



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:52 PM UTC

PDB ID : 9BEX / pdb_00009bex
Title : X-ray crystallography structural model of the immunoglobulin G1 (IgG1) Fc D270C K326C variant
Authors : Shenoy, A.; Barb, A.W.
Deposited on : 2024-04-16
Resolution : 2.25 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

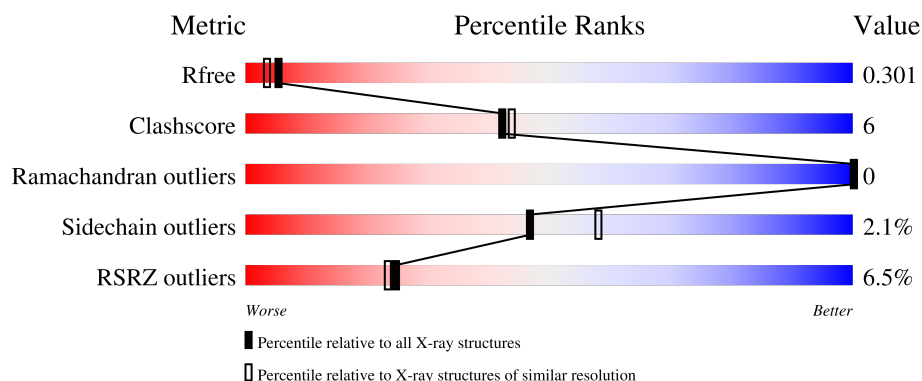
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

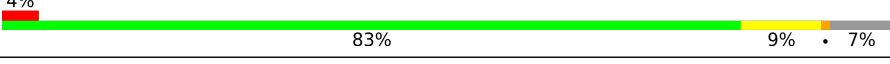
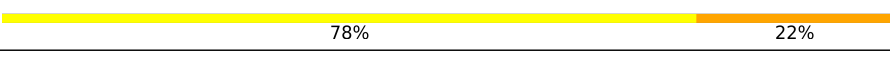
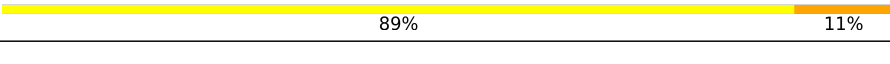
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	232	
1	BBB	232	
2	AaA	9	
2	BaB	9	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUL	AaA	9	X	-	-	-
2	FUL	BaB	9	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3680 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.

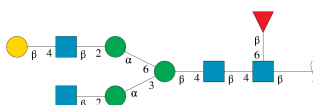
- Molecule 1 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	214	Total	C	N	O	S	0	0	0
			1667	1065	272	321	9			
1	BBB	216	Total	C	N	O	S	0	1	0
			1696	1079	282	326	9			

There are 4 discrepancies between the modelled and reference sequences:

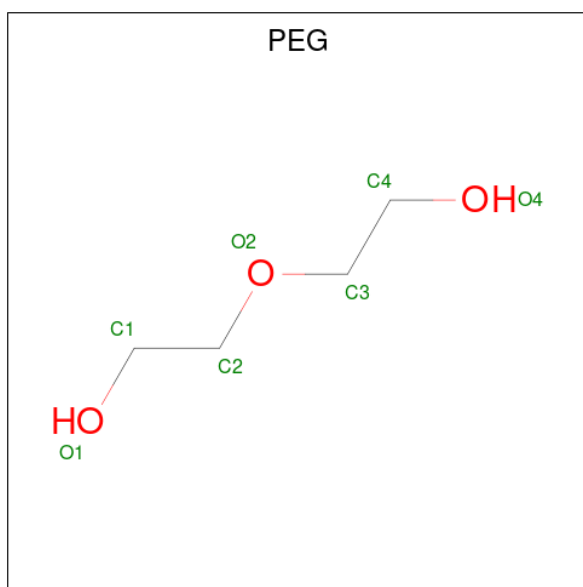
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	270	CYS	ASP	engineered mutation	UNP P0DOX5
AAA	326	CYS	LYS	engineered mutation	UNP P0DOX5
BBB	270	CYS	ASP	engineered mutation	UNP P0DOX5
BBB	326	CYS	LYS	engineered mutation	UNP P0DOX5

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
2	AaA	9	Total	C	N	O	0	0	0
			110	62	4	44			
2	BaB	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			7	4	3		

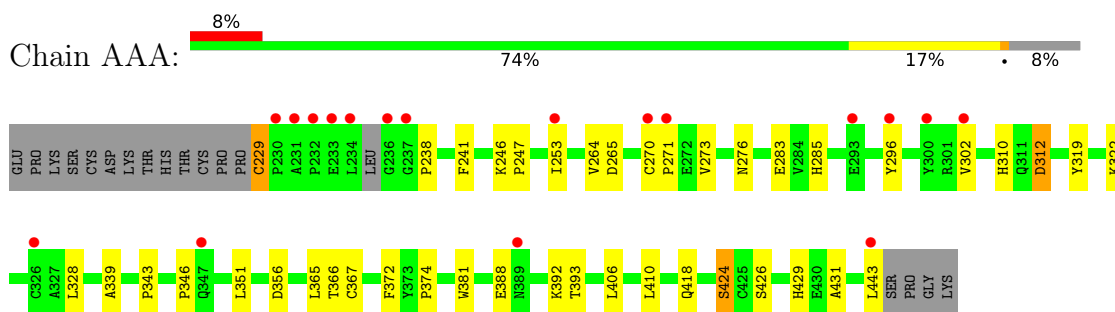
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	38	Total	O	0	0
			38	38		
4	BBB	52	Total	O	0	0
			52	52		

