Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 01:34 PM EST

PDB ID	:	6PDX
Title	:	Crystal structure of C585 Fab in complex with influenza virus hemagglutinin from A/Switzerland/9715293/2013 (H3N2)
Authors	:	Qiu, Y.; Zhou, Y.
Deposited on	:	2019-06-19
Resolution	:	3.99 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

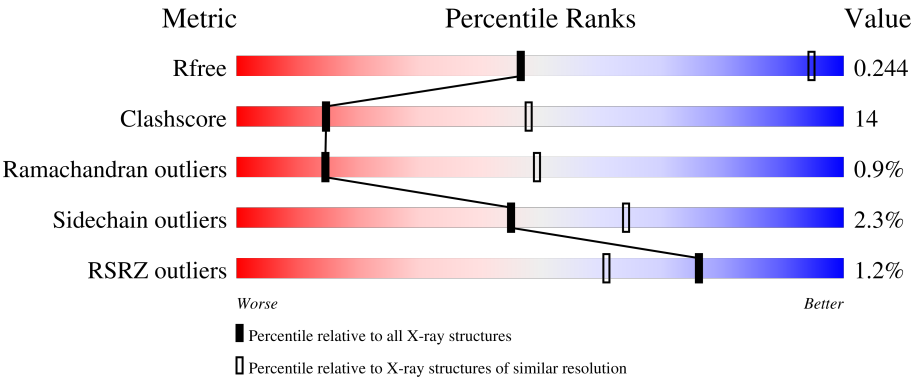
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.99 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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	505	% 75% 21% • •
1	B	505	% 75% 21% • •
1	C	505	75% 21% •
2	H	237	% 69% 22% • 7%
2	M	237	% 72% 19% • 7%

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Mol	Chain	Length	Quality of chain
2	O	237	2% 62% 29% 7%
3	L	215	2% 77% 21%
3	N	215	% 77% 21%
3	P	215	2% 75% 22%
4	D	3	33% 67%
4	E	3	67% 33%
4	G	3	100%
4	I	3	100%
4	J	3	100%
4	K	3	67% 33%
4	Q	3	33% 33% 33%
4	R	3	67% 33%
4	U	3	33% 33% 33%
4	W	3	67% 33%
4	X	3	100%
4	Y	3	67% 33%
4	Z	3	100%
5	F	2	100%
5	S	2	100%
5	T	2	50% 50%
5	V	2	100%
5	a	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	2	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	1	0
			3798	2364	673	742	19			
1	B	488	Total	C	N	O	S	0	0	0
			3684	2290	652	724	18			
1	C	487	Total	C	N	O	S	0	0	0
			3719	2313	651	737	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	SER	-	expression tag	UNP A0A1L3A363
B	505	SER	-	expression tag	UNP A0A1L3A363
C	505	SER	-	expression tag	UNP A0A1L3A363

- Molecule 2 is a protein called C585 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1559	981	265	308	5			
2	M	221	Total	C	N	O	S	0	0	0
			1547	974	261	306	6			
2	O	221	Total	C	N	O	S	0	0	0
			1575	998	263	308	6			

- Molecule 3 is a protein called C585 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1446	902	239	299	6			
3	N	213	Total	C	N	O	S	0	1	0
			1426	897	235	288	6			

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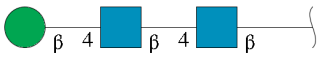
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	214	Total	C	N	O	S	0	0	0
			1481	936	242	298	5			

- Molecule 4 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.

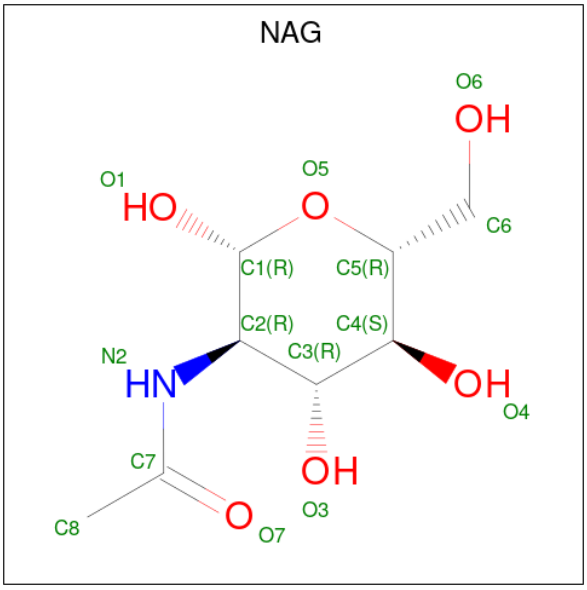


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	F	2	Total C N O 28 16 2 10	0	0	0
5	S	2	Total C N O 28 16 2 10	0	0	0
5	T	2	Total C N O 28 16 2 10	0	0	0
5	V	2	Total C N O 28 16 2 10	0	0	0
5	a	2	Total C N O 28 16 2 10	0	0	0

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



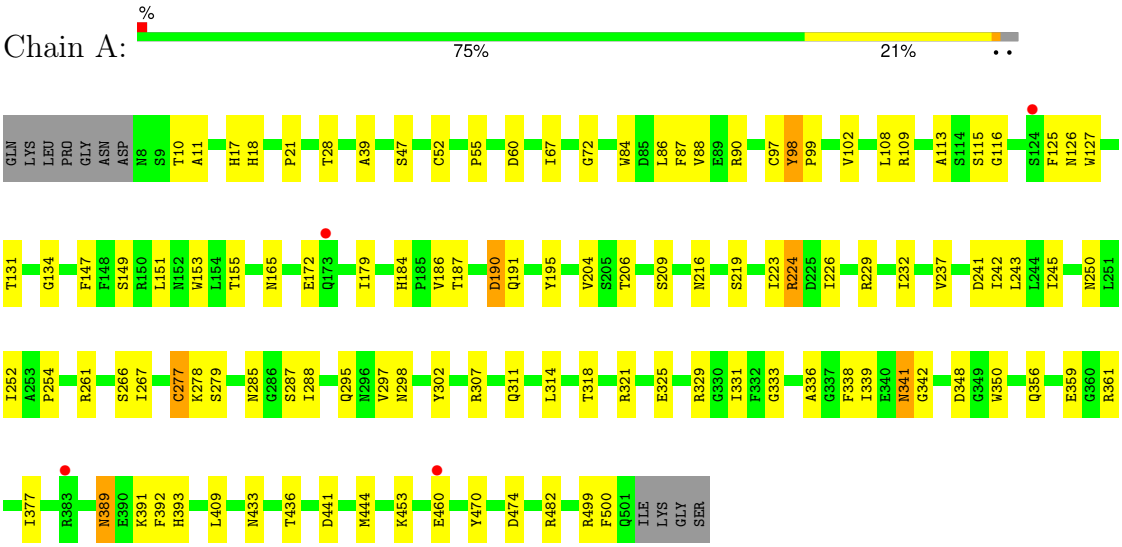
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

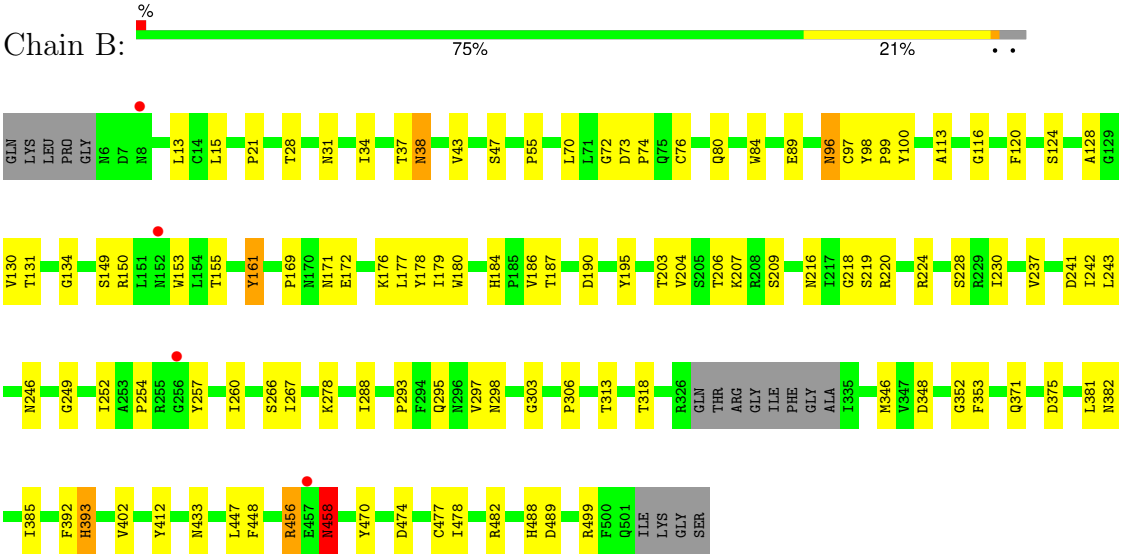
• Molecule 1: Hemagglutinin

Chain A:



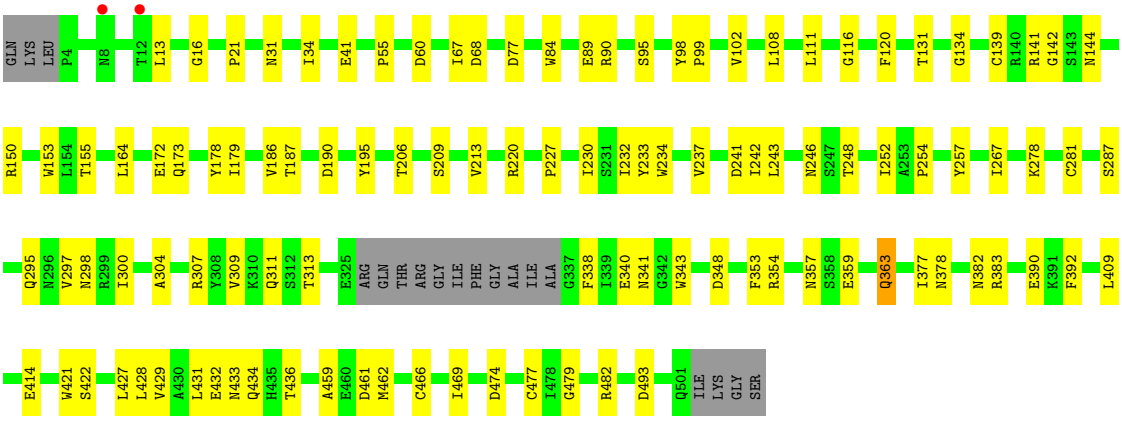
• Molecule 1: Hemagglutinin

Chain B:



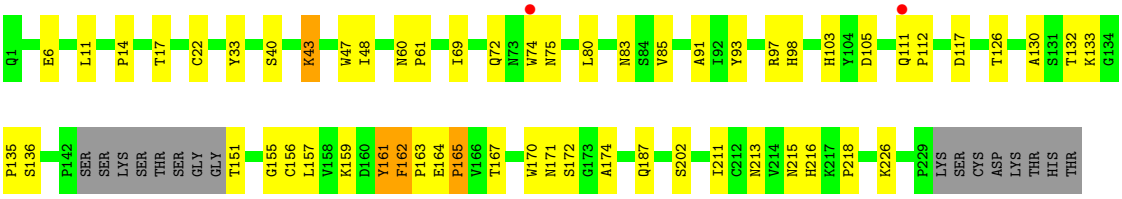
• Molecule 1: Hemagglutinin

Chain C:



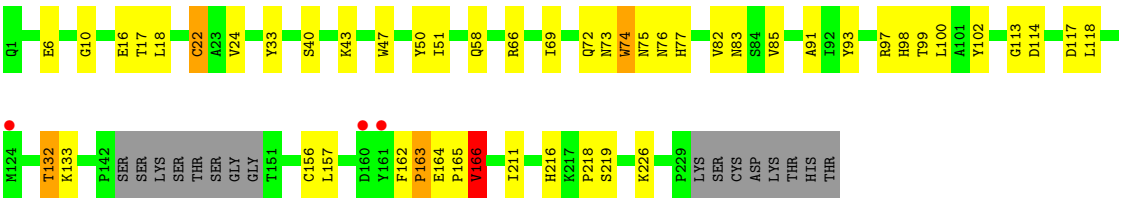
• Molecule 2: C585 Fab heavy chain

Chain H:



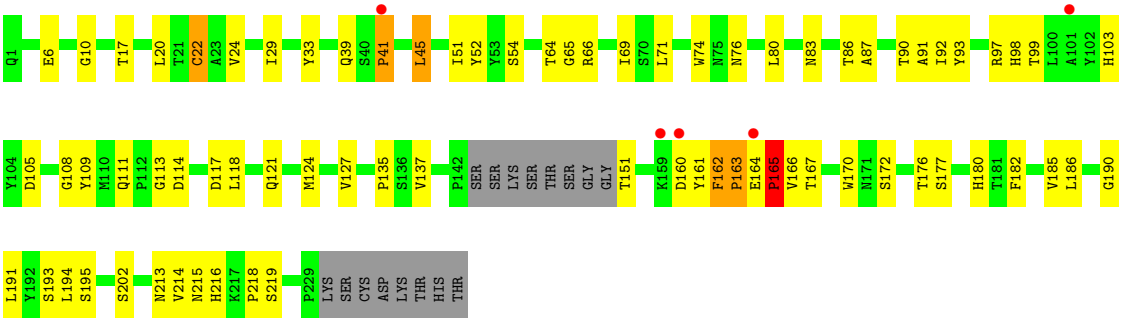
• Molecule 2: C585 Fab heavy chain

Chain M:



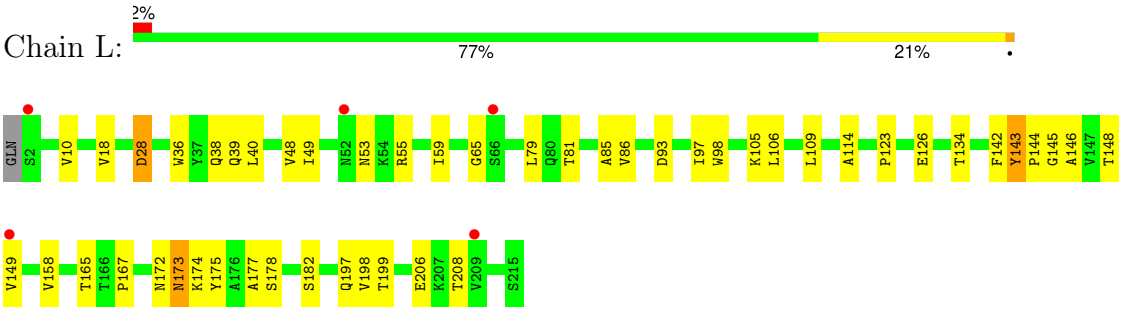
• Molecule 2: C585 Fab heavy chain

Chain O:



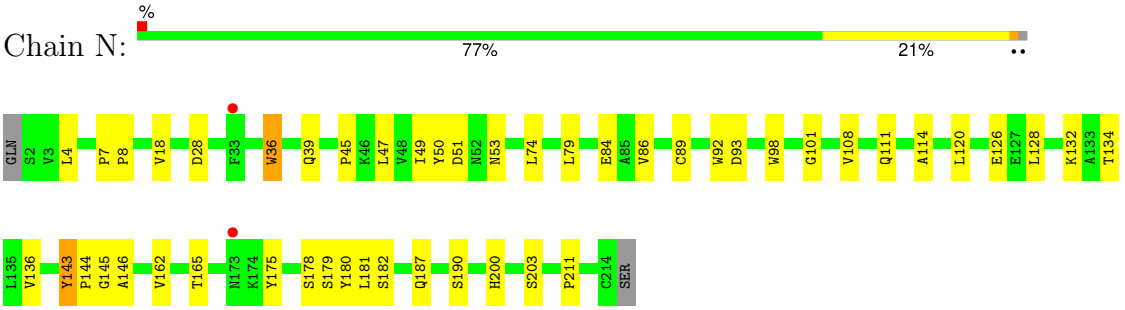
• Molecule 3: C585 Fab light chain

Chain L:



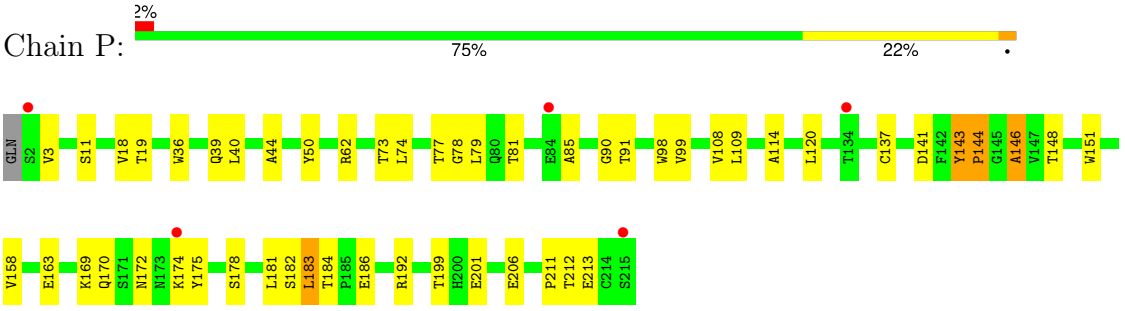
• Molecule 3: C585 Fab light chain

Chain N:



• Molecule 3: C585 Fab light chain

Chain P:



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

Chain D:

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

Chain E:

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

Chain G:

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

Chain I:

