



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 01:30 PM EDT

PDB ID : 6N9T  
Title : Structure of a peptide-based photo-affinity cross-linker with Herceptin Fc  
Authors : Sadowsky, J.; Ultsch, M.; Vance, N.; Wang, W.  
Deposited on : 2018-12-04  
Resolution : 2.58 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

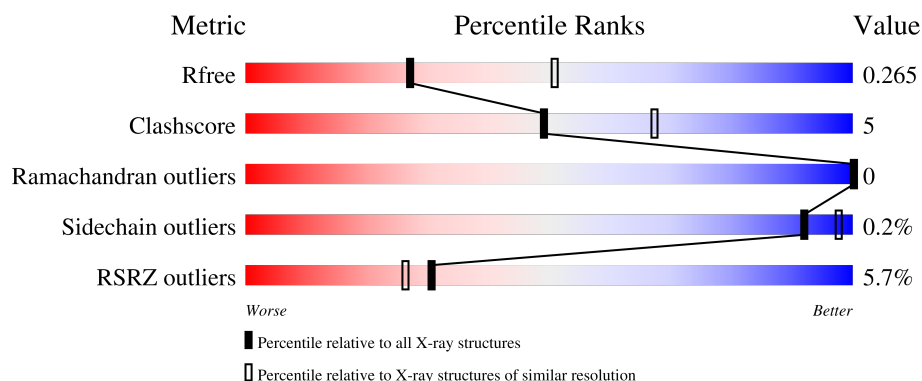
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	224	<div> <div>4%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
1	B	224	<div> <div>5%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
2	E	13	<div> <div>23%</div> <div>77%</div> <div>15%</div> <div>8%</div> </div>
2	F	13	<div> <div>8%</div> <div>85%</div> <div>8%</div> <div>8%</div> </div>
3	C	7	<div> <div>57%</div> <div>43%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	7	<div><div></div><div>29%</div><div>43%</div><div>29%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3894 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.

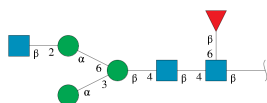
- Molecule 1 is a protein called Immunoglobulin G1 FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1659	1056	279	317	7			
1	B	207	Total	C	N	O	S	0	0	0
			1659	1056	279	317	7			

- Molecule 2 is a protein called Photo-affinity peptide.

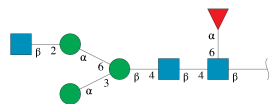
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	S	0	0	0
			118	80	17	19	2			
2	F	13	Total	C	N	O	S	0	0	0
			118	80	17	19	2			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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
3	C	7	Total	C	N	O		0	0	0
			85	48	3	34				

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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
4	D	7	Total	C	N	O	0	0	0
			85	48	3	34			

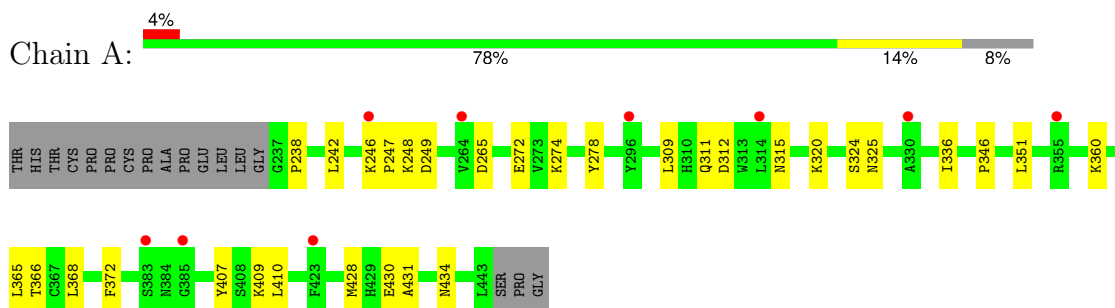
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	E	1	Total	O	0	0
			1	1		
5	B	89	Total	O	0	0
			89	89		
5	F	3	Total	O	0	0
			3	3		

