Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 06:00 AM UTC

PDB ID	:	5NNJ / pdb_00005nnj
Title	:	Dimer structure of Sortilin ectodomain crystal form 3, 4.0 Angstrom
Authors	:	Leloup, N.O.L.; Janssen, B.J.C.
Deposited on	:	2017-04-09
Resolution	:	4.00 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 (i) 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 (i)) were used in the production of this report:

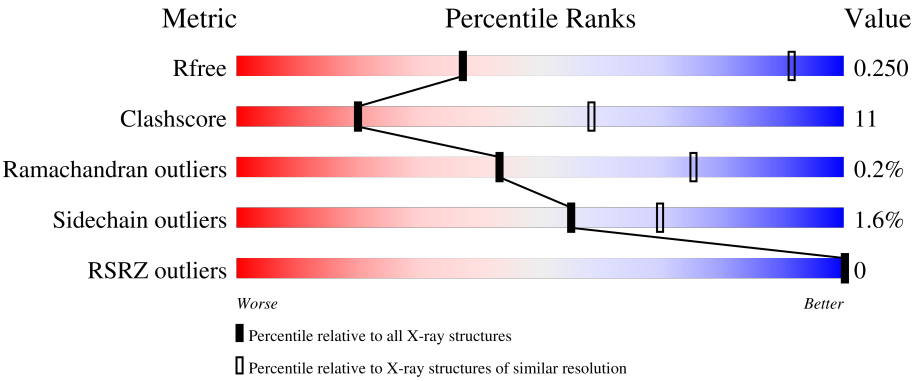
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 <=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	732	64% 24% • 11%
1	B	732	63% 25% • 11%
1	C	732	68% 20% • 12%
1	D	732	65% 23% 11%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	F	3	33% 67%
2	G	3	67% 33%
2	H	3	33% 67%
2	I	3	33% 33% 33%
2	J	3	67% 33%
2	K	3	33% 67%
2	L	3	67% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20730 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	0	0
			5094	3220	855	990	29			
1	B	648	Total	C	N	O	S	0	0	0
			5094	3220	855	990	29			
1	D	648	Total	C	N	O	S	0	0	0
			5094	3220	855	990	29			
1	C	646	Total	C	N	O	S	0	0	0
			5080	3213	853	986	28			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	ALA	-	expression tag	UNP Q6PHU5
A	724	ALA	-	expression tag	UNP Q6PHU5
A	725	ALA	-	expression tag	UNP Q6PHU5
A	726	HIS	-	expression tag	UNP Q6PHU5
A	727	HIS	-	expression tag	UNP Q6PHU5
A	728	HIS	-	expression tag	UNP Q6PHU5
A	729	HIS	-	expression tag	UNP Q6PHU5
A	730	HIS	-	expression tag	UNP Q6PHU5
A	731	HIS	-	expression tag	UNP Q6PHU5
B	723	ALA	-	expression tag	UNP Q6PHU5
B	724	ALA	-	expression tag	UNP Q6PHU5
B	725	ALA	-	expression tag	UNP Q6PHU5
B	726	HIS	-	expression tag	UNP Q6PHU5
B	727	HIS	-	expression tag	UNP Q6PHU5
B	728	HIS	-	expression tag	UNP Q6PHU5
B	729	HIS	-	expression tag	UNP Q6PHU5
B	730	HIS	-	expression tag	UNP Q6PHU5
B	731	HIS	-	expression tag	UNP Q6PHU5
D	723	ALA	-	expression tag	UNP Q6PHU5
D	724	ALA	-	expression tag	UNP Q6PHU5
D	725	ALA	-	expression tag	UNP Q6PHU5

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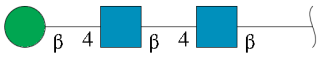
Chain	Residue	Modelled	Actual	Comment	Reference
D	726	HIS	-	expression tag	UNP Q6PHU5
D	727	HIS	-	expression tag	UNP Q6PHU5
D	728	HIS	-	expression tag	UNP Q6PHU5
D	729	HIS	-	expression tag	UNP Q6PHU5
D	730	HIS	-	expression tag	UNP Q6PHU5
D	731	HIS	-	expression tag	UNP Q6PHU5
C	723	ALA	-	expression tag	UNP Q6PHU5
C	724	ALA	-	expression tag	UNP Q6PHU5
C	725	ALA	-	expression tag	UNP Q6PHU5
C	726	HIS	-	expression tag	UNP Q6PHU5
C	727	HIS	-	expression tag	UNP Q6PHU5
C	728	HIS	-	expression tag	UNP Q6PHU5
C	729	HIS	-	expression tag	UNP Q6PHU5
C	730	HIS	-	expression tag	UNP Q6PHU5
C	731	HIS	-	expression tag	UNP Q6PHU5

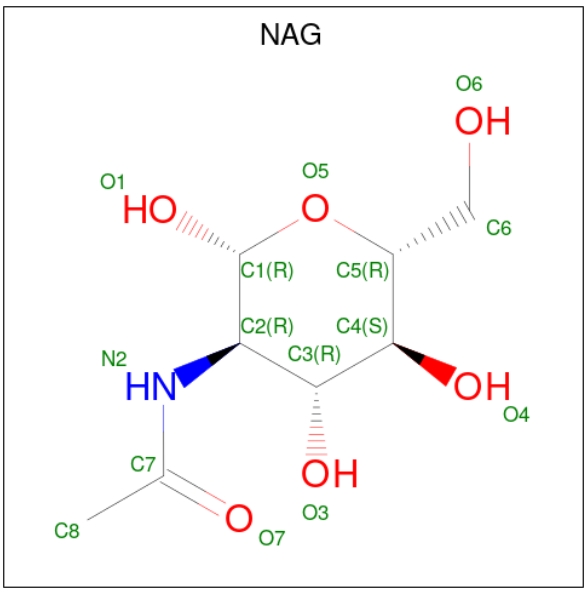
- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	3	Total C N O 39 22 2 15	0	0	0
2	F	3	Total C N O 39 22 2 15	0	0	0
2	G	3	Total C N O 39 22 2 15	0	0	0
2	H	3	Total C N O 39 22 2 15	0	0	0
2	I	3	Total C N O 39 22 2 15	0	0	0
2	J	3	Total C N O 39 22 2 15	0	0	0
2	K	3	Total C N O 39 22 2 15	0	0	0
2	L	3	Total C N O 39 22 2 15	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

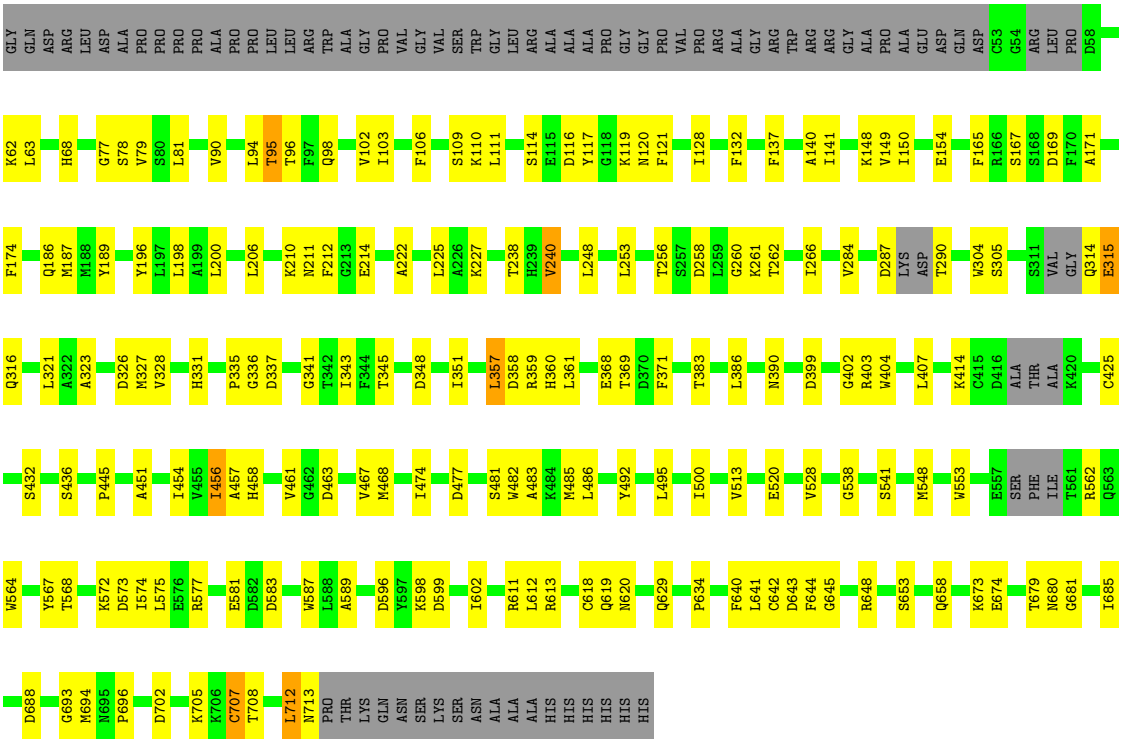
3 Residue-property plots (i)

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: Sortilin

Chain A:

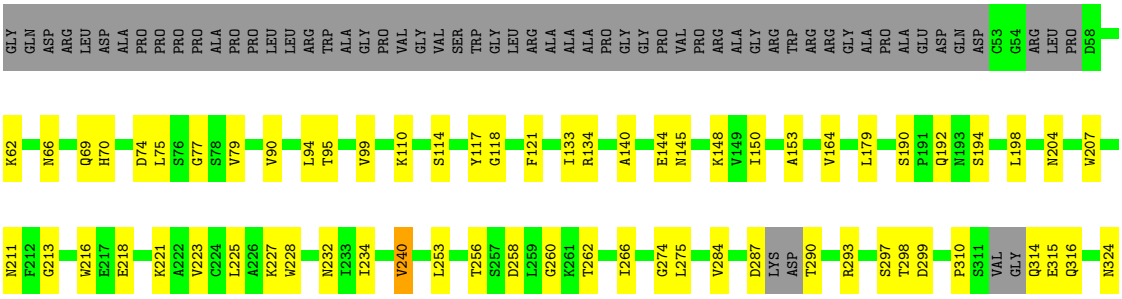


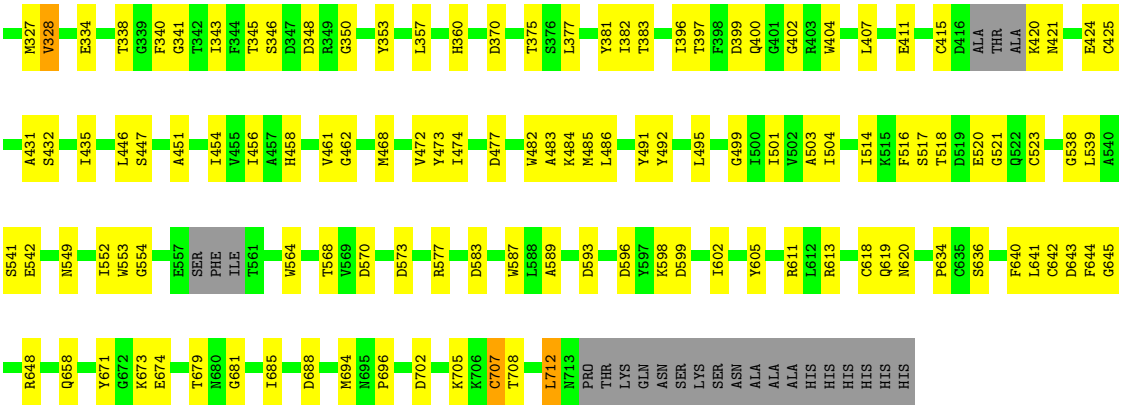


- Molecule 1: Sortilin

Chain B:



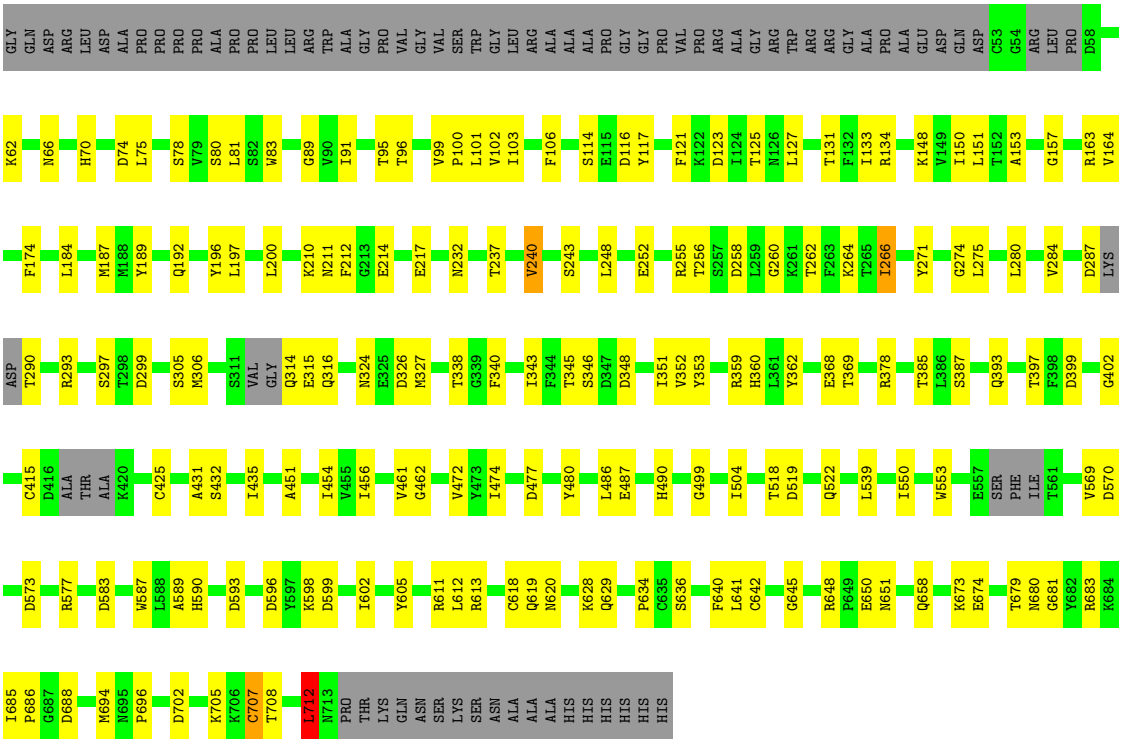




• Molecule 1: Sortilin

Chain D:

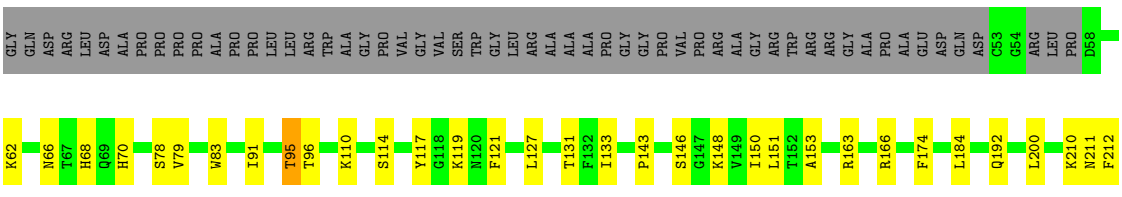


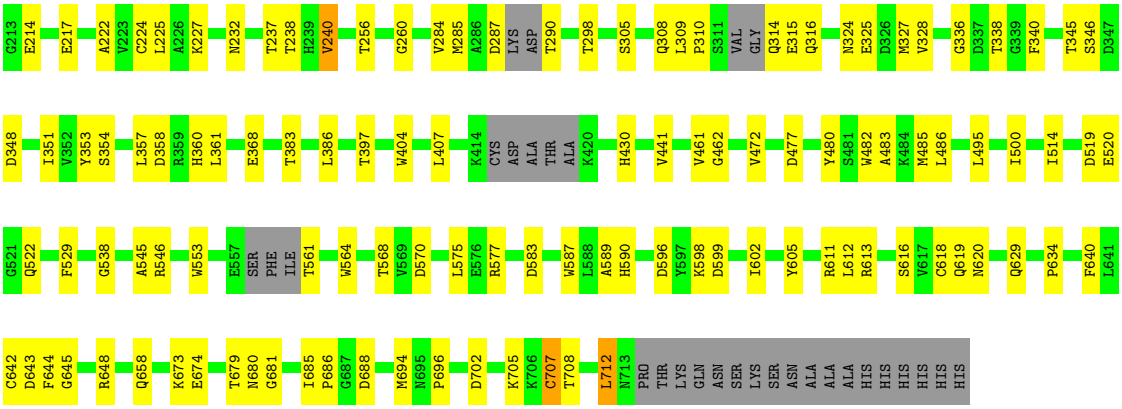


• Molecule 1: Sortilin

Chain C:







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

Chain E:





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

Chain F:





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

Chain G:





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

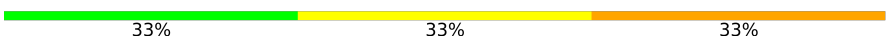
Chain H:





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

Chain I:





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

Chain J:





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

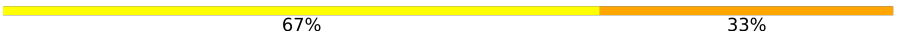
Chain K:





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

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	150.32Å 151.82Å 162.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.72 – 4.00 71.72 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.72-4.00) 99.8 (71.72-4.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 4.01Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.186 , 0.250 0.189 , 0.250	Depositor DCC
R_{free} test set	1436 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	155.7	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 152.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20730	wwPDB-VP
Average B, all atoms (Å^2)	202.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 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	A	0.45	0/5212	0.68	0/7055
1	B	0.43	0/5212	0.63	0/7055
1	C	0.44	1/5198 (0.0%)	0.60	0/7036
1	D	0.47	1/5212 (0.0%)	0.60	0/7055
All	All	0.45	2/20834 (0.0%)	0.63	0/28201

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	712	LEU	C-N	18.84	1.59	1.33
1	C	561	THR	C-N	13.90	1.53	1.33

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	5094	0	4871	132	3
1	B	5094	0	4871	125	0
1	C	5080	0	4864	94	2
1	D	5094	0	4871	115	0
2	E	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	39	0	34	5	0
2	G	39	0	34	6	0
2	H	39	0	34	5	0
2	I	39	0	34	1	0
2	J	39	0	34	3	0
2	K	39	0	33	4	1
2	L	39	0	34	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	4	0
All	All	20730	0	19800	463	3

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 11.