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

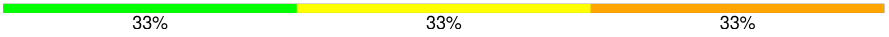
Chain J:

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

Chain K:

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

Chain Q:

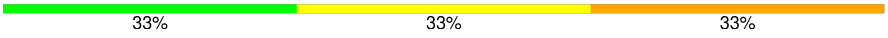


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain U:



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

Chain W:

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

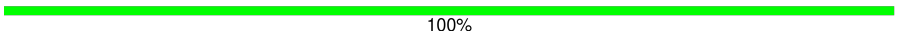
Chain X:

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

Chain Y:

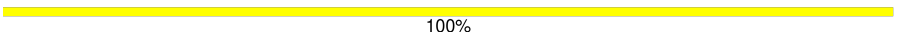
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



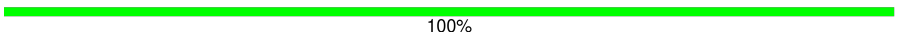
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

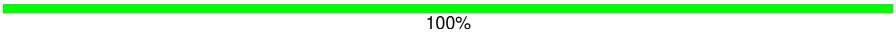
Chain S:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	287.26Å 287.26Å 182.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 3.99 47.88 – 3.99	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.88-3.99) 96.7 (47.88-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.212 , 0.241 0.216 , 0.244	Depositor DCC
R_{free} test set	3625 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	126.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 164.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20896	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/3880	0.47	0/5275
1	B	0.27	0/3761	0.47	1/5126 (0.0%)
1	C	0.27	0/3798	0.47	0/5169
2	H	0.29	0/1602	0.52	0/2210
2	M	0.33	0/1589	0.63	1/2191 (0.0%)
2	O	0.42	0/1619	0.68	5/2231 (0.2%)
3	L	0.30	0/1484	0.50	0/2050
3	N	0.30	0/1465	0.56	0/2027
3	P	0.35	1/1522 (0.1%)	0.59	1/2102 (0.0%)
All	All	0.30	1/20720 (0.0%)	0.53	8/28381 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	144	PRO	N-CD	-5.53	1.40	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	163	PRO	N-CD-CG	-8.25	90.82	103.20
3	P	144	PRO	N-CD-CG	-7.01	92.69	103.20
2	O	162	PHE	CB-CA-C	-6.43	97.54	110.40
2	O	163	PRO	N-CD-CG	-6.13	94.01	103.20
1	B	458	ASN	N-CA-C	5.47	125.78	111.00
2	O	165	PRO	N-CA-CB	-5.32	96.75	102.60
2	O	163	PRO	N-CA-CB	-5.05	97.04	102.60
2	O	41	PRO	N-CA-C	-5.03	99.02	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3560	85	0
1	B	3684	0	3364	74	0
1	C	3719	0	3432	73	0
2	H	1559	0	1379	65	0
2	M	1547	0	1371	45	0
2	O	1575	0	1425	73	0
3	L	1446	0	1255	38	0
3	N	1426	0	1260	46	0
3	P	1481	0	1347	50	0
4	D	39	0	34	9	0
4	E	39	0	34	0	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
4	J	39	0	34	4	0
4	K	39	0	34	1	0
4	Q	39	0	34	2	0
4	R	39	0	34	1	0
4	U	39	0	34	4	0
4	W	39	0	34	2	0
4	X	39	0	34	0	0
4	Y	39	0	34	2	0
4	Z	39	0	34	0	0
5	F	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
5	a	28	0	25	0	0
6	B	14	0	13	0	0
All	All	20896	0	18973	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (545) 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:O:163:PRO:HG3	2:O:216:HIS:CE1	1.13	1.65
2:O:163:PRO:CG	2:O:216:HIS:NE2	1.68	1.53
2:O:163:PRO:CG	2:O:216:HIS:CE1	1.95	1.48
2:O:163:PRO:HG3	2:O:216:HIS:NE2	1.14	1.41
3:N:143:TYR:CD2	3:N:144:PRO:HG3	1.66	1.29
2:H:132:THR:HA	2:H:162:PHE:CD1	1.68	1.28
1:C:429:VAL:O	1:C:433:ASN:ND2	1.68	1.26
3:N:143:TYR:HD2	3:N:144:PRO:CG	1.51	1.23
2:M:163:PRO:HD2	2:M:216:HIS:NE2	1.55	1.20
1:A:131:THR:HB	1:A:155:THR:CG2	1.72	1.18
2:H:163:PRO:HG2	2:H:216:HIS:CE1	1.82	1.15
2:H:163:PRO:HG2	2:H:216:HIS:NE2	1.66	1.09
2:O:163:PRO:HG2	2:O:216:HIS:NE2	1.69	1.08
3:N:143:TYR:HB3	3:N:144:PRO:CD	1.84	1.07
1:A:131:THR:HB	1:A:155:THR:HG22	1.34	1.07
3:N:143:TYR:CB	3:N:144:PRO:HD3	1.82	1.06
3:P:143:TYR:HB3	3:P:144:PRO:HD3	1.42	0.99
2:H:163:PRO:CG	2:H:216:HIS:CE1	2.45	0.99
3:N:143:TYR:HB3	3:N:144:PRO:HD3	0.96	0.96
2:H:162:PHE:HB3	2:H:163:PRO:CD	1.97	0.94
3:P:143:TYR:HD2	3:P:144:PRO:HG3	1.30	0.94
3:N:143:TYR:HD2	3:N:144:PRO:HG3	0.77	0.92
2:O:163:PRO:HG3	2:O:216:HIS:HE1	1.22	0.91
2:H:111:GLN:HB3	2:H:112:PRO:HD2	1.56	0.87
2:H:132:THR:HA	2:H:162:PHE:HD1	1.34	0.87
1:A:131:THR:HB	1:A:155:THR:HG23	1.55	0.86
1:B:456:ARG:NH2	1:B:488:HIS:NE2	2.23	0.85
2:H:132:THR:CA	2:H:162:PHE:CD1	2.57	0.85
2:H:151:THR:N	2:H:202:SER:HG	1.76	0.84
2:O:162:PHE:H	2:O:163:PRO:HD2	1.43	0.84
2:H:74:TRP:CZ3	4:D:2:NAG:H2	2.13	0.83
3:L:199:THR:HA	3:L:206:GLU:HB3	1.61	0.83
1:B:161:TYR:HE2	1:B:249:GLY:HA2	1.44	0.83
2:O:162:PHE:N	2:O:163:PRO:HD2	1.91	0.83
3:N:162:VAL:HG21	3:N:181:LEU:HA	1.61	0.82
3:P:146:ALA:HB1	3:P:201:GLU:CB	2.11	0.81
2:H:74:TRP:CZ3	4:D:2:NAG:H4	2.16	0.80
2:H:74:TRP:CE3	4:D:2:NAG:H2	2.16	0.80
1:C:428:LEU:O	1:C:432:GLU:HB2	1.82	0.80
1:B:206:THR:HG23	1:B:209:SER:H	1.44	0.80
1:B:237:VAL:HG21	1:B:243:LEU:HB2	1.64	0.80
3:N:143:TYR:CD2	3:N:144:PRO:CG	2.43	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:163:PRO:CD	2:M:216:HIS:NE2	2.42	0.79
3:L:143:TYR:HB3	3:L:144:PRO:HD3	1.63	0.79
2:O:163:PRO:CG	2:O:216:HIS:HE1	1.83	0.78
3:P:181:LEU:HG	3:P:183:LEU:HD21	1.66	0.77
3:P:143:TYR:CD2	3:P:144:PRO:HG3	2.17	0.77
2:H:162:PHE:HB3	2:H:163:PRO:HD2	1.66	0.77
1:B:470:TYR:HD2	1:B:499:ARG:HG2	1.49	0.76
2:H:74:TRP:CH2	4:D:2:NAG:H4	2.20	0.76
3:P:169:LYS:HG2	3:P:175:TYR:CE1	2.20	0.76
3:P:91:THR:N	3:P:98:TRP:CZ3	2.53	0.76
1:C:98:TYR:N	1:C:139:CYS:SG	2.58	0.75
3:P:3:VAL:HG22	3:P:99:VAL:HG21	1.68	0.75
3:P:169:LYS:CG	3:P:175:TYR:HE1	1.99	0.75
1:A:499:ARG:CD	1:A:500:PHE:CE1	2.71	0.73
2:H:163:PRO:CG	2:H:216:HIS:NE2	2.45	0.72
2:H:163:PRO:HG2	2:H:216:HIS:HE2	1.52	0.72
3:P:181:LEU:HG	3:P:183:LEU:CD2	2.20	0.71
3:N:143:TYR:CB	3:N:144:PRO:CD	2.52	0.71
2:H:162:PHE:CB	2:H:163:PRO:CD	2.68	0.70
1:B:402:VAL:HG11	1:C:111:LEU:HD13	1.73	0.70
2:H:162:PHE:HB3	2:H:163:PRO:HD3	1.73	0.70
2:M:163:PRO:HD2	2:M:216:HIS:CE1	2.26	0.70
2:O:163:PRO:CB	2:O:216:HIS:NE2	2.54	0.70
1:B:47:SER:HB2	1:B:288:ILE:HG22	1.71	0.70
3:N:143:TYR:O	3:N:175:TYR:CD2	2.45	0.70
1:A:97:CYS:SG	1:A:98:TYR:N	2.65	0.70
1:A:499:ARG:HD2	1:A:500:PHE:CE1	2.26	0.69
1:A:87:PHE:HB3	1:A:267:ILE:HG22	1.73	0.69
2:O:161:TYR:HE2	2:O:194:LEU:H	1.39	0.68
1:B:31:ASN:HD21	1:B:34:ILE:HB	1.59	0.68
1:B:458:ASN:N	1:B:458:ASN:OD1	2.26	0.68
2:O:92:ILE:HG22	2:O:124:MET:HG2	1.75	0.68
4:D:1:NAG:H62	4:D:2:NAG:H83	1.75	0.67
1:A:131:THR:CB	1:A:155:THR:CG2	2.63	0.67
1:B:206:THR:CG2	1:B:209:SER:H	2.08	0.67
1:A:125:PHE:O	1:A:127:TRP:N	2.27	0.66
3:N:143:TYR:CD2	3:N:144:PRO:N	2.63	0.66
2:H:164:GLU:N	2:H:165:PRO:HD2	2.10	0.66
3:L:148:THR:HG23	3:L:199:THR:HB	1.77	0.66
2:O:163:PRO:CD	2:O:216:HIS:CE1	2.77	0.66
3:L:28:ASP:HA	3:L:93:ASP:HA	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:47:LEU:HD21	3:N:50:TYR:HB3	1.77	0.66
1:A:331:ILE:HD13	1:A:331:ILE:N	2.11	0.65
3:N:143:TYR:CD2	3:N:144:PRO:CD	2.78	0.65
2:H:163:PRO:HG3	2:H:216:HIS:CE1	2.33	0.64
1:A:499:ARG:HD2	1:A:500:PHE:CZ	2.33	0.64
3:N:143:TYR:O	3:N:175:TYR:HD2	1.78	0.64
1:C:16:GLY:HA2	1:C:338:PHE:HB3	1.79	0.64
1:A:99:PRO:HB3	1:A:223:ILE:HD11	1.80	0.64
2:H:132:THR:HA	2:H:162:PHE:CG	2.27	0.64
1:A:295:GLN:NE2	1:A:298:ASN:O	2.28	0.64
2:O:10:GLY:HA3	2:O:218:PRO:HB3	1.80	0.64
1:C:295:GLN:NE2	1:C:298:ASN:O	2.28	0.64
3:P:120:LEU:HD13	3:P:211:PRO:HD3	1.79	0.64
1:C:433:ASN:O	1:C:436:THR:N	2.31	0.63
3:P:143:TYR:CB	3:P:144:PRO:HD3	2.18	0.63
2:O:39:GLN:O	2:O:91:ALA:HB1	1.98	0.63
1:A:409:LEU:HD12	1:C:409:LEU:HD21	1.79	0.63
1:B:31:ASN:ND2	1:B:34:ILE:HB	2.12	0.63
1:C:55:PRO:HD3	1:C:278:LYS:HA	1.81	0.63
3:L:18:VAL:HG13	3:L:79:LEU:HD11	1.79	0.63
3:N:36:TRP:CG	3:N:74:LEU:HD12	2.33	0.63
1:C:340:GLU:OE1	1:C:341:ASN:ND2	2.31	0.63
1:A:206:THR:HG23	1:A:209:SER:H	1.64	0.63
2:M:10:GLY:HA3	2:M:218:PRO:HB3	1.81	0.63
2:O:91:ALA:HB3	2:O:93:TYR:HE1	1.64	0.62
1:A:86:LEU:HB2	1:A:302:TYR:HE2	1.64	0.62
2:H:155:GLY:HA2	2:H:170:TRP:HH2	1.63	0.62
3:N:143:TYR:HD2	3:N:144:PRO:CD	2.11	0.62
3:P:169:LYS:HG3	3:P:175:TYR:HE1	1.65	0.62
2:M:216:HIS:HD1	2:M:219:SER:HG	1.45	0.62
2:O:163:PRO:CD	2:O:216:HIS:HE1	2.12	0.62
2:H:133:LYS:H	2:H:162:PHE:HB2	1.65	0.62
1:A:125:PHE:HB2	1:A:127:TRP:CE2	2.33	0.62
1:B:161:TYR:CE2	1:B:249:GLY:HA2	2.32	0.62
2:H:132:THR:HG22	2:H:162:PHE:CE1	2.35	0.62
1:C:429:VAL:C	1:C:433:ASN:ND2	2.51	0.61
2:H:163:PRO:HG3	2:H:216:HIS:HE1	1.65	0.61
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.81	0.61
3:P:40:LEU:HD23	3:P:85:ALA:HB2	1.82	0.61
2:M:74:TRP:CZ2	4:U:2:NAG:H2	2.35	0.61
3:P:169:LYS:CG	3:P:175:TYR:CE1	2.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:163:PRO:CD	2:M:216:HIS:CE1	2.84	0.61
1:C:230:ILE:HD13	1:C:252:ILE:HD13	1.83	0.60
2:H:172:SER:N	2:H:213:ASN:OD1	2.34	0.60
3:N:18:VAL:HG13	3:N:79:LEU:HD11	1.84	0.60
3:P:120:LEU:HD22	3:P:211:PRO:HG3	1.82	0.60
2:H:133:LYS:N	2:H:162:PHE:HB2	2.17	0.60
3:P:170:GLN:HG3	3:P:172:ASN:H	1.67	0.59
3:P:81:THR:HA	3:P:108:VAL:HG21	1.83	0.59
2:H:6:GLU:HG3	2:H:22:CYS:SG	2.42	0.59
1:A:453:LYS:NZ	1:C:461:ASP:OD2	2.34	0.59
4:J:2:NAG:H3	4:J:3:BMA:O5	2.03	0.59
1:B:177:LEU:HB2	1:B:260:ILE:HD11	1.84	0.59
2:M:51:ILE:HB	2:M:69:ILE:HG21	1.85	0.59
1:A:460:GLU:OE1	1:B:456:ARG:NH1	2.36	0.58
2:H:132:THR:CA	2:H:162:PHE:HD1	2.09	0.58
3:N:120:LEU:HD13	3:N:211:PRO:HD3	1.84	0.58
1:A:325:GLU:HA	1:A:341:ASN:HB2	1.85	0.58
1:A:131:THR:CB	1:A:155:THR:HG22	2.23	0.58
2:M:50:TYR:CE1	2:M:58:GLN:HB2	2.38	0.58
2:O:124:MET:SD	2:O:164:GLU:HG2	2.44	0.58
3:N:84:GLU:HG3	3:N:108:VAL:HG12	1.85	0.58
1:A:97:CYS:O	1:A:224:ARG:NH2	2.21	0.58
2:O:166:VAL:O	2:O:166:VAL:HG13	2.02	0.58
1:C:172:GLU:N	1:C:172:GLU:OE1	2.36	0.58
2:O:163:PRO:HG2	2:O:216:HIS:CE1	2.18	0.58
2:H:17:THR:HG22	2:H:83:ASN:HB3	1.84	0.58
1:A:359:GLU:N	1:A:359:GLU:OE1	2.36	0.57
3:N:165:THR:HG22	3:N:178:SER:H	1.69	0.57
3:L:55:ARG:NH1	3:L:59:ILE:O	2.37	0.57
1:C:427:LEU:O	1:C:431:LEU:HB2	2.04	0.57
3:P:192:ARG:O	3:P:212:THR:HG23	2.04	0.57
2:H:163:PRO:HG3	2:H:218:PRO:HB2	1.86	0.57
3:P:11:SER:HB2	3:P:109:LEU:HD11	1.87	0.57
2:H:211:ILE:HA	2:H:226:LYS:HA	1.85	0.57
1:B:15:LEU:HD11	1:B:448:PHE:HD1	1.69	0.57
1:B:70:LEU:HD21	1:B:179:ILE:HG13	1.86	0.57
2:O:51:ILE:HB	2:O:69:ILE:HG21	1.87	0.57
4:K:2:NAG:O7	4:K:2:NAG:O3	2.20	0.57
2:M:18:LEU:HB3	2:M:82:VAL:HG13	1.86	0.56
2:M:166:VAL:HG23	2:M:166:VAL:O	2.05	0.56
3:N:111:GLN:HB2	3:N:143:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:PRO:CD	2:H:216:HIS:HE2	2.17	0.56
3:L:126:GLU:OE1	3:L:126:GLU:N	2.37	0.56
1:A:339:ILE:HD12	1:A:339:ILE:H	1.70	0.56
1:B:89:GLU:HG3	1:B:267:ILE:HD11	1.88	0.56
3:P:143:TYR:HB3	3:P:144:PRO:CD	2.26	0.56
1:A:98:TYR:HD1	1:A:147:PHE:HE1	1.54	0.56
1:B:184:HIS:O	1:B:228:SER:OG	2.22	0.56
2:M:211:ILE:HA	2:M:226:LYS:HA	1.88	0.56
1:C:186:VAL:HG13	1:C:187:THR:HG22	1.87	0.56
2:M:40:SER:HB2	2:M:43:LYS:HB2	1.87	0.56
2:M:74:TRP:HE1	4:U:2:NAG:H83	1.71	0.56
3:P:199:THR:HA	3:P:206:GLU:HA	1.88	0.56
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.86	0.55
2:H:132:THR:HG22	2:H:162:PHE:HE1	1.70	0.55
1:B:172:GLU:OE1	1:B:172:GLU:N	2.39	0.55
1:B:203:THR:N	1:B:246:ASN:O	2.39	0.55
1:A:241:ASP:OD1	1:A:242:ILE:N	2.38	0.55
2:H:111:GLN:HB3	2:H:112:PRO:CD	2.35	0.55
1:B:266:SER:HB2	1:B:393:HIS:HB2	1.89	0.55
1:A:67:ILE:HD12	1:A:108:LEU:HD23	1.88	0.55
1:A:499:ARG:HG2	1:A:500:PHE:CE1	2.42	0.55
2:H:163:PRO:HD2	2:H:216:HIS:HE2	1.72	0.55
3:L:167:PRO:HA	3:L:177:ALA:HB2	1.89	0.55
1:B:187:THR:HG23	1:B:190:ASP:H	1.72	0.55
2:H:163:PRO:CG	2:H:216:HIS:HE2	2.12	0.55
3:P:148:THR:HG1	3:P:199:THR:HG1	1.54	0.55
1:A:102:VAL:HG23	1:A:232:ILE:O	2.07	0.54
3:N:162:VAL:HG22	3:N:180:TYR:O	2.07	0.54
1:A:356:GLN:HB2	1:A:361:ARG:HD3	1.89	0.54
1:A:460:GLU:OE1	1:A:470:TYR:OH	2.23	0.54
1:A:18:HIS:N	1:A:350:TRP:O	2.41	0.54
1:A:307:ARG:NH2	1:A:389:ASN:OD1	2.39	0.54
3:L:144:PRO:C	3:L:146:ALA:H	2.11	0.54
2:O:216:HIS:CD2	2:O:218:PRO:HD2	2.42	0.54
2:O:29:ILE:HD11	2:O:71:LEU:HB2	1.90	0.54
2:O:91:ALA:HB3	2:O:93:TYR:CE1	2.43	0.54
2:O:216:HIS:HD1	2:O:219:SER:HG	1.54	0.54
3:P:143:TYR:CB	3:P:144:PRO:CD	2.85	0.54
3:L:149:VAL:HG22	3:L:198:VAL:HG13	1.90	0.54
1:B:207:LYS:CB	1:B:241:ASP:OD1	2.56	0.54
3:L:123:PRO:HB3	3:L:134:THR:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ALA:HB2	1:C:469:ILE:HD13	1.90	0.53
2:O:6:GLU:N	2:O:6:GLU:OE1	2.41	0.53
1:A:165:ASN:HB2	4:J:1:NAG:H83	1.91	0.53
2:M:91:ALA:HB3	2:M:93:TYR:HE1	1.73	0.53
1:B:124:SER:OG	2:M:73:ASN:OD1	2.22	0.53
3:N:134:THR:HG22	3:N:182:SER:HA	1.88	0.53
2:H:130:ALA:HB3	2:H:162:PHE:CZ	2.44	0.53
1:C:428:LEU:O	1:C:432:GLU:CB	2.55	0.53
2:H:74:TRP:CZ3	4:D:2:NAG:C4	2.90	0.53
3:L:40:LEU:HD23	3:L:85:ALA:HB2	1.91	0.53
1:A:266:SER:HB2	1:A:393:HIS:HB2	1.89	0.53
2:M:162:PHE:HD2	2:M:163:PRO:HG3	1.72	0.53
2:O:185:VAL:HG21	3:P:163:GLU:HB3	1.90	0.53
1:B:295:GLN:NE2	1:B:298:ASN:O	2.38	0.53
1:B:98:TYR:CG	1:B:99:PRO:HD2	2.44	0.53
2:O:74:TRP:CE3	4:W:2:NAG:H2	2.44	0.53
1:A:302:TYR:HE1	1:A:392:PHE:CD1	2.27	0.53
1:A:98:TYR:CE2	1:A:226:ILE:HG12	2.44	0.53
1:A:172:GLU:N	1:A:172:GLU:OE1	2.41	0.52
4:Q:1:NAG:O3	4:Q:2:NAG:O5	2.23	0.52
1:A:55:PRO:HD3	1:A:278:LYS:HA	1.91	0.52
1:A:333:GLY:O	1:A:361:ARG:NH2	2.42	0.52
3:L:38:GLN:HB3	3:L:48:VAL:HG21	1.91	0.52
1:C:354:ARG:HG2	1:C:363:GLN:HB2	1.91	0.52
1:A:499:ARG:HG2	1:A:500:PHE:CD1	2.44	0.52
2:H:47:TRP:CG	3:L:98:TRP:HB3	2.45	0.52
1:C:433:ASN:ND2	1:C:433:ASN:H	2.08	0.52
2:M:133:LYS:H	2:M:162:PHE:HB2	1.75	0.52
3:L:134:THR:HG22	3:L:182:SER:HA	1.91	0.52
2:M:97:ARG:HH21	2:M:118:LEU:HD22	1.73	0.52
1:B:179:ILE:O	1:B:254:PRO:HB3	2.10	0.52
1:C:102:VAL:HG23	1:C:232:ILE:O	2.10	0.52
2:M:6:GLU:N	2:M:6:GLU:OE1	2.43	0.52
3:N:143:TYR:CD2	3:N:144:PRO:CA	2.93	0.52
1:C:248:THR:HG23	4:Y:1:NAG:H82	1.91	0.52
2:O:162:PHE:C	2:O:162:PHE:CD2	2.83	0.52
1:A:325:GLU:OE2	1:A:329:ARG:HG3	2.10	0.52
1:B:37:THR:OG1	1:B:38:ASN:N	2.42	0.52
1:C:462:MET:HE2	1:C:466:CYS:HB3	1.92	0.52
1:A:321:ARG:NH1	1:A:441:ASP:OD2	2.28	0.51
3:L:143:TYR:CB	3:L:144:PRO:HD3	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:HB3	1:B:76:CYS:SG	2.50	0.51
