



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:55 PM UTC

PDB ID : 5O4G / pdb_00005o4g
Title : HER2 in complex with Fab MF3958
Authors : De Nardis, C.; Gros, P.
Deposited on : 2017-05-29
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

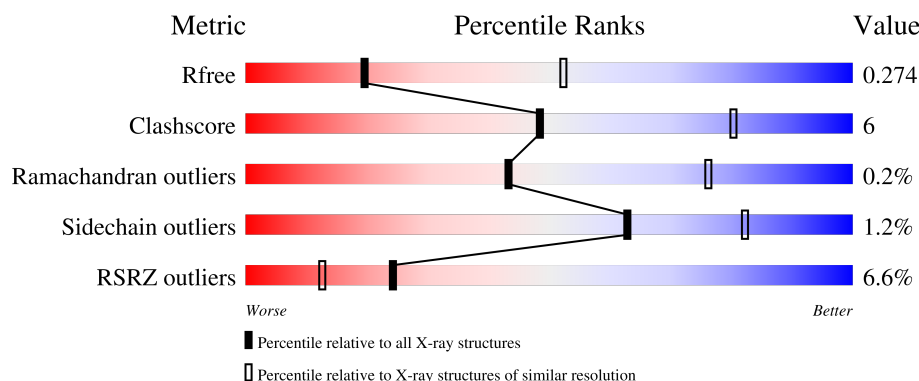
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 ≥ 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	C	606	12% 75% 11% 13%
2	A	214	12% 90% 9%
3	B	247	12% 71% 16% 13%
4	D	6	50% 50%
5	E	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7472 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	530	Total	C	N	O	S	0	0	0
			4100	2549	740	767	44			

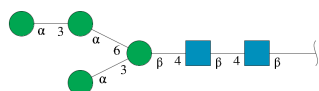
- Molecule 2 is a protein called MF3958 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	214	Total	C	N	O	S	0	0	0
			1636	1020	273	337	6			

- Molecule 3 is a protein called MF3958 FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	216	Total	C	N	O	S	0	0	0
			1622	1033	265	319	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

