



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:44 AM BST

PDB ID : 3D6G
Title : Fc fragment of IgG1 (Herceptin) with protein-A mimetic peptide dendrimer ligand.
Authors : Bujacz, A.D.; Redzynia, I.; Bujacz, G.D.; Dinon, F.; Pengo, P.; Fassina, G.
Deposited on : 2008-05-19
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

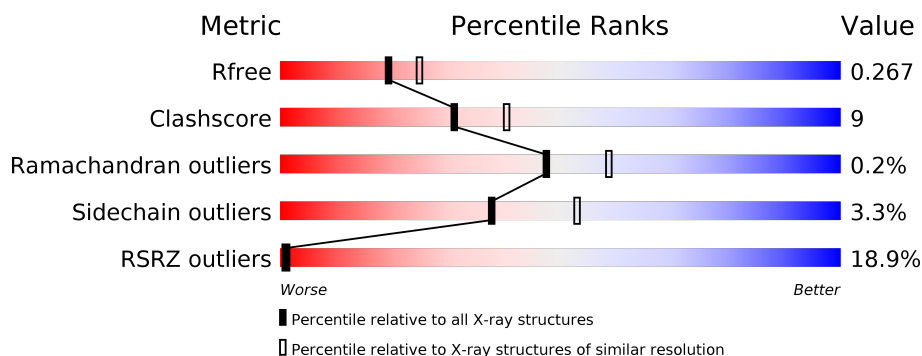
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	B	210	<div> <div>26%</div> <div> <div></div> <div>79%</div> <div>19%</div> </div> </div>
2	C	8	<div> <div>13%</div> <div> <div></div> <div>75%</div> <div>13%</div> </div> </div>
2	D	8	<div> <div>13%</div> <div> <div></div> <div>50%</div> <div>38%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	-	-	-	X
2	NAG	D	2	-	-	-	X
2	NAG	D	5	-	-	-	X
3	X12	B	446	-	-	-	X

2 Entry composition [i](#)

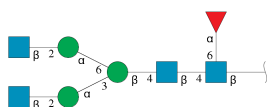
There are 4 unique types of molecules in this entry. The entry contains 4002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ig gamma-1 chain C region.

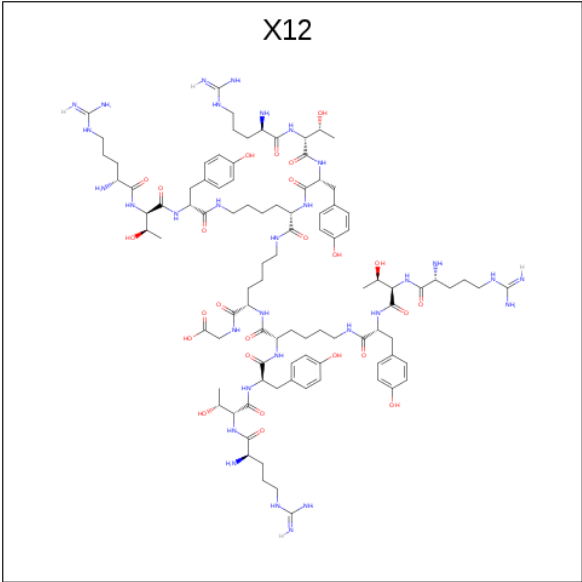
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	4	0
			1702	1084	288	324	6			
1	B	209	Total	C	N	O	S	0	2	0
			1682	1070	285	321	6			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			
2	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 3 is 2-[[[(2S)-2,6-bis[[[(2S)-2,6-bis[[[(2R)-2-[[[(2R,3R)-2-[[[(2R)-2-amino-5-carbamimidamido-pentanoyl]amino]-3-hydroxy-butanoyl]amino]-3-(4-hydroxyphenyl)propanoyl]amino]hexanoyl]amino]hexanoyl]amino]ethanoic acid (three-letter code: X12) (formula: C₉₆H₁₅₃N₃₁O₂₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			152	96	31	25		

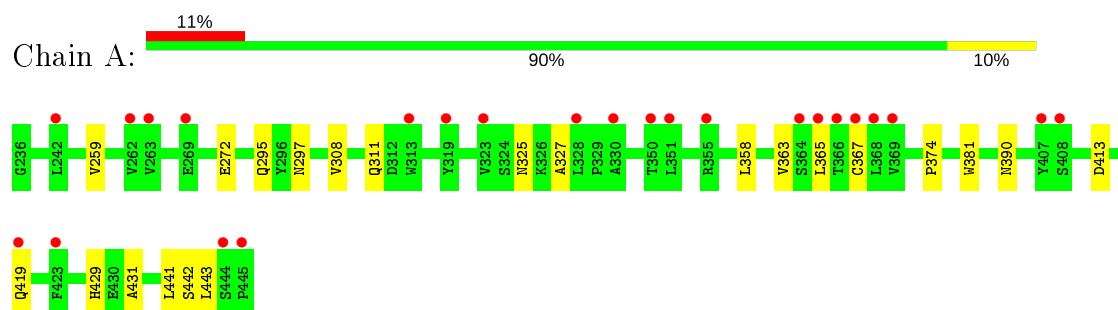
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	123	Total	O	0	0
			123	123		

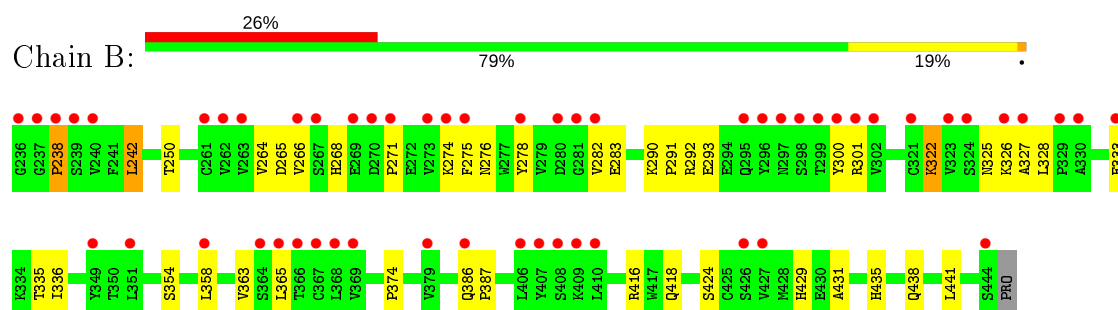
3 Residue-property plots [i](#)