3:P:212:THR:HG22	3:P:213:GLU:N	2.25	0.51
1:B:218:GLY:O	1:B:220:ARG:NH1	2.43	0.51
3:P:90:GLY:C	3:P:98:TRP:CZ3	2.83	0.51
1:A:86:LEU:HB2	1:A:302:TYR:CE2	2.45	0.51
1:A:109:ARG:CZ	1:A:267:ILE:HD11	2.40	0.51
2:H:91:ALA:HB3	2:H:93:TYR:HE1	1.75	0.51
3:P:90:GLY:C	3:P:98:TRP:HZ3	2.13	0.51
2:H:105:ASP:HB3	2:H:111:GLN:HG3	1.92	0.51
1:A:47:SER:HB2	1:A:288:ILE:HG22	1.91	0.51
1:B:295:GLN:OE1	1:B:297:VAL:N	2.43	0.51
1:A:98:TYR:HD2	1:A:99:PRO:CD	2.23	0.51
1:A:348:ASP:OD1	1:A:348:ASP:N	2.38	0.51
1:B:80:GLN:HB2	1:B:150:ARG:NH2	2.26	0.51
3:N:143:TYR:CG	3:N:144:PRO:N	2.77	0.51
1:A:311:GLN:HG2	1:A:314:LEU:HD21	1.92	0.51
3:L:143:TYR:HD2	3:L:144:PRO:CD	2.24	0.51
3:L:142:PHE:O	3:L:175:TYR:HB2	2.11	0.51
1:C:474:ASP:N	1:C:477:CYS:SG	2.84	0.51
2:H:61:PRO:HD3	3:L:97:ILE:HD13	1.93	0.50
1:C:68:ASP:OD2	1:C:95:SER:OG	2.28	0.50
1:C:173:GLN:HG2	2:O:108:GLY:HA2	1.93	0.50
1:C:179:ILE:O	1:C:254:PRO:HB3	2.11	0.50
1:B:186:VAL:HG13	1:B:187:THR:HG22	1.92	0.50
1:A:28:THR:HG22	1:A:433:ASN:HB3	1.93	0.50
1:A:377:ILE:HD12	1:A:436:THR:HG23	1.92	0.50
2:O:105:ASP:HB3	2:O:111:GLN:HG2	1.93	0.50
3:P:141:ASP:HA	3:P:174:LYS:HB3	1.92	0.50
1:A:60:ASP:HA	1:A:88:VAL:HG23	1.93	0.50
3:L:143:TYR:CD2	3:L:144:PRO:CD	2.94	0.50
4:Q:1:NAG:H83	4:R:1:NAG:H82	1.94	0.50
1:A:98:TYR:HD2	1:A:99:PRO:HD2	1.75	0.50
1:B:84:TRP:CE2	1:B:116:GLY:HA2	2.46	0.50
1:A:186:VAL:HG23	1:A:219:SER:HA	1.93	0.50
2:M:99:THR:O	2:M:113:GLY:HA3	2.12	0.50
1:B:474:ASP:N	1:B:477:CYS:SG	2.85	0.50
3:N:187:GLN:HA	3:N:190:SER:HB3	1.94	0.50
1:A:277:CYS:SG	1:A:278:LYS:N	2.84	0.50
3:L:53:ASN:ND2	3:L:53:ASN:O	2.45	0.50
1:C:433:ASN:ND2	1:C:433:ASN:N	2.60	0.50
2:O:54:SER:HB2	2:O:109:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:THR:HA	2:H:83:ASN:HA	1.94	0.50
3:L:114:ALA:HB3	3:L:143:TYR:N	2.27	0.50
2:H:33:TYR:HB2	2:H:98:HIS:HB2	1.93	0.49
1:B:55:PRO:HD3	1:B:278:LYS:HA	1.93	0.49
1:C:178:TYR:CE1	1:C:257:TYR:HB3	2.47	0.49
2:M:47:TRP:CG	3:N:98:TRP:HB3	2.47	0.49
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.95	0.49
3:P:184:THR:HG22	3:P:186:GLU:H	1.77	0.49
3:L:81:THR:O	3:L:173:ASN:ND2	2.44	0.49
1:B:207:LYS:HB2	1:B:241:ASP:OD1	2.10	0.49
1:A:60:ASP:OD2	1:A:90:ARG:NH2	2.44	0.49
1:B:131:THR:OG1	1:B:155:THR:OG1	2.22	0.49
2:M:66:ARG:O	2:M:82:VAL:HA	2.13	0.49
2:H:163:PRO:CG	2:H:216:HIS:HE1	2.10	0.49
3:N:36:TRP:HB2	3:N:49:ILE:HB	1.94	0.49
1:C:187:THR:HG23	1:C:190:ASP:H	1.78	0.49
2:O:24:VAL:HG12	2:O:76:ASN:O	2.13	0.49
1:A:499:ARG:CG	1:A:500:PHE:CE1	2.96	0.49
2:M:162:PHE:C	2:M:162:PHE:CD2	2.85	0.49
2:O:151:THR:N	2:O:202:SER:HG	2.10	0.49
3:N:200:HIS:HB3	3:N:203:SER:CB	2.43	0.49
1:B:134:GLY:HA3	1:B:153:TRP:HB3	1.95	0.49
2:O:17:THR:HA	2:O:83:ASN:HA	1.95	0.49
2:O:163:PRO:HG2	2:O:163:PRO:O	2.13	0.49
2:H:6:GLU:N	2:H:6:GLU:OE1	2.46	0.48
1:C:206:THR:HG23	1:C:209:SER:H	1.78	0.48
3:P:18:VAL:HG13	3:P:79:LEU:HD11	1.94	0.48
1:A:113:ALA:HB1	1:A:267:ILE:HG23	1.95	0.48
3:L:39:GLN:HB3	3:L:86:VAL:HG23	1.94	0.48
1:C:309:VAL:HG12	1:C:311:GLN:H	1.77	0.48
1:A:186:VAL:HG13	1:A:187:THR:HG22	1.94	0.48
2:H:69:ILE:HG12	2:H:80:LEU:HD13	1.93	0.48
1:C:309:VAL:HG13	1:C:422:SER:HA	1.95	0.48
2:O:135:PRO:HB3	2:O:161:TYR:HB3	1.95	0.48
2:M:24:VAL:HG12	2:M:76:ASN:O	2.12	0.48
2:O:39:GLN:HA	2:O:45:LEU:HD23	1.94	0.48
1:A:84:TRP:CZ2	1:A:116:GLY:HA2	2.48	0.48
2:H:103:HIS:O	2:H:103:HIS:ND1	2.47	0.48
2:O:182:PHE:CD2	3:P:178:SER:HB3	2.48	0.48
4:D:1:NAG:H62	4:D:2:NAG:C8	2.44	0.48
1:C:431:LEU:C	1:C:431:LEU:HD23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:10:VAL:HG23	3:L:106:LEU:HD23	1.95	0.48
1:B:456:ARG:CZ	1:B:488:HIS:NE2	2.75	0.48
3:N:128:LEU:HA	3:N:132:LYS:O	2.13	0.48
1:C:429:VAL:HG13	1:C:433:ASN:HD21	1.78	0.48
2:O:160:ASP:HA	2:O:191:LEU:HB3	1.96	0.48
1:C:304:ALA:HA	1:C:390:GLU:HA	1.96	0.48
1:C:348:ASP:N	1:C:348:ASP:OD1	2.46	0.48
1:A:184:HIS:CE1	1:A:216:ASN:H	2.32	0.47
1:B:96:ASN:HA	1:B:224:ARG:CZ	2.43	0.47
3:N:39:GLN:HB2	3:N:45:PRO:HB3	1.95	0.47
3:N:39:GLN:HB3	3:N:86:VAL:HG23	1.94	0.47
1:C:429:VAL:O	1:C:433:ASN:N	2.39	0.47
2:H:74:TRP:CD1	2:H:75:ASN:N	2.82	0.47
2:M:156:CYS:C	2:M:157:LEU:HD12	2.34	0.47
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.49	0.47
1:B:84:TRP:HZ2	1:B:113:ALA:HA	1.79	0.47
1:B:381:LEU:O	1:B:385:ILE:HG22	2.14	0.47
2:O:90:THR:HB	2:O:127:VAL:HG23	1.97	0.47
2:O:162:PHE:N	2:O:163:PRO:CD	2.71	0.47
1:B:43:VAL:HB	1:B:313:THR:HA	1.96	0.47
1:B:184:HIS:CE1	1:B:216:ASN:H	2.32	0.47
1:B:478:ILE:HG22	1:B:482:ARG:HH11	1.80	0.47
1:C:108:LEU:HD23	1:C:234:TRP:CD2	2.49	0.47
1:C:281:CYS:O	1:C:287:SER:OG	2.20	0.47
2:M:100:LEU:H	2:M:100:LEU:HD23	1.80	0.47
3:N:53:ASN:OD1	3:N:53:ASN:N	2.47	0.47
1:C:241:ASP:OD1	1:C:242:ILE:N	2.41	0.47
2:O:162:PHE:CD2	2:O:162:PHE:O	2.68	0.47
2:O:167:THR:OG1	2:O:215:ASN:HB3	2.15	0.47
1:B:28:THR:HG22	1:B:433:ASN:HB3	1.95	0.47
1:B:38:ASN:OD1	1:B:318:THR:OG1	2.32	0.47
1:C:67:ILE:HD12	1:C:108:LEU:HD12	1.96	0.47
2:O:103:HIS:O	2:O:103:HIS:ND1	2.47	0.47
2:O:162:PHE:O	2:O:162:PHE:CG	2.67	0.47
3:P:212:THR:HG22	3:P:213:GLU:O	2.15	0.47
2:H:40:SER:HB2	2:H:43:LYS:HB2	1.95	0.47
1:C:429:VAL:CG1	1:C:433:ASN:HD21	2.27	0.47
1:C:13:LEU:HD11	1:C:353:PHE:HB3	1.97	0.47
2:M:97:ARG:NH2	2:M:118:LEU:HD22	2.29	0.47
2:O:69:ILE:HG12	2:O:80:LEU:HD13	1.95	0.47
4:D:1:NAG:O3	4:D:1:NAG:H83	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASP:OD1	1:A:474:ASP:N	2.42	0.46
3:P:146:ALA:CB	3:P:201:GLU:CB	2.91	0.46
1:A:52:CYS:HB2	1:A:279:SER:HB3	1.97	0.46
3:N:120:LEU:HD13	3:N:211:PRO:CD	2.45	0.46
3:P:36:TRP:CE2	3:P:74:LEU:HB2	2.50	0.46
1:A:18:HIS:HB2	1:A:350:TRP:HA	1.97	0.46
1:B:371:GLN:NE2	1:B:375:ASP:OD1	2.46	0.46
1:C:295:GLN:OE1	1:C:297:VAL:N	2.49	0.46
2:O:66:ARG:HH12	2:O:86:THR:HG22	1.80	0.46
2:H:135:PRO:HA	2:H:161:TYR:HB3	1.98	0.46
3:P:114:ALA:HB3	3:P:143:TYR:N	2.31	0.46
1:A:39:ALA:HA	1:A:318:THR:HG23	1.97	0.46
1:C:343:TRP:CE2	1:C:354:ARG:HD2	2.51	0.46
4:J:2:NAG:C1	4:J:2:NAG:C8	2.94	0.46
2:M:17:THR:HA	2:M:83:ASN:HA	1.97	0.46
2:O:172:SER:N	2:O:213:ASN:OD1	2.48	0.46
1:A:391:LYS:HA	1:A:391:LYS:HD2	1.64	0.45
1:B:98:TYR:CD1	1:B:99:PRO:HD2	2.51	0.45
2:M:6:GLU:HG3	2:M:22:CYS:HB2	1.98	0.45
1:C:246:ASN:CG	4:Y:1:NAG:H83	2.37	0.45
1:C:479:GLY:HA2	1:C:482:ARG:HG2	1.97	0.45
3:L:143:TYR:HD2	3:L:144:PRO:HG3	1.81	0.45
2:M:162:PHE:CD1	2:M:162:PHE:O	2.68	0.45
3:L:143:TYR:CD2	3:L:144:PRO:HD3	2.51	0.45
3:L:172:ASN:O	3:L:174:LYS:N	2.50	0.45
2:O:41:PRO:O	2:O:41:PRO:HG2	2.15	0.45
2:H:171:ASN:HB2	2:H:174:ALA:HB3	1.99	0.45
1:B:169:PRO:HA	1:B:242:ILE:HG22	1.97	0.45
3:N:36:TRP:NE1	3:N:89:CYS:HB3	2.31	0.45
2:O:86:THR:OG1	2:O:87:ALA:N	2.50	0.45
2:H:72:GLN:NE2	2:H:74:TRP:CZ2	2.85	0.45
2:M:72:GLN:HG3	2:M:75:ASN:OD1	2.16	0.45
3:P:19:THR:HG23	3:P:73:THR:HG23	1.99	0.45
3:P:62:ARG:HG3	3:P:77:THR:O	2.17	0.45
2:H:74:TRP:CG	2:H:75:ASN:N	2.84	0.45
3:L:143:TYR:HD2	3:L:144:PRO:HD3	1.81	0.45
2:O:6:GLU:HG3	2:O:22:CYS:HB2	1.98	0.45
2:O:33:TYR:CE1	2:O:52:TYR:HB2	2.52	0.45
2:O:182:PHE:HB2	2:O:195:SER:O	2.16	0.45
3:P:143:TYR:HD2	3:P:144:PRO:CG	2.17	0.45
1:A:109:ARG:NE	1:A:267:ILE:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:SER:HA	1:A:261:ARG:O	2.17	0.45
1:A:179:ILE:O	1:A:254:PRO:HB3	2.17	0.45
2:O:74:TRP:CZ3	4:W:2:NAG:H2	2.52	0.45
1:A:325:GLU:HG2	1:A:342:GLY:O	2.18	0.44
3:L:143:TYR:HB3	3:L:144:PRO:CD	2.40	0.44
1:B:382:ASN:HA	1:B:385:ILE:HG22	2.00	0.44
2:O:161:TYR:CE2	2:O:193:SER:HA	2.52	0.44
1:B:303:GLY:HA2	1:B:392:PHE:HE1	1.81	0.44
1:B:346:MET:HE1	1:B:352:GLY:HA3	2.00	0.44
2:H:14:PRO:HA	2:H:85:VAL:HG23	1.98	0.44
1:B:176:LYS:HE3	1:B:257:TYR:CG	2.53	0.44
2:M:33:TYR:HB2	2:M:98:HIS:HB2	2.00	0.44
2:M:163:PRO:C	2:M:165:PRO:HD2	2.38	0.44
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.99	0.44
2:H:48:ILE:O	2:H:60:ASN:N	2.43	0.44
1:C:41:GLU:OE1	1:C:313:THR:OG1	2.34	0.44
1:C:131:THR:OG1	1:C:155:THR:OG1	2.33	0.44
1:B:178:TYR:CE1	1:B:257:TYR:HB3	2.53	0.44
2:M:162:PHE:O	2:M:162:PHE:CG	2.68	0.44
2:O:161:TYR:OH	2:O:194:LEU:CB	2.65	0.44
1:B:74:PRO:HD2	1:B:97:CYS:HB2	2.00	0.44
1:C:431:LEU:C	1:C:431:LEU:CD2	2.85	0.44
3:P:170:GLN:HG2	3:P:174:LYS:O	2.18	0.44
1:A:295:GLN:OE1	1:A:297:VAL:N	2.50	0.44
1:C:164:LEU:O	1:C:246:ASN:HA	2.17	0.44
4:J:1:NAG:H4	4:J:2:NAG:H82	1.98	0.44
3:N:144:PRO:C	3:N:146:ALA:H	2.21	0.43
1:C:220:ARG:HB2	1:C:227:PRO:O	2.18	0.43
2:O:176:THR:HG23	2:O:177:SER:H	1.82	0.43
1:B:180:TRP:CE2	1:B:204:VAL:HG21	2.53	0.43
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.43
3:P:181:LEU:O	3:P:183:LEU:HD23	2.18	0.43
1:B:230:ILE:HD13	1:B:252:ILE:HD13	2.00	0.43
2:O:97:ARG:HH21	2:O:118:LEU:HD22	1.83	0.43
4:D:2:NAG:O7	4:D:2:NAG:C3	2.66	0.43
1:B:470:TYR:CD2	1:B:499:ARG:HG2	2.40	0.43
2:M:114:ASP:HA	3:N:92:TRP:HE1	1.83	0.43
3:P:182:SER:O	3:P:183:LEU:HD22	2.17	0.43
2:O:97:ARG:O	2:O:117:ASP:N	2.38	0.43
1:B:412:TYR:OH	1:C:414:GLU:OE1	2.28	0.43
1:C:31:ASN:HB2	1:C:34:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:GLY:HA2	2:H:170:TRP:CH2	2.48	0.43
1:B:128:ALA:O	1:B:130:VAL:HG13	2.17	0.43
1:A:10:THR:OG1	1:A:11:ALA:N	2.52	0.43
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.43	0.43
3:L:165:THR:HG22	3:L:178:SER:H	1.84	0.43
1:C:60:ASP:OD2	1:C:90:ARG:NH2	2.48	0.43
3:P:91:THR:N	3:P:98:TRP:HZ3	2.12	0.43
3:L:145:GLY:O	3:L:167:PRO:HG2	2.19	0.43
3:N:143:TYR:CG	3:N:144:PRO:CD	3.02	0.43
1:A:72:GLY:HA3	1:A:149:SER:OG	2.18	0.43
2:H:136:SER:OG	2:H:159:LYS:O	2.29	0.43
1:B:72:GLY:HA3	1:B:149:SER:OG	2.19	0.43
2:M:164:GLU:N	2:M:165:PRO:HD2	2.34	0.43
2:H:97:ARG:O	2:H:117:ASP:N	2.35	0.42
1:C:307:ARG:HD3	1:C:421:TRP:CE2	2.54	0.42
1:A:125:PHE:HB2	1:A:127:TRP:CZ2	2.54	0.42
1:C:98:TYR:CD1	1:C:99:PRO:HD2	2.54	0.42
1:C:428:LEU:O	1:C:432:GLU:N	2.43	0.42
2:M:47:TRP:HZ2	2:M:50:TYR:HD1	1.66	0.42
1:C:77:ASP:CG	1:C:141:ARG:HH21	2.21	0.42
2:O:137:VAL:HG11	2:O:214:VAL:HG21	2.00	0.42
1:B:348:ASP:OD1	1:B:348:ASP:N	2.52	0.42
1:C:431:LEU:HD23	1:C:431:LEU:O	2.20	0.42
3:P:151:TRP:HB2	3:P:158:VAL:HG11	1.99	0.42
2:H:132:THR:CB	2:H:162:PHE:HD1	2.32	0.42
1:C:84:TRP:CZ2	1:C:116:GLY:HA2	2.54	0.42
2:O:20:LEU:CD1	2:O:93:TYR:HD2	2.33	0.42
3:P:137:CYS:HB2	3:P:151:TRP:CH2	2.55	0.42
2:O:33:TYR:HB2	2:O:98:HIS:HB2	2.02	0.42
3:L:86:VAL:HG12	3:L:105:LYS:HA	2.01	0.42
2:M:16:GLU:H	2:M:85:VAL:HG12	1.84	0.42
1:C:357:ASN:HD21	1:C:359:GLU:HB2	1.84	0.42
2:O:20:LEU:HD11	2:O:93:TYR:HD2	1.84	0.42
1:B:13:LEU:HD11	1:B:353:PHE:HB3	2.02	0.42
1:B:15:LEU:HD11	1:B:448:PHE:CD1	2.52	0.42
2:O:121:GLN:HA	3:P:44:ALA:HB2	2.02	0.42
1:A:99:PRO:HB2	1:A:229:ARG:HD3	2.02	0.42
1:A:151:LEU:HD13	1:A:252:ILE:HD12	2.01	0.42
1:B:207:LYS:HB3	1:B:241:ASP:OD1	2.19	0.42
1:B:293:PRO:C	1:B:306:PRO:HB3	2.40	0.42
2:M:74:TRP:CE2	4:U:2:NAG:H2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:151:TRP:CE3	3:P:181:LEU:HD22	2.55	0.42
1:B:186:VAL:HG23	1:B:219:SER:HA	2.02	0.41
1:B:353:PHE:CZ	1:B:447:LEU:HD11	2.55	0.41
2:M:102:TYR:HD1	2:M:102:TYR:HA	1.75	0.41
3:N:143:TYR:O	3:N:175:TYR:CE2	2.73	0.41
2:O:20:LEU:HD23	2:O:20:LEU:HA	1.92	0.41
3:N:36:TRP:CD1	3:N:74:LEU:HD12	2.56	0.41
3:N:136:VAL:HG22	3:N:180:TYR:CD2	2.55	0.41
1:C:98:TYR:HD2	1:C:230:ILE:HD12	1.86	0.41
1:C:120:PHE:CE2	1:C:150:ARG:HD2	2.55	0.41
1:A:17:HIS:HB3	1:A:444:MET:SD	2.61	0.41
3:L:53:ASN:HB3	3:L:65:GLY:O	2.20	0.41
1:B:120:PHE:CE2	1:B:150:ARG:HD2	2.55	0.41
1:C:89:GLU:HG3	1:C:267:ILE:HD11	2.02	0.41
2:O:64:THR:O	2:O:66:ARG:N	2.54	0.41
2:O:216:HIS:HD2	2:O:218:PRO:HD2	1.82	0.41
2:M:132:THR:HA	2:M:162:PHE:CB	2.51	0.41
2:M:97:ARG:O	2:M:117:ASP:N	2.39	0.41
3:N:28:ASP:HA	3:N:93:ASP:HA	2.02	0.41
2:O:186:LEU:HD11	2:O:190:GLY:HA2	2.03	0.41
2:H:167:THR:OG1	2:H:215:ASN:HB3	2.21	0.41
3:L:197:GLN:HA	3:L:208:THR:OG1	2.20	0.41
3:N:4:LEU:HB3	3:N:101:GLY:HA2	2.02	0.41
2:O:64:THR:C	2:O:66:ARG:H	2.23	0.41
1:A:113:ALA:CB	1:A:267:ILE:HG23	2.51	0.41
2:H:156:CYS:C	2:H:157:LEU:HD12	2.41	0.41
3:L:143:TYR:CB	3:L:144:PRO:CD	2.99	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.56	0.41
1:C:300:ILE:HD13	1:C:300:ILE:HA	1.91	0.41
3:L:143:TYR:CD2	3:L:144:PRO:N	2.89	0.41
1:B:176:LYS:HE3	1:B:257:TYR:CD1	2.56	0.41
2:M:132:THR:O	2:M:132:THR:OG1	2.35	0.41
2:M:216:HIS:HD1	2:M:219:SER:H	1.69	0.41
1:C:213:VAL:HG11	1:C:233:TYR:CE1	2.56	0.41
1:C:433:ASN:H	1:C:433:ASN:HD22	1.68	0.41
2:O:99:THR:O	2:O:113:GLY:HA3	2.20	0.41
4:U:2:NAG:H62	4:U:3:BMA:O5	2.20	0.41
1:A:187:THR:HG23	1:A:190:ASP:H	1.85	0.41
2:H:162:PHE:CD1	2:H:163:PRO:HD3	2.55	0.41
1:B:120:PHE:HE2	1:B:150:ARG:HD2	1.86	0.41
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:39:GLN:NE2	3:P:39:GLN:HE22	2.19	0.41
3:P:120:LEU:HD13	3:P:211:PRO:CD	2.48	0.41
1:A:329:ARG:NH2	1:A:336:ALA:HB2	2.36	0.40
1:A:204:VAL:HG22	1:A:245:ILE:HG23	2.03	0.40
2:H:11:LEU:HA	2:H:126:THR:O	2.21	0.40
3:N:7:PRO:HA	3:N:8:PRO:HD3	1.98	0.40
3:N:114:ALA:HB3	3:N:143:TYR:N	2.37	0.40
1:C:429:VAL:C	1:C:433:ASN:HD22	2.08	0.40
2:O:41:PRO:O	2:O:41:PRO:CG	2.68	0.40
3:P:212:THR:CG2	3:P:213:GLU:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/505 (98%)	468 (95%)	23 (5%)	2 (0%)	30	66
1	B	484/505 (96%)	459 (95%)	22 (4%)	3 (1%)	22	58
1	C	483/505 (96%)	453 (94%)	25 (5%)	5 (1%)	13	47
2	H	217/237 (92%)	199 (92%)	16 (7%)	2 (1%)	14	49
2	M	217/237 (92%)	201 (93%)	14 (6%)	2 (1%)	14	49
2	O	217/237 (92%)	202 (93%)	13 (6%)	2 (1%)	14	49
3	L	212/215 (99%)	191 (90%)	18 (8%)	3 (1%)	9	40
3	N	212/215 (99%)	194 (92%)	16 (8%)	2 (1%)	14	49
3	P	212/215 (99%)	194 (92%)	15 (7%)	3 (1%)	9	40
All	All	2747/2871 (96%)	2561 (93%)	162 (6%)	24 (1%)	14	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
3	N	143	TYR
3	P	146	ALA
2	H	162	PHE
2	M	132	THR
2	M	166	VAL
3	N	145	GLY
2	O	65	GLY
3	L	173	ASN
1	B	458	ASN
1	C	21	PRO
3	L	143	TYR
1	B	21	PRO
1	C	434	GLN
2	O	165	PRO
3	P	78	GLY
1	A	21	PRO
1	B	393	HIS
1	C	378	ASN
2	H	165	PRO
1	C	142	GLY
3	P	143	TYR
3	L	158	VAL
1	C	377	ILE