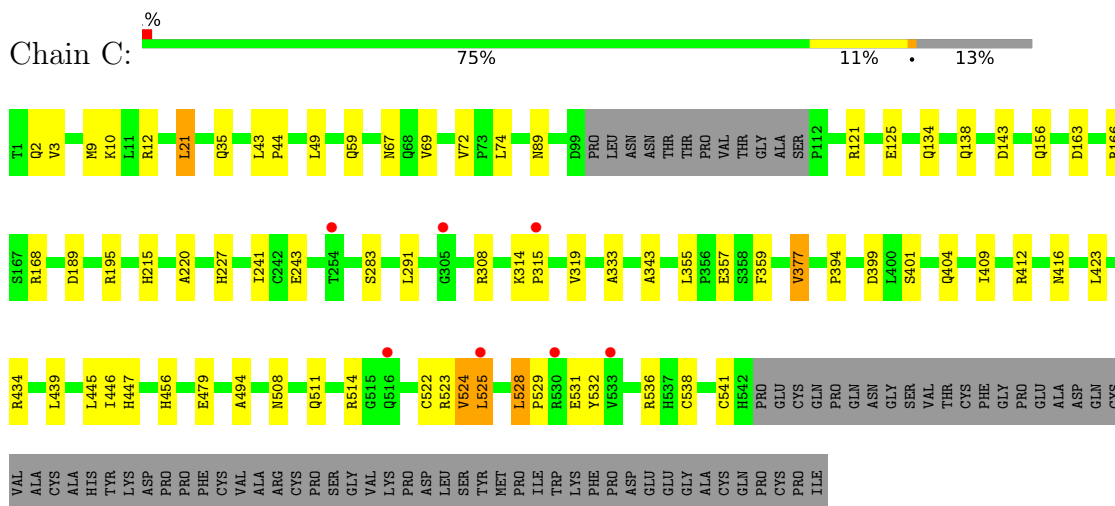


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

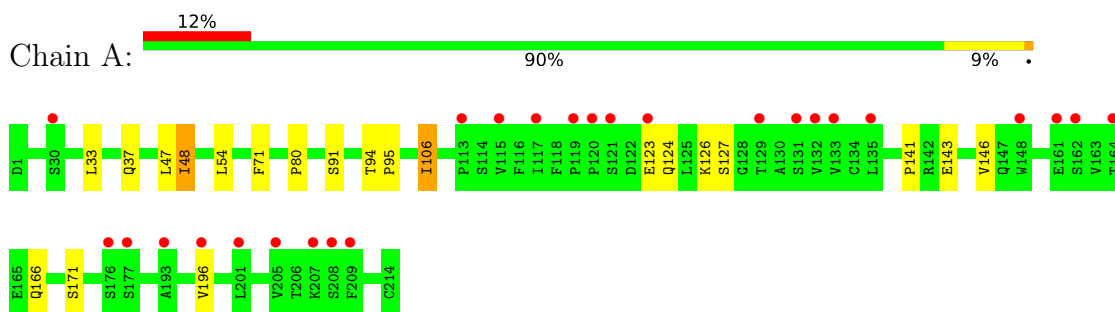
3 Residue-property plots

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.

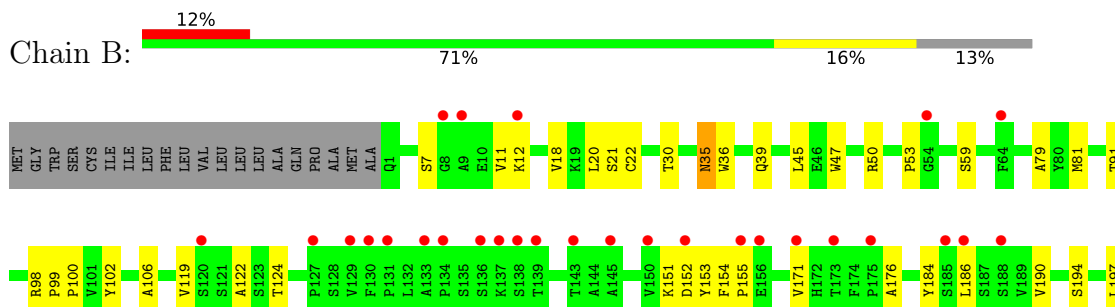
• Molecule 1: Receptor tyrosine-protein kinase erbB-2

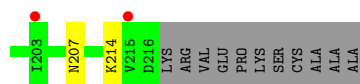


• Molecule 2: MF3958 FAB light chain



• Molecule 3: MF3958 FAB heavy chain





- Molecule 4: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D:
The bar chart for Chain D shows occupancy for residues T203, N207, K214, Y215, and D216. The bar is divided into two segments: a green segment representing 50% occupancy and a yellow segment representing 50% occupancy.



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

Chain E:
The bar chart for Chain E shows occupancy for residues NAG1 and NAG2. The bar is a single green segment representing 100% occupancy.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.79Å 113.50Å 113.49Å 90.00° 101.92° 90.00°	Depositor
Resolution (Å)	35.84 – 3.00 35.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.84-3.00) 97.3 (35.84-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.229 , 0.271 0.234 , 0.274	Depositor DCC
R_{free} test set	1533 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7472	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: BMA, MAN, NAG

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	C	0.28	0/4192	0.73	4/5698 (0.1%)
2	A	0.25	0/1671	0.67	0/2268
3	B	0.26	0/1667	0.68	0/2279
All	All	0.27	0/7530	0.71	4/10245 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	528	LEU	CA-C-N	8.43	130.38	119.84
1	C	528	LEU	C-N-CA	8.43	130.38	119.84
1	C	10	LYS	CB-CA-C	-5.62	110.07	116.54
1	C	89	ASN	CB-CA-C	-5.23	100.97	109.13

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	C	4100	0	3952	43	0
2	A	1636	0	1588	13	0
3	B	1622	0	1573	26	0
4	D	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	25	0	0
6	C	14	0	13	0	0
All	All	7472	0	7212	81	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 6.

