Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:18 PM BST

PDB ID	:	1MQN
Title	:	BHA/LSTc
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Deposited on	:	2002-09-16
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

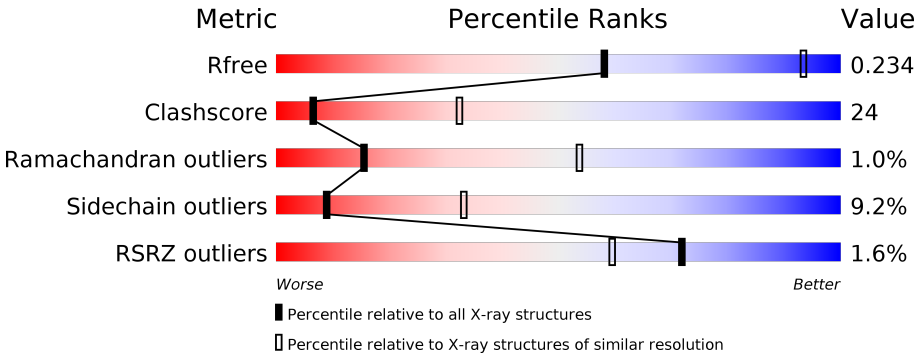
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	329	2% 56% 36% 5%
1	D	329	% 53% 39% 5%
1	G	329	2% 53% 36% 7%
2	B	221	% 54% 21% 22%
2	E	221	2% 47% 29% 22%
2	H	221	% 48% 27% 22%

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Mol	Chain	Length	Quality of chain
3	C	2	100%
3	I	2	100%
4	F	4	50% 25% 25%
4	K	4	25% 50% 25%
4	M	4	50% 50%
5	J	2	50% 50%
5	L	2	50% 50%

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
3	NAG	C	2	-	-	-	X
3	NAG	I	2	-	-	-	X
4	MAN	F	4	-	-	-	X
6	NAG	A	400	-	-	-	X
6	NAG	D	401	-	-	-	X
6	NAG	E	400	-	-	-	X
6	NAG	G	400	-	-	-	X
6	NAG	G	406	-	-	-	X
6	NAG	H	400	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11982 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2425	1522	424	466	13			
1	D	318	Total	C	N	O	S	0	0	0
			2432	1526	425	468	13			
1	G	318	Total	C	N	O	S	0	0	0
			2426	1523	424	466	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1398	867	247	278	6			
2	E	172	Total	C	N	O	S	0	0	0
			1401	869	248	278	6			
2	H	172	Total	C	N	O	S	0	0	0
			1404	871	249	278	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

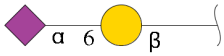
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco

pyranose.

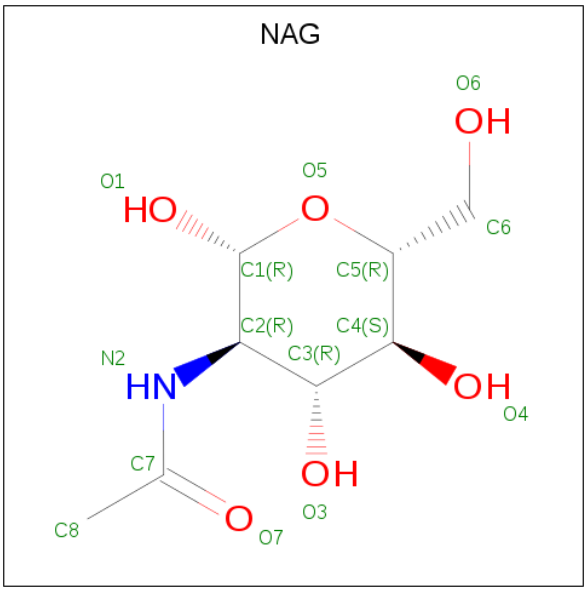
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	2	Total	C	N	O	0	0	0
			32	17	1	14			
5	L	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	H	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	20	Total O 20 20	0	0
7	B	14	Total O 14 14	0	0
7	D	22	Total O 22 22	0	0

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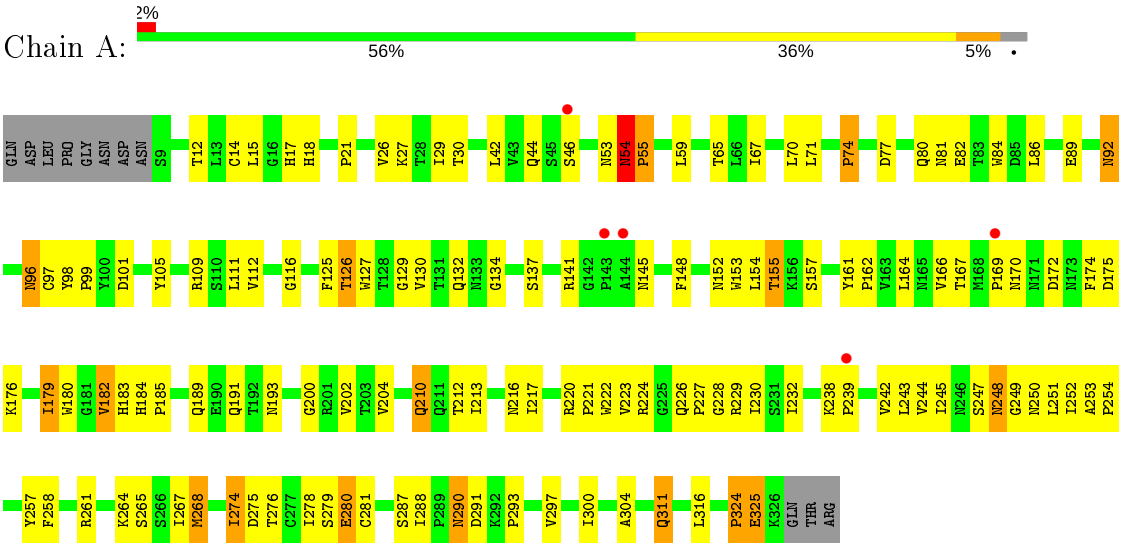
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	12	Total O 12 12	0	0
7	G	22	Total O 22 22	0	0
7	H	10	Total O 10 10	0	0

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.

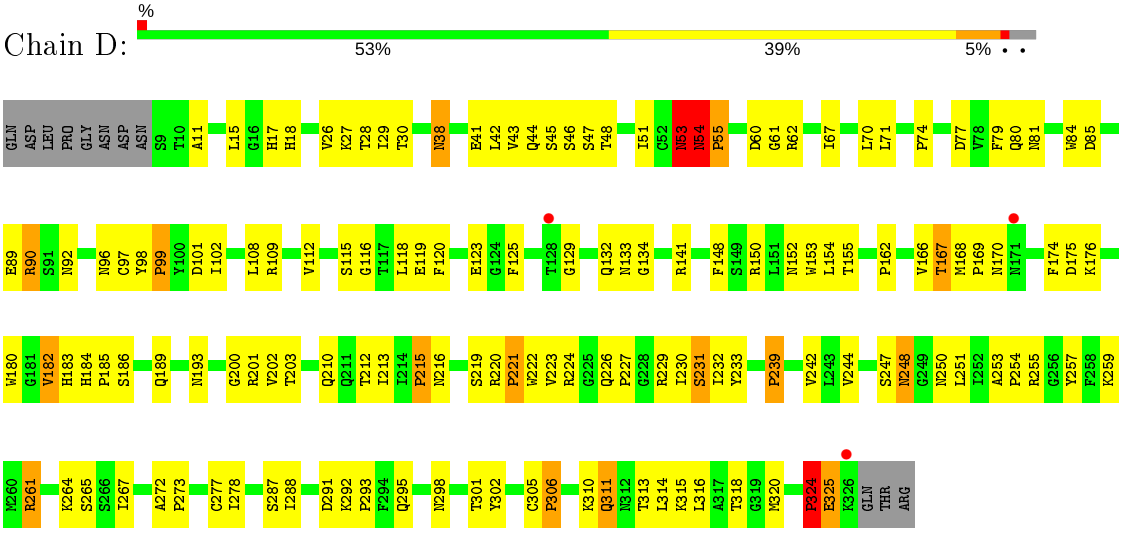
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



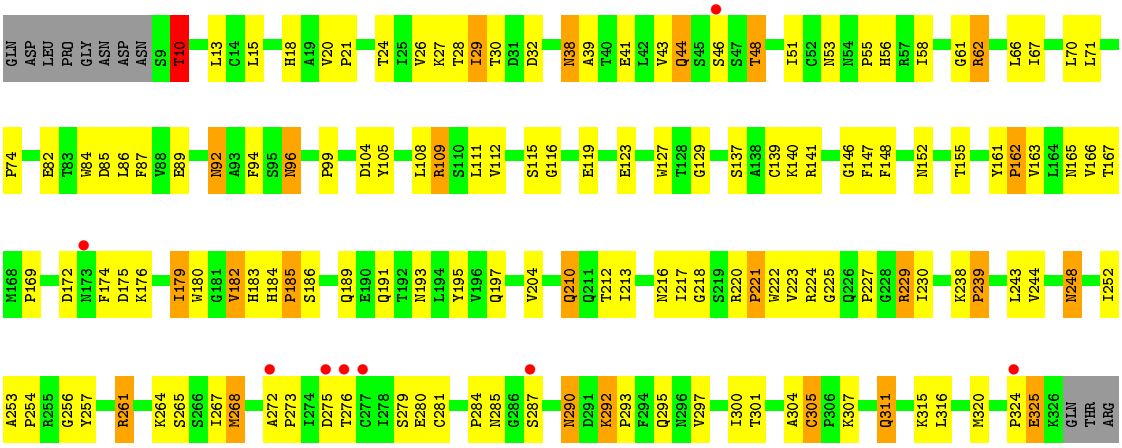
- Molecule 1: Hemagglutinin HA1 chain

Chain D:



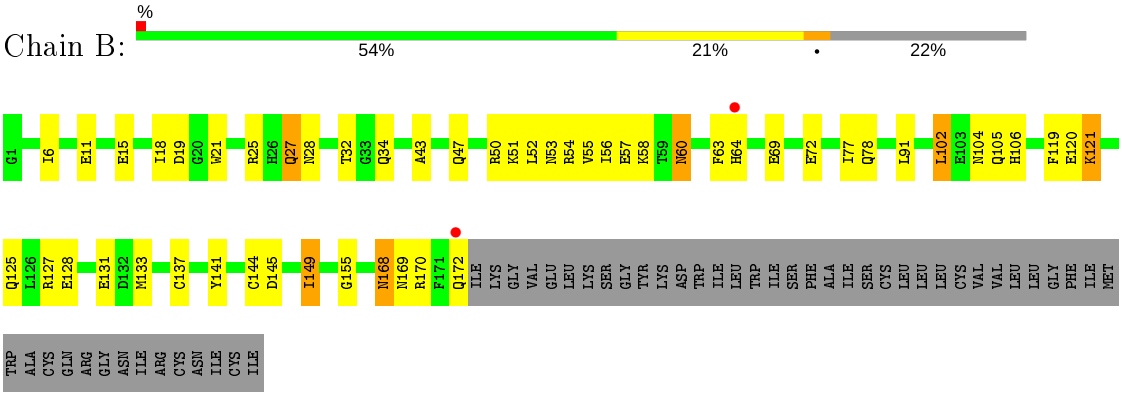
- Molecule 1: Hemagglutinin HA1 chain

Chain G:



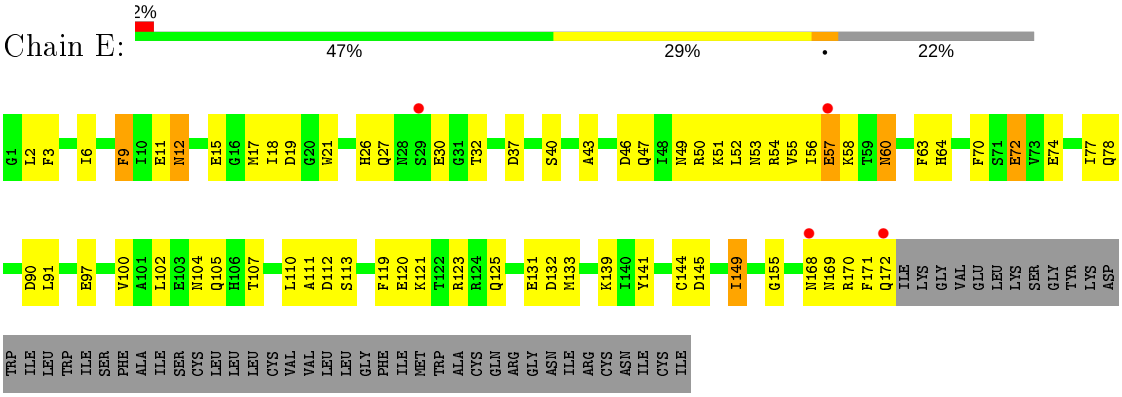
- Molecule 2: Hemagglutinin HA2 chain

Chain B:



