Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:22 AM EDT

PDB ID	:	2GK1
Title	:	X-ray crystal structure of NGT-bound HexA
Authors	:	Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.; James, M.N.
Deposited on	:	2006-03-31
Resolution	:	3.25 Å(reported)

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

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

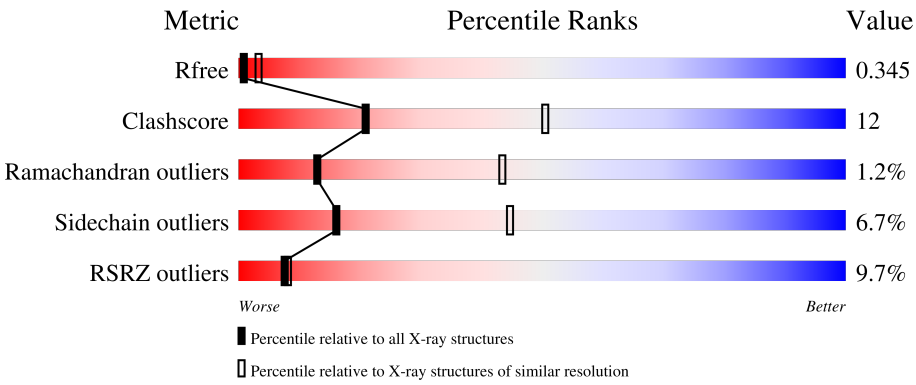
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	52	52% 37% 12%
1	C	52	2% 54% 42% •
1	E	52	10% 62% 35% •
1	G	52	4% 52% 44% •
2	I	440	2% 66% 30% •

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Mol	Chain	Length	Quality of chain
2	J	440	5% 71% 25%
2	K	440	11% 71% 26%
2	L	440	14% 67% 30%
3	B	58	2% 76% 10% 7% 7%
3	D	58	2% 83% 10% 7%
3	F	58	21% 66% 26% 7%
3	H	58	28% 59% 33% 7%
4	M	190	6% 73% 26%
4	O	190	4% 75% 23%
4	Q	190	15% 65% 34%
4	S	190	16% 79% 21%
5	N	237	4% 76% 23%
5	P	237	4% 69% 28%
5	R	237	11% 71% 27%
5	T	237	32% 75% 24%
6	U	3	100%
6	V	3	100%
6	W	3	100%
6	Y	3	33% 67%
6	d	3	33% 67%
7	X	2	50% 50%
7	Z	2	100%
7	a	2	100%
7	b	2	50% 50%
7	c	2	100%

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Mol	Chain	Length	Quality of chain
7	e	2	100%

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
6	NAG	Y	1	-	-	X	-
6	NAG	Y	2	X	-	-	-
6	BMA	Y	3	-	-	-	X
6	NAG	d	2	X	-	-	-
7	NAG	X	1	-	-	-	X
7	NAG	X	2	-	-	-	X
7	NAG	Z	1	X	-	-	-
7	NAG	Z	2	X	-	-	-
7	NAG	a	1	X	-	-	-
7	NAG	a	2	X	-	-	X
7	NAG	b	1	X	-	-	-
7	NAG	b	2	X	-	-	-
7	NAG	c	2	X	-	-	X
7	NAG	e	2	X	-	-	-
8	NGT	A	21	-	-	X	-
8	NGT	C	530	-	-	X	-
8	NGT	E	530	-	-	X	-
8	NGT	G	533	-	-	X	-
8	NGT	H	28	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 32011 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 Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	52	441	286	73	81	1	0	0	0
1	C	52	441	286	73	81	1	0	0	0
1	E	52	441	286	73	81	1	0	0	0
1	G	52	441	286	73	81	1	0	0	0

- Molecule 2 is a protein called Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	440	3565	2312	577	663	13	0	0	0
2	J	440	3565	2312	577	663	13	0	0	0
2	K	440	3565	2312	577	663	13	0	0	0
2	L	440	3565	2312	577	663	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	436	VAL	ILE	variant	UNP P06865
J	436	VAL	ILE	variant	UNP P06865
K	436	VAL	ILE	variant	UNP P06865
L	436	VAL	ILE	variant	UNP P06865

- Molecule 3 is a protein called Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	54	428	281	71	74	2	0	0	0
3	D	54	428	281	71	74	2	0	0	0
3	F	54	428	281	71	74	2	0	0	0
3	H	54	428	281	71	74	2	0	0	0

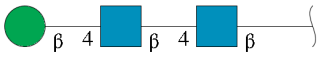
- Molecule 4 is a protein called Beta-hexosaminidase subunit beta chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	190	1528	982	256	286	4	0	0	0
4	O	189	1522	979	255	284	4	0	0	0
4	Q	190	1528	982	256	286	4	0	0	0
4	S	190	1528	982	256	286	4	0	0	0

- Molecule 5 is a protein called Beta-hexosaminidase subunit beta chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	N	236	1921	1242	316	356	7	0	0	0
5	P	236	1921	1242	316	356	7	0	0	0
5	R	236	1921	1242	316	356	7	0	0	0
5	T	236	1921	1242	316	356	7	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	U	3	39	22	2	15	0	0	0

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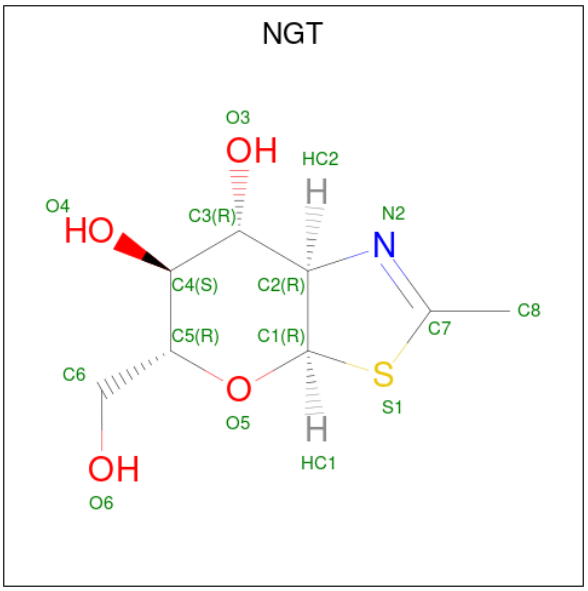
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	V	3	39	22	2	15	0	0	0
6	W	3	39	22	2	15	0	0	0
6	Y	3	39	22	2	15	0	0	0
6	d	3	39	22	2	15	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	X	2	28	16	2	10	0	0	0
7	Z	2	28	16	2	10	0	0	0
7	a	2	28	16	2	10	0	0	0
7	b	2	28	16	2	10	0	0	0
7	c	2	28	16	2	10	0	0	0
7	e	2	28	16	2	10	0	0	0

- Molecule 8 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	A	1	14	8	1	4	1	0	0
8	B	1	14	8	1	4	1	0	0
8	C	1	14	8	1	4	1	0	0
8	D	1	14	8	1	4	1	0	0
8	E	1	14	8	1	4	1	0	0
8	F	1	14	8	1	4	1	0	0
8	G	1	14	8	1	4	1	0	0
8	H	1	14	8	1	4	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	5	5	5	0	0
9	B	1	1	1	0	0
9	C	2	2	2	0	0
9	D	2	2	2	0	0

3 Residue-property plots (i)

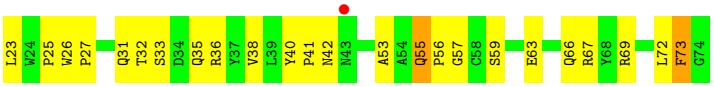
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-hexosaminidase subunit alpha

Chain A:

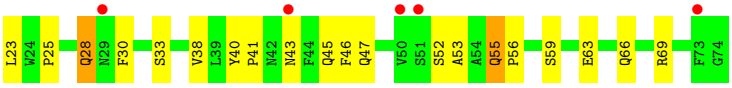
• Molecule 1: Beta-hexosaminidase subunit alpha

Chain C:



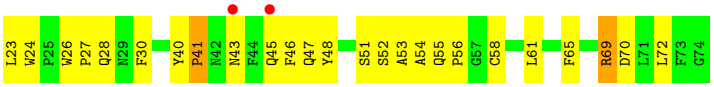
• Molecule 1: Beta-hexosaminidase subunit alpha

Chain E:



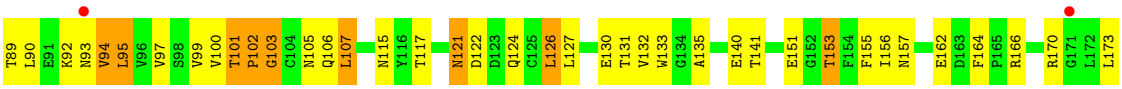
• Molecule 1: Beta-hexosaminidase subunit alpha

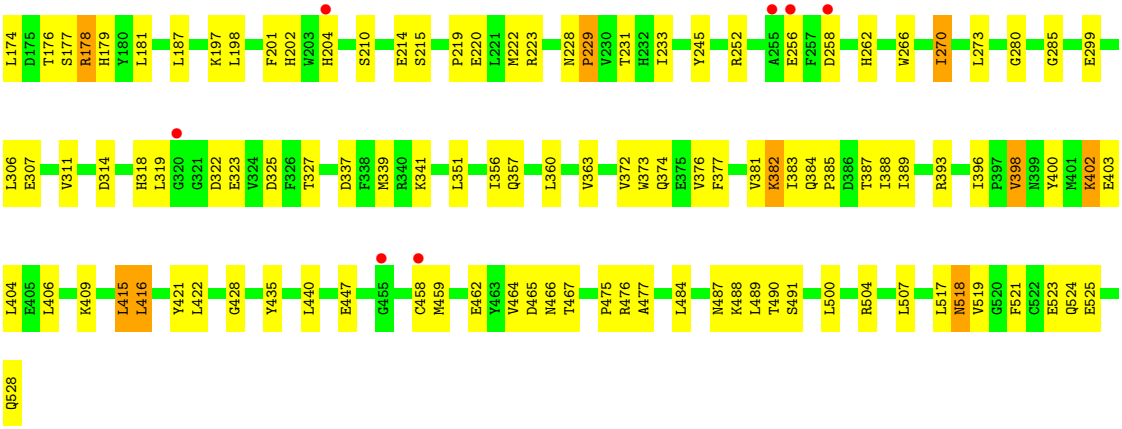
Chain G:



• Molecule 2: Beta-hexosaminidase subunit alpha

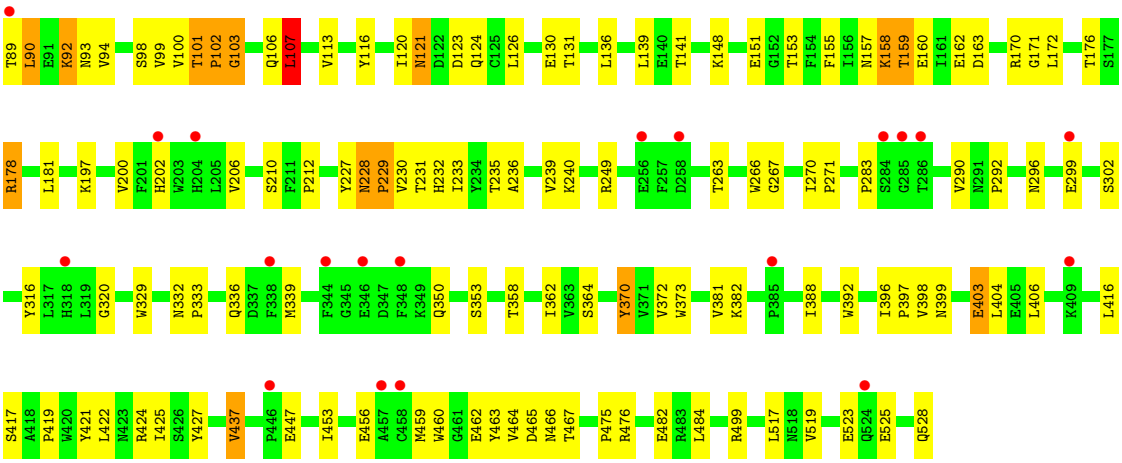
Chain I:





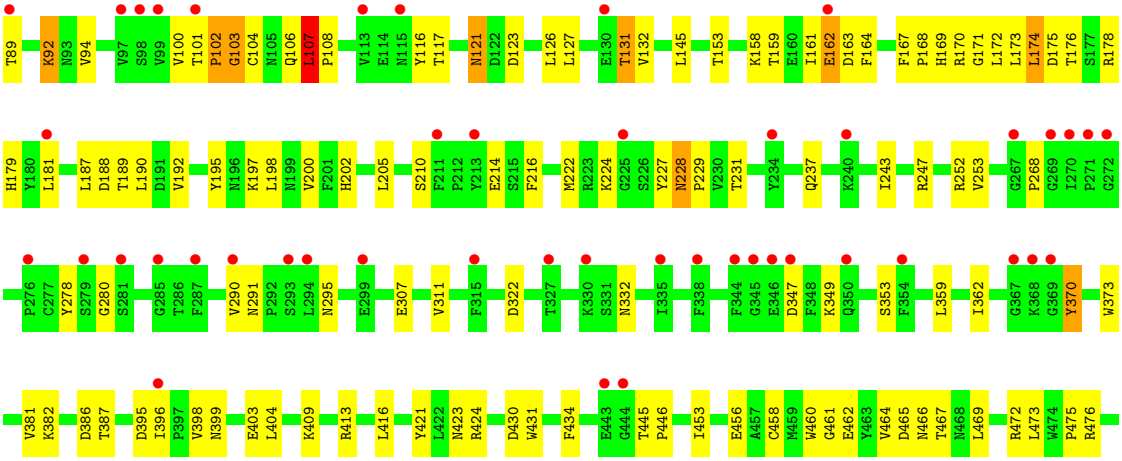
• Molecule 2: Beta-hexosaminidase subunit alpha

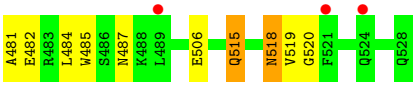
Chain J:



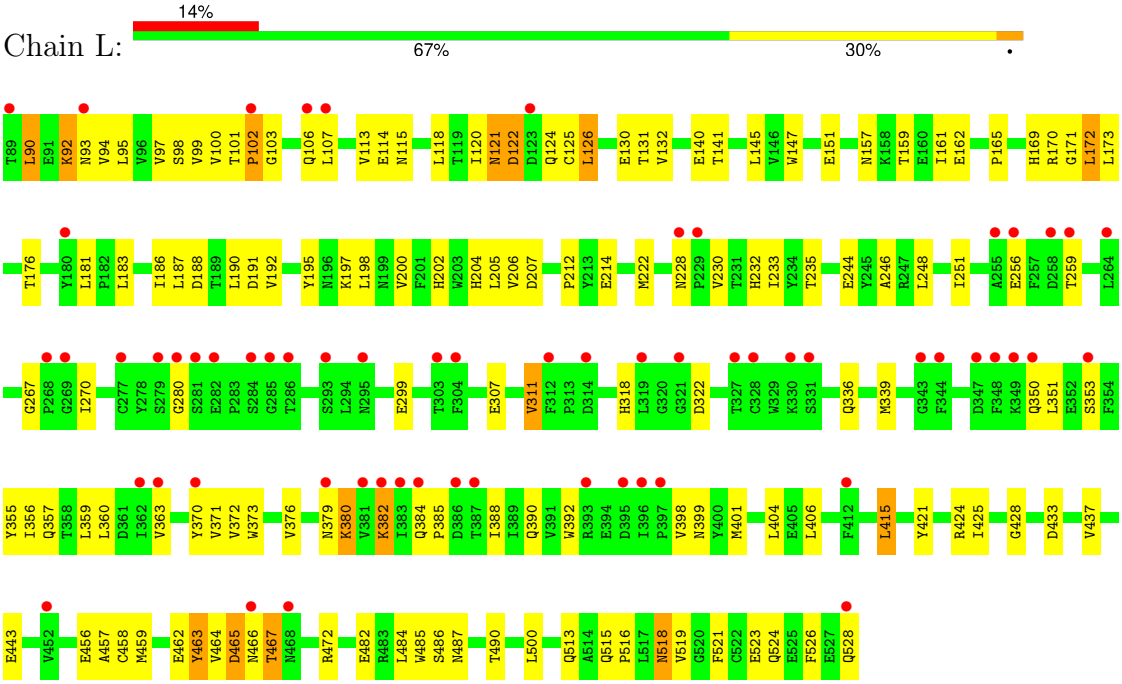
• Molecule 2: Beta-hexosaminidase subunit alpha

Chain K:

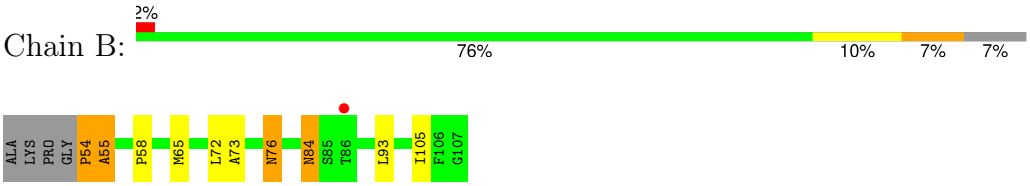




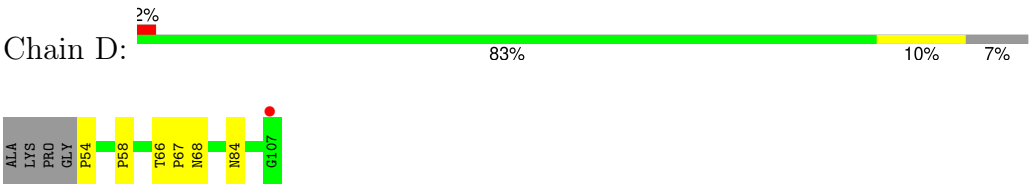
• Molecule 2: Beta-hexosaminidase subunit alpha



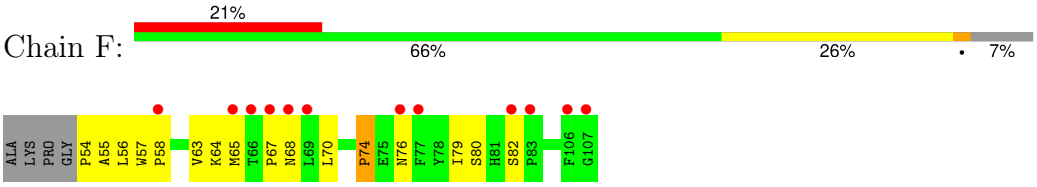
• Molecule 3: Beta-hexosaminidase subunit beta



• Molecule 3: Beta-hexosaminidase subunit beta



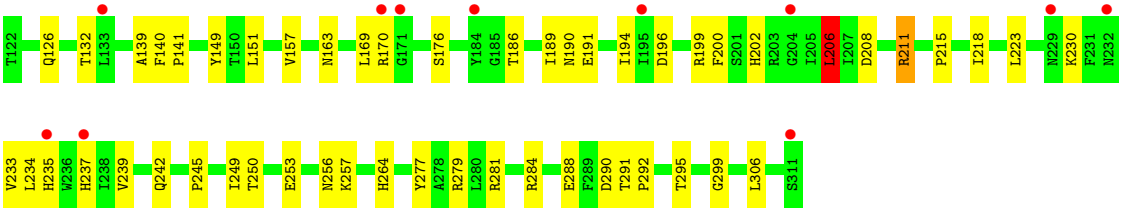
• Molecule 3: Beta-hexosaminidase subunit beta



• Molecule 3: Beta-hexosaminidase subunit beta

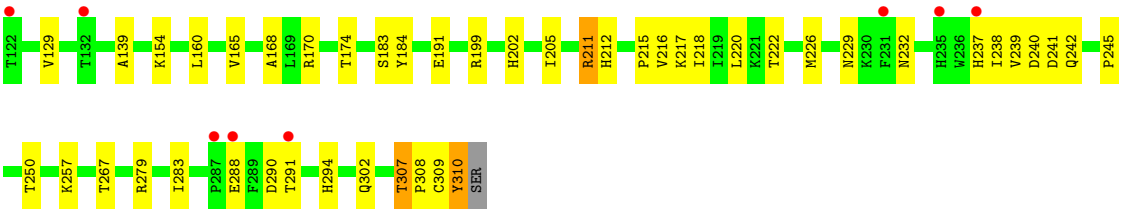
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain M:



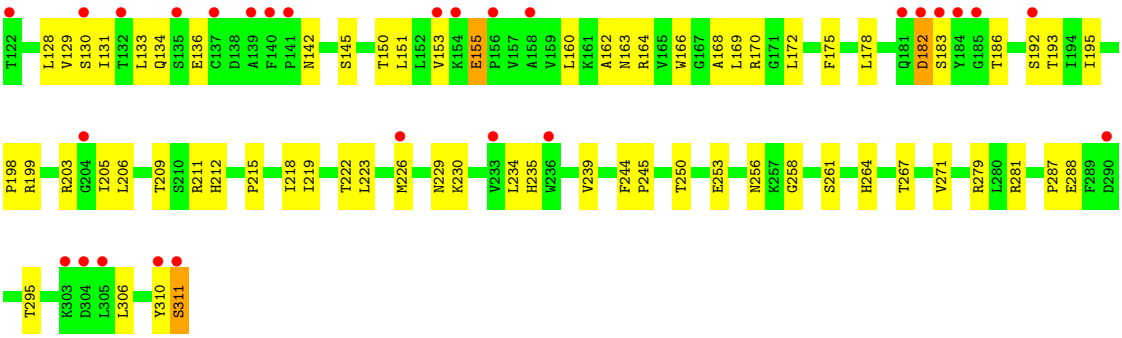
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain O:



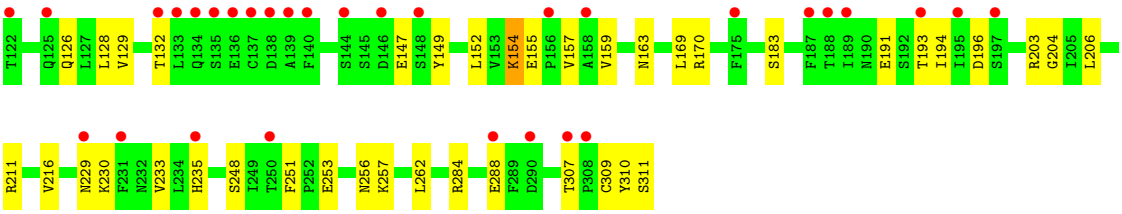
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain Q:



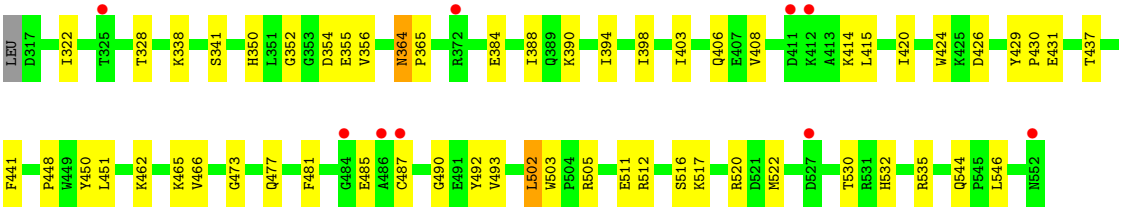
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain S:



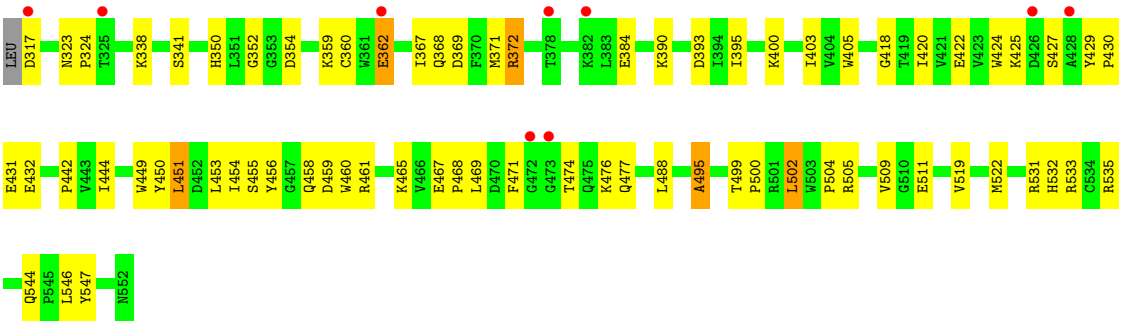
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain N:



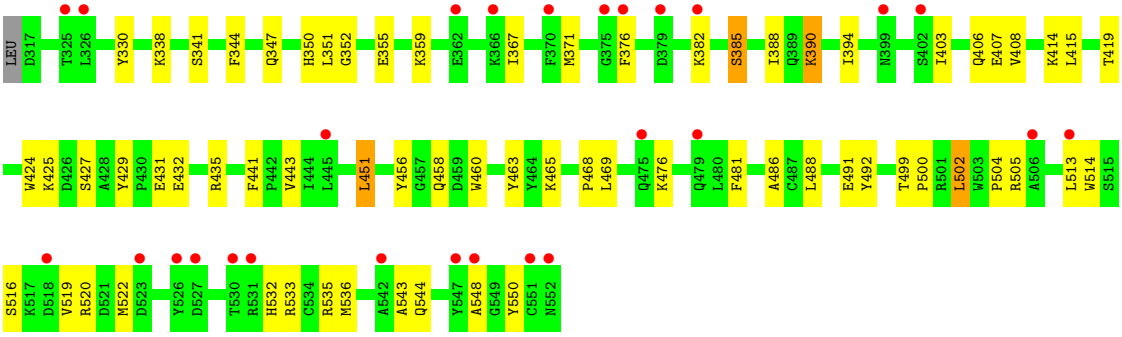
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain P:



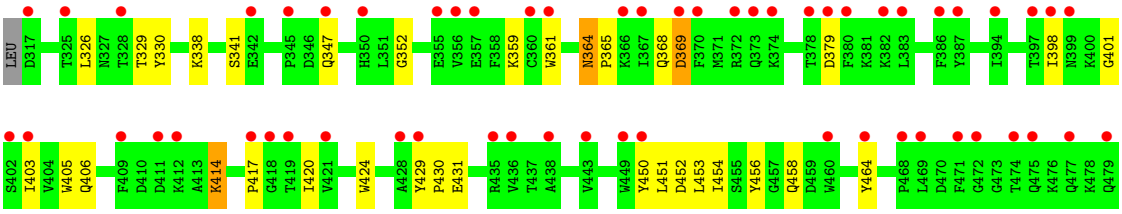
• Molecule 5: Beta-hexosaminidase subunit beta chain A

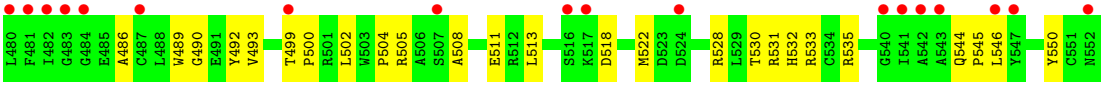
Chain R:



• Molecule 5: Beta-hexosaminidase subunit beta chain A

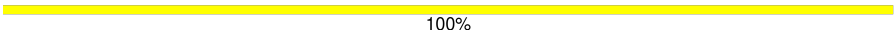
Chain T:





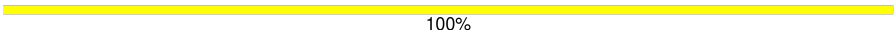
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



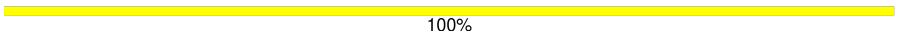
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

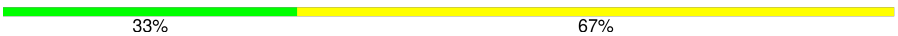


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%

NAG1
NAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

NAG1
NAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 50%

NAG1
NAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 100%

NAG1
NAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	322.25Å 109.80Å 132.76Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	29.99 – 3.25 29.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.99-3.25) 97.8 (29.98-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.274 , 0.322 0.305 , 0.345	Depositor DCC
R_{free} test set	3599 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	89.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 15.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32011	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NGT, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/457	0.63	0/624
1	C	0.43	0/457	0.52	0/624
1	E	0.37	0/457	0.48	0/624
1	G	0.40	0/457	0.51	0/624
2	I	0.38	0/3671	0.56	0/5004
2	J	0.40	0/3671	0.53	1/5004 (0.0%)
2	K	0.40	0/3671	0.54	1/5004 (0.0%)
2	L	0.40	0/3671	0.54	0/5004
3	B	2.59	4/445 (0.9%)	0.78	1/609 (0.2%)
3	D	0.32	0/445	0.49	0/609
3	F	0.39	0/445	0.51	0/609
3	H	0.38	0/445	0.50	0/609
4	M	0.36	0/1567	0.55	1/2134 (0.0%)
4	O	0.39	0/1561	0.59	1/2126 (0.0%)
4	Q	0.39	0/1567	0.54	0/2134
4	S	0.35	0/1567	0.49	0/2134
5	N	0.40	0/1976	0.52	0/2680
5	P	0.41	0/1976	0.54	0/2680
5	R	0.45	0/1976	0.54	0/2680
5	T	0.36	0/1976	0.47	0/2680
All	All	0.50	4/32458 (0.0%)	0.54	5/44196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	O	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	54	PRO	N-CA	42.00	2.18	1.47
3	B	54	PRO	N-CD	32.56	1.93	1.47
3	B	55	ALA	CA-CB	7.07	1.67	1.52
3	B	54	PRO	CG-CD	5.16	1.67	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	54	PRO	CA-N-CD	-12.34	94.23	111.50
4	O	309	CYS	N-CA-C	8.31	133.45	111.00
2	K	107	LEU	CA-CB-CG	5.67	128.33	115.30
2	J	107	LEU	CA-CB-CG	5.21	127.28	115.30
4	M	206	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	O	308	PRO	Peptide

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	441	0	397	28	0
1	C	441	0	397	20	0
1	E	441	0	397	21	0
1	G	441	0	397	27	0
2	I	3565	0	3442	118	0
2	J	3565	0	3441	102	0
2	K	3565	0	3441	94	0
2	L	3565	0	3438	101	1
3	B	428	0	416	10	0
3	D	428	0	416	5	0
3	F	428	0	416	8	0
3	H	428	0	416	18	0
4	M	1528	0	1511	38	0
4	O	1522	0	1504	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1528	0	1509	46	0
4	S	1528	0	1509	27	0
5	N	1921	0	1857	39	0
5	P	1921	0	1857	59	0
5	R	1921	0	1857	52	0
5	T	1921	0	1857	42	1
6	U	39	0	34	5	0
6	V	39	0	34	1	0
6	W	39	0	34	1	0
6	Y	39	0	33	7	0
6	d	39	0	34	0	0
7	X	28	0	25	1	0
7	Z	28	0	25	2	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	e	28	0	25	0	0
8	A	14	0	13	6	0
8	B	14	0	13	3	0
8	C	14	0	13	12	0
8	D	14	0	13	4	0
8	E	14	0	13	6	0
8	F	14	0	13	2	0
8	G	14	0	13	8	0
8	H	14	0	13	6	0
9	A	5	0	0	1	0
9	B	1	0	0	0	0
9	C	2	0	0	1	0
9	D	2	0	0	0	0
All	All	32011	0	30898	743	1

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 12.

