



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:57 AM UTC

PDB ID : 7QVK / pdb_00007qvk
Title : NM-02 in complex with HER2-ECD
Authors : Cowan, R.; Hall, G.; Carr, M.
Deposited on : 2022-01-21
Resolution : 3.10 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

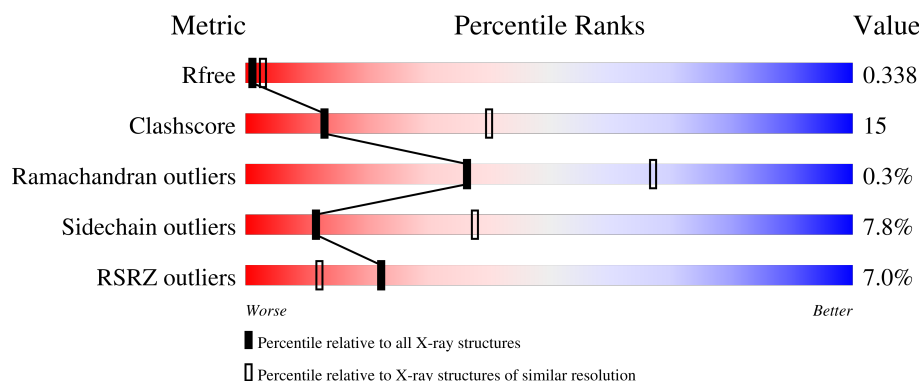
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	AAA	630	 5% 58% 21% • 20%
2	BBB	132	 9% 58% 27% 7% 8%
3	AbA	3	 33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9457 atoms, of which 4621 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	AAA	506	Total	C	H	N	O	S	122	0	0
			7621	2415	3743	692	730	41			

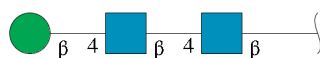
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	647	HIS	-	expression tag	UNP P04626
AAA	648	HIS	-	expression tag	UNP P04626
AAA	649	HIS	-	expression tag	UNP P04626
AAA	650	HIS	-	expression tag	UNP P04626
AAA	651	HIS	-	expression tag	UNP P04626
AAA	652	HIS	-	expression tag	UNP P04626

- Molecule 2 is a protein called NM-02.

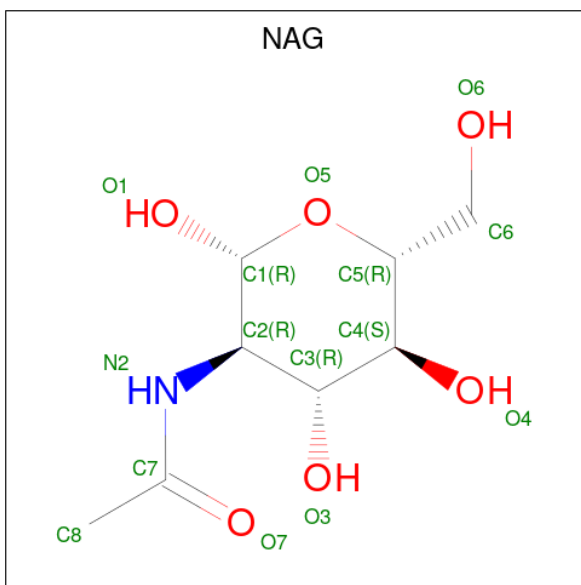
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	121	Total	C	H	N	O	S	37	0	0
			1732	555	827	151	193	6			

- Molecule 3 is an oligosaccharide called 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
3	AbA	3	Total	C	H	N	O		8	0	0
			76	22	37	2	15				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