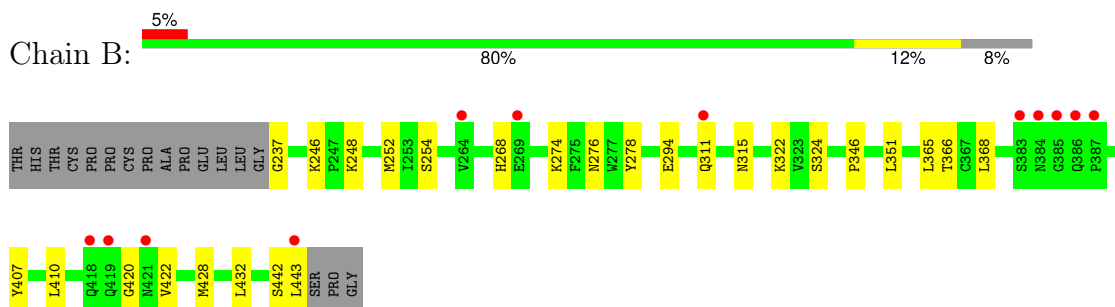
### 3 Residue-property plots [i](#)

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.

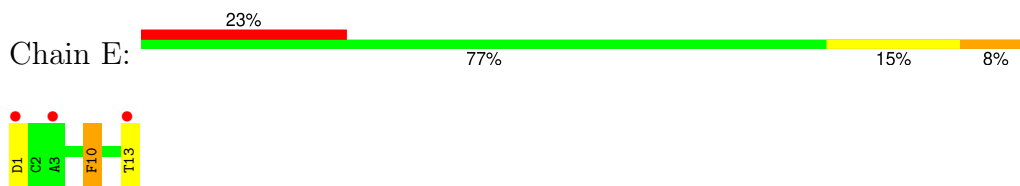
- Molecule 1: Immunoglobulin G1 FC



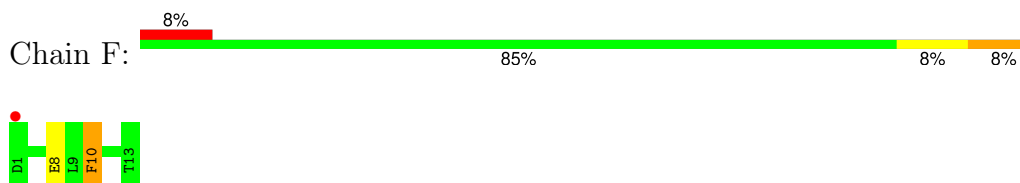
- Molecule 1: Immunoglobulin G1 FC



- Molecule 2: Photo-affinity peptide



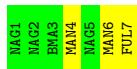
- Molecule 2: Photo-affinity peptide



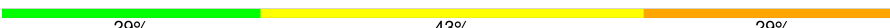
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

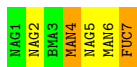
nose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  57% 43%



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

Chain D:  29% 43% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.11Å 60.85Å 68.17Å 90.00° 103.13° 90.00°	Depositor
Resolution (Å)	44.22 – 2.58 44.22 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.22-2.58) 99.9 (44.22-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.12-2829)	Depositor
R, $R_{free}$	0.229 , 0.265 0.230 , 0.265	Depositor DCC
$R_{free}$ test set	872 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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 28.49 % 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 1.8269e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, NAG, FUL, PBF, MAN, FUC

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	0.26	0/1705	0.44	0/2322
1	B	0.26	0/1705	0.44	0/2322
2	E	0.25	0/102	0.39	0/138
2	F	0.24	0/102	0.42	0/138
All	All	0.26	0/3614	0.44	0/4920