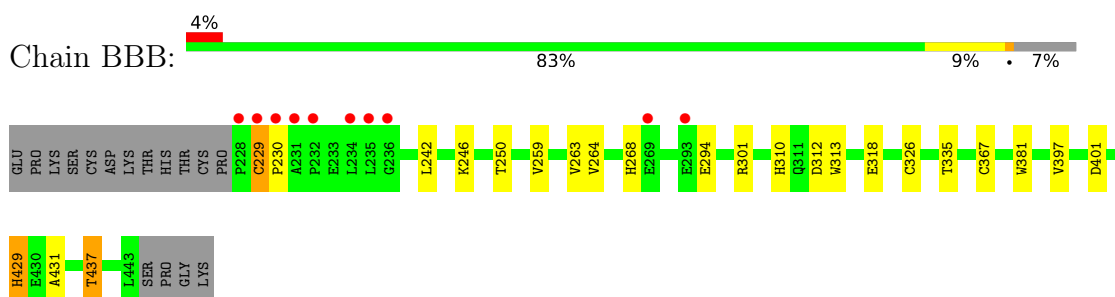
3 Residue-property plots

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.

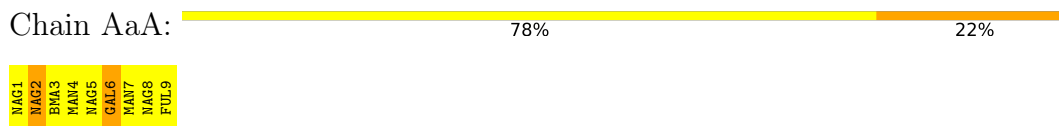
- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



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



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



MAG1
MAG2
BMA3
MAN4
NAG5
GAL6
MAN7
MAG8
FUL9

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 79.74Å 142.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.50 – 2.25 30.50 – 2.25	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.50-2.25) 88.4 (30.50-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.242 , 0.302 0.244 , 0.301	Depositor DCC
R_{free} test set	1213 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3680	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PEG, FUL, GAL, NAG, MAN

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	1.05	0/1714	1.30	3/2342 (0.1%)
1	BBB	1.04	0/1747	1.29	5/2386 (0.2%)
All	All	1.04	0/3461	1.30	8/4728 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	429	HIS	CA-C-N	6.53	129.36	120.54
1	BBB	429	HIS	C-N-CA	6.53	129.36	120.54
1	AAA	343	PRO	CA-C-N	6.22	132.78	122.33
1	AAA	343	PRO	C-N-CA	6.22	132.78	122.33
1	BBB	312	ASP	CA-CB-CG	5.35	117.95	112.60
1	AAA	312	ASP	CA-CB-CG	5.12	117.72	112.60
1	BBB	264	VAL	CA-C-O	-5.09	116.27	121.67
1	BBB	437	THR	CA-CB-OG1	-5.07	101.99	109.60