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: Ig gamma-1 chain C region



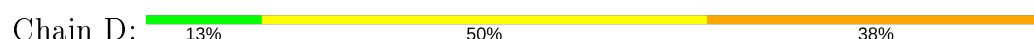
- Molecule 1: Ig gamma-1 chain C region



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



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



MAG1	MAG2	MAN3	MAN4	MAG5	MAN6	MAG7	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.78 Å 79.16 Å 139.22 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 30.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.30) 99.3 (30.11-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.257 0.203 , 0.267	Depositor DCC
R_{free} test set	806 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4002	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, X12, BMA, NAG, 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	0.76	0/1762	0.77	0/2400
1	B	0.76	0/1734	0.74	0/2361
All	All	0.76	0/3496	0.75	0/4761

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	1702	0	1674	12	0
1	B	1682	0	1654	43	0
2	C	99	0	85	2	0
2	D	99	0	85	2	0
3	B	152	0	146	13	0
4	A	145	0	0	0	0
4	B	123	0	0	4	0
All	All	4002	0	3644	67	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.

All (67) 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)
3:B:446:X12:HNBS	3:B:446:X12:HBI	1.29	0.96
1:B:276:ASN:HA	4:B:532:HOH:O	1.65	0.95
1:B:282:VAL:HG12	1:B:283:GLU:N	1.91	0.83
3:B:446:X12:HBI	3:B:446:X12:NBS	1.93	0.83
1:B:429:HIS:HD2	1:B:431:ALA:H	1.32	0.77
1:B:274:LYS:HG2	1:B:275:PHE:N	2.01	0.76
1:B:278:TYR:HD1	1:B:282:VAL:O	1.73	0.72
1:B:282:VAL:HG12	1:B:283:GLU:O	1.90	0.72
1:B:274:LYS:HG2	1:B:275:PHE:H	1.55	0.71
1:B:278:TYR:CD1	1:B:282:VAL:O	2.44	0.70
1:B:242:LEU:HD13	1:B:336:ILE:HB	1.72	0.70
1:A:297:ASN:HD22	2:C:1:NAG:H83	1.58	0.69
1:B:429:HIS:CD2	1:B:431:ALA:H	2.12	0.65
1:B:268:HIS:CD2	1:B:300:TYR:CE1	2.86	0.64
1:B:322:LYS:HG2	1:B:333:GLU:HG2	1.79	0.64
1:B:264:VAL:HG13	1:B:265:ASP:H	1.63	0.64
1:B:268:HIS:CD2	1:B:300:TYR:HE1	2.18	0.61
1:B:278:TYR:HB3	1:B:282:VAL:O	1.99	0.61
1:B:264:VAL:HG13	1:B:265:ASP:N	2.17	0.60
1:B:358:LEU:HD23	1:B:363:VAL:HG11	1.84	0.60
1:B:282:VAL:CG1	1:B:283:GLU:N	2.61	0.59
1:A:374:PRO:O	1:A:429:HIS:HE1	1.86	0.59
1:B:250:THR:O	3:B:446:X12:NDU	2.36	0.58
1:B:325:ASN:HB3	1:B:328:LEU:HG	1.88	0.56
1:B:278:TYR:CB	1:B:282:VAL:O	2.56	0.54
1:B:282:VAL:HG12	1:B:283:GLU:H	1.70	0.53
1:A:272[A]:GLU:HA	1:A:272[A]:GLU:OE1	2.08	0.53
1:B:264:VAL:CG1	1:B:265:ASP:N	2.71	0.53
1:A:429:HIS:CD2	1:A:431:ALA:H	2.27	0.52
3:B:446:X12:HCQ	3:B:446:X12:HB5	1.92	0.52
1:A:295:GLN:HE21	2:C:1:NAG:H62	1.75	0.51
1:A:429:HIS:HD2	1:A:431:ALA:H	1.57	0.51
1:B:274:LYS:CG	1:B:275:PHE:N	2.74	0.50
3:B:446:X12:HCJ	3:B:446:X12:HC6	1.93	0.50
1:A:259:VAL:HG23	1:A:308:VAL:HG11	1.94	0.50
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.48	0.49
1:B:276:ASN:HB2	1:B:322:LYS:HB2	1.95	0.48
1:B:325:ASN:HD21	1:B:327:ALA:HB3	1.79	0.48
1:A:311[B]:GLN:H	1:A:311[B]:GLN:NE2	2.11	0.48
3:B:446:X12:HAW	3:B:446:X12:NBC	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:CG	1:B:275:PHE:H	2.26	0.46
3:B:446:X12:HAT	3:B:446:X12:HAQA	1.48	0.45
3:B:446:X12:HNAG	3:B:446:X12:CC1	2.28	0.45
1:B:435:HIS:HE1	3:B:446:X12:NDT	2.14	0.45
1:B:424:SER:HB3	1:B:438:GLN:HE21	1.82	0.45
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.00	0.44
1:B:325:ASN:ND2	1:B:327:ALA:H	2.15	0.44
1:A:358:LEU:HD23	1:A:363:VAL:HG11	1.98	0.44
1:B:282:VAL:CG1	1:B:283:GLU:H	2.29	0.43
1:B:325:ASN:ND2	1:B:327:ALA:HB3	2.34	0.43
1:B:365:LEU:HB3	1:B:441:LEU:HD23	2.01	0.42
4:B:512:HOH:O	2:D:3:BMA:O4	2.21	0.42
1:B:276:ASN:HB2	1:B:322:LYS:CB	2.48	0.42
1:B:335:THR:HG22	1:B:336:ILE:N	2.34	0.42
1:B:416:ARG:HD3	4:B:509:HOH:O	2.18	0.42
1:B:238:PRO:HB3	1:B:264:VAL:O	2.20	0.41
1:B:271:PRO:HG2	4:B:560:HOH:O	2.20	0.41
1:B:374:PRO:O	1:B:429:HIS:HE1	2.02	0.41
1:B:435:HIS:HE1	3:B:446:X12:CDS	2.33	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.96	0.41
1:B:290:LYS:HA	1:B:291:PRO:HD3	1.79	0.41
3:B:446:X12:HCU	3:B:446:X12:HDH	2.01	0.41
1:A:325:ASN:OD1	1:A:327:ALA:HB3	2.21	0.40
3:B:446:X12:HBP	3:B:446:X12:HNBA	1.86	0.40
2:D:4:MAN:H4	2:D:5:NAG:H83	2.03	0.40
1:A:365:LEU:HB3	1:A:441:LEU:HD23	2.02	0.40
3:B:446:X12:CAW	3:B:446:X12:NBC	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/210 (101%)	210 (99%)	2 (1%)	0	100	100
1	B	209/210 (100%)	202 (97%)	6 (3%)	1 (0%)	29	35
All	All	421/420 (100%)	412 (98%)	8 (2%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	PRO

