Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 09:20 PM EDT

PDB ID	:	2BUA
Title	:	Crystal Structure Of Porcine Dipeptidyl Peptidase IV (Cd26) in Complex With a Low Molecular Weight Inhibitor.
Authors	:	Nordhoff, S.; Cerezo-Galvez, S.; Feurer, A.; Hill, O.; Matassa, V.G.; Metz, G.; Rummey, C.; Thiemann, M.; Edwards, P.J.
Deposited on	:	2005-06-09
Resolution	:	2.56 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:

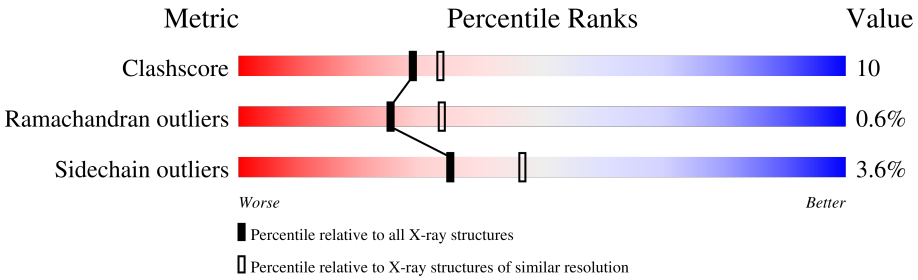
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.56 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))
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	79% 20% •
1	B	728	79% 19% •
1	C	728	79% 20% •
1	D	728	80% 18% •
2	E	2	100%
2	F	2	100%
2	G	2	100%
2	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	I	2	100%
2	J	2	50% 50%
2	K	2	100%
2	L	2	100%
2	M	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
2	NAG	F	1	X	-	-	-
2	NAG	F	2	X	-	-	-
2	NAG	G	1	X	-	-	-
2	NAG	I	2	X	-	-	-
2	NAG	J	1	X	-	-	-
2	NAG	K	1	X	-	-	-
2	NAG	L	1	X	-	-	-
2	NAG	L	2	X	-	-	-
3	NAG	A	1092	X	-	-	-
3	NAG	C	1092	X	-	-	-
3	NAG	D	1085	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25244 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 DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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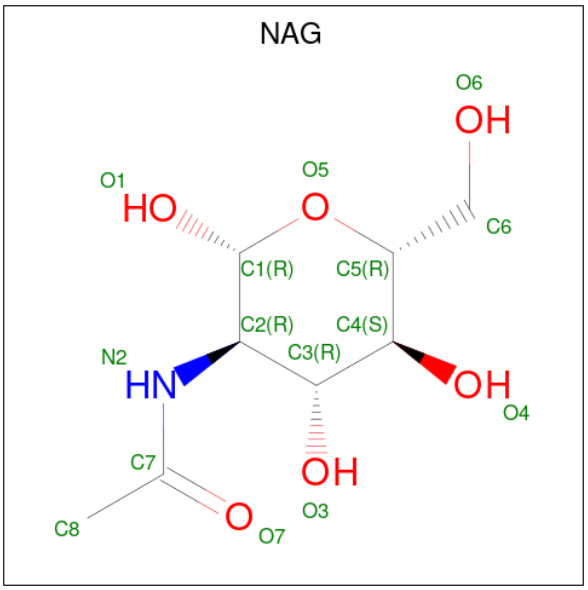
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	M	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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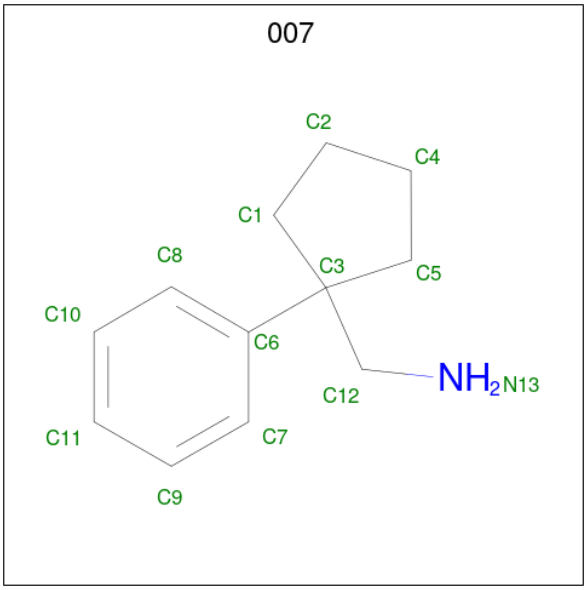
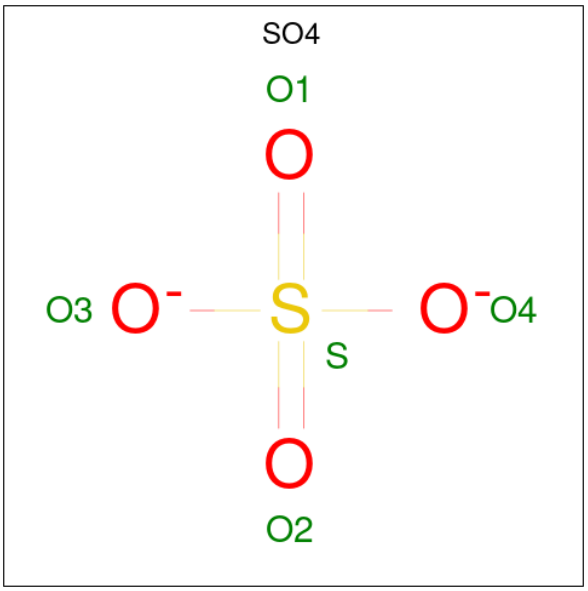
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 1-METHYLAMINE-1-BENZYL-CYCLOPENTANE (three-letter code: 007) (formula: $C_{12}H_{17}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 13 12 1	0	0
4	B	1	Total C N 13 12 1	0	0
4	C	1	Total C N 13 12 1	0	0
4	D	1	Total C N 13 12 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	186	Total O 186 186	0	0
6	B	254	Total O 254 254	0	0
6	C	207	Total O 207 207	0	0
6	D	179	Total O 179 179	0	0

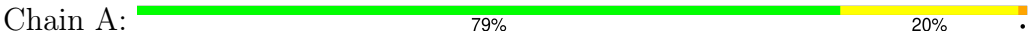
3 Residue-property plots (i)

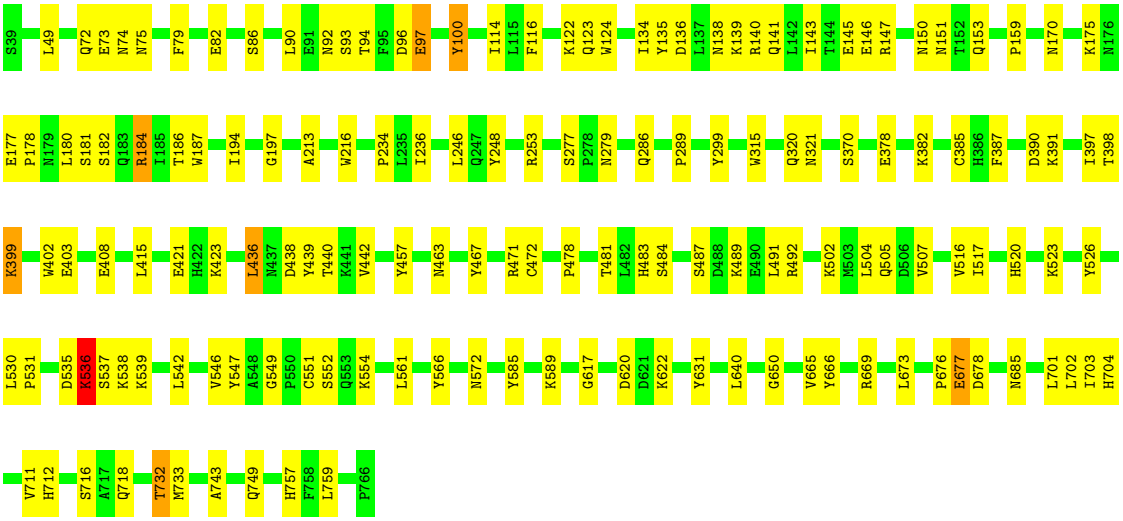
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: DIPEPTIDYL PEPTIDASE IV

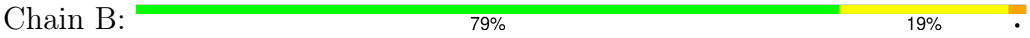
Chain A:

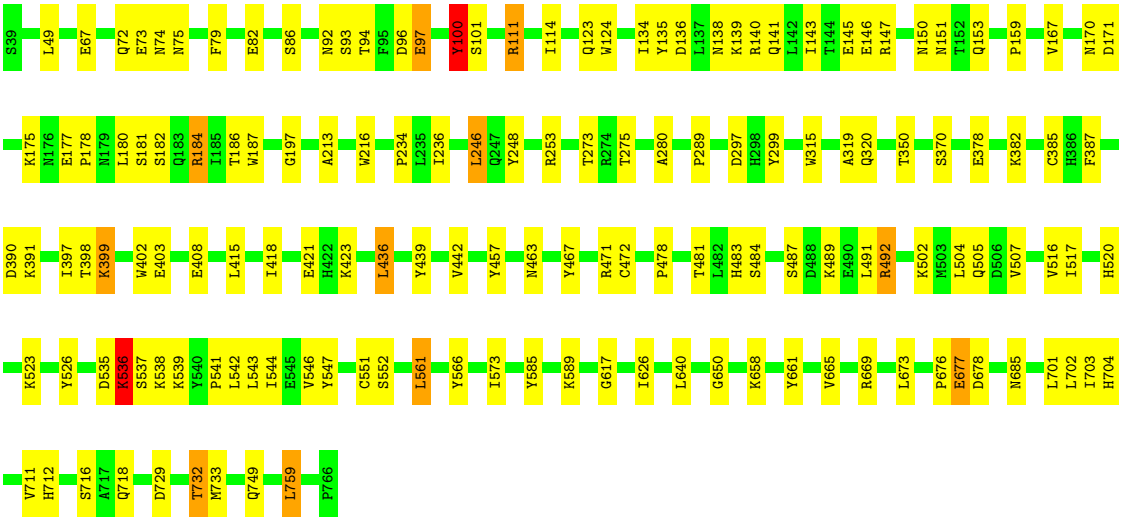




• Molecule 1: DIPEPTIDYL PEPTIDASE IV

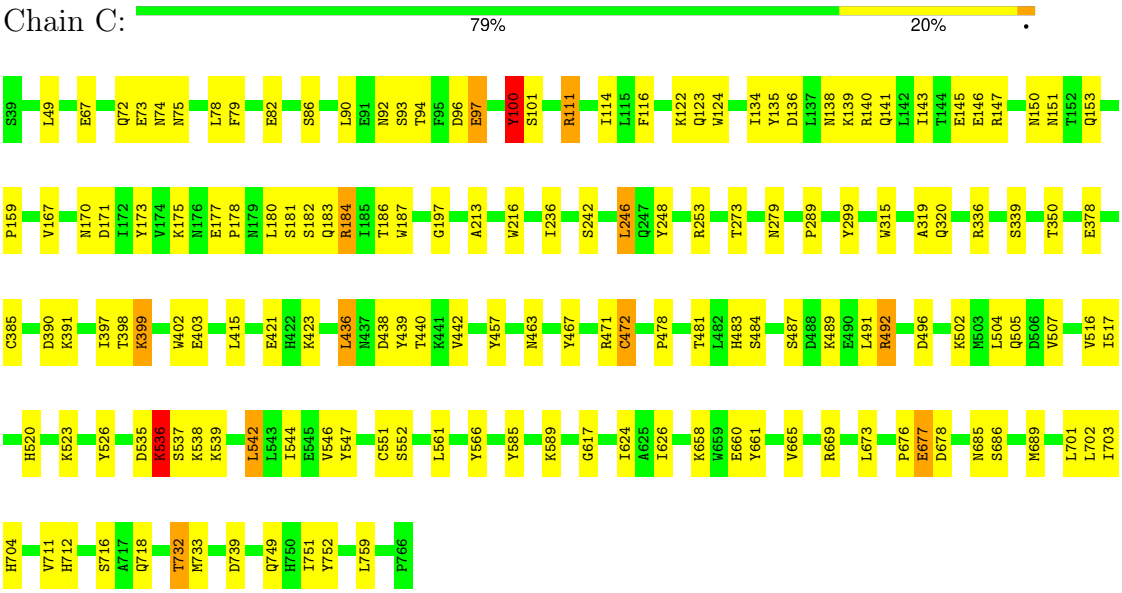
Chain B:





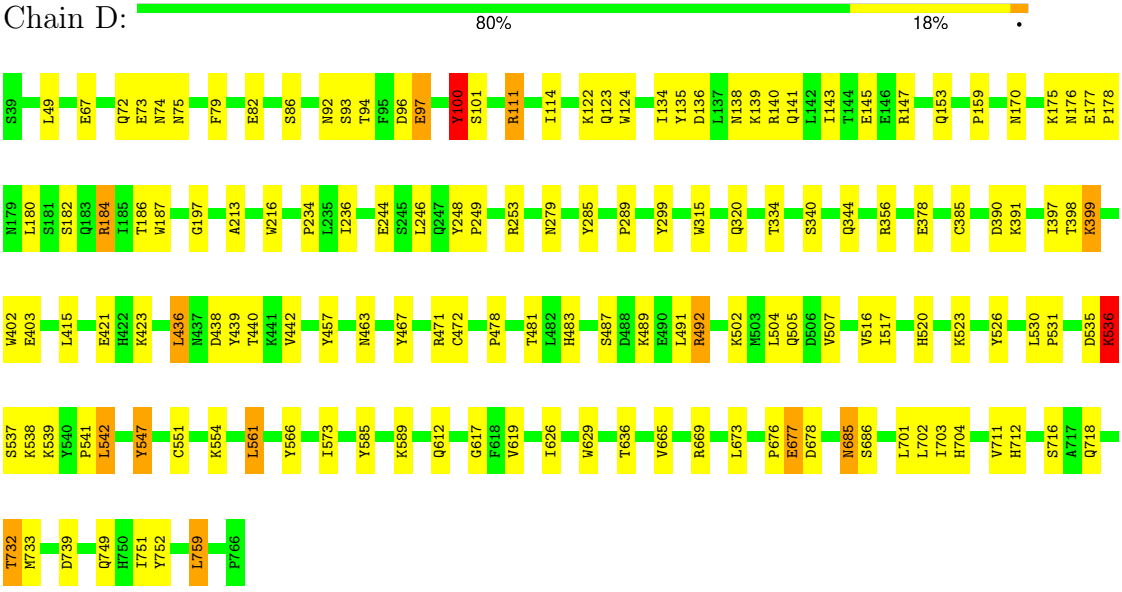
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain C:



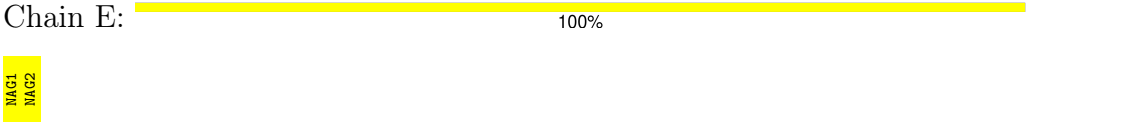
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D:



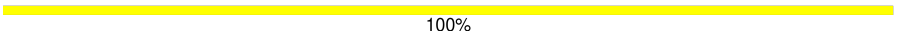
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



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

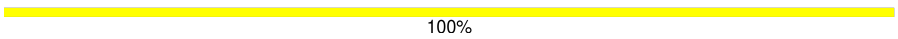
Chain G:

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

Chain H:

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

Chain I:

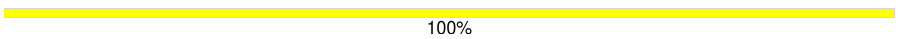


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain K:



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

Chain L:

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

Chain M:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.42Å 118.13Å 133.32Å 112.40° 94.98° 90.99°	Depositor
Resolution (Å)	20.00 – 2.56	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.56)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.220 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25244	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 007, NAG, SO4