All (81) 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:C:522:CYS:SG	1:C:538:CYS:CB	2.16	1.32
1:C:522:CYS:CB	1:C:538:CYS:SG	2.51	0.99
2:A:166:GLN:HE21	2:A:171:SER:HB3	1.54	0.71
1:C:522:CYS:SG	1:C:538:CYS:SG	0.68	0.68
1:C:283:SER:HB2	1:C:308:ARG:HG2	1.75	0.68
2:A:143:GLU:N	2:A:143:GLU:OE2	2.27	0.68
3:B:30:THR:HA	3:B:53:PRO:HB2	1.77	0.67
1:C:511:GLN:HA	1:C:536:ARG:HH21	1.61	0.66
3:B:98:ARG:NH1	3:B:99:PRO:O	2.29	0.64
1:C:143:ASP:OD1	1:C:166:ARG:NH2	2.31	0.64
1:C:523:ARG:HE	1:C:528:LEU:H	1.50	0.59
3:B:151:LYS:NZ	3:B:152:ASP:OD2	2.31	0.59
1:C:2:GLN:HG3	1:C:3:VAL:HG23	1.86	0.58
2:A:123:GLU:HG3	2:A:126:LYS:HE2	1.84	0.57
2:A:146:VAL:HG22	2:A:196:VAL:HG22	1.86	0.57
3:B:39:GLN:HB2	3:B:45:LEU:HD23	1.87	0.57
3:B:12:LYS:HG3	3:B:18:VAL:HB	1.87	0.57
1:C:125:GLU:HB2	1:C:220:ALA:HA	1.87	0.56
2:A:37:GLN:HB2	2:A:47:LEU:HD11	1.89	0.55
1:C:121:ARG:NH1	1:C:189:ASP:OD1	2.40	0.54
1:C:227:HIS:CD2	1:C:241:ILE:HG23	2.43	0.53
1:C:514:ARG:NH1	1:C:531:GLU:OE1	2.42	0.53
3:B:22:CYS:HB3	3:B:79:ALA:HB3	1.91	0.53
1:C:522:CYS:SG	1:C:538:CYS:HB3	2.40	0.53
3:B:176:ALA:HB2	3:B:186:LEU:HD23	1.92	0.52
1:C:494:ALA:HB3	1:C:508:ASN:HB3	1.90	0.52
1:C:12:ARG:NH1	1:C:416:ASN:OD1	2.37	0.52
3:B:171:VAL:HG22	3:B:190:VAL:HG22	1.92	0.52
1:C:67:ASN:HB3	1:C:69:VAL:HG22	1.91	0.51
3:B:194:SER:HA	3:B:197:LEU:HG	1.92	0.51
2:A:141:PRO:HB2	2:A:143:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:HIS:HB2	1:C:479:GLU:OE2	2.11	0.50
1:C:21:LEU:HD23	1:C:43:LEU:HD22	1.94	0.49
3:B:36:TRP:CE2	3:B:81:MET:HB2	2.47	0.49
3:B:7:SER:OG	3:B:21:SER:OG	2.29	0.49
2:A:91:SER:HB2	3:B:106:ALA:HB3	1.95	0.49
1:C:134:GLN:HA	1:C:163:ASP:HB3	1.94	0.48
3:B:176:ALA:HB1	3:B:184:TYR:HB3	1.94	0.48
1:C:399:ASP:OD2	1:C:401:SER:HB3	2.15	0.47
3:B:50:ARG:HG2	3:B:59:SER:HB2	1.96	0.47
1:C:291:LEU:HB3	1:C:412:ARG:HB3	1.97	0.47
1:C:333:ALA:HB2	1:C:355:LEU:HG	1.96	0.47
3:B:207:ASN:CG	3:B:214:LYS:HZ3	2.22	0.47
1:C:35:GLN:OE1	1:C:59:GLN:NE2	2.48	0.47
1:C:156:GLN:HB3	1:C:195:ARG:HH22	1.79	0.47
3:B:151:LYS:HG2	3:B:152:ASP:OD2	2.16	0.46
3:B:124:THR:HG23	3:B:155:PRO:HG2	1.97	0.46
1:C:524:VAL:HG13	1:C:525:LEU:HG	1.96	0.45
1:C:241:ILE:HG22	1:C:243:GLU:HG3	1.97	0.45
3:B:91:THR:HG22	3:B:119:VAL:H	1.82	0.45
1:C:409:ILE:HB	1:C:439:LEU:HD23	1.99	0.45
1:C:404:GLN:OE1	1:C:434:ARG:NH1	2.43	0.45
3:B:122:ALA:HB3	3:B:154:PHE:CZ	2.52	0.45
2:A:124:GLN:O	2:A:127:SER:OG	2.34	0.44
1:C:343:ALA:HA	1:C:377:VAL:HG13	1.98	0.43
1:C:423:LEU:HB2	1:C:446:ILE:HG23	2.01	0.43
1:C:291:LEU:HD22	1:C:412:ARG:HG2	1.99	0.43
1:C:43:LEU:HA	1:C:44:PRO:HD3	1.89	0.43
3:B:47:TRP:CZ2	3:B:50:ARG:HD2	2.54	0.43
1:C:359:PHE:CZ	1:C:394:PRO:HD3	2.54	0.42
1:C:43:LEU:HD13	1:C:49:LEU:HD21	2.01	0.42
1:C:215:HIS:CG	1:C:227:HIS:HB3	2.54	0.42
2:A:94:THR:HA	2:A:95:PRO:HA	1.89	0.42
2:A:106:ILE:HD11	2:A:171:SER:OG	2.19	0.42
3:B:99:PRO:HB2	3:B:102:TYR:O	2.20	0.42
2:A:80:PRO:HA	2:A:106:ILE:HD13	2.01	0.42
1:C:314:LYS:HG3	1:C:315:PRO:HD2	2.00	0.42
1:C:523:ARG:HG3	1:C:528:LEU:HD22	2.01	0.42
2:A:33:LEU:HD22	2:A:71:PHE:CG	2.55	0.42
1:C:355:LEU:HB2	1:C:357:GLU:HG2	2.02	0.42
3:B:35:ASN:HA	3:B:50:ARG:HA	2.01	0.42
3:B:20:LEU:N	3:B:81:MET:O	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:MET:HB3	1:C:416:ASN:HB3	2.01	0.41
1:C:138:GLN:OE1	1:C:168:ARG:HD3	2.19	0.41
3:B:176:ALA:HA	3:B:186:LEU:HB3	2.03	0.41
3:B:47:TRP:HZ2	3:B:50:ARG:HD2	1.85	0.41
1:C:532:TYR:HD1	1:C:541:CYS:HB2	1.85	0.41
2:A:48:ILE:HG23	2:A:54:LEU:HA	2.02	0.41
3:B:20:LEU:O	3:B:81:MET:N	2.51	0.41
1:C:72:VAL:HG12	1:C:74:LEU:HG	2.03	0.41
1:C:445:LEU:HG	1:C:447:HIS:HD2	1.86	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	C	526/606 (87%)	492 (94%)	33 (6%)	1 (0%)	43	76
2	A	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	B	214/247 (87%)	199 (93%)	14 (6%)	1 (0%)	24	60
All	All	952/1067 (89%)	894 (94%)	56 (6%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	529	PRO
3	B	100	PRO

