



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 1WCY / pdb_00001wcy
Title : Crystal Structure Of Human Dipeptidyl Peptidase IV (DPPIV) Complex With Diprotin A
Authors : Hiramatsu, H.; Yamamoto, A.; Kyono, K.; Higashiyama, Y.; Fukushima, C.; Shima, H.; Sugiyama, S.; Inaka, K.; Shimizu, R.
Deposited on : 2004-05-07
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

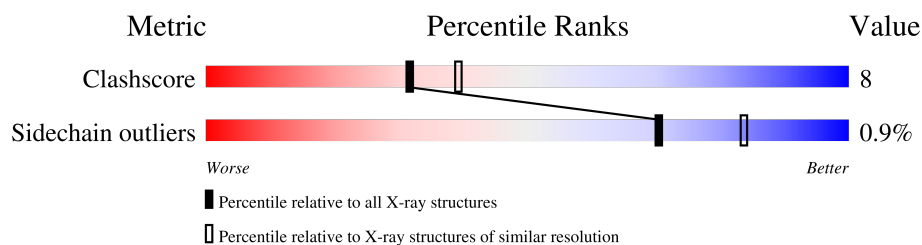
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

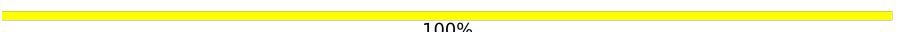
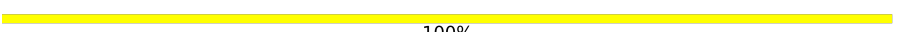
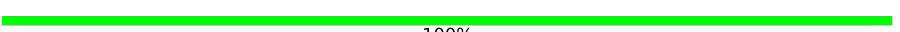
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

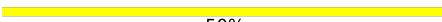
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	740	 78% 20% ..
1	B	740	 78% 20% ..
2	C	3	 100%
2	D	3	 100%
3	E	2	 100%
3	I	2	 50% 50%
4	F	2	 50% 50%
4	G	2	 100%
4	H	2	 100%

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Mol	Chain	Length	Quality of chain
4	J	2	 100%
4	K	2	 50%  50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13485 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	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			
1	B	729	Total	C	N	O	S	0	0	0
			5971	3831	983	1131	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
B	767	HIS	-	expression tag	UNP P27487
B	768	HIS	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487

- Molecule 2 is a protein called Diprotin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			24	17	3	4			
2	D	3	Total	C	N	O	0	0	0
			24	17	3	4			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

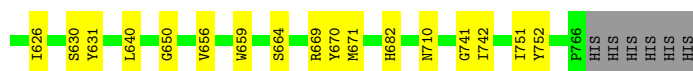
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



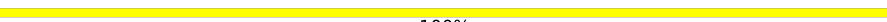
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	602	Total	O	0	0
			602	602		
6	B	631	Total	O	0	0
			631	631		
6	C	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