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	AAA	1667	0	1590	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	1696	0	1625	14	0
2	AaA	110	0	94	4	0
2	BaB	110	0	94	2	0
3	AAA	7	0	10	3	0
4	AAA	38	0	0	0	0
4	BBB	52	0	0	0	0
All	All	3680	0	3413	44	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 (44) 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:253:ILE:H	1:AAA:253:ILE:HD12	1.53	0.73
1:AAA:246:LYS:HE3	2:AaA:6:GAL:O4	1.88	0.73
1:AAA:310:HIS:H	1:AAA:310:HIS:CD2	2.07	0.70
1:BBB:229:CYS:SG	1:BBB:230:PRO:HD2	2.35	0.67
1:BBB:310:HIS:H	1:BBB:310:HIS:CD2	2.10	0.66
1:BBB:318:GLU:HG2	1:BBB:335:THR:CG2	2.35	0.57
1:BBB:246:LYS:HD3	2:BaB:6:GAL:O4	2.05	0.57
1:AAA:229:CYS:HB2	1:AAA:296:TYR:O	2.05	0.56
1:AAA:241:PHE:CE2	2:AaA:2:NAG:H61	2.41	0.56
1:AAA:418:GLN:HA	1:AAA:443:LEU:HD22	1.89	0.55
1:AAA:406:LEU:C	1:AAA:406:LEU:HD12	2.31	0.55
1:AAA:393:THR:N	3:AAA:501:PEG:O1	2.35	0.54
3:AAA:501:PEG:H42	1:BBB:397:VAL:HG13	1.88	0.54
1:BBB:429:HIS:HD2	1:BBB:431:ALA:H	1.57	0.52
1:AAA:238:PRO:HB3	1:AAA:265:ASP:O	2.10	0.51
1:AAA:246:LYS:CE	2:AaA:6:GAL:O4	2.57	0.51
1:AAA:238:PRO:HB2	1:AAA:264:VAL:O	2.10	0.51
1:BBB:246:LYS:HD3	2:BaB:6:GAL:HO4	1.77	0.50
1:AAA:429:HIS:HD2	1:AAA:431:ALA:H	1.58	0.50
1:AAA:351:LEU:HB2	1:AAA:366:THR:HB	1.93	0.49
1:AAA:367:CYS:HB2	1:AAA:381:TRP:CZ2	2.48	0.48
1:AAA:392:LYS:HA	3:AAA:501:PEG:O1	2.14	0.48
1:BBB:242:LEU:HD11	1:BBB:259:VAL:CG1	2.44	0.47
1:AAA:273:VAL:CG2	1:AAA:302:VAL:HG21	2.45	0.47
1:AAA:429:HIS:CD2	1:AAA:431:ALA:H	2.32	0.47
1:AAA:238:PRO:HD2	1:AAA:328:LEU:HD21	1.98	0.46
1:AAA:241:PHE:HE2	2:AaA:2:NAG:H61	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:365:LEU:HD12	1:AAA:410:LEU:HD23	1.98	0.46
1:AAA:276:ASN:HB2	1:AAA:322:LYS:HB3	1.98	0.46
1:BBB:250:THR:HG21	1:BBB:313:TRP:CD1	2.52	0.45
1:AAA:283:GLU:HG2	1:AAA:285:HIS:CE1	2.53	0.44
1:AAA:273:VAL:HG21	1:AAA:302:VAL:HG21	1.98	0.44
1:BBB:401:ASP:C	1:BBB:401:ASP:OD1	2.60	0.44
1:BBB:268:HIS:CE1	1:BBB:294:GLU:OE1	2.71	0.44
1:BBB:429:HIS:CD2	1:BBB:431:ALA:H	2.36	0.42
1:BBB:263:VAL:O	1:BBB:301:ARG:HA	2.20	0.42
1:AAA:388:GLU:HA	1:AAA:388:GLU:OE1	2.20	0.42
1:AAA:339:ALA:HB3	1:AAA:374:PRO:HB3	2.01	0.41
1:AAA:381:TRP:HA	1:AAA:424:SER:O	2.21	0.41
1:AAA:238:PRO:HD2	1:AAA:328:LEU:CD2	2.51	0.40
1:AAA:346:PRO:HB3	1:AAA:372:PHE:HB3	2.03	0.40
1:AAA:270:CYS:N	1:AAA:271:PRO:HD3	2.36	0.40
1:AAA:312:ASP:HB3	1:AAA:319:TYR:OH	2.21	0.40
1:BBB:367:CYS:HB2	1:BBB:381:TRP:CZ2	2.56	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	AAA	210/232 (90%)	200 (95%)	10 (5%)	0	100	100
1	BBB	215/232 (93%)	214 (100%)	1 (0%)	0	100	100
All	All	425/464 (92%)	414 (97%)	11 (3%)	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	AAA	189/215 (88%)	184 (97%)	5 (3%)	40	50
1	BBB	194/215 (90%)	191 (98%)	3 (2%)	57	68
All	All	383/430 (89%)	375 (98%)	8 (2%)	47	58

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	229	CYS
1	AAA	247	PRO
1	AAA	356	ASP
1	AAA	424	SER
1	AAA	426	SER
1	BBB	229	CYS
1	BBB	326	CYS
1	BBB	437	THR

