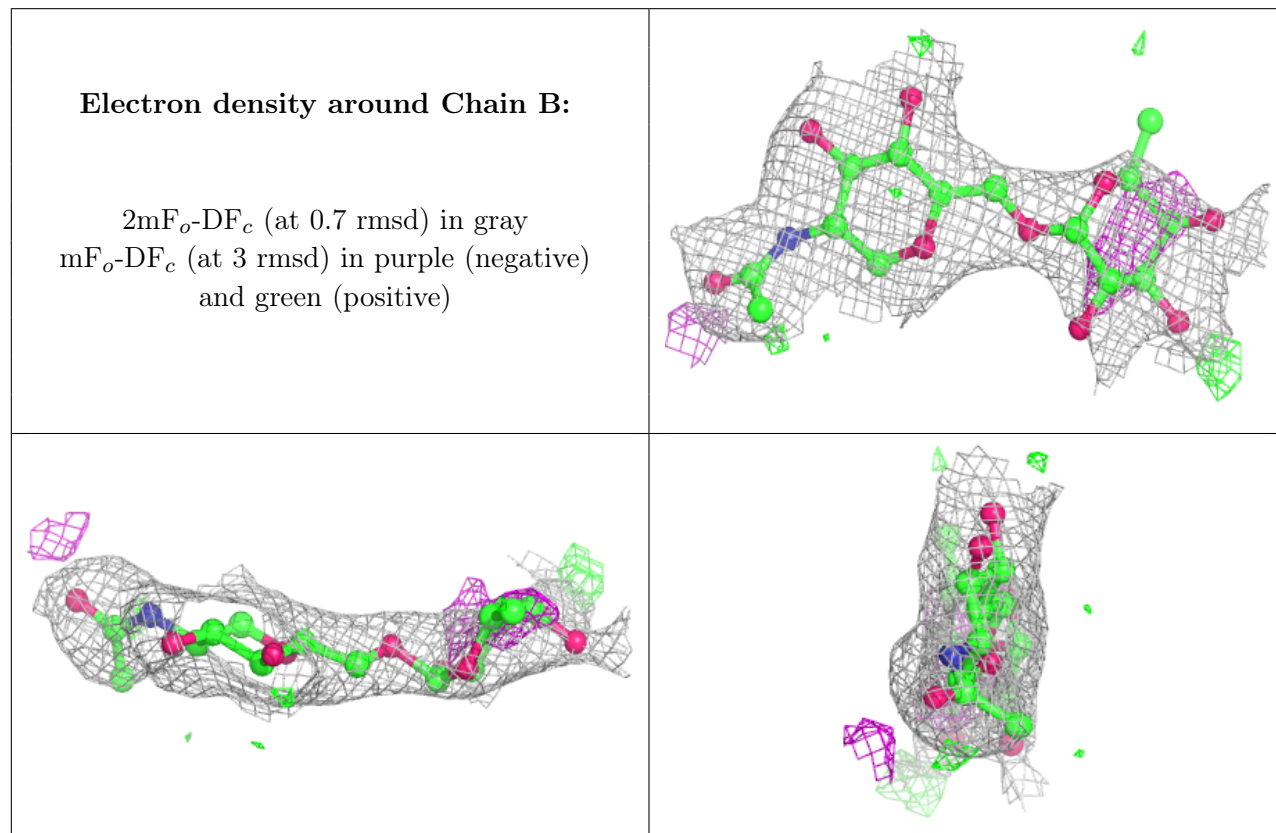
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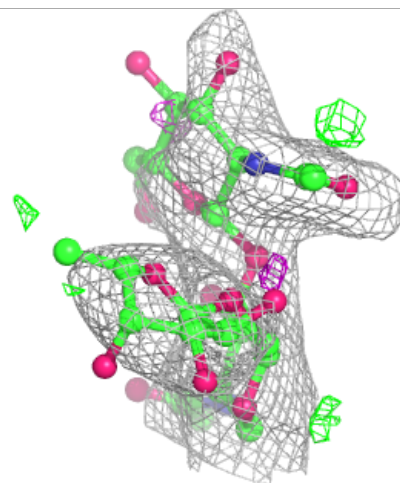
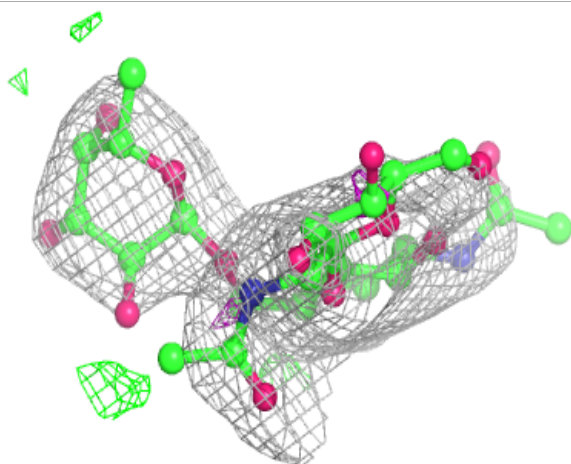
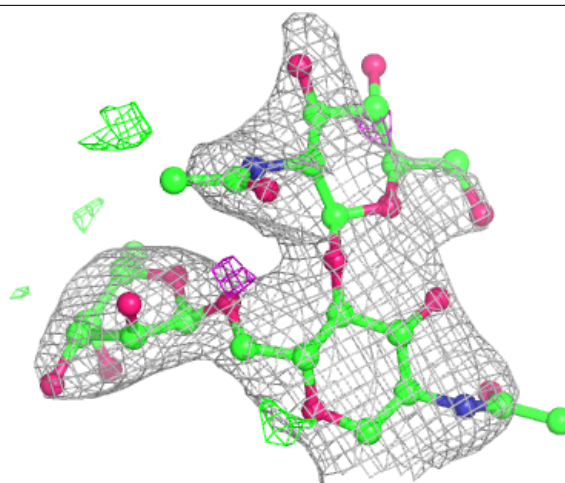
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1	14/15	0.94	0.09	71,76,80,83	0

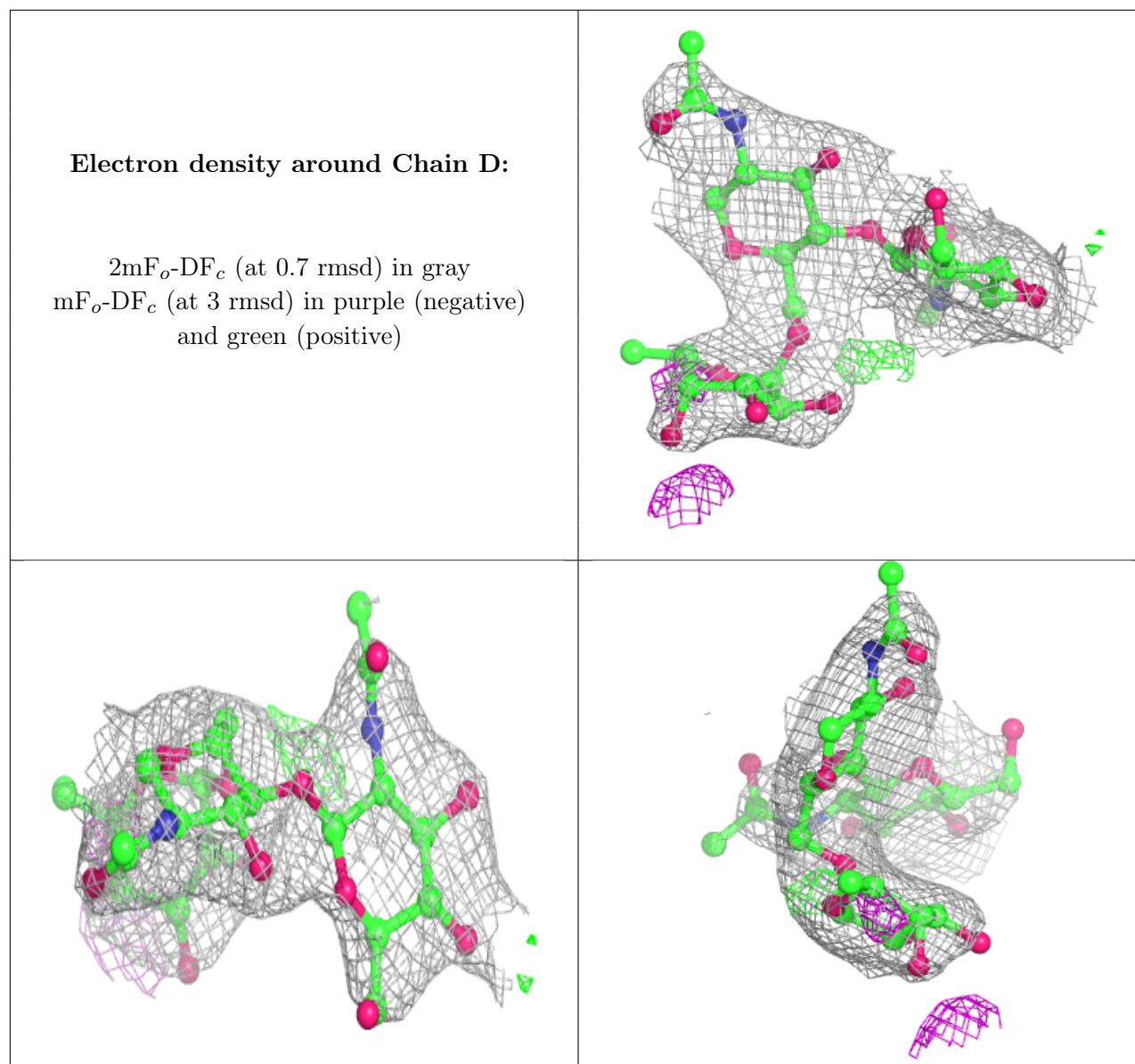
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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(Å <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.54	0.15	99,106,113,113	0