5.3.2 Protein sidechains ⓘ

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	199/195 (102%)	194 (98%)	5 (2%)	47	65
1	B	196/195 (100%)	187 (95%)	9 (5%)	27	38
All	All	395/390 (101%)	381 (96%)	14 (4%)	38	50

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

Mol	Chain	Res	Type
1	A	390	ASN
1	A	413	ASP
1	A	419	GLN
1	A	442	SER
1	A	443	LEU
1	B	242	LEU
1	B	292	ARG
1	B	293	GLU
1	B	301[A]	ARG
1	B	301[B]	ARG
1	B	322	LYS
1	B	326	LYS
1	B	354	SER
1	B	418	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	361	ASN
1	A	386	GLN
1	A	419	GLN
1	A	429	HIS
1	A	438	GLN
1	B	268	HIS
1	B	325	ASN
1	B	389	ASN
1	B	390	ASN
1	B	418	GLN
1	B	419	GLN
1	B	429	HIS
1	B	435	HIS
1	B	438	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 ⓘ

16 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	C	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	1.58	3 (17%)
2	NAG	C	2	2	14,14,15	1.05	1 (7%)	17,19,21	1.86	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	C	3	2	11,11,12	1.12	2 (18%)	15,15,17	1.52	2 (13%)
2	MAN	C	4	2	11,11,12	1.01	1 (9%)	15,15,17	1.94	4 (26%)
2	NAG	C	5	2	14,14,15	0.98	1 (7%)	17,19,21	1.32	3 (17%)
2	MAN	C	6	2	11,11,12	1.31	2 (18%)	15,15,17	1.31	2 (13%)
2	NAG	C	7	2	14,14,15	0.82	1 (7%)	17,19,21	1.56	5 (29%)
2	FUC	C	8	2	10,10,11	0.42	0	14,14,16	1.02	0
2	NAG	D	1	1,2	14,14,15	1.26	2 (14%)	17,19,21	1.46	4 (23%)
2	NAG	D	2	2	14,14,15	0.99	0	17,19,21	1.44	2 (11%)
2	BMA	D	3	2	11,11,12	0.83	0	15,15,17	1.45	3 (20%)
2	MAN	D	4	2	11,11,12	1.13	1 (9%)	15,15,17	1.63	2 (13%)
2	NAG	D	5	2	14,14,15	1.11	2 (14%)	17,19,21	1.35	2 (11%)
2	MAN	D	6	2	11,11,12	1.12	1 (9%)	15,15,17	1.63	1 (6%)
2	NAG	D	7	2	14,14,15	0.81	0	17,19,21	1.01	0
2	FUC	D	8	2	10,10,11	0.59	0	14,14,16	1.43	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	MAN	C	6	2	-	1/2/19/22	0/1/1/1
2	NAG	C	7	2	-	2/6/23/26	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	4/6/23/26	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	7	2	-	2/6/23/26	0/1/1/1
2	FUC	D	8	2	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C2-C3	3.23	1.57	1.52
2	C	1	NAG	O5-C5	2.90	1.49	1.43
2	D	6	MAN	O5-C1	2.75	1.48	1.43
2	C	4	MAN	O5-C5	2.55	1.48	1.43
2	C	1	NAG	C1-C2	2.52	1.56	1.52
2	C	2	NAG	O5-C1	-2.51	1.39	1.43
2	C	5	NAG	C8-C7	2.47	1.55	1.50
2	D	1	NAG	O5-C1	2.44	1.47	1.43
2	D	4	MAN	O5-C1	2.43	1.47	1.43
2	D	1	NAG	C1-C2	2.32	1.55	1.52
2	C	3	BMA	C2-C3	2.28	1.55	1.52
2	C	7	NAG	C8-C7	2.26	1.55	1.50
2	C	6	MAN	O5-C5	2.24	1.48	1.43
2	C	3	BMA	O5-C5	2.20	1.47	1.43
2	D	5	NAG	C4-C5	2.10	1.57	1.53
2	D	5	NAG	C8-C7	2.08	1.54	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	MAN	C1-O5-C5	5.60	119.77	112.19
2	C	1	NAG	O6-C6-C5	-4.40	96.19	111.29
2	C	2	NAG	C3-C4-C5	-4.32	102.53	110.24
2	D	4	MAN	O2-C2-C3	-4.30	101.53	110.14
2	C	4	MAN	C1-O5-C5	4.05	117.69	112.19
2	D	1	NAG	C1-O5-C5	3.77	117.30	112.19
2	D	8	FUC	O5-C1-C2	-3.75	104.99	110.77
2	D	5	NAG	C1-C2-N2	-3.71	104.15	110.49
2	C	4	MAN	O2-C2-C3	-3.71	102.71	110.14
2	D	4	MAN	C1-C2-C3	3.69	114.20	109.67
2	D	2	NAG	C1-O5-C5	3.66	117.15	112.19
2	C	3	BMA	O6-C6-C5	-3.63	98.85	111.29
2	C	7	NAG	O5-C1-C2	-3.41	105.91	111.29
2	C	1	NAG	C6-C5-C4	-3.18	105.56	113.00
2	D	3	BMA	C1-C2-C3	3.15	113.54	109.67
2	C	6	MAN	C1-O5-C5	2.90	116.12	112.19
2	C	3	BMA	O3-C3-C4	-2.89	103.67	110.35
2	C	4	MAN	C2-C3-C4	-2.85	105.97	110.89
2	C	2	NAG	O5-C1-C2	-2.72	107.00	111.29
2	C	2	NAG	C1-O5-C5	2.72	115.87	112.19
2	C	2	NAG	C8-C7-N2	-2.66	111.59	116.10
2	C	7	NAG	C6-C5-C4	2.66	119.24	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	NAG	O5-C5-C6	-2.65	103.05	107.20
2	D	1	NAG	C6-C5-C4	-2.65	106.80	113.00
2	C	4	MAN	C1-C2-C3	2.62	112.88	109.67
2	C	2	NAG	O4-C4-C5	-2.58	102.90	109.30
2	C	2	NAG	O7-C7-N2	2.52	126.58	121.95
2	D	3	BMA	O6-C6-C5	-2.42	103.00	111.29
2	D	3	BMA	C6-C5-C4	-2.39	107.42	113.00
2	D	2	NAG	O4-C4-C5	-2.37	103.40	109.30
2	C	7	NAG	O5-C5-C6	-2.34	103.54	107.20
2	C	6	MAN	O5-C5-C6	2.21	110.66	107.20
2	C	5	NAG	C2-N2-C7	2.17	125.99	122.90
2	C	5	NAG	C1-O5-C5	-2.16	109.27	112.19
2	D	5	NAG	O5-C1-C2	2.10	114.61	111.29
2	C	7	NAG	C1-O5-C5	-2.09	109.36	112.19
2	D	1	NAG	O4-C4-C5	-2.02	104.28	109.30
2	C	1	NAG	C3-C4-C5	-2.01	106.65	110.24
2	C	7	NAG	O5-C5-C4	-2.01	105.93	110.83
2	D	1	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