All (463) 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:D:651:ASN:ND2	3:D:801:NAG:C1	1.70	1.50
1:B:298:THR:OG1	1:D:629:GLN:NE2	1.90	1.04
1:D:570:ASP:HB2	2:J:1:NAG:H82	1.47	0.96
2:H:1:NAG:H62	2:H:2:NAG:HN2	1.35	0.90
1:B:298:THR:HG1	1:D:629:GLN:NE2	1.70	0.89
1:C:472:VAL:HB	1:C:486:LEU:HB2	1.54	0.88
1:D:570:ASP:HB2	2:J:1:NAG:C8	2.06	0.85
1:A:513:VAL:HG22	1:A:528:VAL:HG22	1.60	0.84
1:B:375:THR:HA	2:G:1:NAG:O6	1.79	0.83
1:D:651:ASN:CG	3:D:801:NAG:C1	2.54	0.80
1:D:192:GLN:HB3	1:D:232:ASN:OD1	1.81	0.79
1:B:598:LYS:NZ	1:B:634:PRO:O	2.18	0.76
1:C:325:GLU:HG2	2:K:2:NAG:H81	1.69	0.75
1:A:598:LYS:NZ	1:A:634:PRO:O	2.18	0.74
1:D:598:LYS:NZ	1:D:634:PRO:O	2.18	0.74
1:C:598:LYS:NZ	1:C:634:PRO:O	2.18	0.74
1:A:225:LEU:HD21	1:A:227:LYS:HE3	1.69	0.74
1:A:707:CYS:SG	1:A:708:THR:N	2.62	0.73
2:H:1:NAG:H62	2:H:2:NAG:N2	2.04	0.72
1:B:707:CYS:SG	1:B:708:THR:N	2.62	0.72
1:A:572:LYS:NZ	2:F:2:NAG:H81	2.05	0.72
1:D:148:LYS:HD2	1:D:212:PHE:CE1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:HB2	1:C:290:THR:HG22	1.70	0.72
1:D:707:CYS:SG	1:D:708:THR:N	2.62	0.71
1:C:707:CYS:SG	1:C:708:THR:N	2.62	0.71
1:D:210:LYS:HE2	1:D:217:GLU:OE1	1.90	0.71
1:C:324:ASN:HB2	2:K:2:NAG:H82	1.71	0.71
1:B:504:ILE:HD12	1:B:539:LEU:HD22	1.73	0.71
1:D:184:LEU:HD23	1:D:200:LEU:HD23	1.73	0.71
1:D:287:ASP:HB2	1:D:290:THR:HG22	1.72	0.70
1:C:310:PRO:HD3	1:C:644:PHE:CE1	2.26	0.70
1:C:127:LEU:HD21	1:C:174:PHE:HB2	1.74	0.70
1:C:225:LEU:HD21	1:C:227:LYS:HE3	1.72	0.70
1:A:321:LEU:HD11	1:A:331:HIS:HB2	1.74	0.70
1:D:451:ALA:HB1	1:D:454:ILE:HD12	1.74	0.69
1:A:425:CYS:HA	1:A:461:VAL:HG13	1.75	0.68
1:D:651:ASN:ND2	3:D:801:NAG:C2	2.55	0.68
1:D:66:ASN:HB3	1:D:570:ASP:HB3	1.77	0.67
1:C:712:LEU:HD12	1:C:712:LEU:O	1.96	0.66
1:A:304:TRP:CG	1:A:712:LEU:HD11	2.31	0.66
1:B:287:ASP:HB2	1:B:290:THR:HA	1.78	0.66
1:B:456:ILE:HD12	1:B:474:ILE:HD11	1.77	0.65
1:A:316:GLN:HE21	1:A:335:PRO:HD3	1.63	0.64
1:B:324:ASN:HD22	2:G:1:NAG:H81	1.63	0.63
1:B:483:ALA:HB3	1:B:485:MET:HE2	1.82	0.62
1:B:297:SER:OG	1:B:299:ASP:OD1	2.18	0.62
1:A:477:ASP:OD2	1:A:481:SER:OG	2.09	0.62
1:C:192:GLN:HB3	1:C:232:ASN:OD1	1.99	0.62
1:D:258:ASP:OD2	1:D:262:THR:OG1	2.12	0.62
1:D:324:ASN:HB3	2:I:1:NAG:O7	2.00	0.62
1:A:148:LYS:HB3	1:A:212:PHE:CE1	2.35	0.62
1:B:570:ASP:OD2	2:H:1:NAG:O6	2.17	0.61
1:C:287:ASP:HB2	1:C:290:THR:HA	1.82	0.61
1:D:345:THR:O	1:D:353:TYR:HA	2.00	0.61
1:D:297:SER:OG	1:D:299:ASP:OD1	2.19	0.61
1:A:287:ASP:HB2	1:A:290:THR:HG22	1.81	0.60
1:B:407:LEU:HD11	1:B:482:TRP:HE1	1.67	0.60
1:A:327:MET:HE1	1:A:345:THR:HB	1.83	0.60
1:D:369:THR:O	1:D:432:SER:HB2	2.01	0.60
1:D:402:GLY:O	1:D:648:ARG:NH1	2.35	0.60
1:C:361:LEU:HD21	1:C:386:LEU:HB2	1.84	0.59
1:D:62:LYS:O	1:D:66:ASN:ND2	2.35	0.59
1:A:137:PHE:O	1:A:186:GLN:NE2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:GLU:HG3	1:D:705:LYS:HB2	1.85	0.59
1:B:671:TYR:CD2	1:D:628:LYS:HE2	2.38	0.59
1:B:287:ASP:HB2	1:B:290:THR:HG22	1.83	0.59
1:A:674:GLU:HG3	1:A:705:LYS:HB2	1.85	0.59
1:C:256:THR:HG21	1:C:260:GLY:N	2.17	0.59
1:C:310:PRO:HD3	1:C:644:PHE:HE1	1.67	0.58
1:C:674:GLU:HG3	1:C:705:LYS:HB2	1.85	0.58
1:A:694:MET:HG2	1:A:696:PRO:HD3	1.86	0.58
1:A:359:ARG:NE	1:A:386:LEU:O	2.33	0.58
1:B:674:GLU:HG3	1:B:705:LYS:HB2	1.85	0.58
1:B:425:CYS:HA	1:B:461:VAL:HG13	1.84	0.58
1:C:66:ASN:HB3	1:C:570:ASP:HB3	1.86	0.58
1:A:495:LEU:HD23	1:A:541:SER:OG	2.04	0.58
1:C:694:MET:HG2	1:C:696:PRO:HD3	1.86	0.58
1:B:324:ASN:ND2	2:G:1:NAG:H81	2.19	0.58
2:E:1:NAG:O6	2:E:2:NAG:O5	2.19	0.58
1:A:117:TYR:O	1:A:568:THR:HG21	2.04	0.57
1:A:256:THR:HG21	1:A:260:GLY:N	2.19	0.57
1:B:517:SER:OG	1:B:523:CYS:O	2.16	0.57
2:G:1:NAG:H3	2:G:1:NAG:H83	1.87	0.57
1:B:117:TYR:O	1:B:568:THR:HG21	2.04	0.57
1:D:274:GLY:O	1:D:280:LEU:HD12	2.04	0.57
1:D:519:ASP:OD2	1:D:522:GLN:HB2	2.04	0.57
1:A:538:GLY:HA3	1:A:553:TRP:CZ2	2.39	0.57
1:D:694:MET:HG2	1:D:696:PRO:HD3	1.86	0.57
1:B:99:VAL:O	1:B:134:ARG:NH1	2.37	0.57
1:A:572:LYS:HZ2	2:F:2:NAG:H81	1.69	0.57
1:B:383:THR:HG22	1:B:404:TRP:CZ3	2.39	0.57
1:C:545:ALA:O	1:C:546:ARG:HD3	2.05	0.57
1:C:305:SER:HB3	1:C:351:ILE:HD12	1.86	0.56
1:B:225:LEU:HD21	1:B:227:LYS:HE3	1.87	0.56
1:B:673:LYS:HD3	1:B:702:ASP:OD2	2.06	0.56
1:B:694:MET:HG2	1:B:696:PRO:HD3	1.86	0.56
1:A:673:LYS:HD3	1:A:702:ASP:OD2	2.06	0.56
1:C:673:LYS:HD3	1:C:702:ASP:OD2	2.06	0.56
1:D:211:ASN:ND2	1:D:214:GLU:HB3	2.21	0.56
1:C:222:ALA:O	1:C:238:THR:HA	2.06	0.56
1:D:106:PHE:CE1	1:D:157:GLY:HA2	2.41	0.56
1:D:123:ASP:OD1	1:D:125:THR:OG1	2.17	0.55
1:D:593:ASP:OD2	1:D:636:SER:OG	2.17	0.55
1:D:673:LYS:HD3	1:D:702:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLU:HG3	1:B:340:PHE:CE1	2.42	0.55
1:A:114:SER:HB2	1:A:121:PHE:CD2	2.41	0.55
1:A:287:ASP:HB2	1:A:290:THR:HA	1.88	0.55
1:B:314:GLN:O	1:B:316:GLN:HG3	2.06	0.55
1:B:399:ASP:N	1:B:399:ASP:OD1	2.39	0.55
1:C:211:ASN:ND2	1:C:214:GLU:HB3	2.22	0.55
1:A:150:ILE:HG21	1:A:187:MET:HG3	1.88	0.55
1:B:685:ILE:HB	1:B:688:ASP:HB2	1.89	0.55
1:D:343:ILE:HD11	1:D:360:HIS:CE1	2.42	0.55
1:C:131:THR:HG21	1:C:163:ARG:HD2	1.90	0.54
1:C:461:VAL:HG12	1:C:462:GLY:H	1.71	0.54
1:B:90:VAL:HA	1:B:114:SER:O	2.07	0.54
1:C:685:ILE:HB	1:C:688:ASP:HB2	1.89	0.54
1:A:500:ILE:HD11	1:A:575:LEU:HD12	1.90	0.54
1:B:357:LEU:HD22	1:B:404:TRP:CD2	2.41	0.54
1:D:133:ILE:HD13	1:D:153:ALA:HB2	1.89	0.54
1:C:95:THR:HB	1:C:110:LYS:H	1.71	0.54
1:B:451:ALA:HB1	1:B:454:ILE:HD12	1.89	0.54
1:C:210:LYS:HE2	1:C:217:GLU:OE1	2.08	0.54
1:A:368:GLU:OE1	1:A:368:GLU:N	2.40	0.54
1:A:685:ILE:HB	1:A:688:ASP:HB2	1.89	0.54
1:A:679:THR:OG1	1:A:681:GLY:N	2.37	0.54
1:A:548:MET:HE2	1:A:619:GLN:OE1	2.08	0.54
1:D:255:ARG:HB2	1:D:266:ILE:HD13	1.90	0.54
1:D:685:ILE:HB	1:D:688:ASP:HB2	1.89	0.54
1:D:81:LEU:HB3	1:D:553:TRP:CZ3	2.43	0.53
1:D:650:GLU:OE2	3:D:801:NAG:N2	2.42	0.53
1:B:593:ASP:OD2	1:B:636:SER:OG	2.17	0.53
1:B:256:THR:HG21	1:B:260:GLY:N	2.24	0.53
1:B:402:GLY:HA2	1:B:641:LEU:HD23	1.89	0.53
1:D:402:GLY:HA2	1:D:641:LEU:HD23	1.90	0.53
1:A:258:ASP:OD2	1:A:262:THR:OG1	2.15	0.52
1:A:369:THR:O	1:A:432:SER:HB2	2.09	0.52
1:B:538:GLY:HA3	1:B:553:TRP:CZ2	2.43	0.52
1:A:458:HIS:CE1	1:A:492:TYR:HE2	2.27	0.52
1:A:572:LYS:HZ3	2:F:2:NAG:H81	1.74	0.52
1:A:102:VAL:HG23	1:A:103:ILE:HD12	1.92	0.52
1:B:679:THR:OG1	1:B:681:GLY:N	2.37	0.52
1:D:284:VAL:HG21	1:D:712:LEU:HD23	1.90	0.52
1:C:357:LEU:HD12	1:C:358:ASP:N	2.25	0.52
1:B:69:GLN:HG2	1:B:70:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LYS:HD2	1:A:573:ASP:HB3	1.92	0.52
1:A:68:HIS:O	1:A:567:TYR:HA	2.09	0.52
1:C:324:ASN:HB3	2:K:1:NAG:C7	2.39	0.52
1:C:679:THR:OG1	1:C:681:GLY:N	2.37	0.52
1:A:78:SER:HB2	1:A:96:THR:OG1	2.10	0.52
1:D:74:ASP:O	1:D:75:LEU:HD23	2.09	0.52
1:A:451:ALA:HB1	1:A:454:ILE:HD12	1.92	0.51
1:D:62:LYS:HD2	1:D:573:ASP:HB3	1.92	0.51
1:D:293:ARG:HD2	1:D:306:MET:HE3	1.93	0.51
1:C:62:LYS:O	1:C:66:ASN:ND2	2.43	0.51
1:C:360:HIS:HE2	1:C:383:THR:HG1	1.55	0.51
1:B:293:ARG:NH2	1:B:314:GLN:HA	2.24	0.51
1:A:343:ILE:HD11	1:A:360:HIS:CE1	2.45	0.51
1:B:324:ASN:HB3	2:G:1:NAG:O7	2.10	0.51
1:B:504:ILE:HG12	1:B:514:ILE:HD13	1.92	0.51
1:A:68:HIS:CD2	2:F:1:NAG:H81	2.45	0.51
1:A:106:PHE:HE2	1:B:421:ASN:HD22	1.59	0.51
1:A:148:LYS:HD2	1:A:212:PHE:CE1	2.46	0.51
1:D:196:TYR:O	1:D:197:LEU:HD23	2.11	0.51
1:B:421:ASN:HB3	1:B:424:GLU:HB2	1.92	0.50
1:B:499:GLY:O	1:B:518:THR:HA	2.11	0.50
1:D:679:THR:OG1	1:D:681:GLY:N	2.37	0.50
1:C:83:TRP:CH2	1:C:91:ILE:HD11	2.46	0.50
1:C:519:ASP:HB3	1:C:616:SER:H	1.76	0.50
1:C:224:CYS:HB2	1:C:237:THR:OG1	2.11	0.50
1:A:304:TRP:CB	1:A:712:LEU:HD11	2.42	0.50
1:A:458:HIS:CE1	1:A:492:TYR:CE2	3.00	0.50
1:B:491:TYR:O	1:B:503:ALA:HA	2.12	0.50
1:D:127:LEU:HD21	1:D:174:PHE:HB2	1.94	0.49
1:D:583:ASP:O	1:D:613:ARG:HG3	2.12	0.49
1:C:284:VAL:HG21	1:C:712:LEU:HD23	1.93	0.49
1:A:148:LYS:HB3	1:A:212:PHE:HE1	1.78	0.49
1:B:148:LYS:HE3	1:B:194:SER:OG	2.12	0.49
1:A:314:GLN:O	1:A:316:GLN:HG3	2.12	0.49
1:D:425:CYS:HA	1:D:461:VAL:HG13	1.94	0.49
1:C:645:GLY:O	1:C:658:GLN:HG3	2.13	0.49
1:A:645:GLY:O	1:A:658:GLN:HG3	2.13	0.49
1:D:83:TRP:CZ2	1:D:91:ILE:HD11	2.47	0.49
1:B:334:GLU:HG2	1:B:341:GLY:HA2	1.93	0.49
1:D:131:THR:HG21	1:D:163:ARG:HD2	1.94	0.49
1:D:645:GLY:O	1:D:658:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:CYS:HA	1:A:461:VAL:CG1	2.43	0.49
1:A:583:ASP:O	1:A:613:ARG:HG3	2.12	0.49
1:A:114:SER:HB2	1:A:121:PHE:CE2	2.48	0.49
1:D:399:ASP:N	1:D:399:ASP:OD1	2.42	0.49
1:B:501:ILE:HD12	1:B:521:GLY:N	2.28	0.49
1:B:645:GLY:O	1:B:658:GLN:HG3	2.13	0.49
1:D:326:ASP:O	1:D:348:ASP:HA	2.12	0.49
1:C:166:ARG:HD2	1:C:212:PHE:O	2.13	0.49
1:C:583:ASP:O	1:C:613:ARG:HG3	2.13	0.49
1:B:118:GLY:HA3	1:B:568:THR:OG1	2.13	0.48
1:B:504:ILE:CD1	1:B:539:LEU:HD22	2.41	0.48
1:D:522:GLN:NE2	1:D:612:LEU:O	2.46	0.48
1:A:77:GLY:HA2	1:B:468:MET:HE2	1.94	0.48
1:B:207:TRP:CH2	1:B:218:GLU:HB2	2.48	0.48
1:D:461:VAL:HG12	1:D:462:GLY:H	1.77	0.48
1:B:140:ALA:HB3	1:B:150:ILE:HB	1.94	0.48
1:B:583:ASP:O	1:B:613:ARG:HG3	2.12	0.48
1:D:314:GLN:O	1:D:316:GLN:HG3	2.13	0.48
1:C:308:GLN:C	1:C:309:LEU:HD12	2.39	0.48
1:A:456:ILE:HD12	1:A:474:ILE:HD11	1.95	0.48
1:C:495:LEU:HD12	1:C:500:ILE:HB	1.95	0.48
1:A:116:ASP:OD2	1:A:119:LYS:HB3	2.13	0.48
1:A:361:LEU:O	1:A:369:THR:HG22	2.13	0.48
1:D:305:SER:HB3	1:D:351:ILE:HD12	1.94	0.48
1:C:577:ARG:NH2	1:C:618:CYS:HB3	2.29	0.48
1:D:99:VAL:HG12	1:D:134:ARG:HH12	1.79	0.48
1:C:522:GLN:NE2	1:C:612:LEU:O	2.47	0.48
1:A:110:LYS:HB3	1:A:110:LYS:HE3	1.66	0.48
1:A:327:MET:CE	1:A:345:THR:HB	2.44	0.48
1:B:62:LYS:HD2	1:B:573:ASP:HB3	1.96	0.48
1:D:150:ILE:HG12	1:D:189:TYR:OH	2.14	0.48
1:D:387:SER:HB3	1:D:393:GLN:CD	2.39	0.48
1:B:298:THR:HG1	1:D:629:GLN:HE21	1.59	0.47
1:B:411:GLU:OE1	1:B:411:GLU:N	2.41	0.47
1:B:79:VAL:HB	1:B:564:TRP:CZ3	2.49	0.47
1:D:256:THR:HG21	1:D:260:GLY:N	2.28	0.47
1:B:258:ASP:OD2	1:B:262:THR:OG1	2.30	0.47
1:D:346:SER:HA	1:D:352:VAL:O	2.13	0.47
1:D:577:ARG:NH2	1:D:618:CYS:HB3	2.29	0.47
1:A:304:TRP:CG	1:A:712:LEU:CD1	2.97	0.47
1:A:326:ASP:O	1:A:348:ASP:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLY:HA2	1:A:641:LEU:HD23	1.97	0.47
1:B:324:ASN:HB3	2:G:1:NAG:C7	2.44	0.47
1:C:520:GLU:HG3	1:C:612:LEU:HD12	1.96	0.47
1:A:577:ARG:NH2	1:A:618:CYS:HB3	2.29	0.47
1:C:324:ASN:HB3	2:K:1:NAG:O7	2.15	0.47
1:A:132:PHE:CE1	1:A:154:GLU:HB2	2.50	0.47
1:D:570:ASP:HB2	2:J:1:NAG:H81	1.93	0.47
1:D:589:ALA:CB	1:D:602:ILE:HD11	2.45	0.47
1:B:293:ARG:HH22	1:B:314:GLN:HA	1.80	0.47
1:C:146:SER:HB2	1:C:148:LYS:HG2	1.97	0.47
1:C:589:ALA:CB	1:C:602:ILE:HD11	2.45	0.47
1:A:341:GLY:N	1:A:360:HIS:O	2.41	0.46
1:C:407:LEU:HD11	1:C:482:TRP:HE1	1.80	0.46
1:C:480:TYR:CD1	1:C:590:HIS:CD2	3.03	0.46
1:C:70:HIS:CE1	1:C:121:PHE:HB2	2.50	0.46
1:D:284:VAL:CG2	1:D:712:LEU:HD23	2.45	0.46
1:D:327:MET:HB3	1:D:686:PRO:HG2	1.96	0.46
1:D:352:VAL:HB	1:D:683:ARG:HH12	1.80	0.46
1:A:109:SER:OG	1:A:132:PHE:HA	2.15	0.46
1:A:386:LEU:HD11	1:A:390:ASN:HA	1.97	0.46
1:A:643:ASP:OD1	1:A:644:PHE:N	2.45	0.46
1:B:577:ARG:NH2	1:B:618:CYS:HB3	2.29	0.46
1:B:589:ALA:CB	1:B:602:ILE:HD11	2.45	0.46
1:D:150:ILE:O	1:D:151:LEU:HD12	2.15	0.46
1:D:431:ALA:O	1:D:435:ILE:HG12	2.16	0.46
1:D:504:ILE:HD12	1:D:539:LEU:HD22	1.97	0.46
1:A:463:ASP:O	1:A:467:VAL:HG23	2.15	0.46
1:A:572:LYS:HZ3	2:F:2:NAG:C8	2.27	0.46
1:A:357:LEU:HD12	1:A:358:ASP:N	2.30	0.46
1:C:587:TRP:CD2	1:C:611:ARG:NH2	2.84	0.46
1:A:414:LYS:HE2	1:A:414:LYS:HB3	1.63	0.46
1:D:274:GLY:C	1:D:275:LEU:HD12	2.41	0.46
1:A:589:ALA:CB	1:A:602:ILE:HD11	2.45	0.46
1:B:79:VAL:HG21	1:B:564:TRP:CD2	2.51	0.46
1:B:587:TRP:CD2	1:B:611:ARG:NH2	2.84	0.46
1:D:327:MET:HE1	1:D:345:THR:HG22	1.97	0.46
1:D:415:CYS:HB3	1:D:425:CYS:HB3	1.89	0.46
1:D:100:PRO:HB2	1:D:103:ILE:HD13	1.97	0.46
1:D:477:ASP:OD1	1:D:477:ASP:N	2.48	0.46
1:D:640:PHE:CZ	1:D:696:PRO:HD2	2.51	0.46
1:C:117:TYR:O	1:C:568:THR:HG21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD21	1:B:133:ILE:HG21	1.98	0.46
1:D:164:VAL:HG11	1:D:187:MET:HE3	1.98	0.46
1:A:169:ASP:OD1	1:A:169:ASP:N	2.48	0.45
1:A:640:PHE:CZ	1:A:696:PRO:HD2	2.51	0.45
1:D:100:PRO:O	1:D:134:ARG:NH1	2.50	0.45
1:C:285:MET:HB2	1:C:285:MET:HE3	1.66	0.45
1:C:133:ILE:HD13	1:C:153:ALA:HB2	1.97	0.45
1:C:640:PHE:CZ	1:C:696:PRO:HD2	2.51	0.45
1:A:128:ILE:HG22	1:A:165:PHE:CE2	2.51	0.45
1:D:89:GLY:HA2	1:D:117:TYR:CD1	2.52	0.45
1:D:550:ILE:HD11	1:D:569:VAL:HB	1.98	0.45
1:A:211:ASN:ND2	1:A:214:GLU:HB3	2.31	0.45
1:B:446:LEU:HD12	1:B:447:SER:H	1.82	0.45
1:B:514:ILE:HD13	1:B:514:ILE:HA	1.85	0.45
1:D:255:ARG:NH2	1:D:264:LYS:HD3	2.31	0.45
1:D:587:TRP:CD2	1:D:611:ARG:NH2	2.84	0.45
1:A:111:LEU:HB2	1:A:128:ILE:HD11	1.97	0.45
1:A:357:LEU:HD22	1:A:404:TRP:CG	2.51	0.45
1:A:587:TRP:CD2	1:A:611:ARG:NH2	2.83	0.45
1:B:74:ASP:O	1:B:75:LEU:HD23	2.16	0.45
1:B:284:VAL:HG21	1:B:712:LEU:HD23	1.98	0.45
1:B:458:HIS:CE1	1:B:492:TYR:HE2	2.35	0.45
1:D:340:PHE:O	1:D:362:TYR:HE1	1.99	0.45
1:D:346:SER:HB3	1:D:353:TYR:CE2	2.52	0.45
1:D:378:ARG:HH22	1:D:605:TYR:HB2	1.81	0.45
1:A:119:LYS:HG3	1:A:120:ASN:ND2	2.32	0.45
1:A:407:LEU:HD11	1:A:482:TRP:HE1	1.80	0.45
1:B:192:GLN:HB3	1:B:232:ASN:OD1	2.17	0.45
1:B:640:PHE:CZ	1:B:696:PRO:HD2	2.51	0.45
1:C:345:THR:O	1:C:353:TYR:HA	2.16	0.45
1:B:164:VAL:CG1	1:B:179:LEU:HD11	2.46	0.45
1:B:643:ASP:OD1	1:B:644:PHE:N	2.45	0.45
1:B:110:LYS:HB3	1:B:110:LYS:HE3	1.51	0.45
1:B:461:VAL:HG12	1:B:462:GLY:H	1.81	0.45
1:D:243:SER:HB3	1:C:336:GLY:H	1.82	0.45
1:C:480:TYR:CE1	1:C:590:HIS:CD2	3.05	0.45
1:A:79:VAL:HG21	1:A:564:TRP:CD2	2.52	0.44
1:B:204:ASN:HB3	1:B:223:VAL:O	2.17	0.44
1:D:114:SER:HB2	1:D:121:PHE:CD2	2.52	0.44
1:C:514:ILE:HG12	1:C:529:PHE:CD1	2.52	0.44
1:D:359:ARG:O	1:D:385:THR:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASP:HA	1:C:587:TRP:CZ3	2.53	0.44
1:A:305:SER:HB3	1:A:351:ILE:HD12	2.00	0.44
1:A:323:ALA:CB	1:A:328:VAL:HG22	2.47	0.44
1:A:284:VAL:HG21	1:A:712:LEU:HD23	2.00	0.44
1:D:327:MET:HE1	1:D:345:THR:CG2	2.48	0.44
1:B:501:ILE:O	1:B:516:PHE:HA	2.18	0.44
1:B:520:GLU:OE1	1:B:611:ARG:HG3	2.18	0.44
1:A:141:ILE:HD13	1:A:149:VAL:HG13	1.99	0.44
1:B:190:SER:HB2	1:B:228:TRP:CZ2	2.52	0.44
1:B:415:CYS:O	1:B:420:LYS:NZ	2.25	0.44
1:C:79:VAL:HB	1:C:564:TRP:CZ3	2.53	0.44
1:C:314:GLN:O	1:C:316:GLN:HG3	2.17	0.44
1:A:256:THR:HG21	1:A:260:GLY:CA	2.47	0.44
1:B:596:ASP:HA	1:B:599:ASP:HB2	2.00	0.44
1:D:596:ASP:HA	1:D:599:ASP:HB2	2.00	0.44
1:C:150:ILE:O	1:C:151:LEU:HD12	2.18	0.44
1:C:287:ASP:HB2	1:C:290:THR:CG2	2.45	0.44
1:B:327:MET:HE1	1:B:345:THR:CG2	2.47	0.44
1:D:102:VAL:HG23	1:D:103:ILE:HD12	2.00	0.44
1:A:148:LYS:HD2	1:A:212:PHE:CD1	2.53	0.43
1:A:258:ASP:C	1:A:260:GLY:H	2.25	0.43
1:B:66:ASN:HB3	1:B:570:ASP:HB3	2.00	0.43
1:B:70:HIS:NE2	1:B:121:PHE:HB2	2.33	0.43
1:C:500:ILE:HD11	1:C:575:LEU:HD12	1.99	0.43
1:D:472:VAL:HB	1:D:486:LEU:HB2	2.00	0.43
1:D:645:GLY:C	1:D:658:GLN:HG3	2.43	0.43
1:C:645:GLY:C	1:C:658:GLN:HG3	2.43	0.43
1:B:144:GLU:HG3	1:B:145:ASN:OD1	2.18	0.43
1:C:483:ALA:HB3	1:C:485:MET:HE2	2.00	0.43
1:A:63:LEU:HD21	1:A:574:ILE:HG13	2.01	0.43
1:A:399:ASP:OD1	1:A:399:ASP:N	2.52	0.43
1:B:346:SER:OG	1:B:350:GLY:HA2	2.18	0.43
1:B:382:ILE:HG12	1:B:396:ILE:HB	2.01	0.43
1:B:495:LEU:HD23	1:B:541:SER:OG	2.18	0.43
1:C:284:VAL:CG2	1:C:712:LEU:HD23	2.48	0.43
1:C:430:HIS:HB3	1:C:441:VAL:HG21	2.00	0.43
1:B:694:MET:HE3	1:B:694:MET:HB2	1.86	0.43
1:C:310:PRO:HD3	1:C:644:PHE:CD1	2.53	0.43
1:C:368:GLU:OE1	1:C:368:GLU:N	2.47	0.43
1:C:596:ASP:HA	1:C:599:ASP:HB2	2.00	0.43
1:A:198:LEU:HD13	1:A:206:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASP:OD1	1:B:348:ASP:N	2.51	0.43
1:D:499:GLY:O	1:D:518:THR:HA	2.18	0.43
1:C:78:SER:HB2	1:C:96:THR:OG1	2.19	0.43
1:C:310:PRO:CD	1:C:644:PHE:HE1	2.30	0.43
2:L:1:NAG:H62	2:L:2:NAG:HN2	1.83	0.43
1:A:403:ARG:NH1	1:A:653:SER:HB3	2.34	0.43
1:B:645:GLY:C	1:B:658:GLN:HG3	2.44	0.43
1:C:694:MET:HE3	1:C:694:MET:HB2	1.86	0.43
1:A:95:THR:HB	1:A:110:LYS:H	1.84	0.43
1:A:140:ALA:HB3	1:A:150:ILE:HB	2.01	0.43
1:A:414:LYS:H	1:A:414:LYS:HG2	1.55	0.43
1:A:645:GLY:C	1:A:658:GLN:HG3	2.44	0.43
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.89	0.43
1:A:457:ALA:HA	1:A:492:TYR:OH	2.19	0.43
1:C:114:SER:HB2	1:C:121:PHE:CD2	2.54	0.43
1:A:68:HIS:ND1	1:A:119:LYS:HD3	2.34	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.88	0.42
1:D:101:LEU:HD21	1:D:184:LEU:HA	2.01	0.42
1:A:94:LEU:HD13	1:A:111:LEU:HD13	2.00	0.42
1:A:468:MET:HE2	1:B:77:GLY:HA2	2.01	0.42
1:A:562:ARG:HE	1:A:562:ARG:HB3	1.67	0.42
1:B:198:LEU:HA	1:B:207:TRP:O	2.19	0.42
1:B:253:LEU:O	1:B:266:ILE:HG12	2.19	0.42
1:B:287:ASP:O	1:B:290:THR:HG22	2.19	0.42
1:A:596:ASP:HA	1:A:599:ASP:HB2	2.00	0.42
1:D:116:ASP:OD1	1:D:116:ASP:N	2.49	0.42
1:C:328:VAL:N	1:C:346:SER:OG	2.52	0.42
1:A:371:PHE:HA	1:A:383:THR:HB	2.01	0.42
1:B:211:ASN:OD1	1:B:211:ASN:N	2.52	0.42
1:B:274:GLY:C	1:B:275:LEU:HD12	2.45	0.42
1:C:348:ASP:N	1:C:348:ASP:OD1	2.52	0.42
1:A:361:LEU:HD21	1:A:386:LEU:HB2	2.01	0.42
1:B:228:TRP:CH2	1:B:234:ILE:HD11	2.54	0.42
1:D:148:LYS:HD2	1:D:212:PHE:CD1	2.55	0.42
1:B:133:ILE:HD13	1:B:153:ALA:HB2	2.01	0.42
1:B:370:ASP:HA	1:B:431:ALA:HB3	2.02	0.42
1:C:619:GLN:NE2	1:C:620:ASN:O	2.53	0.42
1:A:368:GLU:HB2	1:A:436:SER:OG	2.20	0.42
1:A:619:GLN:NE2	1:A:620:ASN:O	2.53	0.42
1:D:368:GLU:OE1	1:D:368:GLU:N	2.46	0.42
1:A:90:VAL:HG11	1:A:171:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TYR:CD1	1:A:210:LYS:HA	2.55	0.42
1:A:343:ILE:HD11	1:A:360:HIS:ND1	2.34	0.42
1:A:520:GLU:HG3	1:A:612:LEU:HD12	2.02	0.42
1:B:258:ASP:C	1:B:260:GLY:H	2.28	0.42
1:B:343:ILE:HD11	1:B:360:HIS:ND1	2.34	0.42
1:B:407:LEU:HD11	1:B:482:TRP:NE1	2.31	0.42
1:B:619:GLN:NE2	1:B:620:ASN:O	2.53	0.42
1:A:81:LEU:HB3	1:A:553:TRP:CZ3	2.55	0.42
1:A:483:ALA:HB3	1:A:485:MET:HE2	2.02	0.42
1:B:642:CYS:SG	1:B:648:ARG:HG3	2.60	0.42
1:C:256:THR:HG21	1:C:260:GLY:H	1.83	0.42
1:A:327:MET:HE3	1:A:327:MET:HB2	1.73	0.41
1:A:642:CYS:SG	1:A:648:ARG:HG3	2.60	0.41
1:B:554:GLY:O	1:B:564:TRP:HA	2.20	0.41
1:D:70:HIS:CE1	1:D:121:PHE:HB2	2.55	0.41
1:D:619:GLN:NE2	1:D:620:ASN:O	2.53	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.85	0.41
1:B:164:VAL:HG13	1:B:179:LEU:HD11	2.02	0.41
1:C:538:GLY:HA3	1:C:553:TRP:CZ2	2.56	0.41
1:A:445:PRO:HA	1:A:457:ALA:HB2	2.02	0.41
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.72	0.41
1:B:549:ASN:OD1	2:H:1:NAG:O5	2.38	0.41
1:D:78:SER:HB2	1:D:96:THR:OG1	2.19	0.41
1:D:237:THR:HA	1:D:252:GLU:O	2.21	0.41
1:D:487:GLU:O	1:D:490:HIS:HE1	2.03	0.41
1:A:222:ALA:O	1:A:238:THR:HA	2.21	0.41
1:B:446:LEU:HD12	1:B:447:SER:N	2.36	0.41
1:C:605:TYR:HD1	1:C:605:TYR:HA	1.75	0.41
1:A:140:ALA:O	1:A:189:TYR:OH	2.32	0.41
1:B:431:ALA:O	1:B:435:ILE:HG12	2.20	0.41
1:C:397:THR:HG22	1:C:404:TRP:CZ3	2.55	0.41
1:B:425:CYS:HA	1:B:461:VAL:CG1	2.51	0.41
1:B:605:TYR:HD1	1:B:605:TYR:HA	1.75	0.41
1:D:642:CYS:SG	1:D:648:ARG:HG3	2.60	0.41
1:D:694:MET:HE3	1:D:694:MET:HB2	1.86	0.41
1:A:167:SER:HB2	1:A:174:PHE:CD2	2.55	0.41
1:A:167:SER:HB2	1:A:174:PHE:CE2	2.55	0.41
1:B:381:TYR:HE1	1:B:400:GLN:HG3	1.85	0.41
1:D:210:LYS:HE2	1:D:217:GLU:CD	2.46	0.41
1:C:310:PRO:CD	1:C:644:PHE:CE1	3.01	0.41
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:MET:HE3	1:A:694:MET:HB2	1.86	0.41
1:C:68:HIS:CD2	1:C:119:LYS:HD3	2.56	0.41
1:C:327:MET:HB3	1:C:686:PRO:HG2	2.03	0.41
1:C:327:MET:HE1	1:C:345:THR:HB	2.02	0.41
1:A:256:THR:HG23	1:A:262:THR:O	2.21	0.41
1:A:336:GLY:O	1:A:337:ASP:C	2.64	0.41
1:A:348:ASP:OD1	1:A:348:ASP:N	2.47	0.41
1:A:485:MET:O	1:A:486:LEU:HD23	2.21	0.41
1:B:310:PRO:N	1:B:644:PHE:HE1	2.19	0.41
1:B:542:GLU:CD	2:H:1:NAG:HN2	2.29	0.41
1:D:293:ARG:HH22	1:D:314:GLN:HA	1.86	0.41
1:A:253:LEU:O	1:A:266:ILE:HG12	2.21	0.40
1:B:477:ASP:OD1	1:B:477:ASP:N	2.48	0.40
1:C:184:LEU:HD23	1:C:200:LEU:HD23	2.03	0.40
1:C:340:PHE:HA	1:C:360:HIS:O	2.21	0.40
1:B:213:GLY:HA2	1:B:216:TRP:CZ2	2.56	0.40
1:B:221:LYS:HB3	1:B:221:LYS:HE2	1.72	0.40
1:D:480:TYR:CD1	1:D:590:HIS:CD2	3.08	0.40
1:D:679:THR:OG1	1:D:680:ASN:N	2.54	0.40
1:C:143:PRO:HB2	1:C:146:SER:HB3	2.03	0.40
1:C:679:THR:OG1	1:C:680:ASN:N	2.54	0.40
1:B:472:VAL:HB	1:B:486:LEU:HB2	2.04	0.40
1:C:642:CYS:SG	1:C:648:ARG:HG3	2.60	0.40
1:A:331:HIS:CE1	1:A:341:GLY:HA3	2.57	0.40
1:D:248:LEU:HB3	1:D:271:TYR:CE1	2.57	0.40
1:A:679:THR:OG1	1:A:680:ASN:N	2.54	0.40
1:B:328:VAL:HG11	1:B:353:TYR:OH	2.22	0.40
1:B:473:TYR:CE2	1:B:484:LYS:HB2	2.56	0.40
1:D:343:ILE:HD11	1:D:360:HIS:ND1	2.37	0.40
1:D:456:ILE:HD12	1:D:474:ILE:HD11	2.04	0.40
1:C:643:ASP:OD1	1:C:644:PHE:N	2.45	0.40