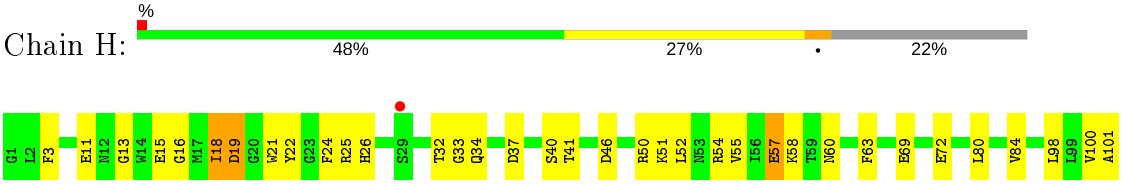
- Molecule 2: Hemagglutinin HA2 chain

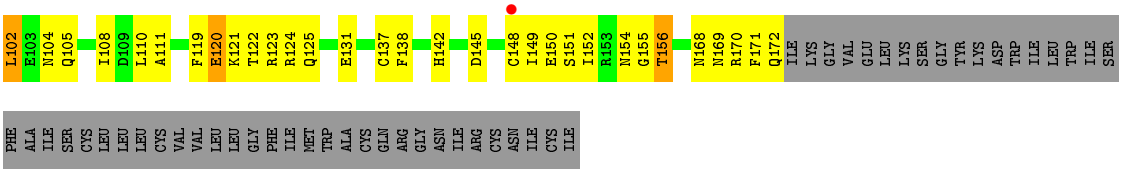
Chain E:



- Molecule 2: Hemagglutinin HA2 chain

Chain H:





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

Chain C:

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

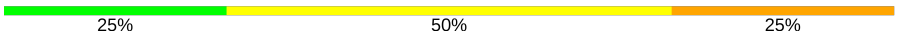
Chain I:

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

Chain F:

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

Chain K:



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

Chain M:

• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain J:

• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	147.32Å 148.43Å 250.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 38.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 93.1 (38.74-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.18Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.243 0.231 , 0.234	Depositor DCC
R_{free} test set	2252 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	1.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11982	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: GAL, SIA, BMA, 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	A	0.48	0/2482	0.81	4/3390 (0.1%)
1	D	0.56	0/2489	0.86	5/3398 (0.1%)
1	G	0.57	1/2483 (0.0%)	0.81	5/3391 (0.1%)
2	B	0.45	0/1422	0.62	0/1912
2	E	0.42	0/1425	0.65	0/1915
2	H	0.47	0/1428	0.73	1/1918 (0.1%)
All	All	0.51	1/11729 (0.0%)	0.77	15/15924 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	GLU	CB-CG	-5.32	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	ASN	C-N-CD	-20.24	76.08	120.60
1	A	54	ASN	C-N-CA	13.61	179.18	122.00
1	D	54	ASN	N-CA-C	11.37	141.70	111.00
1	D	54	ASN	C-N-CD	9.49	148.32	128.40
1	D	54	ASN	C-N-CA	-7.01	92.57	122.00
1	A	54	ASN	N-CA-C	6.93	129.71	111.00
1	G	305	CYS	CA-CB-SG	5.95	124.71	114.00
1	A	55	PRO	CA-N-CD	-5.85	103.31	111.50
2	H	137	CYS	CA-CB-SG	5.81	124.46	114.00
1	G	163	VAL	N-CA-C	-5.79	95.38	111.00
1	G	48	THR	N-CA-C	-5.72	95.56	111.00
1	D	53	ASN	C-N-CA	-5.59	107.72	121.70
1	D	55	PRO	N-CA-C	-5.55	97.67	112.10
1	G	10	THR	N-CA-C	5.17	124.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	141	ARG	N-CA-C	-5.17	97.06	111.00

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	A	2425	0	2334	133	0
1	D	2432	0	2347	149	0
1	G	2426	0	2338	160	0
2	B	1398	0	1308	49	0
2	E	1401	0	1317	79	0
2	H	1404	0	1326	83	0
3	C	28	0	25	2	0
3	I	28	0	25	0	0
4	F	50	0	43	2	0
4	K	50	0	43	1	0
4	M	50	0	43	3	0
5	J	32	0	27	1	0
5	L	32	0	27	2	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	D	28	0	26	0	0
6	E	14	0	13	0	0
6	G	42	0	39	11	0
6	H	14	0	13	2	0
7	A	20	0	0	2	0
7	B	14	0	0	0	0
7	D	22	0	0	2	0
7	E	12	0	0	0	0
7	G	22	0	0	4	0
7	H	10	0	0	1	0
All	All	11982	0	11320	549	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 24.

