



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 07:08 AM EDT

PDB ID : 4Y16  
Title : Crystal structure of the mCD1d/NC-aGC/iNKTTCR ternary complex  
Authors : Zajonc, D.M.; Nemcovic, M.  
Deposited on : 2015-02-06  
Resolution : 2.60 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 ⓘ](#)) 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 : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

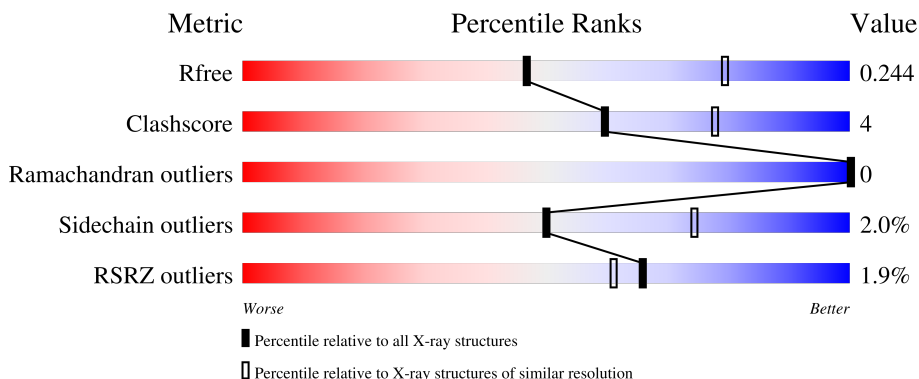
# 1 Overall quality at a glance

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.



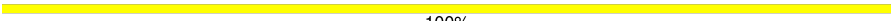
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	285	<div> <div>79%</div> <div>15%</div> <div>6%</div> </div>
2	B	99	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	C	209	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
4	D	241	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
5	E	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	3	 100%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6527 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2118	1353	358	394	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	variant	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			801	511	135	148	7			

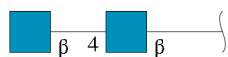
- Molecule 3 is a protein called Chimeric TCR Valpha14/Jalpha18 chain (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	0	0
			1537	952	261	316	8			

- Molecule 4 is a protein called Chimeric TCR Vbeta8.2 chain (mouse variable domain, human constant domain).

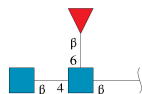
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1872	1175	334	357	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



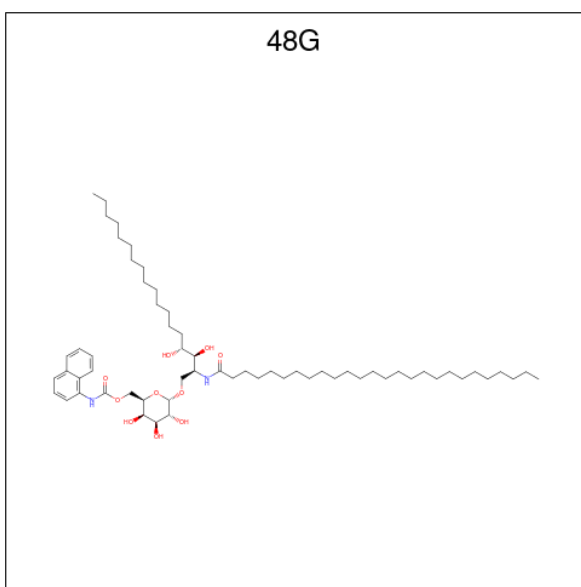
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



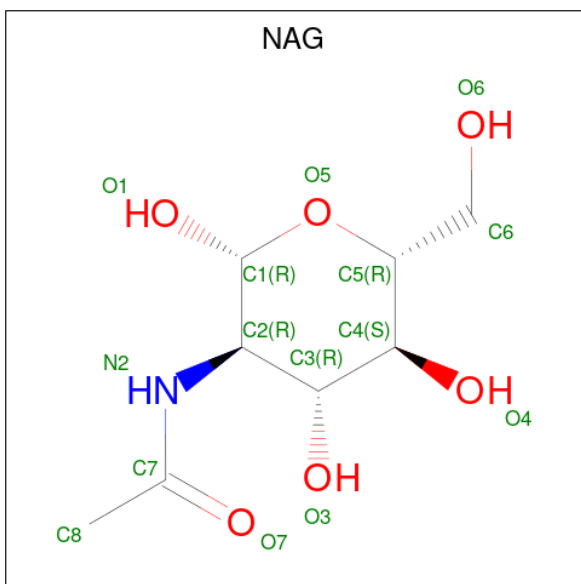
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is N-[(2S,3S,4R)-3,4-dihydroxy-1-{[6-O-(naphthalen-1-ylcarbonyl)-alpha-D-galactopyranosyl]oxy}octadecan-2-yl]hexacosanamide (three-letter code: 48G) (formula: C<sub>61</sub>H<sub>106</sub>N<sub>2</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			73	61	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