All (3) 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:A:629:GLN:NE2	2:K:2:NAG:O4[1_554]	1.84	0.36
1:A:581:GLU:OE2	1:C:298:THR:OG1[1_554]	2.12	0.08
1:A:693:GLY:CA	1:C:629:GLN:NE2[1_554]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/732 (87%)	592 (93%)	42 (7%)	2 (0%)	36	70
1	B	636/732 (87%)	592 (93%)	43 (7%)	1 (0%)	43	75
1	C	634/732 (87%)	596 (94%)	37 (6%)	1 (0%)	43	75
1	D	636/732 (87%)	591 (93%)	44 (7%)	1 (0%)	43	75
All	All	2542/2928 (87%)	2371 (93%)	166 (6%)	5 (0%)	43	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	C	240	VAL
1	B	240	VAL
1	D	240	VAL
1	A	240	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/626 (90%)	556 (98%)	9 (2%)	55	70
1	B	565/626 (90%)	555 (98%)	10 (2%)	51	68
1	C	563/626 (90%)	556 (99%)	7 (1%)	63	73
1	D	565/626 (90%)	556 (98%)	9 (2%)	55	70
All	All	2258/2504 (90%)	2223 (98%)	35 (2%)	55	70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
1	A	98	GLN
1	A	240	VAL
1	A	315	GLU
1	A	357	LEU
1	A	456	ILE
1	A	707	CYS
1	A	712	LEU
1	A	713	ASN
1	B	95	THR
1	B	240	VAL
1	B	315	GLU
1	B	328	VAL
1	B	338	THR
1	B	397	THR
1	B	432	SER
1	B	552	ILE
1	B	707	CYS
1	B	712	LEU
1	D	80	SER
1	D	95	THR
1	D	240	VAL
1	D	266	ILE
1	D	315	GLU
1	D	338	THR
1	D	397	THR
1	D	707	CYS
1	D	712	LEU
1	C	95	THR
1	C	240	VAL
1	C	315	GLU
1	C	338	THR
1	C	354	SER
1	C	707	CYS
1	C	712	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	300	GLN