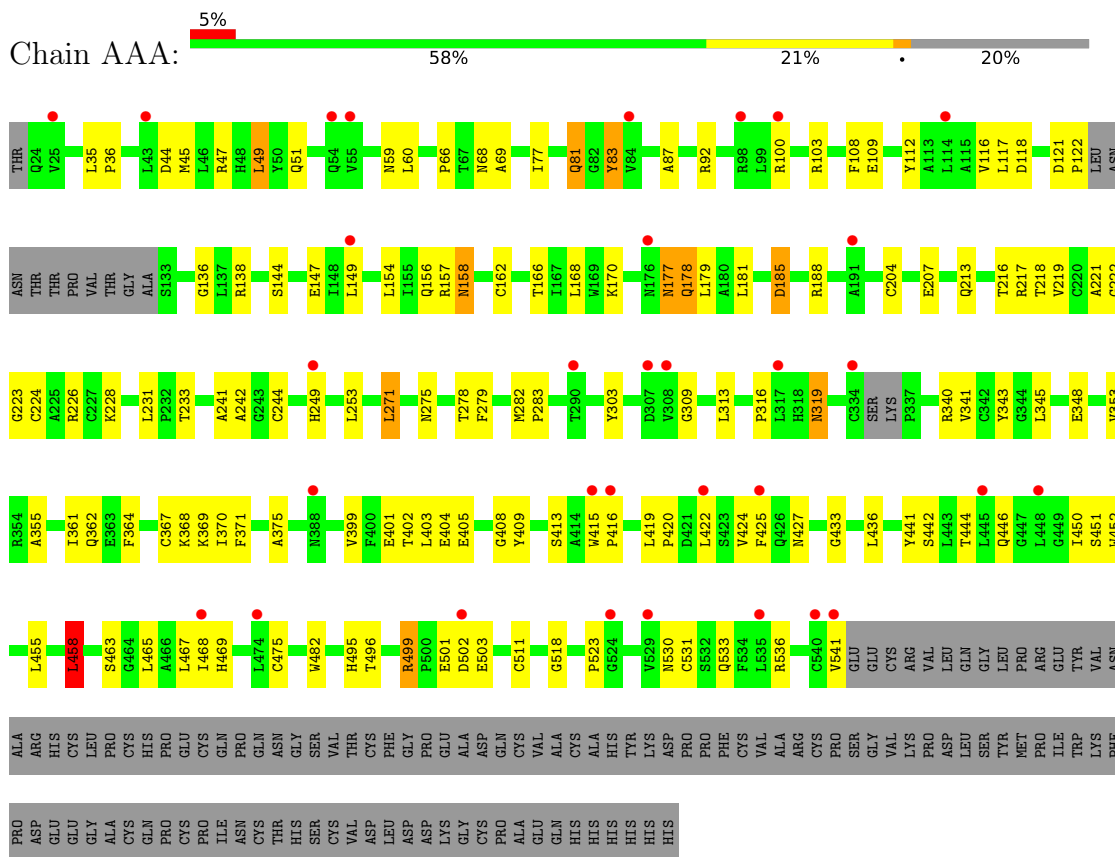


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	AAA	1	28	8	14	1	5	3	0

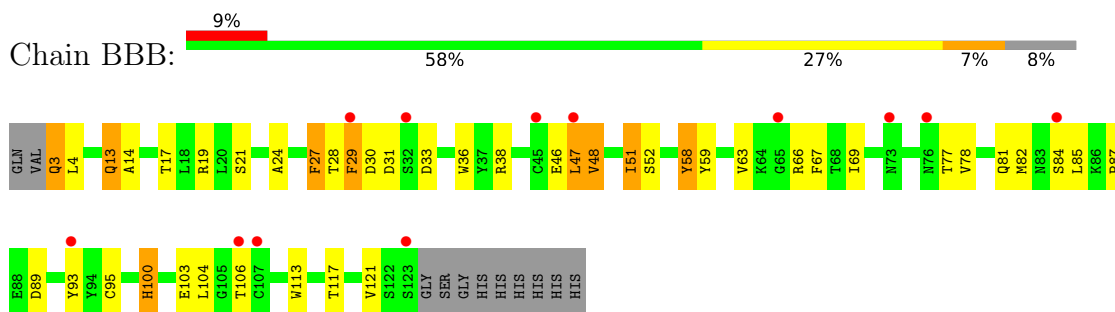
3 Residue-property plots

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: Receptor tyrosine-protein kinase erbB-2



- Molecule 2: NM-02



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AbA:  33% 67%

MAG1
MAG2
EM13

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.77Å 105.77Å 185.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.32 – 3.10 65.32 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.32-3.10) 99.9 (65.32-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.275 , 0.330 0.282 , 0.338	Depositor DCC
R_{free} test set	1186 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	95.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 90.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9457	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: NAG, BMA

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	AAA	1.03	1/3964 (0.0%)	1.39	4/5393 (0.1%)
2	BBB	1.02	0/922	1.39	4/1250 (0.3%)
All	All	1.03	1/4886 (0.0%)	1.39	8/6643 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	158	ASN	C-N	12.36	1.50	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	158	ASN	CA-C-N	15.43	136.18	119.05
1	AAA	158	ASN	C-N-CA	15.43	136.18	119.05
2	BBB	27	PHE	CB-CA-C	-5.68	99.11	110.42
1	AAA	222	GLY	N-CA-C	-5.52	108.41	115.42
1	AAA	368	LYS	N-CA-C	-5.43	106.70	113.38
2	BBB	27	PHE	CA-CB-CG	5.37	119.17	113.80
2	BBB	27	PHE	CA-C-N	5.15	130.40	121.64
2	BBB	27	PHE	C-N-CA	5.15	130.40	121.64

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	AAA	3878	3743	3708	106	2
2	BBB	905	827	821	42	2
3	AbA	39	37	34	0	0
4	AAA	14	14	13	0	0
All	All	4836	4621	4576	141	2

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 15.