All (549) 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)
2:H:154:ASN:OD1	2:H:156:THR:HG22	1.43	1.15
1:D:81:ASN:OD1	1:D:119:GLU:HA	1.67	0.94
1:D:27:LYS:HB3	2:H:54:ARG:HH12	1.34	0.91
1:G:24:THR:OG1	6:G:400:NAG:H62	1.68	0.91
1:D:216:ASN:CB	1:G:212:THR:HG21	2.01	0.91
1:D:293:PRO:HG3	2:E:55:VAL:O	1.70	0.90
2:H:154:ASN:OD1	2:H:156:THR:CG2	2.20	0.89
1:D:216:ASN:CG	1:G:212:THR:HG21	1.92	0.89
1:G:293:PRO:HG3	2:H:55:VAL:O	1.73	0.88
2:H:57:GLU:HG3	2:H:57:GLU:O	1.71	0.88
1:A:29:ILE:HD11	2:B:102:LEU:HD12	1.53	0.87
1:D:29:ILE:HD11	2:E:102:LEU:HD12	1.57	0.87
2:H:151:SER:HA	2:H:156:THR:HG23	1.57	0.86
1:D:129:GLY:HA3	1:D:162:PRO:HG2	1.56	0.85
1:A:167:THR:OG1	4:F:1:NAG:H62	1.77	0.85
1:D:97:CYS:O	1:D:224:ARG:NH1	2.12	0.83
2:E:123:ARG:HH22	2:H:123:ARG:NH2	1.77	0.83
1:G:71:LEU:HD23	1:G:179:ILE:HD11	1.61	0.82
1:G:86:LEU:HD21	1:G:268:MET:HE3	1.62	0.80
2:E:11:GLU:C	2:E:12:ASN:HD22	1.84	0.80
2:E:12:ASN:HD22	2:E:12:ASN:N	1.78	0.80
1:A:29:ILE:H	2:B:105:GLN:HE21	1.29	0.80
1:G:29:ILE:H	2:H:105:GLN:HE21	1.28	0.80
1:A:170:ASN:OD1	1:A:176:LYS:HE3	1.82	0.79
1:D:216:ASN:HB3	1:G:212:THR:HG21	1.61	0.79
1:D:221:PRO:O	1:D:229:ARG:NH2	2.14	0.79
1:G:71:LEU:CD2	1:G:179:ILE:HD11	2.12	0.79
1:G:220:ARG:CB	1:G:229:ARG:HH11	1.97	0.78
2:H:25:ARG:NE	2:H:34:GLN:OE1	2.12	0.77
2:E:6:ILE:HD12	2:E:112:ASP:HA	1.68	0.76
1:D:167:THR:HG22	1:D:242:VAL:CG2	2.16	0.76
1:A:274:ILE:HG12	1:A:274:ILE:O	1.87	0.75
1:A:248:ASN:H	1:A:248:ASN:HD22	1.32	0.74
1:G:189:GLN:O	1:G:193:ASN:HB2	1.86	0.74
2:H:21:TRP:HB2	2:H:41:THR:HG23	1.69	0.73
1:G:38:ASN:ND2	1:G:39:ALA:H	1.86	0.73
2:E:57:GLU:HG3	2:E:57:GLU:O	1.88	0.72
2:E:123:ARG:NH2	2:H:123:ARG:NH2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:ASN:HA	2:E:172:GLN:HE21	1.53	0.72
1:D:302:TYR:CE2	2:E:63:PHE:HD2	2.08	0.72
1:D:325:GLU:OE1	2:E:15:GLU:HB2	1.90	0.71
2:B:57:GLU:O	2:B:57:GLU:HG3	1.90	0.71
1:D:27:LYS:HB3	2:H:54:ARG:NH1	2.04	0.71
2:H:169:ASN:HA	2:H:172:GLN:HE21	1.54	0.71
1:A:71:LEU:CD2	1:A:179:ILE:HD11	2.21	0.71
1:D:77:ASP:O	1:D:80:GLN:HG3	1.90	0.71
1:A:96:ASN:HA	1:A:224:ARG:HE	1.55	0.71
1:G:220:ARG:HB2	1:G:229:ARG:HH11	1.55	0.70
2:B:144:CYS:SG	2:B:149:ILE:HD12	2.31	0.70
1:G:28:THR:HB	2:H:105:GLN:NE2	2.07	0.70
1:D:29:ILE:H	2:E:105:GLN:HE21	1.40	0.69
2:H:120:GLU:HG3	2:H:123:ARG:NH1	2.07	0.69
1:D:170:ASN:OD1	1:D:176:LYS:HE3	1.92	0.69
1:G:29:ILE:HG22	1:G:30:THR:HG23	1.73	0.69
1:A:86:LEU:HD21	1:A:268:MET:HE3	1.74	0.69
1:D:220:ARG:HH11	1:G:210:GLN:HG3	1.57	0.69
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.75	0.68
1:G:248:ASN:HD22	1:G:248:ASN:H	1.41	0.68
2:E:123:ARG:NH2	2:H:123:ARG:HH21	1.91	0.68
1:G:67:ILE:HG13	1:G:105:TYR:CZ	2.29	0.67
1:G:38:ASN:ND2	1:G:39:ALA:N	2.41	0.67
1:G:180:TRP:HB3	1:G:254:PRO:HG3	1.76	0.67
2:H:131:GLU:OE2	2:H:170:ARG:HD2	1.94	0.67
1:D:248:ASN:HD22	1:D:248:ASN:H	1.41	0.67
2:H:151:SER:CA	2:H:156:THR:HG23	2.25	0.67
1:G:222:TRP:CD1	1:G:227:PRO:HG3	2.30	0.67
1:G:44:GLN:N	1:G:292:LYS:HZ2	1.91	0.66
2:H:142:HIS:HE1	2:H:148:CYS:SG	2.18	0.66
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.76	0.66
1:D:167:THR:HG22	1:D:242:VAL:HG21	1.76	0.66
1:D:44:GLN:HG2	1:D:292:LYS:HD2	1.78	0.66
1:A:129:GLY:HA3	1:A:162:PRO:HG2	1.78	0.65
1:D:53:ASN:H	1:D:53:ASN:HD22	1.42	0.65
2:E:11:GLU:HB3	2:E:12:ASN:ND2	2.10	0.65
1:G:223:VAL:HG12	1:G:224:ARG:NH1	2.11	0.65
2:H:120:GLU:HG3	2:H:123:ARG:HH12	1.61	0.65
1:G:29:ILE:H	2:H:105:GLN:NE2	1.94	0.65
2:H:80:LEU:O	2:H:84:VAL:HG23	1.97	0.65
1:D:152:ASN:HB3	1:D:253:ALA:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:LYS:NZ	2:E:90:ASP:OD1	2.30	0.65
1:A:125:PHE:O	1:A:126:THR:HG23	1.96	0.65
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.31	0.65
1:G:43:VAL:C	1:G:292:LYS:NZ	2.51	0.64
2:H:21:TRP:CB	2:H:41:THR:HG23	2.27	0.64
1:G:316:LEU:HD23	2:H:52:LEU:HD13	1.78	0.64
1:G:109:ARG:NH1	1:G:267:ILE:HD13	2.12	0.64
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.32	0.64
2:B:15:GLU:O	2:B:18:ILE:HD11	1.98	0.64
1:D:43:VAL:HG23	1:D:314:LEU:HB2	1.79	0.64
2:B:169:ASN:HA	2:B:172:GLN:HE21	1.63	0.64
2:H:169:ASN:HA	2:H:172:GLN:NE2	2.12	0.64
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.78	0.64
1:G:13:LEU:HD11	2:H:24:PHE:HB3	1.80	0.63
2:B:102:LEU:HD21	2:E:102:LEU:HD23	1.79	0.63
1:D:53:ASN:HD22	1:D:53:ASN:N	1.96	0.63
1:D:55:PRO:HD3	7:D:409:HOH:O	1.97	0.63
1:A:30:THR:O	2:E:50:ARG:HD2	1.98	0.63
1:G:84:TRP:CE2	1:G:116:GLY:HA2	2.33	0.63
2:H:19:ASP:N	2:H:19:ASP:OD1	2.32	0.63
2:E:123:ARG:HH22	2:H:123:ARG:HH22	1.46	0.62
2:B:54:ARG:HA	2:B:58:LYS:NZ	2.15	0.62
1:A:189:GLN:O	1:A:193:ASN:HB2	2.00	0.61
1:D:180:TRP:HB3	1:D:254:PRO:HG3	1.81	0.61
1:G:220:ARG:HB3	1:G:229:ARG:HH11	1.64	0.61
1:G:223:VAL:CG1	1:G:224:ARG:NH1	2.63	0.61
1:D:291:ASP:O	2:E:56:ILE:HG13	1.99	0.61
1:G:127:TRP:CH2	1:G:166:VAL:HG21	2.35	0.61
1:G:316:LEU:HD23	2:H:52:LEU:CD1	2.30	0.61
2:H:11:GLU:OE2	2:H:11:GLU:HA	2.00	0.61
1:D:42:LEU:HD12	2:E:100:VAL:CG1	2.30	0.61
1:A:293:PRO:HG3	2:B:55:VAL:O	2.00	0.61
1:D:182:VAL:HG11	1:D:213:ILE:CG2	2.31	0.61
1:A:71:LEU:HD23	1:A:179:ILE:HD11	1.82	0.61
1:A:221:PRO:HG3	1:D:244:VAL:HG23	1.83	0.61
1:D:134:GLY:HA3	1:D:153:TRP:HB3	1.81	0.61
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.82	0.60
1:D:222:TRP:CD1	1:D:227:PRO:HG3	2.36	0.60
1:D:325:GLU:HG2	1:D:325:GLU:O	2.01	0.60
1:G:275:ASP:CG	1:G:276:THR:H	2.03	0.60
1:G:220:ARG:O	1:G:227:PRO:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:O	2:B:56:ILE:HG13	2.01	0.60
1:D:53:ASN:O	1:D:54:ASN:HB3	2.00	0.60
1:D:38:ASN:OD1	1:D:318:THR:OG1	2.13	0.59
1:G:115:SER:HA	1:G:261:ARG:O	2.01	0.59
1:D:26:VAL:CG1	1:D:27:LYS:N	2.65	0.59
1:G:220:ARG:CB	1:G:229:ARG:NH1	2.64	0.59
2:H:22:TYR:O	2:H:37:ASP:N	2.35	0.59
1:G:56:HIS:O	1:G:58:ILE:HG13	2.02	0.59
1:A:216:ASN:HB3	1:D:212:THR:OG1	2.02	0.59
2:H:26:HIS:O	2:H:32:THR:HA	2.02	0.59
1:G:216:ASN:O	1:G:220:ARG:NH2	2.35	0.59
1:D:201:ARG:HH11	1:D:201:ARG:HG2	1.67	0.59
2:E:51:LYS:HE3	2:E:107:THR:OG1	2.03	0.59
2:E:37:ASP:OD2	2:E:40:SER:HB2	2.02	0.59
1:D:231:SER:HB3	1:D:233:TYR:HE1	1.66	0.59
1:D:278:ILE:HA	7:D:409:HOH:O	2.03	0.58
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.03	0.58
2:B:125:GLN:NE2	2:B:155:GLY:HA2	2.19	0.58
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.69	0.58
1:A:125:PHE:HB2	1:A:127:TRP:CD1	2.39	0.58
2:E:54:ARG:HA	2:E:58:LYS:NZ	2.18	0.58
1:G:53:ASN:HB3	1:G:275:ASP:O	2.04	0.58
1:A:170:ASN:HD22	1:A:238:LYS:C	2.07	0.58
4:K:1:NAG:H61	4:K:2:NAG:H82	1.86	0.58
2:B:25:ARG:NE	2:B:34:GLN:OE1	2.35	0.58
2:H:21:TRP:H	2:H:41:THR:CG2	2.16	0.57
1:A:129:GLY:O	1:A:157:SER:HB3	2.05	0.57
1:D:53:ASN:ND2	1:D:277:CYS:O	2.37	0.57
1:A:96:ASN:HA	1:A:224:ARG:NE	2.19	0.57
1:A:77:ASP:O	1:A:80:GLN:HG3	2.05	0.57
2:E:72:GLU:HG2	1:G:238:LYS:NZ	2.19	0.57
1:G:27:LYS:HG2	1:G:32:ASP:O	2.04	0.57
1:A:74:PRO:HA	1:A:141:ARG:HH21	1.69	0.57
2:E:17:MET:C	2:E:18:ILE:HD13	2.25	0.57
2:B:43:ALA:O	2:B:47:GLN:HG3	2.05	0.57
1:D:216:ASN:CG	1:G:212:THR:CG2	2.69	0.57
1:A:53:ASN:O	1:A:54:ASN:HB3	2.03	0.57
1:D:175:ASP:OD1	1:D:239:PRO:HD3	2.04	0.57
1:D:17:HIS:CD2	2:E:6:ILE:HG12	2.40	0.57
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.04	0.56
2:H:37:ASP:OD2	2:H:40:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:HG23	1:D:244:VAL:HG22	1.86	0.56
1:D:222:TRP:NE1	1:D:227:PRO:HG3	2.19	0.56
1:D:97:CYS:SG	1:D:98:TYR:N	2.76	0.56
1:A:137:SER:HA	1:A:145:ASN:OD1	2.06	0.56
1:A:217:ILE:HD12	1:A:217:ILE:N	2.20	0.56
1:D:182:VAL:HG11	1:D:213:ILE:HG21	1.87	0.56
1:D:324:PRO:O	1:D:325:GLU:CB	2.54	0.56
2:E:12:ASN:ND2	2:E:12:ASN:N	2.51	0.56
1:G:191:GLN:OE1	1:G:217:ILE:HD11	2.05	0.56
1:D:155:THR:HG21	5:L:2:SIA:H111	1.88	0.56
1:D:125:PHE:HD2	1:D:166:VAL:HG11	1.69	0.56
1:G:89:GLU:HG3	1:G:267:ILE:HD11	1.88	0.56
1:G:264:LYS:HB2	2:H:63:PHE:CG	2.41	0.56
1:D:220:ARG:NH1	1:G:210:GLN:HG3	2.21	0.56
1:G:39:ALA:O	6:G:400:NAG:H2	2.06	0.55
1:D:325:GLU:HB3	2:E:15:GLU:OE2	2.06	0.55
1:D:77:ASP:OD2	1:D:141:ARG:NH1	2.39	0.55
1:G:71:LEU:HD23	1:G:179:ILE:CD1	2.34	0.55
1:A:17:HIS:HA	2:B:21:TRP:O	2.06	0.55
2:B:131:GLU:OE2	2:B:170:ARG:HD2	2.07	0.55
2:B:27:GLN:HA	2:B:32:THR:HG22	1.87	0.55
2:E:132:ASP:OD2	2:H:124:ARG:NE	2.35	0.55
1:G:220:ARG:HB3	1:G:229:ARG:NH1	2.22	0.55
2:H:123:ARG:HB2	2:H:138:PHE:CZ	2.42	0.55
1:G:175:ASP:OD1	1:G:239:PRO:HD3	2.07	0.54
2:H:21:TRP:CG	2:H:41:THR:HG23	2.43	0.54
1:D:60:ASP:OD2	1:D:90:ARG:NH1	2.40	0.54
2:E:37:ASP:OD2	2:E:40:SER:CB	2.56	0.54
1:A:169:PRO:HA	1:A:242:VAL:HG23	1.90	0.54
1:A:152:ASN:HB3	1:A:253:ALA:HB3	1.89	0.54
2:E:60:ASN:HD22	2:E:60:ASN:C	2.09	0.54
2:E:144:CYS:SG	2:E:149:ILE:HD12	2.47	0.54
1:G:53:ASN:OD1	1:G:276:THR:HA	2.08	0.53
1:G:275:ASP:CG	1:G:276:THR:N	2.62	0.53
1:G:26:VAL:HG13	2:H:104:ASN:ND2	2.22	0.53
1:A:176:LYS:HD3	1:A:257:TYR:CD2	2.43	0.53
1:A:92:ASN:C	1:A:92:ASN:HD22	2.10	0.53
3:C:2:NAG:H83	3:C:2:NAG:O3	2.09	0.53
2:E:43:ALA:O	2:E:47:GLN:HG3	2.09	0.53
2:E:17:MET:O	2:E:18:ILE:HD13	2.08	0.53
1:G:167:THR:HG22	1:G:169:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:CE1	2:H:33:GLY:HA3	2.44	0.53
2:H:37:ASP:OD2	2:H:40:SER:CB	2.57	0.53
1:A:281:CYS:HB2	1:A:304:ALA:O	2.10	0.52
1:G:27:LYS:CG	1:G:32:ASP:O	2.57	0.52
1:D:184:HIS:HE2	1:D:231:SER:HB2	1.74	0.52
1:D:295:GLN:NE2	1:D:298:ASN:O	2.40	0.52
1:G:220:ARG:HB2	1:G:227:PRO:O	2.08	0.52
1:G:186:SER:HA	1:G:218:GLY:O	2.09	0.52
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.75	0.52
1:D:248:ASN:N	1:D:248:ASN:HD22	2.04	0.52
1:D:302:TYR:HE2	2:E:63:PHE:HB3	1.75	0.52
1:A:96:ASN:ND2	1:A:96:ASN:C	2.63	0.52
1:G:108:LEU:O	1:G:112:VAL:HG23	2.10	0.52
1:A:275:ASP:CG	1:A:276:THR:N	2.63	0.52
1:A:29:ILE:H	2:B:105:GLN:NE2	2.04	0.52
1:A:81:ASN:ND2	3:C:1:NAG:C7	2.73	0.52
1:G:43:VAL:N	7:G:419:HOH:O	2.34	0.52
1:A:77:ASP:HB3	1:A:80:GLN:HE21	1.75	0.52
1:D:99:PRO:HB3	1:D:229:ARG:HE	1.75	0.52
1:G:212:THR:O	1:G:212:THR:HG23	2.10	0.52
1:G:26:VAL:CG1	2:H:104:ASN:ND2	2.73	0.52
1:A:244:VAL:HB	1:G:221:PRO:HD3	1.91	0.52
1:G:297:VAL:HA	6:G:406:NAG:C8	2.40	0.52
1:D:200:GLY:HA3	1:D:250:ASN:OD1	2.10	0.51
2:B:19:ASP:N	2:B:19:ASP:OD1	2.43	0.51
1:G:137:SER:O	1:G:140:LYS:HE3	2.10	0.51
1:G:301:THR:HB	1:G:305:CYS:SG	2.50	0.51
1:D:30:THR:O	2:H:50:ARG:HD2	2.10	0.51
1:A:26:VAL:HG13	2:B:104:ASN:ND2	2.26	0.51
2:B:27:GLN:CB	2:B:32:THR:HG22	2.40	0.51
1:A:223:VAL:HG12	1:A:224:ARG:NH1	2.26	0.51
2:B:50:ARG:HD2	1:G:30:THR:O	2.11	0.51
1:G:281:CYS:HB2	1:G:304:ALA:O	2.10	0.51
1:D:102:ILE:HG12	1:D:232:ILE:HB	1.93	0.51
1:G:139:CYS:HB3	1:G:146:GLY:O	2.10	0.51
1:A:65:THR:HG21	1:A:105:TYR:OH	2.11	0.51
1:A:248:ASN:N	1:A:248:ASN:HD22	1.99	0.51
1:D:84:TRP:HZ3	1:D:118:LEU:HG	1.75	0.51
1:D:47:SER:HA	1:D:288:ILE:HG22	1.93	0.51
1:G:220:ARG:HB2	1:G:229:ARG:NH1	2.24	0.51
1:G:279:SER:OG	1:G:287:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ARG:HD2	1:G:229:ARG:HD3	1.91	0.51
2:B:77:ILE:HG23	2:B:78:GLN:N	2.26	0.50
2:H:58:LYS:HG3	7:H:410:HOH:O	2.10	0.50
1:G:28:THR:HB	2:H:105:GLN:HE21	1.75	0.50
1:G:325:GLU:HG2	2:H:13:GLY:O	2.12	0.50
1:D:316:LEU:HD23	2:E:52:LEU:HD13	1.93	0.50
1:G:172:ASP:HB3	1:G:174:PHE:CE2	2.45	0.50
1:D:302:TYR:CE2	2:E:63:PHE:CD2	2.94	0.50
1:D:15:LEU:CD2	2:E:119:PHE:HA	2.42	0.50
1:G:297:VAL:HG13	6:G:406:NAG:H81	1.92	0.50
1:G:182:VAL:HG11	1:G:213:ILE:HG21	1.93	0.50
2:H:54:ARG:O	2:H:58:LYS:HE3	2.12	0.50
1:A:26:VAL:CG1	1:A:27:LYS:N	2.74	0.50
1:D:189:GLN:O	1:D:193:ASN:HB2	2.12	0.50
1:A:221:PRO:HG3	1:D:244:VAL:CG2	2.41	0.50
1:D:85:ASP:O	1:D:265:SER:HA	2.11	0.50
2:H:168:ASN:O	2:H:172:GLN:HB3	2.12	0.50
1:A:212:THR:HG21	1:G:216:ASN:HB2	1.93	0.50
1:A:183:HIS:O	1:A:185:PRO:HD3	2.11	0.50
1:A:222:TRP:CD1	1:A:227:PRO:HG3	2.47	0.50
1:D:29:ILE:H	2:E:105:GLN:NE2	2.08	0.50
2:H:46:ASP:O	2:H:50:ARG:HG3	2.11	0.50
2:B:27:GLN:HB2	2:B:32:THR:HG22	1.92	0.49
1:D:295:GLN:HB3	1:D:306:PRO:HB2	1.94	0.49
1:D:301:THR:HB	1:D:305:CYS:SG	2.52	0.49
2:E:11:GLU:HB3	2:E:12:ASN:HD22	1.75	0.49
2:E:125:GLN:NE2	2:E:155:GLY:HA2	2.26	0.49
1:A:279:SER:OG	1:A:287:SER:HB3	2.12	0.49
1:D:186:SER:HB3	1:D:227:PRO:HB2	1.94	0.49
1:A:204:VAL:CG1	1:A:243:LEU:HD11	2.42	0.49
1:A:71:LEU:HD21	1:A:179:ILE:HD11	1.92	0.49
1:G:195:TYR:O	1:G:197:GLN:N	2.45	0.49
1:D:174:PHE:HZ	1:D:257:TYR:HH	1.59	0.49
1:G:325:GLU:OE2	2:H:15:GLU:N	2.24	0.49
1:G:222:TRP:CE3	1:G:225:GLY:HA2	2.48	0.49
2:E:30:GLU:OE1	2:E:145:ASP:HB2	2.12	0.49
2:E:54:ARG:O	2:E:58:LYS:HD2	2.13	0.49
2:E:54:ARG:HA	2:E:58:LYS:HZ1	1.78	0.49
1:D:27:LYS:HE2	2:H:54:ARG:NH2	2.28	0.48
1:G:13:LEU:HD13	2:H:26:HIS:HB3	1.94	0.48
2:H:142:HIS:CE1	2:H:148:CYS:SG	3.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:NH1	1:D:267:ILE:HD13	2.27	0.48