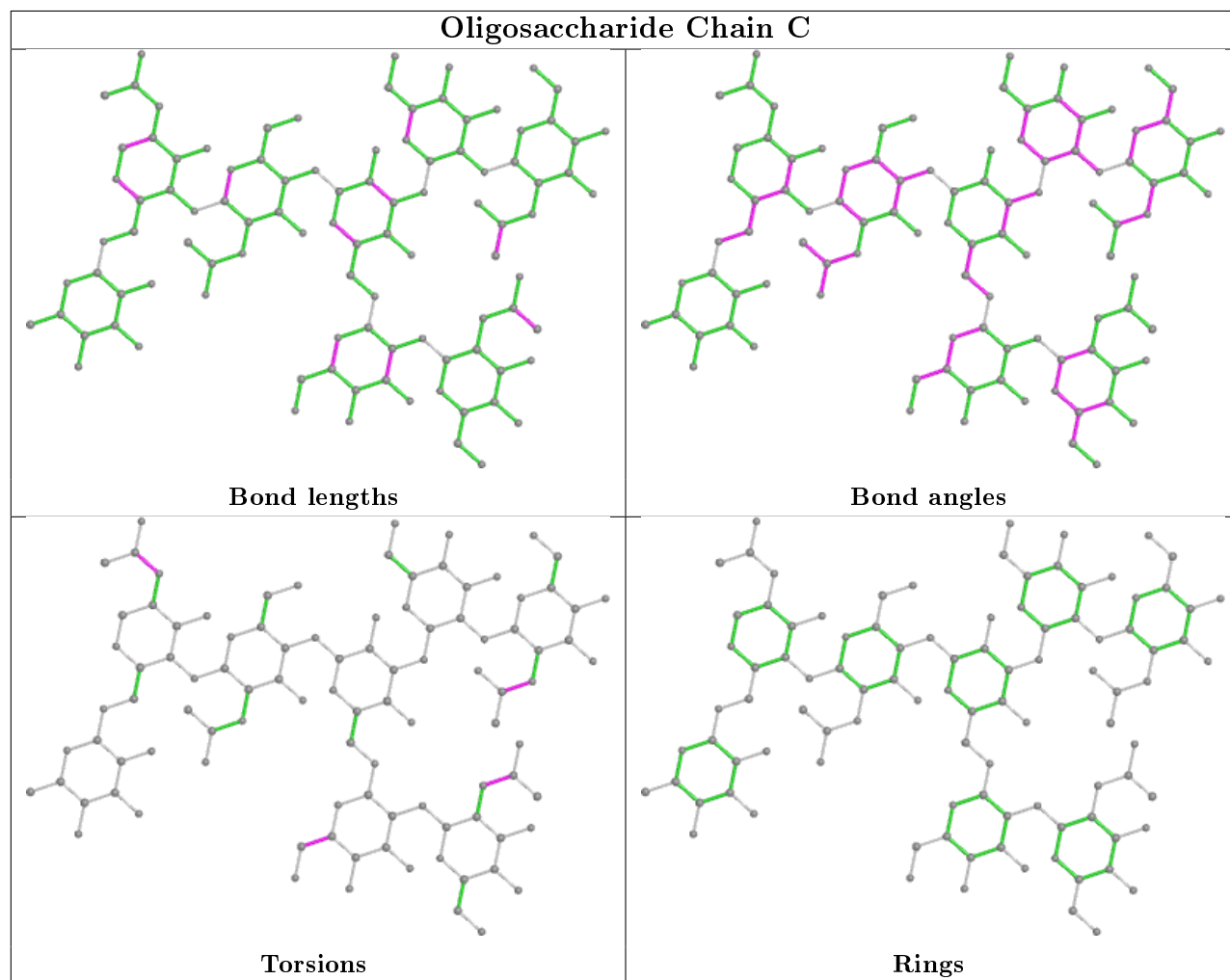
Mol	Chain	Res	Type	Atoms
2	D	4	MAN	C4-C5-C6-O6
2	C	7	NAG	C8-C7-N2-C2
2	C	7	NAG	O7-C7-N2-C2
2	D	7	NAG	C8-C7-N2-C2
2	D	7	NAG	O7-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	4	MAN	O5-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6