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	0.40	0/6141	0.66	3/8353 (0.0%)
1	B	0.39	0/6141	0.66	3/8353 (0.0%)
1	C	0.40	0/6141	0.67	3/8353 (0.0%)
1	D	0.40	0/6141	0.66	3/8353 (0.0%)
All	All	0.40	0/24564	0.66	12/33412 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	492	ARG	NE-CZ-NH1	-15.36	112.62	120.30
1	C	492	ARG	NE-CZ-NH2	14.91	127.76	120.30
1	B	492	ARG	NE-CZ-NH2	-14.49	113.06	120.30
1	A	492	ARG	NE-CZ-NH1	-14.47	113.07	120.30
1	B	492	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	D	492	ARG	NE-CZ-NH2	-14.33	113.13	120.30
1	D	492	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	A	492	ARG	NE-CZ-NH2	14.16	127.38	120.30
1	C	492	ARG	CD-NE-CZ	8.05	134.87	123.60
1	A	492	ARG	CD-NE-CZ	7.93	134.70	123.60
1	B	492	ARG	CD-NE-CZ	7.71	134.40	123.60
1	D	492	ARG	CD-NE-CZ	7.54	134.16	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5663	116	0
1	B	5966	0	5663	120	0
1	C	5966	0	5663	121	0
1	D	5966	0	5660	112	0
2	E	28	0	25	3	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	4	0
2	K	28	0	25	0	0
2	L	28	0	25	3	0
2	M	28	0	25	3	0
3	A	56	0	52	2	0
3	B	56	0	52	1	0
3	C	70	0	65	2	0
3	D	28	0	26	1	0
4	A	13	0	17	1	0
4	B	13	0	17	0	0
4	C	13	0	17	0	0
4	D	13	0	17	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	186	0	0	6	0
6	B	254	0	0	8	0
6	C	207	0	0	10	0
6	D	179	0	0	6	0
All	All	25244	0	23137	459	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 10.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.07	1.00
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.24	0.86
1:A:536:LYS:HD2	1:A:536:LYS:H	1.42	0.84
1:D:536:LYS:H	1:D:536:LYS:HD2	1.45	0.81
1:B:536:LYS:H	1:B:536:LYS:HD2	1.46	0.79
1:C:536:LYS:H	1:C:536:LYS:HD2	1.46	0.78
1:A:536:LYS:HD2	1:A:536:LYS:N	2.01	0.76
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.84	0.75
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.83	0.75
1:C:496:ASP:HB2	6:C:2124:HOH:O	1.87	0.75
1:D:536:LYS:HD2	1:D:536:LYS:N	2.03	0.73
1:C:75:ASN:OD1	1:C:92:ASN:HB3	1.89	0.72
1:A:732:THR:HG22	1:B:732:THR:HG22	1.71	0.72
1:C:536:LYS:HD2	1:C:536:LYS:N	2.03	0.72
1:B:536:LYS:HD2	1:B:536:LYS:N	2.05	0.71
1:A:75:ASN:OD1	1:A:92:ASN:HB3	1.91	0.71
1:D:676:PRO:HG2	1:D:677:GLU:OE1	1.91	0.70
1:C:676:PRO:HG2	1:C:677:GLU:OE1	1.91	0.70
1:B:676:PRO:HG2	1:B:677:GLU:OE1	1.92	0.69
1:A:676:PRO:HG2	1:A:677:GLU:OE1	1.92	0.68
1:D:75:ASN:OD1	1:D:92:ASN:HB3	1.94	0.68
1:A:743:ALA:HB3	6:A:2178:HOH:O	1.92	0.68
1:B:150:ASN:ND2	6:B:2024:HOH:O	2.27	0.67
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.93	0.66
1:B:399:LYS:HD3	1:B:399:LYS:N	2.11	0.66
1:B:75:ASN:OD1	1:B:92:ASN:HB3	1.95	0.66
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.94	0.66
1:A:408:GLU:HG2	6:A:2106:HOH:O	1.96	0.65
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.79	0.65
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.80	0.64
1:B:378:GLU:CD	1:B:378:GLU:H	2.01	0.64
1:D:378:GLU:CD	1:D:378:GLU:H	2.00	0.64
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.64
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.80	0.64
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.95	0.64
1:C:589:LYS:HB3	6:C:2154:HOH:O	1.98	0.63
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.97	0.63
1:A:139:LYS:O	1:A:141:GLN:HG3	1.98	0.63
1:A:378:GLU:CD	1:A:378:GLU:H	2.01	0.63
1:A:382:LYS:HE2	6:A:2140:HOH:O	1.97	0.63
2:J:1:NAG:H62	2:J:2:NAG:HN2	1.64	0.63
2:E:1:NAG:O6	2:E:2:NAG:H82	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.63	0.63
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.80	0.63
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.97	0.63
1:C:378:GLU:H	1:C:378:GLU:CD	2.01	0.63
1:A:589:LYS:HB3	6:A:2139:HOH:O	1.99	0.62
1:C:139:LYS:O	1:C:141:GLN:HG3	2.00	0.62
1:C:492:ARG:NH1	6:C:2135:HOH:O	2.32	0.62
1:B:502:LYS:O	1:B:505:GLN:HG2	1.99	0.62
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.82	0.62
1:A:286:GLN:HB3	1:C:279:ASN:HB3	1.82	0.61
1:D:502:LYS:O	1:D:505:GLN:HG2	1.99	0.61
1:B:139:LYS:O	1:B:141:GLN:HG3	2.00	0.61
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.99	0.61
1:A:535:ASP:OD2	1:A:537:SER:HB3	2.00	0.61
1:A:502:LYS:O	1:A:505:GLN:HG2	2.01	0.61
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.66	0.61
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.01	0.61
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.65	0.61
1:C:502:LYS:O	1:C:505:GLN:HG2	2.01	0.60
1:B:184:ARG:HD3	1:B:186:THR:O	2.02	0.60
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.67	0.60
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.36	0.60
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.59
1:A:535:ASP:C	1:A:537:SER:H	2.06	0.59
3:C:1092:NAG:O3	3:C:1092:NAG:H83	2.02	0.59
1:D:139:LYS:O	1:D:141:GLN:HG3	2.01	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.01	0.59
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.02	0.59
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.85	0.59
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.85	0.59
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.38	0.58
1:C:536:LYS:H	1:C:536:LYS:CD	2.16	0.58
1:A:399:LYS:HD3	1:A:399:LYS:N	2.19	0.58
1:C:399:LYS:HD3	1:C:399:LYS:N	2.19	0.58
1:B:79:PHE:CD1	1:B:86:SER:HB3	2.39	0.58
1:D:399:LYS:HD3	1:D:399:LYS:N	2.19	0.58
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.38	0.58
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.38	0.58
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.39	0.57
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.86	0.57
1:A:546:VAL:HG22	1:A:547:TYR:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.69	0.57
1:D:536:LYS:H	1:D:536:LYS:CD	2.16	0.57
1:A:184:ARG:HD3	1:A:186:THR:O	2.03	0.57
1:B:536:LYS:H	1:B:536:LYS:CD	2.17	0.57
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.40	0.57
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.39	0.57
1:D:535:ASP:C	1:D:537:SER:H	2.09	0.56
1:B:93:SER:HA	1:B:96:ASP:OD2	2.06	0.56
1:C:535:ASP:C	1:C:537:SER:H	2.09	0.56
1:B:516:VAL:HG11	1:B:523:LYS:HB2	1.87	0.56
1:C:184:ARG:HD3	1:C:186:THR:O	2.06	0.56
1:B:399:LYS:N	1:B:399:LYS:CD	2.69	0.56
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.88	0.56
1:D:184:ARG:HD3	1:D:186:THR:O	2.05	0.56
1:A:93:SER:HA	1:A:96:ASP:OD2	2.06	0.56
1:C:491:LEU:HD12	6:C:2135:HOH:O	2.06	0.56
1:C:546:VAL:HG22	1:C:547:TYR:N	2.21	0.56
1:D:739:ASP:HB2	6:D:2169:HOH:O	2.05	0.56
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.88	0.55
1:B:280:ALA:HB2	1:D:285:TYR:CD1	2.42	0.55
1:C:463:ASN:N	1:C:463:ASN:HD22	2.05	0.55
1:C:732:THR:HG22	1:D:732:THR:HG22	1.89	0.55
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.37	0.55
1:B:535:ASP:C	1:B:537:SER:H	2.09	0.55
1:D:93:SER:HA	1:D:96:ASP:OD2	2.07	0.55
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.37	0.55
1:D:249:PRO:HB2	6:D:2055:HOH:O	2.06	0.55
1:B:546:VAL:HG22	1:B:547:TYR:N	2.23	0.54
1:D:279:ASN:OD1	3:D:1279:NAG:N2	2.41	0.54
1:A:546:VAL:CG2	1:A:547:TYR:N	2.71	0.54
1:D:542:LEU:HD12	1:D:619:VAL:HG11	1.88	0.54
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.90	0.54
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.89	0.53
1:C:93:SER:HA	1:C:96:ASP:OD2	2.07	0.53
1:B:143:ILE:HD12	1:B:143:ILE:H	1.74	0.53
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.38	0.53
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.39	0.53
1:D:535:ASP:OD2	1:D:537:SER:HB3	2.08	0.53
1:A:535:ASP:CG	1:A:537:SER:HB3	2.29	0.53
1:C:236:ILE:HG12	1:C:712:HIS:CE1	2.43	0.53
1:D:547:TYR:HB2	1:D:554:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:TYR:CD2	1:B:552:SER:HB2	2.43	0.53
1:A:143:ILE:H	1:A:143:ILE:HD12	1.74	0.53
1:A:733:MET:HE2	1:B:732:THR:HB	1.89	0.53
1:B:535:ASP:OD2	1:B:537:SER:HB3	2.08	0.53
1:C:516:VAL:HG12	1:C:517:ILE:N	2.24	0.53
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.44	0.53
1:A:139:LYS:HD3	1:A:141:GLN:NE2	2.24	0.52
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.45	0.52
1:C:399:LYS:N	1:C:399:LYS:CD	2.73	0.52
1:D:685:ASN:O	2:M:1:NAG:H82	2.09	0.52
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.39	0.52
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.39	0.52
1:B:350:THR:HG22	3:B:1321:NAG:H81	1.92	0.52
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.39	0.52
1:B:382:LYS:HD3	6:B:2128:HOH:O	2.10	0.52
1:B:516:VAL:HG12	1:B:517:ILE:N	2.25	0.52
1:C:73:GLU:O	1:C:74:ASN:HB2	2.10	0.52
1:D:463:ASN:N	1:D:463:ASN:HD22	2.06	0.52
2:G:1:NAG:H62	2:G:2:NAG:H82	1.92	0.52
1:D:704:HIS:HE1	1:D:711:VAL:O	1.94	0.51
1:A:516:VAL:HG12	1:A:517:ILE:N	2.25	0.51
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.24	0.51
1:D:143:ILE:HD12	1:D:143:ILE:H	1.74	0.51
1:A:536:LYS:H	1:A:536:LYS:CD	2.15	0.51
1:B:463:ASN:N	1:B:463:ASN:HD22	2.08	0.51
1:D:399:LYS:N	1:D:399:LYS:CD	2.73	0.51
1:D:516:VAL:HG12	1:D:517:ILE:N	2.26	0.51
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.46	0.51
1:A:399:LYS:N	1:A:399:LYS:CD	2.72	0.51
1:B:147:ARG:HG3	1:B:147:ARG:HH11	1.76	0.51
1:A:535:ASP:O	1:A:537:SER:N	2.44	0.51
1:C:491:LEU:HD22	1:C:491:LEU:H	1.76	0.51
1:C:535:ASP:OD2	1:C:537:SER:HB3	2.09	0.51
2:J:1:NAG:C6	2:J:2:NAG:HN2	2.22	0.51
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.93	0.51
1:C:143:ILE:HD12	1:C:143:ILE:H	1.75	0.51
1:D:589:LYS:HB3	6:D:2131:HOH:O	2.11	0.51
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.41	0.51
1:C:704:HIS:HE1	1:C:711:VAL:O	1.92	0.51
1:A:277:SER:OG	1:C:336:ARG:HD3	2.12	0.50
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:CYS:HB2	6:D:2094:HOH:O	2.11	0.50
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.46	0.50
1:B:535:ASP:CG	1:B:537:SER:HB3	2.32	0.50
1:A:491:LEU:HD22	1:A:491:LEU:H	1.77	0.50
1:D:147:ARG:HG3	1:D:147:ARG:HH11	1.76	0.50
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.92	0.50
2:J:1:NAG:O3	2:J:1:NAG:H83	2.11	0.50
1:C:504:LEU:HA	1:C:507:VAL:HG12	1.94	0.50
1:D:535:ASP:CG	1:D:537:SER:HB3	2.32	0.50
1:D:541:PRO:HG2	1:D:573:ILE:HG12	1.92	0.50
1:B:472:CYS:O	1:B:478:PRO:HA	2.12	0.50
1:B:408:GLU:HG2	6:B:2145:HOH:O	2.12	0.50
1:B:491:LEU:H	1:B:491:LEU:HD22	1.76	0.50
1:C:134:ILE:HG21	1:C:178:PRO:HB3	1.93	0.50
1:A:463:ASN:HD22	1:A:463:ASN:N	2.08	0.50
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.93	0.50
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.93	0.49
1:C:704:HIS:CE1	1:C:711:VAL:O	2.65	0.49
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.94	0.49
1:A:757:HIS:HD2	1:B:729:ASP:OD2	1.96	0.49
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.12	0.49
1:B:704:HIS:HE1	1:B:711:VAL:O	1.95	0.49
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.94	0.49
1:B:589:LYS:HB3	6:B:2199:HOH:O	2.12	0.49
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.94	0.49
1:A:704:HIS:HE1	1:A:711:VAL:O	1.96	0.49
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.27	0.49
1:C:147:ARG:HG3	1:C:147:ARG:HH11	1.76	0.49
1:D:73:GLU:O	1:D:74:ASN:HB2	2.12	0.49
1:D:491:LEU:H	1:D:491:LEU:HD22	1.77	0.49
1:A:194:ILE:CD1	2:E:1:NAG:H82	2.42	0.49
1:B:535:ASP:OD1	1:B:537:SER:HB3	2.13	0.49
1:A:472:CYS:O	1:A:478:PRO:HA	2.13	0.49
1:B:399:LYS:HD3	1:B:399:LYS:H	1.75	0.49
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.27	0.49
1:C:175:LYS:HG2	1:C:182:SER:HB3	1.94	0.49
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.47	0.49
1:A:572:ASN:ND2	6:A:2135:HOH:O	2.40	0.49
1:D:139:LYS:HD3	1:D:141:GLN:NE2	2.28	0.49
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.48	0.49
1:D:704:HIS:CE1	1:D:711:VAL:O	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:MET:HE2	1:D:732:THR:HB	1.94	0.48
1:B:704:HIS:HD2	1:B:716:SER:OG	1.95	0.48
1:C:535:ASP:CG	1:C:537:SER:HB3	2.33	0.48
1:B:73:GLU:O	1:B:74:ASN:HB2	2.13	0.48
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.95	0.48