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Mol	Chain	Res	Type
1	A	308	GLN
1	A	316	GLN
1	A	400	GLN
1	A	506	HIS
1	A	658	GLN
1	B	506	HIS
1	B	658	GLN
1	D	70	HIS
1	D	316	GLN
1	D	331	HIS
1	D	400	GLN
1	D	423	ASN
1	D	437	GLN
1	D	506	HIS
1	D	522	GLN
1	D	525	GLN
1	D	629	GLN
1	D	658	GLN
1	C	68	HIS
1	C	186	GLN
1	C	400	GLN
1	C	437	GLN
1	C	590	HIS
1	C	658	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

24 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	E	1	2,1	14,14,15	0.61	0	17,19,21	2.18	5 (29%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	2.56	7 (41%)
2	BMA	E	3	2	11,11,12	0.52	0	15,15,17	1.51	4 (26%)
2	NAG	F	1	2,1	14,14,15	0.66	0	17,19,21	1.51	4 (23%)
2	NAG	F	2	2	14,14,15	0.43	0	17,19,21	1.36	3 (17%)
2	BMA	F	3	2	11,11,12	0.37	0	15,15,17	1.05	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.58	0	17,19,21	2.46	7 (41%)
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.75	0
2	BMA	G	3	2	11,11,12	0.30	0	15,15,17	0.83	0
2	NAG	H	1	2,1	14,14,15	0.71	0	17,19,21	2.74	6 (35%)
2	NAG	H	2	2	14,14,15	0.36	0	17,19,21	1.14	1 (5%)
2	BMA	H	3	2	11,11,12	0.32	0	15,15,17	0.98	0
2	NAG	I	1	2,1	14,14,15	0.69	0	17,19,21	1.34	3 (17%)
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	1.62	2 (11%)
2	BMA	I	3	2	11,11,12	0.41	0	15,15,17	0.82	0
2	NAG	J	1	2,1	14,14,15	0.48	0	17,19,21	1.66	4 (23%)
2	NAG	J	2	2	14,14,15	0.37	0	17,19,21	1.69	4 (23%)
2	BMA	J	3	2	11,11,12	0.37	0	15,15,17	0.99	1 (6%)
2	NAG	K	1	2,1	14,14,15	0.57	0	17,19,21	1.34	3 (17%)
2	NAG	K	2	2	14,14,15	0.58	0	17,19,21	2.26	4 (23%)
2	BMA	K	3	2	11,11,12	0.68	0	15,15,17	1.43	3 (20%)
2	NAG	L	1	2,1	14,14,15	0.53	0	17,19,21	0.85	0
2	NAG	L	2	2	14,14,15	0.41	0	17,19,21	1.50	4 (23%)
2	BMA	L	3	2	11,11,12	0.53	0	15,15,17	1.38	3 (20%)

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	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	BMA	L	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAG	C2-N2-C7	7.65	133.15	122.90
2	G	1	NAG	C2-N2-C7	7.18	132.52	122.90
2	K	2	NAG	O4-C4-C3	-7.13	93.56	110.38
2	E	2	NAG	C1-O5-C5	6.52	120.92	112.19
2	H	1	NAG	C1-O5-C5	5.32	119.31	112.19
2	E	1	NAG	C4-C3-C2	-4.40	104.56	111.02
2	I	2	NAG	C2-N2-C7	4.40	128.80	122.90
2	E	1	NAG	O4-C4-C3	4.23	120.34	110.38
2	K	2	NAG	C4-C3-C2	4.13	117.07	111.02
2	E	1	NAG	O5-C5-C6	4.05	115.55	107.66
2	E	2	NAG	C3-C4-C5	-3.87	103.22	110.23
2	J	2	NAG	O5-C1-C2	-3.83	105.37	111.29
2	G	1	NAG	O6-C6-C5	-3.81	98.35	111.33
2	F	1	NAG	O5-C5-C6	-3.60	100.66	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	C1-O5-C5	3.44	116.80	112.19
2	H	2	NAG	C2-N2-C7	3.35	127.39	122.90
2	E	2	NAG	O4-C4-C3	3.34	118.25	110.38
2	J	1	NAG	C2-N2-C7	3.29	127.31	122.90
2	E	2	NAG	C1-C2-N2	3.27	115.59	110.43
2	H	1	NAG	C1-C2-N2	3.25	115.56	110.43
2	E	2	NAG	O5-C1-C2	-3.22	106.31	111.29
2	L	2	NAG	C2-N2-C7	3.21	127.20	122.90
2	E	2	NAG	O3-C3-C4	3.07	117.61	110.38
2	E	3	BMA	O3-C3-C2	3.06	116.31	110.05
2	L	3	BMA	C1-O5-C5	-2.99	108.19	112.19
2	J	1	NAG	O4-C4-C5	2.95	116.58	109.32
2	J	2	NAG	C1-C2-N2	2.91	115.02	110.43
2	H	1	NAG	O5-C1-C2	-2.89	106.82	111.29
2	J	1	NAG	C6-C5-C4	2.88	120.10	113.02
2	E	1	NAG	O5-C5-C4	-2.85	103.89	110.83
2	G	1	NAG	C8-C7-N2	2.79	120.75	116.12
2	F	1	NAG	O4-C4-C3	2.78	116.93	110.38
2	F	2	NAG	C1-O5-C5	2.76	115.88	112.19
2	L	2	NAG	O4-C4-C5	-2.75	102.54	109.32
2	E	3	BMA	O4-C4-C3	-2.74	103.92	110.38
2	G	1	NAG	O5-C1-C2	-2.67	107.15	111.29
2	K	3	BMA	O2-C2-C3	-2.61	104.74	110.15
2	K	1	NAG	O3-C3-C2	2.61	114.82	109.40
2	L	3	BMA	O5-C5-C6	2.59	112.70	107.66
2	E	2	NAG	C4-C3-C2	-2.58	107.23	111.02
2	H	1	NAG	C8-C7-N2	2.54	120.33	116.12
2	K	3	BMA	C1-O5-C5	-2.54	108.78	112.19
2	H	1	NAG	O5-C5-C6	-2.50	102.79	107.66
2	G	1	NAG	O7-C7-N2	-2.50	117.56	121.98
2	E	1	NAG	O4-C4-C5	2.45	115.35	109.32
2	L	3	BMA	C1-C2-C3	-2.43	106.10	109.64
2	I	1	NAG	C2-N2-C7	-2.42	119.66	122.90
2	K	3	BMA	C6-C5-C4	2.42	118.95	113.02
2	L	2	NAG	O4-C4-C3	-2.38	104.76	110.38
2	G	1	NAG	O5-C5-C6	-2.38	103.03	107.66
2	K	1	NAG	C2-N2-C7	2.35	126.05	122.90
2	J	3	BMA	C1-C2-C3	-2.34	106.23	109.64
2	I	1	NAG	O4-C4-C3	2.34	115.88	110.38
2	F	1	NAG	O6-C6-C5	-2.27	103.59	111.33
2	I	2	NAG	C1-O5-C5	2.26	115.22	112.19
2	F	3	BMA	O2-C2-C3	-2.20	105.59	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	C3-C4-C5	-2.17	106.30	110.23
2	I	1	NAG	C1-O5-C5	2.17	115.09	112.19
2	J	1	NAG	O5-C1-C2	2.17	114.64	111.29
2	K	2	NAG	C2-N2-C7	2.13	125.75	122.90
2	K	2	NAG	C1-C2-N2	2.12	113.78	110.43
2	K	1	NAG	O5-C1-C2	-2.11	108.02	111.29
2	E	3	BMA	O3-C3-C4	-2.09	105.46	110.38
2	G	1	NAG	O4-C4-C3	-2.07	105.49	110.38
2	F	2	NAG	O5-C1-C2	-2.06	108.10	111.29
2	L	2	NAG	O5-C1-C2	-2.06	108.10	111.29
2	F	2	NAG	C3-C4-C5	-2.06	106.50	110.23
2	F	1	NAG	O4-C4-C5	-2.06	104.25	109.32
2	E	3	BMA	O4-C4-C5	2.02	114.31	109.32

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	I	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	L	3	BMA	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C4-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7

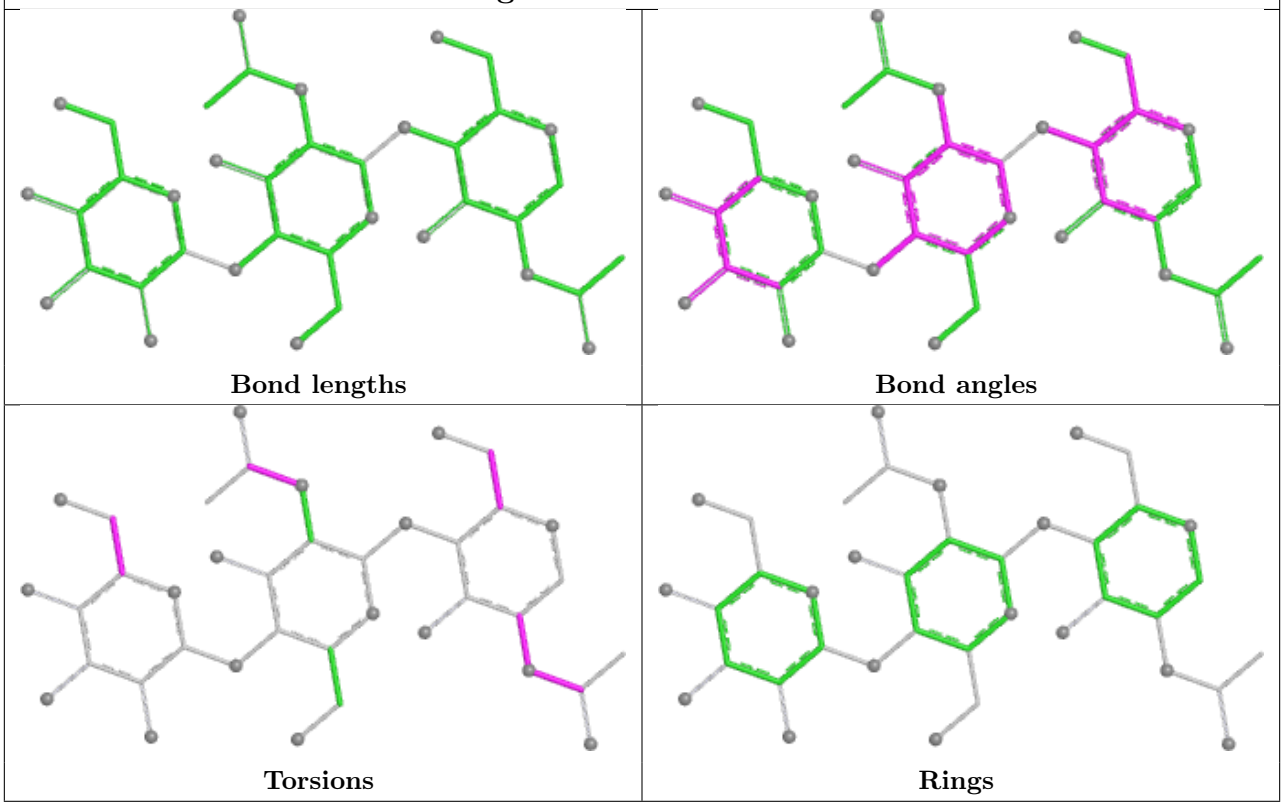
There are no ring outliers.