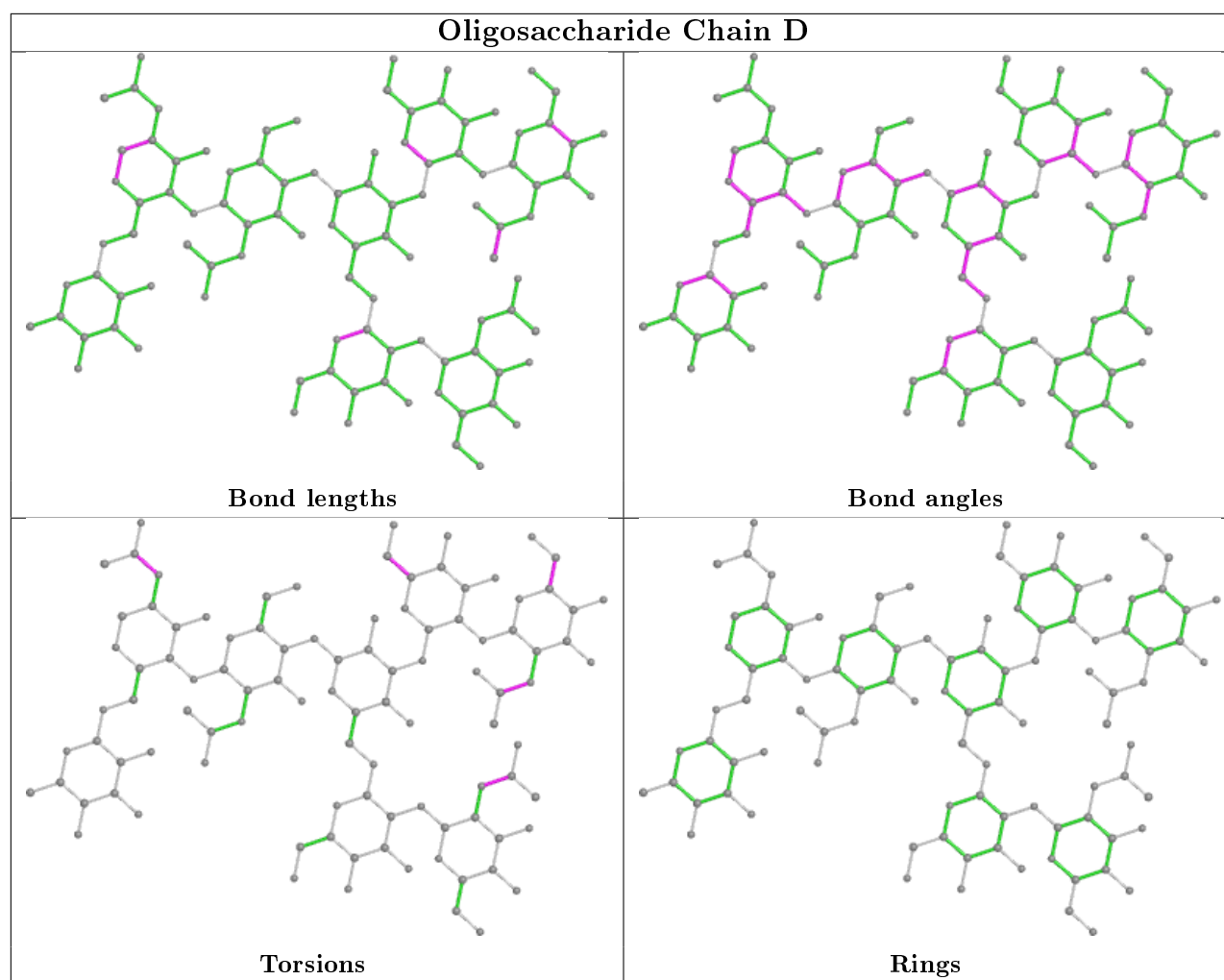
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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





5.6 Ligand geometry [i](#)

1 ligand is 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	X12	B	446	-	152,155,155	0.96	3 (1%)	198,205,205	1.16	14 (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	X12	B	446	-	-	69/191/193/193	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	446	X12	CB2-NBK	5.22	1.53	1.32
3	B	446	X12	CBG-NBH	5.01	1.57	1.46
3	B	446	X12	CB2-NBH	2.45	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	446	X12	CBH-NBG-CBX	6.21	134.99	121.67
3	B	446	X12	CBD-CB1-NAV	3.79	121.41	116.15
3	B	446	X12	CDG-NDF-CDV	3.55	130.94	121.89
3	B	446	X12	CAT-NAU-C	3.40	128.66	122.59
3	B	446	X12	CAW-NAV-CB1	3.36	130.46	121.89
3	B	446	X12	CAP-NAO-CBE	3.31	128.76	121.67
3	B	446	X12	CBT-CBX-NBG	3.15	123.27	116.48
3	B	446	X12	NBJ-CB2-NBH	-3.07	112.11	119.19
3	B	446	X12	CCU-NCT-CDK	2.94	127.97	121.67
3	B	446	X12	CB5-NBW-CCN	2.84	127.76	121.67
3	B	446	X12	CDN-CDV-NDF	2.34	119.40	116.15
3	B	446	X12	CBI-CBH-NBG	2.03	115.06	110.79
3	B	446	X12	CBQ-CBH-NBG	-2.02	105.67	111.16
3	B	446	X12	CAY-NAX-CBQ	2.01	125.98	121.67

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	446	X12	NBS-CBT-CBU-CBW
3	B	446	X12	NBS-CBT-CBU-OBV
3	B	446	X12	CBX-CBT-CBU-CBW
3	B	446	X12	CBX-CBT-CBU-OBV
3	B	446	X12	CAV-CAP-NAO-CBE
3	B	446	X12	CDD-CCU-CCV-CCW
3	B	446	X12	CBF-CB3-CBD-NBC
3	B	446	X12	CBF-CB3-CBD-CB1
3	B	446	X12	CAS-CAT-NAU-C