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	405/440 (92%)	394 (97%)	11 (3%)	40	60
1	B	382/440 (87%)	373 (98%)	9 (2%)	44	63
1	C	395/440 (90%)	388 (98%)	7 (2%)	54	71
2	H	154/200 (77%)	151 (98%)	3 (2%)	52	70
2	M	152/200 (76%)	148 (97%)	4 (3%)	41	61
2	O	159/200 (80%)	153 (96%)	6 (4%)	28	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	141/181 (78%)	139 (99%)	2 (1%)	62 75
3	N	137/181 (76%)	134 (98%)	3 (2%)	47 65
3	P	152/181 (84%)	150 (99%)	2 (1%)	65 77
All	All	2077/2463 (84%)	2030 (98%)	47 (2%)	45 64

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	TYR
1	A	190	ASP
1	A	195	TYR
1	A	224	ARG
1	A	277	CYS
1	A	285	ASN
1	A	287	SER
1	A	338	PHE
1	A	341	ASN
1	A	389	ASN
1	A	482	ARG
2	H	43	LYS
2	H	161	TYR
2	H	187	GLN
3	L	28	ASP
3	L	109	LEU
1	B	38	ASN
1	B	96	ASN
1	B	100	TYR
1	B	161	TYR
1	B	171	ASN
1	B	195	TYR
1	B	456	ARG
1	B	458	ASN
1	B	489	ASP
2	M	22	CYS
2	M	74	TRP
2	M	77	HIS
2	M	166	VAL
3	N	36	TRP
3	N	51	ASP
3	N	179	SER
1	C	144	ASN

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Mol	Chain	Res	Type
1	C	195	TYR
1	C	363	GLN
1	C	382	ASN
1	C	383	ARG
1	C	392	PHE
1	C	493	ASP
2	O	22	CYS
2	O	45	LEU
2	O	114	ASP
2	O	165	PRO
2	O	170	TRP
2	O	180	HIS
3	P	50	TYR
3	P	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	C	341	ASN
2	O	39	GLN
3	P	39	GLN

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)