All (141) 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:AAA:343:TYR:CE2	1:AAA:348:GLU:OE1	1.65	1.46
1:AAA:343:TYR:CD2	1:AAA:348:GLU:OE1	1.68	1.45
1:AAA:59:ASN:ND2	1:AAA:83:TYR:HE1	1.57	1.01
1:AAA:59:ASN:CG	1:AAA:83:TYR:HE1	1.70	0.98
1:AAA:59:ASN:CG	1:AAA:83:TYR:CE1	2.42	0.98
1:AAA:345:LEU:HD22	1:AAA:353:VAL:HG12	1.45	0.97
1:AAA:343:TYR:HD2	1:AAA:348:GLU:OE1	1.43	0.92
1:AAA:343:TYR:HE2	1:AAA:348:GLU:OE1	1.39	0.90
2:BBB:3:GLN:N	2:BBB:3:GLN:OE1	2.08	0.86
1:AAA:83:TYR:CD2	1:AAA:108:PHE:HB2	2.12	0.85
1:AAA:83:TYR:HD2	1:AAA:108:PHE:HB2	1.43	0.83
1:AAA:355:ALA:HB1	1:AAA:375:ALA:O	1.79	0.82
1:AAA:345:LEU:HD22	1:AAA:353:VAL:CG1	2.10	0.82
1:AAA:178:GLN:HE21	1:AAA:178:GLN:HA	1.46	0.81
1:AAA:112:TYR:CD1	1:AAA:154:LEU:HB2	2.19	0.78
1:AAA:408:GLY:O	1:AAA:433:GLY:HA2	1.85	0.77
1:AAA:231:LEU:CD2	2:BBB:27:PHE:HZ	1.99	0.75
1:AAA:475:CYS:SG	1:AAA:499:ARG:HD3	2.26	0.75
1:AAA:231:LEU:HD22	2:BBB:27:PHE:HZ	1.54	0.72
1:AAA:401:GLU:O	1:AAA:427:ASN:ND2	2.23	0.71
1:AAA:345:LEU:CD2	1:AAA:353:VAL:CG1	2.69	0.71
2:BBB:66:ARG:NH1	2:BBB:84:SER:O	2.26	0.69
2:BBB:13:GLN:HE21	2:BBB:13:GLN:H	1.41	0.68
1:AAA:436:LEU:HD21	1:AAA:463:SER:O	1.95	0.67
1:AAA:361:ILE:HD11	1:AAA:399:VAL:HG11	1.77	0.67
1:AAA:168:LEU:H	1:AAA:213:GLN:HE22	1.44	0.65
1:AAA:59:ASN:ND2	1:AAA:83:TYR:CE1	2.50	0.64
1:AAA:118:ASP:HA	1:AAA:157:ARG:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:147:GLU:HB2	1:AAA:242:ALA:HB2	1.80	0.64
1:AAA:468:ILE:O	1:AAA:495:HIS:HA	1.98	0.63
1:AAA:361:ILE:HD12	1:AAA:361:ILE:O	1.99	0.63
2:BBB:4:LEU:CD2	2:BBB:27:PHE:CE2	2.82	0.62
2:BBB:4:LEU:HD21	2:BBB:27:PHE:CZ	2.34	0.62
2:BBB:19:ARG:HH11	2:BBB:81:GLN:HE21	1.48	0.61
1:AAA:345:LEU:CD2	1:AAA:353:VAL:HG11	2.31	0.61
1:AAA:108:PHE:CD2	1:AAA:109:GLU:HG3	2.36	0.61
1:AAA:166:THR:CG2	1:AAA:204:CYS:O	2.50	0.60
1:AAA:45:MET:SD	1:AAA:49:LEU:HD12	2.42	0.60
1:AAA:362:GLN:HA	1:AAA:362:GLN:OE1	2.01	0.59
2:BBB:4:LEU:HD21	2:BBB:27:PHE:CE2	2.37	0.59
2:BBB:100:HIS:O	2:BBB:100:HIS:ND1	2.35	0.59
1:AAA:316:PRO:O	1:AAA:319:ASN:HB2	2.03	0.59
1:AAA:452:TRP:CE2	1:AAA:523:PRO:HD2	2.38	0.58
1:AAA:166:THR:HG21	1:AAA:204:CYS:O	2.02	0.58
1:AAA:536:ARG:HB2	1:AAA:541:VAL:HG22	1.85	0.58
1:AAA:231:LEU:HD22	2:BBB:27:PHE:CZ	2.38	0.57