All (743) 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:J:157:ASN:HD21	6:Y:1:NAG:C1	1.16	1.58
2:I:115:ASN:HD21	6:U:1:NAG:C1	1.18	1.53
2:I:157:ASN:HD21	6:V:1:NAG:C1	1.34	1.40
3:B:54:PRO:N	3:B:54:PRO:CD	1.93	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:530:NGT:HC62	2:K:462:GLU:OE1	1.19	1.29
8:H:28:NGT:S1	5:T:450:TYR:HE2	1.61	1.23
1:A:66:GLN:HE21	1:A:66:GLN:HA	0.98	1.13
8:C:530:NGT:HC81	2:J:421:TYR:OH	1.47	1.12
2:I:100:VAL:HG12	2:I:102:PRO:HD2	1.33	1.10
2:K:170:ARG:HG2	2:K:484:LEU:HB3	1.35	1.09
3:B:54:PRO:N	3:B:54:PRO:CA	2.18	1.06
1:G:55:GLN:HG3	1:G:56:PRO:HD2	1.36	1.04
8:H:28:NGT:S1	5:T:450:TYR:CE2	2.52	1.03
2:I:459:MET:HE1	2:I:464:VAL:HG11	1.45	0.98
8:E:530:NGT:C6	2:K:462:GLU:OE1	2.13	0.96
5:N:532:HIS:HD2	5:N:535:ARG:HH21	1.10	0.95
1:A:66:GLN:HA	1:A:66:GLN:NE2	1.82	0.94
8:H:28:NGT:HC62	5:T:452:ASP:OD2	1.68	0.92
1:G:55:GLN:HG3	1:G:56:PRO:CD	1.99	0.91
5:N:532:HIS:CD2	5:N:535:ARG:HH21	1.88	0.90
2:K:178:ARG:HD2	2:K:462:GLU:OE2	1.71	0.90
1:A:66:GLN:HE21	1:A:66:GLN:CA	1.81	0.89
2:J:427:TYR:CD1	5:P:453:LEU:HA	2.08	0.89
2:J:157:ASN:CG	6:Y:1:NAG:C1	2.43	0.87
2:I:170:ARG:HG2	2:I:484:LEU:HB3	1.56	0.85
5:N:364:ASN:HD22	5:N:365:PRO:HD2	1.41	0.85
3:D:58:PRO:HB3	5:P:511:GLU:HA	1.58	0.85
2:I:100:VAL:CG1	2:I:102:PRO:HD2	2.07	0.85
1:G:30:PHE:HD2	2:L:161:ILE:HG12	1.42	0.84
8:F:26:NGT:HC2	5:R:355:GLU:OE1	1.78	0.84
4:O:307:THR:HG21	5:P:367:ILE:HD11	1.60	0.83
8:G:533:NGT:C8	2:L:373:TRP:CE2	2.62	0.82
4:Q:142:ASN:HB2	5:R:347:GLN:OE1	1.79	0.82
8:E:530:NGT:HC62	2:K:462:GLU:CD	2.00	0.81
2:K:465:ASP:OD2	2:K:467:THR:HG22	1.81	0.81
8:C:530:NGT:C8	2:J:421:TYR:OH	2.28	0.81
4:O:239:VAL:HG12	4:O:245:PRO:HD2	1.63	0.80
4:Q:205:ILE:HD13	5:R:486:ALA:HB3	1.62	0.80
5:R:350:HIS:HD2	5:R:352:GLY:H	1.30	0.79
5:P:420:ILE:HD13	5:P:442:PRO:HB2	1.63	0.79
2:L:90:LEU:HD13	2:L:92:LYS:HE3	1.64	0.79
1:C:53:ALA:HB1	2:J:101:THR:HA	1.65	0.79
5:N:406:GLN:NE2	5:N:424:TRP:H	1.80	0.79
1:E:55:GLN:HG3	1:E:56:PRO:HD2	1.63	0.79
2:I:467:THR:HG21	5:N:544:GLN:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:24:NGT:S1	5:P:450:TYR:OH	2.43	0.75
5:P:532:HIS:HD2	5:P:535:ARG:HH21	1.32	0.75
8:A:21:NGT:N2	2:I:322:ASP:OD2	2.20	0.75
2:L:100:VAL:HG12	2:L:102:PRO:HD2	1.67	0.75
2:L:121:ASN:HD21	2:L:124:GLN:HG2	1.51	0.74
2:J:424:ARG:HA	5:P:456:TYR:CD1	2.22	0.74
2:K:467:THR:HG21	5:R:544:GLN:HA	1.69	0.74
5:R:432:GLU:HG2	5:R:435:ARG:HH21	1.51	0.74
2:I:131:THR:HG22	2:I:133:TRP:H	1.54	0.73
2:I:117:THR:HG22	2:I:162:GLU:HG3	1.69	0.73
5:P:532:HIS:CD2	5:P:535:ARG:HH21	2.05	0.73
2:J:100:VAL:HG12	2:J:102:PRO:HD2	1.68	0.73
5:R:504:PRO:HG3	5:R:533:ARG:HG3	1.70	0.73
2:I:170:ARG:NH2	2:I:197:LYS:O	2.22	0.73
8:B:22:NGT:O4	4:M:211:ARG:NH2	2.22	0.73
5:T:365:PRO:HA	5:T:368:GLN:HB2	1.71	0.72
5:N:451:LEU:O	5:N:505:ARG:NH2	2.22	0.72
2:I:229:PRO:HA	2:I:233:ILE:HD11	1.70	0.72
4:O:170:ARG:NH2	4:O:232:ASN:HB3	2.04	0.72
4:O:211:ARG:HD2	4:O:242:GLN:OE1	1.89	0.72
4:S:203:ARG:HG2	5:T:513:LEU:HB3	1.71	0.72
2:I:115:ASN:CG	6:U:1:NAG:C1	2.58	0.71
2:J:121:ASN:ND2	2:J:124:GLN:H	1.88	0.71
2:I:151:GLU:HG2	1:C:38:VAL:HG11	1.71	0.71
9:A:534:HOH:O	2:I:421:TYR:HB2	1.90	0.70
2:J:398:VAL:HG12	2:J:403:GLU:HG2	1.73	0.70
5:N:406:GLN:HE21	5:N:424:TRP:H	1.36	0.70
8:C:530:NGT:HC83	2:J:392:TRP:CD2	2.26	0.70
2:I:89:THR:HG22	2:I:90:LEU:H	1.56	0.70
2:K:214:GLU:HG3	2:K:222:MET:HE2	1.74	0.70
5:R:451:LEU:O	5:R:505:ARG:NH2	2.25	0.70
2:J:427:TYR:HD1	5:P:453:LEU:HA	1.57	0.69
2:K:107:LEU:HB2	2:K:108:PRO:HD2	1.74	0.69
4:M:141:PRO:O	4:M:284:ARG:HG2	1.92	0.69
4:M:295:THR:HG21	5:N:322:ILE:HD11	1.73	0.69
4:M:235:HIS:HB2	5:N:485:GLU:OE2	1.93	0.69
2:K:178:ARG:CD	2:K:462:GLU:OE2	2.42	0.68
2:K:100:VAL:HG12	2:K:102:PRO:HD2	1.73	0.68
1:E:43:ASN:HD22	2:K:92:LYS:HG2	1.59	0.68
1:E:45:GLN:HB3	4:S:262:LEU:HD23	1.76	0.68
4:S:229:ASN:OD1	5:T:532:HIS:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:192:VAL:HA	2:K:195:TYR:CD2	2.28	0.67
4:Q:229:ASN:OD1	5:R:532:HIS:HE1	1.78	0.67
1:A:55:GLN:HG3	1:A:56:PRO:HD2	1.76	0.67
2:I:377:PHE:HB2	2:I:389:ILE:HD12	1.75	0.67
8:C:530:NGT:O4	2:J:178:ARG:NH1	2.26	0.67
2:K:170:ARG:NH2	2:K:197:LYS:O	2.27	0.67
2:J:157:ASN:OD1	6:Y:1:NAG:C1	2.43	0.67
2:L:99:VAL:HG22	2:L:130:GLU:HA	1.76	0.67
4:O:307:THR:CG2	5:P:367:ILE:HD11	2.25	0.67
4:Q:183:SER:O	3:H:74:PRO:HD2	1.94	0.67
2:L:228:ASN:HD22	2:L:230:VAL:H	1.42	0.66
2:K:101:THR:N	2:K:102:PRO:HD2	2.11	0.66
4:M:215:PRO:O	4:M:218:ILE:HG22	1.96	0.66
1:E:45:GLN:HB3	4:S:262:LEU:CD2	2.26	0.66
2:L:459:MET:HE1	2:L:464:VAL:HG21	1.78	0.66
5:R:390:LYS:O	5:R:394:ILE:HD12	1.96	0.65
4:Q:136:GLU:OE2	4:Q:166:TRP:NE1	2.26	0.65
8:C:530:NGT:S1	2:J:421:TYR:HE1	2.20	0.65
4:O:307:THR:HG21	5:P:367:ILE:CD1	2.26	0.65
2:L:94:VAL:HA	2:L:125:CYS:SG	2.37	0.65
2:L:173:LEU:HA	2:L:202:HIS:HB3	1.78	0.65
2:I:447:GLU:CD	2:I:447:GLU:H	2.00	0.65
2:I:121:ASN:HD21	2:I:124:GLN:HG2	1.60	0.65
1:G:30:PHE:CD2	2:L:161:ILE:HG12	2.30	0.64
2:L:371:VAL:HG22	2:L:388:ILE:HD12	1.79	0.64
2:I:115:ASN:ND2	6:U:1:NAG:C2	2.59	0.64
2:I:465:ASP:OD2	2:I:467:THR:HG22	1.97	0.64
5:P:451:LEU:O	5:P:505:ARG:NH2	2.30	0.64
8:G:533:NGT:HC82	2:L:373:TRP:CE2	2.33	0.64
1:A:49:ASP:OD1	1:A:51:SER:N	2.24	0.64
2:K:121:ASN:HD22	2:K:123:ASP:H	1.44	0.64
1:G:58:CYS:SG	1:G:61:LEU:HG	2.37	0.64
4:Q:166:TRP:HA	4:Q:169:LEU:HD12	1.79	0.64
2:J:170:ARG:HG2	2:J:484:LEU:HB3	1.80	0.63
8:G:533:NGT:C8	2:L:373:TRP:CD2	2.82	0.63
2:J:89:THR:HG22	2:J:90:LEU:H	1.62	0.63
5:R:425:LYS:O	5:R:429:TYR:HB3	1.98	0.63
3:D:67:PRO:HA	7:Z:1:NAG:O5	1.98	0.63
4:S:310:TYR:HE1	5:T:364:ASN:ND2	1.96	0.63
3:H:58:PRO:HB3	5:T:511:GLU:HA	1.79	0.63
2:L:173:LEU:HB3	2:L:458:CYS:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:415:LEU:HB2	5:R:441:PHE:CZ	2.33	0.62
2:J:206:VAL:HG12	2:J:212:PRO:HD2	1.82	0.62
5:R:533:ARG:HA	5:R:536:MET:CE	2.29	0.62
5:R:499:THR:HB	5:R:500:PRO:HD3	1.81	0.61
2:J:102:PRO:O	2:J:103:GLY:O	2.18	0.61
1:E:53:ALA:HB1	2:K:101:THR:HA	1.83	0.61
4:M:132:THR:HB	4:M:163:ASN:HA	1.83	0.61
8:H:28:NGT:HC5	5:T:489:TRP:CD1	2.34	0.61
3:B:58:PRO:HB3	5:N:511:GLU:HA	1.81	0.61
5:P:372:ARG:HH11	5:P:372:ARG:CG	2.14	0.61
8:A:21:NGT:O4	2:I:178:ARG:NH1	2.34	0.61
1:G:46:PHE:CD2	2:L:94:VAL:HG11	2.36	0.61
1:G:48:TYR:CZ	1:G:65:PHE:HE2	2.19	0.61
2:L:463:TYR:O	5:T:545:PRO:HG2	2.01	0.61
2:I:153:THR:HG23	2:J:151:GLU:HB3	1.83	0.60
3:D:67:PRO:HB3	7:Z:1:NAG:O6	2.01	0.60
1:G:43:ASN:HD22	2:L:92:LYS:HG2	1.66	0.60
2:I:101:THR:N	2:I:102:PRO:HD2	2.16	0.60
2:I:121:ASN:ND2	2:I:124:GLN:HG2	2.16	0.60
2:L:359:LEU:O	2:L:363:VAL:HG23	2.02	0.60
4:M:126:GLN:HB3	4:M:157:VAL:HG13	1.83	0.60
1:G:52:SER:HA	2:L:97:VAL:HG23	1.83	0.60
2:I:151:GLU:HB3	2:J:153:THR:HG23	1.82	0.60
2:L:131:THR:HG22	2:L:132:VAL:H	1.66	0.60
2:L:339:MET:SD	2:L:351:LEU:HD22	2.41	0.60
4:M:239:VAL:HG12	4:M:245:PRO:HD2	1.84	0.60
5:T:424:TRP:HB2	5:T:450:TYR:OH	2.02	0.60
4:O:222:THR:O	4:O:226:MET:HG3	2.00	0.59
1:E:55:GLN:HG3	1:E:56:PRO:CD	2.32	0.59
4:Q:206:LEU:HA	4:Q:235:HIS:HB3	1.82	0.59
2:J:157:ASN:ND2	6:Y:1:NAG:C2	2.63	0.59
1:A:45:GLN:HG3	2:I:93:ASN:ND2	2.17	0.59
4:M:190:ASN:ND2	6:W:1:NAG:C1	2.66	0.59
5:P:372:ARG:NH1	5:P:372:ARG:HG3	2.16	0.59
2:J:467:THR:HG21	5:P:544:GLN:HA	1.84	0.59
2:I:459:MET:HE1	2:I:464:VAL:CG1	2.27	0.59
5:P:372:ARG:HH11	5:P:372:ARG:HG3	1.66	0.59
5:N:465:LYS:O	5:N:520:ARG:NH2	2.36	0.59
2:J:417:SER:O	2:J:421:TYR:CE2	2.56	0.59
2:L:515:GLN:HB2	2:L:516:PRO:HD2	1.84	0.59
5:P:403:ILE:HG12	5:P:420:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:490:GLY:HA2	5:N:493:VAL:HB	1.86	0.58
5:N:532:HIS:HD2	5:N:535:ARG:NH2	1.92	0.58
5:N:473:GLY:HA2	5:N:477:GLN:NE2	2.19	0.58
2:K:170:ARG:HG2	2:K:484:LEU:CB	2.22	0.58
2:J:121:ASN:HD21	2:J:124:GLN:H	1.50	0.58
2:K:169:HIS:NE2	2:K:200:VAL:HG11	2.19	0.58
4:Q:310:TYR:O	4:Q:311:SER:HB2	2.02	0.58
2:I:404:LEU:HD11	2:I:416:LEU:HG	1.84	0.57
5:N:403:ILE:HG23	5:N:420:ILE:HB	1.86	0.57
2:J:422:LEU:O	2:J:476:ARG:NH2	2.34	0.57
2:I:459:MET:CE	2:I:464:VAL:HG11	2.28	0.57
2:J:228:ASN:HD22	2:J:230:VAL:H	1.52	0.57
5:N:415:LEU:HB2	5:N:441:PHE:CE1	2.40	0.57
2:J:101:THR:O	2:J:102:PRO:C	2.42	0.57
2:K:108:PRO:HG2	2:K:252:ARG:HG2	1.86	0.57
4:Q:229:ASN:OD1	5:R:532:HIS:CE1	2.56	0.57
2:J:171:GLY:HA3	2:J:456:GLU:HG2	1.86	0.57
1:E:25:PRO:HD2	2:K:197:LYS:HD2	1.86	0.56
4:S:149:TYR:CZ	4:S:196:ASP:HB3	2.40	0.56
8:A:21:NGT:O3	2:I:262:HIS:CE1	2.58	0.56
2:K:145:LEU:HD11	2:K:161:ILE:HD11	1.88	0.56
8:A:21:NGT:HC82	2:I:373:TRP:CE2	2.41	0.56
8:E:530:NGT:O4	2:K:462:GLU:OE2	2.21	0.56
1:G:48:TYR:HH	1:G:65:PHE:HE2	1.51	0.56
5:P:488:LEU:HD22	5:P:502:LEU:HG	1.88	0.56
2:J:171:GLY:HA2	2:J:200:VAL:O	2.06	0.56
5:R:350:HIS:CD2	5:R:352:GLY:H	2.17	0.56
5:N:341:SER:OG	5:N:398:ILE:HD12	2.05	0.56
2:K:398:VAL:HG12	2:K:403:GLU:HG2	1.88	0.56
4:O:215:PRO:O	4:O:218:ILE:HG22	2.05	0.55
2:L:183:LEU:HA	2:L:186:ILE:HD12	1.87	0.55
4:S:132:THR:HB	4:S:163:ASN:HA	1.87	0.55
2:I:319:LEU:HD12	2:I:360:LEU:HD23	1.89	0.55
2:I:467:THR:CG2	5:N:544:GLN:HA	2.36	0.55
2:J:463:TYR:CE1	5:P:547:TYR:HD1	2.24	0.55
2:L:318:HIS:HE1	2:L:373:TRP:CD1	2.23	0.55
8:C:530:NGT:HO4	2:J:178:ARG:HH12	1.54	0.55
4:Q:129:VAL:HG22	4:Q:160:LEU:HD23	1.89	0.55
3:H:73:ALA:HB3	3:H:76:ASN:HB3	1.87	0.55
3:B:58:PRO:HD2	4:M:230:LYS:HD2	1.88	0.55
2:J:90:LEU:HD13	2:J:92:LYS:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:518:ASN:ND2	5:R:492:TYR:CE1	2.74	0.55
5:R:533:ARG:HA	5:R:536:MET:HE2	1.89	0.55
5:T:341:SER:OG	5:T:398:ILE:HD12	2.07	0.55
2:L:204:HIS:HE1	2:L:207:ASP:OD1	1.89	0.55
1:E:38:VAL:HG11	2:L:151:GLU:HG2	1.89	0.54
5:R:443:VAL:HG12	5:R:481:PHE:HA	1.88	0.54
4:M:170:ARG:HB3	4:M:230:LYS:HE3	1.88	0.54
2:K:176:THR:OG1	2:K:205:LEU:HA	2.07	0.54
1:G:52:SER:HB3	1:G:55:GLN:HE22	1.73	0.54
8:H:28:NGT:O6	5:T:450:TYR:HD2	1.90	0.54
8:C:530:NGT:HC83	2:J:392:TRP:CE3	2.42	0.54
2:J:170:ARG:NH2	2:J:197:LYS:O	2.40	0.54
2:K:100:VAL:HG12	2:K:102:PRO:CD	2.38	0.54
5:P:424:TRP:CZ2	5:P:425:LYS:HE2	2.43	0.54
8:D:24:NGT:S1	5:P:450:TYR:CZ	3.00	0.54
2:L:101:THR:N	2:L:102:PRO:HD2	2.23	0.54
2:I:170:ARG:HG2	2:I:484:LEU:CB	2.33	0.54
2:I:228:ASN:HD22	2:I:231:THR:H	1.56	0.54
1:A:38:VAL:HG22	2:I:155:PHE:HE1	1.72	0.53
2:J:136:LEU:HA	2:J:139:LEU:HD12	1.88	0.53
8:C:530:NGT:HC81	2:J:421:TYR:HH	1.67	0.53
2:K:519:VAL:HG12	5:R:491:GLU:HA	1.90	0.53
6:Y:1:NAG:H61	6:Y:2:NAG:N2	2.24	0.53
1:A:23:LEU:HD21	2:I:141:THR:HG23	1.89	0.53
2:L:372:VAL:HG21	2:L:376:VAL:HG21	1.90	0.53
4:M:211:ARG:HD2	4:M:242:GLN:OE1	2.09	0.53
5:T:352:GLY:HA2	5:T:405:TRP:CD1	2.44	0.53
5:P:424:TRP:HB2	5:P:450:TYR:OH	2.09	0.53
2:L:467:THR:HG21	5:T:544:GLN:HA	1.91	0.53
3:H:81:HIS:HE1	3:H:95:GLU:OE2	1.91	0.53
1:A:45:GLN:HG3	2:I:93:ASN:HD21	1.74	0.53
1:G:23:LEU:HD11	2:L:141:THR:HG23	1.91	0.53
1:G:28:GLN:NE2	2:L:487:ASN:HD22	2.07	0.53
2:I:102:PRO:O	2:I:103:GLY:O	2.27	0.53
2:K:423:ASN:HB3	2:K:460:TRP:H	1.74	0.53
8:D:24:NGT:S1	5:P:450:TYR:CE2	3.03	0.52
2:L:228:ASN:ND2	2:L:230:VAL:H	2.07	0.52
2:J:99:VAL:HG22	2:J:130:GLU:HA	1.90	0.52
8:G:533:NGT:HC81	2:L:373:TRP:CD2	2.44	0.52
3:H:58:PRO:HD2	4:S:230:LYS:HD2	1.91	0.52
2:K:173:LEU:HA	2:K:202:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:170:ARG:HG2	2:L:484:LEU:HB3	1.91	0.52
5:N:390:LYS:O	5:N:394:ILE:HG13	2.09	0.52
8:C:530:NGT:HC83	2:J:392:TRP:CG	2.45	0.52
2:L:147:TRP:NE1	2:L:157:ASN:OD1	2.39	0.52
1:A:61:LEU:HD11	2:I:135:ALA:CB	2.40	0.52
2:I:525:GLU:OE1	4:M:264:HIS:HE1	1.93	0.52
2:J:417:SER:O	2:J:421:TYR:HE2	1.93	0.52
5:R:406:GLN:HE21	5:R:424:TRP:H	1.57	0.52
2:L:459:MET:HE1	2:L:464:VAL:HG11	1.92	0.52
5:T:429:TYR:N	5:T:430:PRO:CD	2.72	0.52
5:R:415:LEU:HD22	5:R:419:THR:HG21	1.92	0.52
5:R:465:LYS:O	5:R:520:ARG:NH2	2.43	0.52
5:T:451:LEU:O	5:T:505:ARG:NH2	2.32	0.52
2:I:402:LYS:HD2	2:I:406:LEU:HD13	1.92	0.51
5:P:459:ASP:OD1	5:P:505:ARG:HD2	2.10	0.51
5:P:504:PRO:HG3	5:P:533:ARG:HG3	1.92	0.51
4:Q:267:THR:O	4:Q:271:VAL:HG23	2.09	0.51
2:J:210:SER:HB2	2:J:227:TYR:CE2	2.45	0.51
2:K:467:THR:CG2	5:R:544:GLN:HA	2.39	0.51
5:R:407:GLU:OE2	5:R:424:TRP:HZ2	1.92	0.51
4:S:310:TYR:CE1	5:T:364:ASN:ND2	2.77	0.51
2:I:101:THR:N	2:I:102:PRO:CD	2.73	0.51
4:Q:170:ARG:HD2	4:Q:230:LYS:HG2	1.92	0.51
2:L:518:ASN:ND2	2:L:519:VAL:H	2.09	0.51
8:C:530:NGT:S1	2:J:460:TRP:NE1	2.83	0.51
2:J:320:GLY:HA2	2:J:373:TRP:CD1	2.44	0.51
2:J:392:TRP:HE3	2:J:421:TYR:HH	1.57	0.51
2:J:396:ILE:HG13	2:J:397:PRO:HA	1.92	0.51
5:P:395:ILE:HG22	5:P:400:LYS:O	2.09	0.51
3:F:55:ALA:O	5:R:535:ARG:NH2	2.40	0.51
4:S:235:HIS:NE2	4:S:288:GLU:OE1	2.38	0.51
1:A:61:LEU:N	1:A:61:LEU:HD23	2.25	0.51
5:P:499:THR:HB	5:P:500:PRO:HD3	1.93	0.51
2:K:107:LEU:HB3	2:K:247:ARG:HG3	1.91	0.51
3:H:55:ALA:HB1	5:T:531:ARG:HG3	1.92	0.51
8:D:24:NGT:O3	4:O:294:HIS:CE1	2.64	0.51
4:Q:199:ARG:HH21	5:R:469:LEU:HD12	1.76	0.51
4:Q:203:ARG:HG2	5:R:513:LEU:HB3	1.92	0.51
4:Q:235:HIS:NE2	4:Q:288:GLU:OE1	2.37	0.51
3:H:64:LYS:HE3	4:S:193:THR:HB	1.93	0.51
2:I:97:VAL:HG12	2:I:126:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:524:GLN:O	2:I:524:GLN:HG2	2.10	0.51
4:M:299:GLY:HA3	4:M:306:LEU:HD12	1.93	0.51
2:J:113:VAL:HG21	7:X:1:NAG:H82	1.93	0.51
1:G:46:PHE:CD2	2:L:94:VAL:CG1	2.93	0.51
2:L:172:LEU:HD23	2:L:457:ALA:HB3	1.93	0.51
2:I:252:ARG:HB3	2:I:314:ASP:OD1	2.10	0.51
5:N:364:ASN:HD22	5:N:365:PRO:CD	2.19	0.51
4:M:151:LEU:HD23	4:M:194:ILE:HD13	1.94	0.50
4:M:202:HIS:CD2	4:M:233:VAL:HG21	2.46	0.50
5:P:362:GLU:O	5:P:368:GLN:NE2	2.44	0.50
5:T:504:PRO:HG3	5:T:533:ARG:HG3	1.92	0.50
5:T:530:THR:HG23	5:T:546:LEU:HD12	1.92	0.50
2:J:101:THR:N	2:J:102:PRO:HD2	2.26	0.50
2:J:202:HIS:ND1	2:J:456:GLU:OE1	2.44	0.50
2:K:424:ARG:HA	5:R:456:TYR:CD1	2.47	0.50
1:A:55:GLN:HG3	1:A:56:PRO:CD	2.42	0.50
2:I:99:VAL:CG2	2:I:100:VAL:N	2.74	0.50
2:J:350:GLN:HA	2:J:353:SER:HB2	1.94	0.50
2:J:475:PRO:HG2	2:J:517:LEU:CD1	2.41	0.50
4:O:302:GLN:HE21	4:O:302:GLN:HA	1.76	0.50
5:P:474:THR:H	5:P:477:GLN:NE2	2.09	0.50
4:S:126:GLN:HB3	4:S:157:VAL:HG13	1.94	0.50
5:T:326:LEU:O	5:T:329:THR:HG22	2.11	0.50
5:R:367:ILE:O	5:R:371:MET:HG2	2.12	0.50
1:C:23:LEU:HD11	2:J:141:THR:HG23	1.94	0.50
5:P:430:PRO:O	5:P:471:PHE:HB2	2.12	0.50
4:M:249:ILE:HG12	1:C:57:GLY:HA2	1.93	0.50
1:E:30:PHE:CD2	2:K:161:ILE:HG12	2.47	0.50
2:K:353:SER:HA	2:K:381:VAL:HG13	1.93	0.50
2:L:214:GLU:HA	2:L:222:MET:HB2	1.94	0.50
4:M:223:LEU:HD21	4:M:234:LEU:HD22	1.94	0.50
2:K:187:LEU:HA	2:K:190:LEU:HD12	1.93	0.50
2:K:228:ASN:HD22	2:K:231:THR:H	1.58	0.50
2:I:319:LEU:HD11	2:I:363:VAL:HG21	1.94	0.50
1:C:55:GLN:HG3	1:C:56:PRO:HD2	1.93	0.50
2:J:235:THR:O	2:J:239:VAL:HG23	2.12	0.50
1:E:30:PHE:HD2	2:K:161:ILE:HG12	1.75	0.50
1:A:39:LEU:HD11	2:I:156:ILE:HB	1.94	0.49
1:E:46:PHE:CD2	2:K:94:VAL:CG1	2.94	0.49
1:G:53:ALA:HB1	2:L:101:THR:HG23	1.94	0.49
4:S:248:SER:HB3	4:S:251:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:388:ILE:HG21	5:R:408:VAL:HG13	1.94	0.49
2:L:357:GLN:CD	2:L:382:LYS:HB3	2.32	0.49
2:I:428:GLY:HA2	5:N:492:TYR:CE2	2.47	0.49
5:P:461:ARG:O	5:P:465:LYS:HB2	2.13	0.49
2:K:198:LEU:HD11	2:K:481:ALA:HB2	1.94	0.49
2:L:307:GLU:O	2:L:311:VAL:HG23	2.11	0.49
2:I:101:THR:O	2:I:103:GLY:N	2.46	0.49
2:I:220:GLU:HA	2:I:223:ARG:HB2	1.95	0.49
2:K:178:ARG:HD3	5:R:548:ALA:HB2	1.94	0.49
2:K:409:LYS:HZ2	2:K:409:LYS:HB2	1.77	0.49
8:F:26:NGT:C2	5:R:355:GLU:OE1	2.56	0.49
1:G:55:GLN:CG	1:G:56:PRO:HD2	2.26	0.49
2:I:325:ASP:OD2	2:I:327:THR:HB	2.13	0.49
1:C:25:PRO:HB3	2:J:482:GLU:HA	1.95	0.49
2:K:421:TYR:HA	2:K:458:CYS:HB2	1.94	0.49
4:Q:253:GLU:HA	4:Q:256:ASN:HB2	1.94	0.49
5:T:329:THR:HG23	5:T:330:TYR:CD2	2.48	0.49
2:I:101:THR:H	2:I:102:PRO:HD2	1.77	0.49
2:L:176:THR:HG22	2:L:181:LEU:HB2	1.94	0.49
5:T:504:PRO:HD3	5:T:544:GLN:O	2.13	0.49
1:A:28:GLN:HE22	2:I:487:ASN:HD22	1.60	0.49
2:I:100:VAL:HG23	2:I:130:GLU:HG3	1.95	0.49
2:K:347:ASP:HB2	2:K:349:LYS:HE3	1.94	0.49
5:R:460:TRP:HA	5:R:463:TYR:HD2	1.77	0.49
2:L:169:HIS:HE1	2:L:456:GLU:OE2	1.96	0.49
2:I:151:GLU:CG	1:C:38:VAL:HG11	2.39	0.48
5:N:350:HIS:HD2	5:N:352:GLY:H	1.61	0.48
5:T:451:LEU:HD11	5:T:486:ALA:HB1	1.94	0.48
2:I:101:THR:H	2:I:102:PRO:CD	2.26	0.48
1:G:24:TRP:CZ3	2:L:500:LEU:HB2	2.48	0.48
1:G:48:TYR:HE2	1:G:61:LEU:HD12	1.79	0.48
2:I:131:THR:HG21	2:I:133:TRP:CD1	2.48	0.48
4:Q:175:PHE:O	4:Q:178:LEU:HB2	2.14	0.48
4:M:277:TYR:O	4:M:281:ARG:NH1	2.45	0.48
4:Q:142:ASN:CB	5:R:347:GLN:OE1	2.56	0.48
2:L:318:HIS:CE1	2:L:373:TRP:CD1	3.01	0.48
5:P:459:ASP:OD2	5:P:505:ARG:NH1	2.45	0.48
5:R:533:ARG:HG2	5:R:543:ALA:HB3	1.96	0.48