49 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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	2.99	8 (57%)	17,19,21	4.16	9 (52%)
4	NAG	D	2	4	14,14,15	1.66	4 (28%)	17,19,21	4.06	10 (58%)
4	BMA	D	3	4	11,11,12	1.31	2 (18%)	15,15,17	2.77	8 (53%)
4	NAG	E	1	1,4	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.45	0
4	BMA	E	3	4	11,11,12	0.57	0	15,15,17	0.74	0
5	NAG	F	1	1,5	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
4	NAG	G	1	1,4	14,14,15	0.34	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.66	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	0.69	0
4	NAG	I	1	1,4	14,14,15	0.38	0	17,19,21	0.67	0
4	NAG	I	2	4	14,14,15	0.20	0	17,19,21	0.39	0
4	BMA	I	3	4	11,11,12	0.51	0	15,15,17	0.69	0
4	NAG	J	1	1,4	14,14,15	0.59	0	17,19,21	1.04	2 (11%)
4	NAG	J	2	4	14,14,15	1.37	2 (14%)	17,19,21	2.71	5 (29%)
4	BMA	J	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.10	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	K	2	4	14,14,15	0.32	0	17,19,21	0.76	1 (5%)
4	BMA	K	3	4	11,11,12	0.70	0	15,15,17	0.68	0
4	NAG	Q	1	1,4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	Q	2	4	14,14,15	0.23	0	17,19,21	0.61	1 (5%)
4	BMA	Q	3	4	11,11,12	0.61	0	15,15,17	0.66	0
4	NAG	R	1	1,4	14,14,15	0.42	0	17,19,21	0.62	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	BMA	R	3	4	11,11,12	0.62	0	15,15,17	0.68	0
5	NAG	S	1	1,5	14,14,15	0.30	0	17,19,21	0.37	0
5	NAG	S	2	5	14,14,15	0.48	0	17,19,21	0.48	0
5	NAG	T	1	1,5	14,14,15	0.48	0	17,19,21	0.52	0
5	NAG	T	2	5	14,14,15	1.60	2 (14%)	17,19,21	1.39	1 (5%)
4	NAG	U	1	1,4	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.60	0
4	BMA	U	3	4	11,11,12	1.09	1 (9%)	15,15,17	0.96	0
5	NAG	V	1	1,5	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	W	1	1,4	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	W	2	4	14,14,15	0.22	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	W	3	4	11,11,12	0.78	0	15,15,17	0.81	0
4	NAG	X	1	1,4	14,14,15	0.17	0	17,19,21	0.61	0
4	NAG	X	2	4	14,14,15	0.24	0	17,19,21	0.65	0
4	BMA	X	3	4	11,11,12	0.63	0	15,15,17	0.73	0
4	NAG	Y	1	1,4	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	BMA	Y	3	4	11,11,12	0.65	0	15,15,17	0.69	0
4	NAG	Z	1	1,4	14,14,15	0.25	0	17,19,21	0.67	0
4	NAG	Z	2	4	14,14,15	0.32	0	17,19,21	0.39	0
4	BMA	Z	3	4	11,11,12	0.56	0	15,15,17	0.82	0
5	NAG	a	1	1,5	14,14,15	0.17	0	17,19,21	0.83	0
5	NAG	a	2	5	14,14,15	0.60	1 (7%)	17,19,21	1.39	2 (11%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	1/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
4	BMA	U	3	4	-	2/2/19/22	0/1/1/1
5	NAG	V	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	4/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Y	3	4	-	2/2/19/22	0/1/1/1
4	NAG	Z	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	a	2	5	-	6/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	-5.68	1.44	1.52
4	D	1	NAG	O5-C1	-5.10	1.35	1.43
4	D	1	NAG	C2-N2	-4.76	1.38	1.46
5	T	2	NAG	O5-C1	4.40	1.51	1.43
5	T	2	NAG	C1-C2	3.96	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	C1-C2	3.67	1.57	1.52
4	D	1	NAG	C3-C2	-3.52	1.45	1.52
4	D	2	NAG	C2-N2	-3.26	1.40	1.46
4	J	2	NAG	O5-C1	-2.95	1.38	1.43
4	J	3	BMA	C1-C2	2.94	1.59	1.52
4	D	2	NAG	C1-C2	-2.87	1.48	1.52
4	D	1	NAG	O5-C5	-2.68	1.38	1.43
4	D	3	BMA	C4-C5	-2.65	1.47	1.53
4	U	3	BMA	C1-C2	2.58	1.58	1.52
4	D	1	NAG	C4-C5	-2.44	1.47	1.53
4	D	1	NAG	C4-C3	-2.20	1.46	1.52
4	D	2	NAG	C3-C2	-2.18	1.47	1.52
4	D	2	NAG	C4-C3	-2.10	1.46	1.52
4	D	3	BMA	C4-C3	-2.06	1.47	1.52
4	D	1	NAG	O4-C4	-2.06	1.37	1.43
5	a	2	NAG	C1-C2	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	C2-N2-C7	-11.40	107.62	122.90
4	D	2	NAG	C3-C4-C5	-9.90	92.28	110.23
4	J	2	NAG	C2-N2-C7	8.21	133.90	122.90
4	D	1	NAG	O5-C1-C2	-7.59	99.55	111.29
4	D	2	NAG	O4-C4-C5	6.61	125.60	109.32
4	D	2	NAG	C4-C3-C2	-6.53	101.45	111.02
4	D	3	BMA	C1-O5-C5	5.57	119.65	112.19
4	D	2	NAG	C8-C7-N2	-5.51	106.97	116.12
4	J	2	NAG	C1-C2-N2	5.47	119.06	110.43
4	D	1	NAG	C4-C3-C2	-5.33	103.20	111.02
4	D	2	NAG	O5-C1-C2	-5.24	103.18	111.29
5	T	2	NAG	C1-O5-C5	5.17	119.11	112.19
4	D	3	BMA	C1-C2-C3	4.59	116.33	109.64
5	a	2	NAG	C2-N2-C7	4.56	129.01	122.90
4	D	3	BMA	C3-C4-C5	-4.29	102.45	110.23
4	D	1	NAG	O4-C4-C3	-3.84	101.33	110.38
4	D	1	NAG	O3-C3-C4	-3.79	101.45	110.38
4	D	1	NAG	O5-C5-C4	-3.78	101.62	110.83
4	D	1	NAG	O3-C3-C2	-3.78	101.55	109.40
4	D	2	NAG	O7-C7-N2	3.43	128.05	121.98
4	D	3	BMA	O3-C3-C4	-3.16	102.94	110.38
4	D	3	BMA	O4-C4-C3	-3.13	103.00	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	3	BMA	C1-C2-C3	3.11	114.17	109.64
4	J	2	NAG	C4-C3-C2	3.10	115.56	111.02
4	D	1	NAG	C3-C4-C5	-2.99	104.81	110.23
4	J	1	NAG	C2-N2-C7	2.88	126.76	122.90
4	D	2	NAG	C2-N2-C7	-2.82	119.12	122.90
4	D	3	BMA	O3-C3-C2	2.79	115.75	110.05
5	F	1	NAG	C1-O5-C5	2.50	115.53	112.19
4	D	2	NAG	O3-C3-C2	2.41	114.40	109.40
4	D	3	BMA	O5-C5-C4	-2.37	105.05	110.83
4	K	2	NAG	C2-N2-C7	2.37	126.07	122.90
4	D	3	BMA	O5-C5-C6	2.33	112.20	107.66
5	a	2	NAG	C1-C2-N2	2.30	114.06	110.43
4	E	1	NAG	C1-O5-C5	2.25	115.21	112.19
4	J	2	NAG	O4-C4-C3	2.24	115.65	110.38
4	D	2	NAG	O3-C3-C4	2.22	115.61	110.38
4	W	2	NAG	C1-O5-C5	2.06	114.95	112.19
4	D	1	NAG	C1-O5-C5	-2.05	109.44	112.19
4	J	2	NAG	C1-O5-C5	-2.01	109.49	112.19
4	Q	2	NAG	C1-O5-C5	2.01	114.88	112.19
5	F	2	NAG	C1-O5-C5	2.01	114.88	112.19
4	J	1	NAG	C1-C2-N2	2.01	113.60	110.43
4	D	2	NAG	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
5	a	1	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	U	2	NAG	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	U	3	BMA	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	Y	3	BMA	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	U	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
4	K	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	R	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7
4	X	2	NAG	C4-C5-C6-O6
4	Y	3	BMA	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	W	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7
5	F	2	NAG	C3-C2-N2-C7
5	a	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C1-C2-N2-C7
4	Z	1	NAG	C1-C2-N2-C7
5	a	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
5	S	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

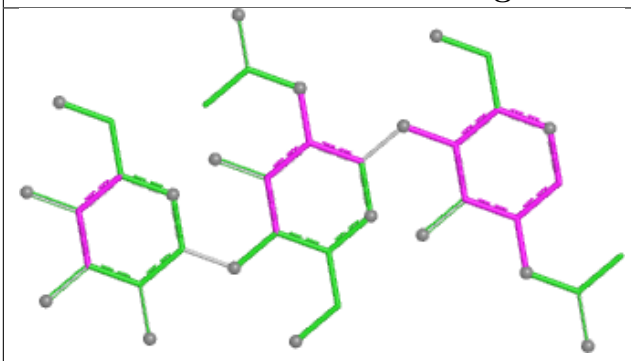
There are no ring outliers.

13 monomers are involved in 24 short contacts:

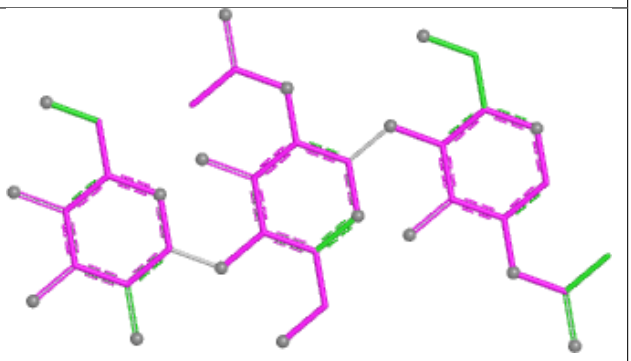
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	2	0
4	U	2	NAG	4	0
4	Y	1	NAG	2	0
4	Q	2	NAG	1	0
4	J	2	NAG	3	0
4	Q	1	NAG	2	0
4	U	3	BMA	1	0
4	R	1	NAG	1	0
4	W	2	NAG	2	0
4	D	2	NAG	8	0
4	D	1	NAG	3	0
4	K	2	NAG	1	0
4	J	3	BMA	1	0