1:G:26:VAL:CG1	1:G:27:LYS:N	2.75	0.48
1:G:71:LEU:HB3	1:G:148:PHE:CD2	2.48	0.48
1:D:221:PRO:HD3	1:G:244:VAL:HB	1.96	0.48
1:A:155:THR:HG21	5:J:2:SIA:H111	1.96	0.48
1:A:70:LEU:HD12	1:A:258:PHE:CE2	2.48	0.48
1:A:99:PRO:HG3	1:A:223:VAL:CG1	2.43	0.48
2:B:11:GLU:HA	2:B:11:GLU:OE1	2.13	0.48
1:G:127:TRP:CZ3	1:G:166:VAL:HG21	2.47	0.48
1:G:24:THR:OG1	6:G:400:NAG:C6	2.54	0.48
1:A:316:LEU:HD23	2:B:52:LEU:CD1	2.44	0.48
1:D:219:SER:HB2	1:G:165:ASN:OD1	2.14	0.48
1:D:26:VAL:HG13	1:D:27:LYS:N	2.29	0.48
1:D:320:MET:CE	2:E:21:TRP:HB3	2.44	0.48
2:H:25:ARG:HG2	2:H:34:GLN:HB2	1.96	0.48
1:A:125:PHE:HD1	1:A:127:TRP:H	1.57	0.48
1:A:210:GLN:HG3	1:G:220:ARG:NH1	2.28	0.48
1:G:26:VAL:HG12	1:G:27:LYS:N	2.28	0.48
2:H:150:GLU:HG2	6:H:400:NAG:O6	2.13	0.48
1:D:293:PRO:HG2	2:E:55:VAL:HG12	1.96	0.48
1:D:320:MET:HB3	2:E:111:ALA:HB1	1.96	0.48
2:H:151:SER:HA	2:H:156:THR:CG2	2.35	0.48
1:G:152:ASN:HB3	1:G:253:ALA:HB3	1.95	0.48
1:G:176:LYS:HE2	1:G:257:TYR:CE2	2.49	0.48
1:G:180:TRP:CE2	1:G:204:VAL:HG21	2.49	0.48
2:H:100:VAL:HG23	2:H:101:ALA:N	2.29	0.48
2:E:141:TYR:CG	2:E:170:ARG:HG2	2.49	0.48
1:A:71:LEU:HD21	1:A:232:ILE:HD13	1.96	0.47
1:D:220:ARG:HB2	1:D:227:PRO:O	2.14	0.47
6:G:400:NAG:H83	6:G:400:NAG:O3	2.14	0.47
1:D:231:SER:HB3	1:D:233:TYR:CE1	2.48	0.47
1:D:67:ILE:O	1:D:70:LEU:HB3	2.14	0.47
2:B:102:LEU:HD21	2:E:102:LEU:CD2	2.43	0.47
1:D:320:MET:HE3	2:E:21:TRP:HB3	1.96	0.47
1:A:210:GLN:HE21	1:A:210:GLN:HB3	1.53	0.47
2:B:54:ARG:O	2:B:58:LYS:HD2	2.14	0.47
2:E:3:PHE:CE1	2:E:113:SER:HB2	2.49	0.47
2:E:131:GLU:OE2	2:E:170:ARG:HD2	2.13	0.47
1:A:125:PHE:O	1:A:126:THR:CG2	2.62	0.47
1:D:183:HIS:O	1:D:185:PRO:HD3	2.15	0.47
1:A:274:ILE:CG1	1:A:274:ILE:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:TYR:CD1	1:D:233:TYR:N	2.83	0.47
2:B:141:TYR:CG	2:B:170:ARG:HG2	2.49	0.47
2:B:168:ASN:O	2:B:172:GLN:HB3	2.14	0.47
1:D:176:LYS:HD3	1:D:257:TYR:CD2	2.50	0.47
1:G:44:GLN:N	1:G:292:LYS:NZ	2.63	0.47
1:D:226:GLN:NE2	5:L:2:SIA:O1B	2.48	0.47
1:A:169:PRO:CA	1:A:242:VAL:HG23	2.45	0.47
1:A:164:LEU:N	1:A:247:SER:O	2.48	0.47
1:A:249:GLY:O	1:A:250:ASN:HB2	2.14	0.47
1:A:12:THR:HG23	2:B:133:MET:CE	2.44	0.47
1:D:324:PRO:O	1:D:325:GLU:HB3	2.15	0.47
1:G:55:PRO:HG2	1:G:280:GLU:OE1	2.15	0.47
2:H:125:GLN:NE2	2:H:155:GLY:HA2	2.30	0.47
1:A:166:VAL:HG22	1:A:245:ILE:HB	1.97	0.47
4:F:1:NAG:H83	4:F:1:NAG:O3	2.15	0.47
1:G:221:PRO:O	1:G:229:ARG:NH2	2.48	0.47
1:G:176:LYS:HD3	1:G:257:TYR:CD2	2.50	0.47
2:E:2:LEU:HB3	2:H:3:PHE:CZ	2.49	0.47
1:A:12:THR:HG23	2:B:133:MET:HE3	1.97	0.46
1:D:28:THR:HB	2:E:105:GLN:NE2	2.30	0.46
1:G:223:VAL:HG23	1:G:229:ARG:NH2	2.30	0.46
1:D:53:ASN:O	1:D:54:ASN:CB	2.55	0.46
2:H:150:GLU:HG3	6:H:400:NAG:O5	2.15	0.46
1:D:99:PRO:HG3	1:D:223:VAL:CG1	2.45	0.46
2:E:74:GLU:HG3	2:E:78:GLN:NE2	2.30	0.46
1:G:109:ARG:NH1	1:G:267:ILE:CD1	2.77	0.46
2:E:77:ILE:HG22	7:G:424:HOH:O	2.15	0.46
1:A:222:TRP:NE1	1:A:227:PRO:HG3	2.31	0.46
1:D:133:ASN:OD1	1:D:255:ARG:NH2	2.48	0.46
1:G:139:CYS:SG	1:G:147:PHE:HA	2.56	0.46
1:G:41:GLU:HA	1:G:41:GLU:OE1	2.15	0.46
1:A:14:CYS:HA	2:B:137:CYS:HA	1.98	0.46
1:A:74:PRO:HG3	1:A:141:ARG:NH2	2.31	0.46
2:E:125:GLN:HE22	2:E:155:GLY:HA2	1.80	0.46
2:E:26:HIS:O	2:E:32:THR:HG22	2.16	0.46
2:E:55:VAL:O	2:E:55:VAL:HG12	2.15	0.46
1:G:220:ARG:HD2	1:G:229:ARG:CD	2.46	0.46
1:G:15:LEU:HD22	2:H:119:PHE:HA	1.98	0.46
1:D:125:PHE:CD2	1:D:166:VAL:HG11	2.51	0.46
1:D:61:GLY:O	1:D:79:PHE:CZ	2.69	0.46
1:A:182:VAL:HG11	1:A:213:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:HG22	1:D:242:VAL:HG22	1.96	0.46
1:A:210:GLN:HG3	1:G:220:ARG:HH11	1.80	0.46
1:A:42:LEU:O	1:A:293:PRO:HD2	2.16	0.46
4:M:1:NAG:H61	4:M:2:NAG:C7	2.46	0.46
1:A:71:LEU:HB3	1:A:148:PHE:CD2	2.51	0.45
1:D:180:TRP:HH2	1:D:213:ILE:CD1	2.28	0.45
1:G:285:ASN:ND2	6:G:406:NAG:C7	2.79	0.45
4:M:1:NAG:H61	4:M:2:NAG:N2	2.31	0.45
1:G:44:GLN:O	1:G:295:GLN:HA	2.16	0.45
2:H:98:LEU:HG	2:H:102:LEU:HD22	1.97	0.45
2:E:77:ILE:HG23	2:E:78:GLN:N	2.31	0.45
1:G:204:VAL:CG1	1:G:243:LEU:HD11	2.46	0.45
1:G:84:TRP:CZ2	1:G:116:GLY:HA2	2.51	0.45
1:G:129:GLY:HA3	1:G:162:PRO:HG2	1.99	0.45
1:G:67:ILE:O	1:G:70:LEU:N	2.50	0.45
1:G:167:THR:OG1	4:M:1:NAG:H62	2.15	0.45
1:D:123:GLU:HB3	1:D:168:MET:CE	2.47	0.45
1:D:54:ASN:O	1:D:55:PRO:C	2.43	0.45
1:A:26:VAL:CG1	2:B:104:ASN:ND2	2.79	0.45
2:E:133:MET:SD	2:E:139:LYS:HB2	2.57	0.45
1:A:80:GLN:O	1:A:81:ASN:HB2	2.17	0.45
1:G:99:PRO:HG3	1:G:223:VAL:CG1	2.46	0.45
1:A:96:ASN:HD22	1:A:96:ASN:C	2.20	0.45
1:D:30:THR:HG22	2:H:51:LYS:HB2	1.99	0.45
1:A:220:ARG:NH1	1:D:203:THR:HG21	2.32	0.45
1:A:67:ILE:HG13	1:A:105:TYR:CZ	2.52	0.45
1:A:97:CYS:SG	1:A:98:TYR:N	2.86	0.45
2:B:102:LEU:HD23	2:H:102:LEU:HD21	1.99	0.45
1:D:180:TRP:CZ3	1:D:202:VAL:HG11	2.52	0.45
1:D:202:VAL:HG22	1:D:251:LEU:HB2	1.98	0.45
1:G:139:CYS:O	1:G:146:GLY:N	2.50	0.45
1:G:183:HIS:ND1	1:G:195:TYR:OH	2.36	0.45
1:D:27:LYS:HE2	2:H:54:ARG:NH1	2.32	0.45
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.98	0.45
1:A:26:VAL:HG12	1:A:27:LYS:N	2.31	0.44
1:D:108:LEU:O	1:D:112:VAL:HG23	2.18	0.44
2:E:46:ASP:HB3	2:E:50:ARG:NH2	2.33	0.44
2:H:110:LEU:HD23	2:H:110:LEU:C	2.37	0.44
1:G:94:PHE:HE1	1:G:96:ASN:HB2	1.82	0.44
1:D:302:TYR:CD2	2:E:63:PHE:HA	2.52	0.44
1:G:82:GLU:HA	1:G:82:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:HIS:HB3	1:A:220:ARG:NH2	2.32	0.44
1:A:17:HIS:CE1	2:B:6:ILE:HG23	2.52	0.44
2:B:54:ARG:HD3	1:G:32:ASP:HB3	1.99	0.44
1:G:48:THR:HG23	7:G:415:HOH:O	2.18	0.44
1:D:90:ARG:NH2	1:D:272:ALA:O	2.50	0.44
1:D:29:ILE:O	1:D:29:ILE:HG22	2.17	0.44
1:A:89:GLU:OE2	1:A:109:ARG:NH1	2.50	0.44
1:G:212:THR:CG2	1:G:212:THR:O	2.64	0.44
1:G:123:GLU:HB2	1:G:256:GLY:HA2	2.00	0.44
1:G:311:GLN:HG2	1:G:311:GLN:H	1.37	0.44
2:H:123:ARG:HB2	2:H:138:PHE:CE2	2.53	0.44
1:A:53:ASN:O	1:A:54:ASN:CB	2.63	0.44
7:A:417:HOH:O	1:D:212:THR:HG21	2.18	0.44
1:G:184:HIS:HB3	1:G:220:ARG:NH2	2.33	0.44
1:A:264:LYS:HB2	2:B:63:PHE:CG	2.53	0.43
1:A:300:ILE:HD11	2:B:69:GLU:HG3	2.00	0.43
1:G:66:LEU:HD22	1:G:267:ILE:HD12	1.99	0.43
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.18	0.43
1:A:116:GLY:HA3	1:A:265:SER:OG	2.19	0.43
1:D:11:ALA:CB	2:E:144:CYS:HB3	2.48	0.43
1:D:53:ASN:ND2	1:D:277:CYS:H	2.16	0.43
1:D:26:VAL:HG13	2:E:104:ASN:ND2	2.33	0.43
1:A:111:LEU:HD12	1:A:111:LEU:C	2.39	0.43
1:A:228:GLY:O	1:A:229:ARG:HG2	2.19	0.43
1:G:183:HIS:O	1:G:185:PRO:HD3	2.17	0.43
1:G:297:VAL:HG13	6:G:406:NAG:C8	2.48	0.43
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.01	0.43
1:G:300:ILE:HD11	2:H:69:GLU:HG3	2.00	0.43
1:A:74:PRO:HG3	1:A:141:ARG:HH21	1.84	0.43
1:D:134:GLY:CA	1:D:153:TRP:HB3	2.47	0.43
1:D:17:HIS:HA	2:E:21:TRP:O	2.19	0.43
2:E:72:GLU:HG2	1:G:238:LYS:HZ3	1.83	0.43
1:G:85:ASP:O	1:G:265:SER:HA	2.19	0.43
1:A:161:TYR:CE2	1:A:249:GLY:N	2.87	0.43
1:A:98:TYR:CD2	1:A:230:ILE:HG12	2.53	0.43
1:D:51:ILE:HA	1:D:287:SER:OG	2.18	0.43
2:E:171:PHE:CE1	2:H:171:PHE:HE2	2.36	0.43
1:G:174:PHE:O	1:G:239:PRO:HG3	2.19	0.43
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.54	0.43
2:B:60:ASN:HD22	2:B:60:ASN:C	2.22	0.43
1:G:15:LEU:HD11	2:H:122:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:GLY:O	1:G:62:ARG:HB2	2.19	0.43
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.00	0.43
1:A:130:VAL:HG13	1:A:162:PRO:HD2	2.01	0.43
1:A:311:GLN:HG2	1:A:311:GLN:H	1.37	0.43
1:D:325:GLU:CG	1:D:325:GLU:O	2.65	0.43
1:G:24:THR:HG21	1:G:39:ALA:HB3	2.01	0.43
1:G:41:GLU:HG3	1:G:292:LYS:HZ3	1.84	0.43
1:D:119:GLU:HB2	1:D:259:LYS:CG	2.48	0.42
1:A:221:PRO:HD3	1:D:244:VAL:HB	2.01	0.42
1:G:84:TRP:CD1	1:G:87:PHE:HB2	2.54	0.42
1:D:182:VAL:HG23	1:D:215:PRO:HG3	2.02	0.42
1:D:221:PRO:HG3	1:G:244:VAL:HG23	2.00	0.42
1:D:28:THR:HB	2:E:105:GLN:HE21	1.85	0.42
1:G:67:ILE:HG13	1:G:105:TYR:CE1	2.54	0.42
2:H:21:TRP:H	2:H:41:THR:HG23	1.84	0.42
2:B:54:ARG:HA	2:B:58:LYS:HZ1	1.82	0.42
1:D:182:VAL:CG2	1:D:215:PRO:HG3	2.49	0.42
1:D:264:LYS:HB2	2:E:63:PHE:CG	2.54	0.42
1:G:92:ASN:HD22	1:G:92:ASN:HA	1.55	0.42
1:A:275:ASP:CG	1:A:276:THR:H	2.21	0.42
1:A:74:PRO:HA	1:A:77:ASP:OD2	2.19	0.42
1:D:221:PRO:HG3	1:G:244:VAL:CG2	2.49	0.42
1:A:42:LEU:HD22	1:A:293:PRO:HG2	2.01	0.42
1:D:26:VAL:HG22	1:D:315:LYS:HB2	2.01	0.42
1:G:297:VAL:CG1	6:G:406:NAG:H82	2.48	0.42
1:G:320:MET:HB3	2:H:111:ALA:HB1	2.01	0.42
1:D:27:LYS:HE2	2:H:54:ARG:CZ	2.49	0.42
1:A:74:PRO:CA	1:A:141:ARG:HH21	2.33	0.42
1:D:132:GLN:HG2	1:D:154:LEU:CD2	2.50	0.42
1:D:26:VAL:HG13	1:D:27:LYS:H	1.84	0.42
1:D:89:GLU:OE2	1:D:109:ARG:NH1	2.52	0.42
1:G:223:VAL:CG1	1:G:224:ARG:HH12	2.30	0.42
1:A:71:LEU:O	1:A:148:PHE:HB3	2.20	0.42
1:A:288:ILE:HG21	1:A:297:VAL:HG21	2.01	0.42
2:E:2:LEU:HB3	2:H:3:PHE:HZ	1.85	0.42
2:H:11:GLU:OE2	2:H:11:GLU:CA	2.68	0.42
2:H:16:GLY:O	2:H:18:ILE:HG13	2.19	0.42
1:A:92:ASN:C	1:A:92:ASN:ND2	2.73	0.42
1:D:316:LEU:HD23	2:E:52:LEU:CD1	2.49	0.42
1:A:324:PRO:O	1:A:325:GLU:CB	2.67	0.42
1:A:67:ILE:HG13	1:A:105:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PHE:CD2	1:D:150:ARG:HD2	2.54	0.42
1:A:290:ASN:HD22	1:A:290:ASN:C	2.23	0.42
2:B:18:ILE:O	2:B:18:ILE:HG22	2.19	0.42
1:A:134:GLY:CA	1:A:153:TRP:HB3	2.51	0.41
1:A:172:ASP:HB3	1:A:174:PHE:CE2	2.54	0.41
1:A:216:ASN:CB	1:D:212:THR:OG1	2.67	0.41
1:A:202:VAL:HG22	1:A:251:LEU:HB2	2.02	0.41
1:G:99:PRO:HG3	1:G:223:VAL:HB	2.02	0.41
1:G:221:PRO:O	1:G:229:ARG:NH1	2.54	0.41
1:A:132:GLN:HG2	1:A:154:LEU:CD2	2.50	0.41
2:E:18:ILE:HG22	2:E:18:ILE:O	2.19	0.41
1:G:297:VAL:HG12	6:G:406:NAG:H82	2.02	0.41
2:H:125:GLN:HE22	2:H:155:GLY:HA2	1.84	0.41
1:D:71:LEU:HB3	1:D:148:PHE:CD2	2.56	0.41
2:E:53:ASN:HA	2:E:56:ILE:CG2	2.51	0.41
2:E:70:PHE:CD1	2:E:70:PHE:N	2.89	0.41
1:G:279:SER:CB	1:G:287:SER:HB3	2.50	0.41
2:B:27:GLN:CA	2:B:32:THR:HG22	2.49	0.41
1:D:115:SER:HA	1:D:261:ARG:O	2.20	0.41
1:D:42:LEU:CD1	2:E:100:VAL:CG1	2.99	0.41
1:G:43:VAL:C	1:G:292:LYS:HZ2	2.19	0.41
1:D:311:GLN:HE22	2:E:97:GLU:HB2	1.86	0.41
1:G:182:VAL:HG11	1:G:213:ILE:CG2	2.50	0.41
2:E:9:PHE:C	2:E:9:PHE:CD1	2.94	0.41
1:G:222:TRP:NE1	1:G:227:PRO:HG3	2.36	0.41
1:G:290:ASN:C	1:G:290:ASN:HD22	2.23	0.41
1:A:111:LEU:HD12	1:A:112:VAL:N	2.36	0.41
2:E:110:LEU:HD23	2:E:110:LEU:C	2.41	0.41
1:G:51:ILE:CD1	1:G:272:ALA:HB3	2.51	0.41
1:G:24:THR:HG21	6:G:400:NAG:O6	2.20	0.41
2:B:121:LYS:HB3	2:B:121:LYS:HE3	1.84	0.41
1:D:216:ASN:OD1	1:G:212:THR:CG2	2.69	0.41
1:G:325:GLU:H	1:G:325:GLU:HG3	1.64	0.41
2:B:53:ASN:HA	2:B:56:ILE:CG2	2.51	0.41
1:G:284:PRO:HG2	1:G:300:ILE:HB	2.03	0.41
1:G:44:GLN:HG2	7:G:411:HOH:O	2.21	0.41
1:A:226:GLN:HA	1:A:227:PRO:HD3	1.77	0.40
1:A:167:THR:CG2	1:A:242:VAL:HG21	2.51	0.40
1:A:54:ASN:O	1:A:278:ILE:HA	2.22	0.40
2:B:127:ARG:HB3	2:B:128:GLU:H	1.67	0.40
1:D:109:ARG:NH1	1:D:267:ILE:CD1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:THR:HG21	2:H:108:ILE:HD12	2.03	0.40
1:G:99:PRO:HB3	1:G:229:ARG:HE	1.85	0.40
2:H:131:GLU:OE2	2:H:170:ARG:CD	2.67	0.40
1:A:125:PHE:HD1	1:A:127:TRP:CD1	2.38	0.40
1:A:184:HIS:HB3	1:A:220:ARG:HH21	1.86	0.40
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.20	0.40
1:A:54:ASN:HA	7:A:422:HOH:O	2.21	0.40
1:D:226:GLN:HA	1:D:227:PRO:HD3	1.86	0.40
2:H:145:ASP:O	2:H:148:CYS:N	2.55	0.40
1:A:59:LEU:CD1	1:A:82:GLU:HG2	2.51	0.40
2:B:51:LYS:NZ	2:B:106:HIS:ND1	2.59	0.40
1:D:248:ASN:ND2	1:D:248:ASN:H	2.15	0.40
1:A:65:THR:HG23	1:A:89:GLU:OE1	2.20	0.40
1:D:84:TRP:CZ2	1:D:116:GLY:HA2	2.57	0.40
1:D:202:VAL:HA	1:D:247:SER:HB2	2.02	0.40
1:G:264:LYS:HB2	2:H:63:PHE:CD1	2.57	0.40
1:G:30:THR:H	2:H:105:GLN:HE22	1.68	0.40
2:H:148:CYS:O	2:H:152:ILE:HG13	2.21	0.40
1:A:216:ASN:O	1:A:220:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	316/329 (96%)	282 (89%)	29 (9%)	5 (2%)	9 43
1	D	316/329 (96%)	289 (92%)	23 (7%)	4 (1%)	12 47
1	G	316/329 (96%)	292 (92%)	20 (6%)	4 (1%)	12 47
2	B	170/221 (77%)	155 (91%)	15 (9%)	0	100 100
2	E	170/221 (77%)	155 (91%)	14 (8%)	1 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	170/221 (77%)	153 (90%)	17 (10%)	0	100 100
All	All	1458/1650 (88%)	1326 (91%)	118 (8%)	14 (1%)	15 54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PRO
1	A	324	PRO
1	A	325	GLU
1	D	324	PRO
1	D	325	GLU
1	G	10	THR
1	A	126	THR
1	D	62	ARG
1	G	21	PRO
1	G	62	ARG
1	G	104	ASP
1	D	54	ASN
2	E	57	GLU
1	A	21	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/288 (93%)	249 (93%)	19 (7%)	14 47
1	D	270/288 (94%)	241 (89%)	29 (11%)	6 27
1	G	268/288 (93%)	234 (87%)	34 (13%)	4 20
2	B	145/190 (76%)	135 (93%)	10 (7%)	15 49
2	E	146/190 (77%)	133 (91%)	13 (9%)	9 35
2	H	147/190 (77%)	137 (93%)	10 (7%)	16 49
All	All	1244/1434 (87%)	1129 (91%)	115 (9%)	9 33