13 monomers are involved in 27 short contacts:

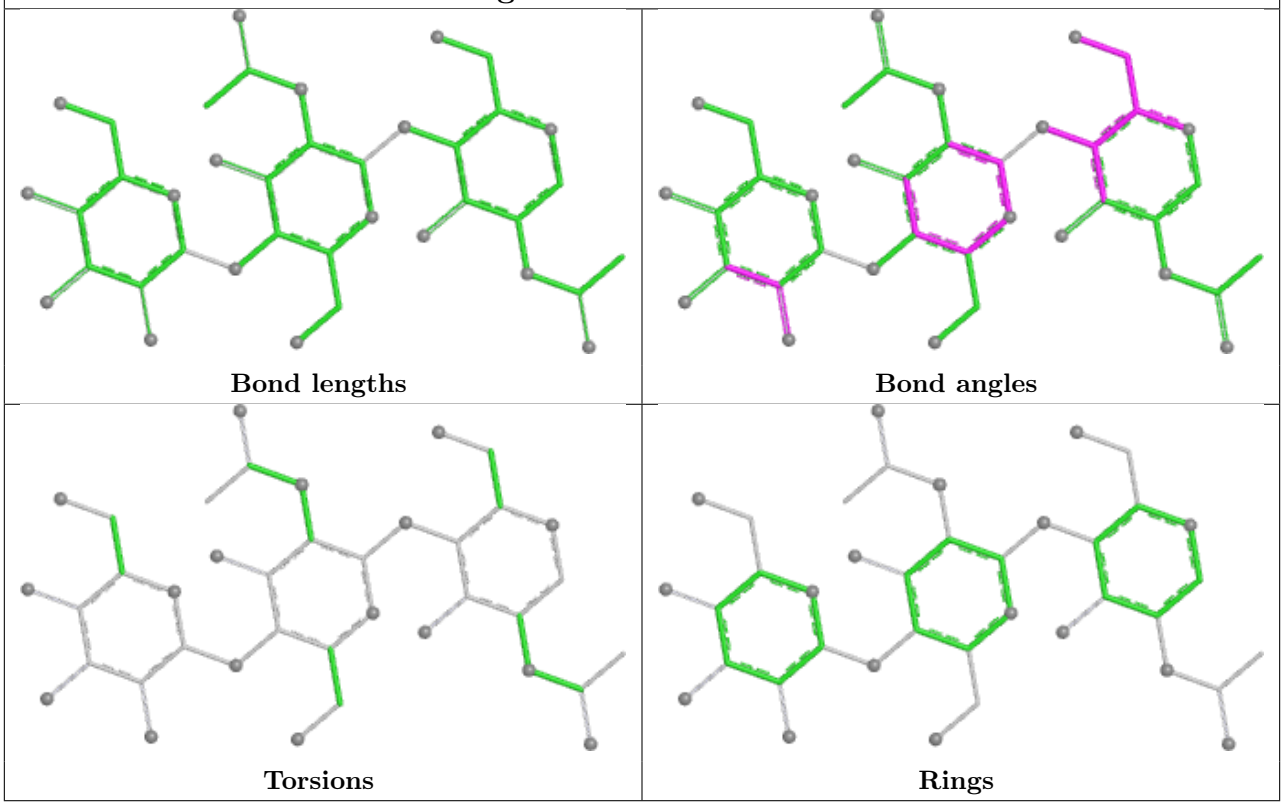
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	2	0
2	L	1	NAG	1	0
2	J	1	NAG	3	0
2	F	1	NAG	1	0
2	L	2	NAG	1	0
2	F	2	NAG	4	0
2	K	2	NAG	2	1
2	G	1	NAG	6	0
2	E	2	NAG	1	0
2	H	1	NAG	5	0
2	I	1	NAG	1	0
2	K	1	NAG	2	0
2	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