2:L:425:ILE:HB	5:T:454:ILE:HD12	1.96	0.48
1:A:43:ASN:CG	1:A:43:ASN:O	2.52	0.48
2:I:422:LEU:O	2:I:476:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:7:HOH:O	2:J:421:TYR:HB2	2.13	0.48
2:J:107:LEU:HD22	2:J:107:LEU:H	1.78	0.48
4:O:170:ARG:HH21	4:O:232:ASN:HB3	1.77	0.48
1:E:43:ASN:ND2	2:K:92:LYS:HG2	2.28	0.48
2:I:204:HIS:CD2	2:I:256:GLU:OE1	2.66	0.48
2:J:419:PRO:HB2	2:J:437:VAL:HG21	1.95	0.48
2:K:117:THR:HG22	2:K:162:GLU:HG2	1.94	0.48
2:I:307:GLU:O	2:I:311:VAL:HG23	2.14	0.48
8:C:530:NGT:C8	2:J:421:TYR:HH	2.24	0.48
2:L:114:GLU:CD	2:L:170:ARG:HH12	2.17	0.48
2:I:518:ASN:ND2	2:I:519:VAL:H	2.12	0.48
4:O:310:TYR:N	4:O:310:TYR:CD1	2.81	0.48
4:M:139:ALA:O	4:M:279:ARG:HD2	2.14	0.47
5:N:530:THR:HG22	5:N:546:LEU:HD12	1.96	0.47
4:S:233:VAL:HG22	4:S:284:ARG:HD3	1.95	0.47
8:G:533:NGT:HC81	2:L:373:TRP:CE2	2.48	0.47
2:I:156:ILE:HG13	2:I:157:ASN:N	2.29	0.47
2:I:176:THR:HG22	2:I:181:LEU:HD12	1.97	0.47
1:C:36:ARG:HD3	6:Y:1:NAG:H62	1.96	0.47
2:L:222:MET:HG2	2:L:233:ILE:HD12	1.96	0.47
2:L:259:THR:HB	2:L:355:TYR:OH	2.13	0.47
2:I:115:ASN:ND2	6:U:1:NAG:N2	2.62	0.47
2:I:377:PHE:HB2	2:I:389:ILE:CD1	2.44	0.47
2:I:500:LEU:HG	2:I:517:LEU:HD11	1.96	0.47
4:O:232:ASN:HA	4:O:283:ILE:HG13	1.96	0.47
2:K:237:GLN:HB2	3:H:92:THR:CG2	2.45	0.47
5:T:406:GLN:HE21	5:T:424:TRP:H	1.62	0.47
1:A:52:SER:HB2	2:I:97:VAL:HA	1.97	0.47
2:J:157:ASN:O	2:J:159:THR:HG22	2.15	0.47
2:J:398:VAL:CG1	2:J:403:GLU:HG2	2.41	0.47
2:K:243:ILE:HA	2:K:253:VAL:HG21	1.97	0.47
3:F:82:SER:HA	4:Q:128:LEU:HD22	1.95	0.47
2:L:390:GLN:HG3	2:L:415:LEU:HB2	1.96	0.47
5:P:354:ASP:OD1	5:P:405:TRP:CD1	2.67	0.47
2:L:120:ILE:HB	2:L:159:THR:HG22	1.95	0.47
2:I:99:VAL:HG23	2:I:100:VAL:N	2.29	0.47
4:M:292:PRO:HA	5:N:322:ILE:HD12	1.96	0.47
2:J:116:TYR:CZ	2:J:163:ASP:HB3	2.50	0.47
4:O:216:VAL:O	4:O:220:LEU:HG	2.14	0.47
5:P:425:LYS:O	5:P:429:TYR:HB3	2.15	0.47
1:E:46:PHE:HD2	2:K:94:VAL:CG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:107:LEU:H	2:K:107:LEU:HD13	1.79	0.47
2:L:113:VAL:HG12	2:L:115:ASN:H	1.80	0.47
2:L:356:ILE:O	2:L:360:LEU:HG	2.14	0.47
2:J:364:SER:HB2	2:J:370:TYR:HE1	1.80	0.47
4:Q:222:THR:O	4:Q:226:MET:HG3	2.15	0.47
2:L:131:THR:HG22	2:L:132:VAL:N	2.29	0.47
2:L:244:GLU:O	2:L:248:LEU:HG	2.15	0.47
2:I:187:LEU:HD22	2:I:245:TYR:CG	2.50	0.47
2:L:424:ARG:HA	5:T:456:TYR:CD1	2.50	0.47
1:A:28:GLN:NE2	2:I:487:ASN:HD22	2.13	0.47
2:I:422:LEU:HD11	2:I:477:ALA:HB2	1.96	0.47
2:K:307:GLU:O	2:K:311:VAL:HG23	2.14	0.47
2:J:170:ARG:HG2	2:J:484:LEU:CB	2.45	0.46
5:R:388:ILE:HG12	5:R:408:VAL:HG11	1.96	0.46
5:T:490:GLY:HA2	5:T:493:VAL:HB	1.98	0.46
2:I:174:LEU:HB2	2:I:201:PHE:HE1	1.80	0.46
4:M:290:ASP:OD2	5:N:354:ASP:OD1	2.33	0.46
4:O:238:ILE:HG23	4:O:239:VAL:HG13	1.96	0.46
2:J:176:THR:HG22	2:J:181:LEU:HD12	1.97	0.46
2:J:302:SER:HA	2:J:362:ILE:HG21	1.96	0.46
5:P:372:ARG:CG	5:P:372:ARG:NH1	2.75	0.46
2:I:270:ILE:HG13	2:I:270:ILE:O	2.15	0.46
2:I:402:LYS:HD2	2:I:406:LEU:CD1	2.46	0.46
8:B:22:NGT:HC2	5:N:355:GLU:OE1	2.15	0.46
8:E:530:NGT:HC82	2:K:460:TRP:CH2	2.49	0.46
2:L:206:VAL:HG12	2:L:212:PRO:HD2	1.96	0.46
2:J:290:VAL:O	2:J:292:PRO:HD3	2.15	0.46
4:S:152:LEU:HB2	4:S:159:VAL:HB	1.97	0.46
2:J:266:TRP:N	2:J:266:TRP:CD1	2.84	0.46
5:R:330:TYR:CG	5:R:390:LYS:HE2	2.50	0.46
3:H:56:LEU:O	5:T:528:ARG:NH1	2.46	0.46
2:I:398:VAL:HG12	2:I:403:GLU:HG2	1.98	0.46
2:J:235:THR:HG22	2:J:236:ALA:N	2.31	0.46
2:K:175:ASP:HB3	2:K:461:GLY:N	2.30	0.46
2:K:210:SER:HB2	2:K:227:TYR:CE2	2.51	0.46
2:K:224:LYS:HB3	2:K:268:PRO:HB2	1.98	0.46
1:G:28:GLN:HE22	2:L:487:ASN:HD22	1.61	0.46
8:G:533:NGT:HC82	2:L:373:TRP:CZ2	2.50	0.46
4:M:253:GLU:HA	4:M:256:ASN:HB2	1.97	0.46
2:K:404:LEU:HD11	2:K:416:LEU:HD13	1.97	0.46
2:K:424:ARG:HA	5:R:456:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:392:TRP:HB2	2:L:421:TYR:OH	2.15	0.46
3:H:54:PRO:HB2	3:H:56:LEU:HG	1.97	0.46
2:I:270:ILE:HG13	2:I:273:LEU:HB2	1.98	0.46
4:M:140:PHE:CE1	4:M:279:ARG:HD3	2.51	0.46
2:J:519:VAL:HA	4:O:212:HIS:CE1	2.51	0.46
4:Q:198:PRO:HB3	5:R:514:TRP:CE3	2.51	0.46
4:Q:261:SER:OG	4:Q:264:HIS:CD2	2.68	0.46
5:N:388:ILE:HG12	5:N:408:VAL:HG21	1.97	0.45
2:J:228:ASN:HD22	2:J:231:THR:H	1.65	0.45
2:J:232:HIS:O	2:J:233:ILE:HD13	2.16	0.45
2:K:216:PHE:CE2	2:K:307:GLU:HG3	2.51	0.45
4:Q:244:PHE:N	4:Q:258:GLY:O	2.42	0.45
8:G:533:NGT:C8	2:L:373:TRP:CZ2	2.97	0.45
2:J:100:VAL:HG12	2:J:102:PRO:CD	2.44	0.45
2:J:350:GLN:HA	2:J:353:SER:CB	2.46	0.45
5:R:533:ARG:HA	5:R:536:MET:HE3	1.98	0.45
8:B:22:NGT:S1	5:N:450:TYR:OH	2.69	0.45
8:C:530:NGT:HC62	2:J:462:GLU:CD	2.37	0.45
4:O:240:ASP:OD1	4:O:241:ASP:N	2.35	0.45
2:L:187:LEU:HA	2:L:190:LEU:HD12	1.97	0.45
4:S:307:THR:HG21	5:T:361:TRP:HD1	1.81	0.45
8:A:21:NGT:C8	2:I:373:TRP:CE2	3.00	0.45
2:I:173:LEU:HA	2:I:202:HIS:HB3	1.98	0.45
1:C:66:GLN:HE22	1:C:69:ARG:HD3	1.81	0.45
1:E:25:PRO:HB3	2:K:482:GLU:HA	1.97	0.45
4:O:288:GLU:HG3	5:P:350:HIS:CD2	2.52	0.45
2:L:101:THR:N	2:L:102:PRO:CD	2.79	0.45
2:L:170:ARG:NH2	2:L:197:LYS:O	2.50	0.45
2:K:322:ASP:HB3	2:K:373:TRP:CD1	2.51	0.45
1:G:52:SER:OG	1:G:54:ALA:O	2.34	0.45
2:I:100:VAL:CG1	2:I:102:PRO:CD	2.90	0.45
2:I:101:THR:O	2:I:102:PRO:C	2.54	0.45
5:R:376:PHE:CD1	5:R:382:LYS:HD3	2.52	0.45
2:L:482:GLU:HG3	2:L:486:SER:OG	2.16	0.45
3:H:82:SER:HA	4:S:128:LEU:HD22	1.98	0.45
5:T:499:THR:HB	5:T:500:PRO:HD3	1.99	0.45
1:A:46:PHE:HD2	2:I:94:VAL:HG12	1.82	0.45
5:N:429:TYR:N	5:N:430:PRO:CD	2.80	0.45
2:K:171:GLY:HA2	2:K:200:VAL:O	2.17	0.45
2:K:188:ASP:O	2:K:192:VAL:HG23	2.17	0.45
2:I:475:PRO:HG3	2:I:504:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:65:MET:CE	4:M:190:ASN:HD22	2.30	0.45
2:K:116:TYR:CZ	2:K:163:ASP:HB3	2.52	0.45
2:K:179:HIS:CE1	5:R:548:ALA:HA	2.52	0.45
2:K:464:VAL:HG21	2:K:472:ARG:HD2	1.99	0.45
4:S:204:GLY:HA2	4:S:233:VAL:O	2.16	0.45
4:Q:175:PHE:HA	4:Q:178:LEU:HD12	1.98	0.45
2:L:246:ALA:HB1	2:L:251:ILE:HB	1.98	0.45
2:I:131:THR:HG22	2:I:132:VAL:N	2.32	0.44
2:I:166:ARG:HH21	2:I:440:LEU:HD12	1.82	0.44
2:I:393:ARG:O	2:I:400:TYR:HB3	2.17	0.44
4:M:199:ARG:NH1	5:N:517:LYS:HA	2.32	0.44
2:J:467:THR:CG2	5:P:544:GLN:HA	2.46	0.44
2:I:258:ASP:OD2	2:I:322:ASP:OD1	2.35	0.44
1:G:69:ARG:HG3	1:G:70:ASP:N	2.32	0.44
2:I:140:GLU:O	2:I:141:THR:C	2.55	0.44
5:N:448:PRO:HB2	5:N:466:VAL:HG21	1.99	0.44
2:K:179:HIS:HB3	2:K:465:ASP:HB3	2.00	0.44
2:J:404:LEU:HD11	2:J:416:LEU:HD13	1.98	0.44
2:J:388:ILE:HG21	2:J:453:ILE:HD11	1.99	0.44
4:O:288:GLU:HB2	5:P:350:HIS:HB3	1.98	0.44
2:L:188:ASP:O	2:L:192:VAL:HG23	2.18	0.44
4:Q:145:SER:HB3	4:Q:166:TRP:CD1	2.53	0.44
5:R:376:PHE:HD1	5:R:382:LYS:HD3	1.83	0.44
5:R:488:LEU:HD22	5:R:502:LEU:HG	1.99	0.44
1:G:40:TYR:HA	1:G:41:PRO:HD2	1.79	0.44
2:I:214:GLU:HA	2:I:222:MET:HB2	1.99	0.44
2:K:506:GLU:OE1	2:K:506:GLU:HA	2.18	0.44
8:H:28:NGT:O6	5:T:453:LEU:HG	2.18	0.44
5:T:403:ILE:HG12	5:T:420:ILE:HB	2.00	0.44
2:I:173:LEU:HB3	2:I:458:CYS:HA	2.00	0.44
1:C:36:ARG:HH11	6:Y:1:NAG:H62	1.83	0.44
4:O:215:PRO:HD2	5:P:495:ALA:HB2	1.99	0.44
2:K:168:PRO:HD2	2:K:453:ILE:O	2.18	0.44
2:K:178:ARG:NE	2:K:462:GLU:OE2	2.51	0.44
2:K:237:GLN:HB2	3:H:92:THR:HG21	1.99	0.44
4:Q:151:LEU:HD13	4:Q:160:LEU:HD13	1.99	0.44
4:M:200:PHE:CE1	5:N:481:PHE:CD1	3.06	0.44
5:N:502:LEU:HD13	5:N:503:TRP:CE2	2.52	0.44
1:C:41:PRO:HB3	1:C:73:PHE:HB3	1.99	0.44
5:P:429:TYR:O	5:P:432:GLU:HB2	2.17	0.44
2:K:445:THR:HB	2:K:446:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:118:LEU:HB3	2:L:161:ILE:HD12	1.99	0.44
5:T:464:TYR:HB2	5:T:508:ALA:HB1	2.00	0.44
2:I:215:SER:O	2:I:219:PRO:HA	2.17	0.43
2:I:339:MET:SD	2:I:351:LEU:HD22	2.58	0.43
4:O:199:ARG:HH21	5:P:469:LEU:HD12	1.82	0.43
2:K:520:GLY:O	4:Q:212:HIS:HD2	2.00	0.43
2:L:120:ILE:HB	2:L:159:THR:CG2	2.48	0.43
2:I:435:TYR:HE2	2:I:491:SER:HA	1.82	0.43
2:J:392:TRP:HB2	2:J:421:TYR:OH	2.18	0.43
2:L:122:ASP:OD1	2:L:122:ASP:N	2.49	0.43
2:L:140:GLU:OE1	2:L:195:TYR:HD1	2.01	0.43
4:M:206:LEU:HB3	5:N:487:CYS:HA	1.99	0.43
2:L:205:LEU:H	2:L:205:LEU:HD12	1.83	0.43
4:M:149:TYR:CZ	4:M:196:ASP:HB3	2.53	0.43
2:J:229:PRO:HA	2:J:233:ILE:HD11	2.00	0.43
4:O:302:GLN:HA	4:O:302:GLN:NE2	2.34	0.43
1:E:40:TYR:HA	1:E:41:PRO:HD2	1.79	0.43
8:E:530:NGT:C8	2:K:460:TRP:CH2	3.01	0.43
2:J:463:TYR:HE1	5:P:547:TYR:HD1	1.64	0.43
1:E:52:SER:O	1:E:55:GLN:NE2	2.51	0.43
2:K:171:GLY:HA3	2:K:456:GLU:HG2	2.00	0.43
3:F:57:TRP:HA	3:F:58:PRO:C	2.38	0.43
3:F:63:VAL:HG12	3:F:65:MET:HG2	2.01	0.43
1:G:55:GLN:HG3	1:G:56:PRO:HD3	1.95	0.43
8:G:533:NGT:HC81	2:L:373:TRP:CE3	2.54	0.43
2:L:513:GLN:HG3	2:L:526:PHE:CZ	2.54	0.43
2:I:357:GLN:OE1	2:I:382:LYS:HB3	2.18	0.43
3:B:105:ILE:HG12	4:M:176:SER:HA	2.01	0.43
1:C:59:SER:O	1:C:63:GLU:HG2	2.19	0.43
4:O:139:ALA:O	4:O:279:ARG:NH2	2.46	0.43
5:P:467:GLU:HA	5:P:468:PRO:HD2	1.88	0.43
2:L:97:VAL:HG12	2:L:126:LEU:HD21	2.01	0.43
2:L:99:VAL:CG2	2:L:130:GLU:HA	2.47	0.43
2:L:356:ILE:HD13	2:L:376:VAL:HG22	2.01	0.43
2:I:107:LEU:HD22	2:I:107:LEU:H	1.84	0.43
2:I:356:ILE:HD13	2:I:376:VAL:HG22	2.00	0.43
4:M:200:PHE:HE1	5:N:481:PHE:HD1	1.67	0.43
2:J:332:ASN:HA	2:J:333:PRO:HD3	1.80	0.43
4:O:202:HIS:CE1	5:P:444:ILE:HD13	2.54	0.43
4:Q:134:GLN:O	4:Q:164:ARG:NH1	2.41	0.43
4:Q:153:VAL:HB	4:Q:192:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:516:SER:HB2	5:R:519:VAL:HG23	2.00	0.43
1:A:40:TYR:HA	1:A:41:PRO:HD2	1.88	0.43
2:I:95:LEU:HB2	2:I:126:LEU:HD23	2.00	0.43
2:I:177:SER:O	2:I:210:SER:HB3	2.18	0.43
4:M:200:PHE:CE1	5:N:481:PHE:HD1	2.36	0.43
2:J:235:THR:HG22	2:J:236:ALA:H	1.83	0.43
2:K:370:TYR:HD2	2:K:387:THR:HG23	1.84	0.43
3:F:54:PRO:HB2	3:F:56:LEU:HG	1.99	0.43
2:L:171:GLY:HA2	2:L:200:VAL:O	2.18	0.43
4:M:208:ASP:OD1	4:M:208:ASP:C	2.56	0.43
4:Q:215:PRO:O	4:Q:218:ILE:HG22	2.18	0.43
5:R:468:PRO:HB2	5:R:481:PHE:CZ	2.54	0.43
4:S:154:LYS:HD2	4:S:155:GLU:O	2.18	0.43
4:S:206:LEU:HA	4:S:235:HIS:O	2.19	0.43
2:I:384:GLN:HG3	2:I:385:PRO:HD2	2.00	0.43
4:O:237:HIS:CD2	4:O:288:GLU:OE1	2.72	0.43
3:H:63:VAL:HA	4:S:194:ILE:HG13	2.01	0.43
2:I:387:THR:HG22	2:I:388:ILE:N	2.33	0.42
5:P:323:ASN:HA	5:P:324:PRO:HD3	1.94	0.42
2:K:101:THR:O	2:K:103:GLY:N	2.52	0.42
2:K:430:ASP:OD2	2:K:476:ARG:NH1	2.51	0.42
2:L:192:VAL:HA	2:L:195:TYR:CD2	2.54	0.42
1:A:42:ASN:H	1:A:42:ASN:ND2	2.17	0.42
2:J:316:TYR:CE2	2:J:388:ILE:HD11	2.53	0.42
2:K:469:LEU:HG	2:K:473:LEU:HD12	2.00	0.42
2:L:99:VAL:HG23	2:L:100:VAL:H	1.83	0.42
3:B:73:ALA:HB3	3:B:76:ASN:HB3	2.01	0.42
4:Q:287:PRO:HB3	5:R:344:PHE:CZ	2.54	0.42
2:L:183:LEU:O	2:L:187:LEU:HG	2.19	0.42
3:H:55:ALA:CB	5:T:531:ARG:HG3	2.48	0.42
1:A:69:ARG:HB2	1:A:69:ARG:CZ	2.50	0.42
1:E:33:SER:HB3	2:K:158:LYS:O	2.19	0.42
3:F:74:PRO:HD2	4:S:183:SER:O	2.19	0.42
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.20	0.42
3:B:72:LEU:HD11	4:M:189:ILE:HG22	2.02	0.42
4:O:211:ARG:HD3	4:O:211:ARG:N	2.34	0.42
2:K:485:TRP:CD1	2:K:485:TRP:C	2.91	0.42
4:Q:142:ASN:HB2	5:R:347:GLN:CD	2.38	0.42
4:Q:182:ASP:OD1	4:Q:186:THR:N	2.52	0.42
1:G:69:ARG:CZ	1:G:69:ARG:HB2	2.48	0.42
2:I:388:ILE:CG2	2:I:415:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:353:SER:HA	2:J:381:VAL:HG13	2.00	0.42
5:P:422:GLU:HA	5:P:444:ILE:O	2.19	0.42
2:K:167:PHE:HA	2:K:168:PRO:HD3	1.94	0.42
4:Q:239:VAL:HG12	4:Q:245:PRO:HD2	2.02	0.42
2:L:169:HIS:CE1	2:L:456:GLU:OE2	2.73	0.42
3:H:93:LEU:HD21	4:S:169:LEU:HD11	1.99	0.42
2:I:381:VAL:O	2:I:383:ILE:HG22	2.20	0.42
4:O:129:VAL:HG22	4:O:160:LEU:HD23	2.02	0.42
4:O:237:HIS:HD2	4:O:288:GLU:OE1	2.01	0.42
5:P:429:TYR:HA	5:P:432:GLU:HB2	2.02	0.42
1:E:30:PHE:HE2	2:K:159:THR:OG1	2.01	0.42
2:K:172:LEU:CD1	2:K:174:LEU:HD13	2.50	0.42
1:G:45:GLN:HG2	2:L:93:ASN:OD1	2.19	0.42
3:H:98:PHE:CE1	4:S:129:VAL:HG21	2.55	0.42
2:J:121:ASN:HD21	2:J:124:GLN:HG2	1.84	0.42
2:K:176:THR:HG22	2:K:181:LEU:HD12	2.00	0.42
4:Q:205:ILE:CD1	5:R:486:ALA:HB3	2.44	0.42
4:Q:279:ARG:C	4:Q:281:ARG:H	2.22	0.42
4:O:205:ILE:HG21	5:P:502:LEU:HD11	2.02	0.42
2:L:379:ASN:O	2:L:380:LYS:C	2.58	0.42
3:B:54:PRO:N	3:B:54:PRO:CG	2.81	0.42
1:C:26:TRP:HA	1:C:27:PRO:HD3	1.95	0.42
2:J:459:MET:HE3	2:J:464:VAL:HG11	2.02	0.42
2:L:256:GLU:HB2	2:L:318:HIS:HB3	2.01	0.42
4:S:253:GLU:HA	4:S:256:ASN:HB2	2.02	0.42
1:C:33:SER:CB	2:J:158:LYS:HG2	2.49	0.41
1:C:40:TYR:HA	1:C:41:PRO:HD2	1.94	0.41
2:J:148:LYS:HA	2:J:153:THR:O	2.20	0.41
1:E:28:GLN:HE22	2:K:487:ASN:HD22	1.67	0.41
4:Q:168:ALA:O	4:Q:172:LEU:HG	2.20	0.41
2:L:165:PRO:HB3	2:L:485:TRP:CE3	2.55	0.41
2:L:188:ASP:O	2:L:191:ASP:HB2	2.20	0.41
4:M:126:GLN:HE21	4:M:126:GLN:HB2	1.71	0.41
2:J:121:ASN:HD22	2:J:123:ASP:H	1.67	0.41
1:E:28:GLN:HG3	2:K:164:PHE:O	2.19	0.41
2:L:145:LEU:HD23	2:L:145:LEU:HA	1.95	0.41
2:L:384:GLN:HG3	2:L:385:PRO:HD2	2.01	0.41
3:H:68:ASN:HB3	4:S:191:GLU:HG2	2.02	0.41
5:T:452:ASP:OD2	5:T:489:TRP:HB2	2.20	0.41
8:A:21:NGT:HC2	2:I:323:GLU:OE1	2.19	0.41
5:N:424:TRP:HB2	5:N:450:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:350:HIS:HD2	5:P:352:GLY:H	1.68	0.41
5:P:350:HIS:HA	5:P:403:ILE:O	2.20	0.41
2:K:131:THR:HG22	2:K:132:VAL:H	1.85	0.41
2:K:359:LEU:HA	2:K:362:ILE:HD12	2.02	0.41
2:K:386:ASP:O	2:K:413:ARG:NH1	2.54	0.41
2:L:350:GLN:HA	2:L:353:SER:HB3	2.02	0.41
3:H:66:THR:HA	3:H:67:PRO:HD3	1.95	0.41
2:I:202:HIS:CE1	2:I:318:HIS:CD2	3.09	0.41
2:I:337:ASP:O	2:I:341:LYS:HG2	2.20	0.41
1:C:38:VAL:HG22	2:J:155:PHE:CE1	2.55	0.41
2:J:160:GLU:OE2	2:J:160:GLU:HA	2.19	0.41
2:J:292:PRO:HG3	2:J:329:TRP:CZ2	2.55	0.41
5:P:449:TRP:CD1	5:P:509:VAL:HG22	2.55	0.41
1:G:55:GLN:CG	1:G:56:PRO:CD	2.84	0.41
2:L:433:ASP:O	2:L:437:VAL:HG23	2.20	0.41
2:L:524:GLN:HG2	2:L:524:GLN:O	2.20	0.41
1:A:66:GLN:HE22	1:A:69:ARG:HD3	1.84	0.41
2:I:99:VAL:HG22	2:I:130:GLU:HA	2.02	0.41
2:I:164:PHE:CD2	6:U:1:NAG:H62	2.55	0.41
2:I:383:ILE:HD11	2:I:387:THR:HG21	2.03	0.41
5:P:532:HIS:HD2	5:P:535:ARG:NH2	2.08	0.41
4:Q:131:ILE:HA	4:Q:162:ALA:O	2.20	0.41
4:Q:133:LEU:HD12	4:Q:163:ASN:HB3	2.02	0.41
1:A:52:SER:HA	2:I:97:VAL:HG23	2.02	0.41
3:B:84:ASN:C	3:B:84:ASN:HD22	2.24	0.41
3:D:54:PRO:HB2	5:P:531:ARG:NH2	2.36	0.41
5:P:350:HIS:CD2	5:P:352:GLY:H	2.38	0.41
5:P:371:MET:H	5:P:371:MET:HG2	1.70	0.41
5:R:504:PRO:HD3	5:R:544:GLN:O	2.20	0.41
5:T:414:LYS:HD3	5:T:414:LYS:HA	1.97	0.41
1:A:26:TRP:HA	1:A:27:PRO:HD3	1.95	0.41
1:C:26:TRP:HB2	2:J:499:ARG:NH1	2.36	0.41
2:J:228:ASN:ND2	2:J:230:VAL:H	2.16	0.41
3:D:68:ASN:HB3	4:O:191:GLU:HG2	2.01	0.41
1:E:59:SER:O	1:E:63:GLU:HG2	2.21	0.41
2:K:278:TYR:CD1	2:K:332:ASN:HA	2.55	0.41
1:A:61:LEU:HD11	2:I:135:ALA:HB3	2.02	0.41
2:I:374:GLN:HA	2:I:389:ILE:HG23	2.03	0.41
2:J:425:ILE:HB	5:P:454:ILE:HD12	2.03	0.41
2:K:475:PRO:HD3	2:K:515:GLN:O	2.20	0.41
2:L:464:VAL:HG22	2:L:472:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG12	1:A:61:LEU:HD23	2.02	0.41
2:I:523:GLU:HG3	1:C:42:ASN:ND2	2.36	0.41
1:C:31:GLN:HB3	2:J:160:GLU:HB3	2.02	0.41
2:J:120:ILE:O	2:J:158:LYS:HA	2.20	0.41
4:O:160:LEU:HD21	4:O:168:ALA:HA	2.02	0.41
2:K:290:VAL:HG12	2:K:291:ASN:N	2.36	0.41
2:K:431:TRP:HA	2:K:434:PHE:CD2	2.55	0.41
4:Q:223:LEU:HD21	4:Q:234:LEU:HD22	2.02	0.41
4:Q:295:THR:O	4:Q:306:LEU:HD21	2.21	0.41
4:O:237:HIS:HE1	4:O:240:ASP:OD2	2.04	0.41
4:O:290:ASP:HA	5:P:352:GLY:HA3	2.03	0.41
2:L:428:GLY:HA2	5:T:492:TYR:CZ	2.56	0.41
5:T:532:HIS:CD2	5:T:535:ARG:HH21	2.39	0.41
2:I:90:LEU:HD13	2:I:92:LYS:HD2	2.02	0.40
2:I:266:TRP:CD1	2:I:266:TRP:N	2.89	0.40
4:M:186:THR:HA	4:O:184:TYR:O	2.21	0.40
2:J:270:ILE:HA	2:J:271:PRO:HD2	1.99	0.40
2:J:459:MET:CE	2:J:464:VAL:HG11	2.51	0.40
2:L:232:HIS:NE2	5:T:550:TYR:HB2	2.36	0.40
2:L:401:MET:HA	2:L:404:LEU:HD12	2.02	0.40
1:A:46:PHE:CD2	2:I:94:VAL:HG12	2.55	0.40
4:O:229:ASN:OD1	5:P:532:HIS:HE1	2.03	0.40
4:Q:209:THR:O	4:Q:245:PRO:HG2	2.21	0.40
2:L:465:ASP:C	2:L:467:THR:H	2.24	0.40
5:T:347:GLN:O	5:T:401:GLY:N	2.43	0.40
2:J:228:ASN:HA	2:J:229:PRO:HD3	1.77	0.40
2:K:423:ASN:OD1	2:K:460:TRP:HD1	2.05	0.40
3:F:70:LEU:HD21	4:Q:155:GLU:HB3	2.04	0.40
5:R:382:LYS:HA	5:R:385:SER:HB2	2.04	0.40
1:G:26:TRP:HA	1:G:27:PRO:HD3	1.85	0.40
2:I:179:HIS:HE1	2:I:462:GLU:O	2.05	0.40
5:N:437:THR:O	5:N:477:GLN:HG2	2.21	0.40
1:C:67:ARG:HD2	2:J:249:ARG:NH2	2.36	0.40
2:J:100:VAL:HG23	2:J:130:GLU:HG3	2.04	0.40
2:J:447:GLU:OE2	2:J:447:GLU:N	2.50	0.40
5:P:460:TRP:CD1	5:P:546:LEU:HD22	2.56	0.40
3:F:64:LYS:HE3	4:Q:193:THR:O	2.21	0.40
4:Q:150:THR:HG22	4:Q:195:ILE:HG12	2.02	0.40
4:S:147:GLU:HB3	4:S:170:ARG:HG3	2.02	0.40
4:M:235:HIS:NE2	4:M:288:GLU:OE1	2.42	0.40
4:M:291:THR:HG22	5:N:322:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:219:ILE:O	4:Q:222:THR:HB	2.21	0.40