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 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	AaA	1	2,1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
2	NAG	AaA	2	2	14,14,15	0.50	0	17,19,21	1.40	2 (11%)
2	BMA	AaA	3	2	11,11,12	0.36	0	15,15,17	1.45	3 (20%)
2	MAN	AaA	4	2	11,11,12	0.51	0	15,15,17	1.46	1 (6%)
2	NAG	AaA	5	2	14,14,15	0.88	0	17,19,21	1.69	2 (11%)
2	GAL	AaA	6	2	11,11,12	0.78	0	15,15,17	1.31	3 (20%)
2	MAN	AaA	7	2	11,11,12	0.38	0	15,15,17	1.35	2 (13%)
2	NAG	AaA	8	2	14,14,15	0.57	0	17,19,21	1.30	2 (11%)
2	FUL	AaA	9	2	10,10,11	0.68	0	14,14,16	1.89	4 (28%)
2	NAG	BaB	1	2,1	14,14,15	0.61	0	17,19,21	1.08	1 (5%)
2	NAG	BaB	2	2	14,14,15	0.67	0	17,19,21	1.56	4 (23%)
2	BMA	BaB	3	2	11,11,12	0.89	1 (9%)	15,15,17	1.65	3 (20%)
2	MAN	BaB	4	2	11,11,12	0.72	0	15,15,17	1.30	1 (6%)
2	NAG	BaB	5	2	14,14,15	0.74	0	17,19,21	1.49	3 (17%)
2	GAL	BaB	6	2	11,11,12	0.90	1 (9%)	15,15,17	1.12	1 (6%)
2	MAN	BaB	7	2	11,11,12	0.56	0	15,15,17	1.46	2 (13%)
2	NAG	BaB	8	2	14,14,15	0.66	0	17,19,21	2.12	4 (23%)
2	FUL	BaB	9	2	10,10,11	0.36	0	14,14,16	1.11	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	AaA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AaA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AaA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	4	2	-	1/2/19/22	0/1/1/1
2	NAG	AaA	5	2	-	2/6/23/26	0/1/1/1
2	GAL	AaA	6	2	-	2/2/19/22	0/1/1/1
2	MAN	AaA	7	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	AaA	8	2	-	1/6/23/26	0/1/1/1
2	FUL	AaA	9	2	1/1/4/5	-	0/1/1/1
2	NAG	BaB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BaB	2	2	-	0/6/23/26	0/1/1/1
2	BMA	BaB	3	2	-	0/2/19/22	0/1/1/1
2	MAN	BaB	4	2	-	0/2/19/22	0/1/1/1
2	NAG	BaB	5	2	-	0/6/23/26	0/1/1/1
2	GAL	BaB	6	2	-	1/2/19/22	0/1/1/1
2	MAN	BaB	7	2	-	0/2/19/22	0/1/1/1
2	NAG	BaB	8	2	-	0/6/23/26	0/1/1/1
2	FUL	BaB	9	2	1/1/4/5	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	6	GAL	C2-C3	2.31	1.56	1.52
2	BaB	3	BMA	O5-C1	-2.02	1.40	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AaA	9	FUL	C1-C2-C3	-4.66	102.85	109.64
2	BaB	8	NAG	C4-C3-C2	4.39	117.45	111.02
2	BaB	8	NAG	C3-C4-C5	4.13	117.72	110.23
2	AaA	8	NAG	O5-C1-C2	4.04	117.55	111.29
2	BaB	8	NAG	C1-O5-C5	-4.00	106.82	112.19
2	BaB	4	MAN	O2-C2-C3	-3.96	101.95	110.15
2	AaA	5	NAG	O4-C4-C3	-3.91	101.16	110.38
2	AaA	2	NAG	C1-C2-N2	3.89	116.57	110.43
2	BaB	8	NAG	O5-C1-C2	3.88	117.30	111.29
2	AaA	5	NAG	O5-C1-C2	3.65	116.94	111.29
2	BaB	7	MAN	O2-C2-C3	-3.65	102.59	110.15
2	AaA	4	MAN	O2-C2-C3	-3.60	102.70	110.15
2	BaB	5	NAG	C4-C3-C2	3.28	115.83	111.02
2	AaA	7	MAN	O2-C2-C3	-3.20	103.52	110.15
2	AaA	6	GAL	O4-C4-C5	3.07	116.89	109.32
2	AaA	9	FUL	O2-C2-C1	3.01	116.12	109.22
2	BaB	2	NAG	C1-C2-N2	3.01	115.17	110.43
2	AaA	1	NAG	O5-C1-C2	-2.95	106.72	111.29
2	BaB	2	NAG	O4-C4-C5	-2.93	102.10	109.32
2	AaA	7	MAN	C1-O5-C5	2.87	116.03	112.19
2	AaA	3	BMA	O4-C4-C3	-2.87	103.62	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BaB	6	GAL	O5-C1-C2	2.85	117.58	110.79
2	BaB	3	BMA	O6-C6-C5	-2.79	101.85	111.33
2	BaB	2	NAG	C2-N2-C7	-2.74	119.23	122.90
2	BaB	9	FUL	C1-C2-C3	-2.72	105.69	109.64
2	BaB	5	NAG	C1-O5-C5	-2.67	108.61	112.19
2	BaB	3	BMA	O3-C3-C2	2.59	115.35	110.05
2	AaA	6	GAL	O5-C1-C2	2.46	116.66	110.79
2	BaB	3	BMA	O2-C2-C1	-2.38	103.77	109.22
2	BaB	2	NAG	C1-O5-C5	-2.36	109.02	112.19
2	AaA	2	NAG	O4-C4-C5	-2.33	103.59	109.32
2	AaA	8	NAG	C1-O5-C5	-2.29	109.11	112.19
2	AaA	6	GAL	C2-C3-C4	2.29	114.88	110.86
2	AaA	3	BMA	C1-O5-C5	-2.27	109.14	112.19
2	BaB	1	NAG	C3-C4-C5	-2.24	106.18	110.23
2	BaB	5	NAG	O5-C5-C6	-2.23	103.31	107.66
2	AaA	9	FUL	O5-C5-C4	2.20	113.51	109.55
2	AaA	9	FUL	C2-C3-C4	-2.19	107.01	110.86
2	BaB	7	MAN	O2-C2-C1	2.18	114.22	109.22
2	AaA	3	BMA	C2-C3-C4	2.12	114.59	110.86
2	AaA	1	NAG	C1-O5-C5	2.06	114.94	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AaA	9	FUL	C1
2	BaB	9	FUL	C1

All (9) torsion outliers are listed below:

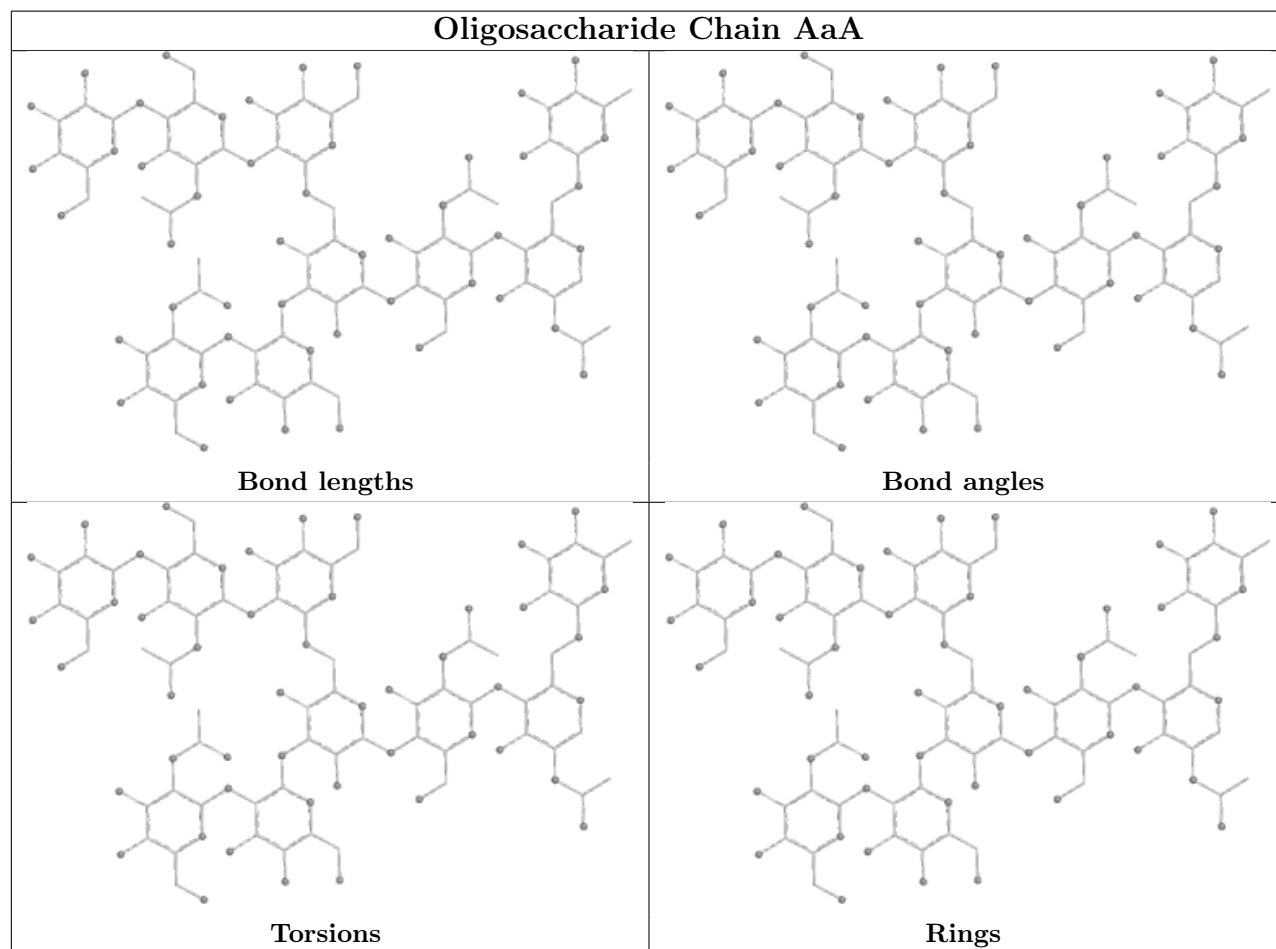
Mol	Chain	Res	Type	Atoms
2	AaA	6	GAL	O5-C5-C6-O6
2	AaA	1	NAG	O5-C5-C6-O6
2	AaA	1	NAG	C4-C5-C6-O6
2	AaA	6	GAL	C4-C5-C6-O6
2	BaB	6	GAL	O5-C5-C6-O6
2	AaA	8	NAG	C4-C5-C6-O6
2	AaA	5	NAG	C1-C2-N2-C7
2	AaA	5	NAG	C8-C7-N2-C2
2	AaA	4	MAN	C4-C5-C6-O6