1:AAA:116:VAL:HG12	1:AAA:158:ASN:ND2	2.18	0.57
1:AAA:59:ASN:CG	1:AAA:83:TYR:CD1	2.82	0.57
1:AAA:87:ALA:HA	1:AAA:117:LEU:O	2.03	0.57
2:BBB:13:GLN:H	2:BBB:13:GLN:NE2	2.02	0.57
2:BBB:104:LEU:HD12	2:BBB:104:LEU:O	2.05	0.56
1:AAA:149:LEU:O	1:AAA:177:ASN:HB2	2.05	0.56
1:AAA:271:LEU:HD11	1:AAA:309:GLY:HA2	1.88	0.56
2:BBB:29:PHE:CD1	2:BBB:29:PHE:N	2.73	0.56
1:AAA:35:LEU:HD12	1:AAA:36:PRO:HD2	1.87	0.56
1:AAA:369:LYS:HD3	1:AAA:371:PHE:CE1	2.41	0.56
1:AAA:364:PHE:CD2	1:AAA:364:PHE:N	2.73	0.56
1:AAA:112:TYR:CE1	1:AAA:154:LEU:HB2	2.41	0.56
1:AAA:369:LYS:HE3	1:AAA:405:GLU:CD	2.31	0.56
1:AAA:116:VAL:HG12	1:AAA:158:ASN:HD21	1.72	0.55
2:BBB:4:LEU:HD23	2:BBB:27:PHE:CE2	2.43	0.54
1:AAA:409:TYR:C	1:AAA:409:TYR:CD1	2.85	0.54
1:AAA:403:LEU:HD12	1:AAA:404:GLU:N	2.22	0.54
1:AAA:458:LEU:HD12	1:AAA:458:LEU:C	2.33	0.54
1:AAA:511:CYS:SG	1:AAA:518:GLY:O	2.67	0.53
1:AAA:367:CYS:O	1:AAA:402:THR:OG1	2.26	0.53
2:BBB:4:LEU:CD2	2:BBB:27:PHE:CZ	2.93	0.52
1:AAA:158:ASN:N	1:AAA:158:ASN:OD1	2.42	0.52
1:AAA:345:LEU:CD2	1:AAA:353:VAL:HG12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:224:CYS:SG	1:AAA:224:CYS:O	2.68	0.52
1:AAA:536:ARG:O	1:AAA:536:ARG:HG3	2.11	0.51
1:AAA:45:MET:SD	1:AAA:49:LEU:CD1	2.98	0.51
1:AAA:221:ALA:C	1:AAA:223:GLY:H	2.18	0.50
2:BBB:48:VAL:HG23	2:BBB:63:VAL:HG11	1.93	0.50
1:AAA:59:ASN:CB	1:AAA:83:TYR:CE1	2.94	0.50
2:BBB:28:THR:HG22	2:BBB:30:ASP:HB2	1.94	0.49
2:BBB:51:ILE:HG22	2:BBB:69:ILE:CG2	2.41	0.49
1:AAA:408:GLY:O	1:AAA:433:GLY:CA	2.58	0.49
2:BBB:13:GLN:NE2	2:BBB:13:GLN:N	2.60	0.49
1:AAA:81:GLN:HA	1:AAA:103:ARG:HB2	1.94	0.48
1:AAA:531:CYS:HB3	1:AAA:533:GLN:O	2.14	0.48
2:BBB:87:PRO:HA	2:BBB:121:VAL:HB	1.96	0.48
2:BBB:38:ARG:HH22	2:BBB:89:ASP:HA	1.79	0.48
2:BBB:38:ARG:HD3	2:BBB:93:TYR:CE2	2.49	0.48
1:AAA:244:CYS:HA	1:AAA:253:LEU:HD13	1.96	0.48
1:AAA:118:ASP:CA	1:AAA:157:ARG:O	2.62	0.47
1:AAA:422:LEU:HB2	1:AAA:455:LEU:HD21	1.96	0.47
2:BBB:3:GLN:N	2:BBB:27:PHE:HE2	2.12	0.47
1:AAA:170:LYS:O	1:AAA:217:ARG:NH2	2.46	0.47
2:BBB:47:LEU:C	2:BBB:47:LEU:HD12	2.39	0.47
1:AAA:44:ASP:OD1	1:AAA:47:ARG:NH1	2.47	0.47
1:AAA:415:TRP:CG	1:AAA:416:PRO:HD2	2.49	0.47
1:AAA:420:PRO:O	1:AAA:451:SER:N	2.47	0.47