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	1659	0	1625	19	0
1	B	1659	0	1625	17	0
2	E	118	0	96	3	0
2	F	118	0	96	3	0
3	C	85	0	73	0	0
4	D	85	0	73	3	0
5	A	77	0	0	3	0
5	B	89	0	0	2	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	3	0	0	0	0
All	All	3894	0	3588	39	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 (39) 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:346:PRO:HB3	1:A:372:PHE:HB3	1.72	0.71
1:A:360:LYS:NZ	5:A:603:HOH:O	2.25	0.68
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.76	0.67
1:B:351:LEU:HB2	1:B:366:THR:HB	1.77	0.65
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.82	0.62
1:A:320:LYS:NZ	5:A:607:HOH:O	2.34	0.61
1:B:237:GLY:N	5:B:610:HOH:O	2.34	0.60
1:B:422:VAL:HA	1:B:442:SER:HB3	1.85	0.58
4:D:2:NAG:HN2	4:D:7:FUC:H61	1.70	0.56
1:B:254:SER:OG	2:F:8:GLU:OE1	2.24	0.56
1:B:248:LYS:HE2	2:F:10:PBF:HI2	1.87	0.56
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.88	0.56
1:A:242:LEU:HG	1:A:336:ILE:HG12	1.89	0.55
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.89	0.54
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.90	0.54
1:B:268:HIS:NE2	1:B:294:GLU:OE1	2.42	0.53
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.44	0.53
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.44	0.52
2:E:1:ASP:OD2	2:E:1:ASP:N	2.44	0.51
1:B:246:LYS:NZ	4:D:5:NAG:O3	2.43	0.51
1:A:351:LEU:HB2	1:A:366:THR:HB	1.92	0.51
1:B:346:PRO:HD2	1:B:432:LEU:HG	1.96	0.48
1:B:278:TYR:OH	5:B:601:HOH:O	2.20	0.48
1:B:248:LYS:HG2	1:B:252:MET:HE3	1.98	0.46
1:A:272:GLU:O	1:A:325:ASN:ND2	2.45	0.45
1:A:434:ASN:OD1	2:E:13:THR:HG23	2.16	0.45
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.98	0.45
1:A:409:LYS:HE2	5:A:613:HOH:O	2.17	0.45
4:D:4:MAN:O3	4:D:5:NAG:O7	2.25	0.45
1:A:246:LYS:HD2	1:A:247:PRO:HD2	1.99	0.44
1:B:428:MET:HG3	2:F:10:PBF:HE1	2.00	0.44
1:B:420:GLY:HA2	1:B:443:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLN:HG2	1:B:315:ASN:ND2	2.33	0.43
1:A:309:LEU:HB2	1:A:312:ASP:HB2	2.00	0.43
1:A:428:MET:HG3	2:E:10:PBF:HE1	2.02	0.41
1:A:311:GLN:HG2	1:A:315:ASN:OD1	2.20	0.41
1:A:246:LYS:HG3	1:A:248:LYS:H	1.86	0.40
1:A:430:GLU:HG3	1:A:431:ALA:N	2.35	0.40
1:A:238:PRO:HA	1:A:265:ASP:HB2	2.01	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	205/224 (92%)	201 (98%)	4 (2%)	0	100	100
1	B	205/224 (92%)	201 (98%)	4 (2%)	0	100	100
2	E	10/13 (77%)	10 (100%)	0	0	100	100
2	F	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
All	All	430/474 (91%)	421 (98%)	9 (2%)	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	193/207 (93%)	192 (100%)	1 (0%)	86	95
1	B	193/207 (93%)	193 (100%)	0	100	100
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
All	All	406/434 (94%)	405 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PBF	F	10	1,2	19,20,21	3.62	1 (5%)	21,26,28	2.42	2 (9%)
2	PBF	E	10	1,2	19,20,21	3.65	1 (5%)	21,26,28	2.55	2 (9%)

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	PBF	F	10	1,2	-	6/13/14/16	0/2/2/2
2	PBF	E	10	1,2	-	4/13/14/16	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10	PBF	ON2-CN1	15.68	1.50	1.22
2	F	10	PBF	ON2-CN1	15.57	1.50	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	10	PBF	ON2-CN1-CZ	-7.77	107.72	120.15
2	E	10	PBF	ON2-CN1-CT	-7.62	107.95	120.15
2	F	10	PBF	ON2-CN1-CT	-7.40	108.31	120.15
2	F	10	PBF	ON2-CN1-CZ	-7.19	108.65	120.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	10	PBF	C-CA-CB-CG
2	F	10	PBF	N-CA-CB-CG
2	F	10	PBF	C-CA-CB-CG
2	E	10	PBF	ON2-CN1-CT-CI1
2	F	10	PBF	ON2-CN1-CT-CI1
2	E	10	PBF	ON2-CN1-CT-CI2
2	F	10	PBF	ON2-CN1-CT-CI2
2	E	10	PBF	N-CA-CB-CG
2	F	10	PBF	CT-CN1-CZ-CE1
2	F	10	PBF	CT-CN1-CZ-CE2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	10	PBF	2	0
2	E	10	PBF	1	0