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	C	457/522 (88%)	452 (99%)	5 (1%)	65	83
2	A	189/189 (100%)	187 (99%)	2 (1%)	65	83
3	B	178/202 (88%)	175 (98%)	3 (2%)	53	78
All	All	824/913 (90%)	814 (99%)	10 (1%)	63	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	C	319	VAL
1	C	377	VAL
1	C	524	VAL
1	C	525	LEU
2	A	48	ILE
2	A	106	ILE
3	B	11	VAL
3	B	35	ASN
3	B	153	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	C	217	GLN
1	C	451	HIS
1	C	491	GLN
2	A	137	ASN
2	A	147	GLN
3	B	172	HIS

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 ⓘ

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$
4	NAG	D	1	1,4	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	0.74	0
4	MAN	D	4	4	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
4	MAN	D	5	4	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
4	MAN	D	6	4	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
5	NAG	E	1	5,1	14,14,15	0.37	0	17,19,21	0.40	0
5	NAG	E	2	5	14,14,15	0.19	0	17,19,21	0.44	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	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	MAN	C1-O5-C5	2.54	115.59	112.19
4	D	5	MAN	O2-C2-C3	-2.32	105.35	110.15
4	D	6	MAN	O2-C2-C3	-2.22	105.56	110.15
4	D	4	MAN	C1-O5-C5	2.20	115.14	112.19
4	D	4	MAN	O2-C2-C3	-2.15	105.70	110.15
4	D	5	MAN	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