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.94	0.48
1:D:535:ASP:O	1:D:537:SER:N	2.47	0.48
1:C:472:CYS:O	1:C:478:PRO:HA	2.14	0.48
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.27	0.48
1:A:538:LYS:HG2	1:A:539:LYS:N	2.28	0.48
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.48	0.48
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.14	0.48
2:L:1:NAG:HO3	2:L:2:NAG:C1	2.26	0.48
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.78	0.48
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.95	0.48
1:C:739:ASP:HB2	6:C:2182:HOH:O	2.14	0.48
1:D:535:ASP:OD1	1:D:537:SER:HB3	2.14	0.48
1:A:73:GLU:O	1:A:74:ASN:HB2	2.13	0.48
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.96	0.48
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.14	0.48
1:C:535:ASP:O	1:C:537:SER:N	2.47	0.47
1:B:517:ILE:HG23	1:B:526:TYR:CE2	2.49	0.47
1:A:547:TYR:HD2	1:A:552:SER:HB2	1.80	0.47
1:B:704:HIS:CE1	1:B:711:VAL:O	2.67	0.47
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.15	0.47
1:B:139:LYS:HD3	1:B:141:GLN:NE2	2.29	0.47
1:B:275:THR:HA	1:D:334:THR:O	2.14	0.47
1:D:356:ARG:HB3	1:D:551:CYS:SG	2.54	0.47
1:D:704:HIS:HD2	1:D:716:SER:OG	1.97	0.47
1:C:542:LEU:HB3	1:C:624:ILE:HG23	1.97	0.47
1:C:673:LEU:O	1:C:678:ASP:HB3	2.14	0.47
1:B:535:ASP:O	1:B:537:SER:N	2.47	0.47
2:L:2:NAG:H83	2:L:2:NAG:O3	2.14	0.47
1:C:535:ASP:OD1	1:C:537:SER:HB3	2.13	0.47
1:D:517:ILE:HG23	1:D:526:TYR:CE2	2.50	0.47
1:A:175:LYS:HG2	1:A:182:SER:HB3	1.97	0.47
1:B:97:GLU:OE1	1:B:97:GLU:N	2.45	0.47
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.97	0.47
1:A:704:HIS:HD2	1:A:716:SER:OG	1.98	0.47
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.15	0.47
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HD12	1:A:143:ILE:N	2.31	0.46
1:B:289:PRO:HB3	1:B:315:TRP:CD2	2.49	0.46
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.49	0.46
1:C:516:VAL:CG1	1:C:517:ILE:N	2.78	0.46
1:C:718:GLN:HE21	1:C:718:GLN:CA	2.25	0.46
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.97	0.46
1:A:415:LEU:HD23	1:A:415:LEU:C	2.35	0.46
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.98	0.46
1:B:297:ASP:HA	6:B:2103:HOH:O	2.14	0.46
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.24	0.46
1:B:516:VAL:CG1	1:B:517:ILE:N	2.79	0.46
1:D:175:LYS:HG2	1:D:182:SER:HB3	1.97	0.46
1:D:538:LYS:HG2	1:D:539:LYS:N	2.31	0.46
1:A:279:ASN:OD1	3:A:1279:NAG:O5	2.33	0.46
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.51	0.46
1:C:273:THR:HB	6:C:2024:HOH:O	2.15	0.46
1:D:703:ILE:HG12	1:D:733:MET:HB3	1.98	0.46
1:B:82:GLU:HG2	1:B:467:TYR:OH	2.16	0.46
1:D:143:ILE:HD12	1:D:143:ILE:N	2.31	0.46
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.97	0.46
1:A:150:ASN:O	1:A:151:ASN:HB2	2.15	0.46
1:A:704:HIS:CE1	1:A:711:VAL:O	2.68	0.46
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.98	0.46
1:C:538:LYS:HG2	1:C:539:LYS:N	2.31	0.46
1:D:516:VAL:CG1	1:D:517:ILE:N	2.79	0.46
1:B:100:TYR:HB2	1:B:101:SER:H	1.57	0.45
1:C:150:ASN:O	1:C:151:ASN:HB2	2.16	0.45
1:D:97:GLU:OE1	1:D:97:GLU:N	2.46	0.45
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.51	0.45
1:A:516:VAL:CG1	1:A:517:ILE:N	2.79	0.45
1:B:72:GLN:O	1:B:73:GLU:HB2	2.16	0.45
1:B:457:TYR:HA	1:B:471:ARG:O	2.16	0.45
1:C:82:GLU:HG2	1:C:467:TYR:OH	2.15	0.45
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.50	0.45
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.80	0.45
1:A:535:ASP:C	1:A:537:SER:N	2.68	0.45
1:C:97:GLU:OE1	1:C:97:GLU:N	2.46	0.45
1:D:536:LYS:N	1:D:536:LYS:CD	2.78	0.45
1:A:732:THR:HB	1:B:733:MET:HE2	1.98	0.45
1:C:299:TYR:CZ	1:C:665:VAL:HG22	2.51	0.45
1:D:72:GLN:O	1:D:73:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:SER:C	1:D:489:LYS:N	2.70	0.45
2:L:1:NAG:O3	2:L:2:NAG:C1	2.65	0.45
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.16	0.45
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.98	0.45
1:B:197:GLY:C	1:B:213:ALA:HB3	2.37	0.45
1:D:686:SER:HA	2:M:1:NAG:H82	1.98	0.45
1:A:97:GLU:OE1	1:A:97:GLU:N	2.46	0.45
1:A:194:ILE:HD12	2:E:1:NAG:H82	1.99	0.45
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.52	0.45
1:B:535:ASP:C	1:B:537:SER:N	2.70	0.45
1:B:538:LYS:HG2	1:B:539:LYS:N	2.32	0.45
1:C:487:SER:C	1:C:489:LYS:N	2.70	0.45
1:D:487:SER:C	1:D:489:LYS:H	2.19	0.45
1:A:72:GLN:O	1:A:73:GLU:HB2	2.17	0.45
1:A:321:ASN:ND2	3:A:1321:NAG:C7	2.80	0.45
1:B:546:VAL:CG2	1:B:547:TYR:N	2.79	0.45
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.82	0.45
2:M:2:NAG:H83	2:M:2:NAG:H2	1.89	0.45
1:A:399:LYS:HD3	1:A:399:LYS:H	1.81	0.45
1:B:143:ILE:HD12	1:B:143:ILE:N	2.31	0.45
1:C:177:GLU:HB2	1:C:180:LEU:HB2	1.99	0.45
1:D:397:ILE:HG22	1:D:439:TYR:CE2	2.51	0.45
1:D:535:ASP:C	1:D:537:SER:N	2.70	0.45
1:C:350:THR:HA	3:C:1321:NAG:H81	1.99	0.44
1:C:397:ILE:HG22	1:C:439:TYR:CE2	2.53	0.44
1:D:530:LEU:HA	1:D:531:PRO:HD3	1.89	0.44
1:B:418:ILE:HD12	6:B:2144:HOH:O	2.17	0.44
1:C:704:HIS:HD2	1:C:716:SER:OG	2.00	0.44
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.99	0.44
1:D:197:GLY:C	1:D:213:ALA:HB3	2.38	0.44
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.00	0.44
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.98	0.44
1:C:551:CYS:HB2	6:C:2094:HOH:O	2.16	0.44
1:C:689:MET:HE3	1:D:244:GLU:HG3	2.00	0.44
1:C:535:ASP:C	1:C:537:SER:N	2.71	0.44
1:B:97:GLU:N	1:B:97:GLU:CD	2.71	0.44
1:B:718:GLN:HE21	1:B:718:GLN:CA	2.26	0.44
1:C:159:PRO:HD3	1:C:216:TRP:HB3	2.00	0.44
1:C:487:SER:C	1:C:489:LYS:H	2.20	0.44
1:C:546:VAL:CG2	1:C:547:TYR:N	2.81	0.44
1:B:138:ASN:C	1:B:140:ARG:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ASN:N	1:C:463:ASN:ND2	2.65	0.44
1:D:457:TYR:HA	1:D:471:ARG:O	2.18	0.43
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.27	0.43
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.88	0.43
1:B:418:ILE:CD1	6:B:2144:HOH:O	2.67	0.43
1:C:660:GLU:HG3	6:C:2167:HOH:O	2.17	0.43
1:D:463:ASN:N	1:D:463:ASN:ND2	2.66	0.43
1:A:547:TYR:HB2	1:A:554:LYS:HD3	1.99	0.43
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.82	0.43
1:C:167:VAL:HA	1:C:171:ASP:O	2.18	0.43
1:B:167:VAL:HA	1:B:171:ASP:O	2.19	0.43
1:C:72:GLN:O	1:C:73:GLU:HB2	2.18	0.43
1:B:487:SER:C	1:B:489:LYS:H	2.21	0.43
1:B:487:SER:C	1:B:489:LYS:N	2.71	0.43
1:C:97:GLU:N	1:C:97:GLU:CD	2.72	0.43
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.49	0.43
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.99	0.43
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.00	0.43
1:A:620:ASP:OD1	1:A:622:LYS:HB2	2.19	0.43
1:C:457:TYR:HA	1:C:471:ARG:O	2.19	0.43
1:D:97:GLU:N	1:D:97:GLU:CD	2.71	0.43
1:D:612:GLN:NE2	6:D:2138:HOH:O	2.52	0.43
1:B:177:GLU:HB2	1:B:180:LEU:HB2	1.99	0.43
1:B:319:ALA:O	1:B:320:GLN:HB2	2.19	0.43
1:B:544:ILE:O	1:B:626:ILE:HA	2.19	0.43
1:B:673:LEU:O	1:B:678:ASP:HB3	2.18	0.43
1:C:547:TYR:HD2	1:C:552:SER:HB2	1.83	0.43
1:A:487:SER:C	1:A:489:LYS:N	2.71	0.43
1:B:123:GLN:HG2	1:B:124:TRP:CD2	2.54	0.43
1:C:197:GLY:C	1:C:213:ALA:HB3	2.39	0.43
1:A:138:ASN:C	1:A:140:ARG:H	2.22	0.43
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.65	0.43
1:A:516:VAL:CG1	1:A:523:LYS:HB2	2.49	0.42
1:A:673:LEU:O	1:A:678:ASP:HB3	2.18	0.42
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.54	0.42
1:C:399:LYS:HD3	1:C:399:LYS:H	1.83	0.42
1:C:143:ILE:HD12	1:C:143:ILE:N	2.33	0.42
1:C:703:ILE:HG12	1:C:733:MET:HB3	2.01	0.42
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.39	0.42
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.54	0.42
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.54	0.42
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.82	0.42
1:C:319:ALA:O	1:C:320:GLN:HB2	2.20	0.42
1:D:177:GLU:HB2	1:D:180:LEU:HB2	2.00	0.42
1:D:399:LYS:HD3	1:D:399:LYS:H	1.82	0.42
1:A:97:GLU:N	1:A:97:GLU:CD	2.72	0.42
1:A:457:TYR:HA	1:A:471:ARG:O	2.19	0.42
1:A:487:SER:C	1:A:489:LYS:H	2.21	0.42
1:C:686:SER:HA	2:I:1:NAG:H82	2.01	0.42
1:B:415:LEU:C	1:B:415:LEU:HD23	2.40	0.42
1:D:123:GLN:HG2	1:D:124:TRP:CD2	2.54	0.42
1:A:90:LEU:HD21	1:A:116:PHE:HZ	1.85	0.42
1:A:177:GLU:HB2	1:A:180:LEU:HB2	2.01	0.42
1:A:732:THR:CG2	1:B:732:THR:HG22	2.45	0.42
1:B:551:CYS:SG	1:B:551:CYS:O	2.77	0.42
1:D:138:ASN:C	1:D:140:ARG:H	2.22	0.42
1:D:176:ASN:ND2	6:D:2028:HOH:O	2.47	0.42
1:D:187:TRP:CD1	1:D:187:TRP:N	2.87	0.42
1:C:138:ASN:C	1:C:140:ARG:H	2.22	0.42
1:C:398:THR:HA	6:C:2109:HOH:O	2.20	0.42
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.19	0.42
1:C:415:LEU:HD23	1:C:415:LEU:C	2.40	0.42
1:D:438:ASP:OD1	1:D:440:THR:HB	2.20	0.42
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.55	0.42
1:D:516:VAL:CG1	1:D:523:LYS:HB2	2.50	0.42
1:D:673:LEU:O	1:D:678:ASP:HB3	2.19	0.42
1:B:150:ASN:O	1:B:151:ASN:HB2	2.20	0.42
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.54	0.42
1:B:463:ASN:N	1:B:463:ASN:ND2	2.67	0.42
1:C:183:GLN:HE21	1:C:183:GLN:HB2	1.71	0.42
1:C:438:ASP:OD1	1:C:440:THR:HB	2.20	0.42
1:B:484:SER:HB2	1:B:491:LEU:HD21	2.02	0.41
1:C:67:GLU:CD	1:C:111:ARG:HH12	2.22	0.41
1:D:67:GLU:CD	1:D:111:ARG:HH12	2.23	0.41
1:D:561:LEU:HD12	1:D:561:LEU:HA	1.84	0.41
1:A:197:GLY:C	1:A:213:ALA:HB3	2.41	0.41
1:B:541:PRO:HG2	1:B:573:ILE:HG12	2.02	0.41
1:B:561:LEU:HD12	1:B:561:LEU:HA	1.85	0.41
1:B:759:LEU:HD23	1:B:759:LEU:HA	1.90	0.41
1:C:175:LYS:CG	1:C:182:SER:HB3	2.50	0.41
1:A:463:ASN:N	1:A:463:ASN:ND2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.55	0.41
1:C:122:LYS:HG2	1:C:123:GLN:N	2.34	0.41
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.56	0.41
1:B:146:GLU:OE1	1:B:181:SER:HA	2.20	0.41
1:B:187:TRP:CD1	1:B:187:TRP:N	2.88	0.41
1:A:122:LYS:HG2	1:A:123:GLN:N	2.35	0.41
1:A:551:CYS:HB2	6:A:2090:HOH:O	2.21	0.41
1:B:390:ASP:O	1:B:391:LYS:HD2	2.21	0.41
1:A:666:TYR:CZ	4:A:1767:007:H8	2.56	0.41
1:B:732:THR:HG23	1:B:733:MET:N	2.36	0.41
1:C:187:TRP:CD1	1:C:187:TRP:N	2.88	0.41
1:D:751:ILE:HG23	1:D:752:TYR:N	2.36	0.41
2:J:2:NAG:O3	2:J:2:NAG:C7	2.69	0.41
1:C:146:GLU:OE1	1:C:181:SER:HA	2.20	0.41
1:D:122:LYS:HG2	1:D:123:GLN:N	2.35	0.41
1:D:759:LEU:HD23	1:D:759:LEU:HA	1.90	0.41
1:A:484:SER:HB2	1:A:491:LEU:HD21	2.02	0.41
1:B:273:THR:HB	6:B:2037:HOH:O	2.21	0.41
1:B:516:VAL:CG1	1:B:523:LYS:HB2	2.51	0.41
1:D:390:ASP:O	1:D:391:LYS:HD2	2.21	0.41
1:A:146:GLU:OE1	1:A:181:SER:HA	2.21	0.41
1:A:390:ASP:O	1:A:391:LYS:HD2	2.21	0.41
1:A:438:ASP:OD1	1:A:440:THR:HB	2.21	0.41
1:B:370:SER:HB2	1:B:387:PHE:O	2.21	0.41
1:C:242:SER:HB3	1:C:246:LEU:HD12	2.03	0.41
1:C:484:SER:HB2	1:C:491:LEU:HD21	2.03	0.41
1:C:751:ILE:HG23	1:C:752:TYR:N	2.35	0.41
1:C:339:SER:HB2	6:C:2085:HOH:O	2.20	0.41
1:C:390:ASP:O	1:C:391:LYS:HD2	2.21	0.41
1:D:100:TYR:HB2	1:D:101:SER:H	1.57	0.41
1:A:123:GLN:HG2	1:A:124:TRP:CD2	2.56	0.40
1:A:150:ASN:O	1:A:151:ASN:CB	2.69	0.40
1:B:246:LEU:HD13	1:B:248:TYR:O	2.21	0.40
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.42	0.40
1:A:438:ASP:C	1:A:440:THR:H	2.25	0.40
1:C:100:TYR:HB2	1:C:101:SER:H	1.57	0.40
1:C:544:ILE:O	1:C:626:ILE:HA	2.20	0.40
1:C:658:LYS:HB3	1:C:661:TYR:CD2	2.56	0.40
1:D:248:TYR:HA	1:D:249:PRO:HD3	1.97	0.40
1:B:67:GLU:CD	1:B:111:ARG:HH12	2.25	0.40
1:B:153:GLN:HE22	1:B:170:ASN:HD21	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.42	0.40
1:D:340:SER:O	1:D:344:GLN:HG3	2.22	0.40
1:A:370:SER:HB2	1:A:387:PHE:O	2.21	0.40
1:C:67:GLU:HB3	1:C:78:LEU:HD11	2.03	0.40
1:C:90:LEU:HD21	1:C:116:PHE:HZ	1.86	0.40
1:C:150:ASN:O	1:C:151:ASN:CB	2.70	0.40
2:G:1:NAG:H62	2:G:2:NAG:C8	2.51	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	726/728 (100%)	677 (93%)	45 (6%)	4 (1%)	25	33
1	B	726/728 (100%)	678 (93%)	44 (6%)	4 (1%)	25	33
1	C	726/728 (100%)	676 (93%)	46 (6%)	4 (1%)	25	33
1	D	726/728 (100%)	676 (93%)	46 (6%)	4 (1%)	25	33
All	All	2904/2912 (100%)	2707 (93%)	181 (6%)	16 (1%)	25	33