## 5.5 Carbohydrates ⓘ

14 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	1,3	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	C	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	BMA	C	3	3	11,11,12	0.61	0	15,15,17	0.67	0
3	MAN	C	4	3	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
3	NAG	C	5	3	14,14,15	0.28	0	17,19,21	0.50	0
3	MAN	C	6	3	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
3	FUL	C	7	3	10,10,11	1.63	2 (20%)	14,14,16	1.28	2 (14%)
4	NAG	D	1	4,1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	D	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	BMA	D	3	4	11,11,12	0.50	0	15,15,17	0.78	0
4	MAN	D	4	4	11,11,12	0.75	0	15,15,17	1.04	2 (13%)
4	NAG	D	5	4	14,14,15	0.32	0	17,19,21	0.45	0
4	MAN	D	6	4	11,11,12	0.76	0	15,15,17	0.96	2 (13%)
4	FUC	D	7	4	10,10,11	1.19	1 (10%)	14,14,16	1.08	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
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	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
3	FUL	C	7	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	NAG	D	5	4	-	1/6/23/26	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	FUC	D	7	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7	FUL	O5-C1	3.78	1.50	1.43
4	D	7	FUC	C2-C3	2.41	1.56	1.52
3	C	7	FUL	C2-C3	-2.36	1.48	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	2.69	115.79	112.19
4	D	4	MAN	C1-O5-C5	2.48	115.51	112.19
3	C	7	FUL	C3-C4-C5	2.40	113.47	109.81
3	C	6	MAN	O2-C2-C3	-2.36	105.26	110.15
3	C	7	FUL	C1-C2-C3	2.36	113.08	109.64
3	C	6	MAN	C1-O5-C5	2.31	115.28	112.19
4	D	6	MAN	O2-C2-C3	-2.30	105.39	110.15
4	D	4	MAN	O2-C2-C3	-2.26	105.47	110.15
4	D	6	MAN	C1-O5-C5	2.15	115.06	112.19
4	D	7	FUC	C1-C2-C3	2.06	112.64	109.64
3	C	4	MAN	O2-C2-C3	-2.05	105.89	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	5	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	5	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