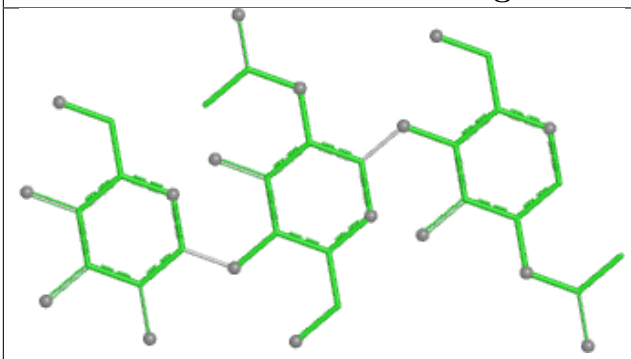
Oligosaccharide Chain E



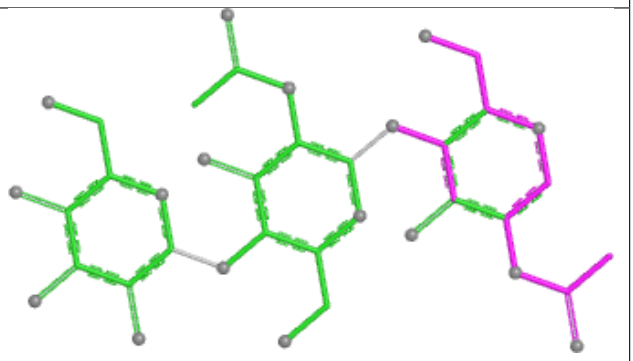
Oligosaccharide Chain F



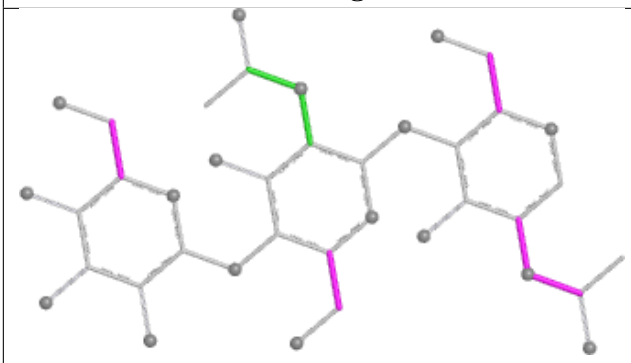
Oligosaccharide Chain G



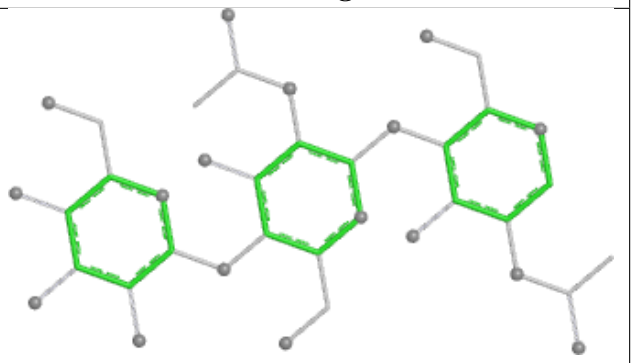
Bond lengths



Bond angles

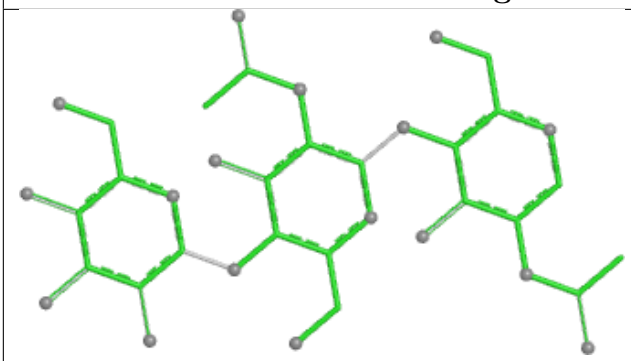


Torsions

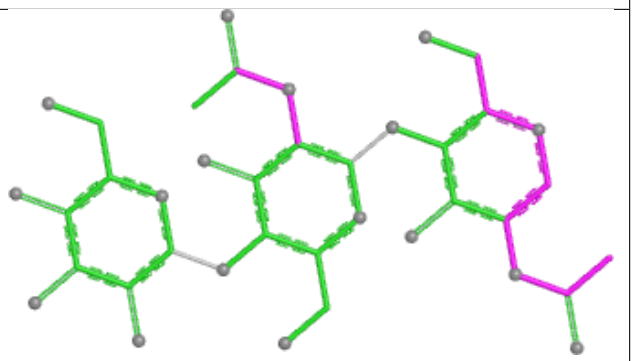


Rings

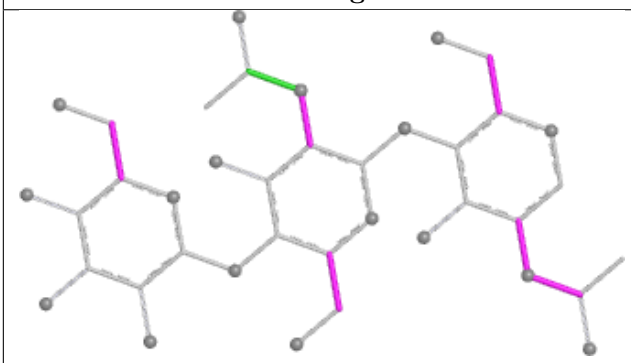
Oligosaccharide Chain H



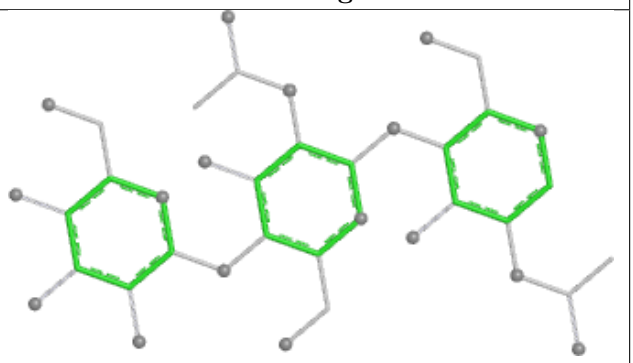
Bond lengths



Bond angles

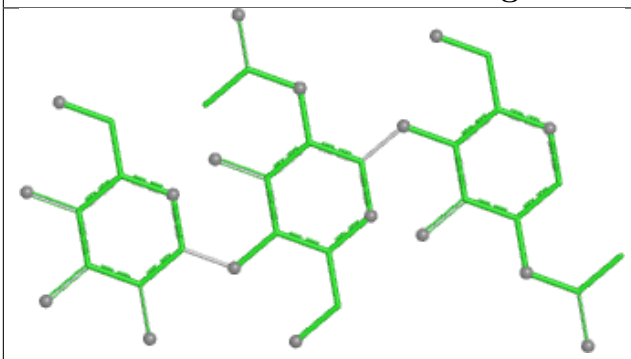


Torsions

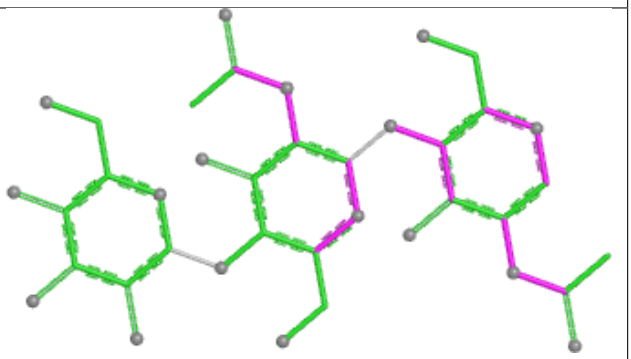


Rings

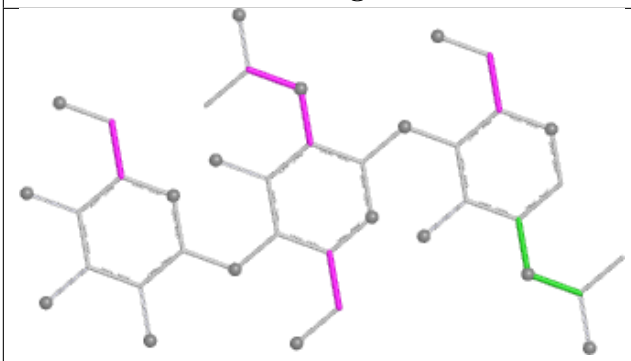
Oligosaccharide Chain I



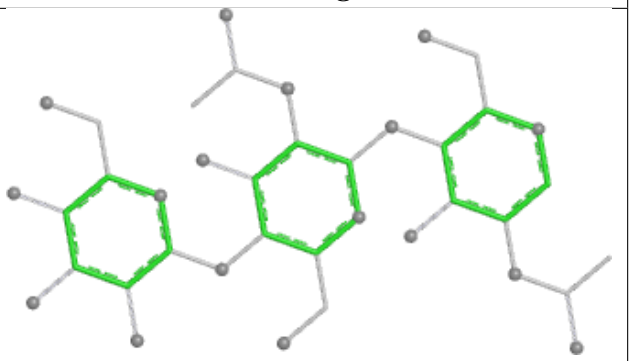
Bond lengths



Bond angles

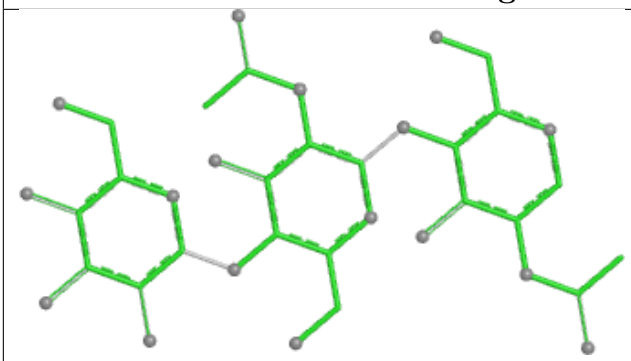


Torsions

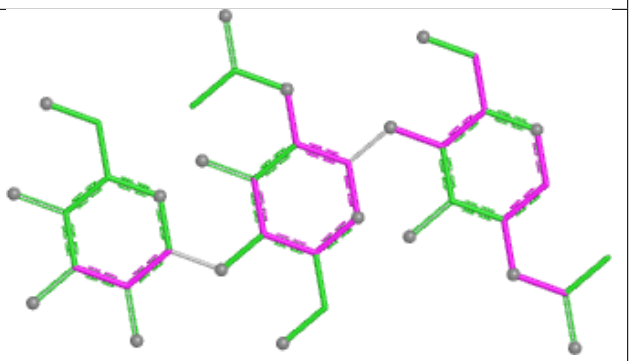


Rings

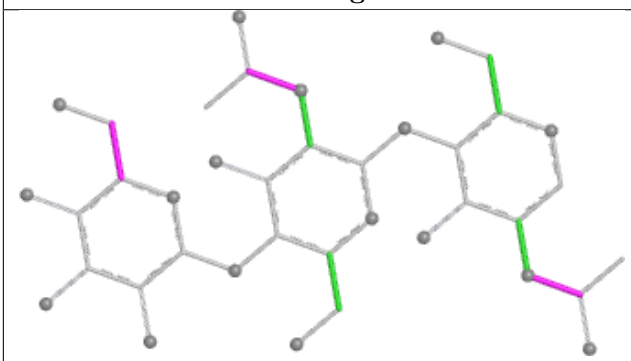
Oligosaccharide Chain J



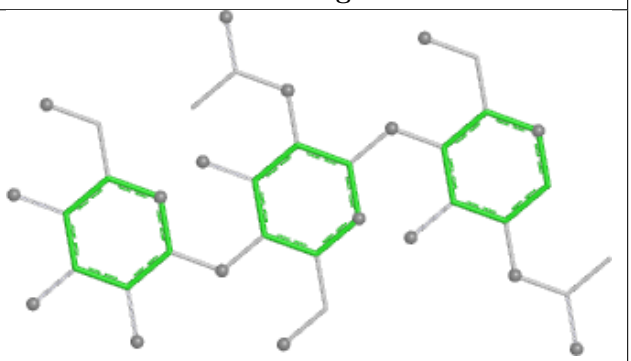
Bond lengths



Bond angles

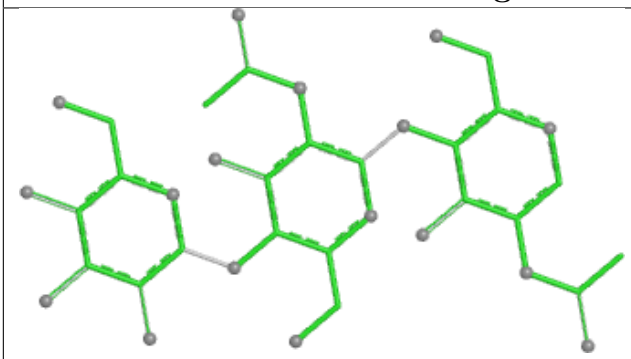


Torsions

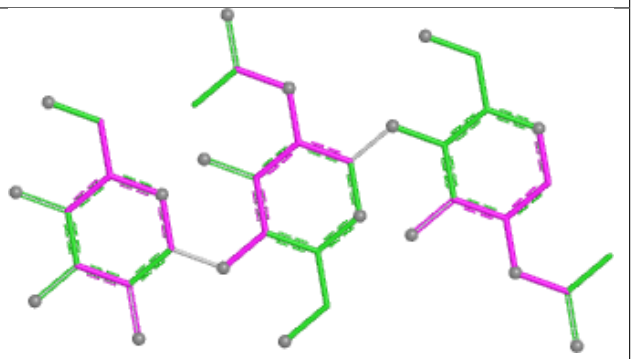


Rings

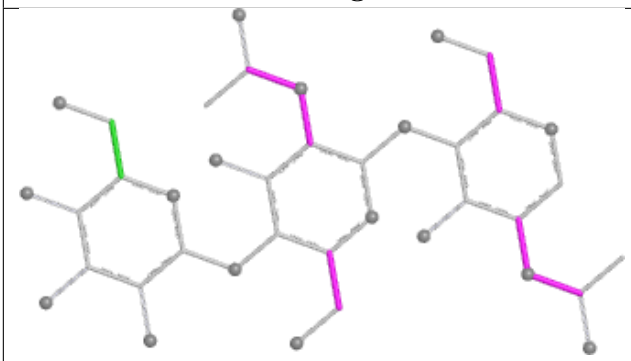
Oligosaccharide Chain K



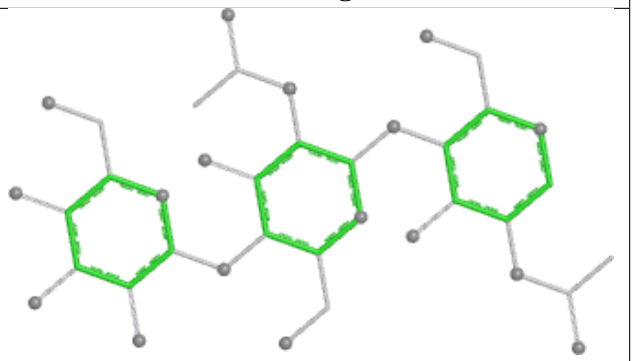
Bond lengths



Bond angles

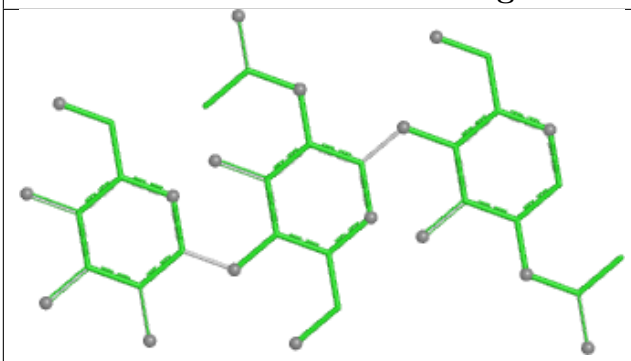


Torsions

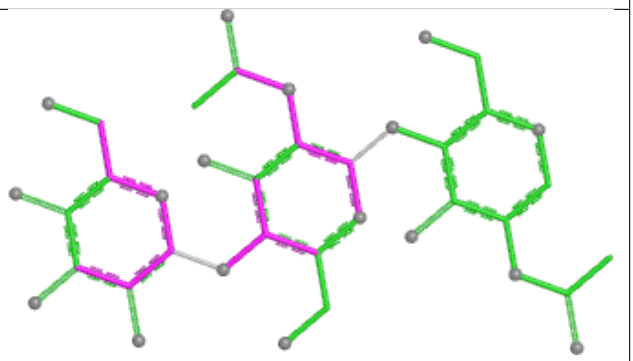


Rings

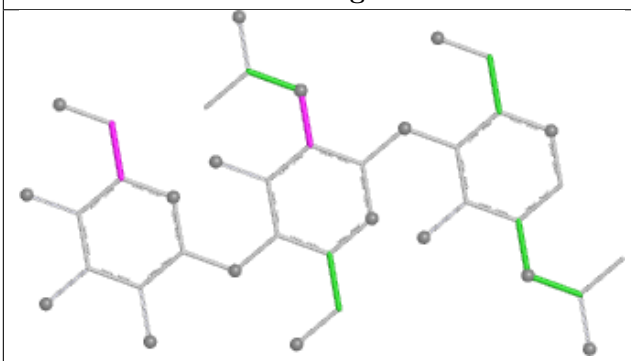
Oligosaccharide Chain L



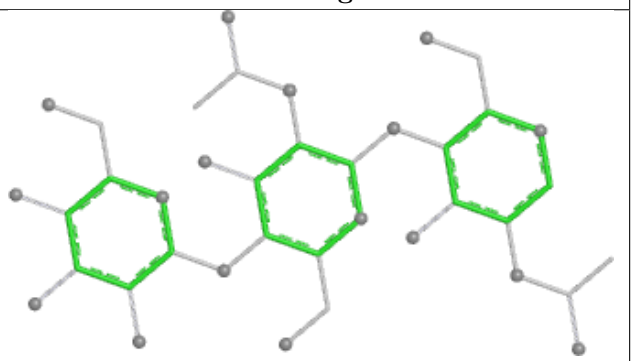
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	801	1	14,14,15	0.51	0	17,19,21	1.68	5 (29%)
3	NAG	B	801	1	14,14,15	0.36	0	17,19,21	0.63	0
3	NAG	D	801	-	14,14,15	0.47	0	17,19,21	0.92	0
3	NAG	A	801	1	14,14,15	0.44	0	17,19,21	0.78	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	C	801	1	-	1/6/23/26	0/1/1/1
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	801	-	-	3/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	801	NAG	C1-C2-N2	3.58	116.08	110.43
3	C	801	NAG	O5-C5-C6	2.70	112.91	107.66
3	C	801	NAG	C6-C5-C4	-2.56	106.74	113.02
3	C	801	NAG	C2-N2-C7	2.38	126.08	122.90
3	C	801	NAG	O3-C3-C2	-2.06	105.12	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	801	NAG	O5-C5-C6-O6
3	D	801	NAG	C4-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6
3	D	801	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	648/732 (88%)	-0.79	0	100	100	107, 178, 239, 297	0
1	B	648/732 (88%)	-0.88	0	100	100	107, 190, 259, 330	0
1	C	646/732 (88%)	-0.85	0	100	100	115, 205, 289, 342	0
1	D	648/732 (88%)	-0.86	0	100	100	133, 224, 288, 377	0
All	All	2590/2928 (88%)	-0.84	0	100	100	107, 198, 279, 377	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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	BMA	I	3	11/12	-0.08	0.12	261,279,288,288	0
2	BMA	E	3	11/12	-0.03	0.12	206,230,249,249	0
2	BMA	L	3	11/12	0.36	0.09	278,289,293,296	0
2	BMA	K	3	11/12	0.38	0.09	152,196,221,225	0
2	BMA	H	3	11/12	0.49	0.07	291,303,307,307	0
2	BMA	G	3	11/12	0.57	0.08	298,309,326,334	0
2	BMA	J	3	11/12	0.58	0.05	261,306,326,336	0
2	NAG	J	2	14/15	0.62	0.05	278,294,311,313	0
2	BMA	F	3	11/12	0.65	0.05	234,273,285,294	0

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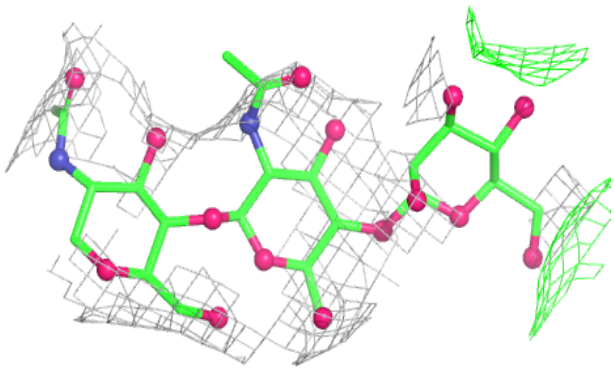
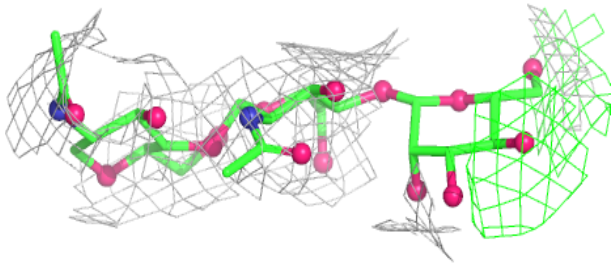
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.67	0.05	257,282,301,305	0
2	NAG	L	2	14/15	0.72	0.06	247,259,269,275	0
2	NAG	J	1	14/15	0.79	0.05	251,284,301,311	0
2	NAG	K	2	14/15	0.81	0.07	176,203,223,227	0
2	NAG	H	1	14/15	0.84	0.08	265,276,320,355	0
2	NAG	L	1	14/15	0.84	0.06	229,252,264,284	0
2	NAG	E	2	14/15	0.87	0.07	175,211,235,238	0
2	NAG	F	2	14/15	0.87	0.04	208,231,258,275	0
2	NAG	I	2	14/15	0.90	0.05	210,227,245,261	0
2	NAG	G	1	14/15	0.90	0.07	179,207,223,228	0
2	NAG	G	2	14/15	0.92	0.07	178,204,242,277	0
2	NAG	F	1	14/15	0.93	0.04	152,186,216,223	0
2	NAG	K	1	14/15	0.95	0.05	154,172,182,186	0
2	NAG	I	1	14/15	0.95	0.08	142,168,192,207	0
2	NAG	E	1	14/15	0.98	0.05	128,153,176,202	0

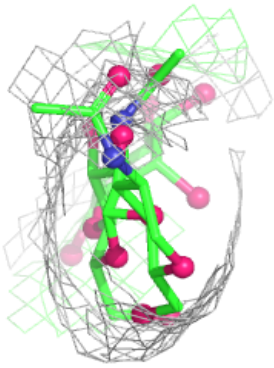
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