2:BBB:24:ALA:HB1	2:BBB:27:PHE:CD2	2.50	0.47
1:AAA:468:ILE:HD11	1:AAA:482:TRP:CH2	2.50	0.46
2:BBB:38:ARG:NH2	2:BBB:89:ASP:HA	2.30	0.46
1:AAA:424:VAL:HG23	1:AAA:425:PHE:CD2	2.50	0.46
2:BBB:3:GLN:N	2:BBB:3:GLN:CD	2.72	0.46
1:AAA:178:GLN:HA	1:AAA:178:GLN:NE2	2.23	0.46
1:AAA:364:PHE:HA	1:AAA:367:CYS:SG	2.55	0.46
1:AAA:231:LEU:CD2	2:BBB:27:PHE:CZ	2.90	0.45
1:AAA:103:ARG:HG2	1:AAA:149:LEU:HD12	1.97	0.45
2:BBB:67:PHE:CE1	2:BBB:82:MET:HB3	2.50	0.45
1:AAA:218:THR:HB	2:BBB:104:LEU:HB2	1.97	0.45
1:AAA:444:THR:HG23	1:AAA:467:LEU:HD23	1.99	0.45
1:AAA:156:GLN:HA	1:AAA:185:ASP:HB3	1.99	0.44
1:AAA:275:ASN:HD22	1:AAA:278:THR:H	1.64	0.44
1:AAA:370:ILE:CD1	1:AAA:403:LEU:HD13	2.47	0.44
1:AAA:441:TYR:HA	1:AAA:465:LEU:O	2.18	0.44
1:AAA:100:ARG:HA	1:AAA:144:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:82:MET:HE3	2:BBB:85:LEU:HD21	1.99	0.44
1:AAA:60:LEU:HD22	1:AAA:77:ILE:HD13	2.00	0.44
2:BBB:33:ASP:HB3	2:BBB:52:SER:HA	2.00	0.43
1:AAA:59:ASN:HB3	1:AAA:83:TYR:CE1	2.54	0.43
1:AAA:413:SER:HA	1:AAA:446:GLN:O	2.18	0.43
1:AAA:216:THR:O	1:AAA:226:ARG:HA	2.18	0.43
2:BBB:58:TYR:CD1	2:BBB:58:TYR:C	2.96	0.43
1:AAA:66:PRO:HG2	1:AAA:69:ALA:HB2	2.01	0.43
1:AAA:409:TYR:HB2	1:AAA:442:SER:O	2.18	0.43
1:AAA:446:GLN:HA	1:AAA:469:HIS:O	2.19	0.42
2:BBB:36:TRP:HE1	2:BBB:78:VAL:HG12	1.84	0.42
2:BBB:59:TYR:HB3	2:BBB:63:VAL:HG23	2.01	0.42
2:BBB:51:ILE:HG13	2:BBB:52:SER:O	2.19	0.42
1:AAA:83:TYR:CD1	1:AAA:83:TYR:N	2.88	0.42
1:AAA:121:ASP:CG	1:AAA:122:PRO:HD2	2.44	0.42
1:AAA:345:LEU:HD21	1:AAA:353:VAL:HG11	2.01	0.42
1:AAA:92:ARG:HB3	1:AAA:138:ARG:HG3	2.02	0.42
2:BBB:13:GLN:HE21	2:BBB:13:GLN:N	2.10	0.42
2:BBB:51:ILE:HG22	2:BBB:69:ILE:HD13	2.01	0.42
1:AAA:47:ARG:O	1:AAA:51:GLN:HB2	2.20	0.41
1:AAA:228:LYS:C	2:BBB:113:TRP:CH2	2.99	0.41
1:AAA:370:ILE:HD13	1:AAA:403:LEU:HD22	2.02	0.41
1:AAA:162:CYS:HA	1:AAA:188:ARG:HH21	1.85	0.41
1:AAA:241:ALA:O	1:AAA:242:ALA:HB3	2.20	0.41
2:BBB:14:ALA:HB2	2:BBB:121:VAL:HG12	2.03	0.41
1:AAA:92:ARG:HA	1:AAA:136:GLY:O	2.20	0.41
1:AAA:83:TYR:HD1	1:AAA:83:TYR:H	1.67	0.41
1:AAA:271:LEU:O	1:AAA:283:PRO:HA	2.21	0.41
1:AAA:355:ALA:CB	1:AAA:375:ALA:O	2.62	0.41
1:AAA:219:VAL:HG12	2:BBB:104:LEU:HD23	2.03	0.41
1:AAA:303:TYR:CE2	1:AAA:313:LEU:HD21	2.56	0.40