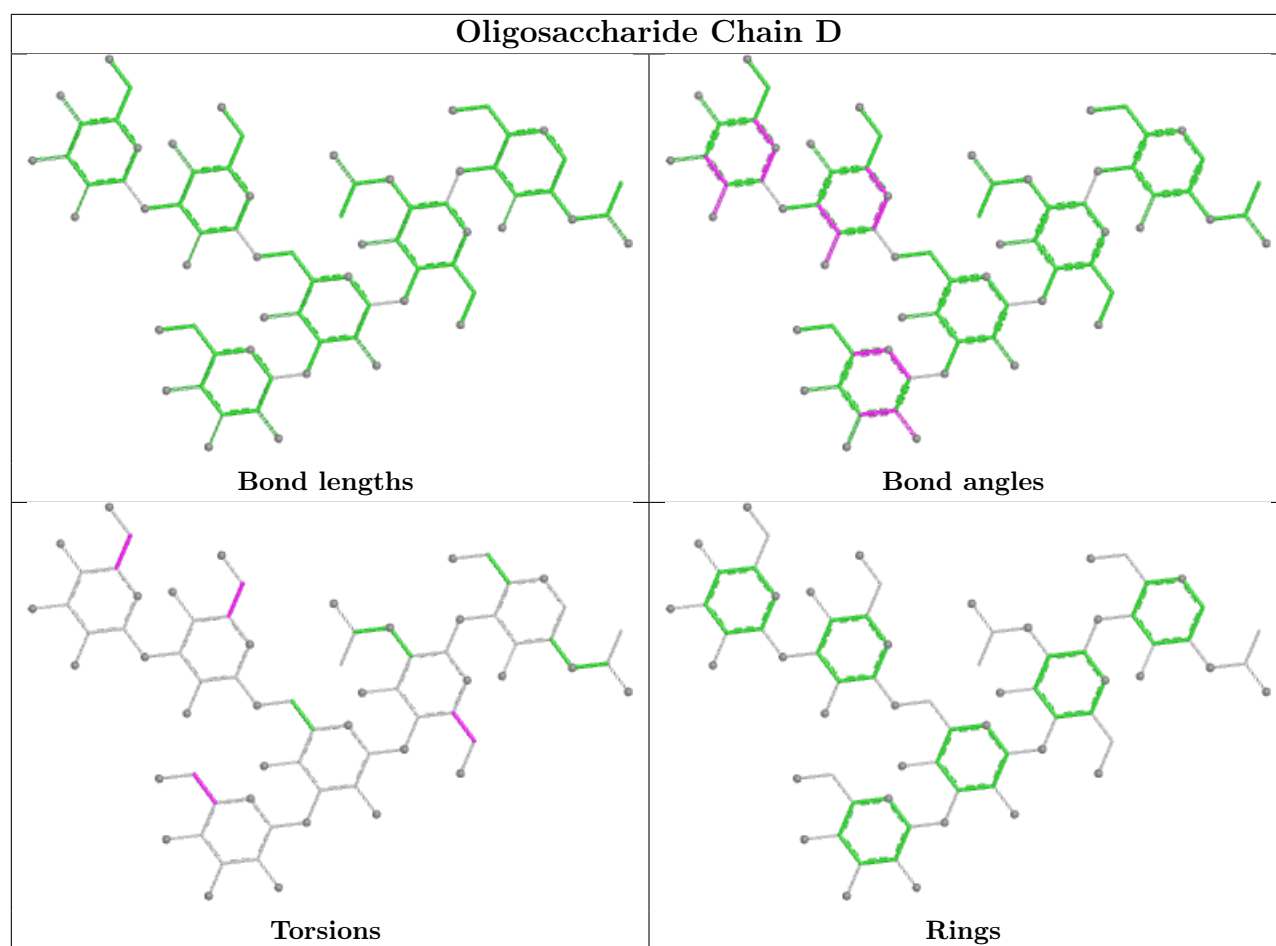
All (7) torsion outliers are listed below:

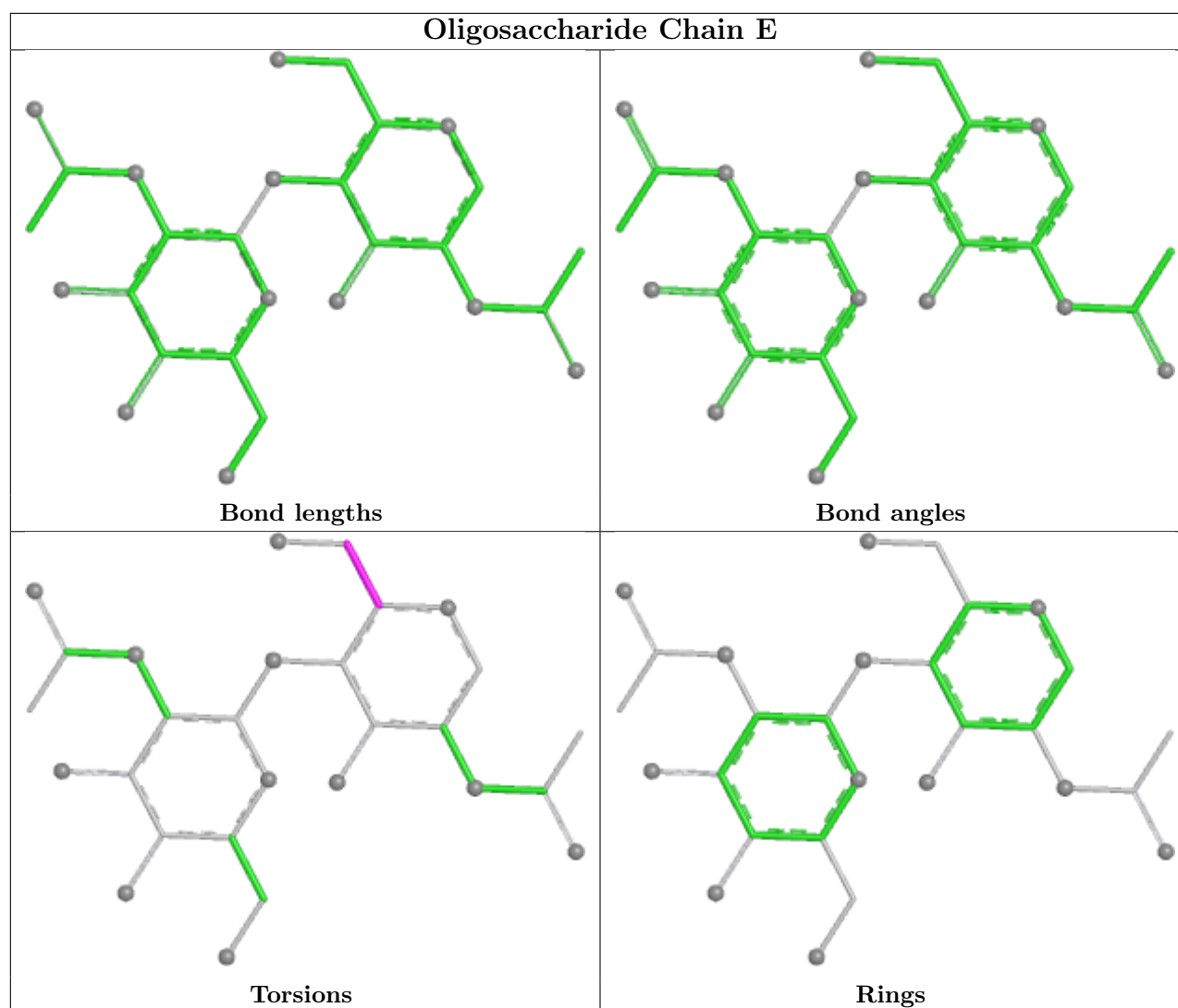
Mol	Chain	Res	Type	Atoms
4	D	6	MAN	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
6	NAG	C	707	1	14,14,15	0.22	0	17,19,21	0.42	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
6	NAG	C	707	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	707	NAG	O5-C5-C6-O6
6	C	707	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	C	530/606 (87%)	-0.08	7 (1%) 75 53	22, 47, 111, 138	0
2	A	214/214 (100%)	0.93	26 (12%) 8 5	65, 108, 173, 181	0
3	B	216/247 (87%)	1.02	30 (13%) 6 4	45, 111, 182, 194	0
All	All	960/1067 (89%)	0.40	63 (6%) 24 12	22, 73, 164, 194	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	138	SER	5.1
2	A	30	SER	4.5
3	B	131	PRO	3.9
2	A	129	THR	3.6
2	A	201	LEU	3.6
3	B	9	ALA	3.5
1	C	254	THR	3.2
3	B	129	VAL	3.1
2	A	207	LYS	3.1
2	A	209	PHE	2.9
3	B	186	LEU	2.8
3	B	203	ILE	2.8
2	A	115	VAL	2.7
2	A	120	PRO	2.7
2	A	121	SER	2.7
1	C	315	PRO	2.7
2	A	131	SER	2.7
3	B	137	LYS	2.7
1	C	530	ARG	2.6
3	B	155	PRO	2.6
2	A	133	VAL	2.6
3	B	139	THR	2.6
2	A	208	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	133	ALA	2.6
3	B	130	PHE	2.5
2	A	177	SER	2.5
2	A	135	LEU	2.5
2	A	113	PRO	2.5
3	B	8	GLY	2.5
2	A	205	VAL	2.5
1	C	516	GLN	2.4
2	A	132	VAL	2.4
2	A	117	ILE	2.4
2	A	119	PRO	2.4
3	B	152	ASP	2.4
3	B	120	SER	2.4
3	B	188	SER	2.4
2	A	196	VAL	2.4
3	B	215	VAL	2.3
2	A	161	GLU	2.3
1	C	533	VAL	2.3
3	B	175	PRO	2.3
3	B	54	GLY	2.3
3	B	185	SER	2.3
3	B	127	PRO	2.2
2	A	148	TRP	2.2
1	C	525	LEU	2.2
3	B	173	THR	2.2
3	B	64	PHE	2.2
3	B	171	VAL	2.1
3	B	134	PRO	2.1
3	B	143	THR	2.1
2	A	162	SER	2.1
2	A	176	SER	2.1
3	B	156	GLU	2.1
2	A	193	ALA	2.1
3	B	136	SER	2.1
3	B	150	VAL	2.0
2	A	164	THR	2.0
3	B	145	ALA	2.0
1	C	305	GLY	2.0
2	A	123	GLU	2.0
3	B	12	LYS	2.0