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	44	GLN
1	A	46	SER
1	A	54	ASN
1	A	74	PRO
1	A	92	ASN
1	A	96	ASN
1	A	101	ASP
1	A	155	THR
1	A	179	ILE
1	A	182	VAL
1	A	210	GLN
1	A	248	ASN
1	A	261	ARG
1	A	268	MET
1	A	274	ILE
1	A	280	GLU
1	A	290	ASN
1	A	311	GLN
2	B	27	GLN
2	B	60	ASN
2	B	64	HIS
2	B	72	GLU
2	B	91	LEU
2	B	102	LEU
2	B	120	GLU
2	B	121	LYS
2	B	149	ILE
2	B	168	ASN
1	D	18	HIS
1	D	38	ASN
1	D	41	GLU
1	D	45	SER
1	D	46	SER
1	D	48	THR
1	D	53	ASN
1	D	74	PRO
1	D	90	ARG
1	D	92	ASN
1	D	96	ASN
1	D	99	PRO
1	D	101	ASP

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Mol	Chain	Res	Type
1	D	167	THR
1	D	169	PRO
1	D	182	VAL
1	D	210	GLN
1	D	215	PRO
1	D	221	PRO
1	D	230	ILE
1	D	231	SER
1	D	239	PRO
1	D	248	ASN
1	D	261	ARG
1	D	273	PRO
1	D	306	PRO
1	D	311	GLN
1	D	313	THR
1	D	324	PRO
2	E	9	PHE
2	E	12	ASN
2	E	19	ASP
2	E	27	GLN
2	E	49	ASN
2	E	60	ASN
2	E	64	HIS
2	E	72	GLU
2	E	91	LEU
2	E	120	GLU
2	E	121	LYS
2	E	149	ILE
2	E	168	ASN
1	G	10	THR
1	G	18	HIS
1	G	20	VAL
1	G	29	ILE
1	G	38	ASN
1	G	44	GLN
1	G	46	SER
1	G	74	PRO
1	G	92	ASN
1	G	96	ASN
1	G	109	ARG
1	G	111	LEU
1	G	155	THR

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Mol	Chain	Res	Type
1	G	161	TYR
1	G	162	PRO
1	G	179	ILE
1	G	182	VAL
1	G	185	PRO
1	G	210	GLN
1	G	221	PRO
1	G	229	ARG
1	G	230	ILE
1	G	239	PRO
1	G	248	ASN
1	G	261	ARG
1	G	268	MET
1	G	273	PRO
1	G	290	ASN
1	G	292	LYS
1	G	307	LYS
1	G	311	GLN
1	G	315	LYS
1	G	324	PRO
1	G	325	GLU
2	H	18	ILE
2	H	19	ASP
2	H	57	GLU
2	H	60	ASN
2	H	72	GLU
2	H	102	LEU
2	H	120	GLU
2	H	121	LYS
2	H	149	ILE
2	H	156	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	92	ASN
1	A	96	ASN
1	A	171	ASN
1	A	210	GLN
1	A	211	GLN
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	248	ASN
1	A	290	ASN
1	A	296	ASN
2	B	27	GLN
2	B	60	ASN
2	B	105	GLN
2	B	168	ASN
2	B	172	GLN
1	D	18	HIS
1	D	53	ASN
1	D	54	ASN
1	D	92	ASN
1	D	96	ASN
1	D	171	ASN
1	D	210	GLN
1	D	226	GLN
1	D	248	ASN
1	D	296	ASN
1	D	311	GLN
2	E	12	ASN
2	E	26	HIS
2	E	27	GLN
2	E	53	ASN
2	E	60	ASN
2	E	105	GLN
2	E	125	GLN
2	E	168	ASN
2	E	172	GLN
1	G	92	ASN
1	G	96	ASN
1	G	171	ASN
1	G	211	GLN
1	G	248	ASN
1	G	290	ASN
1	G	296	ASN
2	H	12	ASN
2	H	26	HIS
2	H	27	GLN
2	H	60	ASN
2	H	105	GLN
2	H	142	HIS
2	H	168	ASN

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Mol	Chain	Res	Type
2	H	172	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