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

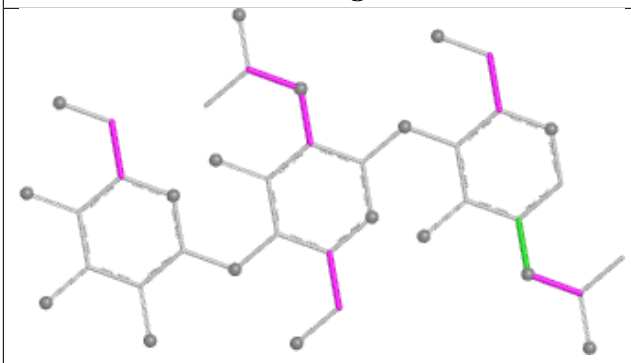
Oligosaccharide Chain D



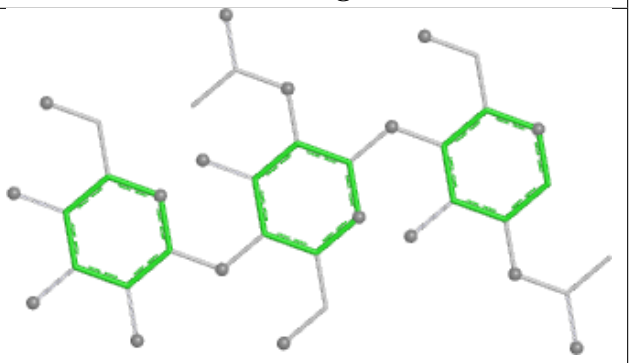
Bond lengths



Bond angles

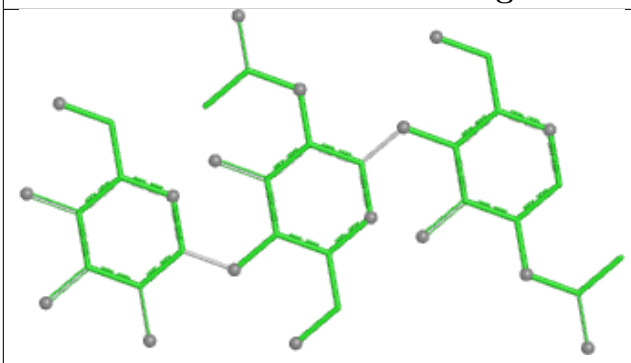


Torsions

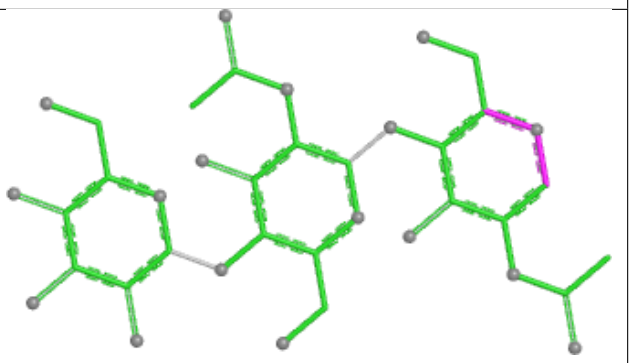


Rings

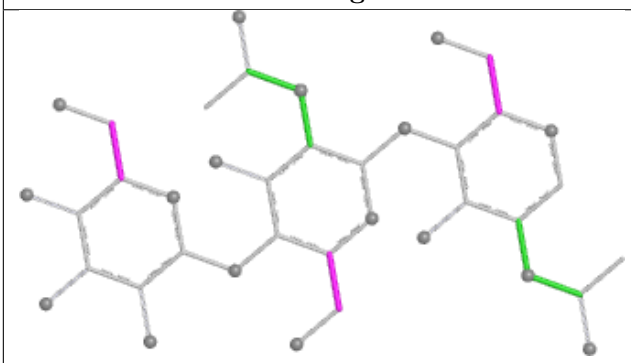
Oligosaccharide Chain E



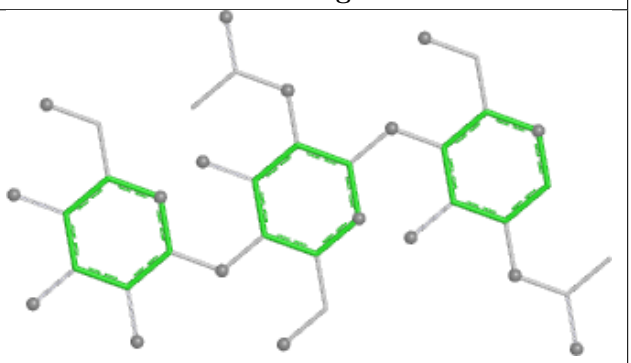
Bond lengths



Bond angles

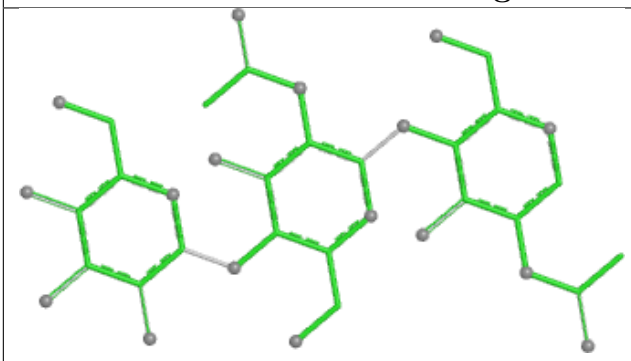


Torsions

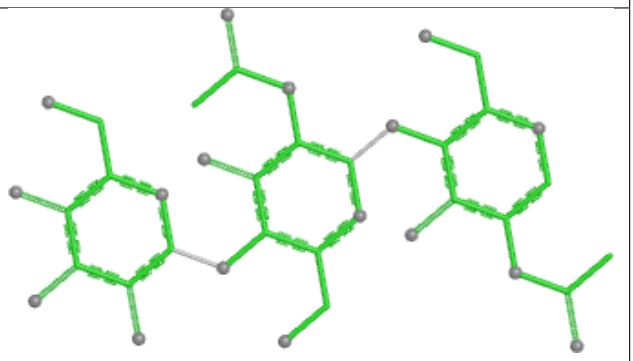


Rings

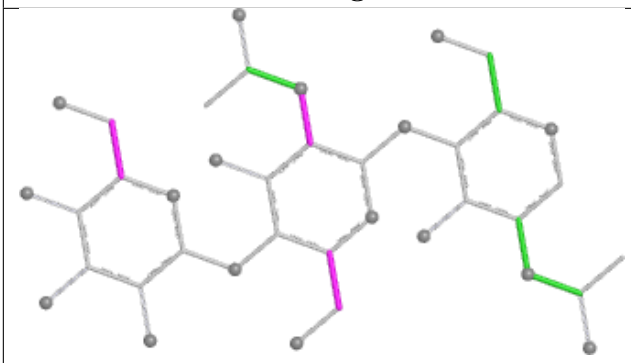
Oligosaccharide Chain G



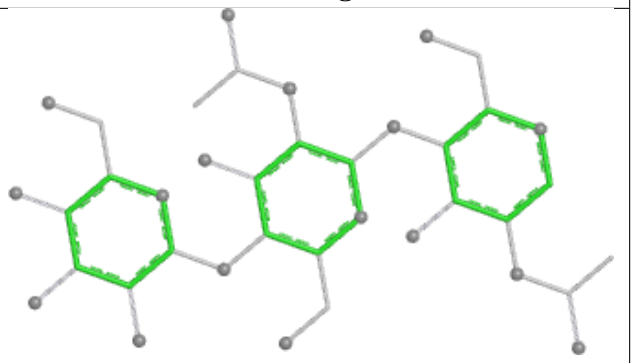
Bond lengths



Bond angles

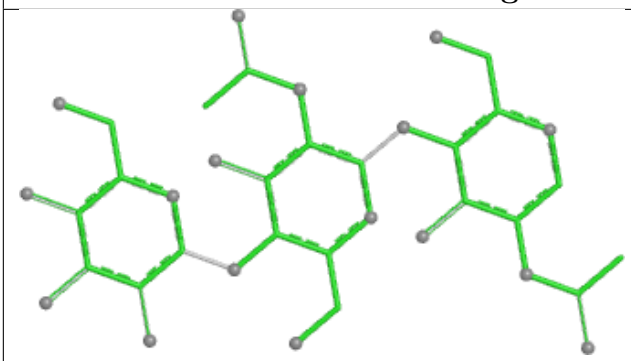


Torsions

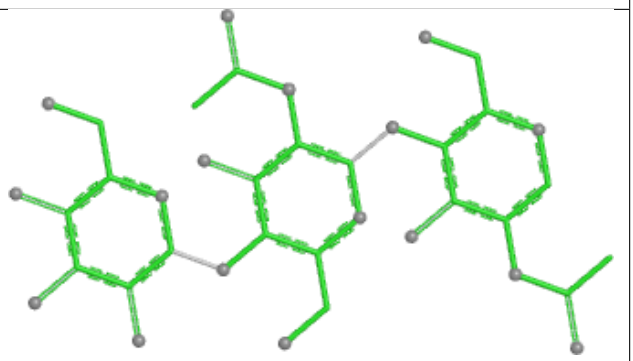


Rings

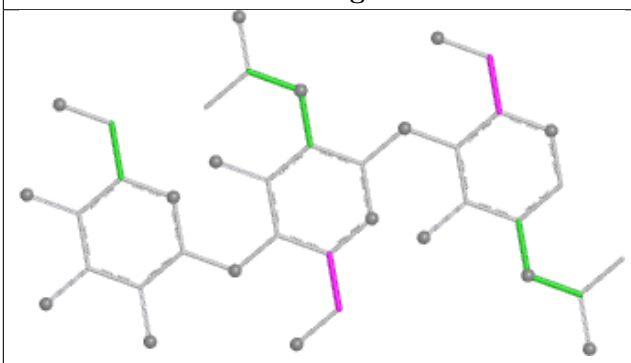
Oligosaccharide Chain I



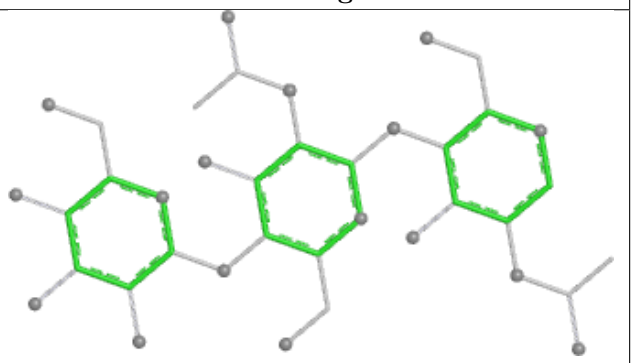
Bond lengths



Bond angles

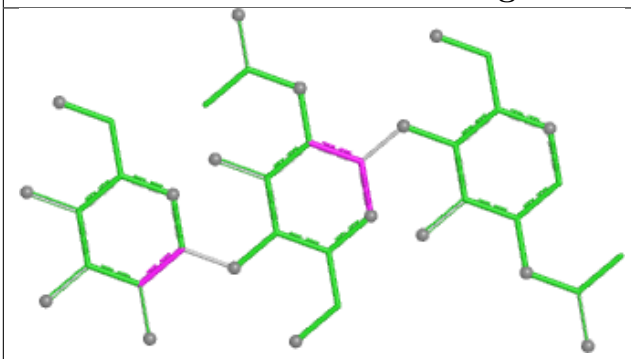


Torsions

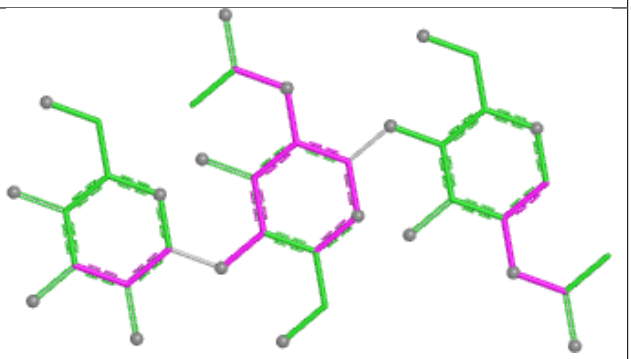


Rings

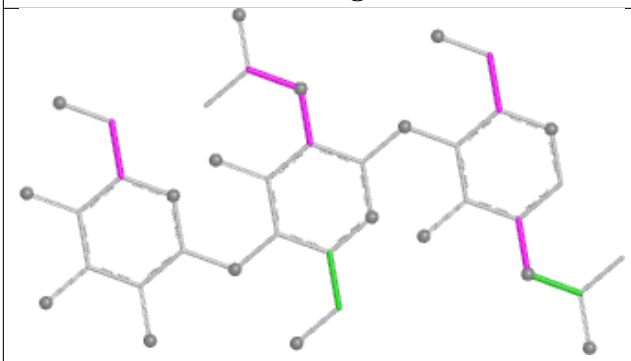
Oligosaccharide Chain J



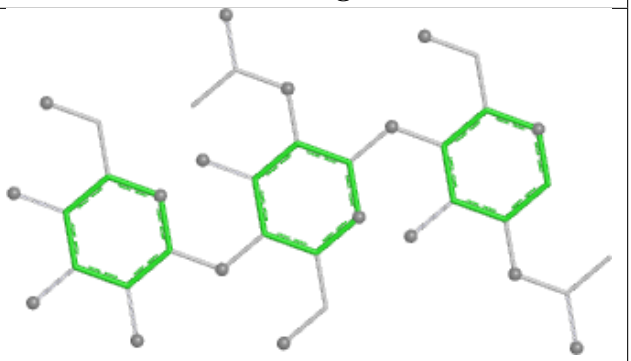
Bond lengths



Bond angles

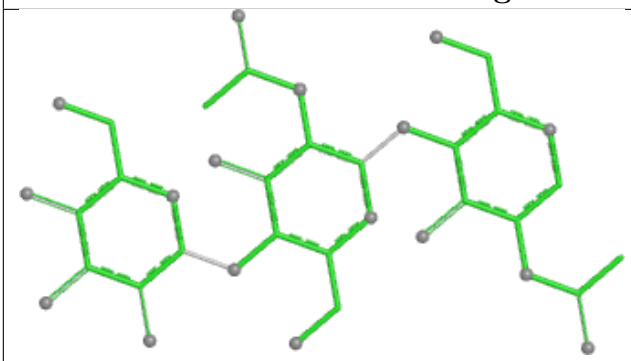


Torsions

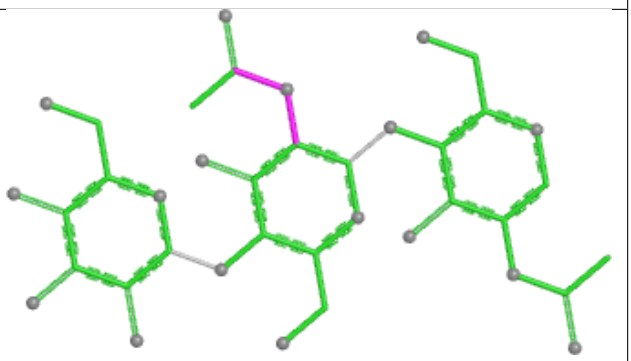


Rings

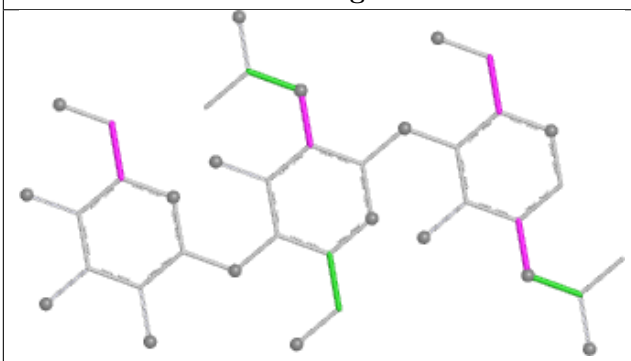
Oligosaccharide Chain K



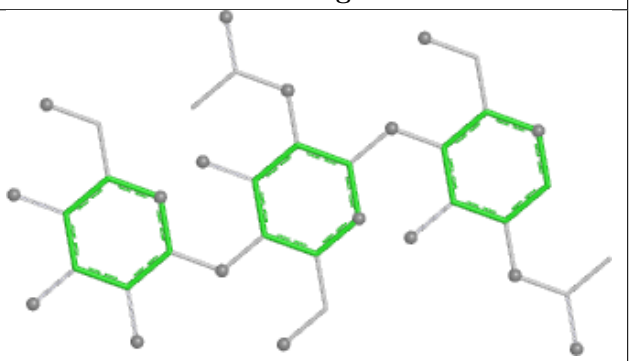
Bond lengths



Bond angles

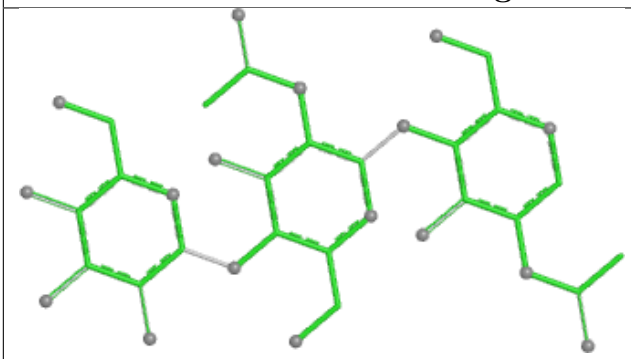


Torsions

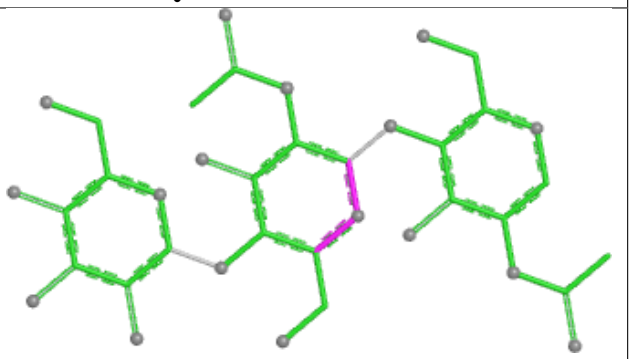


Rings

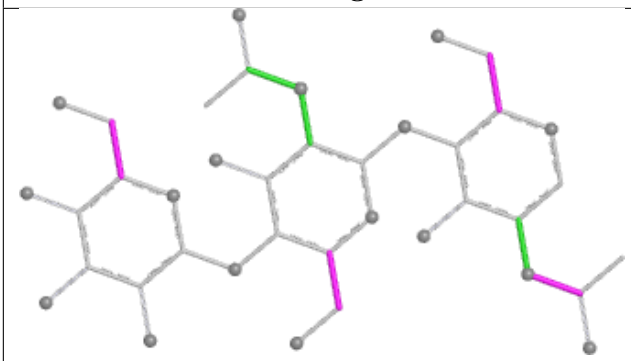
Oligosaccharide Chain Q



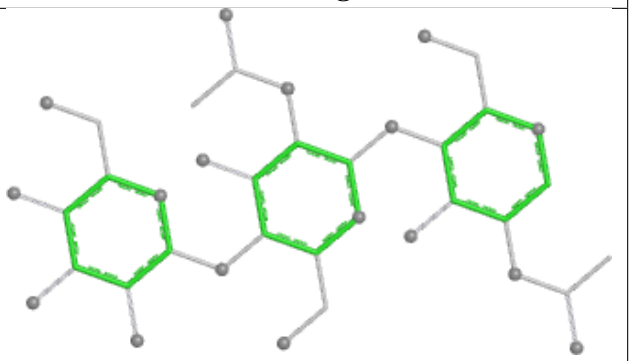
Bond lengths



Bond angles

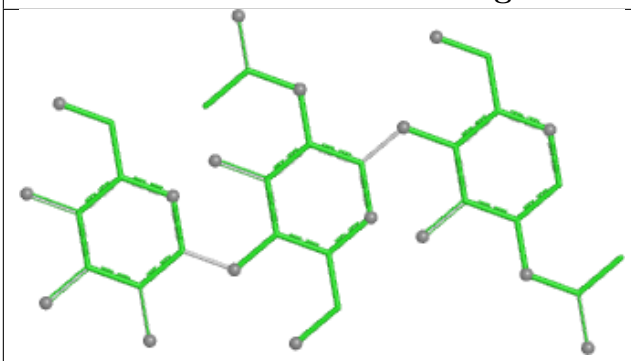


Torsions

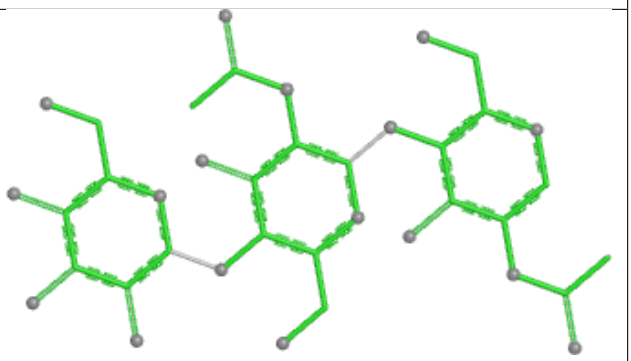


Rings

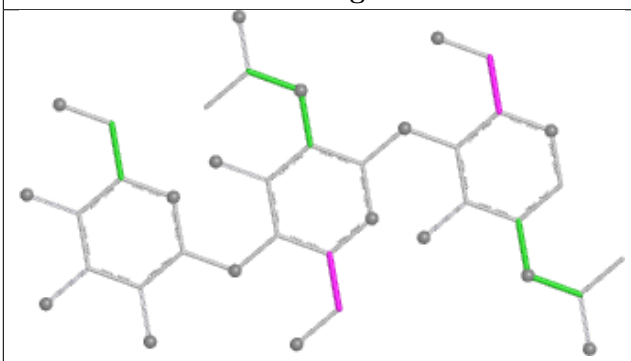
Oligosaccharide Chain R



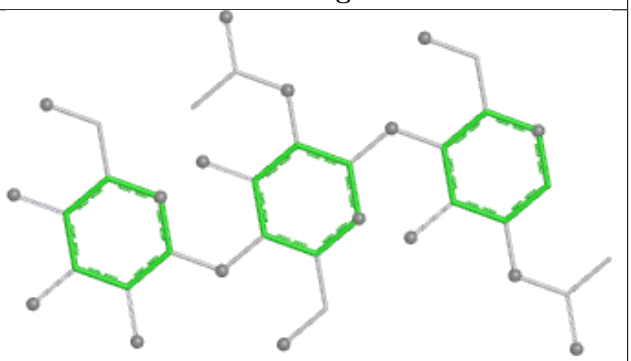
Bond lengths



Bond angles

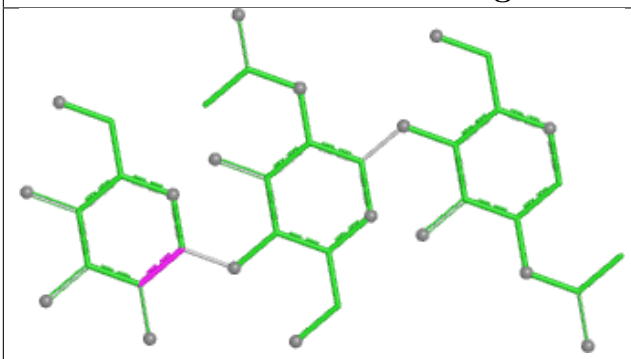