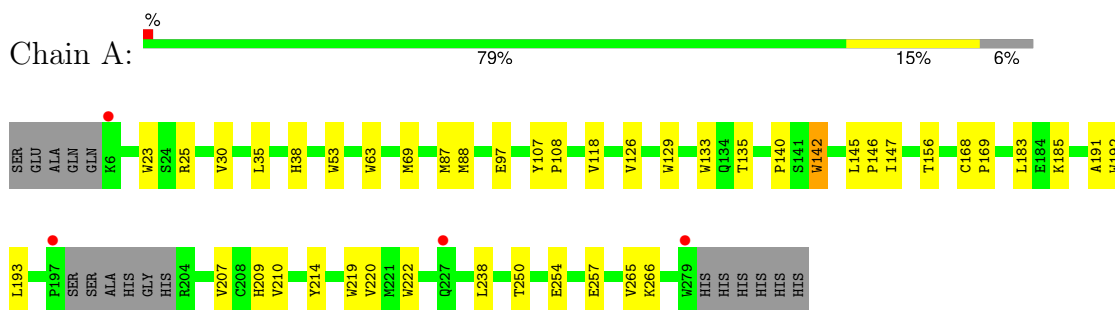
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	14	Total 14	O 14	0	0
9	B	4	Total 4	O 4	0	0
9	C	11	Total 11	O 11	0	0
9	D	17	Total 17	O 17	0	0

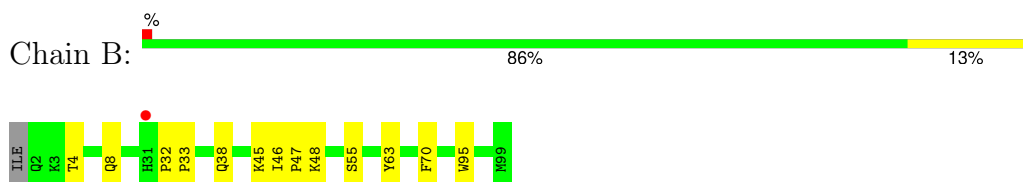
### 3 Residue-property plots

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.

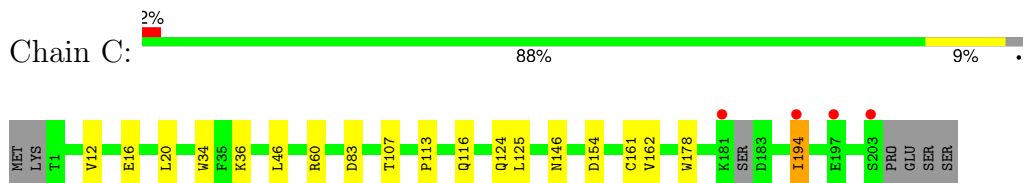
- Molecule 1: Antigen-presenting glycoprotein CD1d1



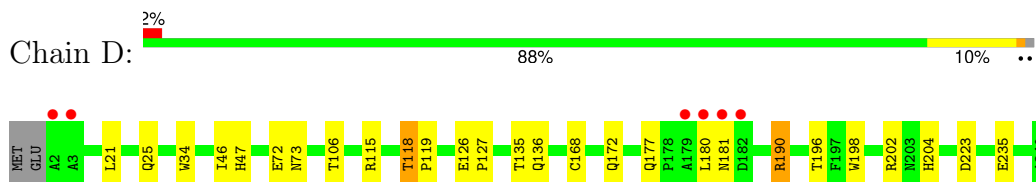
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Chimeric TCR Valpha14/Jalpha18 chain (mouse variable domain, human constant domain)



- Molecule 4: Chimeric TCR Vbeta8.2 chain (mouse variable domain, human constant domain)



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

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

Chain F:

100%

MAG1  
MAG2  
FUL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.64Å 191.91Å 151.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.88-2.60) 93.2 (19.88-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, $R_{free}$	0.211 , 0.244 0.210 , 0.244	Depositor DCC
$R_{free}$ test set	970 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: NAG, FUL, 48G

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	0.71	8/2178 (0.4%)	0.62	0/2963
2	B	0.65	1/827 (0.1%)	0.61	0/1125
3	C	0.59	2/1564 (0.1%)	0.61	0/2130
4	D	0.63	2/1923 (0.1%)	0.61	0/2622
All	All	0.65	13/6492 (0.2%)	0.61	0/8840

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	34	TRP	CD2-CE2	5.66	1.48	1.41
1	A	23	TRP	CD2-CE2	5.63	1.48	1.41
4	D	34	TRP	CD2-CE2	5.52	1.48	1.41
1	A	133	TRP	CD2-CE2	5.35	1.47	1.41
1	A	192	TRP	CD2-CE2	5.20	1.47	1.41
3	C	178	TRP	CD2-CE2	5.16	1.47	1.41
2	B	95	TRP	CD2-CE2	5.11	1.47	1.41
1	A	142	TRP	CD2-CE2	5.10	1.47	1.41
1	A	129	TRP	CD2-CE2	5.10	1.47	1.41
4	D	198	TRP	CD2-CE2	5.09	1.47	1.41
1	A	53	TRP	CD2-CE2	5.07	1.47	1.41
1	A	222	TRP	CD2-CE2	5.07	1.47	1.41
1	A	63	TRP	CD2-CE2	5.07	1.47	1.41