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Mol	Chain	Res	Type	Atoms
3	B	446	X12	NCT-CCU-CCV-CCW
3	B	446	X12	CAQ-CAR-CAS-CAT
3	B	446	X12	CCV-CCU-CDD-ODE
3	B	446	X12	CCV-CCU-CDD-NBD
3	B	446	X12	NAO-CAP-CAQ-CAR
3	B	446	X12	N-CA-CB-CAD
3	B	446	X12	CAD-CAE-CAF-NAG
3	B	446	X12	CAV-CAP-CAQ-CAR
3	B	446	X12	C-CA-CB-CAD
3	B	446	X12	CBI-CBH-NBG-CBX
3	B	446	X12	CA-C-NAU-CAT
3	B	446	X12	CBA-CBB-CBC-NBD
3	B	446	X12	CDG-CDK-NCT-CCU
3	B	446	X12	CDN-CDV-NDF-CDG
3	B	446	X12	NBW-CB5-CBY-CBZ
3	B	446	X12	CBD-CB1-NAV-CAW
3	B	446	X12	CCQ-CC5-NCI-CCJ
3	B	446	X12	OBY-CBX-NBG-CBH
3	B	446	X12	ODL-CDK-NCT-CCU
3	B	446	X12	ODW-CDV-NDF-CDG
3	B	446	X12	OBM-CB1-NAV-CAW
3	B	446	X12	OCO-CCN-NBW-CB5
3	B	446	X12	OCZ-CC5-NCI-CCJ
3	B	446	X12	CA4-CAK-CAL-CAM
3	B	446	X12	CBT-CBX-NBG-CBH
3	B	446	X12	CCJ-CCN-NBW-CB5
3	B	446	X12	O-C-NAU-CAT
3	B	446	X12	CBY-CB5-CCG-OCH
3	B	446	X12	CDO-CDP-CDQ-NDR
3	B	446	X12	CDN-CDO-CDP-CDQ
3	B	446	X12	CBD-CB3-CBF-CBG
3	B	446	X12	CBY-CB5-CCG-NAG
3	B	446	X12	CAP-CAQ-CAR-CAS
3	B	446	X12	CAZ-CAY-NAX-CBQ
3	B	446	X12	NAJ-CAK-CAL-CAM
3	B	446	X12	CCQ-CCR-CCS-CCT
3	B	446	X12	CBH-CBI-CBJ-CBK
3	B	446	X12	CAZ-CBA-CBB-CBC
3	B	446	X12	CBH-CBI-CBJ-CBP
3	B	446	X12	CAE-CAD-CB-CA
3	B	446	X12	CCG-CB5-CBY-CBZ
3	B	446	X12	C-CA-N-CA4

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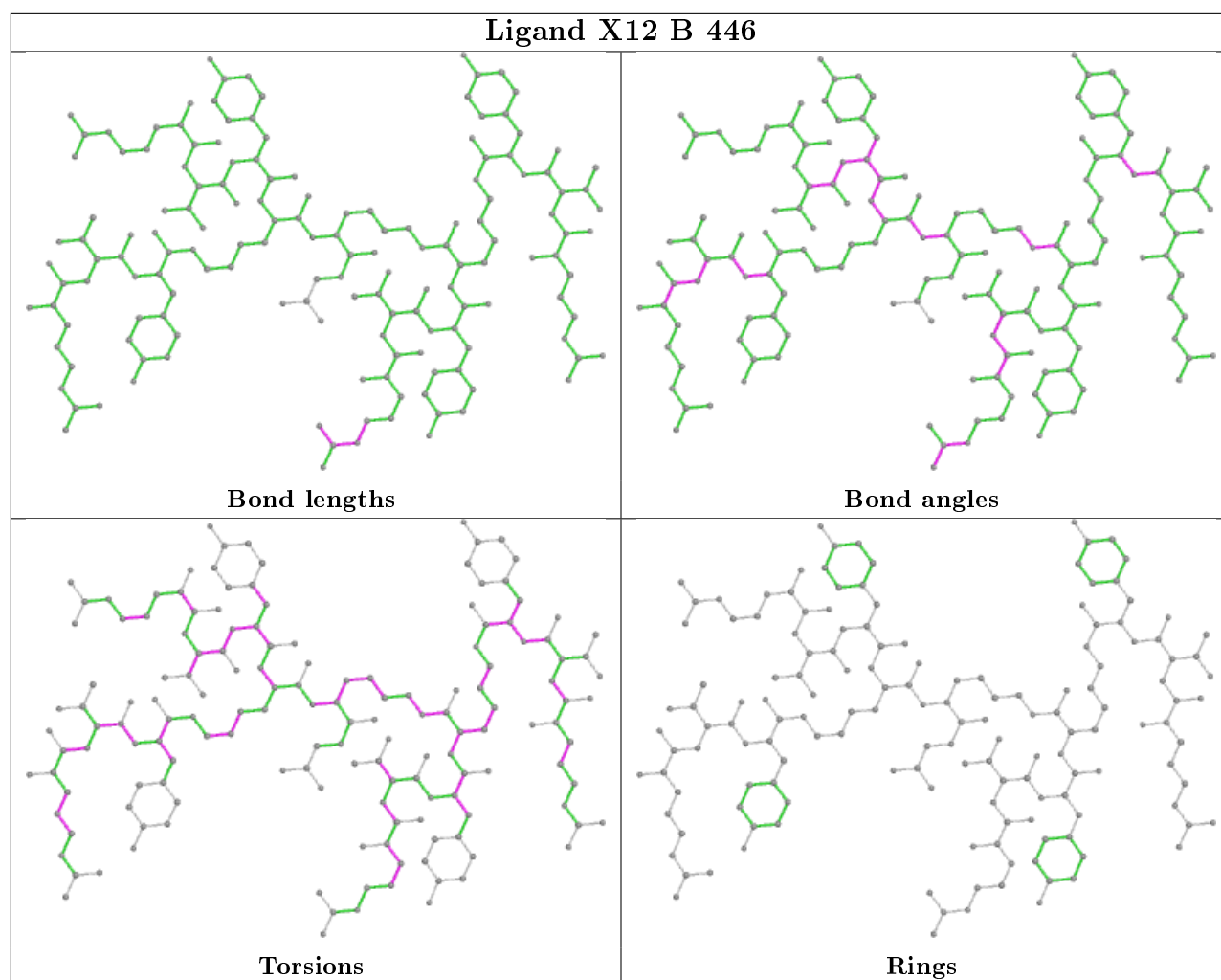
Mol	Chain	Res	Type	Atoms
3	B	446	X12	OAU-CA4-CAK-CAL
3	B	446	X12	N-CA4-CAK-CAL
3	B	446	X12	OAU-CA4-CAK-NAJ
3	B	446	X12	N-CA4-CAK-NAJ
3	B	446	X12	CCB-CCC-CCD-NCE
3	B	446	X12	CBQ-CBH-NBG-CBX
3	B	446	X12	CB4-CAW-CAX-OAY
3	B	446	X12	NBS-CBT-CBX-OBY
3	B	446	X12	CCB-CCA-CCI-NBS
3	B	446	X12	CCG-CB5-NBW-CCN
3	B	446	X12	NBW-CB5-CCG-OCH
3	B	446	X12	NCT-CCU-CDD-ODE
3	B	446	X12	NCT-CCU-CDD-NBD
3	B	446	X12	CBI-CBH-CBQ-OBX
3	B	446	X12	NBW-CB5-CCG-NAG
3	B	446	X12	NBS-CBT-CBX-NBG
3	B	446	X12	CBI-CBH-CBQ-NAX
3	B	446	X12	NDF-CDG-CDK-ODL