All (2) 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)
1:AAA:340:ARG:HH21	2:BBB:17:THR:O[3_665]	1.48	0.12
1:AAA:340:ARG:NH2	2:BBB:17:THR:O[3_665]	2.18	0.02

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	AAA	500/630 (79%)	448 (90%)	50 (10%)	2 (0%)	30	61
2	BBB	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
All	All	619/762 (81%)	555 (90%)	62 (10%)	2 (0%)	36	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	279	PHE
1	AAA	458	LEU

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	AAA	429/544 (79%)	404 (94%)	25 (6%)	18	48
2	BBB	96/107 (90%)	80 (83%)	16 (17%)	2	10
All	All	525/651 (81%)	484 (92%)	41 (8%)	11	38

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	49	LEU
1	AAA	68	ASN
1	AAA	81	GLN
1	AAA	83	TYR

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Mol	Chain	Res	Type
1	AAA	177	ASN
1	AAA	178	GLN
1	AAA	179	LEU
1	AAA	181	LEU
1	AAA	185	ASP
1	AAA	207	GLU
1	AAA	233	THR
1	AAA	249	HIS
1	AAA	271	LEU
1	AAA	282	MET
1	AAA	319	ASN
1	AAA	341	VAL
1	AAA	419	LEU
1	AAA	450	ILE
1	AAA	458	LEU
1	AAA	496	THR
1	AAA	499	ARG
1	AAA	501	GLU
1	AAA	502	ASP
1	AAA	503	GLU
1	AAA	530	ASN
2	BBB	3	GLN
2	BBB	13	GLN
2	BBB	21	SER
2	BBB	29	PHE
2	BBB	31	ASP
2	BBB	46	GLU
2	BBB	47	LEU
2	BBB	48	VAL
2	BBB	51	ILE
2	BBB	58	TYR
2	BBB	77	THR
2	BBB	95	CYS
2	BBB	100	HIS
2	BBB	103	GLU
2	BBB	106	THR
2	BBB	117	THR

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 ⓘ

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

5.5 Carbohydrates ⓘ

3 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	AbA	1	1,3	14,14,15	0.40	0	17,19,21	1.33	2 (11%)
3	NAG	AbA	2	3	14,14,15	0.38	0	17,19,21	1.31	2 (11%)
3	BMA	AbA	3	3	11,11,12	0.41	0	15,15,17	0.93	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
3	NAG	AbA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	AbA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	AbA	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AbA	1	NAG	C4-C3-C2	-3.36	106.10	111.02
3	AbA	2	NAG	C4-C3-C2	-3.30	106.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AbA	1	NAG	O4-C4-C3	2.95	117.34	110.38
3	AbA	2	NAG	C8-C7-N2	2.13	119.65	116.12

There are no chirality outliers.