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	2118	0	2008	25	0
2	B	801	0	761	6	0
3	C	1537	0	1449	12	0
4	D	1872	0	1776	14	0
5	E	28	0	25	1	0
6	F	38	0	34	0	0
7	A	73	0	106	4	0
8	A	14	0	13	0	0
9	A	14	0	0	1	1
9	B	4	0	0	0	0
9	C	11	0	0	0	0
9	D	17	0	0	1	0
All	All	6527	0	6172	53	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (53) 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:168:CYS:HB3	1:A:169:PRO:HD3	1.64	0.80
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.69	0.73
1:A:69:MET:HB3	7:A:301:48G:CCI	2.19	0.72
3:C:20:LEU:HD22	3:C:107:THR:HG21	1.72	0.71
3:C:161:CYS:HB3	4:D:190:ARG:NH1	2.05	0.70
1:A:118:VAL:HG11	7:A:301:48G:H78	1.77	0.66
4:D:202:ARG:HH11	4:D:202:ARG:HG3	1.60	0.65
3:C:60:ARG:NH2	3:C:83:ASP:OD2	2.34	0.61
4:D:73:ASN:HB3	9:D:311:HOH:O	2.01	0.61
1:A:88:MET:HE1	1:A:146:PRO:HD3	1.83	0.60
1:A:220:VAL:HG22	1:A:265:VAL:HG22	1.86	0.57
1:A:135:THR:HG23	1:A:147:ILE:HG13	1.88	0.56
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.89	0.54
3:C:36:LYS:HB2	3:C:46:LEU:HD11	1.89	0.54
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:CYS:HB3	4:D:190:ARG:HH12	1.74	0.51
1:A:87:MET:HB3	1:A:88:MET:HE2	1.93	0.50
1:A:30:VAL:HB	1:A:38:HIS:HB2	1.94	0.50
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.40	0.50
2:B:55:SER:HB3	2:B:63:TYR:CZ	2.48	0.49
4:D:202:ARG:HG3	4:D:202:ARG:NH1	2.27	0.48
2:B:38:GLN:HE21	2:B:45:LYS:HE2	1.78	0.48
1:A:207:VAL:HG22	1:A:250:THR:HG22	1.95	0.48
4:D:118:THR:HG22	4:D:119:PRO:HD2	1.96	0.47
2:B:48:LYS:HA	2:B:48:LYS:HE2	1.96	0.47
1:A:35:LEU:HD12	1:A:183:LEU:HD23	1.95	0.47
1:A:69:MET:HB3	7:A:301:48G:CCJ	2.44	0.47
1:A:118:VAL:HB	1:A:126:VAL:HB	1.97	0.47
4:D:46:ILE:HG22	4:D:47:HIS:CD2	2.51	0.46
1:A:156:THR:HG23	7:A:301:48G:H55	1.98	0.46
1:A:185:LYS:HE3	1:A:214:TYR:CD1	2.51	0.46
3:C:12:VAL:HG13	3:C:16:GLU:HB2	1.98	0.45
4:D:21:LEU:HD22	4:D:106:THR:HG21	1.97	0.45
1:A:25:ARG:HB3	5:E:1:NAG:H82	1.99	0.45
4:D:177:GLN:HG2	4:D:180:LEU:HD12	1.98	0.44
3:C:113:PRO:HG3	3:C:162:VAL:HG11	1.98	0.44
4:D:204:HIS:NE2	4:D:235:GLU:CG	2.81	0.44
1:A:238:LEU:HD21	2:B:8:GLN:HE22	1.82	0.44
3:C:161:CYS:CB	4:D:190:ARG:HH12	2.30	0.44
1:A:254:GLU:O	1:A:257:GLU:HG2	2.17	0.43
1:A:210:VAL:HG21	1:A:220:VAL:HG21	1.99	0.43
3:C:124:GLN:C	3:C:125:LEU:HD12	2.39	0.43
1:A:97:GLU:HG2	9:A:407:HOH:O	2.19	0.43
1:A:140:PRO:HB2	1:A:142:TRP:CD1	2.53	0.42
1:A:107:TYR:HB3	1:A:108:PRO:HD2	2.00	0.42
3:C:116:GLN:HE21	3:C:116:GLN:HA	1.82	0.42
4:D:72:GLU:H	4:D:72:GLU:CD	2.23	0.42
4:D:135:THR:O	4:D:136:GLN:HB2	2.19	0.42
3:C:146:ASN:HB2	3:C:194:ILE:HD11	2.02	0.41
1:A:191:ALA:HA	1:A:209:HIS:O	2.21	0.40
3:C:194:ILE:H	3:C:194:ILE:HG13	1.57	0.40
4:D:126:GLU:HA	4:D:127:PRO:HD3	1.86	0.40
2:B:46:ILE:HA	2:B:47:PRO:HD3	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:411:HOH:O	9:A:411:HOH:O[3_654]	1.59	0.61

## 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	264/285 (93%)	255 (97%)	9 (3%)	0	100	100
2	B	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
3	C	198/209 (95%)	192 (97%)	6 (3%)	0	100	100
4	D	237/241 (98%)	228 (96%)	9 (4%)	0	100	100
All	All	795/834 (95%)	766 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	227/249 (91%)	226 (100%)	1 (0%)	89	96
2	B	90/93 (97%)	88 (98%)	2 (2%)	47	72
3	C	175/188 (93%)	173 (99%)	2 (1%)	70	86
4	D	202/208 (97%)	193 (96%)	9 (4%)	23	47
All	All	694/738 (94%)	680 (98%)	14 (2%)	50	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
2	B	4	THR
2	B	70	PHE
3	C	154	ASP
3	C	194	ILE
4	D	25	GLN
4	D	115	ARG
4	D	118	THR
4	D	168	CYS
4	D	172	GLN
4	D	181	ASN
4	D	190	ARG
4	D	196	THR
4	D	223	ASP