All (1) 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)
2:L:424:ARG:NH2	5:T:369:ASP:OD1[2_456]	1.93	0.27

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	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	33
1	C	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	E	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	G	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	7	33
2	I	438/440 (100%)	400 (91%)	30 (7%)	8 (2%)	8	35
2	J	438/440 (100%)	402 (92%)	29 (7%)	7 (2%)	9	37
2	K	438/440 (100%)	402 (92%)	31 (7%)	5 (1%)	14	46
2	L	438/440 (100%)	404 (92%)	25 (6%)	9 (2%)	7	32
3	B	52/58 (90%)	42 (81%)	8 (15%)	2 (4%)	3	19
3	D	52/58 (90%)	42 (81%)	10 (19%)	0	100	100
3	F	52/58 (90%)	45 (86%)	4 (8%)	3 (6%)	1	10
3	H	52/58 (90%)	45 (86%)	6 (12%)	1 (2%)	8	34
4	M	188/190 (99%)	177 (94%)	10 (5%)	1 (0%)	29	62
4	O	187/190 (98%)	175 (94%)	12 (6%)	0	100	100
4	Q	188/190 (99%)	170 (90%)	17 (9%)	1 (0%)	29	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
5	N	234/237 (99%)	215 (92%)	19 (8%)	0	100	100
5	P	234/237 (99%)	213 (91%)	16 (7%)	5 (2%)	7	32
5	R	234/237 (99%)	210 (90%)	22 (9%)	2 (1%)	17	50
5	T	234/237 (99%)	217 (93%)	15 (6%)	2 (1%)	17	50
All	All	3847/3908 (98%)	3523 (92%)	276 (7%)	48 (1%)	13	43

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	103	GLY
3	B	55	ALA
2	J	102	PRO
2	J	103	GLY
2	K	102	PRO
5	R	458	GLN
2	L	102	PRO
2	L	380	LYS
2	L	462	GLU
2	J	466	ASN
5	P	427	SER
2	K	103	GLY
2	K	104	CYS
2	K	229	PRO
5	R	427	SER
2	I	488	LYS
4	M	237	HIS
5	P	458	GLN
5	P	495	ALA
3	F	76	ASN
2	I	102	PRO
2	I	280	GLY
1	G	41	PRO
2	L	490	THR
3	H	74	PRO
1	A	41	PRO
2	I	285	GLY
2	I	490	THR
3	B	76	ASN
2	J	229	PRO

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Mol	Chain	Res	Type
2	J	283	PRO
2	K	280	GLY
4	Q	182	ASP
2	L	267	GLY
2	L	466	ASN
5	T	417	PRO
5	T	458	GLN
2	J	437	VAL
5	P	519	VAL
3	F	67	PRO
2	L	103	GLY
2	L	465	ASP
5	P	418	GLY
3	F	74	PRO
2	L	280	GLY
2	I	229	PRO
2	I	101	THR
2	J	267	GLY

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	47/47 (100%)	39 (83%)	8 (17%)	2 9
1	C	47/47 (100%)	42 (89%)	5 (11%)	6 25
1	E	47/47 (100%)	41 (87%)	6 (13%)	4 18
1	G	47/47 (100%)	43 (92%)	4 (8%)	10 34
2	I	393/394 (100%)	364 (93%)	29 (7%)	13 40
2	J	393/394 (100%)	359 (91%)	34 (9%)	10 34
2	K	393/394 (100%)	371 (94%)	22 (6%)	21 52
2	L	393/394 (100%)	362 (92%)	31 (8%)	12 37
3	B	47/49 (96%)	45 (96%)	2 (4%)	29 59
3	D	47/49 (96%)	45 (96%)	2 (4%)	29 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	47/49 (96%)	44 (94%)	3 (6%)	17	47
3	H	47/49 (96%)	45 (96%)	2 (4%)	29	59
4	M	174/174 (100%)	168 (97%)	6 (3%)	37	64
4	O	173/174 (99%)	161 (93%)	12 (7%)	15	43
4	Q	174/174 (100%)	169 (97%)	5 (3%)	42	68
4	S	174/174 (100%)	168 (97%)	6 (3%)	37	64
5	N	205/206 (100%)	192 (94%)	13 (6%)	18	47
5	P	205/206 (100%)	188 (92%)	17 (8%)	11	36
5	R	205/206 (100%)	191 (93%)	14 (7%)	16	44
5	T	205/206 (100%)	195 (95%)	10 (5%)	25	55
All	All	3463/3480 (100%)	3232 (93%)	231 (7%)	16	45