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	TYR
1	A	536	LYS
1	A	617	GLY
1	B	100	TYR
1	B	536	LYS
1	B	617	GLY
1	C	100	TYR
1	C	536	LYS

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Mol	Chain	Res	Type
1	C	617	GLY
1	D	100	TYR
1	D	536	LYS
1	D	617	GLY
1	A	94	THR
1	B	94	THR
1	C	94	THR
1	D	94	THR

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	652/652 (100%)	631 (97%)	21 (3%)	39	51
1	B	652/652 (100%)	628 (96%)	24 (4%)	34	45
1	C	652/652 (100%)	629 (96%)	23 (4%)	36	48
1	D	652/652 (100%)	627 (96%)	25 (4%)	33	44
All	All	2608/2608 (100%)	2515 (96%)	93 (4%)	35	47

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	100	TYR
1	A	145	GLU
1	A	184	ARG
1	A	246	LEU
1	A	385	CYS
1	A	399	LYS
1	A	423	LYS
1	A	436	LEU
1	A	442	VAL
1	A	520	HIS
1	A	536	LYS
1	A	542	LEU

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Mol	Chain	Res	Type
1	A	561	LEU
1	A	566	TYR
1	A	677	GLU
1	A	685	ASN
1	A	701	LEU
1	A	702	LEU
1	A	732	THR
1	A	759	LEU
1	B	97	GLU
1	B	100	TYR
1	B	111	ARG
1	B	145	GLU
1	B	184	ARG
1	B	246	LEU
1	B	385	CYS
1	B	399	LYS
1	B	423	LYS
1	B	436	LEU
1	B	442	VAL
1	B	492	ARG
1	B	520	HIS
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	561	LEU
1	B	566	TYR
1	B	677	GLU
1	B	685	ASN
1	B	701	LEU
1	B	702	LEU
1	B	732	THR
1	B	759	LEU
1	C	97	GLU
1	C	100	TYR
1	C	111	ARG
1	C	145	GLU
1	C	184	ARG
1	C	246	LEU
1	C	385	CYS
1	C	399	LYS
1	C	423	LYS
1	C	436	LEU

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Mol	Chain	Res	Type
1	C	442	VAL
1	C	472	CYS
1	C	520	HIS
1	C	536	LYS
1	C	542	LEU
1	C	561	LEU
1	C	566	TYR
1	C	677	GLU
1	C	685	ASN
1	C	701	LEU
1	C	702	LEU
1	C	732	THR
1	C	759	LEU
1	D	97	GLU
1	D	100	TYR
1	D	111	ARG
1	D	145	GLU
1	D	184	ARG
1	D	246	LEU
1	D	385	CYS
1	D	399	LYS
1	D	423	LYS
1	D	436	LEU
1	D	442	VAL
1	D	492	ARG
1	D	520	HIS
1	D	536	LYS
1	D	542	LEU
1	D	547	TYR
1	D	561	LEU
1	D	566	TYR
1	D	629	TRP
1	D	677	GLU
1	D	685	ASN
1	D	701	LEU
1	D	702	LEU
1	D	732	THR
1	D	759	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	72	GLN
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	183	GLN
1	A	192	ASN
1	A	247	GLN
1	A	369	ASN
1	A	435	GLN
1	A	463	ASN
1	A	483	HIS
1	A	505	GLN
1	A	520	HIS
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	A	757	HIS
1	B	61	GLN
1	B	72	GLN
1	B	141	GLN
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN
1	B	219	ASN
1	B	247	GLN
1	B	369	ASN
1	B	435	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	520	HIS
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN

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Mol	Chain	Res	Type
1	B	745	ASN
1	B	757	HIS
1	C	61	GLN
1	C	72	GLN
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	183	GLN
1	C	192	ASN
1	C	247	GLN
1	C	369	ASN
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	520	HIS
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	757	HIS
1	D	61	GLN
1	D	72	GLN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	247	GLN
1	D	369	ASN
1	D	435	GLN
1	D	463	ASN
1	D	483	HIS
1	D	505	GLN
1	D	520	HIS
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN

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Mol	Chain	Res	Type
1	D	704	HIS
1	D	718	GLN
1	D	745	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.52	0	17,19,21	0.66	0
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	0.70	0
2	NAG	F	1	2,1	14,14,15	0.90	0	17,19,21	1.48	3 (17%)
2	NAG	F	2	2	14,14,15	0.86	1 (7%)	17,19,21	0.84	0
2	NAG	G	1	2,1	14,14,15	0.79	0	17,19,21	1.14	3 (17%)
2	NAG	G	2	2	14,14,15	0.63	0	17,19,21	1.14	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.60	0	17,19,21	0.66	0
2	NAG	H	2	2	14,14,15	0.59	0	17,19,21	0.81	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.74	0	17,19,21	0.59	0
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.79	0
2	NAG	J	1	2,1	14,14,15	0.90	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	0.70	0
2	NAG	K	1	2,1	14,14,15	0.71	0	17,19,21	1.55	4 (23%)
2	NAG	K	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	L	1	2,1	14,14,15	1.03	1 (7%)	17,19,21	1.34	3 (17%)
2	NAG	L	2	2	14,14,15	0.87	1 (7%)	17,19,21	0.87	0
2	NAG	M	1	2,1	14,14,15	0.62	0	17,19,21	0.73	0
2	NAG	M	2	2	14,14,15	0.58	0	17,19,21	0.97	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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	NAG	K	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	L	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	NAG	C1-C2	2.77	1.56	1.52
2	J	1	NAG	C1-C2	2.73	1.56	1.52
2	F	2	NAG	C1-C2	2.37	1.55	1.52
2	I	2	NAG	C1-C2	2.34	1.55	1.52
2	L	2	NAG	C1-C2	2.34	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	NAG	C1-C2	2.27	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C4-C3-C2	-4.18	104.90	111.02
2	K	1	NAG	C1-O5-C5	3.85	117.34	112.19
2	K	1	NAG	O5-C1-C2	3.32	116.43	111.29
2	L	1	NAG	O5-C1-C2	2.94	115.85	111.29
2	G	2	NAG	C4-C3-C2	-2.88	106.79	111.02
2	F	1	NAG	C2-N2-C7	-2.70	119.28	122.90
2	G	2	NAG	C2-N2-C7	-2.69	119.29	122.90
2	L	1	NAG	C3-C4-C5	-2.65	105.42	110.23
2	G	1	NAG	O5-C1-C2	2.53	115.20	111.29
2	L	1	NAG	C1-O5-C5	2.52	115.57	112.19
2	M	2	NAG	C2-N2-C7	-2.48	119.58	122.90
2	G	1	NAG	C1-O5-C5	2.44	115.45	112.19
2	F	1	NAG	O4-C4-C3	2.35	115.92	110.38
2	H	2	NAG	C2-N2-C7	-2.30	119.81	122.90
2	G	1	NAG	C2-N2-C7	-2.26	119.87	122.90
2	K	1	NAG	C2-N2-C7	-2.25	119.89	122.90
2	J	1	NAG	O5-C1-C2	2.21	114.72	111.29
2	K	1	NAG	C3-C4-C5	-2.02	106.57	110.23

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1
2	F	2	NAG	C1
2	G	1	NAG	C1
2	I	2	NAG	C1
2	J	1	NAG	C1
2	K	1	NAG	C1
2	L	1	NAG	C1
2	L	2	NAG	C1

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2

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

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Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

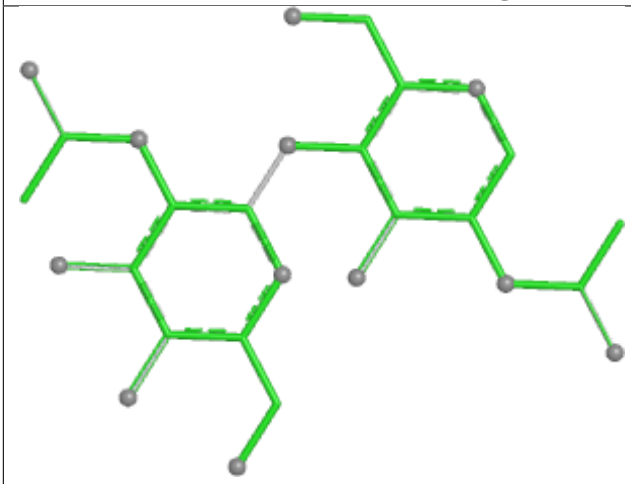
There are no ring outliers.

11 monomers are involved in 16 short contacts:

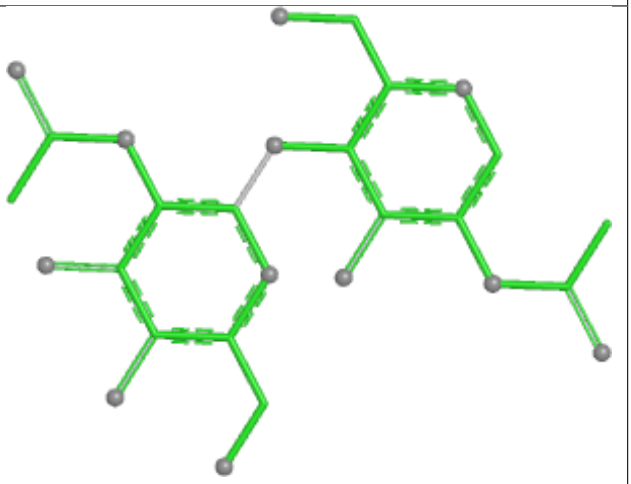
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	2	0
2	L	1	NAG	2	0
2	G	1	NAG	2	0
2	I	1	NAG	1	0
2	M	2	NAG	1	0
2	M	1	NAG	2	0
2	E	2	NAG	1	0
2	E	1	NAG	3	0
2	L	2	NAG	3	0
2	J	2	NAG	3	0
2	J	1	NAG	3	0