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	110	ASN
2	B	8	GLN
2	B	29	GLN
2	B	38	GLN
3	C	30	ASN
3	C	116	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 ⓘ

5 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	$\# Z  > 2$
5	NAG	E	1	1,5	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
5	NAG	E	2	5	14,14,15	0.56	0	17,19,21	1.21	2 (11%)
6	NAG	F	1	1,6	14,14,15	0.39	0	17,19,21	1.52	2 (11%)
6	NAG	F	2	6	14,14,15	0.49	0	17,19,21	1.61	1 (5%)
6	FUL	F	3	6	10,10,11	0.54	0	14,14,16	1.51	1 (7%)

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	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	FUL	F	3	6	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2	NAG	C1-O5-C5	5.61	119.71	112.19
6	F	3	FUL	C1-C2-C3	-4.13	103.63	109.64
6	F	1	NAG	O5-C5-C6	3.59	114.65	107.66
5	E	2	NAG	C2-N2-C7	3.23	127.23	122.90
5	E	1	NAG	C2-N2-C7	-2.91	119.01	122.90
5	E	2	NAG	O5-C1-C2	-2.20	107.88	111.29
6	F	1	NAG	C1-C2-N2	2.04	113.64	110.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C3-C2-N2-C7

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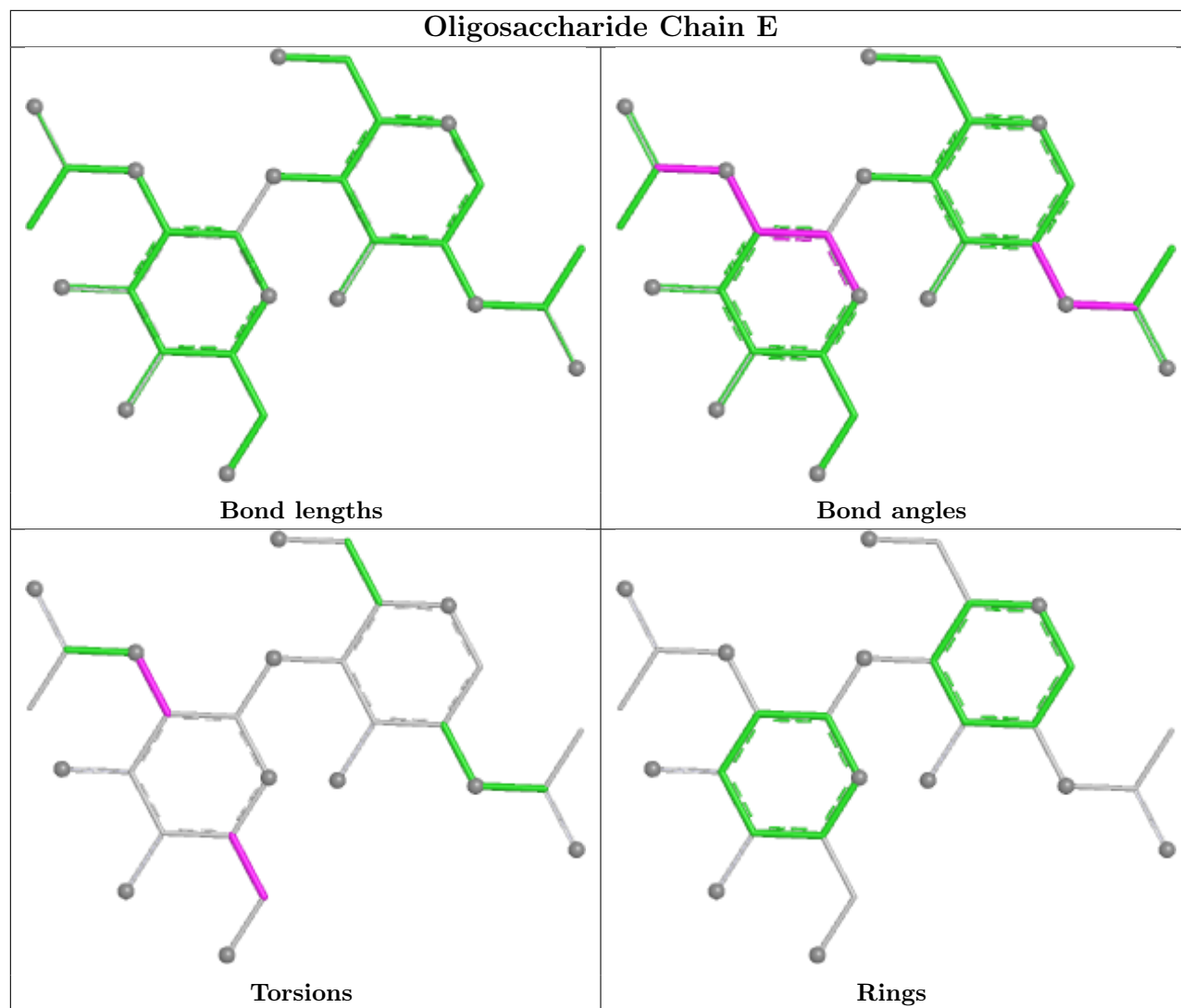
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