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	35	GLN
1	A	42	ASN
1	A	45	GLN
1	A	47	GLN
1	A	66	GLN
1	A	69	ARG
1	A	72	LEU
2	I	94	VAL
2	I	95	LEU
2	I	105	ASN
2	I	106	GLN
2	I	107	LEU
2	I	121	ASN
2	I	122	ASP
2	I	126	LEU
2	I	127	LEU
2	I	153	THR
2	I	178	ARG
2	I	198	LEU
2	I	270	ILE
2	I	299	GLU
2	I	306	LEU

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Mol	Chain	Res	Type
2	I	372	VAL
2	I	382	LYS
2	I	396	ILE
2	I	398	VAL
2	I	402	LYS
2	I	409	LYS
2	I	415	LEU
2	I	416	LEU
2	I	466	ASN
2	I	489	LEU
2	I	507	LEU
2	I	518	ASN
2	I	521	PHE
2	I	528	GLN
3	B	84	ASN
3	B	93	LEU
4	M	169	LEU
4	M	191	GLU
4	M	206	LEU
4	M	211	ARG
4	M	250	THR
4	M	257	LYS
5	N	328	THR
5	N	338	LYS
5	N	356	VAL
5	N	364	ASN
5	N	384	GLU
5	N	414	LYS
5	N	426	ASP
5	N	431	GLU
5	N	462	LYS
5	N	502	LEU
5	N	512	ARG
5	N	516	SER
5	N	522	MET
1	C	32	THR
1	C	35	GLN
1	C	55	GLN
1	C	72	LEU
1	C	73	PHE
2	J	90	LEU
2	J	92	LYS

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Mol	Chain	Res	Type
2	J	93	ASN
2	J	94	VAL
2	J	98	SER
2	J	101	THR
2	J	106	GLN
2	J	107	LEU
2	J	121	ASN
2	J	126	LEU
2	J	131	THR
2	J	158	LYS
2	J	159	THR
2	J	162	GLU
2	J	172	LEU
2	J	178	ARG
2	J	228	ASN
2	J	240	LYS
2	J	263	THR
2	J	296	ASN
2	J	299	GLU
2	J	336	GLN
2	J	339	MET
2	J	358	THR
2	J	370	TYR
2	J	372	VAL
2	J	382	LYS
2	J	399	ASN
2	J	403	GLU
2	J	406	LEU
2	J	465	ASP
2	J	523	GLU
2	J	525	GLU
2	J	528	GLN
3	D	66	THR
3	D	84	ASN
4	O	154	LYS
4	O	165	VAL
4	O	174	THR
4	O	183	SER
4	O	211	ARG
4	O	217	LYS
4	O	250	THR
4	O	257	LYS

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Mol	Chain	Res	Type
4	O	267	THR
4	O	291	THR
4	O	307	THR
4	O	310	TYR
5	P	317	ASP
5	P	338	LYS
5	P	341	SER
5	P	359	LYS
5	P	360	CYS
5	P	362	GLU
5	P	369	ASP
5	P	372	ARG
5	P	384	GLU
5	P	390	LYS
5	P	393	ASP
5	P	431	GLU
5	P	451	LEU
5	P	455	SER
5	P	476	LYS
5	P	502	LEU
5	P	522	MET
1	E	23	LEU
1	E	28	GLN
1	E	47	GLN
1	E	55	GLN
1	E	66	GLN
1	E	69	ARG
2	K	89	THR
2	K	92	LYS
2	K	106	GLN
2	K	107	LEU
2	K	121	ASN
2	K	126	LEU
2	K	127	LEU
2	K	131	THR
2	K	153	THR
2	K	162	GLU
2	K	174	LEU
2	K	189	THR
2	K	228	ASN
2	K	295	ASN
2	K	370	TYR

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Mol	Chain	Res	Type
2	K	382	LYS
2	K	395	ASP
2	K	396	ILE
2	K	399	ASN
2	K	466	ASN
2	K	515	GLN
2	K	518	ASN
3	F	68	ASN
3	F	79	ILE
3	F	80	SER
4	Q	130	SER
4	Q	155	GLU
4	Q	211	ARG
4	Q	250	THR
4	Q	311	SER
5	R	338	LYS
5	R	341	SER
5	R	351	LEU
5	R	359	LYS
5	R	385	SER
5	R	390	LYS
5	R	403	ILE
5	R	414	LYS
5	R	431	GLU
5	R	451	LEU
5	R	476	LYS
5	R	502	LEU
5	R	522	MET
5	R	550	TYR
1	G	47	GLN
1	G	51	SER
1	G	69	ARG
1	G	72	LEU
2	L	90	LEU
2	L	92	LYS
2	L	95	LEU
2	L	98	SER
2	L	106	GLN
2	L	107	LEU
2	L	121	ASN
2	L	122	ASP
2	L	126	LEU

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Mol	Chain	Res	Type
2	L	162	GLU
2	L	172	LEU
2	L	198	LEU
2	L	235	THR
2	L	270	ILE
2	L	299	GLU
2	L	311	VAL
2	L	322	ASP
2	L	336	GLN
2	L	370	TYR
2	L	382	LYS
2	L	398	VAL
2	L	399	ASN
2	L	406	LEU
2	L	415	LEU
2	L	443	GLU
2	L	463	TYR
2	L	467	THR
2	L	518	ASN
2	L	521	PHE
2	L	523	GLU
2	L	528	GLN
3	H	65	MET
3	H	84	ASN
4	S	154	LYS
4	S	211	ARG
4	S	216	VAL
4	S	257	LYS
4	S	309	CYS
4	S	311	SER
5	T	338	LYS
5	T	359	LYS
5	T	364	ASN
5	T	369	ASP
5	T	379	ASP
5	T	414	LYS
5	T	431	GLU
5	T	502	LEU
5	T	518	ASP
5	T	522	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	42	ASN
1	A	47	GLN
1	A	55	GLN
1	A	66	GLN
2	I	93	ASN
2	I	115	ASN
2	I	121	ASN
2	I	157	ASN
2	I	204	HIS
2	I	228	ASN
2	I	262	HIS
2	I	336	GLN
2	I	384	GLN
2	I	466	ASN
2	I	518	ASN
2	I	528	GLN
3	B	76	ASN
3	B	84	ASN
3	B	102	HIS
4	M	123	GLN
4	M	126	GLN
4	M	190	ASN
4	M	237	HIS
4	M	264	HIS
4	M	302	GLN
5	N	347	GLN
5	N	350	HIS
5	N	364	ASN
5	N	406	GLN
5	N	532	HIS
1	C	28	GLN
1	C	55	GLN
1	C	66	GLN
2	J	106	GLN
2	J	121	ASN
2	J	124	GLN
2	J	204	HIS
2	J	228	ASN
2	J	336	GLN
2	J	350	GLN
2	J	466	ASN
2	J	518	ASN

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Mol	Chain	Res	Type
3	D	76	ASN
3	D	81	HIS
3	D	84	ASN
3	D	102	HIS
4	O	123	GLN
4	O	126	GLN
4	O	237	HIS
4	O	302	GLN
5	P	373	GLN
5	P	406	GLN
5	P	477	GLN
5	P	532	HIS
1	E	28	GLN
1	E	43	ASN
1	E	47	GLN
1	E	55	GLN
2	K	106	GLN
2	K	121	ASN
2	K	124	GLN
2	K	228	ASN
2	K	336	GLN
2	K	399	ASN
2	K	448	GLN
2	K	515	GLN
2	K	518	ASN
3	F	76	ASN
3	F	84	ASN
4	Q	123	GLN
4	Q	126	GLN
4	Q	237	HIS
4	Q	264	HIS
5	R	350	HIS
5	R	406	GLN
5	R	477	GLN
5	R	532	HIS
1	G	28	GLN
1	G	29	ASN
1	G	43	ASN
1	G	55	GLN
2	L	105	ASN
2	L	121	ASN
2	L	169	HIS

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Mol	Chain	Res	Type
2	L	204	HIS
2	L	228	ASN
2	L	336	GLN
2	L	350	GLN
2	L	384	GLN
2	L	399	ASN
2	L	466	ASN
2	L	518	ASN
3	H	76	ASN
3	H	81	HIS
3	H	84	ASN
4	S	123	GLN
4	S	237	HIS
4	S	264	HIS
4	S	302	GLN
5	T	364	ASN
5	T	406	GLN
5	T	532	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

27 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	$\#\|Z\| > 2$
6	NAG	U	1	6,2	14,14,15	0.75	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	U	2	6	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
6	BMA	U	3	6	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
6	NAG	V	1	6,2	14,14,15	0.53	0	17,19,21	0.61	0
6	NAG	V	2	6	14,14,15	0.58	0	17,19,21	1.22	1 (5%)
6	BMA	V	3	6	11,11,12	0.76	0	15,15,17	2.17	3 (20%)
6	NAG	W	1	6	14,14,15	0.59	0	17,19,21	0.62	0
6	NAG	W	2	6	14,14,15	0.64	0	17,19,21	1.13	1 (5%)
6	BMA	W	3	6	11,11,12	2.26	2 (18%)	15,15,17	3.09	6 (40%)
7	NAG	X	1	7,2	14,14,15	0.65	0	17,19,21	0.89	1 (5%)
7	NAG	X	2	7	14,14,15	0.53	0	17,19,21	0.77	0
6	NAG	Y	1	6,2	14,14,15	1.02	2 (14%)	17,19,21	0.63	0
6	NAG	Y	2	6	14,14,15	1.14	2 (14%)	17,19,21	4.11	6 (35%)
6	BMA	Y	3	6	11,11,12	0.61	0	15,15,17	1.79	2 (13%)
7	NAG	Z	1	7,4	14,14,15	0.48	0	17,19,21	0.62	0
7	NAG	Z	2	7	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
7	NAG	a	1	7,2	14,14,15	2.76	5 (35%)	17,19,21	0.77	1 (5%)
7	NAG	a	2	7	14,14,15	1.20	1 (7%)	17,19,21	1.93	3 (17%)
7	NAG	b	1	7,4	14,14,15	0.64	0	17,19,21	0.61	0
7	NAG	b	2	7	14,14,15	0.69	0	17,19,21	1.22	2 (11%)
7	NAG	c	1	7,2	14,14,15	2.01	3 (21%)	17,19,21	0.64	0
7	NAG	c	2	7	14,14,15	0.66	0	17,19,21	1.34	3 (17%)
6	NAG	d	1	6,2	14,14,15	0.58	0	17,19,21	0.61	0
6	NAG	d	2	6	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
6	BMA	d	3	6	11,11,12	0.62	0	15,15,17	0.98	1 (6%)
7	NAG	e	1	7,4	14,14,15	1.07	1 (7%)	17,19,21	0.61	0
7	NAG	e	2	7	14,14,15	0.65	0	17,19,21	1.21	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	U	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1
6	NAG	W	1	6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	5/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
7	NAG	X	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	5/6/23/26	0/1/1/1
6	NAG	Y	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	1/1/5/7	4/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
7	NAG	Z	1	7,4	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	a	1	7,2	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	a	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	b	1	7,4	1/1/5/7	6/6/23/26	0/1/1/1
7	NAG	b	2	7	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	c	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	d	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	1/1/5/7	5/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,4	-	3/6/23/26	0/1/1/1
7	NAG	e	2	7	1/1/5/7	4/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	3	BMA	O2-C2	6.61	1.57	1.43
7	a	1	NAG	O4-C4	-6.22	1.27	1.43
7	c	1	NAG	C2-N2	6.17	1.56	1.46
7	a	1	NAG	C1-C2	4.48	1.58	1.52
7	a	1	NAG	O5-C1	-4.37	1.36	1.43
7	a	1	NAG	C4-C5	-4.29	1.43	1.53
7	a	2	NAG	C1-C2	3.62	1.57	1.52
6	Y	2	NAG	O5-C1	-3.11	1.38	1.43
7	c	1	NAG	C1-C2	-2.73	1.48	1.52
6	W	3	BMA	C2-C3	2.60	1.56	1.52
7	e	1	NAG	C2-N2	2.54	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	1	NAG	C2-N2	-2.41	1.42	1.46
6	Y	1	NAG	C1-C2	2.29	1.55	1.52
6	Y	2	NAG	O5-C5	-2.28	1.39	1.43
6	Y	1	NAG	C2-N2	2.07	1.49	1.46
7	c	1	NAG	O5-C5	2.03	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Y	2	NAG	O5-C5-C6	10.51	128.11	107.66
6	Y	2	NAG	O5-C1-C2	10.45	127.45	111.29
6	W	3	BMA	C1-C2-C3	6.51	119.12	109.64
6	W	3	BMA	C1-O5-C5	-5.99	104.16	112.19
7	a	2	NAG	C1-O5-C5	5.93	120.13	112.19
6	V	3	BMA	C1-C2-C3	-5.71	101.33	109.64
6	Y	3	BMA	O5-C5-C6	5.00	117.40	107.66
6	V	3	BMA	C1-O5-C5	-4.74	105.84	112.19
6	W	3	BMA	O5-C5-C6	4.40	116.23	107.66
6	W	3	BMA	O2-C2-C1	4.26	118.98	109.22
6	W	3	BMA	O2-C2-C3	4.18	118.81	110.15
6	Y	2	NAG	C3-C4-C5	4.02	117.52	110.23
6	U	2	NAG	C2-N2-C7	3.79	127.98	122.90
6	Y	3	BMA	C1-O5-C5	-3.67	107.26	112.19
6	Y	2	NAG	C2-N2-C7	3.62	127.76	122.90
6	Y	2	NAG	O5-C5-C4	3.59	119.56	110.83
6	Y	2	NAG	C4-C3-C2	3.52	116.18	111.02
6	U	3	BMA	C1-O5-C5	3.49	116.87	112.19
7	e	2	NAG	C2-N2-C7	3.28	127.29	122.90
7	c	2	NAG	C4-C3-C2	3.11	115.57	111.02
7	a	2	NAG	C2-N2-C7	3.02	126.94	122.90
6	V	2	NAG	C4-C3-C2	2.73	115.02	111.02
6	d	2	NAG	C4-C3-C2	2.69	114.96	111.02
6	d	3	BMA	C1-O5-C5	-2.57	108.75	112.19
7	b	2	NAG	C4-C3-C2	2.56	114.77	111.02
6	W	2	NAG	C2-N2-C7	2.52	126.28	122.90
7	c	2	NAG	C2-N2-C7	2.45	126.18	122.90
6	U	3	BMA	C1-C2-C3	2.37	113.09	109.64
7	b	2	NAG	C2-N2-C7	2.34	126.04	122.90
7	c	2	NAG	C1-O5-C5	2.19	115.12	112.19
7	X	1	NAG	C1-O5-C5	2.15	115.06	112.19
7	a	2	NAG	O4-C4-C5	2.09	114.48	109.32
6	W	3	BMA	C2-C3-C4	-2.05	107.25	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	2	NAG	C4-C3-C2	2.04	114.01	111.02
6	V	3	BMA	O5-C5-C6	2.03	111.61	107.66
6	d	2	NAG	C2-N2-C7	2.02	125.61	122.90
7	a	1	NAG	O7-C7-C8	-2.00	118.49	122.05

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	Y	2	NAG	C5
6	d	2	NAG	C1
7	Z	1	NAG	C1
7	Z	2	NAG	C1
7	a	1	NAG	C1
7	a	2	NAG	C1
7	b	1	NAG	C1
7	b	2	NAG	C1
7	c	2	NAG	C1
7	e	2	NAG	C1

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	W	2	NAG	C3-C2-N2-C7
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	d	2	NAG	C3-C2-N2-C7
6	d	2	NAG	C8-C7-N2-C2
6	d	2	NAG	O7-C7-N2-C2
7	Z	2	NAG	C3-C2-N2-C7
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2
7	b	1	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
7	b	2	NAG	C3-C2-N2-C7
7	c	2	NAG	C3-C2-N2-C7
7	e	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	Y	3	BMA	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6
6	Y	2	NAG	C4-C5-C6-O6
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
6	d	2	NAG	O5-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
6	W	3	BMA	C4-C5-C6-O6
6	d	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	X	2	NAG	C8-C7-N2-C2
7	Z	1	NAG	C8-C7-N2-C2
7	c	2	NAG	C8-C7-N2-C2
7	X	2	NAG	O7-C7-N2-C2
6	U	3	BMA	O5-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
6	U	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	c	2	NAG	O7-C7-N2-C2
6	W	1	NAG	C8-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	Y	2	NAG	C3-C2-N2-C7
6	V	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
6	W	2	NAG	O5-C5-C6-O6
7	b	1	NAG	C1-C2-N2-C7
7	b	1	NAG	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
6	V	2	NAG	O7-C7-N2-C2
7	X	2	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
7	b	1	NAG	C3-C2-N2-C7
7	e	2	NAG	C3-C2-N2-C7
6	U	2	NAG	C4-C5-C6-O6
6	V	1	NAG	O7-C7-N2-C2
7	e	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	U	2	NAG	O5-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
7	a	2	NAG	C1-C2-N2-C7
7	e	2	NAG	C1-C2-N2-C7
7	e	2	NAG	O5-C5-C6-O6
6	U	2	NAG	C3-C2-N2-C7
6	V	1	NAG	C8-C7-N2-C2

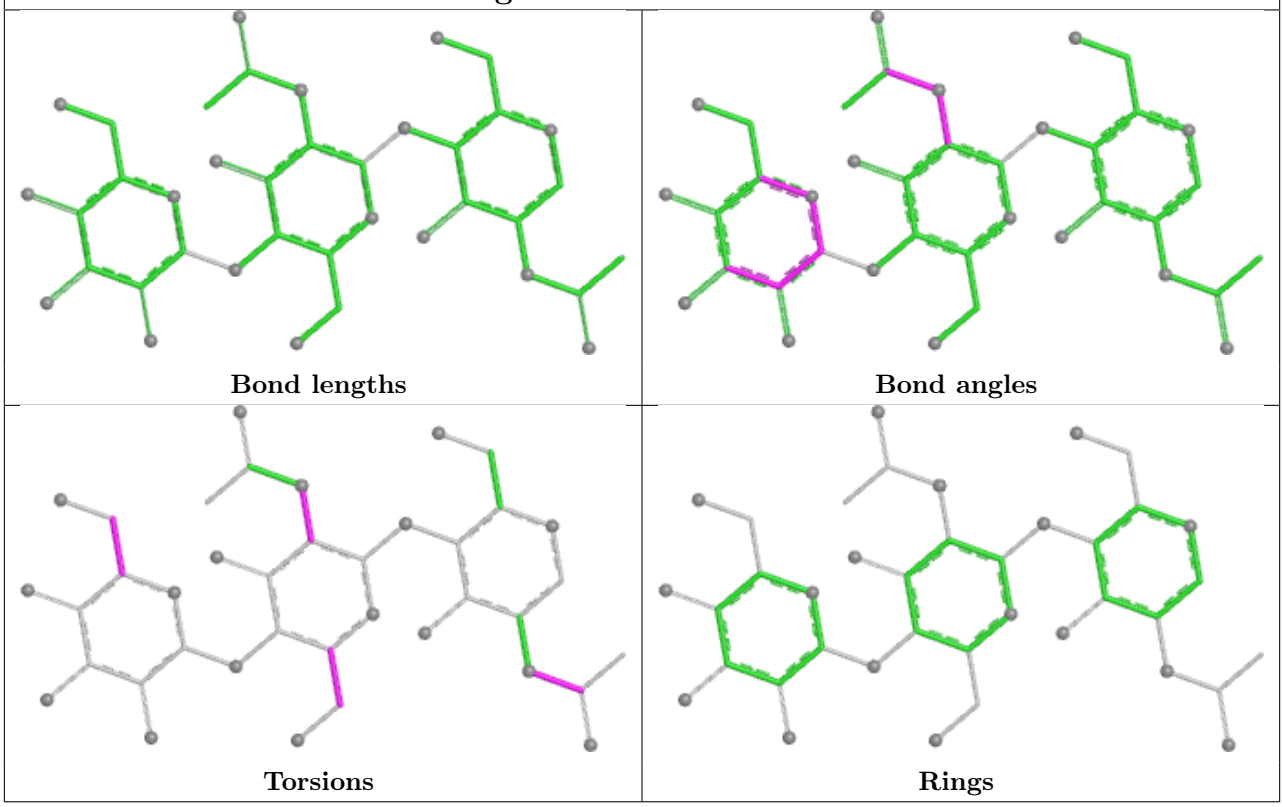
There are no ring outliers.

7 monomers are involved in 17 short contacts:

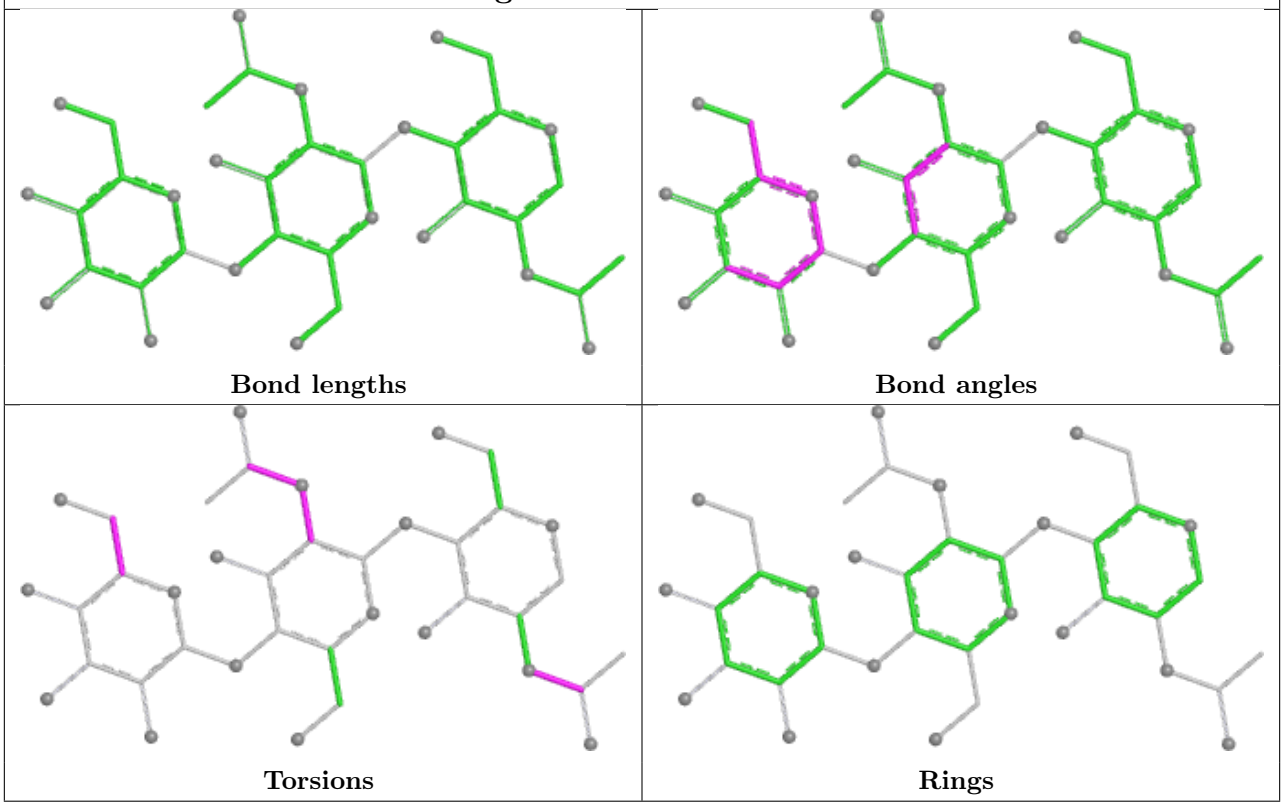
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Y	1	NAG	7	0
6	W	1	NAG	1	0
7	X	1	NAG	1	0
7	Z	1	NAG	2	0
6	Y	2	NAG	1	0
6	U	1	NAG	5	0
6	V	1	NAG	1	0