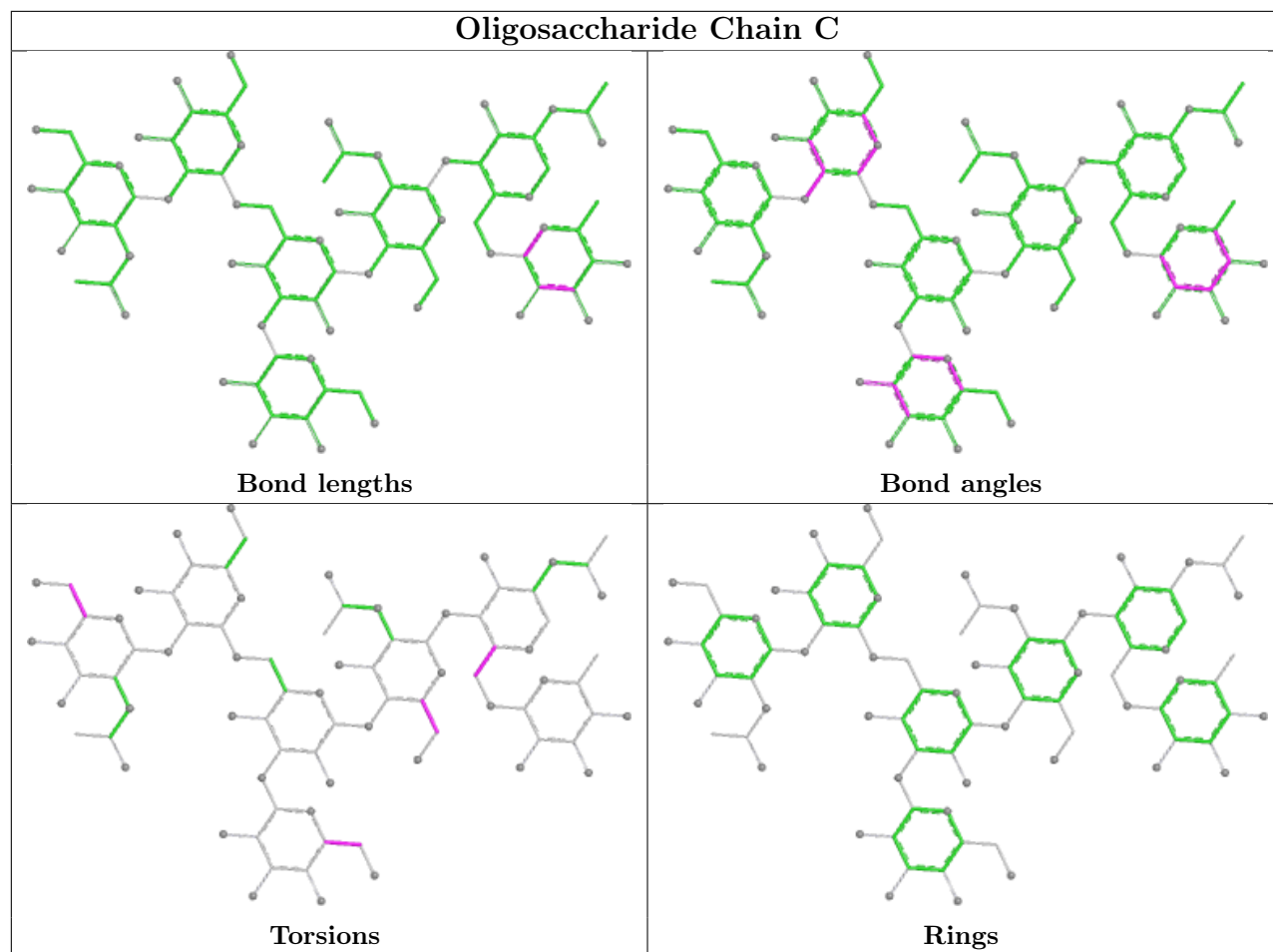
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