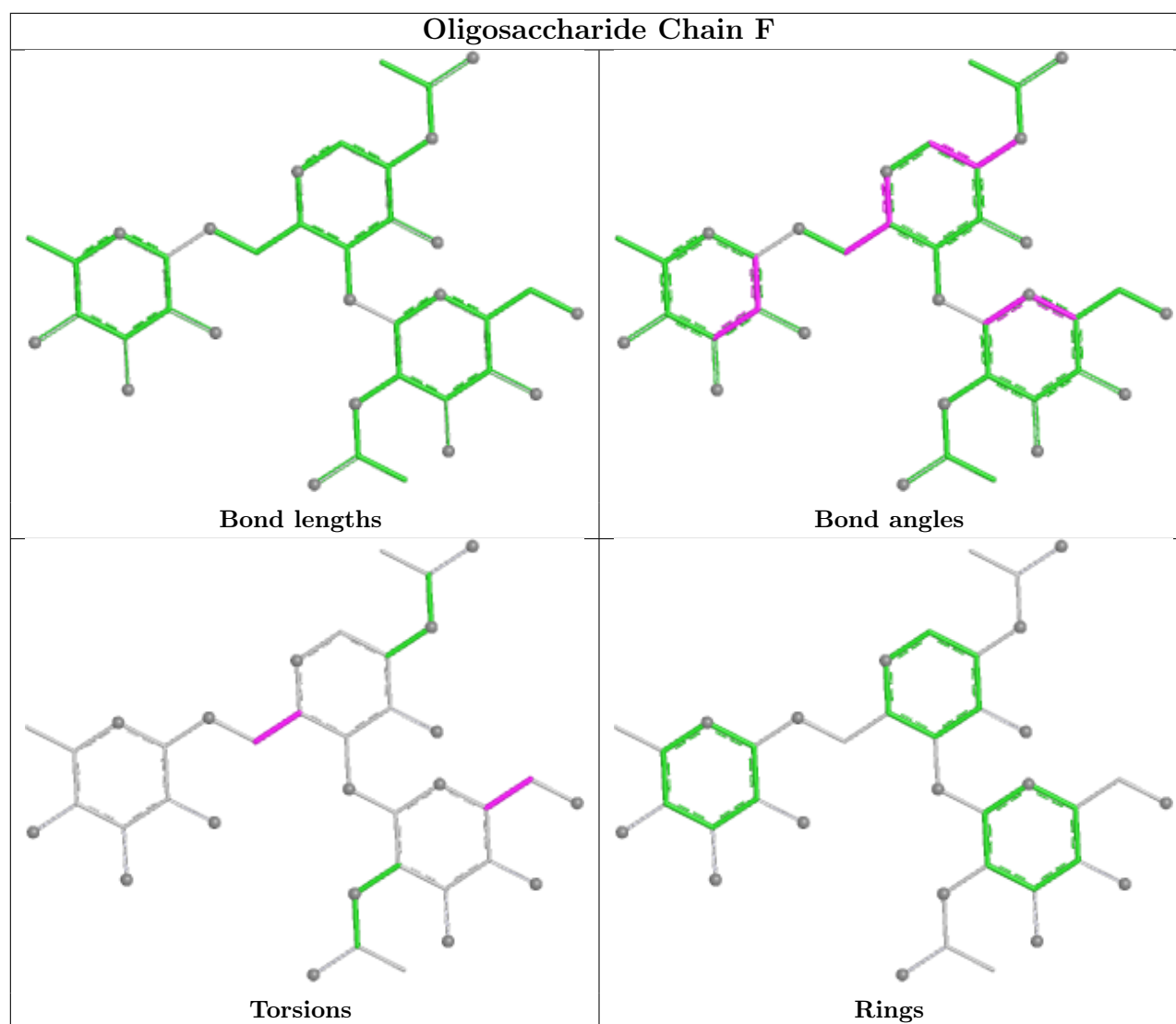
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	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](#)

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$
8	NAG	A	302	1	14,14,15	0.72	1 (7%)	17,19,21	1.02	1 (5%)
7	48G	A	301	-	75,75,75	0.82	2 (2%)	87,90,90	1.05	2 (2%)

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
8	NAG	A	302	1	-	0/6/23/26	0/1/1/1
7	48G	A	301	-	-	24/65/85/85	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	301	48G	O1-C1	2.08	1.43	1.40
7	A	301	48G	CBQ-CBM	2.03	1.56	1.52
8	A	302	NAG	C1-C2	2.03	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	301	48G	O6-CCH-NCS	5.34	117.74	109.35
7	A	301	48G	OCT-CCH-NCS	-2.55	120.70	126.12
8	A	302	NAG	C1-O5-C5	2.16	115.08	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	301	48G	CCC-CCD-CCE-CCF
7	A	301	48G	CAQ-CAR-CAS-CAT
7	A	301	48G	CAK-CAL-CAM-CAN
7	A	301	48G	CAP-CAQ-CAR-CAS
7	A	301	48G	CAH-CAI-CAJ-CAK
7	A	301	48G	CAN-CAO-CAP-CAQ
7	A	301	48G	CAI-CAJ-CAK-CAL
7	A	301	48G	CAE-CAF-CAG-CAH
7	A	301	48G	CAT-CAU-CAV-CAW
7	A	301	48G	CAM-CAN-CAO-CAP
7	A	301	48G	CBX-CBY-CBZ-CCA
7	A	301	48G	CBS-CBV-CBW-CBX
7	A	301	48G	CAU-CAV-CAW-CAX
7	A	301	48G	CAO-CAP-CAQ-CAR
7	A	301	48G	CAV-CAW-CAX-CAY
7	A	301	48G	CBZ-CCA-CCB-CCC