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

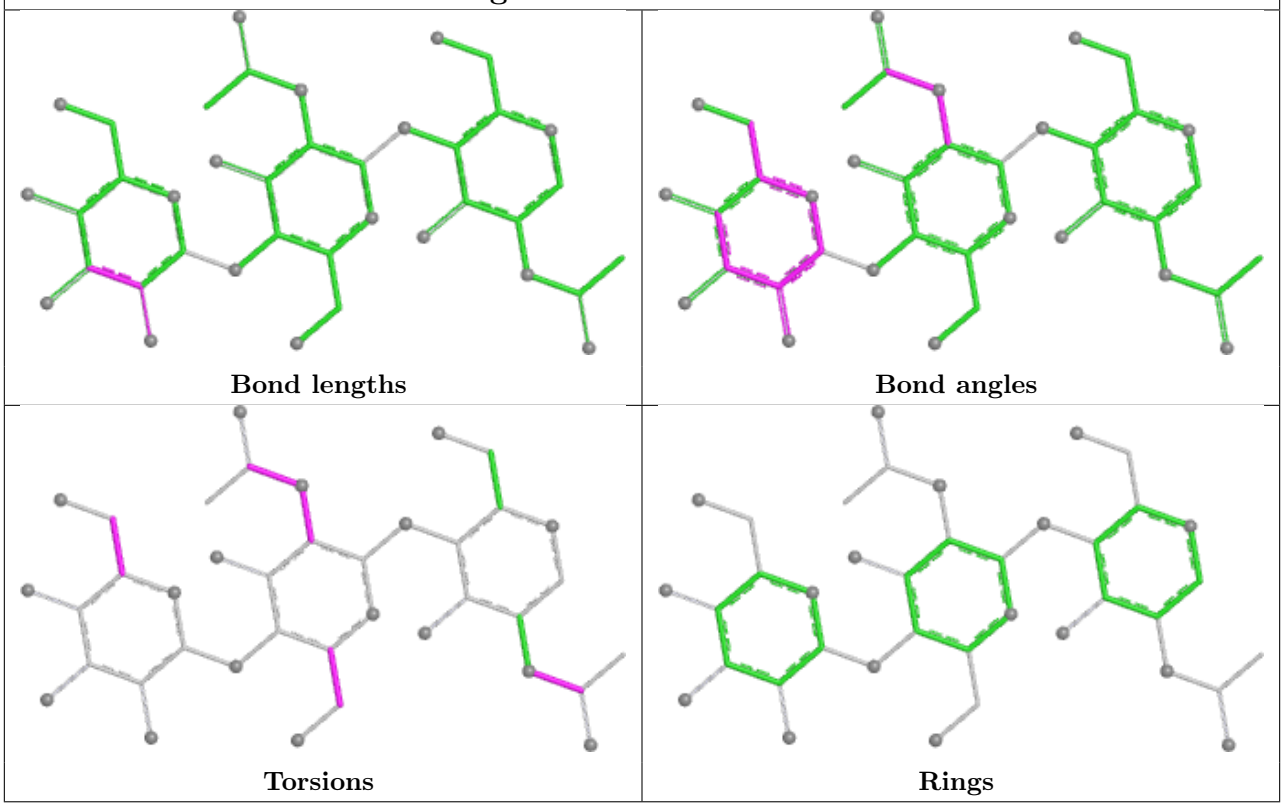
Oligosaccharide Chain U



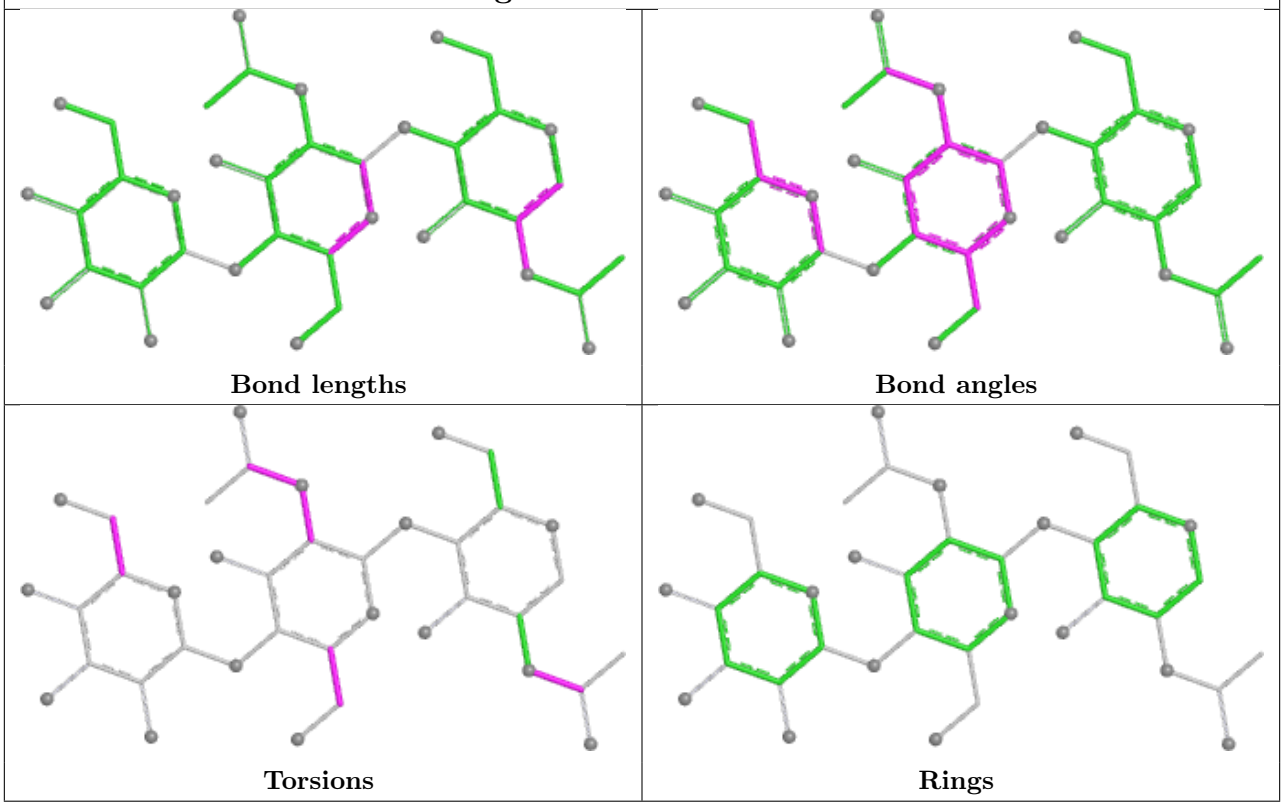
Oligosaccharide Chain V



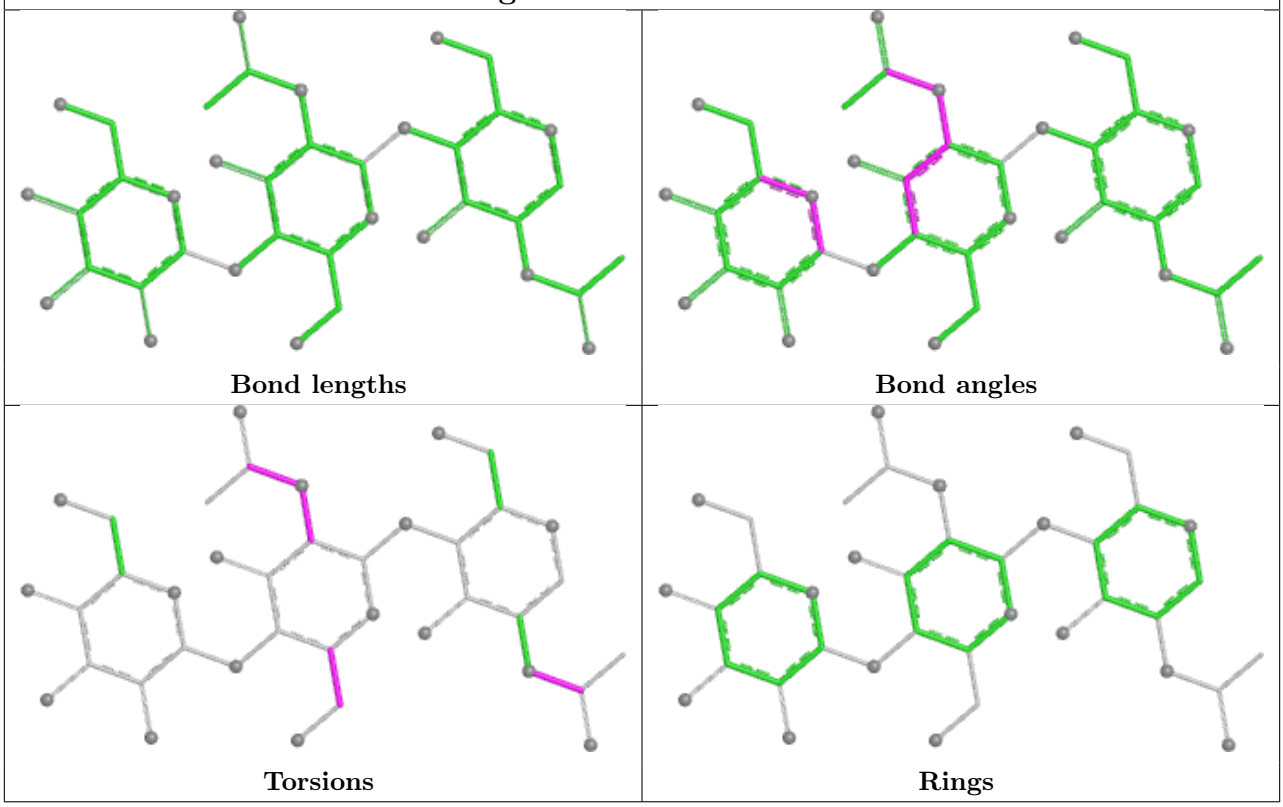
Oligosaccharide Chain W



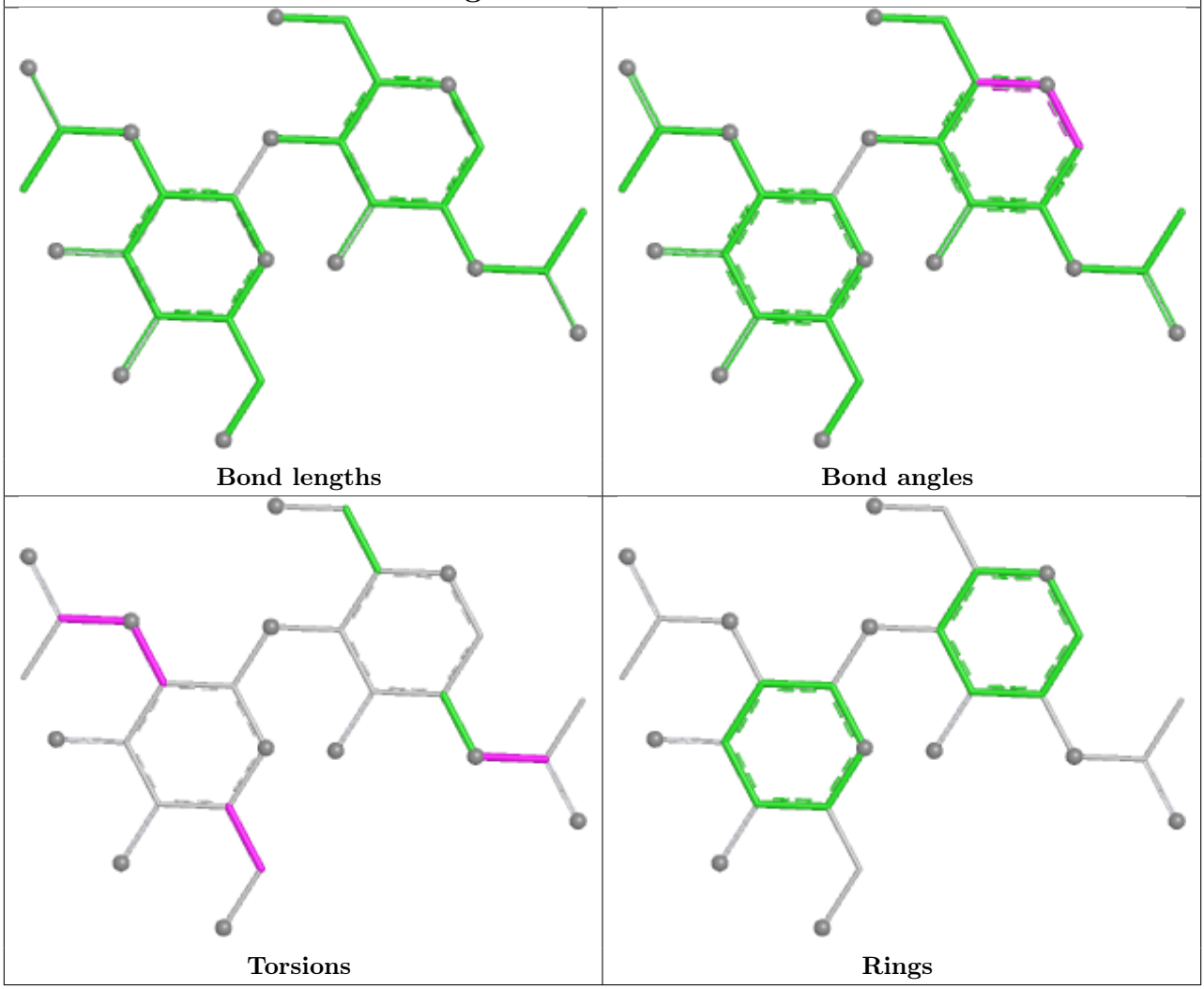
Oligosaccharide Chain Y



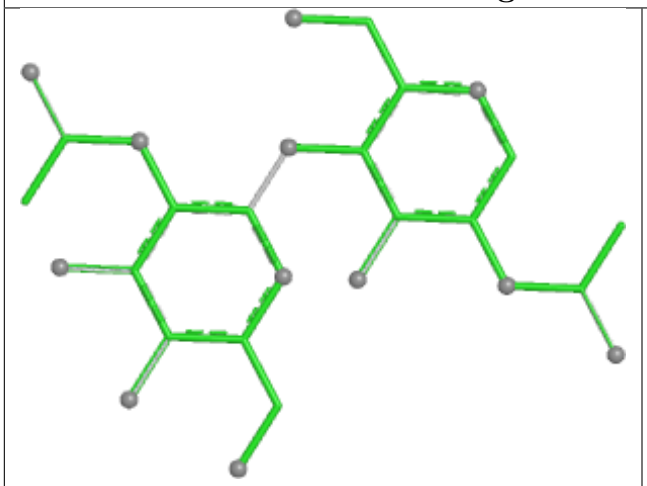
Oligosaccharide Chain d



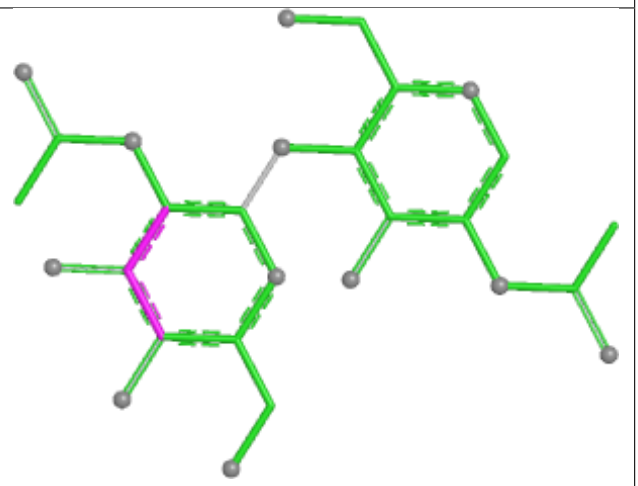
Oligosaccharide Chain X



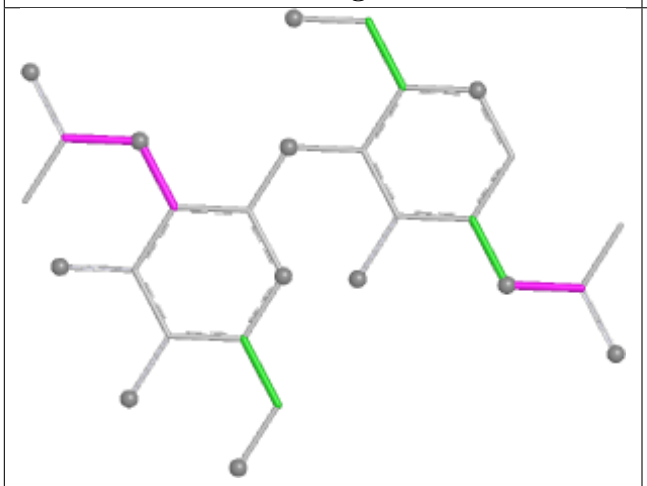
Oligosaccharide Chain Z



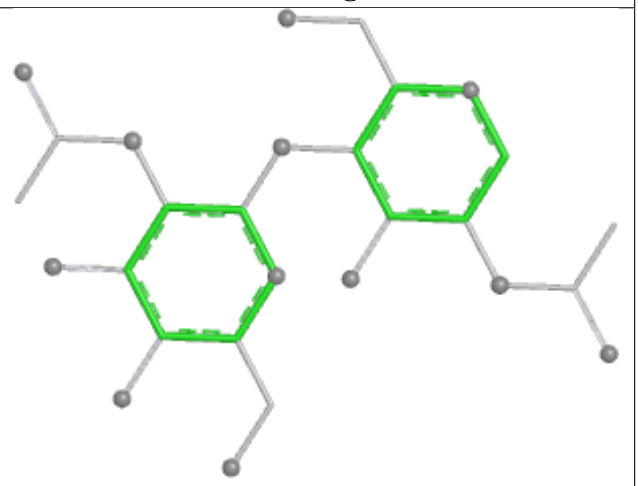
Bond lengths



Bond angles

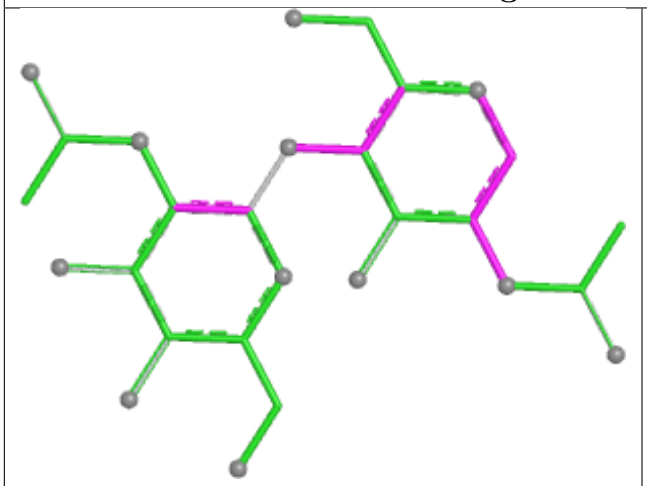


Torsions

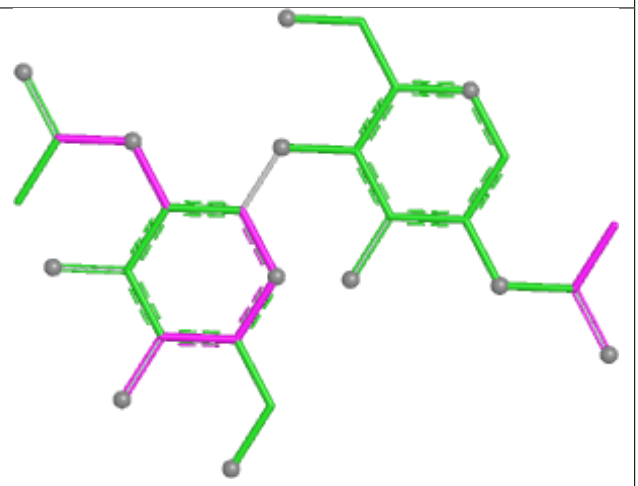


Rings

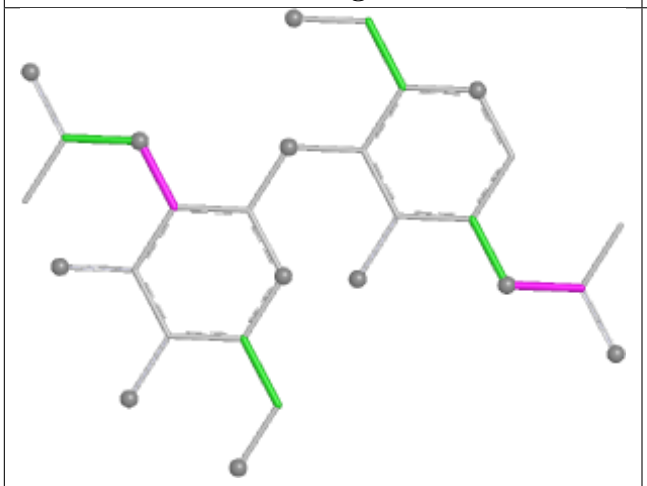
Oligosaccharide Chain a



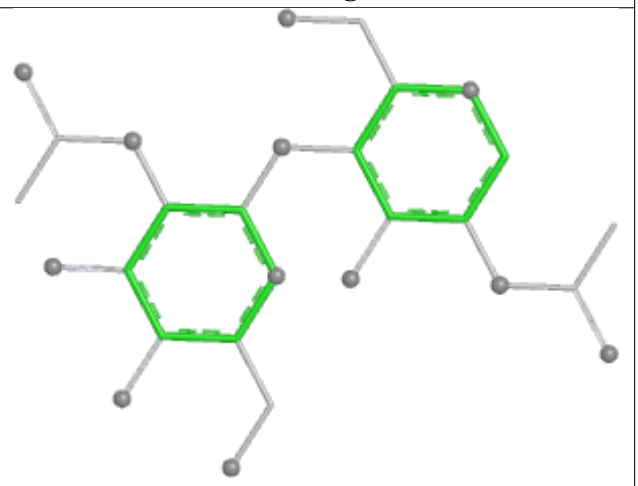
Bond lengths



Bond angles

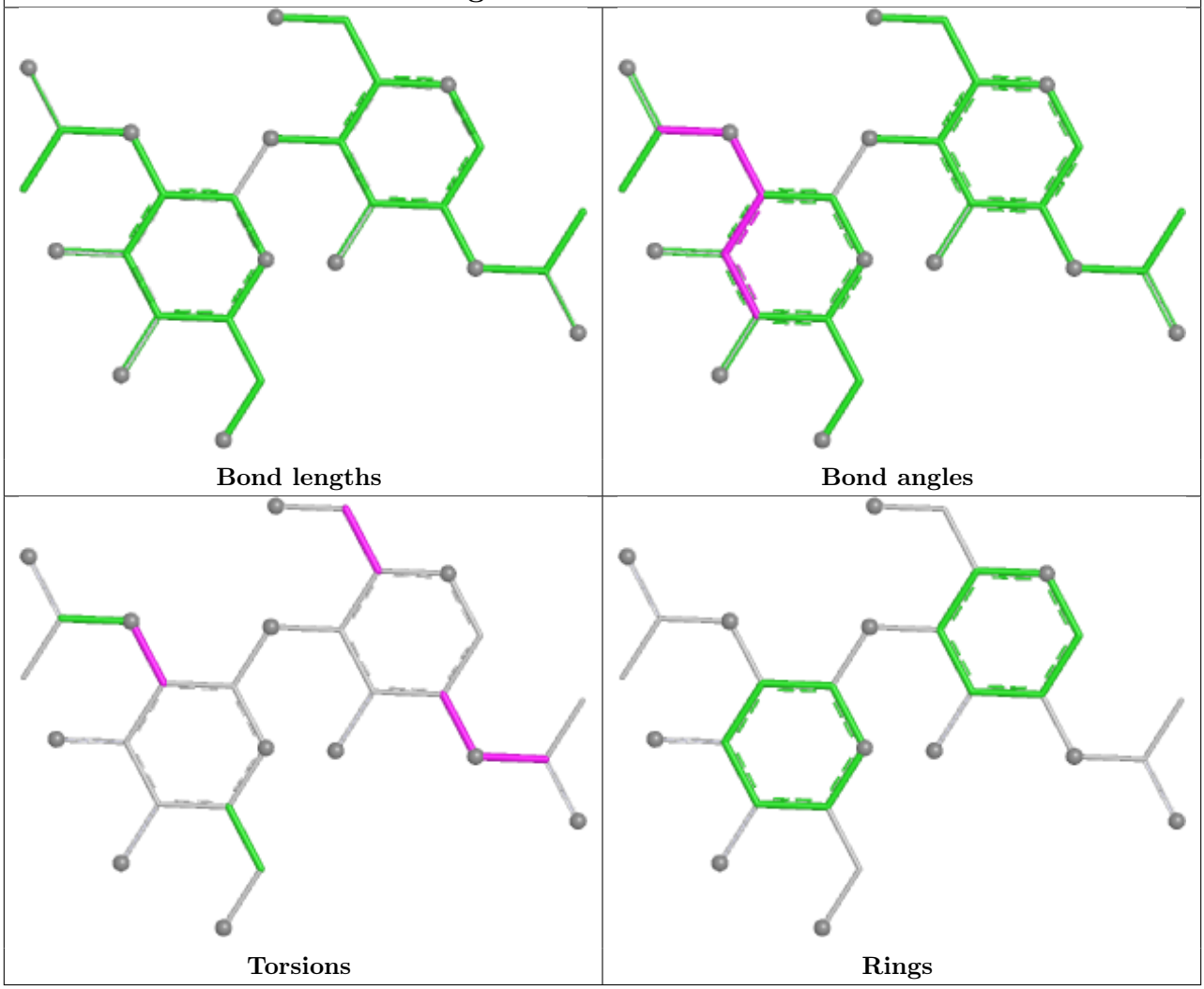


Torsions

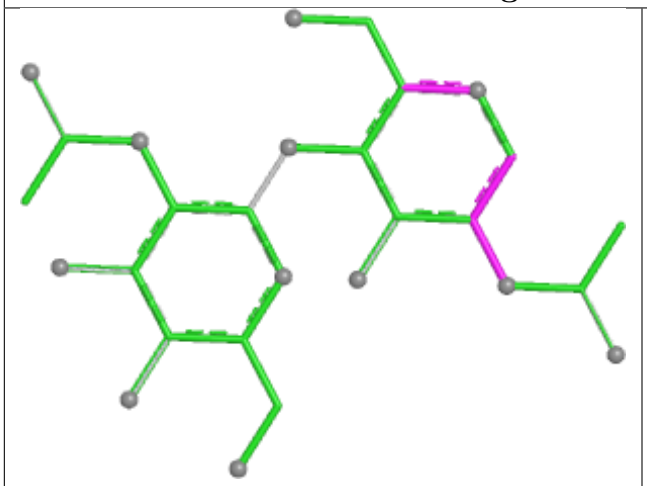


Rings

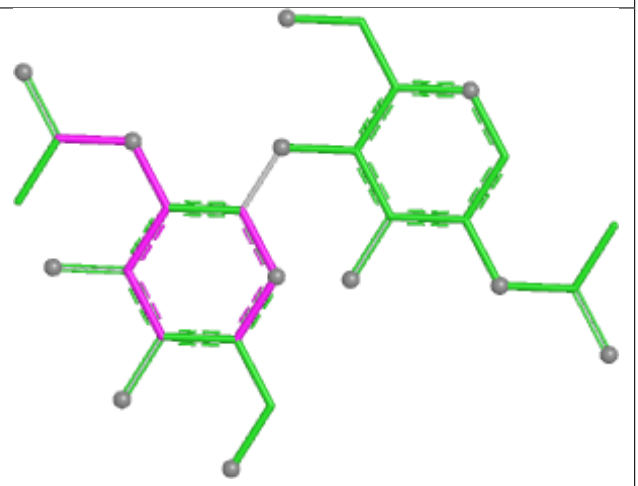
Oligosaccharide Chain b



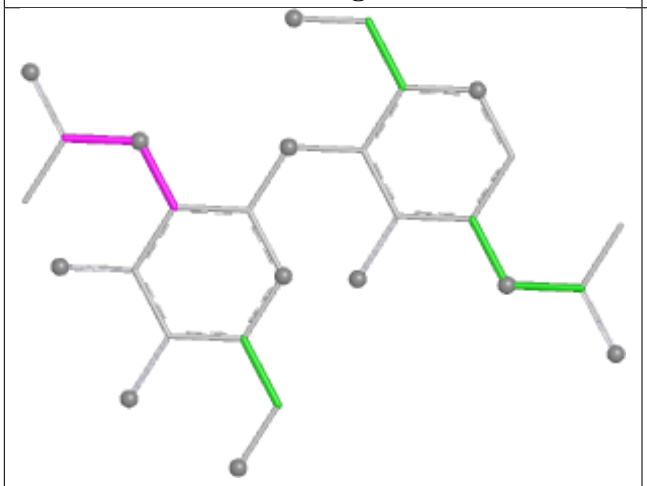
Oligosaccharide Chain c



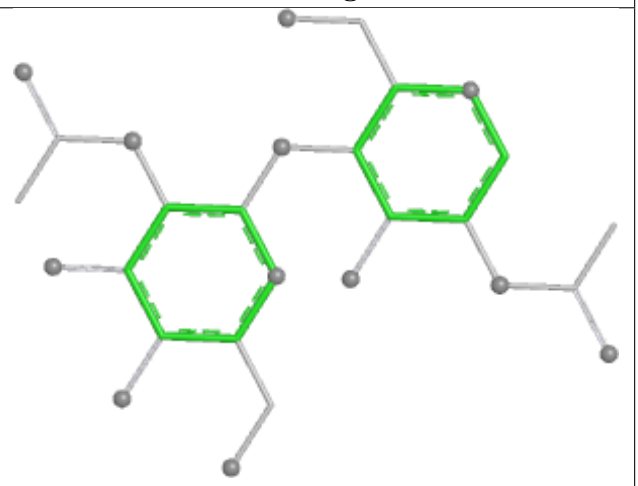
Bond lengths



Bond angles

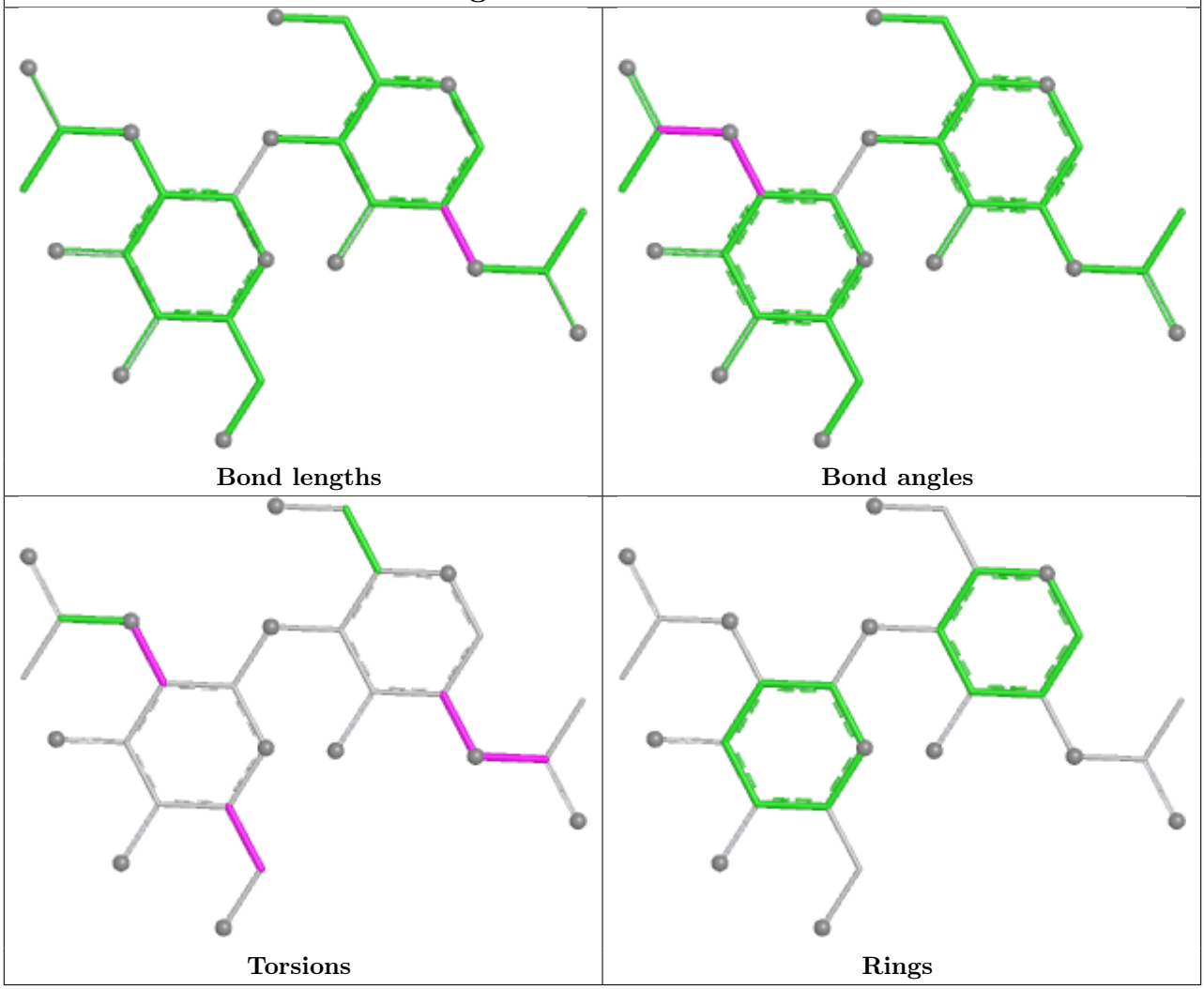


Torsions



Rings

Oligosaccharide Chain e



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
8	NGT	F	26	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	C	530	-	13,15,15	1.45	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	E	530	-	13,15,15	1.39	3 (23%)	14,22,22	0.88	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NGT	A	21	-	13,15,15	1.25	1 (7%)	14,22,22	0.88	1 (7%)
8	NGT	B	22	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	G	533	-	13,15,15	1.34	2 (15%)	14,22,22	0.87	1 (7%)
8	NGT	H	28	-	13,15,15	1.42	4 (30%)	14,22,22	0.88	1 (7%)
8	NGT	D	24	-	13,15,15	1.38	2 (15%)	14,22,22	0.88	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NGT	F	26	-	-	0/2/30/30	0/2/2/2
8	NGT	C	530	-	-	0/2/30/30	0/2/2/2
8	NGT	E	530	-	-	0/2/30/30	0/2/2/2
8	NGT	A	21	-	-	0/2/30/30	0/2/2/2
8	NGT	B	22	-	-	2/2/30/30	0/2/2/2
8	NGT	G	533	-	-	0/2/30/30	0/2/2/2
8	NGT	H	28	-	-	0/2/30/30	0/2/2/2
8	NGT	D	24	-	-	0/2/30/30	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	530	NGT	C3-C2	3.60	1.59	1.53
8	G	533	NGT	C3-C2	3.31	1.59	1.53
8	B	22	NGT	C3-C2	3.22	1.59	1.53
8	A	21	NGT	C3-C2	3.20	1.58	1.53
8	F	26	NGT	C3-C2	3.15	1.58	1.53
8	E	530	NGT	C3-C2	3.05	1.58	1.53
8	D	24	NGT	C3-C2	2.96	1.58	1.53
8	H	28	NGT	C3-C2	2.90	1.58	1.53
8	D	24	NGT	C2-N2	-2.70	1.45	1.47
8	F	26	NGT	C2-N2	-2.45	1.45	1.47
8	B	22	NGT	C2-N2	-2.41	1.45	1.47
8	C	530	NGT	C2-N2	-2.40	1.45	1.47
8	H	28	NGT	O5-C1	-2.39	1.38	1.42
8	E	530	NGT	C7-S1	2.20	1.78	1.77
8	H	28	NGT	C2-N2	-2.14	1.45	1.47
8	G	533	NGT	C2-N2	-2.13	1.45	1.47
8	E	530	NGT	C2-N2	-2.12	1.45	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	28	NGT	C7-S1	2.06	1.78	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	22	NGT	C1-O5-C5	2.36	116.80	112.56
8	C	530	NGT	C1-O5-C5	2.36	116.80	112.56
8	A	21	NGT	C1-O5-C5	2.36	116.79	112.56
8	E	530	NGT	C1-O5-C5	2.35	116.77	112.56
8	F	26	NGT	C1-O5-C5	2.35	116.77	112.56
8	H	28	NGT	C1-O5-C5	2.35	116.77	112.56
8	G	533	NGT	C1-O5-C5	2.34	116.76	112.56
8	D	24	NGT	C1-O5-C5	2.34	116.76	112.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	22	NGT	C4-C5-C6-O6
8	B	22	NGT	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	26	NGT	2	0
8	C	530	NGT	12	0
8	E	530	NGT	6	0
8	A	21	NGT	6	0
8	B	22	NGT	3	0
8	G	533	NGT	8	0
8	H	28	NGT	6	0
8	D	24	NGT	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	52/52 (100%)	0.19	0	100	100	31, 56, 60, 63	0
1	C	52/52 (100%)	0.11	1 (1%)	66	64	31, 55, 62, 62	0
1	E	52/52 (100%)	0.43	5 (9%)	8	8	32, 54, 57, 59	0
1	G	52/52 (100%)	0.30	2 (3%)	40	37	31, 54, 59, 60	0
2	I	440/440 (100%)	0.34	9 (2%)	65	63	41, 53, 60, 66	0
2	J	440/440 (100%)	0.35	20 (4%)	33	31	42, 57, 62, 66	0
2	K	440/440 (100%)	0.68	49 (11%)	5	5	43, 57, 62, 64	0
2	L	440/440 (100%)	0.80	62 (14%)	2	2	42, 56, 60, 61	0
3	B	54/58 (93%)	0.18	1 (1%)	66	64	50, 58, 60, 60	0
3	D	54/58 (93%)	0.31	1 (1%)	66	64	51, 57, 59, 60	0
3	F	54/58 (93%)	1.02	12 (22%)	0	1	57, 60, 62, 63	0
3	H	54/58 (93%)	1.74	16 (29%)	0	0	56, 58, 60, 61	0
4	M	190/190 (100%)	0.54	11 (5%)	23	22	48, 55, 59, 63	0
4	O	189/190 (99%)	0.43	8 (4%)	36	33	28, 54, 57, 60	0
4	Q	190/190 (100%)	0.88	28 (14%)	2	2	54, 57, 61, 63	0
4	S	190/190 (100%)	1.00	31 (16%)	1	2	50, 56, 59, 61	0
5	N	236/237 (99%)	0.36	9 (3%)	40	37	21, 56, 60, 62	0
5	P	236/237 (99%)	0.44	9 (3%)	40	37	21, 57, 61, 62	0
5	R	236/237 (99%)	0.80	27 (11%)	5	5	21, 59, 63, 64	0
5	T	236/237 (99%)	1.59	75 (31%)	0	0	21, 57, 58, 59	0
All	All	3887/3908 (99%)	0.64	376 (9%)	7	8	21, 56, 61, 66	0

All (376) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	107	GLY	10.3
2	L	279	SER	9.2
3	H	54	PRO	7.3
5	T	480	LEU	6.7
5	T	483	GLY	6.5
5	T	484	GLY	6.4
5	R	362	GLU	6.3
5	R	548	ALA	6.0
2	L	327	THR	6.0
5	T	482	ILE	5.8
3	F	67	PRO	5.8
2	K	344	PHE	5.5
5	T	552	ASN	5.4
2	L	382	LYS	5.4
5	R	479	GLN	5.3
2	L	328	CYS	5.3
3	F	68	ASN	5.3
4	Q	122	THR	5.3
4	Q	311	SER	5.1
2	L	280	GLY	5.0
3	H	106	PHE	5.0
3	H	90	SER	4.9
5	T	380	PHE	4.8
4	S	122	THR	4.8
5	T	361	TRP	4.7
4	Q	140	PHE	4.7
3	H	84	ASN	4.6
2	K	367	GLY	4.6
2	K	115	ASN	4.6
5	R	399	ASN	4.4
4	M	204	GLY	4.4
2	L	331	SER	4.4
5	T	418	GLY	4.4
2	K	89	THR	4.3
5	T	397	THR	4.3
4	Q	154	LYS	4.3
2	L	396	ILE	4.3
2	L	362	ILE	4.3
5	P	317	ASP	4.2
5	T	409	PHE	4.2
4	S	135	SER	4.2
5	T	383	LEU	4.2
5	R	542	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	107	LEU	4.1
4	Q	181	GLN	4.1
5	R	325	THR	4.1
4	S	193	THR	4.0
4	S	250	THR	4.0
2	L	347	ASP	4.0
3	H	85	SER	3.9
4	S	136	GLU	3.9
2	L	349	LYS	3.8
5	T	402	SER	3.8
2	K	489	LEU	3.8
4	Q	204	GLY	3.8
5	T	479	GLN	3.7
2	L	180	TYR	3.7
5	T	507	SER	3.7
2	L	344	PHE	3.7
3	F	69	LEU	3.7
5	T	356	VAL	3.6
5	T	317	ASP	3.6
5	T	411	ASP	3.6
5	T	547	TYR	3.6
5	P	382	LYS	3.6
4	S	137	CYS	3.6
2	L	303	THR	3.6
2	J	344	PHE	3.6
5	T	542	ALA	3.6
1	C	43	ASN	3.5
5	T	379	ASP	3.5
4	S	140	PHE	3.5
2	L	381	VAL	3.5
2	L	395	ASP	3.5
5	T	370	PHE	3.5
4	S	288	GLU	3.5
5	T	436	VAL	3.4
2	K	98	SER	3.4
4	S	235	HIS	3.4
4	S	175	PHE	3.4
5	T	350	HIS	3.4
5	T	472	GLY	3.4
5	R	552	ASN	3.4
1	E	43	ASN	3.4
4	S	134	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
4	Q	303	LYS	3.4
5	N	412	LYS	3.4
2	K	293	SER	3.3
3	H	62	SER	3.3
2	K	113	VAL	3.3
3	H	86	THR	3.3
4	Q	184	TYR	3.3
5	T	398	ILE	3.3
5	T	328	THR	3.3
4	S	138	ASP	3.3
5	R	379	ASP	3.3
4	S	188	THR	3.3
5	N	325	THR	3.3
5	T	474	THR	3.3
2	K	285	GLY	3.3
4	S	146	ASP	3.3
3	F	66	THR	3.2
2	I	258	ASP	3.2
3	H	69	LEU	3.2
3	H	83	PRO	3.2
2	K	270	ILE	3.2
2	K	130	GLU	3.2
2	L	285	GLY	3.2
5	T	417	PRO	3.2
5	T	471	PHE	3.2
5	R	530	THR	3.2
5	T	372	ARG	3.2
5	T	429	TYR	3.2
2	J	284	SER	3.2
2	L	284	SER	3.2
2	K	444	GLY	3.2
5	T	468	PRO	3.2
3	H	91	CYS	3.2
2	K	338	PHE	3.2
5	T	546	LEU	3.1
2	L	293	SER	3.1
4	S	132	THR	3.1
4	Q	130	SER	3.1
5	T	460	TRP	3.1
2	L	384	GLN	3.1
4	Q	182	ASP	3.1
5	T	386	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	43	ASN	3.1
3	H	68	ASN	3.1
5	T	345	PRO	3.0
2	K	350	GLN	3.0
4	Q	183	SER	3.0
5	R	382	LYS	3.0
2	L	281	SER	3.0
5	R	551	CYS	3.0
2	K	396	ILE	3.0
5	T	387	TYR	3.0
2	K	287	PHE	3.0
2	J	89	THR	3.0
2	K	369	GLY	3.0
2	L	259	THR	3.0
2	L	348	PHE	3.0
5	T	373	GLN	3.0
5	N	411	ASP	3.0
5	T	325	THR	3.0
2	K	162	GLU	3.0
2	K	101	THR	3.0
5	T	374	LYS	3.0
4	S	156	PRO	3.0
4	Q	305	LEU	2.9
2	L	228	ASN	2.9
5	T	357	GLU	2.9
2	L	363	VAL	2.9
4	O	235	HIS	2.9
5	T	541	ILE	2.9
2	J	346	GLU	2.9
5	R	527	ASP	2.9
5	R	402	SER	2.9
5	R	445	LEU	2.9
2	K	271	PRO	2.9
5	T	524	ASP	2.9
2	L	353	SER	2.9
4	S	148	SER	2.9
5	P	426	ASP	2.9
2	I	458	CYS	2.9
5	T	355	GLU	2.8
5	T	443	VAL	2.8
4	Q	290	ASP	2.8
3	F	83	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	385	PRO	2.8
3	F	82	SER	2.8
2	L	379	ASN	2.8
5	R	526	TYR	2.8
2	K	347	ASP	2.8
2	L	258	ASP	2.8
2	L	412	PHE	2.8
2	J	285	GLY	2.8
4	Q	153	VAL	2.8
4	Q	226	MET	2.7
4	Q	158	ALA	2.7
2	L	330	LYS	2.7
2	L	282	GLU	2.7
5	P	428	ALA	2.7
5	T	342	GLU	2.7
5	T	450	TYR	2.7
5	T	464	TYR	2.7
5	T	412	LYS	2.7
2	L	314	ASP	2.6
5	T	516	SER	2.6
2	L	286	THR	2.6
2	L	343	GLY	2.6
5	T	378	THR	2.6
4	S	187	PHE	2.6
4	Q	132	THR	2.6
5	T	477	GLN	2.6
2	L	295	ASN	2.6
5	T	394	ILE	2.6
2	I	320	GLY	2.6
4	S	125	GLN	2.6
4	M	229	ASN	2.6
2	L	89	THR	2.6
4	S	133	LEU	2.6
2	K	443	GLU	2.6
3	H	102	HIS	2.6
4	M	311	SER	2.6
5	R	376	PHE	2.6
2	L	256	GLU	2.6
2	K	213	TYR	2.6
5	T	438	ALA	2.6
2	K	276	PRO	2.6
2	L	393	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
4	O	287	PRO	2.6
5	T	487	CYS	2.6
2	I	204	HIS	2.6
1	G	45	GLN	2.5
2	K	225	GLY	2.5
1	E	29	ASN	2.5
5	P	325	THR	2.5
5	T	360	CYS	2.5
5	R	326	LEU	2.5
4	Q	156	PRO	2.5
2	L	264	LEU	2.5
2	I	256	GLU	2.5
1	E	50	VAL	2.5
3	H	87	ALA	2.5
4	M	232	ASN	2.5
4	S	229	ASN	2.5
2	J	446	PRO	2.5
4	Q	135	SER	2.5
5	R	475	GLN	2.5
4	S	231	PHE	2.5
2	L	387	THR	2.5
2	L	229	PRO	2.5
5	N	527	ASP	2.5
1	E	73	PHE	2.5
2	K	267	GLY	2.4
4	O	288	GLU	2.4
4	S	189	ILE	2.4
2	K	211	PHE	2.4
2	K	234	TYR	2.4
2	K	354	PHE	2.4
5	N	552	ASN	2.4
5	T	382	LYS	2.4
5	T	481	PHE	2.4
2	L	268	PRO	2.4
2	K	345	GLY	2.4
5	T	419	THR	2.4
2	L	383	ILE	2.4
2	K	99	VAL	2.4
5	P	378	THR	2.4
4	Q	304	ASP	2.4
4	M	170	ARG	2.4
5	T	421	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	240	LYS	2.4
5	R	523	ASP	2.4
2	J	524	GLN	2.4
5	T	347	GLN	2.4
2	L	123	ASP	2.4
2	L	386	ASP	2.4
5	R	518	ASP	2.4
5	R	513	LEU	2.4
4	Q	192	SER	2.4
2	J	458	CYS	2.4
2	L	528	GLN	2.3
2	K	330	LYS	2.3
5	T	366	LYS	2.3
4	S	290	ASP	2.3
5	T	475	GLN	2.3
4	M	237	HIS	2.3
2	K	181	LEU	2.3
4	M	195	ILE	2.3
2	I	171	GLY	2.3
5	T	540	GLY	2.3
5	P	362	GLU	2.3
4	S	144	SER	2.3
5	P	473	GLY	2.3
2	L	106	GLN	2.3
2	L	468	ASN	2.3
3	F	106	PHE	2.3
5	N	487	CYS	2.3
4	Q	141	PRO	2.3
3	H	88	GLY	2.3
5	T	469	LEU	2.3
2	K	521	PHE	2.3
4	Q	233	VAL	2.3
5	T	543	ALA	2.3
2	K	281	SER	2.3
4	Q	310	TYR	2.3
5	T	428	ALA	2.3
2	J	299	GLU	2.2
2	J	286	THR	2.2
2	J	409	LYS	2.2
1	E	51	SER	2.2
5	T	449	TRP	2.2
5	T	399	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	139	ALA	2.2
5	P	472	GLY	2.2
2	L	93	ASN	2.2
5	R	370	PHE	2.2
2	J	256	GLU	2.2
2	K	272	GLY	2.2
2	L	255	ALA	2.2
2	K	290	VAL	2.2
3	F	58	PRO	2.2
3	H	89	PRO	2.2
5	N	486	ALA	2.2
2	K	294	LEU	2.2
4	O	237	HIS	2.2
4	Q	236	TRP	2.2
2	L	397	PRO	2.2
2	L	319	LEU	2.2
5	T	367	ILE	2.2
5	N	484	GLY	2.2
2	J	258	ASP	2.2
2	K	279	SER	2.2
2	J	204	HIS	2.2
2	I	255	ALA	2.2
5	T	435	ARG	2.2
3	F	107	GLY	2.2
4	M	235	HIS	2.2
2	L	370	TYR	2.2
4	M	133	LEU	2.2
4	S	139	ALA	2.2
4	S	197	SER	2.2
2	K	299	GLU	2.2
5	T	369	ASP	2.2
5	T	403	ILE	2.2
4	Q	137	CYS	2.1
3	F	76	ASN	2.1
2	J	457	ALA	2.1
5	R	547	TYR	2.1
2	J	202	HIS	2.1
2	J	338	PHE	2.1
2	K	327	THR	2.1
2	K	368	LYS	2.1
2	L	350	GLN	2.1
2	K	269	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	185	GLY	2.1
2	K	315	PHE	2.1
3	B	86	THR	2.1
4	O	132	THR	2.1
4	O	291	THR	2.1
2	J	318	HIS	2.1
2	L	466	ASN	2.1
5	T	499	THR	2.1
2	L	269	GLY	2.1
4	M	184	TYR	2.1
2	K	524	GLN	2.1
3	F	65	MET	2.1
4	O	122	THR	2.1
2	K	335	ILE	2.1
2	I	93	ASN	2.1
2	J	348	PHE	2.1
2	L	312	PHE	2.1
4	S	195	ILE	2.1
5	N	372	ARG	2.1
5	R	375	GLY	2.1
4	S	308	PRO	2.1
5	R	531	ARG	2.1
2	K	346	GLU	2.1
5	T	517	LYS	2.1
2	L	452	VAL	2.1
5	R	506	ALA	2.1
4	M	171	GLY	2.1
4	O	231	PHE	2.0
4	S	307	THR	2.0
2	L	321	GLY	2.0
3	D	107	GLY	2.0
2	I	455	GLY	2.0
4	S	158	ALA	2.0
5	R	366	LYS	2.0
2	L	277	CYS	2.0
2	K	97	VAL	2.0
2	L	304	PHE	2.0
3	F	77	PHE	2.0
2	L	102	PRO	2.0