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

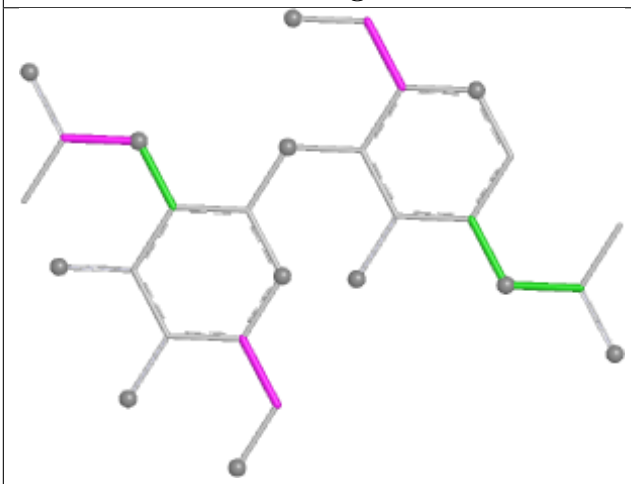
Oligosaccharide Chain E



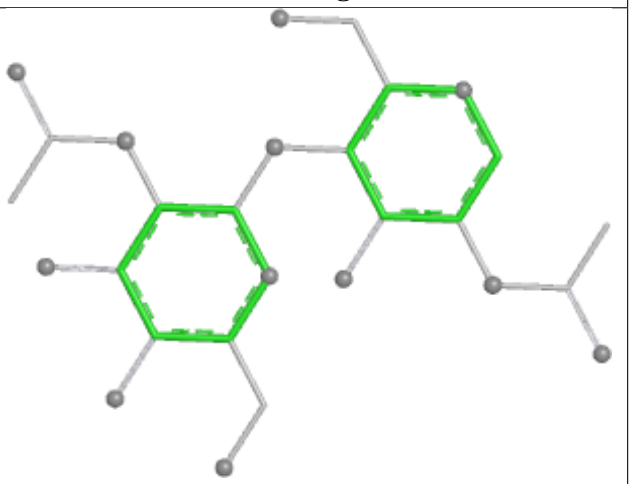
Bond lengths



Bond angles

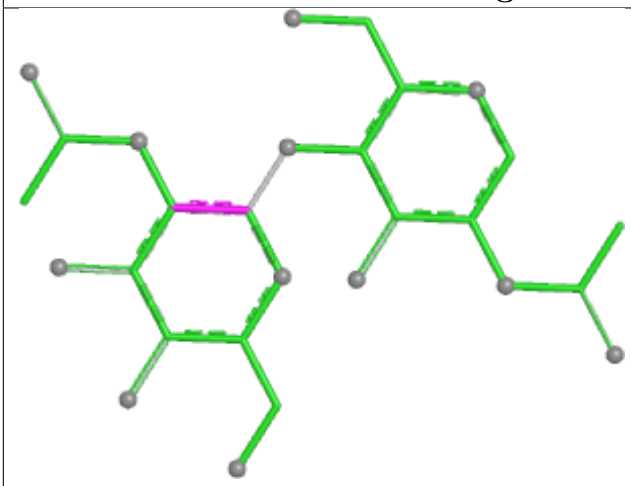


Torsions

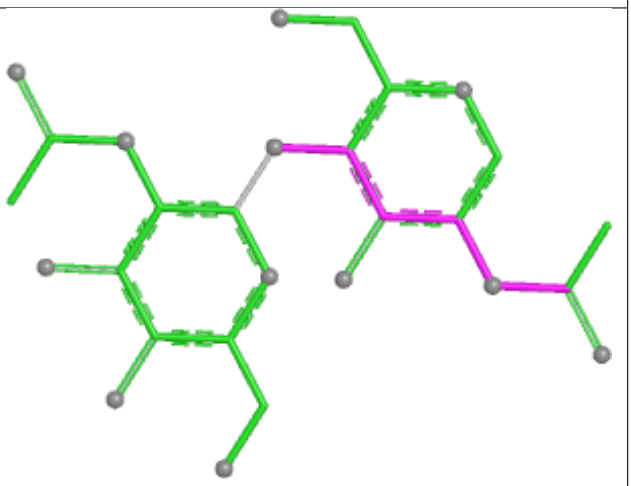


Rings

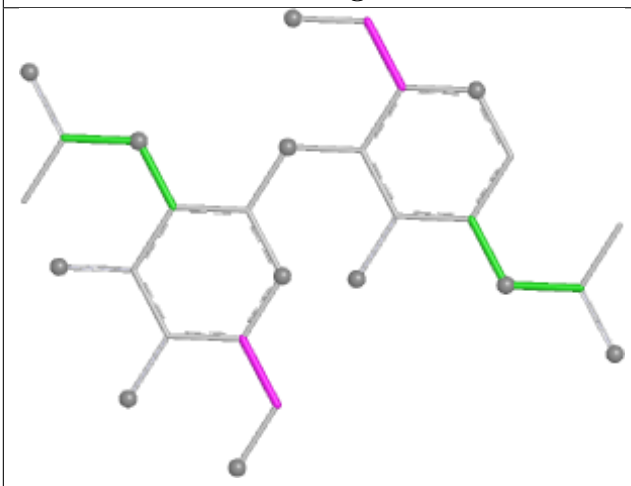
Oligosaccharide Chain F



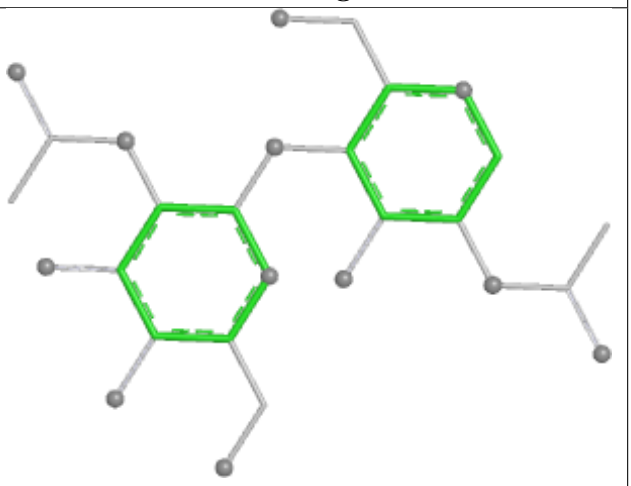
Bond lengths



Bond angles

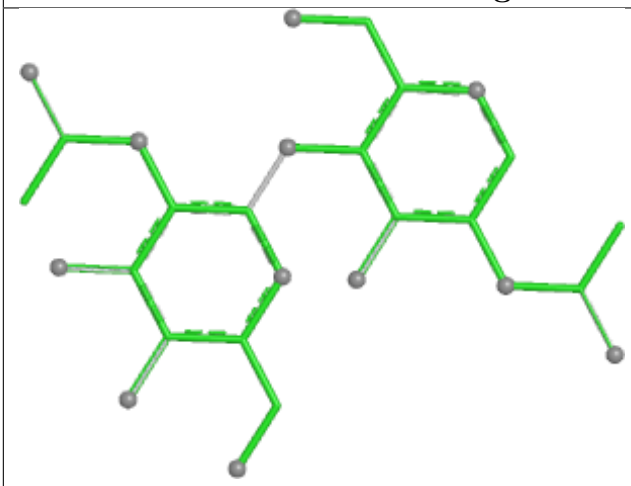


Torsions

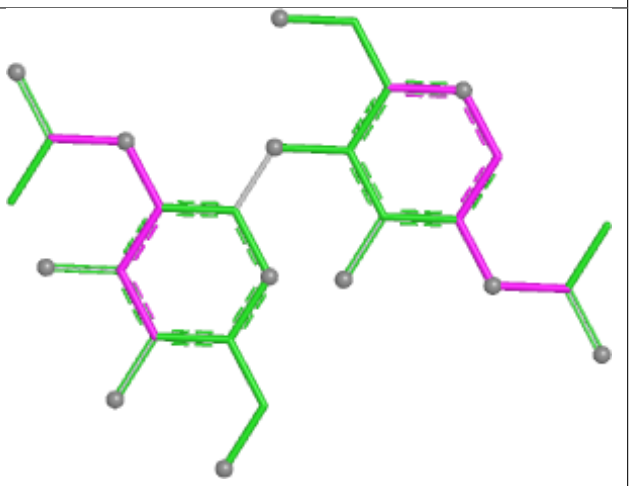


Rings

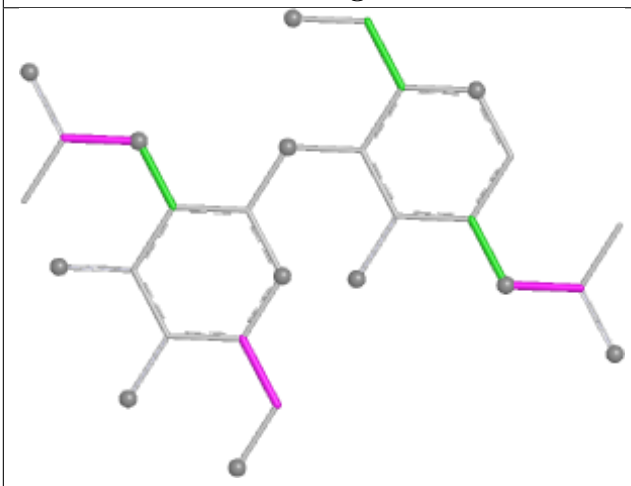
Oligosaccharide Chain G



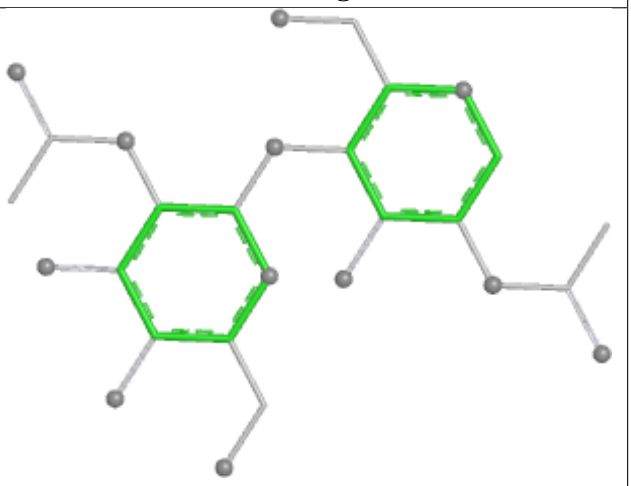
Bond lengths



Bond angles

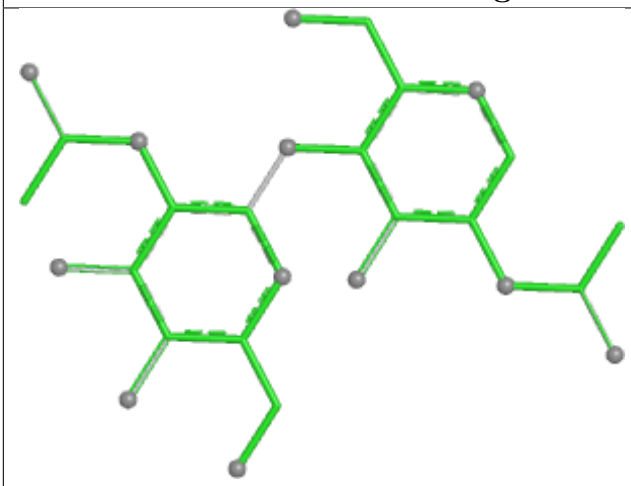


Torsions

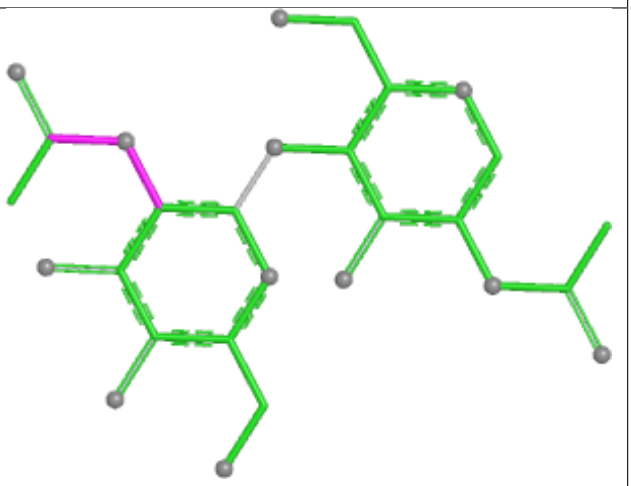


Rings

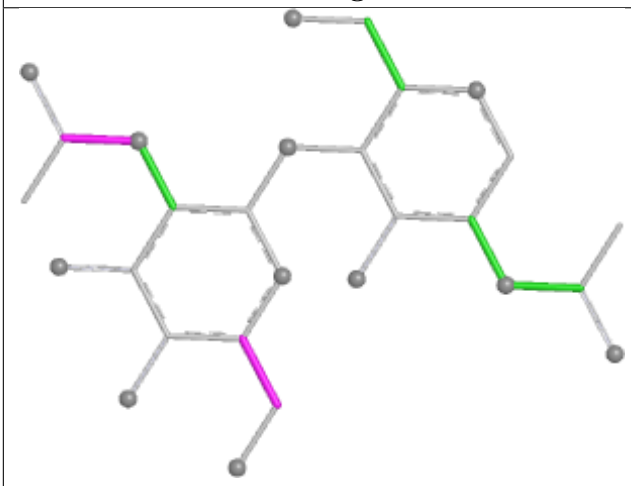
Oligosaccharide Chain H



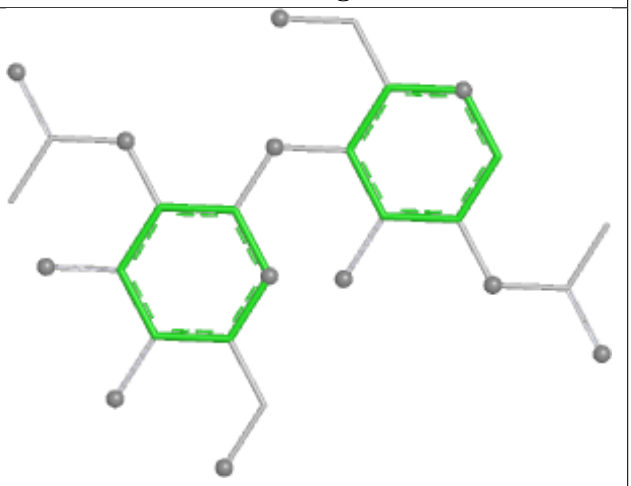
Bond lengths



Bond angles

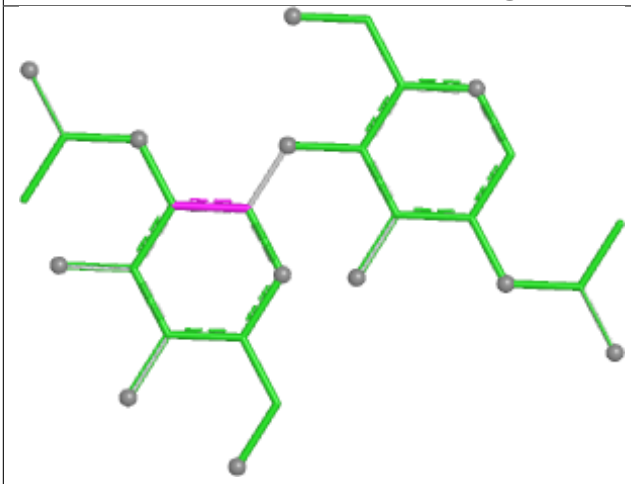


Torsions

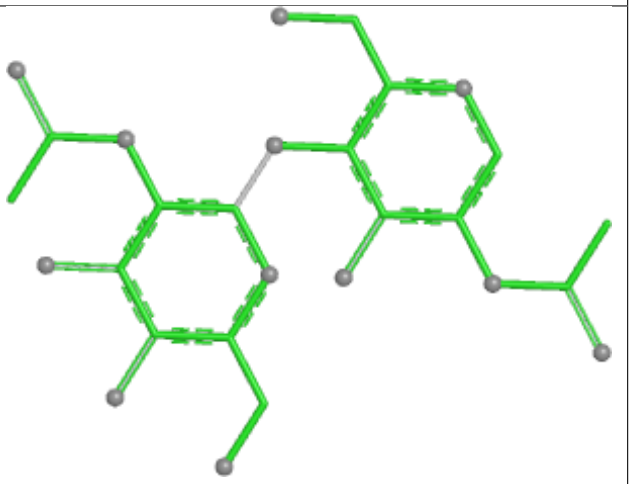


Rings

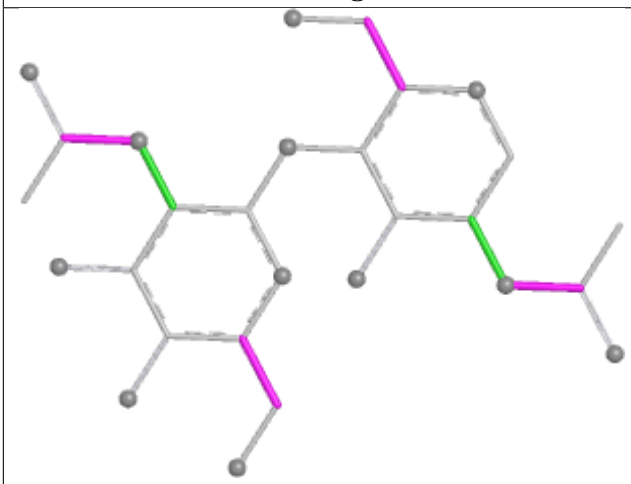
Oligosaccharide Chain I



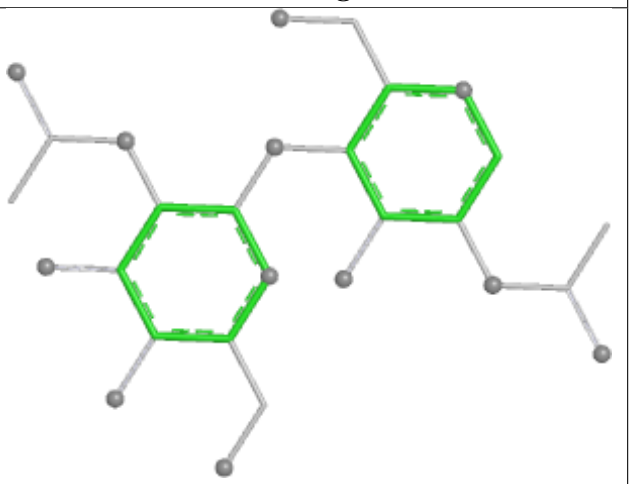
Bond lengths



Bond angles

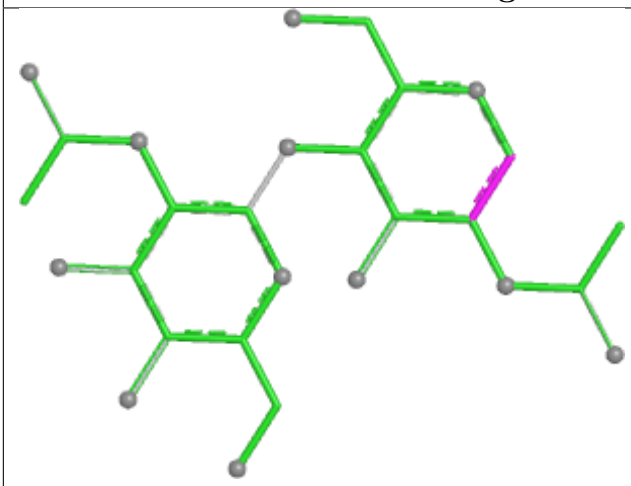


Torsions

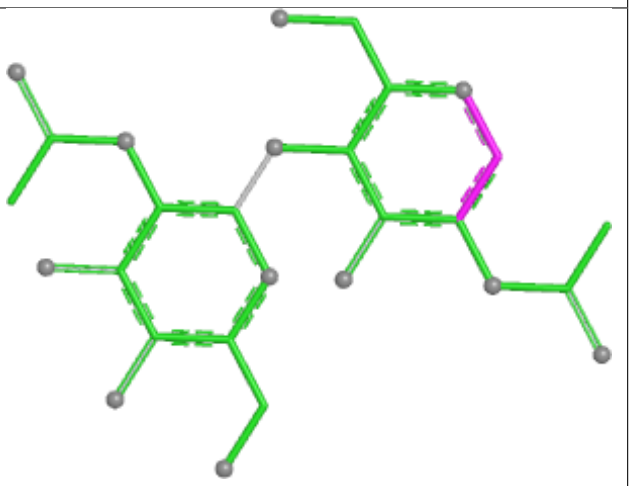


Rings

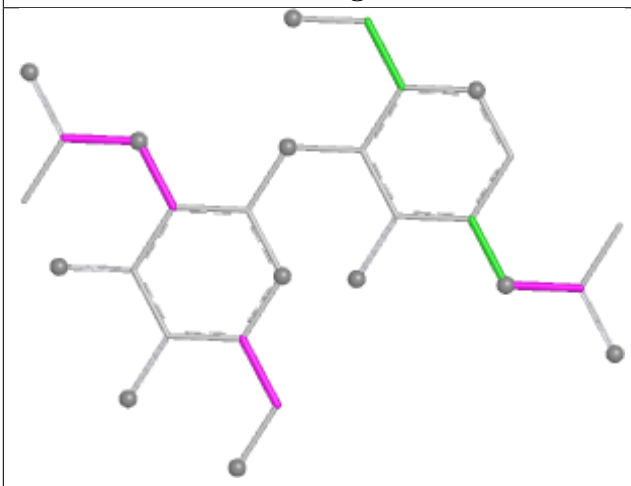
Oligosaccharide Chain J



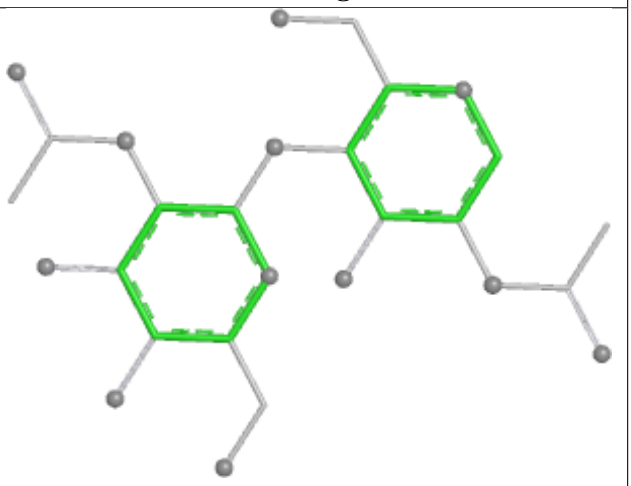
Bond lengths



Bond angles

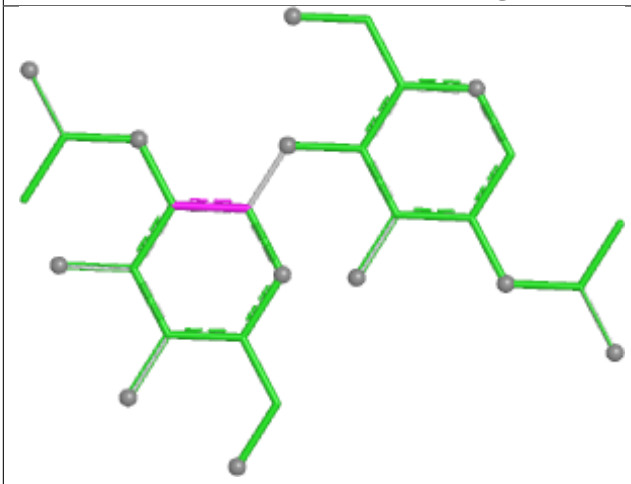


Torsions

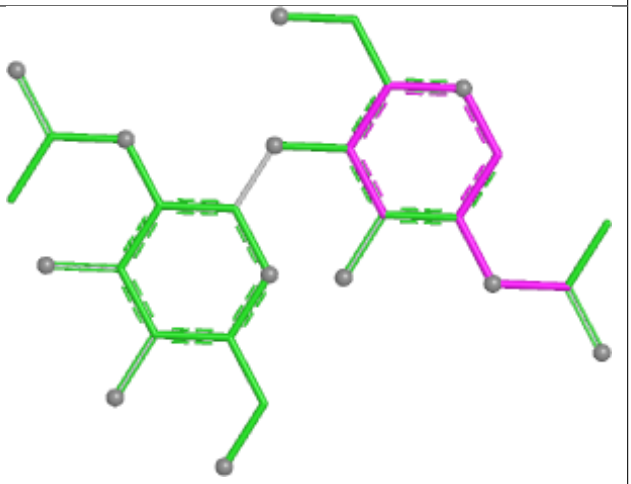


Rings

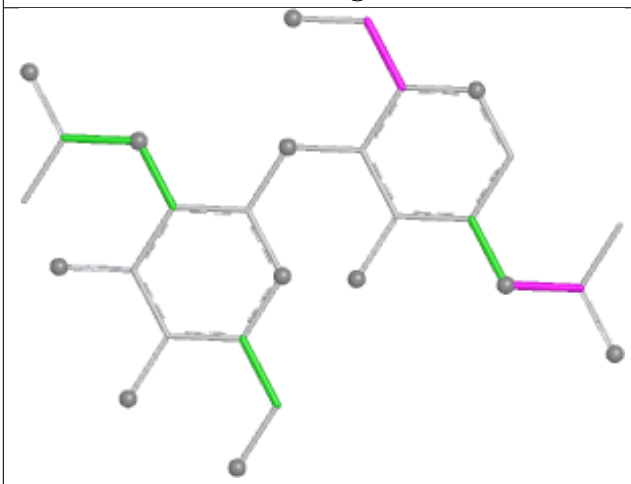
Oligosaccharide Chain K



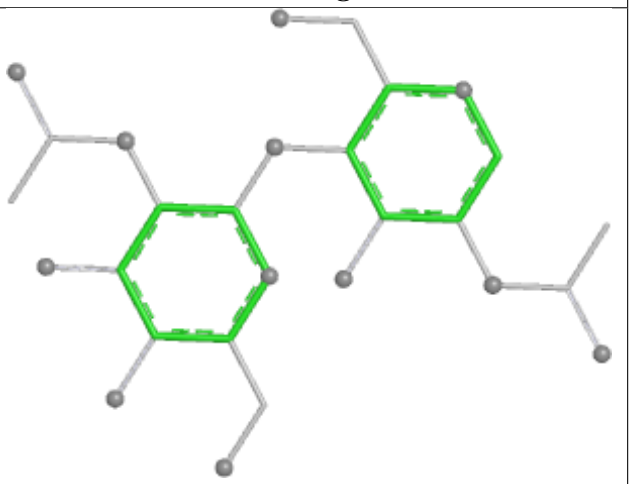
Bond lengths



Bond angles

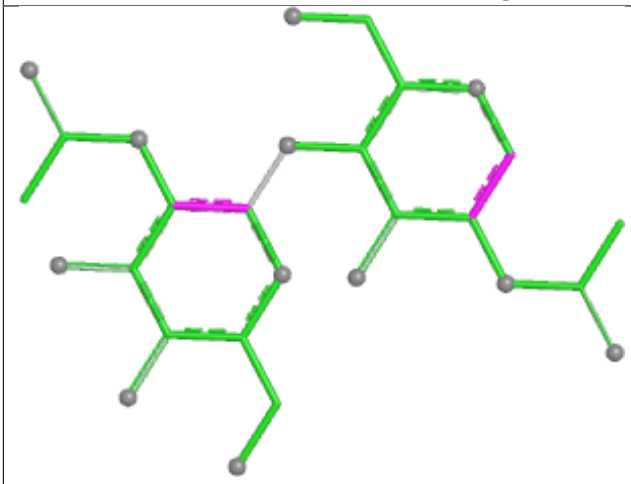


Torsions

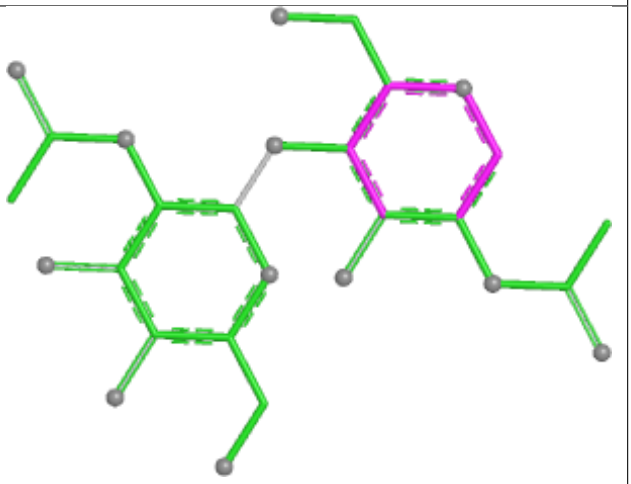


Rings

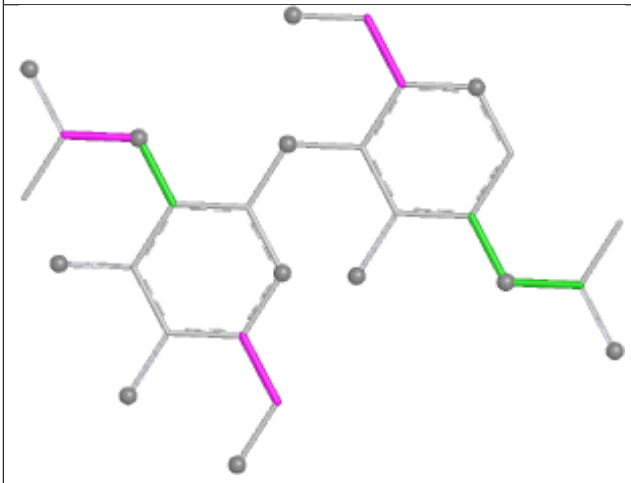
Oligosaccharide Chain L



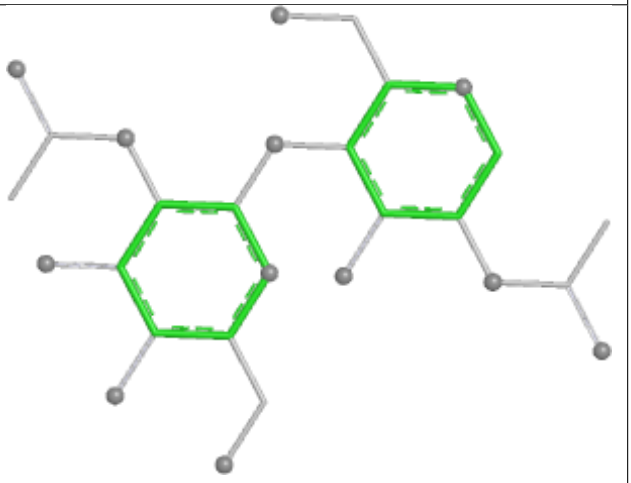
Bond lengths



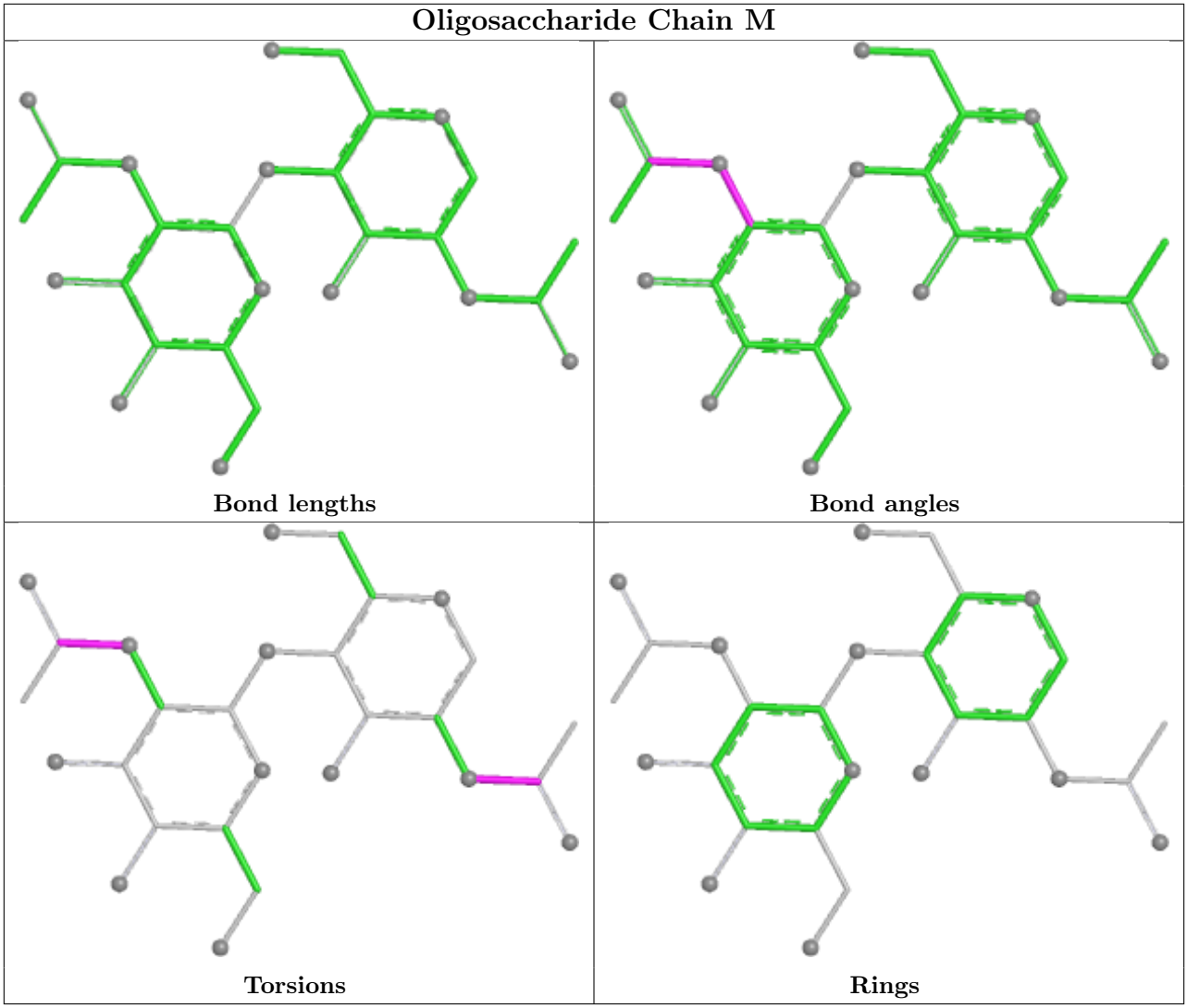
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1085	1	14,14,15	0.53	0	17,19,21	0.81	0
3	NAG	A	1321	1	14,14,15	0.60	0	17,19,21	1.12	2 (11%)
3	NAG	C	1321	1	14,14,15	0.61	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1085	1	14,14,15	0.72	0	17,19,21	0.56	0