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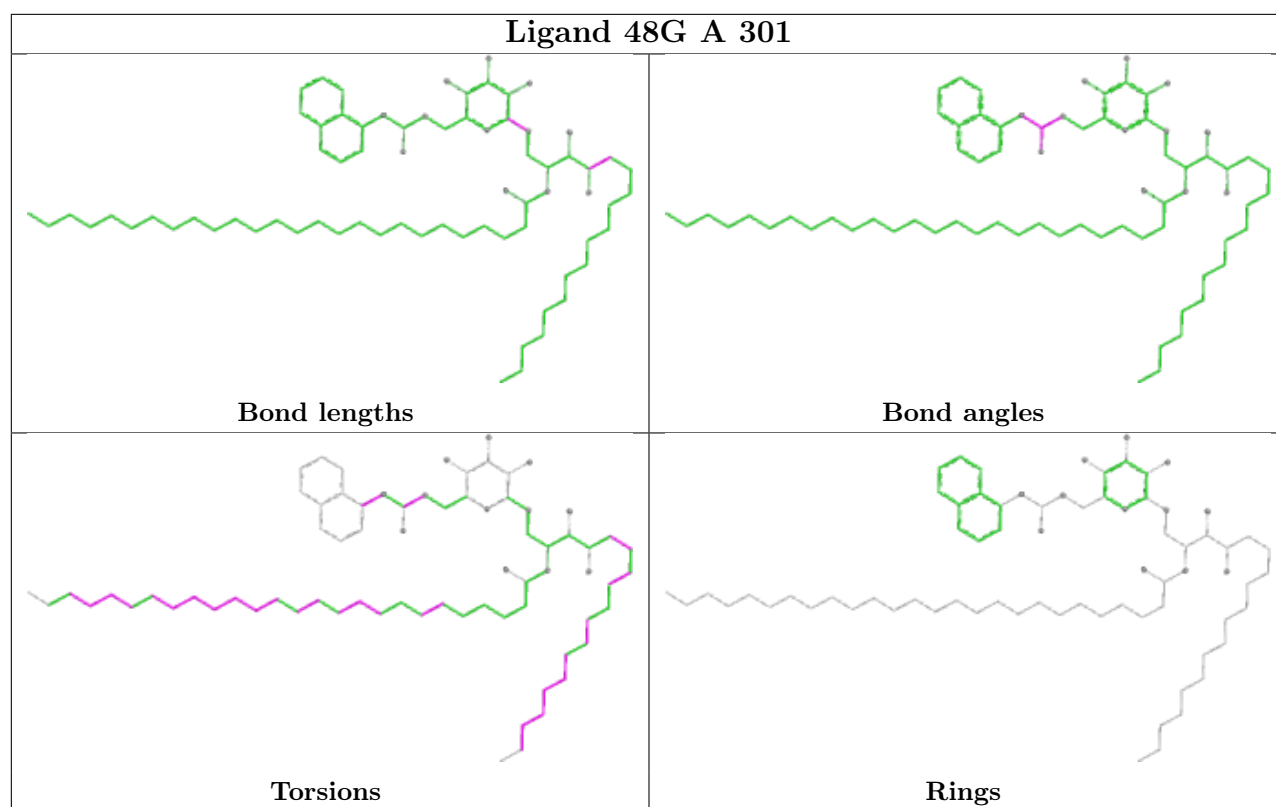
Mol	Chain	Res	Type	Atoms
7	A	301	48G	CCB-CCC-CCD-CCE
7	A	301	48G	OCT-CCH-O6-C6
7	A	301	48G	NCS-CCH-O6-C6
7	A	301	48G	CAR-CAS-CAT-CAU
7	A	301	48G	CCD-CCE-CCF-CCG
7	A	301	48G	CCA-CCB-CCC-CCD
7	A	301	48G	CCQ-CCR-NCS-CCH
7	A	301	48G	CBM-CBQ-CBS-CBV

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	301	48G	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	268/285 (94%)	-0.41	4 (1%) 71 67	21, 33, 76, 91	0
2	B	98/99 (98%)	-0.34	1 (1%) 79 75	17, 42, 66, 87	1 (1%)
3	C	202/209 (96%)	-0.29	4 (1%) 64 59	19, 39, 84, 95	0
4	D	239/241 (99%)	-0.48	6 (2%) 58 53	23, 36, 61, 97	0
All	All	807/834 (96%)	-0.39	15 (1%) 66 61	17, 37, 78, 97	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	31	HIS	5.9
4	D	182	ASP	4.0
4	D	180	LEU	3.7
3	C	194	ILE	3.4
1	A	6	LYS	3.1
1	A	197	PRO	3.1
3	C	203	SER	3.0
3	C	197	GLU	2.9
1	A	279	TRP	2.8
4	D	2	ALA	2.5
4	D	179	ALA	2.4
4	D	181	ASN	2.2
4	D	3	ALA	2.1
3	C	181	LYS	2.1
1	A	227	GLN	2.1