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

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

6.3 Carbohydrates (i)

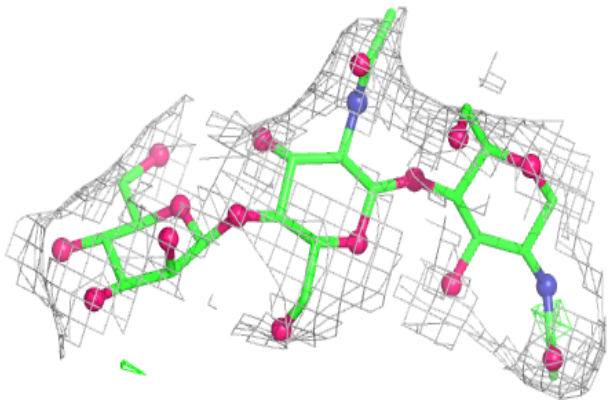
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

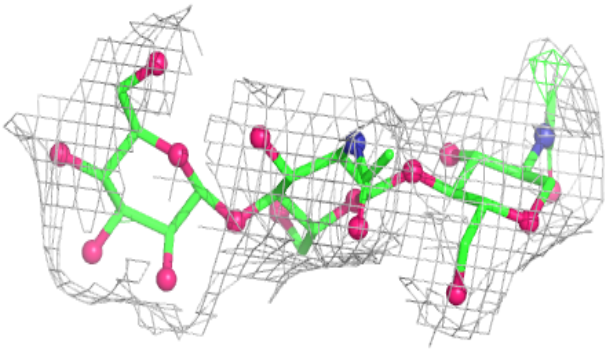
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	a	2	14/15	0.50	0.46	73,76,78,79	0
7	NAG	c	2	14/15	0.64	0.46	72,75,76,76	0
6	BMA	Y	3	11/12	0.65	0.41	46,49,51,51	0
7	NAG	X	2	14/15	0.67	0.48	65,68,69,69	0
6	NAG	Y	2	14/15	0.71	0.32	55,59,63,63	0
7	NAG	X	1	14/15	0.72	0.43	51,56,60,62	0
7	NAG	Z	1	14/15	0.74	0.33	60,62,67,67	0
7	NAG	b	2	14/15	0.75	0.38	73,76,77,77	0
7	NAG	b	1	14/15	0.77	0.32	61,62,62,66	0
7	NAG	c	1	14/15	0.80	0.55	59,60,63,65	0
7	NAG	a	1	14/15	0.80	0.31	58,59,62,64	0
6	NAG	V	2	14/15	0.81	0.45	61,66,71,71	0
7	NAG	e	1	14/15	0.81	0.26	61,62,63,66	0
6	BMA	V	3	11/12	0.82	0.26	52,53,55,56	0
6	NAG	W	2	14/15	0.82	0.34	61,66,68,68	0
6	BMA	W	3	11/12	0.82	0.18	48,54,56,57	0
7	NAG	e	2	14/15	0.82	0.27	73,76,76,76	0
6	NAG	Y	1	14/15	0.83	0.21	45,47,48,51	0
6	NAG	W	1	14/15	0.83	0.30	47,50,53,56	0
6	NAG	d	2	14/15	0.84	0.35	57,63,64,65	0
6	BMA	d	3	11/12	0.85	0.20	48,48,50,52	0
6	NAG	U	1	14/15	0.86	0.21	45,47,50,51	0
7	NAG	Z	2	14/15	0.86	0.46	74,76,78,78	0
6	NAG	V	1	14/15	0.87	0.24	54,55,58,60	0
6	BMA	U	3	11/12	0.88	0.29	50,52,54,55	0
6	NAG	U	2	14/15	0.91	0.31	58,61,63,63	0
6	NAG	d	1	14/15	0.91	0.16	52,54,57,58	0

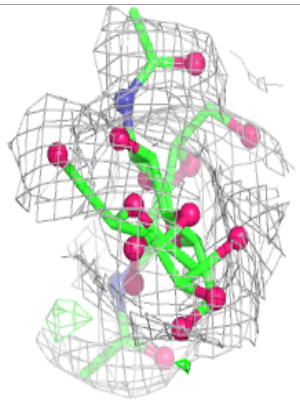
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

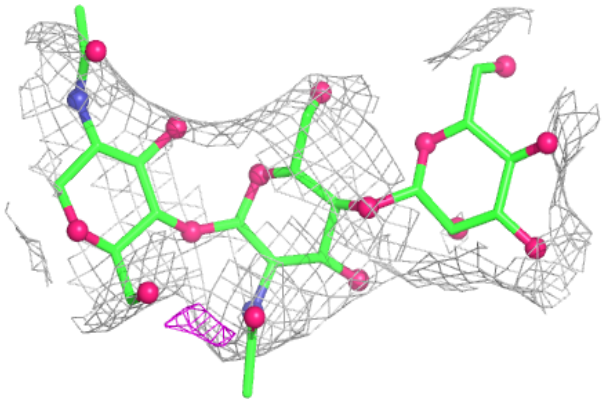


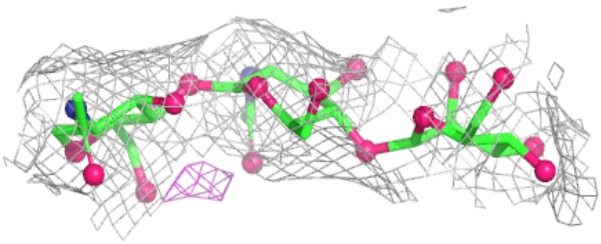


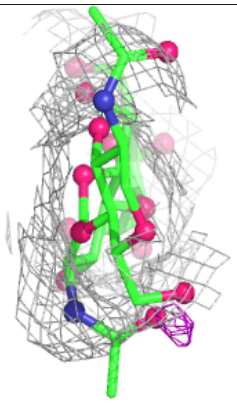


Electron density around Chain V:

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

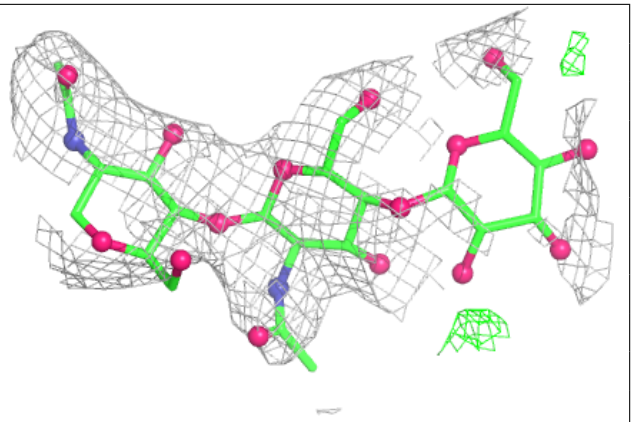


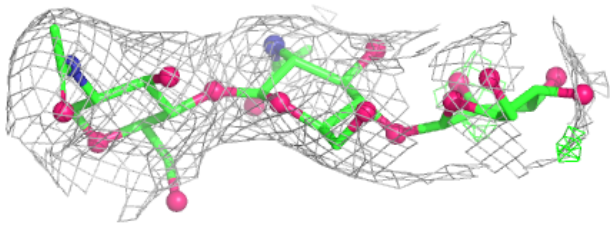


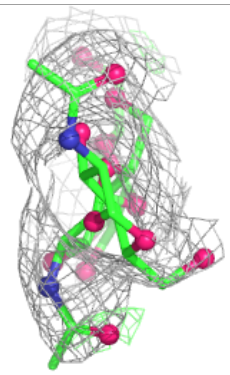


Electron density around Chain W:

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

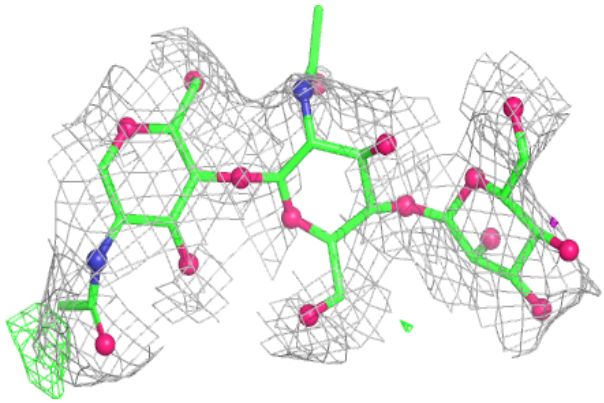


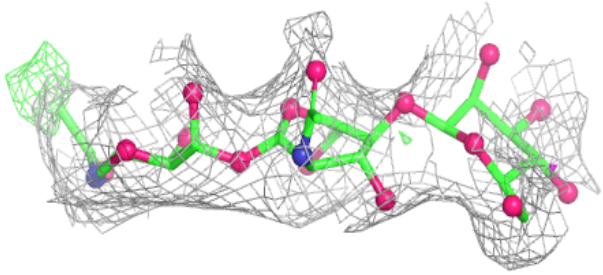


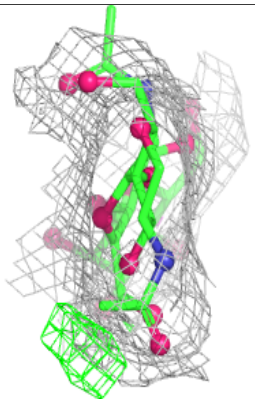


Electron density around Chain Y:

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

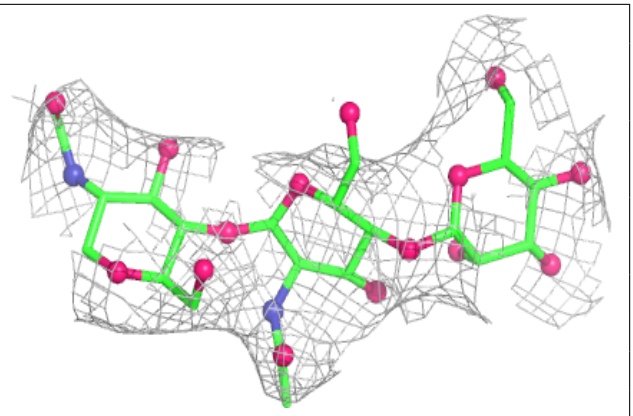


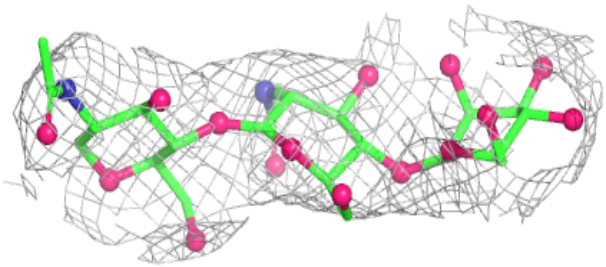


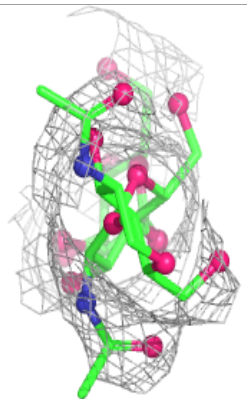


Electron density around Chain d:

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

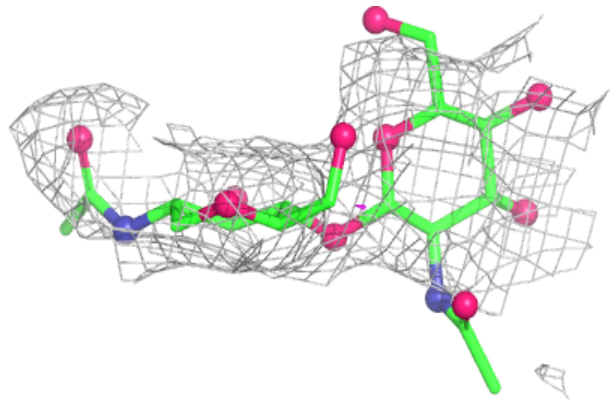


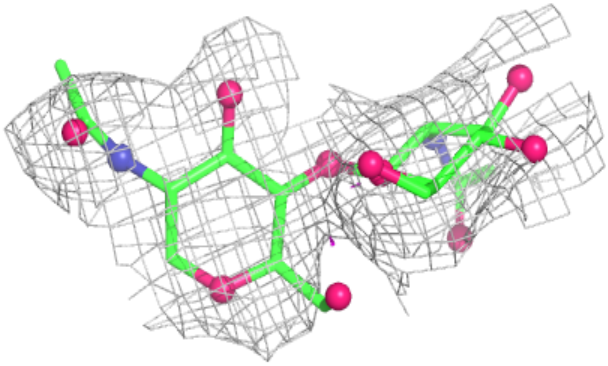


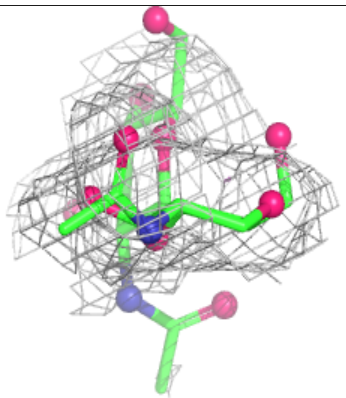


Electron density around Chain X:

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

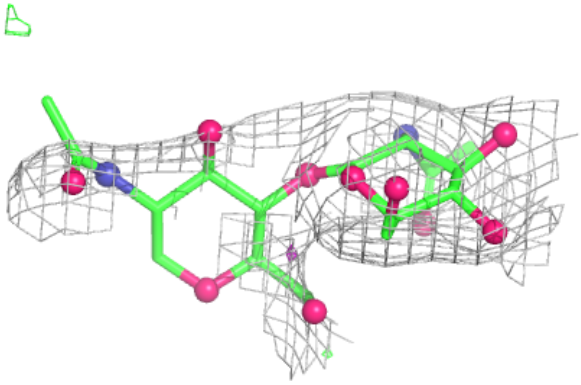


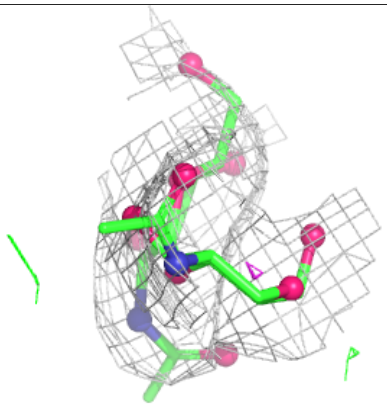




Electron density around Chain Z:

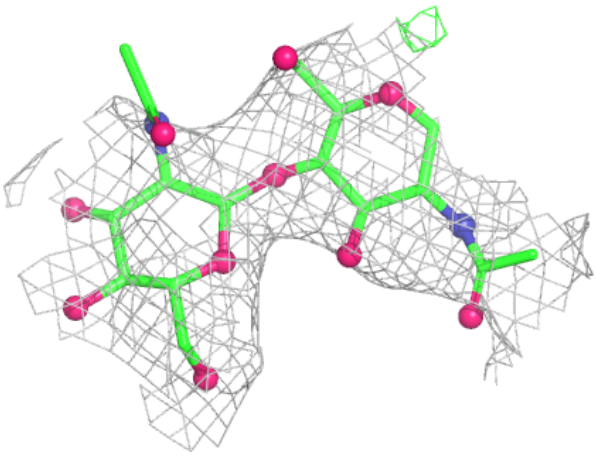
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

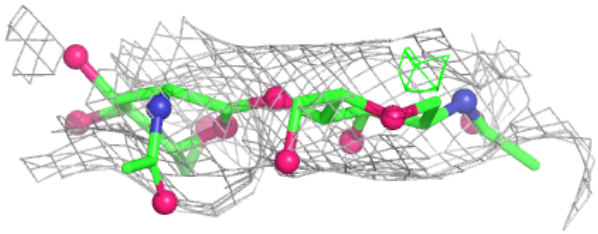


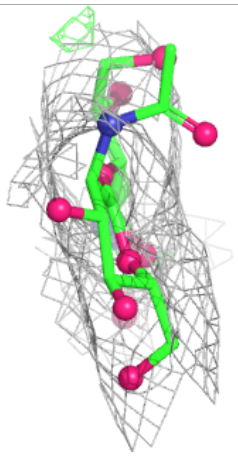


Electron density around Chain a:

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

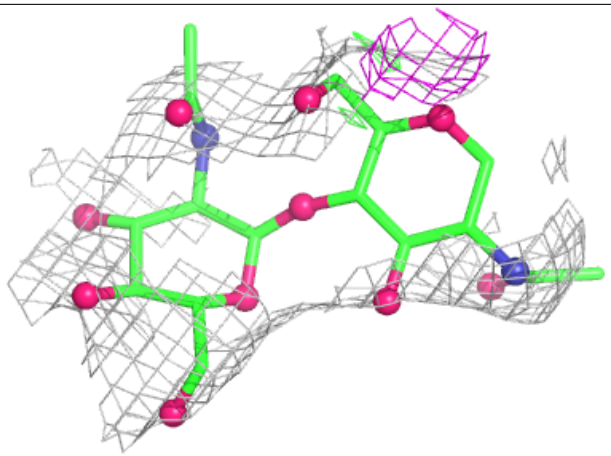


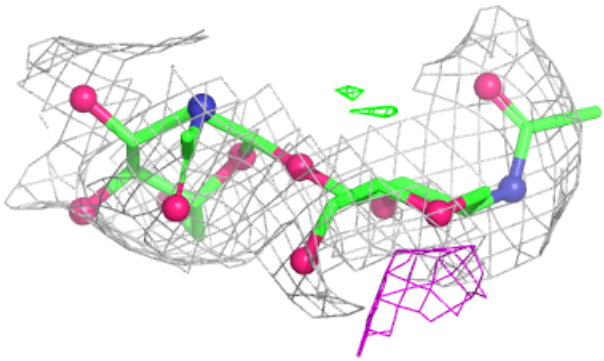


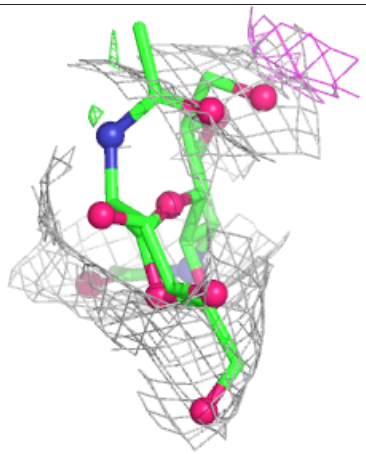


Electron density around Chain b:

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

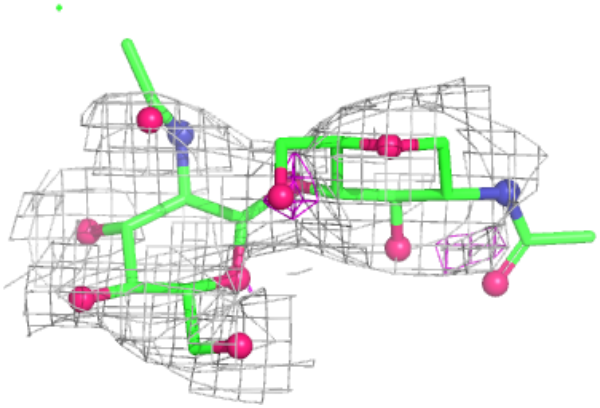


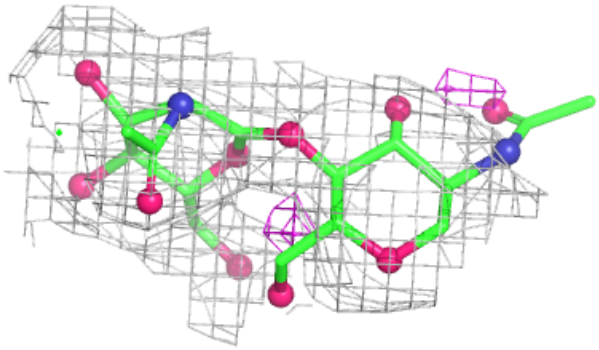


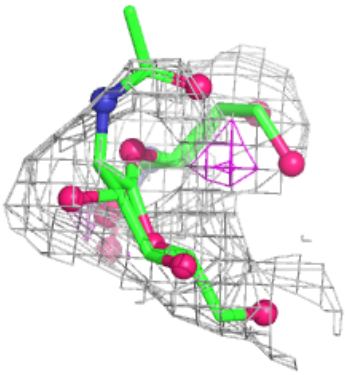


Electron density around Chain c:

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

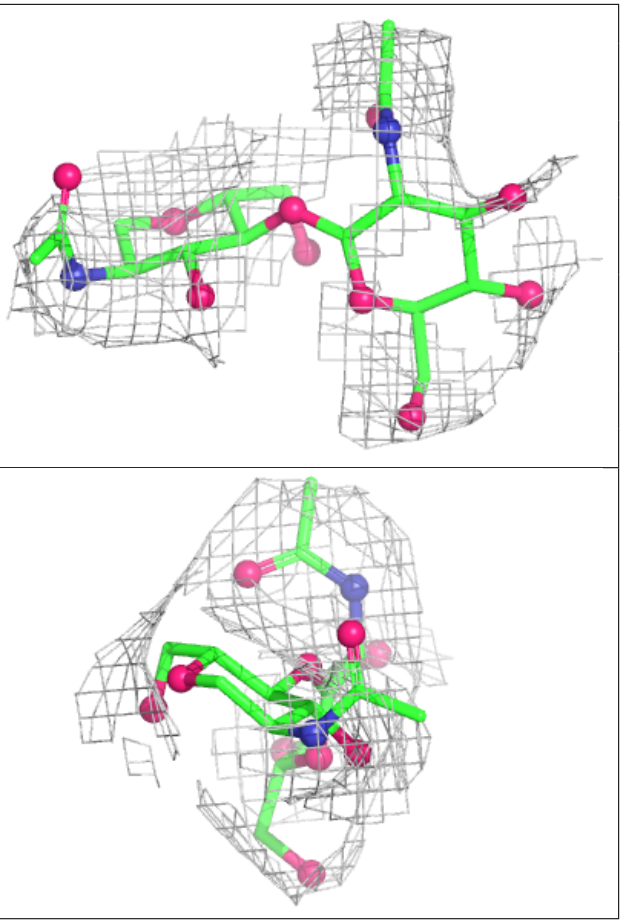






Electron density around Chain e:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NGT	H	28	14/14	0.73	0.33	48,50,53,54	0
8	NGT	G	533	14/14	0.75	0.35	47,47,49,50	0
8	NGT	E	530	14/14	0.77	0.25	47,49,52,53	0
8	NGT	C	530	14/14	0.81	0.25	44,46,49,50	0
8	NGT	F	26	14/14	0.85	0.23	40,41,42,43	0
8	NGT	B	22	14/14	0.90	0.23	38,39,41,44	0
8	NGT	D	24	14/14	0.93	0.18	39,41,43,43	0
8	NGT	A	21	14/14	0.94	0.17	33,35,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.