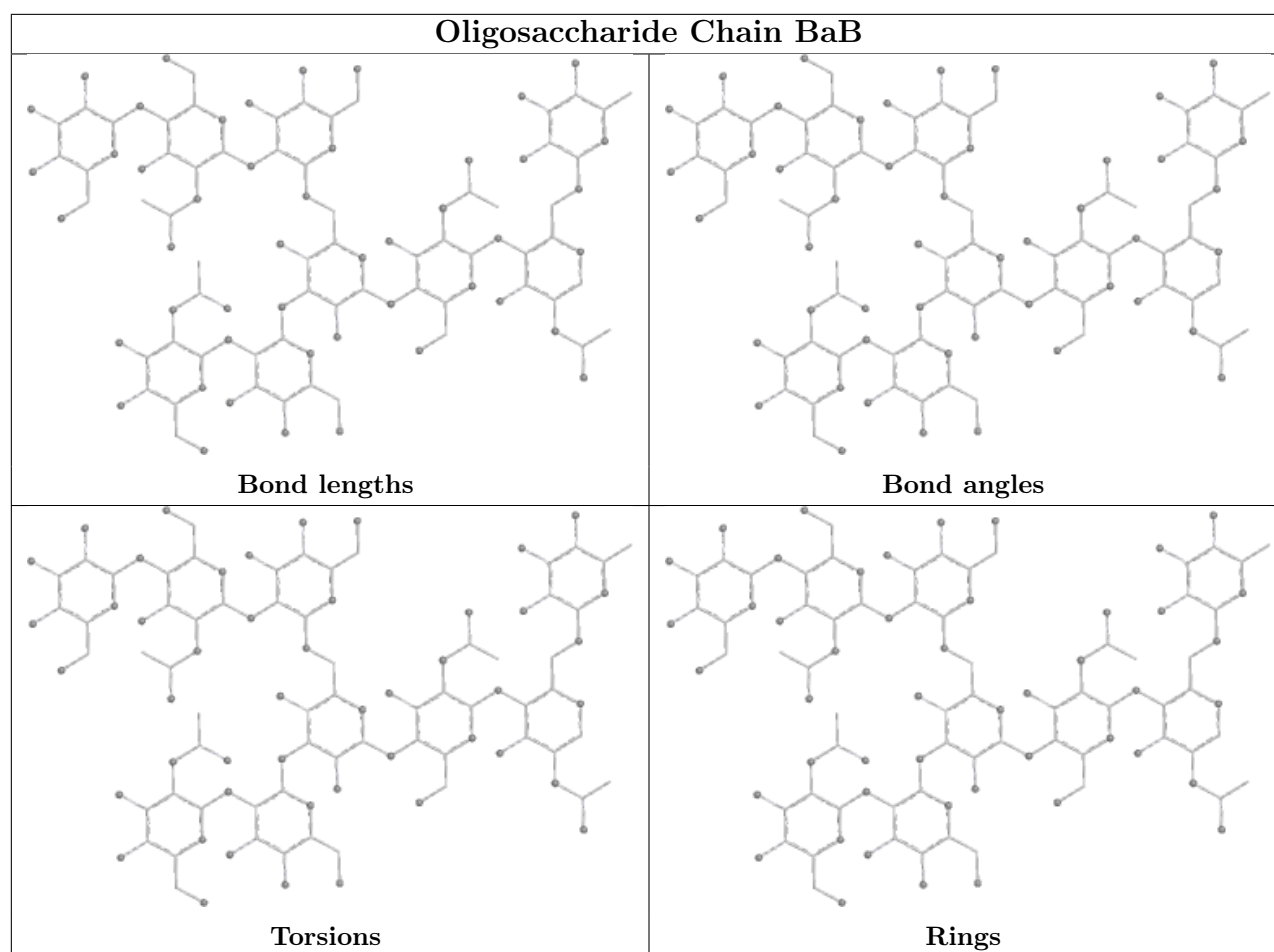
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AaA	6	GAL	2	0
2	BaB	6	GAL	2	0
2	AaA	2	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	PEG	AAA	501	-	6,6,6	0.43	0	5,5,5	0.26	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	PEG	AAA	501	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