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

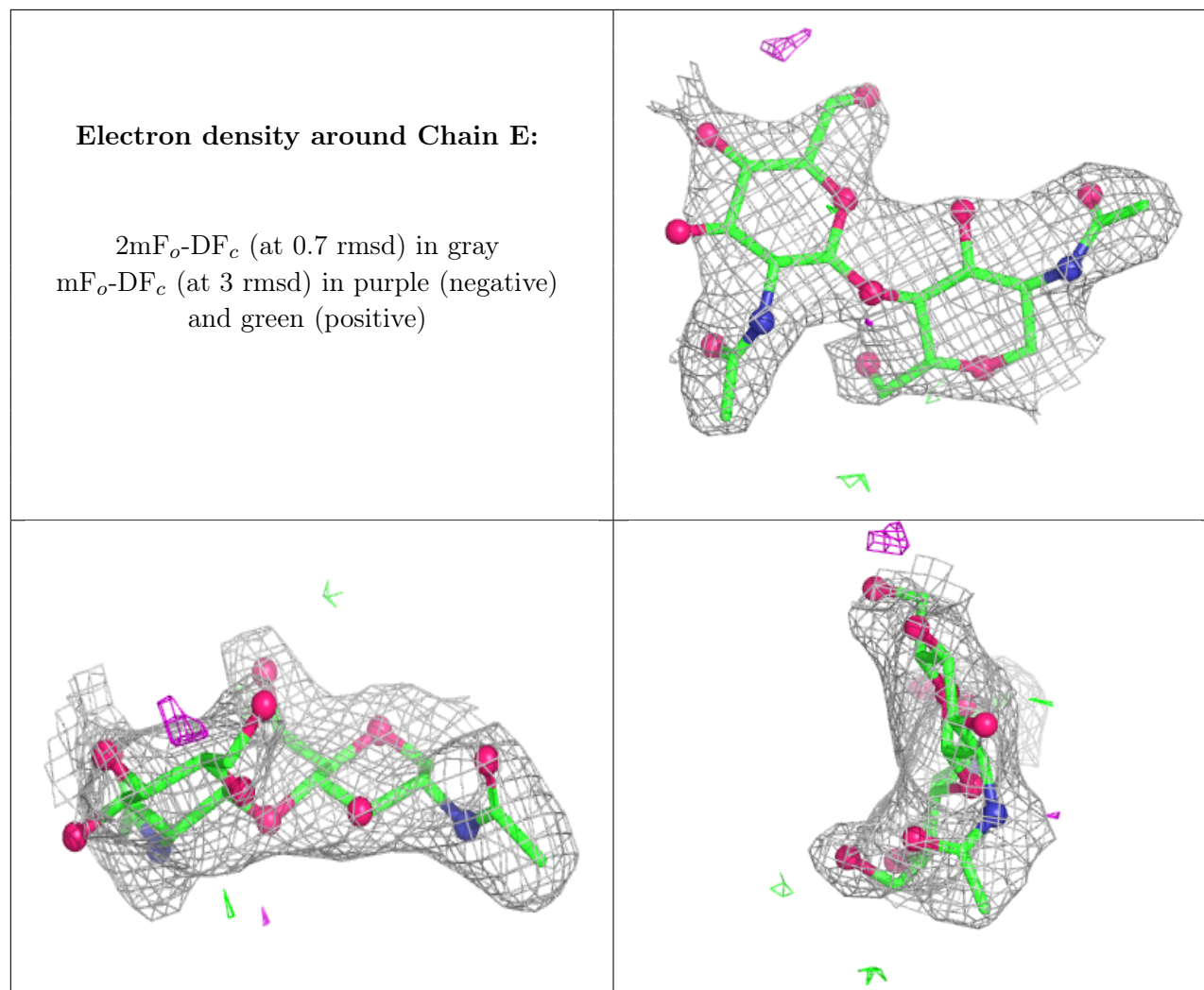
There are no non-standard protein/DNA/RNA residues in this entry.