4	007	A	1767	-	13,14,14	1.51	3 (23%)	13,19,19	1.05	2 (15%)
5	SO4	C	1768	-	4,4,4	0.42	0	6,6,6	0.18	0
3	NAG	B	1279	1	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
5	SO4	B	1769	-	4,4,4	0.48	0	6,6,6	0.10	0
3	NAG	C	1092	1	14,14,15	1.01	1 (7%)	17,19,21	0.84	0
4	007	B	1767	-	13,14,14	1.24	1 (7%)	13,19,19	0.71	0
3	NAG	B	1229	1	14,14,15	0.55	0	17,19,21	0.73	0
4	007	D	1767	-	13,14,14	1.45	3 (23%)	13,19,19	0.93	1 (7%)
3	NAG	D	1085	1	14,14,15	0.78	0	17,19,21	0.84	0
3	NAG	A	1092	1	14,14,15	0.79	1 (7%)	17,19,21	0.76	0
5	SO4	D	1768	-	4,4,4	0.40	0	6,6,6	0.11	0
4	007	C	1767	-	13,14,14	1.42	3 (23%)	13,19,19	0.76	1 (7%)
3	NAG	D	1279	1	14,14,15	0.71	1 (7%)	17,19,21	0.62	0
3	NAG	A	1279	1	14,14,15	0.71	0	17,19,21	0.61	0
5	SO4	C	1769	-	4,4,4	0.46	0	6,6,6	0.08	0
3	NAG	C	1279	1	14,14,15	0.66	0	17,19,21	0.77	0
5	SO4	A	1769	-	4,4,4	0.52	0	6,6,6	0.23	0
3	NAG	C	1085	1	14,14,15	0.62	0	17,19,21	0.68	0
5	SO4	B	1768	-	4,4,4	0.42	0	6,6,6	0.23	0
5	SO4	A	1768	-	4,4,4	0.38	0	6,6,6	0.08	0
3	NAG	B	1321	1	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
3	NAG	C	1229	1	14,14,15	0.53	0	17,19,21	0.84	0
5	SO4	D	1769	-	4,4,4	0.47	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1085	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1321	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1321	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1085	1	-	4/6/23/26	0/1/1/1
4	007	A	1767	-	-	0/6/18/18	0/2/2/2
3	NAG	B	1279	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1092	1	1/1/5/7	4/6/23/26	0/1/1/1
4	007	B	1767	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1229	1	-	0/6/23/26	0/1/1/1
4	007	D	1767	-	-	0/6/18/18	0/2/2/2
3	NAG	D	1085	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	A	1092	1	1/1/5/7	4/6/23/26	0/1/1/1
4	007	C	1767	-	-	0/6/18/18	0/2/2/2
3	NAG	D	1279	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1279	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1279	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1085	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1321	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1229	1	-	1/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1092	NAG	C1-C2	3.44	1.57	1.52
4	A	1767	007	C3-C6	2.78	1.59	1.53