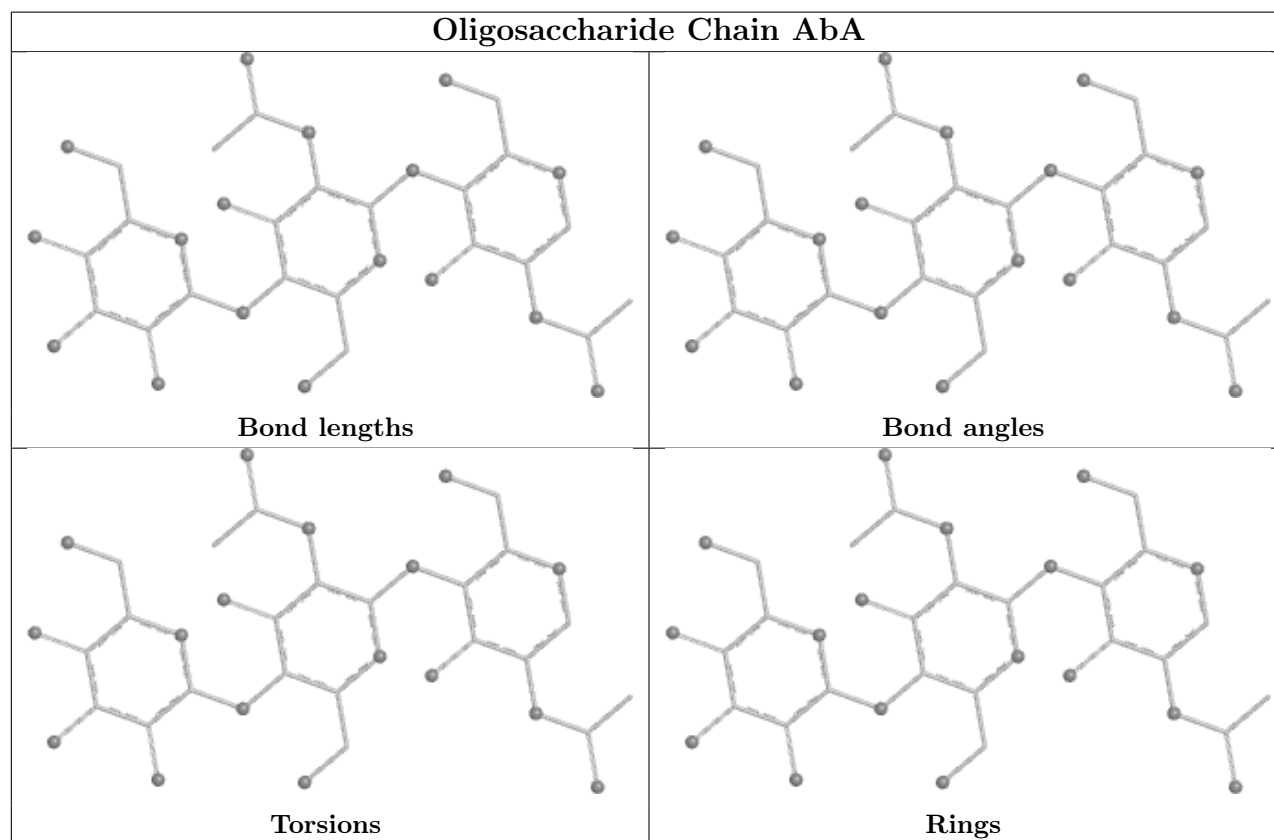
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AbA	2	NAG	C8-C7-N2-C2
3	AbA	2	NAG	O7-C7-N2-C2
3	AbA	1	NAG	O5-C5-C6-O6
3	AbA	1	NAG	C4-C5-C6-O6
3	AbA	1	NAG	C3-C2-N2-C7
3	AbA	1	NAG	C1-C2-N2-C7

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

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
4	NAG	AAA	700	1	14,14,15	0.64	1 (7%)	17,19,21	1.18	2 (11%)

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	AAA	700	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	700	NAG	C1-C2	2.16	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	700	NAG	C1-O5-C5	2.82	115.97	112.19
4	AAA	700	NAG	C1-C2-N2	2.79	114.82	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	700	NAG	O5-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	AAA	506/630 (80%)	0.32	32 (6%) 26 14	75, 108, 148, 183	0
2	BBB	121/132 (91%)	0.36	12 (9%) 13 7	86, 115, 154, 189	0
All	All	627/762 (82%)	0.33	44 (7%) 22 12	75, 110, 151, 189	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	415	TRP	6.1
1	AAA	176	ASN	6.0
1	AAA	25	VAL	5.3
1	AAA	149	LEU	3.6
1	AAA	317	LEU	3.4
1	AAA	55	VAL	3.3
1	AAA	502	ASP	3.3
1	AAA	416	PRO	3.2
1	AAA	541	VAL	3.2
2	BBB	123	SER	3.1
1	AAA	54	GLN	3.1
2	BBB	65	GLY	3.0
1	AAA	445	LEU	2.9
1	AAA	468	ILE	2.9
2	BBB	45	CYS	2.9
1	AAA	307	ASP	2.8
1	AAA	334	CYS	2.8
1	AAA	308	VAL	2.7
2	BBB	29	PHE	2.6
1	AAA	535	LEU	2.6
1	AAA	540	CYS	2.6
1	AAA	388	ASN	2.6
1	AAA	448	LEU	2.5
2	BBB	106	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	100	ARG	2.5
1	AAA	114	LEU	2.3
1	AAA	290	THR	2.3
2	BBB	107	CYS	2.3
2	BBB	76	ASN	2.3
1	AAA	524	GLY	2.3
1	AAA	422	LEU	2.2
2	BBB	84	SER	2.2
2	BBB	73	ASN	2.2
1	AAA	191	ALA	2.2
1	AAA	249	HIS	2.2
1	AAA	84	VAL	2.2
2	BBB	32	SER	2.2
2	BBB	93	TYR	2.1
1	AAA	43	LEU	2.1
1	AAA	425	PHE	2.1
2	BBB	47	LEU	2.0
1	AAA	529	VAL	2.0
1	AAA	98	ARG	2.0
1	AAA	474	LEU	2.0