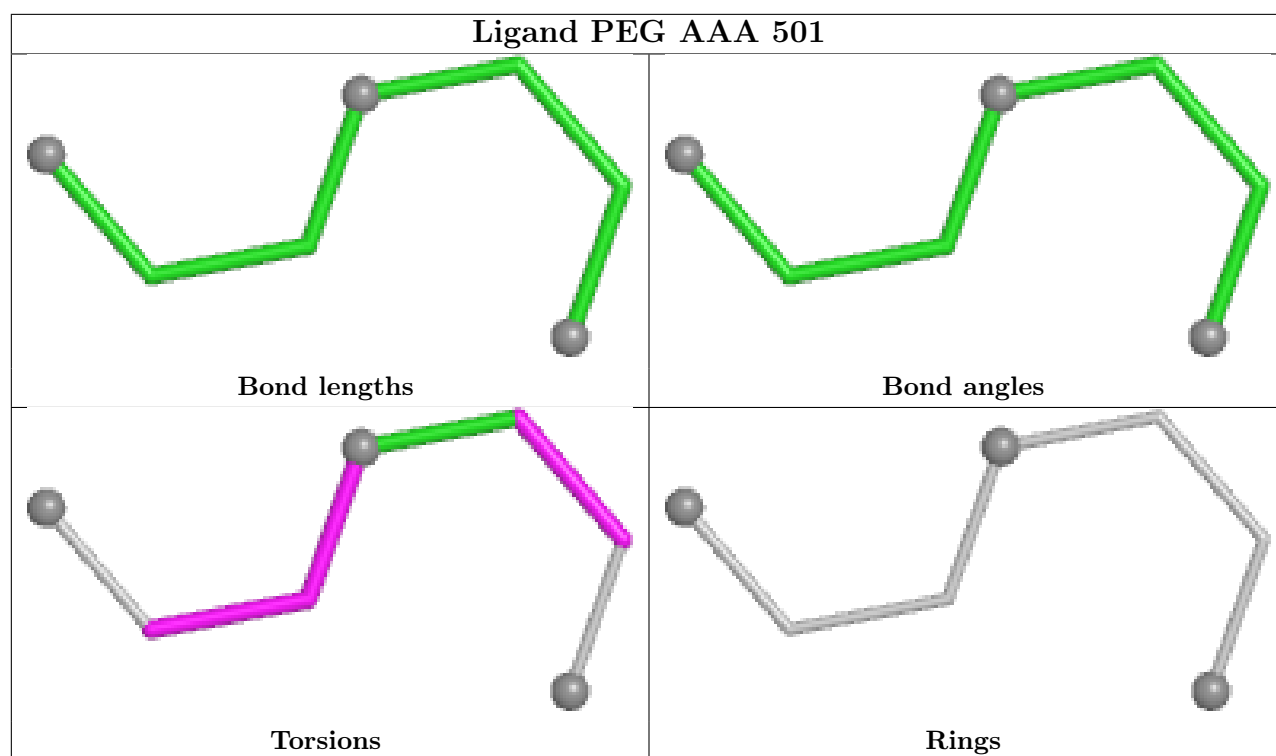
Mol	Chain	Res	Type	Atoms
3	AAA	501	PEG	O2-C3-C4-O4
3	AAA	501	PEG	O1-C1-C2-O2
3	AAA	501	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	501	PEG	3	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	AAA	214/232 (92%)	0.66	18 (8%)	17 15	30, 50, 96, 132	0
1	BBB	216/232 (93%)	0.30	10 (4%)	37 36	30, 45, 84, 112	1 (0%)
All	All	430/464 (92%)	0.48	28 (6%)	25 23	30, 46, 91, 132	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	236	GLY	5.1
1	BBB	234	LEU	4.3
1	AAA	231	ALA	3.9
1	AAA	326	CYS	3.6
1	BBB	235	LEU	3.4
1	AAA	300	TYR	3.4
1	AAA	233	GLU	3.3
1	AAA	232	PRO	3.1
1	BBB	236	GLY	3.1
1	BBB	228	PRO	3.1
1	AAA	443	LEU	3.0
1	AAA	253	ILE	2.8
1	AAA	230	PRO	2.8
1	AAA	270	CYS	2.7
1	AAA	237	GLY	2.6
1	BBB	230	PRO	2.6
1	AAA	296	TYR	2.5
1	AAA	271	PRO	2.5
1	AAA	302	VAL	2.5
1	BBB	231	ALA	2.4
1	BBB	232	PRO	2.4
1	AAA	347	GLN	2.4
1	AAA	293	GLU	2.4
1	BBB	293[A]	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	234	LEU	2.1
1	BBB	269	GLU	2.1
1	BBB	229	CYS	2.1
1	AAA	389	ASN	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](#)

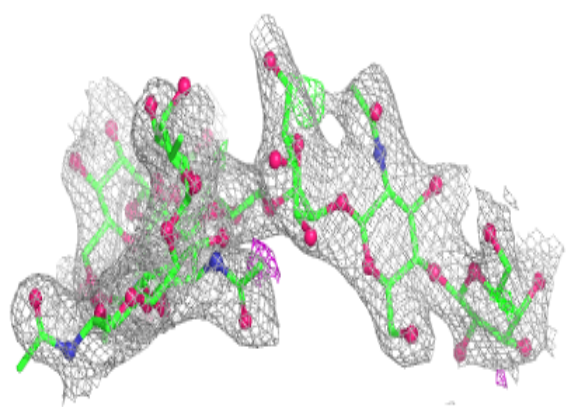
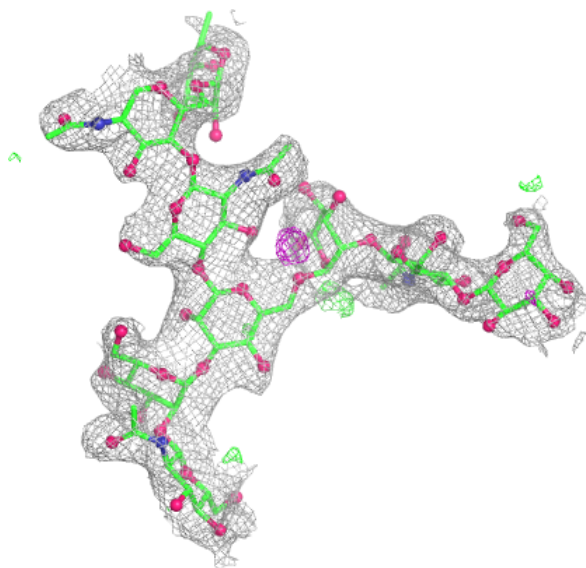
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NAG	AaA	1	14/15	-	-	82,93,97,98	0
2	NAG	AaA	2	14/15	-	-	57,75,81,83	0
2	BMA	AaA	3	11/12	-	-	61,64,66,67	0
2	MAN	AaA	4	11/12	-	-	62,72,77,78	0
2	NAG	AaA	5	14/15	-	-	51,57,64,65	0
2	GAL	AaA	6	11/12	-	-	70,72,74,74	0
2	MAN	AaA	7	11/12	-	-	60,64,69,76	0
2	NAG	AaA	8	14/15	-	-	83,93,99,100	0
2	FUL	AaA	9	10/11	-	-	106,112,119,119	0
2	NAG	BaB	1	14/15	-	-	58,63,65,65	0
2	NAG	BaB	2	14/15	-	-	40,48,52,53	0
2	BMA	BaB	3	11/12	-	-	46,50,54,55	0
2	MAN	BaB	4	11/12	-	-	49,56,59,64	0
2	NAG	BaB	5	14/15	-	-	48,55,62,64	0
2	GAL	BaB	6	11/12	-	-	55,64,66,66	0
2	MAN	BaB	7	11/12	-	-	54,63,71,79	0
2	NAG	BaB	8	14/15	-	-	77,91,96,100	0
2	FUL	BaB	9	10/11	-	-	78,81,83,84	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.