4	A	1767	007	C7-C6	2.57	1.43	1.39
4	C	1767	007	C3-C6	2.52	1.58	1.53
4	D	1767	007	C7-C6	2.50	1.43	1.39
4	A	1767	007	C8-C6	2.50	1.43	1.39
4	D	1767	007	C8-C6	2.48	1.43	1.39
4	C	1767	007	C8-C6	2.47	1.43	1.39
4	D	1767	007	C3-C6	2.43	1.58	1.53
3	A	1092	NAG	C1-C2	2.34	1.55	1.52
4	B	1767	007	C8-C6	2.19	1.43	1.39
4	C	1767	007	C7-C6	2.16	1.42	1.39
3	D	1279	NAG	C1-C2	2.04	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1321	NAG	C2-N2-C7	-2.95	118.94	122.90
4	A	1767	007	C4-C5-C3	2.71	108.31	105.00
4	D	1767	007	C2-C1-C3	2.69	108.28	105.00
3	A	1321	NAG	C4-C3-C2	-2.41	107.49	111.02
4	A	1767	007	C2-C1-C3	2.32	107.83	105.00
3	B	1321	NAG	C2-N2-C7	-2.14	120.04	122.90
4	C	1767	007	C2-C1-C3	2.11	107.57	105.00
3	B	1279	NAG	C2-N2-C7	-2.02	120.20	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1092	NAG	C1
3	C	1092	NAG	C1
3	D	1085	NAG	C1

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1085	NAG	C8-C7-N2-C2
3	A	1085	NAG	O7-C7-N2-C2
3	A	1092	NAG	C8-C7-N2-C2
3	A	1092	NAG	O7-C7-N2-C2
3	A	1279	NAG	C8-C7-N2-C2
3	A	1279	NAG	O7-C7-N2-C2
3	B	1085	NAG	C8-C7-N2-C2
3	B	1085	NAG	O7-C7-N2-C2
3	C	1085	NAG	C8-C7-N2-C2
3	C	1085	NAG	O7-C7-N2-C2
3	C	1092	NAG	C8-C7-N2-C2
3	C	1092	NAG	O7-C7-N2-C2
3	C	1279	NAG	C8-C7-N2-C2
3	C	1279	NAG	O7-C7-N2-C2
3	C	1321	NAG	C8-C7-N2-C2
3	C	1321	NAG	O7-C7-N2-C2
3	D	1085	NAG	C8-C7-N2-C2
3	D	1085	NAG	O7-C7-N2-C2
3	D	1279	NAG	C8-C7-N2-C2
3	D	1279	NAG	O7-C7-N2-C2
3	B	1321	NAG	C4-C5-C6-O6
3	C	1321	NAG	C4-C5-C6-O6
3	B	1321	NAG	O5-C5-C6-O6
3	B	1279	NAG	C8-C7-N2-C2
3	B	1279	NAG	O7-C7-N2-C2
3	A	1321	NAG	O5-C5-C6-O6
3	A	1085	NAG	C4-C5-C6-O6
3	C	1321	NAG	O5-C5-C6-O6
3	A	1085	NAG	O5-C5-C6-O6
3	A	1321	NAG	C8-C7-N2-C2
3	A	1092	NAG	O5-C5-C6-O6
3	A	1321	NAG	O7-C7-N2-C2
3	B	1321	NAG	C8-C7-N2-C2
3	C	1092	NAG	O5-C5-C6-O6
3	B	1321	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1321	NAG	C4-C5-C6-O6
3	C	1085	NAG	C1-C2-N2-C7
3	A	1092	NAG	C4-C5-C6-O6
3	C	1229	NAG	C4-C5-C6-O6
3	C	1085	NAG	C3-C2-N2-C7
3	C	1092	NAG	C4-C5-C6-O6
3	C	1321	NAG	C1-C2-N2-C7
3	C	1279	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1321	NAG	1	0
3	C	1321	NAG	1	0
4	A	1767	007	1	0
3	C	1092	NAG	1	0
3	D	1279	NAG	1	0
3	A	1279	NAG	1	0
3	B	1321	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.