Torsions

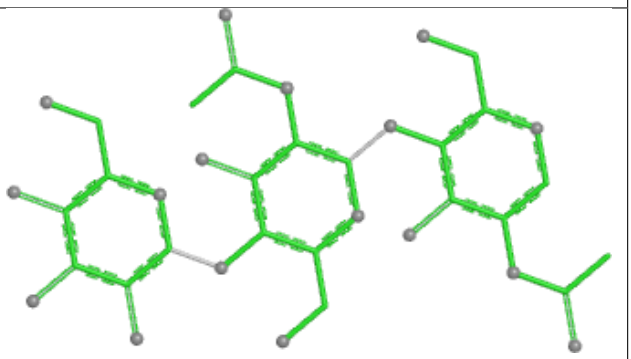


Rings

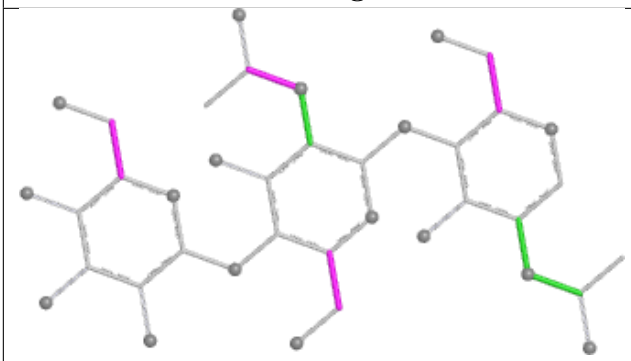
Oligosaccharide Chain U



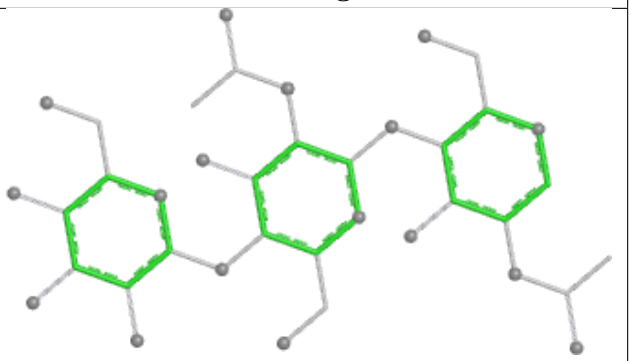
Bond lengths



Bond angles

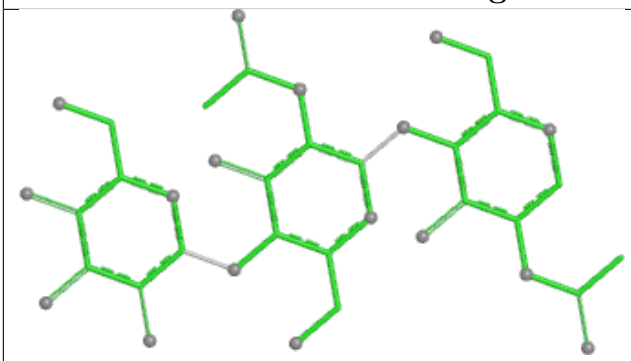


Torsions

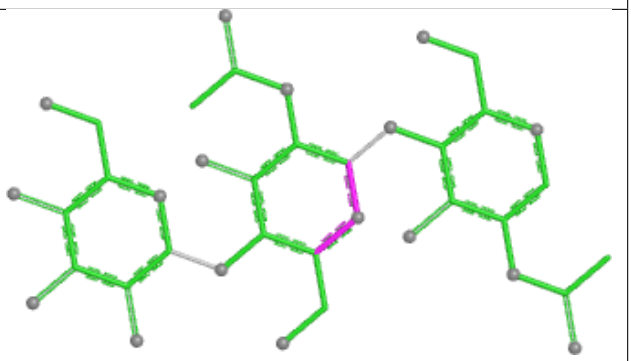


Rings

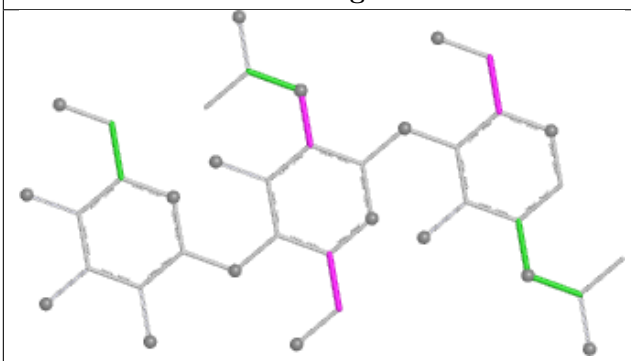
Oligosaccharide Chain W



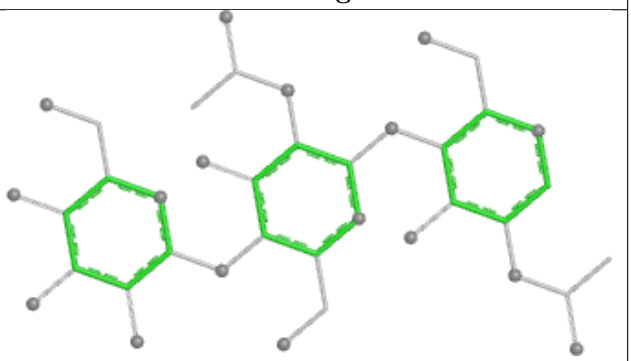
Bond lengths



Bond angles

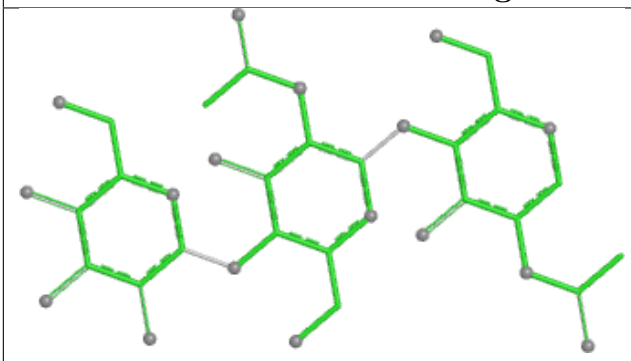


Torsions

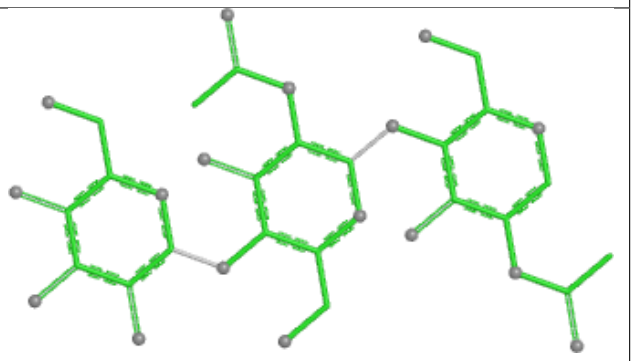


Rings

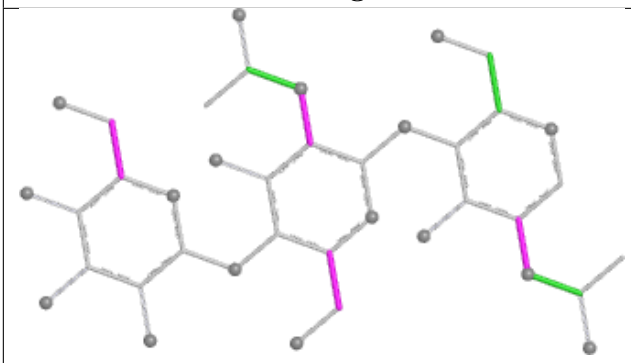
Oligosaccharide Chain X



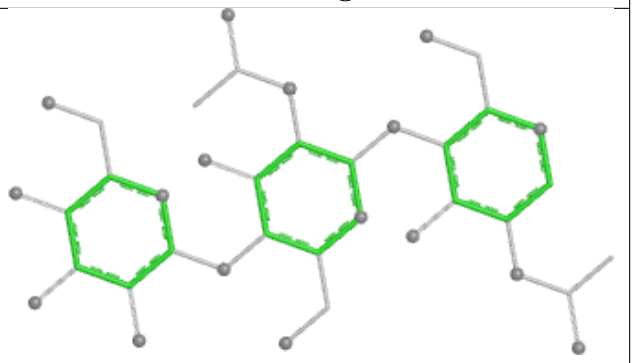
Bond lengths



Bond angles

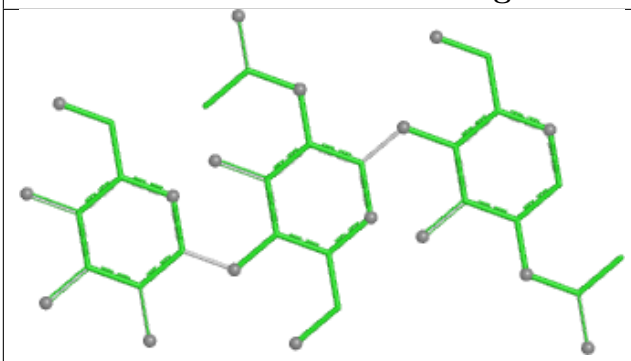


Torsions

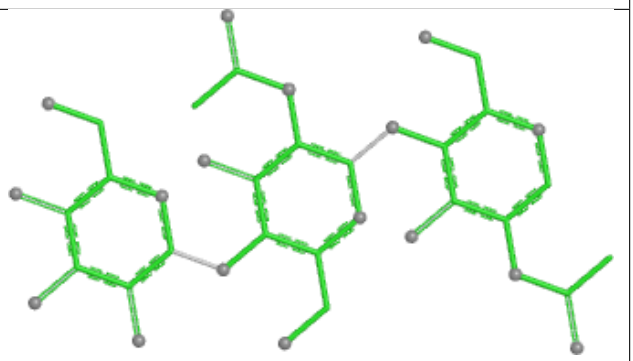


Rings

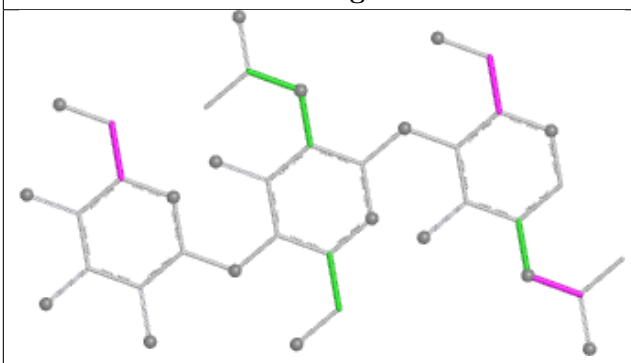
Oligosaccharide Chain Y



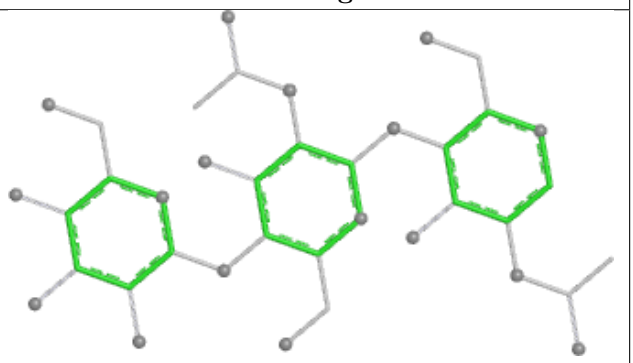
Bond lengths



Bond angles

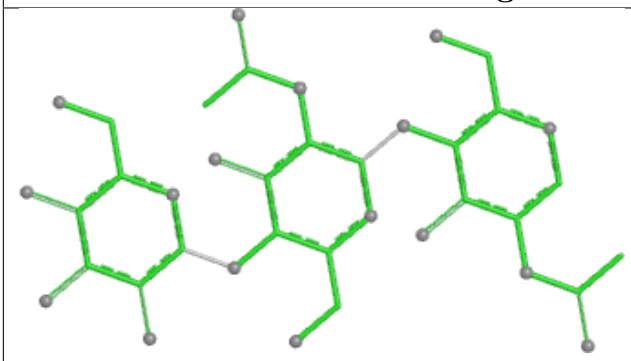


Torsions

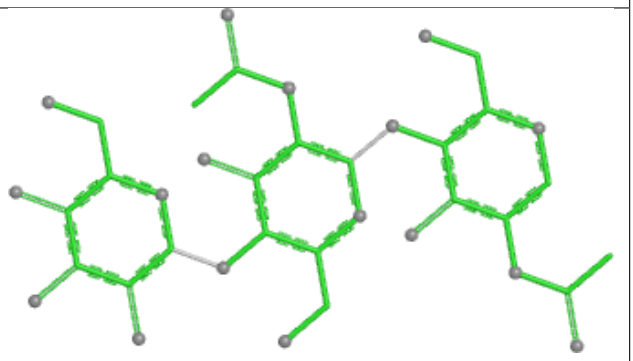


Rings

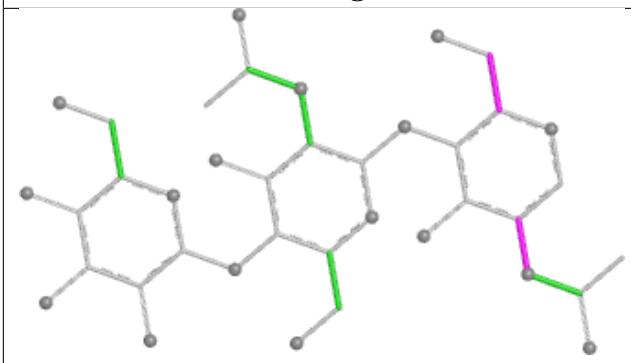
Oligosaccharide Chain Z



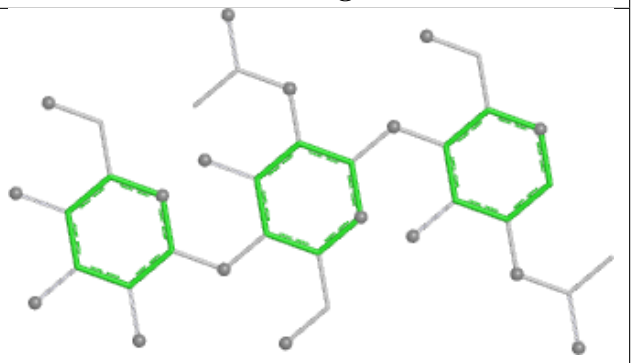
Bond lengths



Bond angles

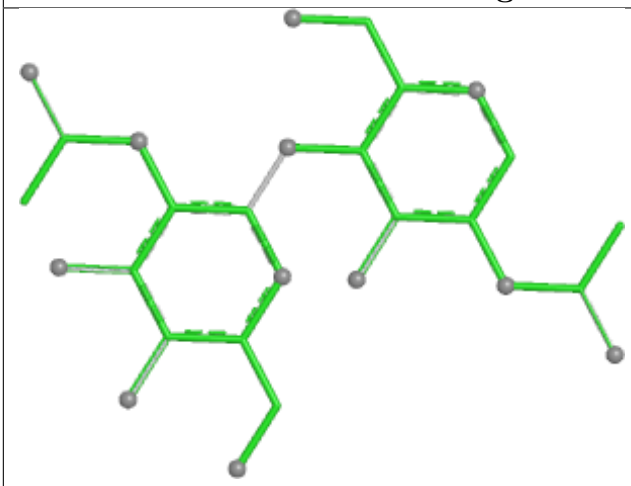


Torsions

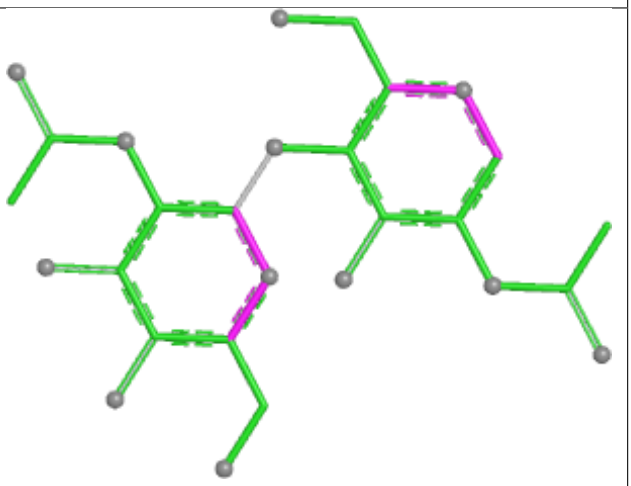


Rings

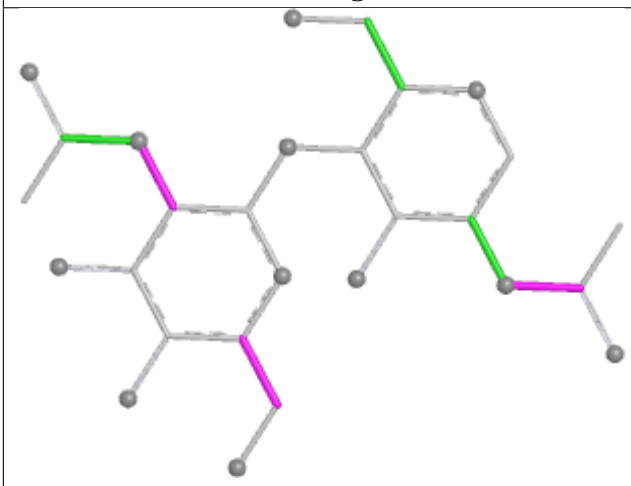
Oligosaccharide Chain F



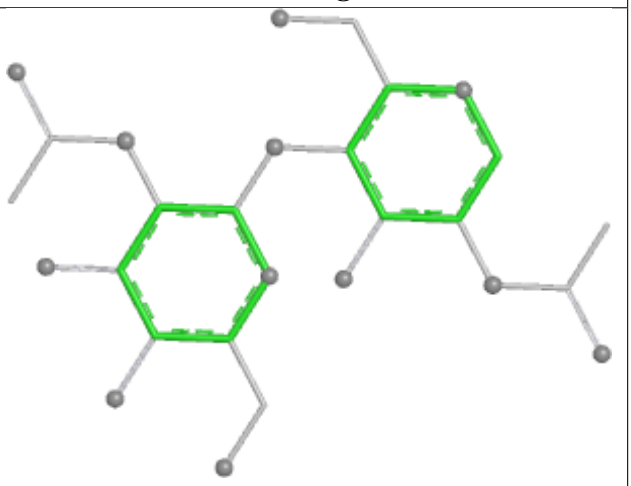
Bond lengths



Bond angles

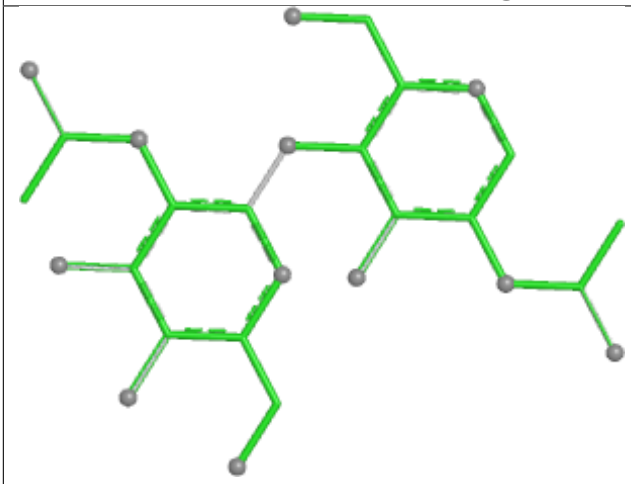


Torsions

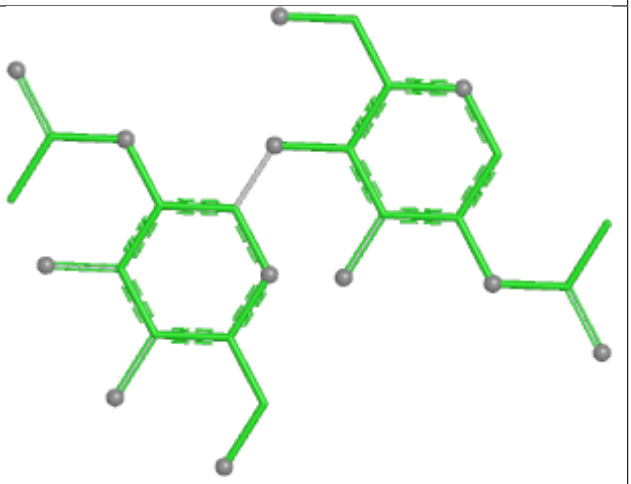


Rings

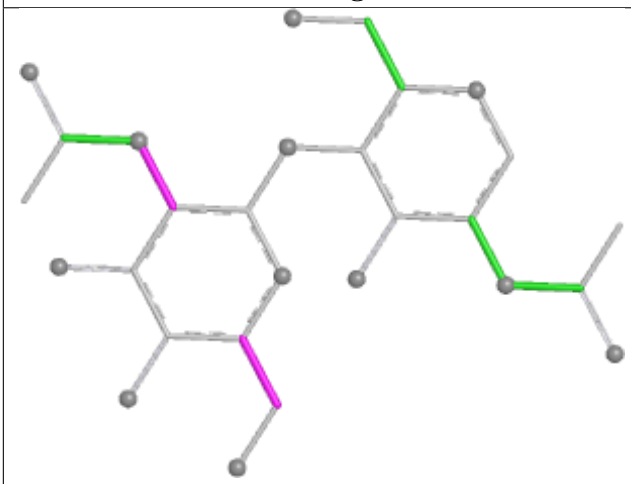
Oligosaccharide Chain S



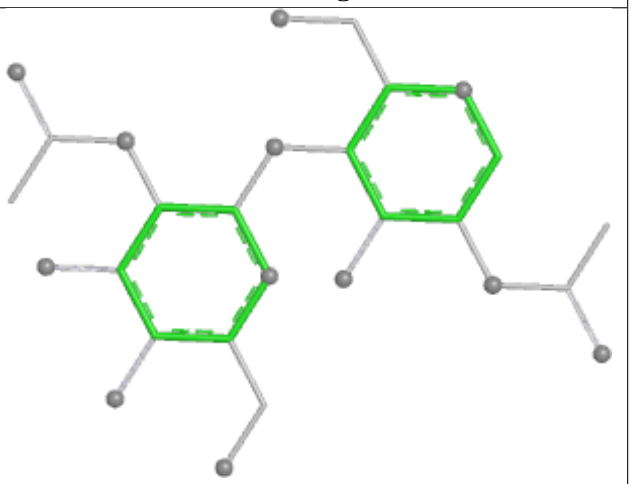
Bond lengths



Bond angles

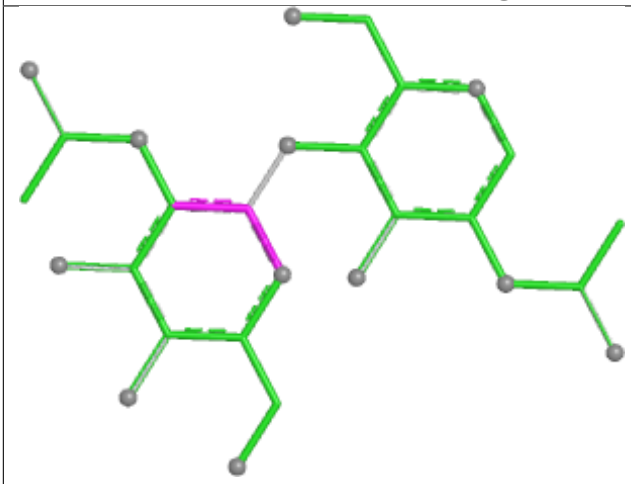


Torsions

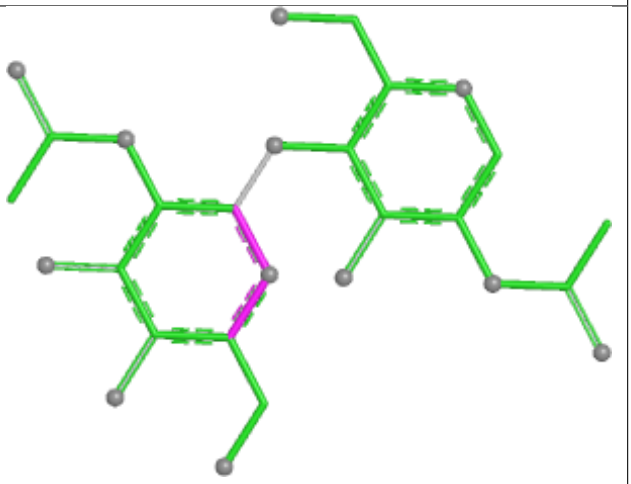


Rings

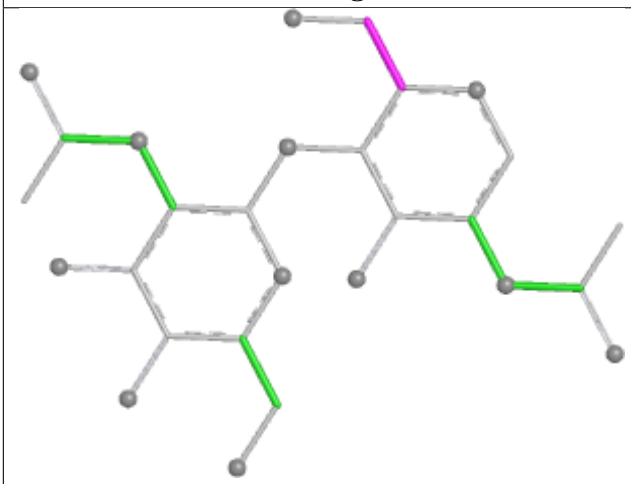
Oligosaccharide Chain T



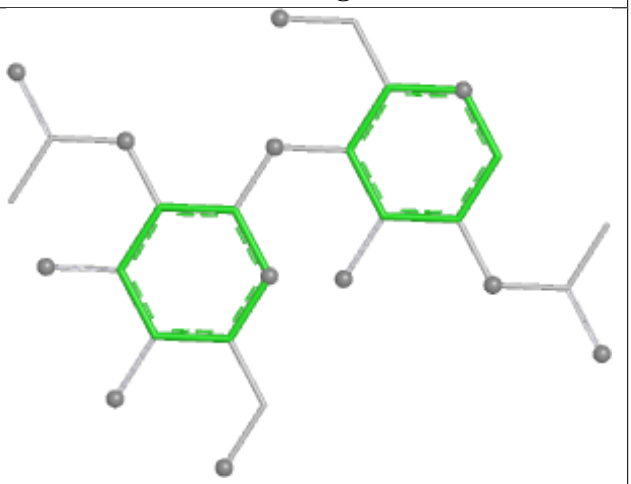
Bond lengths



Bond angles