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.59	0	17,19,21	0.61	0
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	0.61	0
4	NAG	F	1	1,4	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	0.67	0
4	BMA	F	3	4	11,11,12	0.81	0	15,15,17	1.31	1 (6%)
4	MAN	F	4	4	11,11,12	0.59	0	15,15,17	0.62	0
3	NAG	I	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	1.29	1 (5%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
5	GAL	J	1	5	12,12,12	0.83	1 (8%)	17,17,17	0.85	1 (5%)
5	SIA	J	2	5	17,20,21	0.63	0	21,28,31	0.84	1 (4%)
4	NAG	K	1	1,4	14,14,15	0.66	0	17,19,21	0.85	1 (5%)
4	NAG	K	2	4	14,14,15	0.74	0	17,19,21	0.73	0
4	BMA	K	3	4	11,11,12	0.51	0	15,15,17	1.53	4 (26%)
4	MAN	K	4	4	11,11,12	0.63	0	15,15,17	0.71	0
5	GAL	L	1	5	12,12,12	0.83	1 (8%)	17,17,17	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SIA	L	2	5	17,20,21	0.64	0	21,28,31	0.84	1 (4%)
4	NAG	M	1	1,4	14,14,15	0.46	0	17,19,21	0.86	1 (5%)
4	NAG	M	2	4	14,14,15	0.51	0	17,19,21	1.07	1 (5%)
4	BMA	M	3	4	11,11,12	0.79	0	15,15,17	1.21	1 (6%)
4	MAN	M	4	4	11,11,12	1.21	1 (9%)	15,15,17	1.29	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
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
5	GAL	J	1	5	-	0/2/22/22	0/1/1/1
5	SIA	J	2	5	-	0/14/34/38	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
5	GAL	L	1	5	-	0/2/22/22	0/1/1/1
5	SIA	L	2	5	-	0/14/34/38	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	4	MAN	O5-C5	2.71	1.48	1.43
5	L	1	GAL	O1-C1	-2.69	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	GAL	O1-C1	-2.67	1.31	1.39
3	I	1	NAG	C1-C2	2.64	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	3	BMA	C3-C4-C5	3.85	117.11	110.24
3	I	1	NAG	C4-C3-C2	-3.23	106.29	111.02
4	K	3	BMA	C1-C2-C3	-2.95	106.04	109.67
4	M	2	NAG	C2-N2-C7	-2.88	118.80	122.90
4	M	4	MAN	C2-C3-C4	2.84	115.81	110.89
4	M	3	BMA	C2-C3-C4	-2.58	106.43	110.89
4	F	1	NAG	C2-N2-C7	-2.52	119.31	122.90
4	M	4	MAN	O2-C2-C1	2.42	114.10	109.15
4	K	3	BMA	O3-C3-C2	2.36	114.51	109.99
4	M	1	NAG	C1-C2-N2	-2.28	106.59	110.49
4	K	3	BMA	C2-C3-C4	2.24	114.78	110.89
5	L	1	GAL	O1-C1-C2	2.22	115.29	109.03
5	J	1	GAL	O1-C1-C2	2.21	115.26	109.03
4	K	1	NAG	C1-C2-N2	-2.20	106.74	110.49
5	J	2	SIA	C8-C7-C6	-2.19	108.88	113.03
5	L	2	SIA	C8-C7-C6	-2.17	108.92	113.03
4	K	3	BMA	C6-C5-C4	-2.10	108.08	113.00
3	I	2	NAG	C2-N2-C7	-2.05	119.99	122.90
4	M	4	MAN	O5-C5-C6	2.04	110.41	107.20

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7
4	K	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	4	MAN	C4-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	K	4	MAN	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	F	4	MAN	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	M	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6

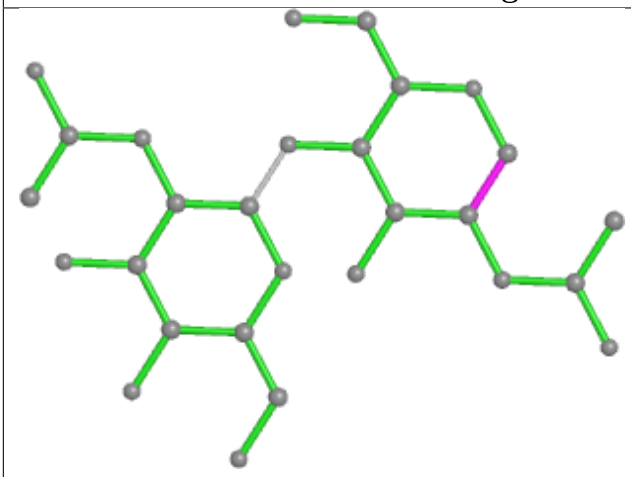
There are no ring outliers.

9 monomers are involved in 11 short contacts:

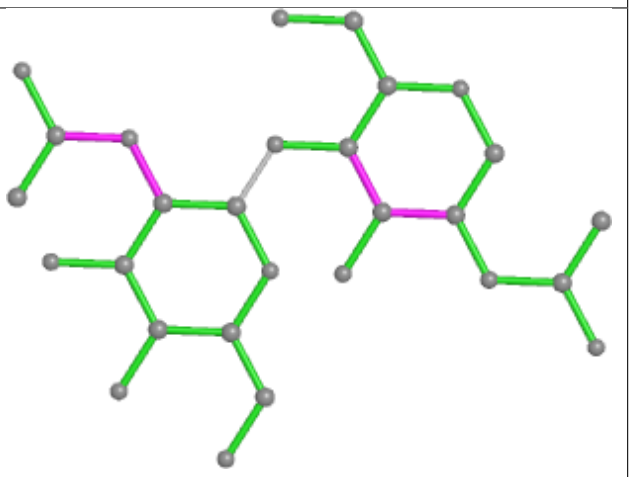
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
4	F	1	NAG	2	0
5	L	2	SIA	2	0
5	J	2	SIA	1	0
4	M	2	NAG	2	0
4	K	1	NAG	1	0
4	K	2	NAG	1	0
4	M	1	NAG	3	0
3	C	1	NAG	1	0