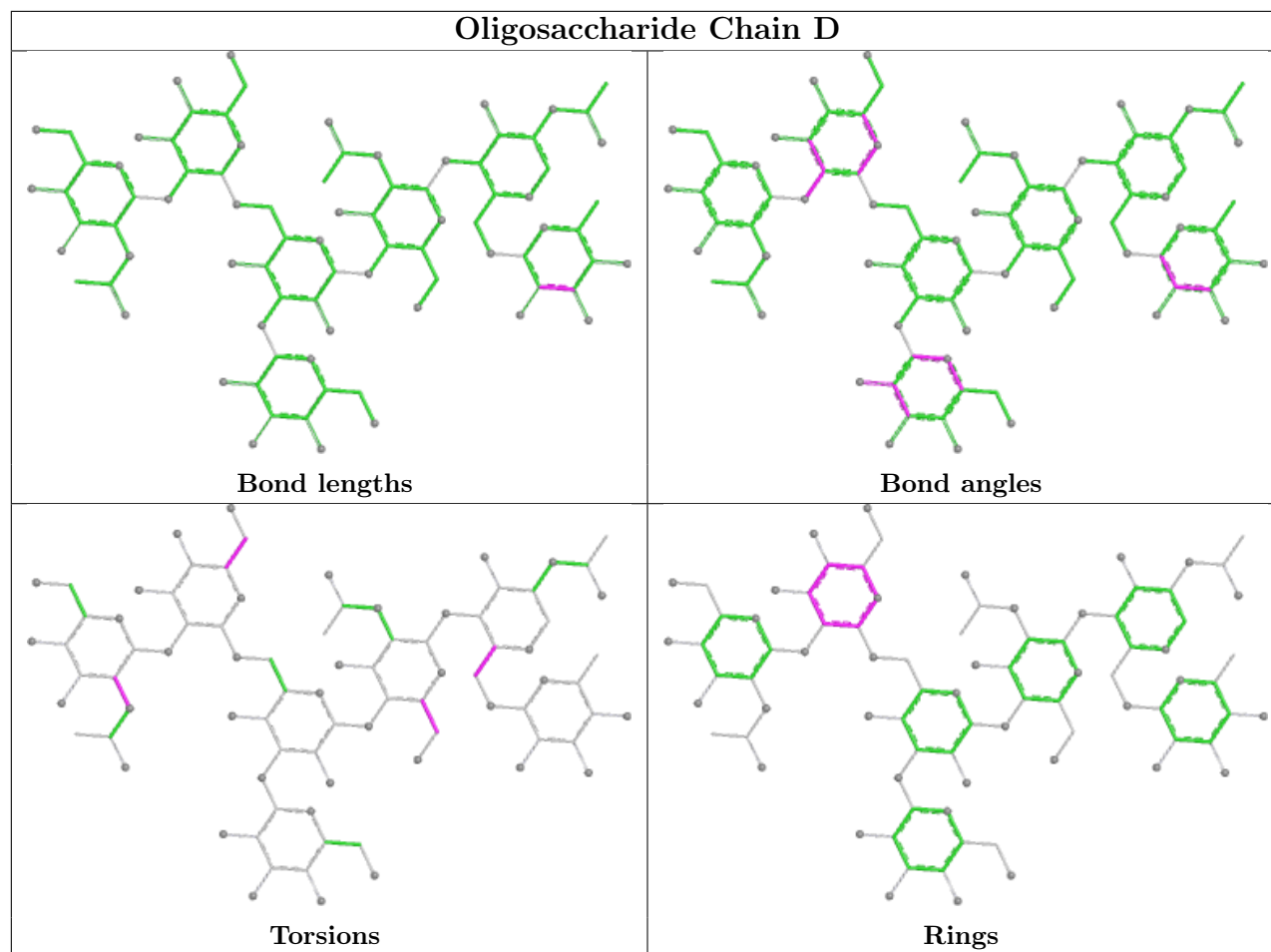
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5	NAG	2	0
4	D	4	MAN	1	0
4	D	7	FUC	1	0
4	D	2	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](#)

There are no ligands in this entry.

## 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, 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	207/224 (92%)	0.49	9 (4%) 40 36	28, 43, 65, 86	0
1	B	207/224 (92%)	0.53	12 (5%) 30 26	28, 41, 70, 111	0
2	E	12/13 (92%)	1.62	3 (25%) 2 2	49, 63, 78, 100	0
2	F	12/13 (92%)	1.38	1 (8%) 19 16	44, 56, 67, 105	0
All	All	438/474 (92%)	0.56	25 (5%) 30 26	28, 42, 69, 111	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	LEU	6.7
1	B	385	GLY	5.5
2	F	1	ASP	4.8
1	A	355	ARG	3.7
2	E	13	THR	3.1
2	E	1	ASP	3.1
1	B	386	GLN	3.0
1	B	384	ASN	2.8
1	B	269	GLU	2.8
1	A	383	SER	2.7
1	A	314	LEU	2.7
1	A	246	LYS	2.7
1	A	423	PHE	2.6
1	A	296	TYR	2.5
1	B	418	GLN	2.4
1	B	311	GLN	2.3
1	A	385	GLY	2.3
2	E	3	ALA	2.3
1	B	264	VAL	2.2
1	B	421	ASN	2.1
1	B	387	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	419	GLN	2.1
1	A	330	ALA	2.0
1	A	264	VAL	2.0
1	B	383	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PBF	E	10	19/20	0.83	0.15	42,47,55,55	0
2	PBF	F	10	19/20	0.83	0.17	48,55,60,62	0

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.