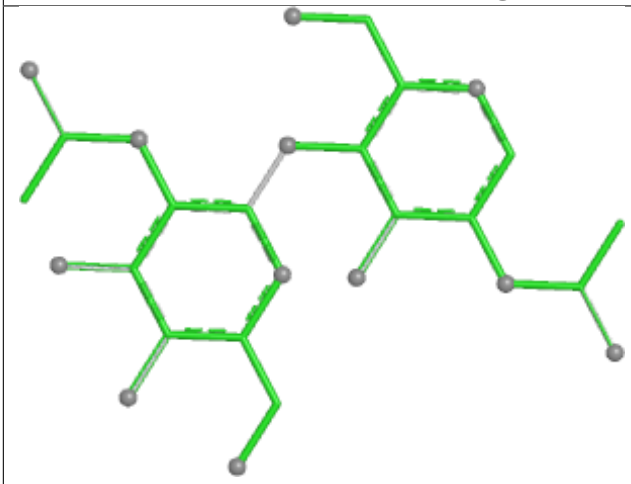


Torsions

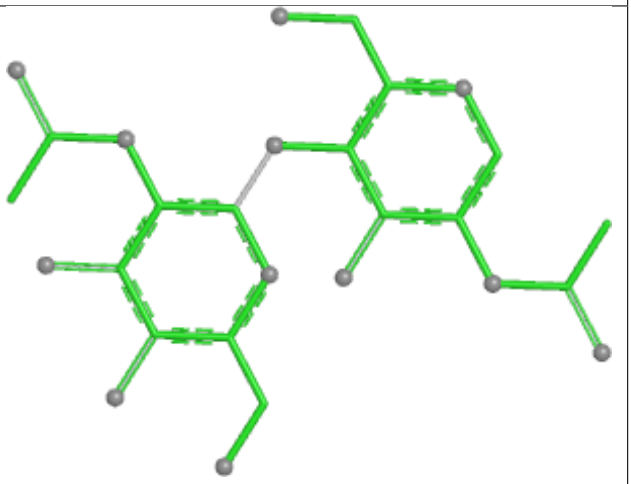


Rings

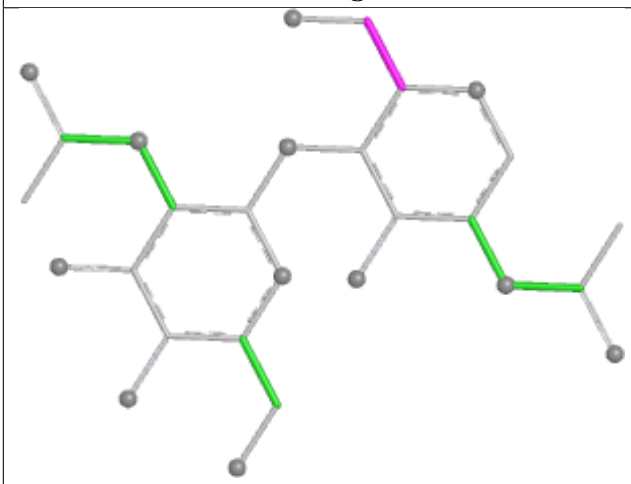
Oligosaccharide Chain V



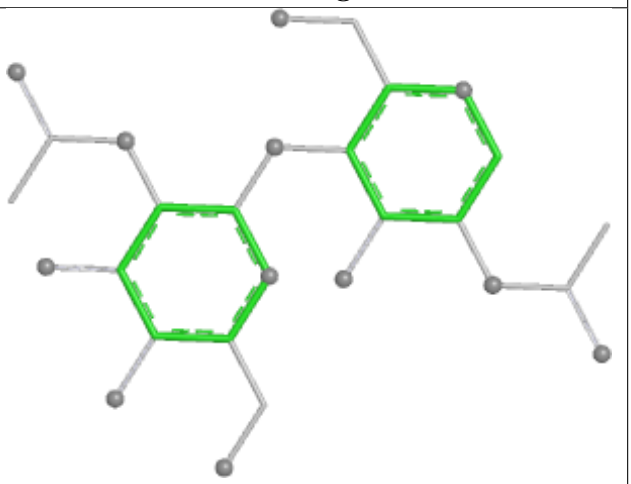
Bond lengths



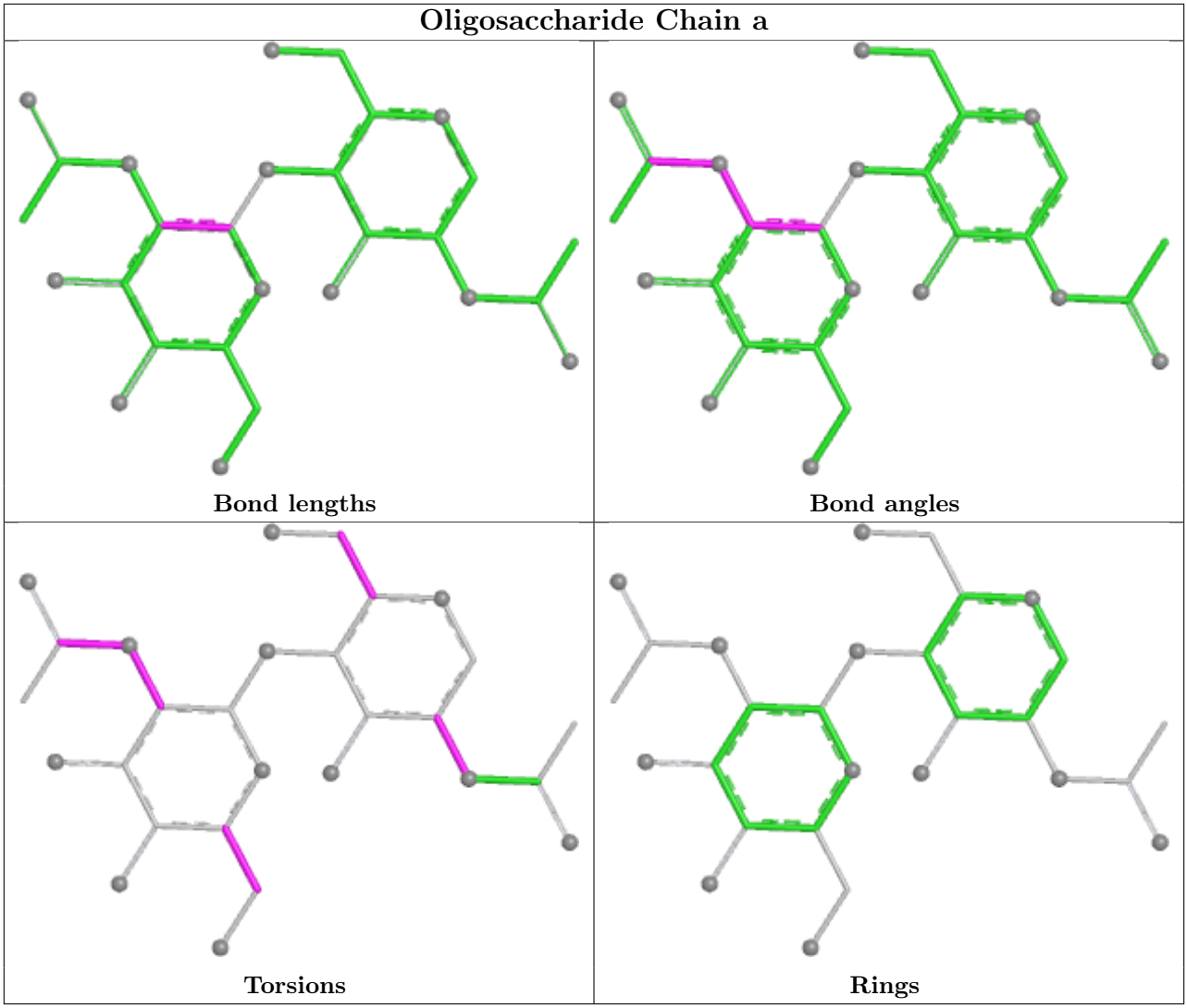
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	601	1	14,14,15	0.47	0	17,19,21	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	NAG	C8-C7-N2-C2
6	B	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	494/505 (97%)	-0.35	4 (0%)	82	69	71, 121, 164, 252	1 (0%)
1	B	488/505 (96%)	-0.33	4 (0%)	82	69	82, 131, 177, 223	0
1	C	487/505 (96%)	-0.34	2 (0%)	89	79	87, 127, 181, 238	0
2	H	221/237 (93%)	-0.07	2 (0%)	81	67	60, 159, 230, 292	0
2	M	221/237 (93%)	-0.04	3 (1%)	73	57	85, 163, 219, 247	0
2	O	221/237 (93%)	-0.13	5 (2%)	61	45	67, 131, 184, 233	0
3	L	214/215 (99%)	-0.01	5 (2%)	61	45	95, 164, 271, 320	0
3	N	213/215 (99%)	-0.07	2 (0%)	81	67	69, 157, 230, 294	1 (0%)
3	P	214/215 (99%)	-0.17	5 (2%)	61	45	77, 142, 180, 305	0
All	All	2773/2871 (96%)	-0.22	32 (1%)	76	61	60, 136, 213, 320	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	164	GLU	8.0
2	M	161	TYR	5.1
3	P	2	SER	4.5
2	M	124	MET	4.2
1	A	460	GLU	3.8
3	P	215	SER	3.6
2	H	74	TRP	3.5
3	P	84	GLU	3.5
3	N	33	PHE	3.4
3	L	2	SER	3.4
1	B	457	GLU	3.0
2	M	160	ASP	2.8
3	L	66	SER	2.8
3	P	134	THR	2.6
1	A	383	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	111	GLN	2.3
2	O	41	PRO	2.3
1	B	152	ASN	2.3
1	C	12	THR	2.3
3	L	209	VAL	2.2
1	A	124	SER	2.2
3	L	149	VAL	2.1
2	O	160	ASP	2.1
1	B	8	ASN	2.1
1	A	173	GLN	2.1
2	O	159	LYS	2.1
1	C	8	ASN	2.1
3	N	173	ASN	2.1
2	O	101	ALA	2.1
1	B	256	GLY	2.0
3	P	174	LYS	2.0
3	L	52	ASN	2.0

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

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

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	601	14/15	0.71	0.12	149,188,209,226	0

6.5 Other polymers (i)

There are no such residues in this entry.