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](#)

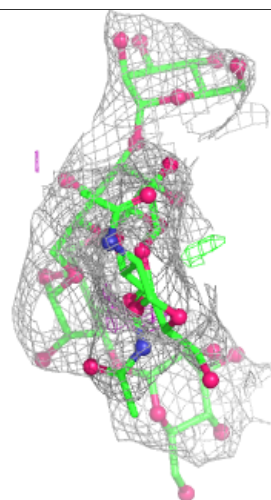
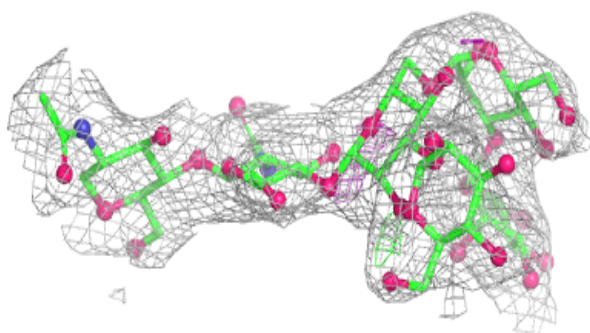
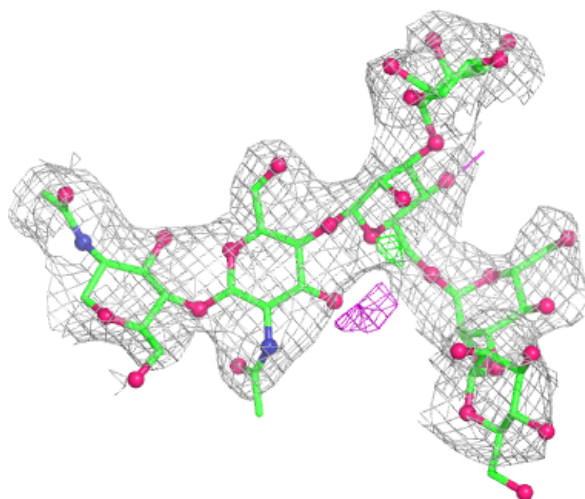
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