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

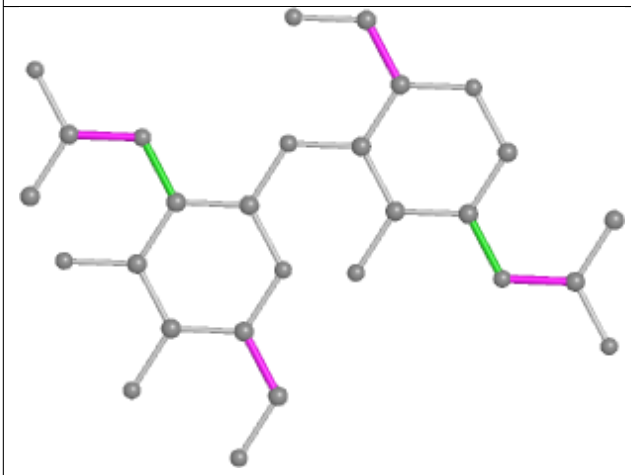
Oligosaccharide Chain I



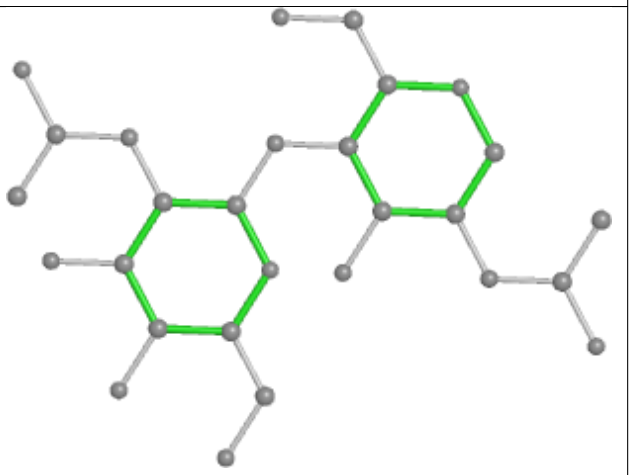
Bond lengths



Bond angles

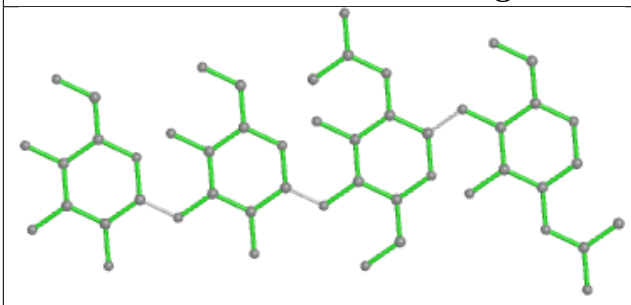


Torsions

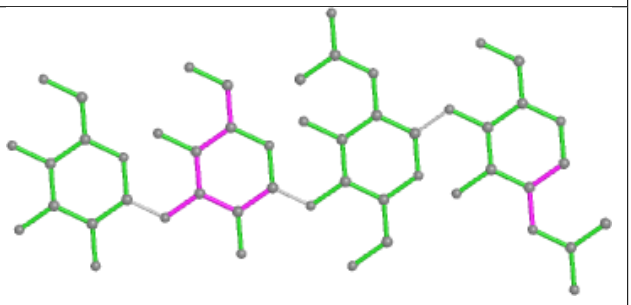


Rings

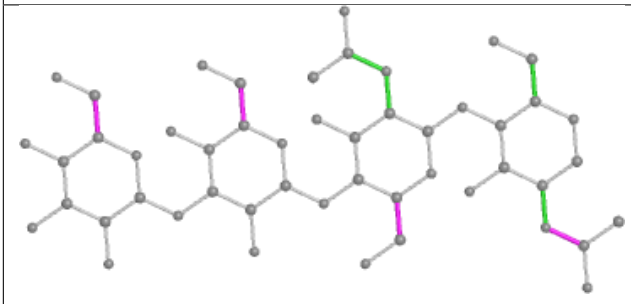
Oligosaccharide Chain K



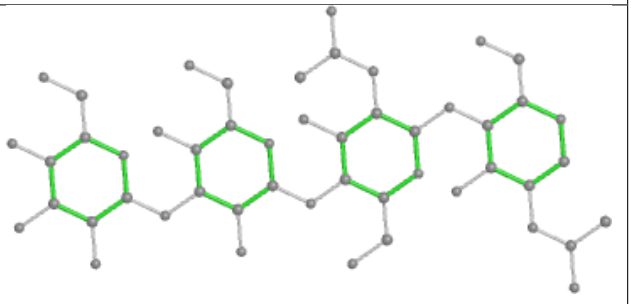
Bond lengths



Bond angles

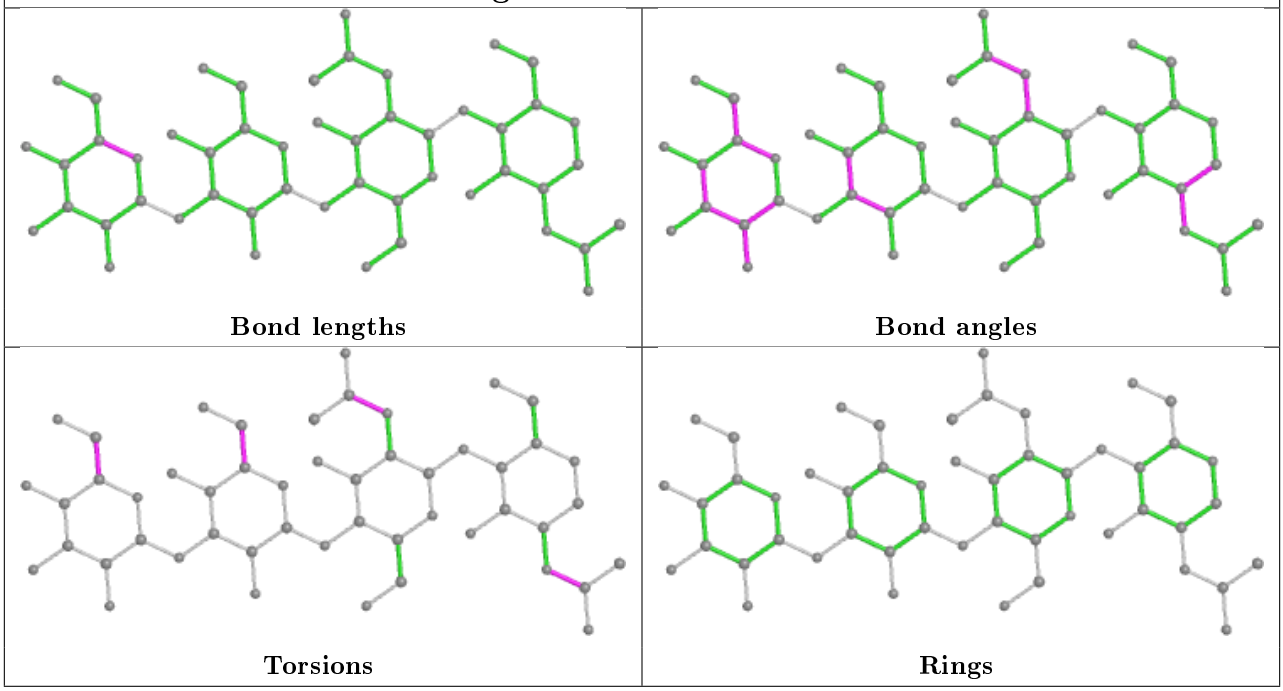


Torsions

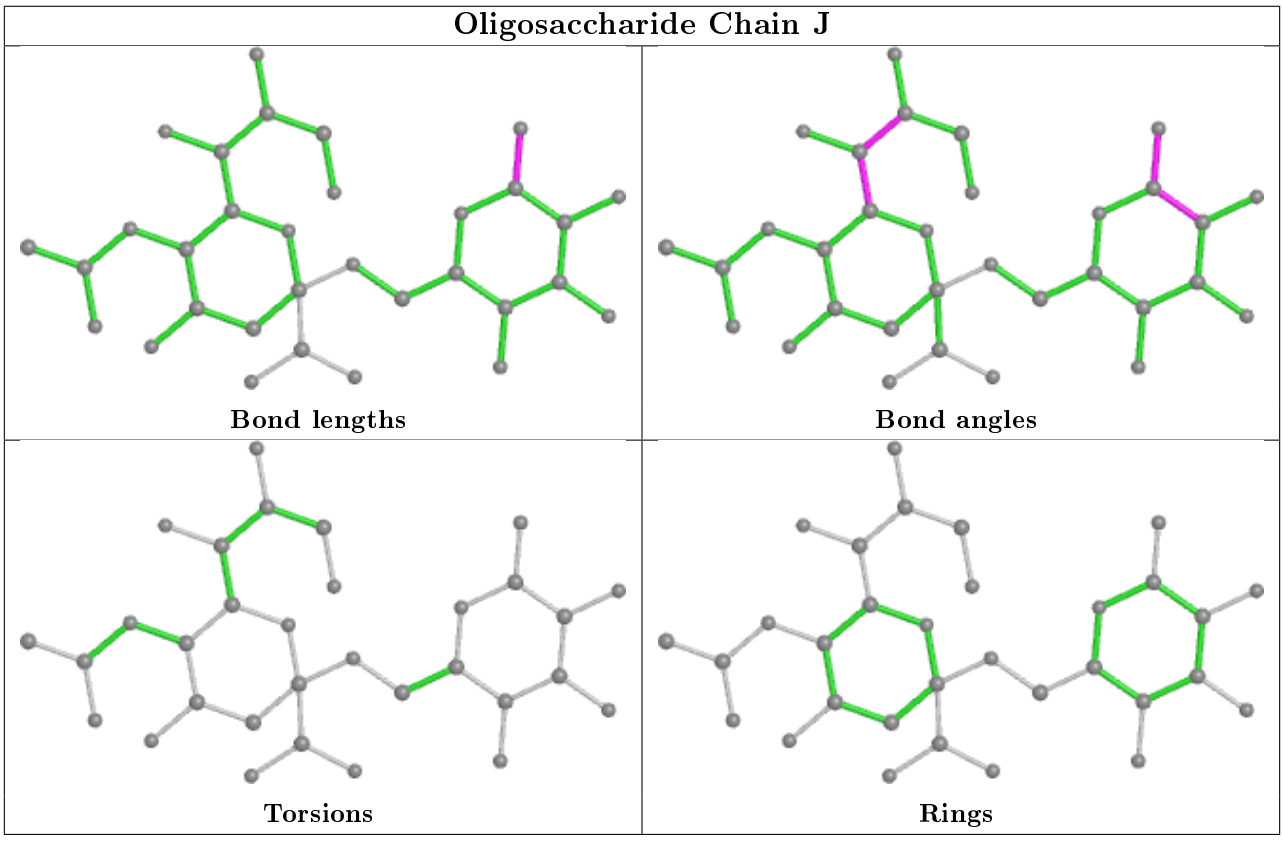


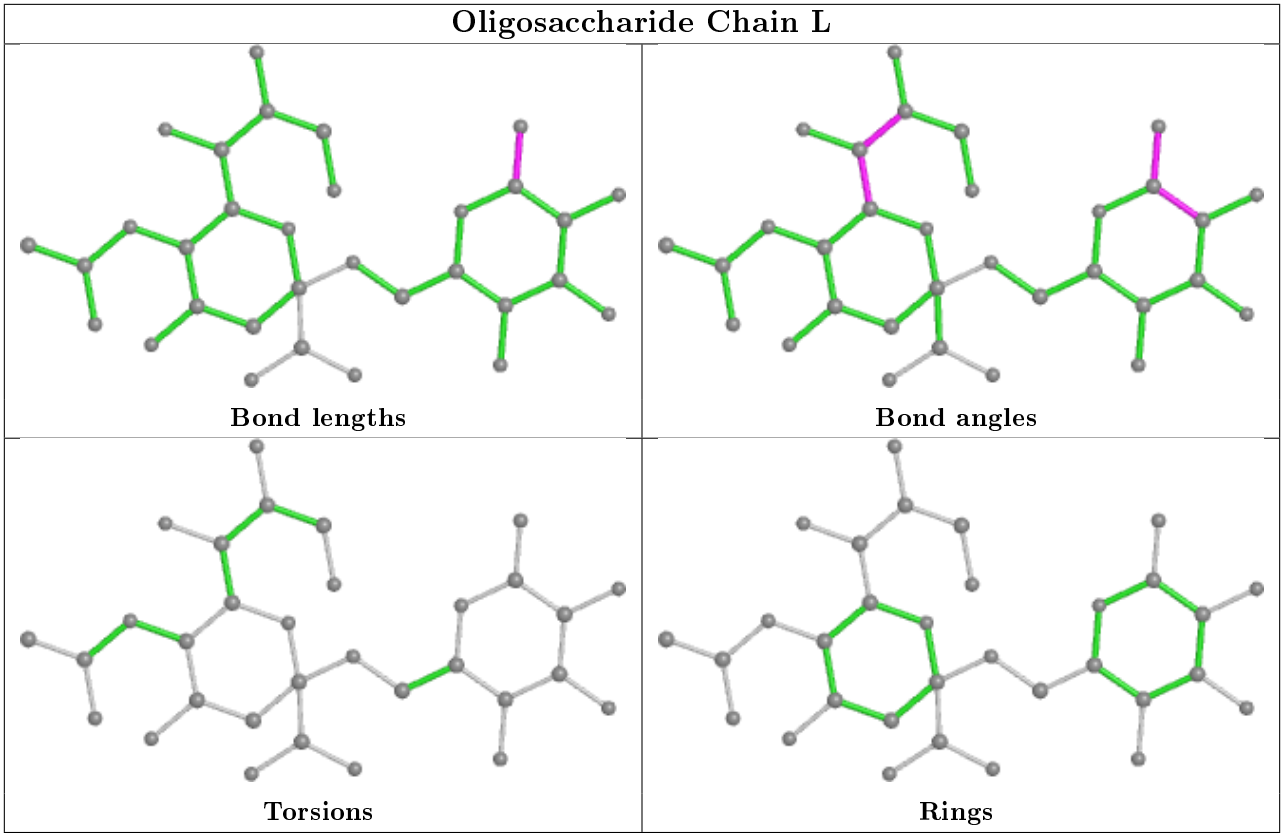
Rings

Oligosaccharide Chain M



Oligosaccharide Chain J





5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
6	NAG	H	400	2	14,14,15	1.32	3 (21%)	17,19,21	1.25	2 (11%)
6	NAG	G	400	1	14,14,15	1.22	1 (7%)	17,19,21	2.56	5 (29%)
6	NAG	D	400	1	14,14,15	1.17	2 (14%)	17,19,21	2.01	4 (23%)
6	NAG	B	400	2	14,14,15	0.66	0	17,19,21	0.89	1 (5%)
6	NAG	G	406	1	14,14,15	0.86	1 (7%)	17,19,21	1.14	1 (5%)
6	NAG	G	401	1	14,14,15	0.73	0	17,19,21	1.27	2 (11%)
6	NAG	D	401	1	14,14,15	0.94	1 (7%)	17,19,21	1.40	3 (17%)
6	NAG	E	400	2	14,14,15	0.61	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	400	1	14,14,15	0.72	0	17,19,21	0.75	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	400	2	-	4/6/23/26	0/1/1/1
6	NAG	G	400	1	-	2/6/23/26	0/1/1/1
6	NAG	D	400	1	-	6/6/23/26	0/1/1/1
6	NAG	B	400	2	-	2/6/23/26	0/1/1/1
6	NAG	G	406	1	-	3/6/23/26	0/1/1/1
6	NAG	G	401	1	-	1/6/23/26	0/1/1/1
6	NAG	D	401	1	-	4/6/23/26	0/1/1/1
6	NAG	E	400	2	-	2/6/23/26	0/1/1/1
6	NAG	A	400	1	-	6/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	400	NAG	C1-C2	3.24	1.57	1.52
6	D	400	NAG	O5-C5	2.94	1.49	1.43
6	G	400	NAG	C1-C2	2.76	1.56	1.52
6	H	400	NAG	C8-C7	2.35	1.55	1.50
6	H	400	NAG	C4-C5	2.24	1.57	1.53
6	G	406	NAG	O5-C5	2.18	1.47	1.43
6	D	401	NAG	O5-C5	2.17	1.47	1.43
6	D	400	NAG	C3-C2	2.09	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	400	NAG	C6-C5-C4	-6.09	98.73	113.00
6	D	400	NAG	C1-C2-N2	-4.88	102.15	110.49
6	D	400	NAG	O5-C5-C6	4.38	114.07	107.20
6	G	400	NAG	C1-O5-C5	4.28	117.99	112.19
6	G	400	NAG	C2-N2-C7	-3.91	117.33	122.90
6	G	401	NAG	C2-N2-C7	-3.82	117.47	122.90
6	G	400	NAG	C4-C3-C2	-3.61	105.72	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	406	NAG	C3-C4-C5	-3.16	104.61	110.24
6	G	400	NAG	O5-C1-C2	3.15	116.26	111.29
6	H	400	NAG	C8-C7-N2	3.12	121.39	116.10
6	D	400	NAG	C1-O5-C5	-3.12	107.97	112.19
6	D	401	NAG	O7-C7-N2	2.93	127.34	121.95
6	B	400	NAG	C2-N2-C7	-2.84	118.86	122.90
6	G	401	NAG	C1-O5-C5	2.55	115.65	112.19
6	D	400	NAG	C2-N2-C7	-2.47	119.39	122.90
6	H	400	NAG	O7-C7-C8	-2.24	117.90	122.06
6	A	400	NAG	C2-N2-C7	-2.20	119.78	122.90
6	D	401	NAG	O5-C5-C6	2.17	110.61	107.20
6	D	401	NAG	C3-C4-C5	-2.17	106.38	110.24

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	400	NAG	C8-C7-N2-C2
6	G	400	NAG	O7-C7-N2-C2
6	D	400	NAG	C1-C2-N2-C7
6	D	400	NAG	O7-C7-N2-C2
6	B	400	NAG	C8-C7-N2-C2
6	B	400	NAG	O7-C7-N2-C2
6	G	406	NAG	C8-C7-N2-C2
6	G	406	NAG	O7-C7-N2-C2
6	D	401	NAG	C8-C7-N2-C2
6	D	401	NAG	O7-C7-N2-C2
6	A	400	NAG	C8-C7-N2-C2
6	A	400	NAG	O7-C7-N2-C2
6	D	400	NAG	C8-C7-N2-C2
6	A	400	NAG	O5-C5-C6-O6
6	D	400	NAG	O5-C5-C6-O6
6	A	400	NAG	C4-C5-C6-O6
6	H	400	NAG	C8-C7-N2-C2
6	D	400	NAG	C4-C5-C6-O6
6	D	401	NAG	C1-C2-N2-C7
6	H	400	NAG	O7-C7-N2-C2
6	A	400	NAG	C1-C2-N2-C7
6	H	400	NAG	O5-C5-C6-O6
6	G	406	NAG	C3-C2-N2-C7
6	D	401	NAG	C3-C2-N2-C7
6	H	400	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	G	401	NAG	C8-C7-N2-C2
6	E	400	NAG	C4-C5-C6-O6
6	D	400	NAG	C3-C2-N2-C7
6	E	400	NAG	O5-C5-C6-O6
6	A	400	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	400	NAG	2	0
6	G	400	NAG	5	0
6	G	406	NAG	6	0

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, 95^{th} 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	318/329 (96%)	-0.03	5 (1%)	72	59	23, 41, 61, 79	0
1	D	318/329 (96%)	-0.14	3 (0%)	84	75	13, 35, 54, 77	0
1	G	318/329 (96%)	-0.02	8 (2%)	57	43	19, 38, 59, 93	0
2	B	172/221 (77%)	-0.27	2 (1%)	79	67	10, 37, 57, 85	0
2	E	172/221 (77%)	-0.05	4 (2%)	60	47	16, 40, 64, 82	0
2	H	172/221 (77%)	-0.04	2 (1%)	79	67	15, 39, 61, 84	0
All	All	1470/1650 (89%)	-0.08	24 (1%)	72	59	10, 38, 60, 93	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	PRO	3.4
2	E	57	GLU	3.0
2	H	29	SER	2.9
1	G	277	CYS	2.7
1	A	144	ALA	2.7
1	G	46	SER	2.7
1	G	275	ASP	2.6
1	D	326	LYS	2.5
1	G	272	ALA	2.5
1	G	287	SER	2.4
2	H	148	CYS	2.4
1	D	171	ASN	2.4
1	G	276	THR	2.3
2	E	168	ASN	2.3
1	A	46	SER	2.2
1	A	239	PRO	2.2
1	G	324	PRO	2.1
2	B	172	GLN	2.1
2	E	29	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	173	ASN	2.1
1	A	169	PRO	2.1
1	D	128	THR	2.1
2	E	172	GLN	2.0
2	B	64	HIS	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)