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

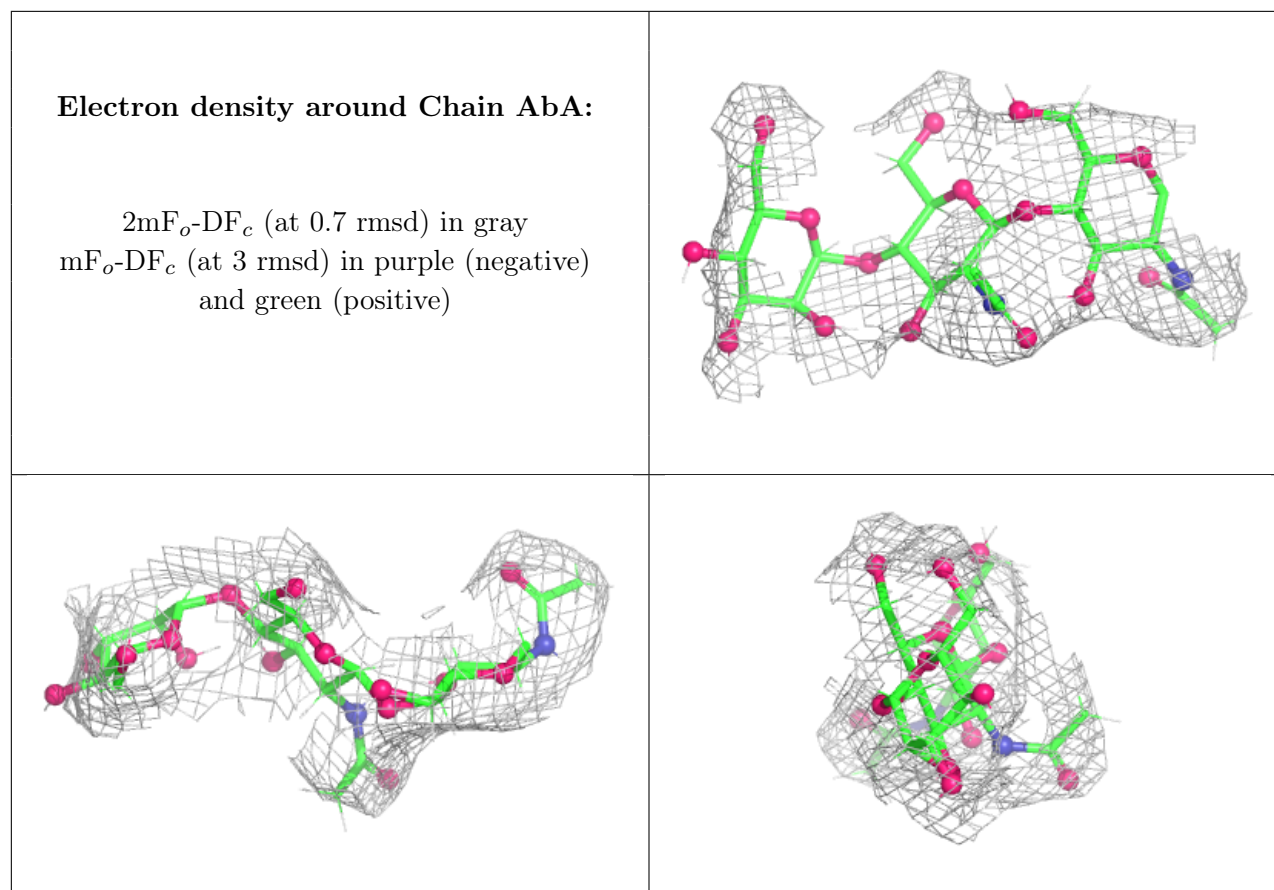
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	NAG	AbA	1	14/15	-	-	105,126,143,151	2
3	NAG	AbA	2	14/15	-	-	141,160,182,192	2
3	BMA	AbA	3	11/12	-	-	155,187,191,198	4

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, 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
4	NAG	AAA	700	14/15	0.60	0.10	152,171,173,176	3

6.5 Other polymers [i](#)

There are no such residues in this entry.