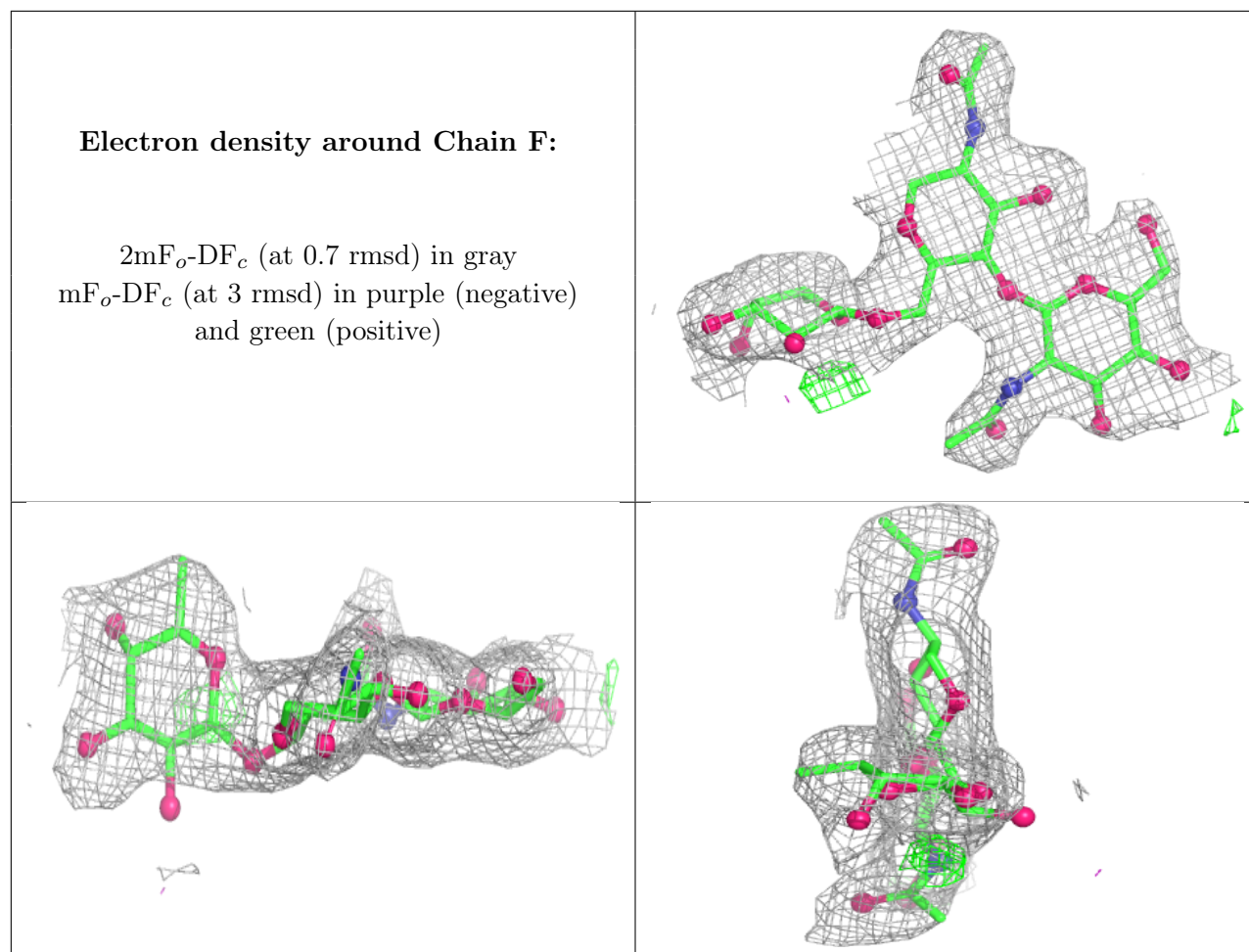
### 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	2	14/15	0.83	0.12	60,67,72,72	0
6	FUL	F	3	10/11	0.86	0.13	56,58,59,62	0
6	NAG	F	2	14/15	0.89	0.11	48,53,57,57	0
5	NAG	E	1	14/15	0.93	0.08	37,41,47,56	0
6	NAG	F	1	14/15	0.95	0.07	34,39,48,51	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.





## 6.4 Ligands [i](#)

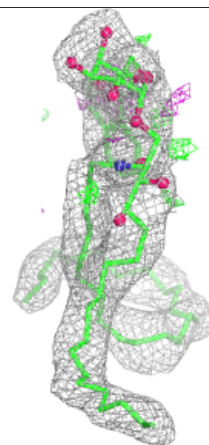
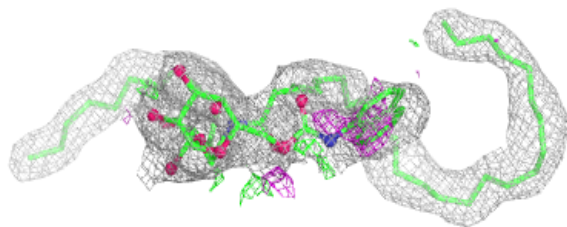
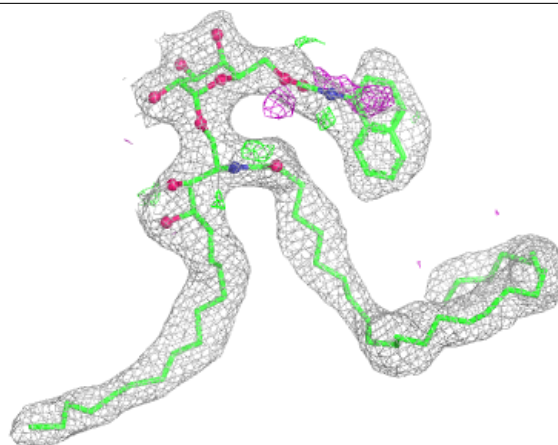
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	NAG	A	302	14/15	0.84	0.12	60,63,66,67	0
7	48G	A	301	73/73	0.94	0.09	24,31,49,50	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 48G A 301:**

$2mF_o-DF_c$  (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.