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	446	X12	13	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	210/210 (100%)	0.73	24 (11%) 5 7	65, 71, 79, 86	0
1	B	209/210 (99%)	1.36	55 (26%) 0 0	65, 72, 78, 84	0
All	All	419/420 (99%)	1.04	79 (18%) 1 1	65, 72, 79, 86	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	10.3
1	A	444	SER	6.7
1	A	445	PRO	6.6
1	B	366	THR	6.4
1	B	330	ALA	6.2
1	B	240	VAL	6.1
1	B	368	LEU	5.8
1	B	300	TYR	5.8
1	B	299	THR	5.0
1	B	351	LEU	4.9
1	B	297	ASN	4.8
1	B	326	LYS	4.8
1	B	367	CYS	4.5
1	B	295	GLN	4.4
1	B	407	TYR	4.4
1	B	406	LEU	4.4
1	B	323	VAL	4.3
1	B	281	GLY	4.3
1	A	366	THR	4.3
1	B	408	SER	4.3
1	A	368	LEU	4.2
1	B	278	TYR	4.2
1	B	267	SER	4.1
1	A	407	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	369	VAL	3.9
1	B	238	PRO	3.9
1	B	324	SER	3.8
1	B	236	GLY	3.8
1	B	270	ASP	3.7
1	B	444	SER	3.7
1	B	379	VAL	3.7
1	A	365	LEU	3.6
1	B	327	ALA	3.6
1	A	355[A]	ARG	3.5
1	B	365	LEU	3.5
1	B	301[A]	ARG	3.3
1	A	269	GLU	3.3
1	B	302	VAL	3.2
1	B	427	VAL	3.1
1	A	369	VAL	3.1
1	B	266	VAL	3.0
1	B	364	SER	3.0
1	A	364	SER	3.0
1	B	333	GLU	3.0
1	B	321	CYS	3.0
1	B	329	PRO	2.9
1	B	261	CYS	2.9
1	A	367	CYS	2.8
1	B	273	VAL	2.8
1	B	349	TYR	2.8
1	B	275	PHE	2.8
1	B	358	LEU	2.7
1	B	409	LYS	2.7
1	A	263	VAL	2.7
1	B	262	VAL	2.7
1	B	237	GLY	2.7
1	A	408	SER	2.7
1	B	239	SER	2.6
1	A	242	LEU	2.5
1	B	263	VAL	2.5
1	A	328	LEU	2.4
1	A	351	LEU	2.4
1	A	323	VAL	2.4
1	A	319	TYR	2.4
1	B	386	GLN	2.4
1	A	419	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	280	ASP	2.3
1	B	298	SER	2.3
1	B	426	SER	2.3
1	A	262	VAL	2.3
1	B	274	LYS	2.3
1	B	282	VAL	2.3
1	B	271	PRO	2.2
1	A	350	THR	2.2
1	A	423	PHE	2.2
1	B	269	GLU	2.2
1	B	410	LEU	2.2
1	A	313	TRP	2.1
1	A	330	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.59	0.47	62,68,71,71	0
2	NAG	D	1	14/15	0.67	0.58	59,65,66,68	0
2	NAG	D	5	14/15	0.67	0.45	76,78,79,79	0
2	NAG	C	5	14/15	0.78	0.30	82,86,89,90	0
2	NAG	C	7	14/15	0.83	0.20	65,69,73,74	0
2	FUC	D	8	10/11	0.83	0.63	69,70,71,71	0
2	FUC	C	8	10/11	0.84	0.31	71,75,75,76	0
2	BMA	D	3	11/12	0.85	0.40	62,65,66,68	0
2	MAN	D	6	11/12	0.88	0.28	65,67,69,70	0
2	MAN	C	4	11/12	0.89	0.24	64,68,72,77	0
2	MAN	D	4	11/12	0.90	0.23	61,64,67,72	0
2	NAG	D	7	14/15	0.91	0.33	64,66,68,70	0
2	BMA	C	3	11/12	0.91	0.15	64,68,71,71	0
2	NAG	C	1	14/15	0.92	0.14	66,69,74,79	0
2	MAN	C	6	11/12	0.94	0.16	66,69,70,72	0

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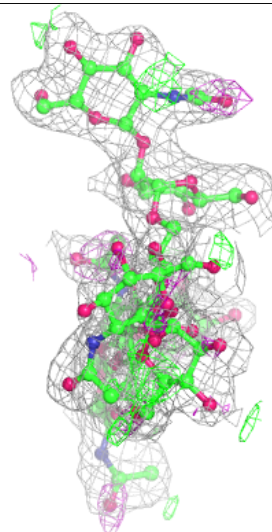
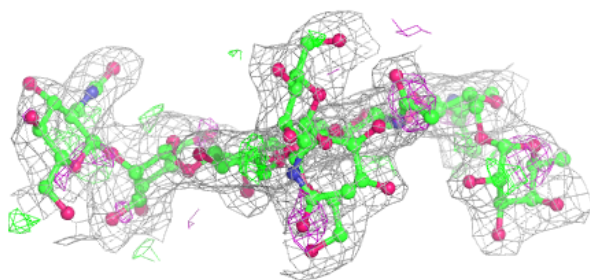
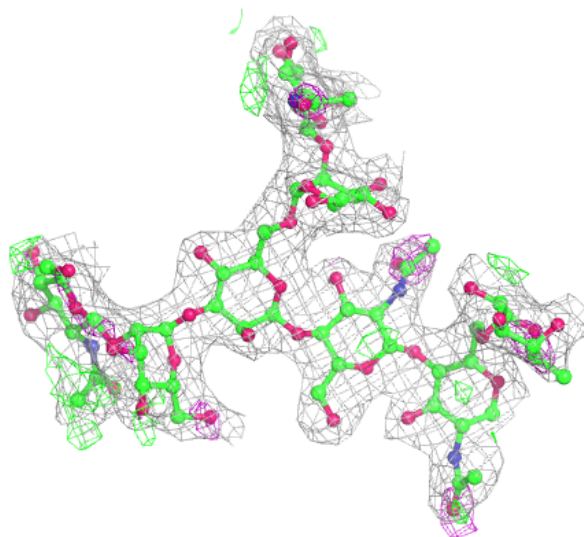
Continued from previous page...