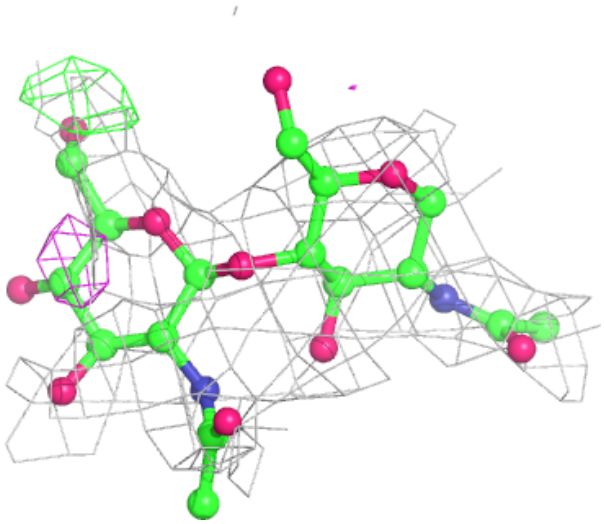
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

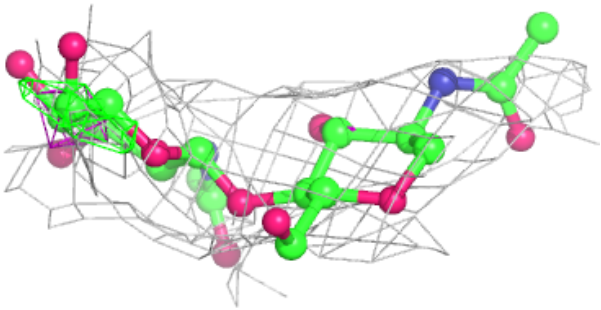
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.55	0.58	103,105,107,107	0
3	NAG	I	2	14/15	0.58	0.49	100,104,106,107	0
4	MAN	K	4	11/12	0.65	0.39	92,96,99,99	0
4	MAN	F	4	11/12	0.69	0.51	93,95,97,97	0
3	NAG	C	1	14/15	0.79	0.33	87,92,98,99	0
4	MAN	M	4	11/12	0.82	0.38	84,87,88,88	0
4	BMA	F	3	11/12	0.82	0.36	77,80,83,89	0
4	BMA	M	3	11/12	0.83	0.30	62,66,70,77	0
5	GAL	J	1	12/12	0.83	0.37	65,82,83,84	0
5	GAL	L	1	12/12	0.85	0.46	59,78,81,82	0
4	BMA	K	3	11/12	0.87	0.32	78,81,83,88	0
4	NAG	F	1	14/15	0.87	0.29	52,55,58,61	0
5	SIA	J	2	20/21	0.89	0.28	53,56,64,64	0
3	NAG	I	1	14/15	0.89	0.46	76,81,90,93	0
4	NAG	M	1	14/15	0.92	0.27	28,31,36,38	0
4	NAG	K	1	14/15	0.92	0.32	49,53,57,59	0
5	SIA	L	2	20/21	0.92	0.28	40,45,53,55	0
4	NAG	K	2	14/15	0.92	0.26	60,62,64,71	0
4	NAG	F	2	14/15	0.93	0.36	61,63,68,74	0
4	NAG	M	2	14/15	0.95	0.19	38,42,45,53	0

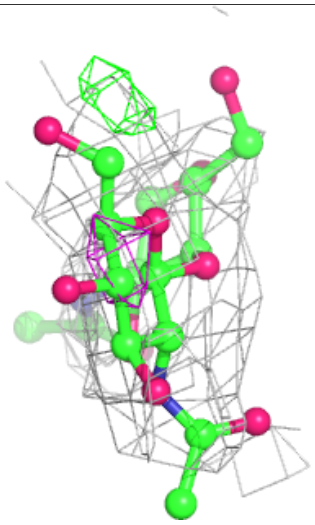
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

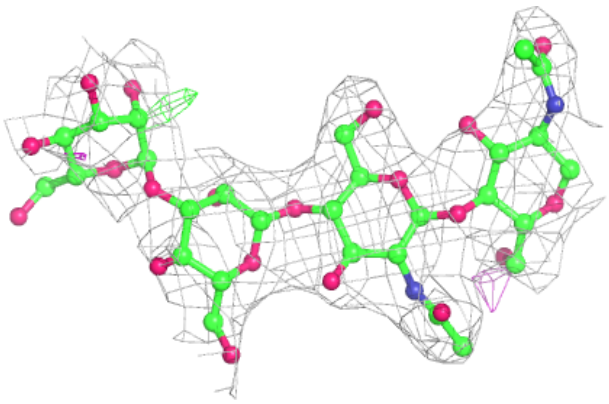


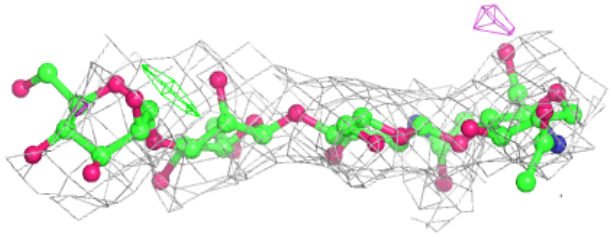


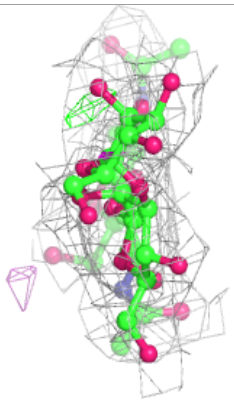


Electron density around Chain K:

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

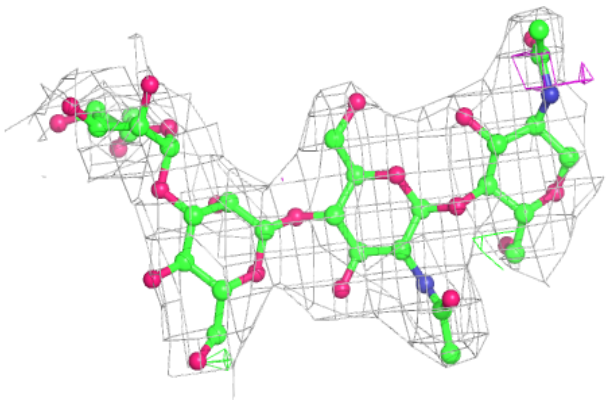


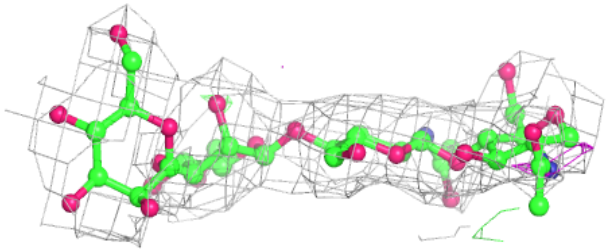


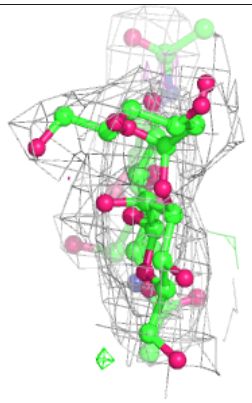


Electron density around Chain M:

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

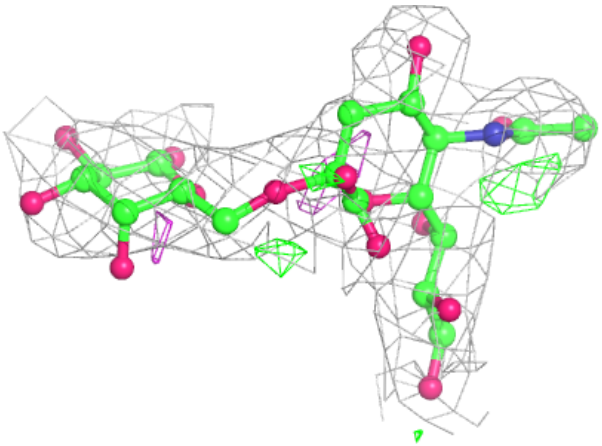


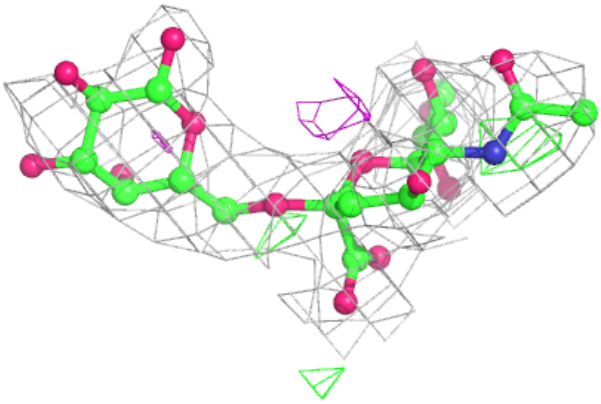


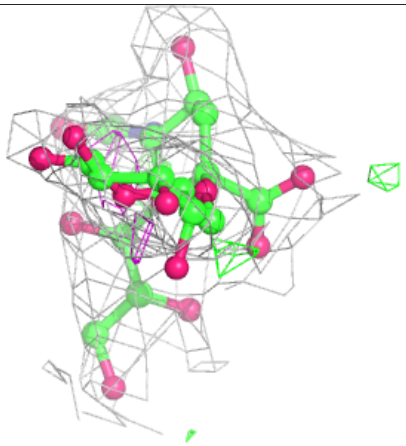


Electron density around Chain J:

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

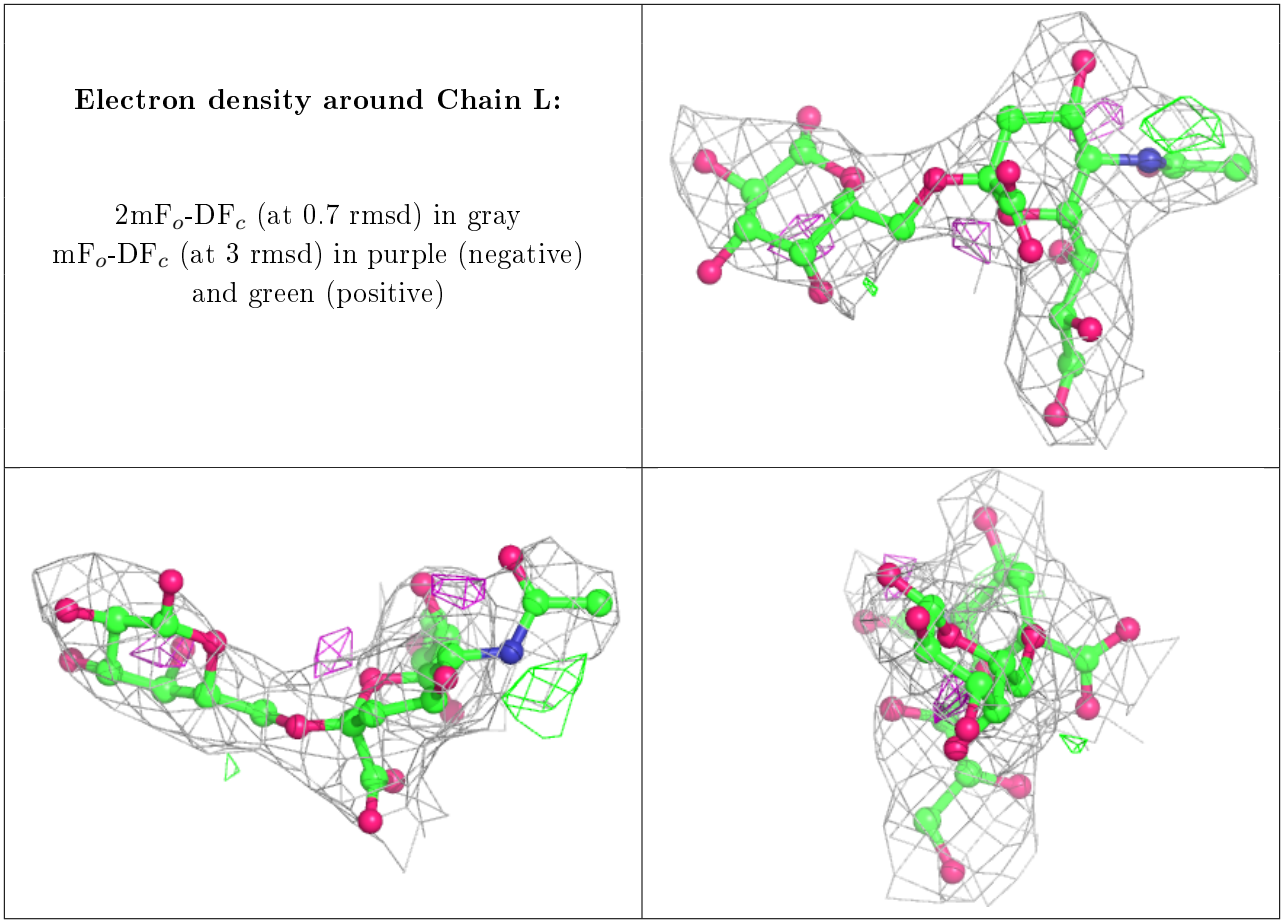






Electron density around Chain L:

$2mF_o$-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, 95^{th} 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
6	NAG	G	400	14/15	0.53	0.52	90,97,99,101	0
6	NAG	G	406	14/15	0.74	0.44	75,79,83,84	0
6	NAG	D	401	14/15	0.74	0.45	82,88,92,93	0
6	NAG	E	400	14/15	0.74	0.72	88,93,95,96	0
6	NAG	H	400	14/15	0.77	0.55	86,89,90,92	0
6	NAG	A	400	14/15	0.77	0.48	74,79,83,83	0
6	NAG	G	401	14/15	0.78	0.34	64,68,70,72	0
6	NAG	D	400	14/15	0.81	0.27	71,74,77,78	0
6	NAG	B	400	14/15	0.86	0.59	77,82,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.