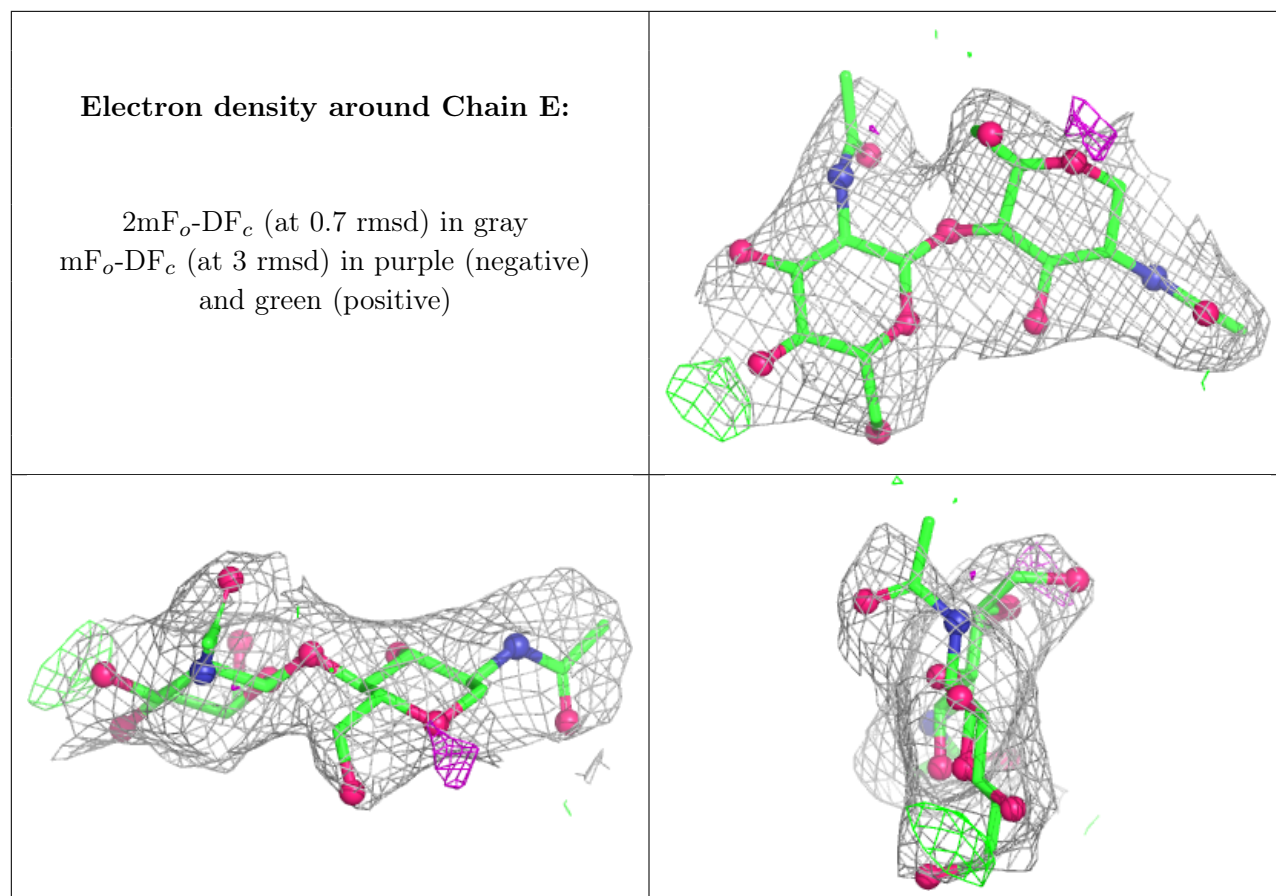
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	1	14/15	0.64	0.13	80,98,108,111	0
4	BMA	D	3	11/12	0.71	0.11	83,104,111,112	0
5	NAG	E	2	14/15	0.74	0.12	74,85,102,103	0
4	NAG	D	2	14/15	0.77	0.12	87,96,105,111	0
4	MAN	D	4	11/12	0.78	0.10	90,96,111,116	0
4	MAN	D	6	11/12	0.79	0.10	82,103,114,115	0
4	MAN	D	5	11/12	0.80	0.13	88,102,120,121	0
5	NAG	E	1	14/15	0.91	0.09	32,59,75,76	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 D:

$2mF_o-DF_c$ (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, 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($\text{\AA}^2$)	Q<0.9
6	NAG	C	707	14/15	0.41	0.16	92,111,122,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.