8	SO4	A	611	5/5	0.69	0.11	91,93,114,124	0
4	NAG	A	603	14/15	0.80	0.14	64,90,99,101	0
4	NAG	A	602	14/15	0.81	0.10	97,103,107,110	0
9	CL	A	613	1/1	0.83	0.14	101,101,101,101	0

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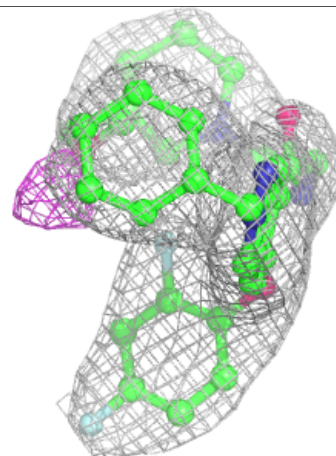
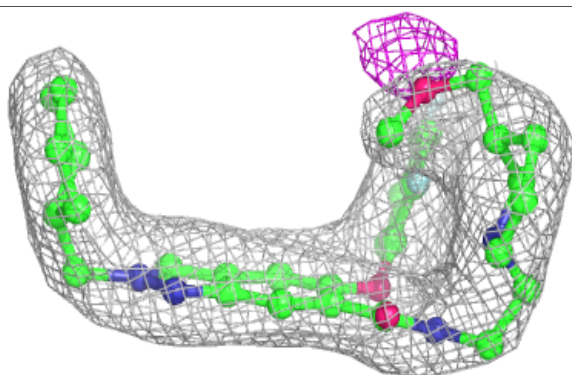
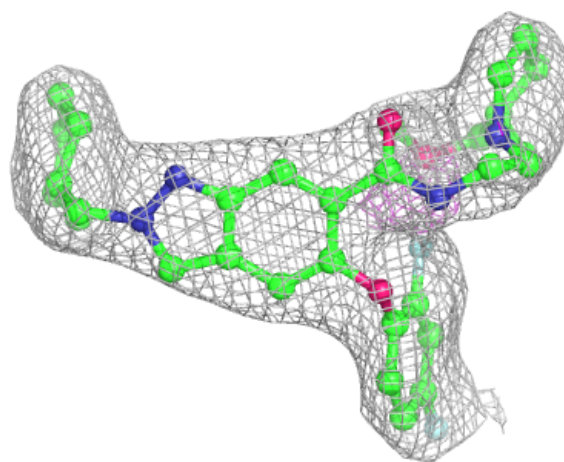
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MES	A	606	12/12	0.85	0.13	69,80,89,90	0
8	SO4	A	612	5/5	0.86	0.07	90,97,108,108	0
5	GOL	A	607	6/6	0.90	0.14	72,77,78,82	0
5	GOL	A	608	6/6	0.90	0.13	50,61,66,66	0
8	SO4	A	610	5/5	0.91	0.13	69,74,79,86	0
5	GOL	A	604	6/6	0.92	0.12	61,65,68,70	0
9	CL	A	614	1/1	0.92	0.13	95,95,95,95	0
8	SO4	A	609	5/5	0.93	0.17	63,70,80,81	0
9	CL	A	615	1/1	0.93	0.20	104,104,104,104	0
6	A1IZ3	A	605	39/39	0.95	0.10	41,55,62,68	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 A1IZ3 A 605:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.