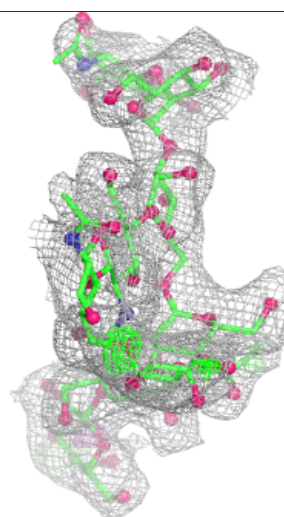
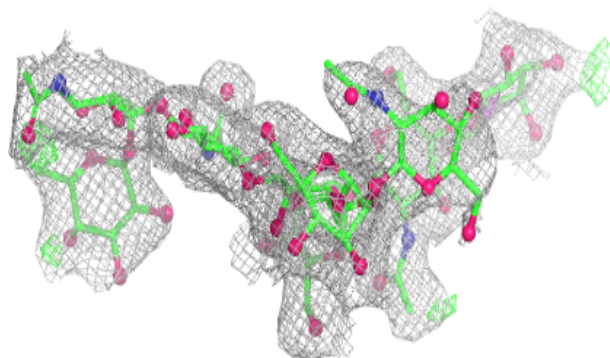
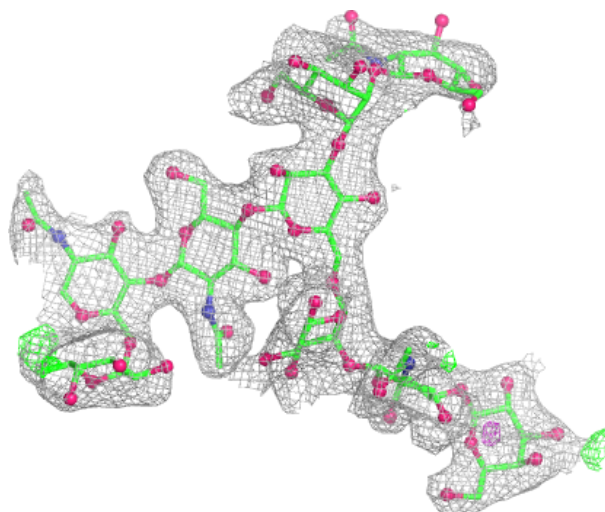
Electron density around Chain AaA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain BaB:

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** ⓘ

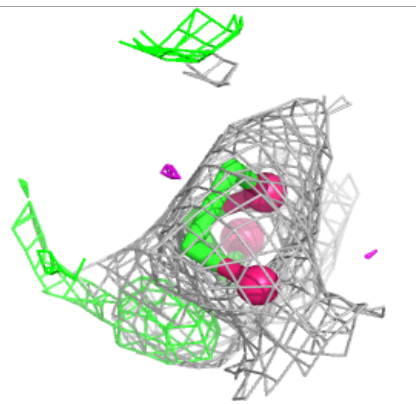
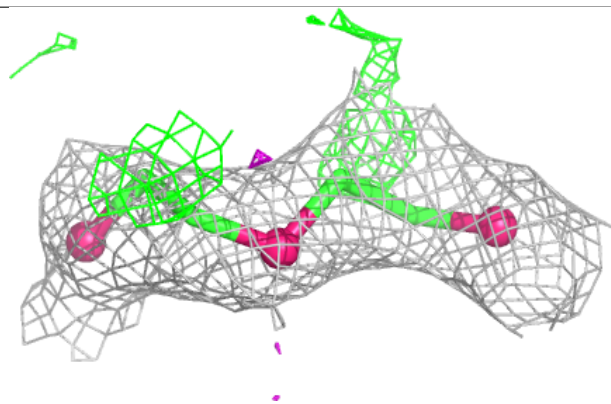
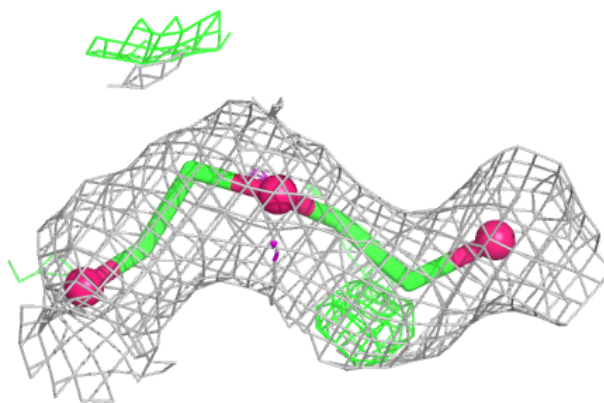
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	PEG	AAA	501	7/7	0.78	0.17	54,60,64,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEG AAA 501:

$2mF_o-DF_c$ (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.