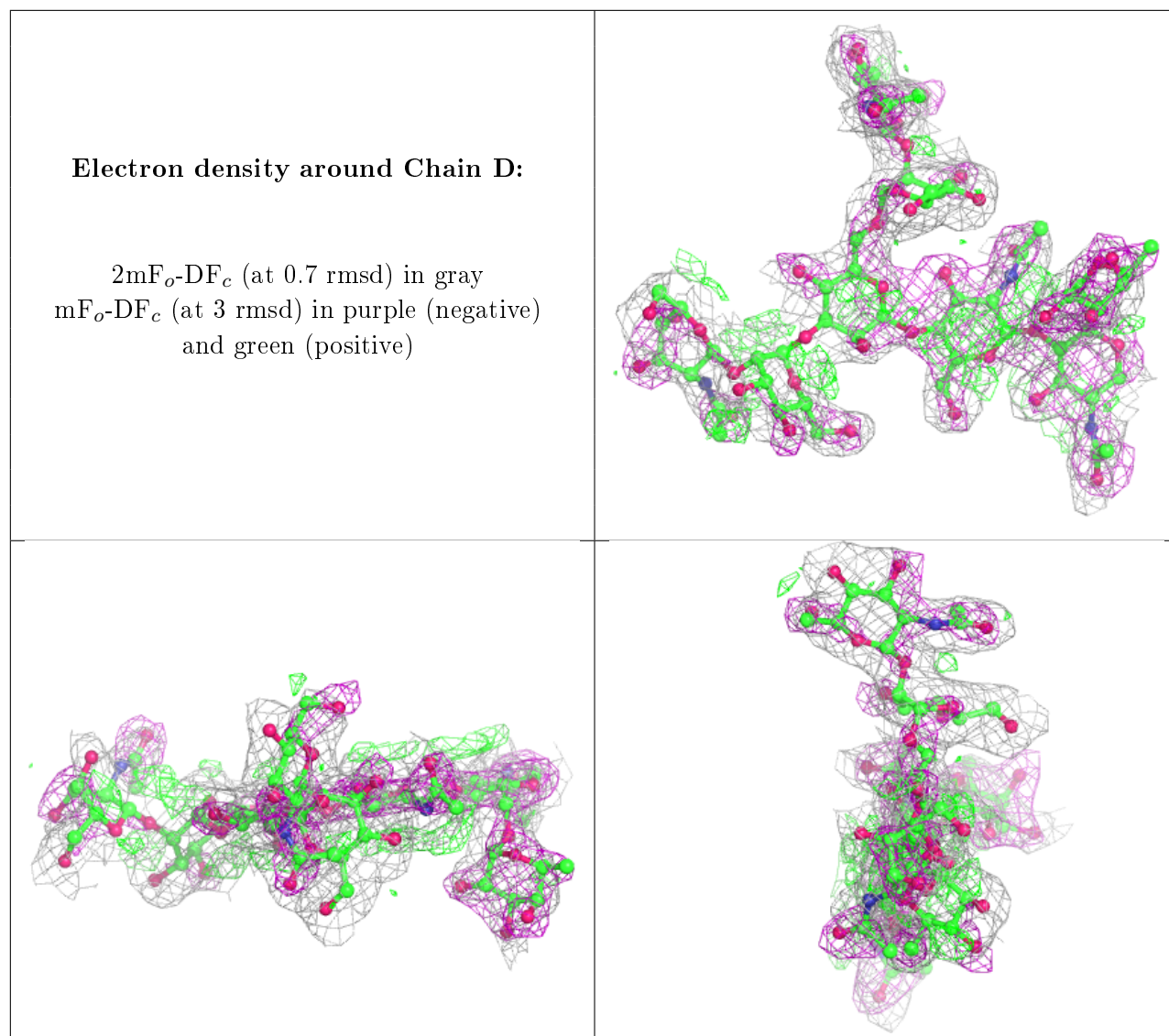
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.95	0.15	67,69,70,73	0

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 ⓘ

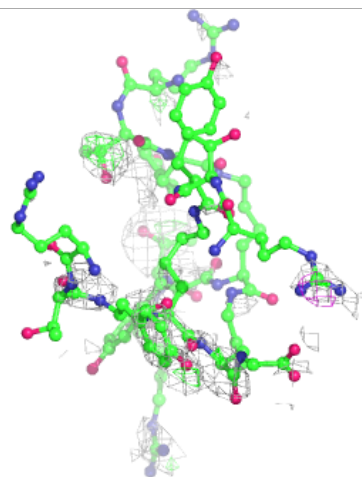
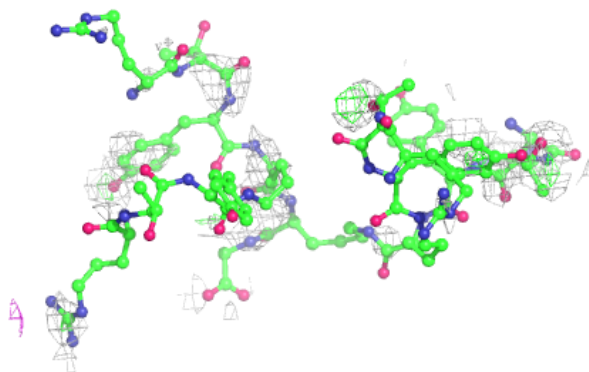
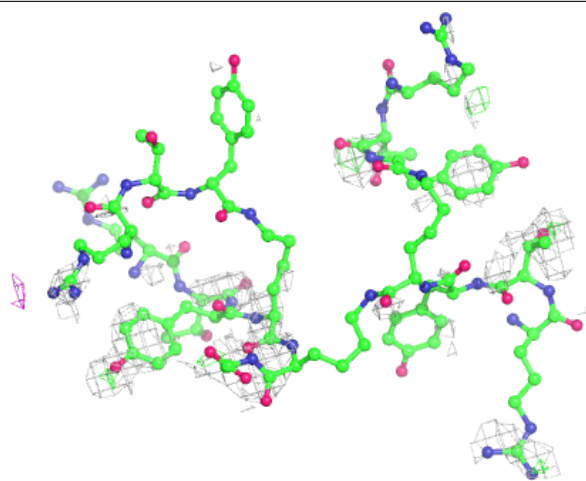
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	X12	B	446	152/152	0.25	0.72	51,79,83,83	152

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 X12 B 446:

$2mF_o-DF_c$ (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.