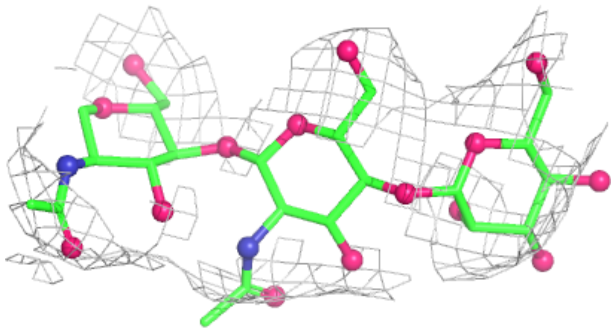


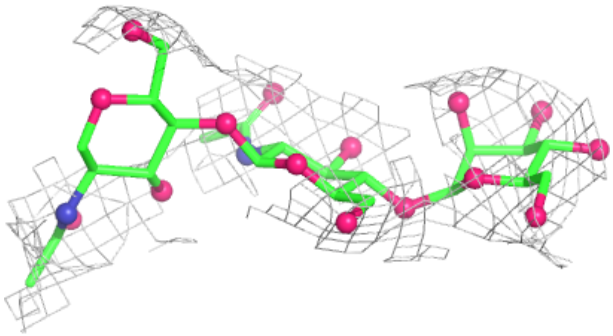


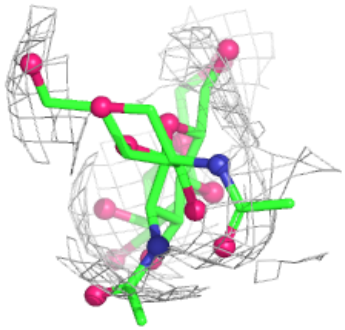


Electron density around Chain F:

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

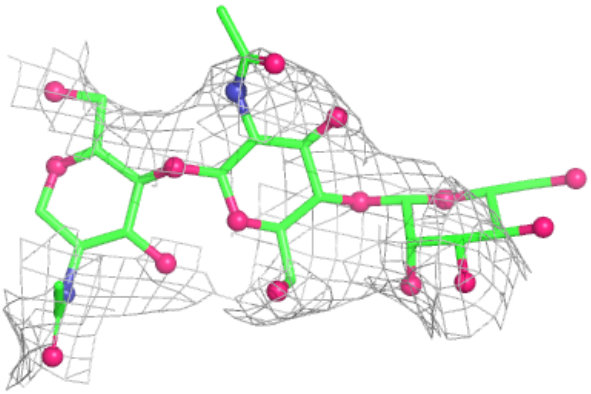


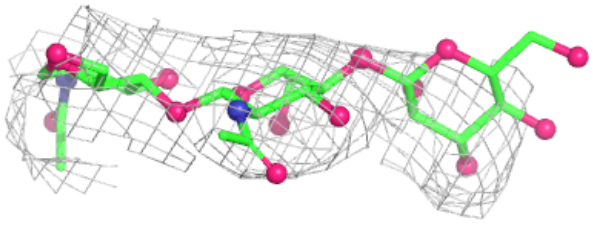


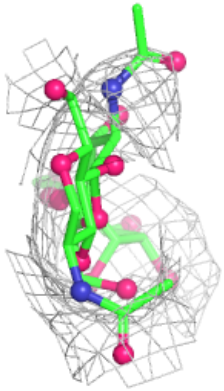


Electron density around Chain G:

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

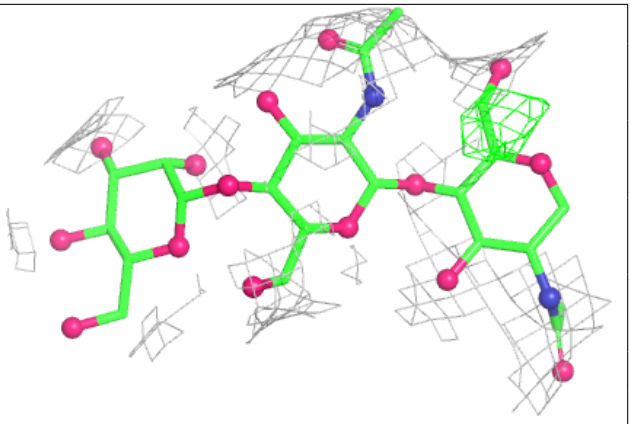


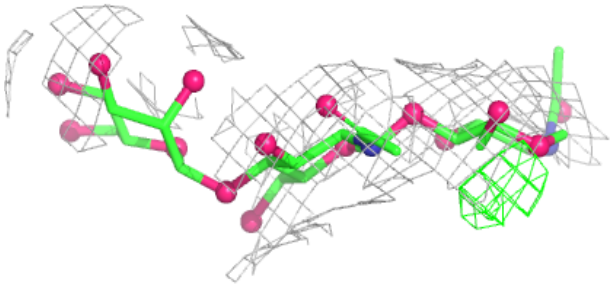


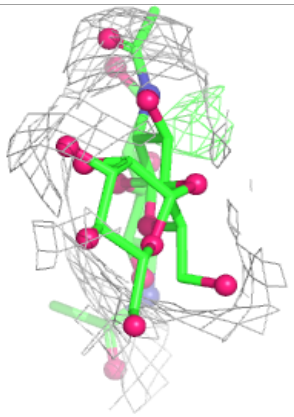


Electron density around Chain H:

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

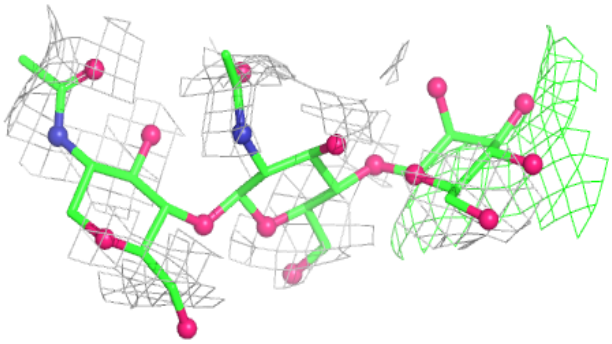


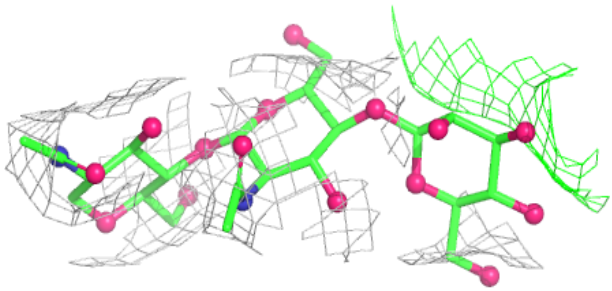


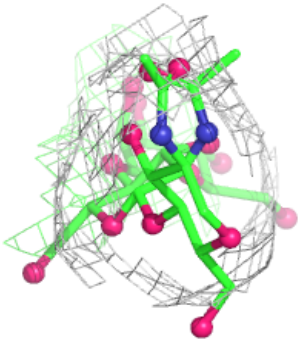


Electron density around Chain I:

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

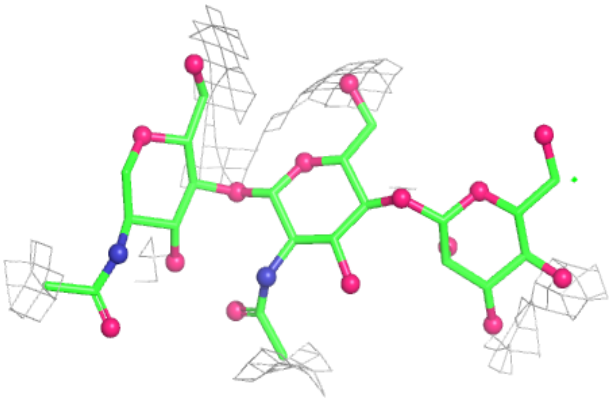


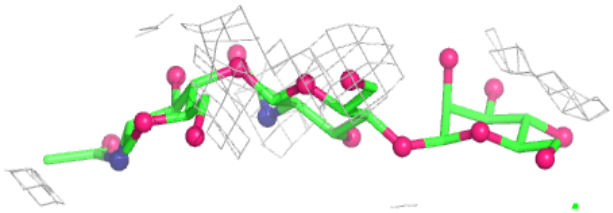


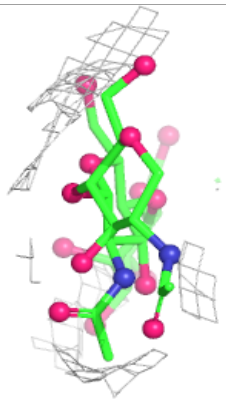


Electron density around Chain J:

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

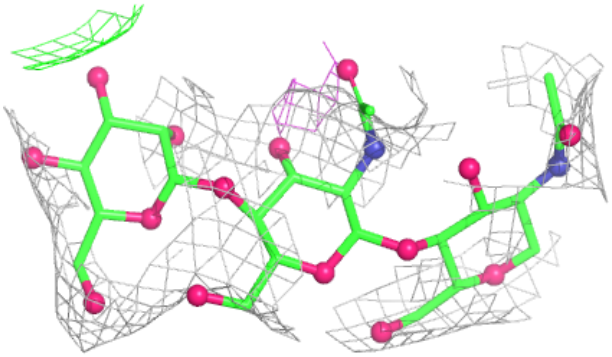


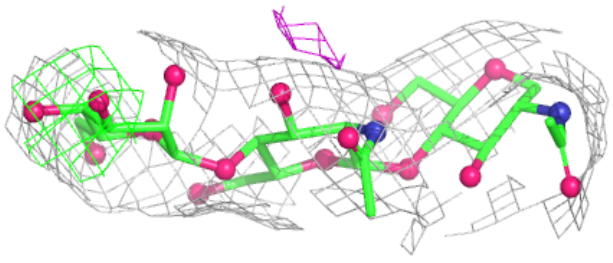


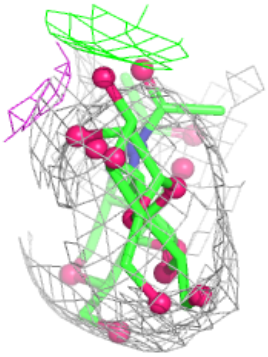


Electron density around Chain K:

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

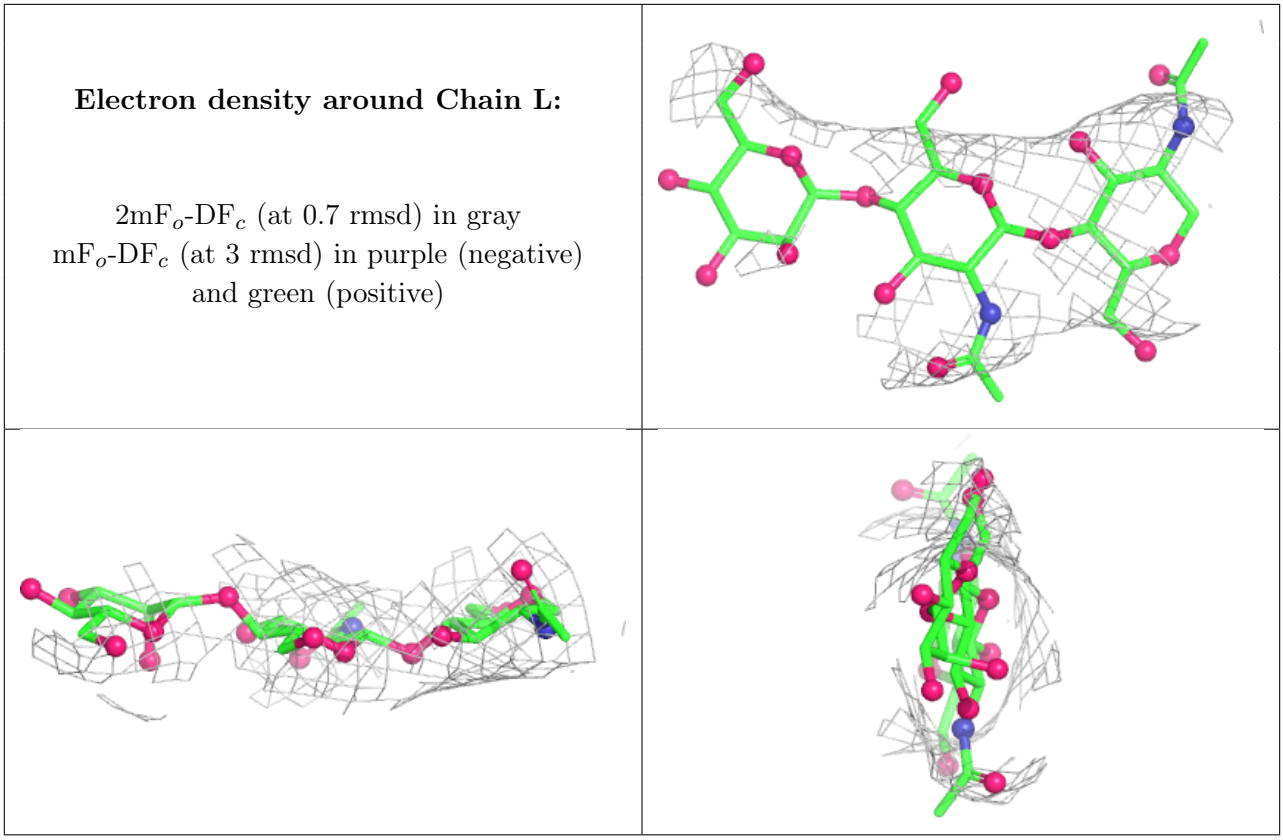






Electron density around Chain L:

$2mF_o$-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	NAG	C	801	14/15	0.81	0.07	170,217,226,230	0
3	NAG	D	801	14/15	0.84	0.07	182,190,213,220	0
3	NAG	A	801	14/15	0.84	0.07	173,194,205,220	0
3	NAG	B	801	14/15	0.92	0.04	157,185,210,222	0

6.5 Other polymers

There are no such residues in this entry.