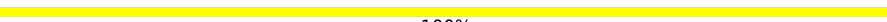


- Molecule 2: Diprotin A

Chain C:  100%

I1
P2
I3

- Molecule 2: Diprotin A

Chain D:  100%

I1
P2
I3

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
FUC2

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
FUC2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.02Å 126.06Å 136.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.8 (20.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.224 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13485	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/6143	0.89	25/8355 (0.3%)
1	B	0.33	0/6143	0.88	21/8355 (0.3%)
2	C	0.51	0/24	0.77	0/31
2	D	0.51	0/24	0.79	0/31
All	All	0.32	0/12334	0.88	46/16772 (0.3%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	VAL	N-CA-C	-8.30	98.10	109.55
1	A	388	GLN	N-CA-C	-8.21	96.30	109.76
1	B	656	VAL	N-CA-C	-7.76	98.65	109.21
1	B	458	SER	N-CA-C	-7.74	97.55	109.24
1	A	300	LEU	N-CA-C	-7.40	96.67	108.73
1	A	458	SER	N-CA-C	-7.18	98.10	109.23
1	B	300	LEU	N-CA-C	-7.07	97.21	108.73
1	A	148	ILE	N-CA-C	-6.82	102.26	108.95
1	A	450	ASN	CA-C-N	6.72	126.98	119.32
1	A	450	ASN	C-N-CA	6.72	126.98	119.32
1	A	664	SER	N-CA-C	6.23	117.73	111.07
1	A	320	GLN	N-CA-C	6.16	123.92	110.80
1	A	548	ALA	N-CA-C	6.13	120.34	112.86
1	B	664	SER	N-CA-C	6.05	117.55	111.07
1	B	485	SER	N-CA-C	6.00	118.78	111.82
1	B	206	GLU	N-CA-C	5.93	120.80	113.50
1	B	320	GLN	N-CA-C	5.92	123.42	110.80
1	A	236	ILE	N-CA-C	-5.78	100.08	108.87
1	B	425	MET	CA-C-N	5.71	125.56	119.28
1	B	425	MET	C-N-CA	5.71	125.56	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-5.67	102.50	110.50
1	B	158	SER	N-CA-C	-5.62	101.96	110.39
1	B	388	GLN	N-CA-C	-5.55	100.14	109.07
1	A	364	PHE	N-CA-C	5.54	118.67	110.48
1	B	319	ILE	N-CA-C	-5.53	98.69	107.15
1	B	546	VAL	N-CA-C	5.48	117.28	108.85
1	A	454	CYS	N-CA-C	5.45	117.28	108.34
1	A	63	ILE	N-CA-C	-5.39	107.72	112.90
1	B	541	PRO	N-CA-C	-5.38	103.34	111.41
1	A	546	VAL	N-CA-C	5.38	117.13	108.85
1	B	450	ASN	CA-C-N	5.33	125.66	119.47
1	B	450	ASN	C-N-CA	5.33	125.66	119.47
1	B	454	CYS	N-CA-C	5.28	117.42	108.02
1	B	659	TRP	N-CA-C	5.27	117.78	111.71
1	A	631	TYR	N-CA-C	-5.25	105.68	111.71
1	A	744	SER	N-CA-C	-5.23	103.24	110.35
1	A	206	GLU	N-CA-C	5.23	119.93	113.50
1	B	631	TYR	N-CA-C	-5.20	105.73	111.71
1	A	403	GLU	N-CA-C	5.18	117.69	109.50
1	A	617	GLY	N-CA-C	5.17	121.24	115.08
1	A	328	CYS	N-CA-C	5.14	117.35	109.07
1	B	414	TYR	N-CA-C	5.09	117.12	109.23
1	A	177	GLU	CA-C-N	5.07	125.35	119.47
1	A	177	GLU	C-N-CA	5.07	125.35	119.47
1	B	548	ALA	N-CA-C	5.07	119.04	112.86
1	A	667	THR	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5971	0	5683	92	0
1	B	5971	0	5683	100	0
2	C	24	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	24	0	31	3	0
3	E	24	0	22	0	0
3	I	24	0	22	0	0
4	F	28	0	25	2	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	1	0
5	A	28	0	26	2	0
5	B	42	0	39	0	0
6	A	602	0	0	5	0
6	B	631	0	0	2	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	13485	0	11662	194	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 8.

All (194) 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:A:253:ARG:HH21	1:B:253:ARG:HH21	1.06	0.93
1:B:142:LEU:HD23	1:B:142:LEU:H	1.42	0.83
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.62	0.82
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.61	0.82
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.51	0.75
1:A:513:LYS:HE3	1:A:515:ASP:HB2	1.68	0.74
4:F:1:NAG:H61	4:F:2:NAG:H82	1.67	0.74
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.69	0.72
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.87	0.72
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.72	0.72
1:A:75:ASN:HD22	1:A:92:ASN:HD22	1.39	0.68
1:B:551:CYS:SG	1:B:591:MET:SD	2.90	0.66
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.77	0.66
1:A:106:SER:HB3	1:A:115:LEU:HB3	1.77	0.66
1:B:600:THR:O	1:B:604:GLU:HG3	1.96	0.65
1:B:105:TYR:HD2	1:B:114:ILE:HD11	1.61	0.65
1:B:535:ASP:OD1	1:B:538:LYS:HE3	1.97	0.65
1:B:277:SER:OG	1:B:279:VAL:HG22	1.98	0.63
1:B:105:TYR:CD2	1:B:114:ILE:HD11	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD12	1:A:57:LEU:N	2.14	0.62
1:B:142:LEU:H	1:B:142:LEU:CD2	2.12	0.62
1:B:95:PHE:HB3	1:B:98:PHE:HB2	1.81	0.62
1:B:272:ASN:HD21	4:J:2:NAG:H81	1.64	0.62
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.34	0.62
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.31	0.60
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.36	0.60
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.01	0.60
1:B:107:ILE:HD12	1:B:107:ILE:N	2.16	0.60
1:B:536:LYS:HG3	1:B:618:PHE:HD2	1.67	0.59
1:B:95:PHE:CE2	1:B:116:LEU:HD11	2.38	0.58
1:B:291:ALA:O	1:B:295:ILE:HG23	2.04	0.58
1:A:107:ILE:HD12	1:A:107:ILE:N	2.19	0.58
1:A:621:ASN:HD22	1:A:621:ASN:N	2.02	0.57
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.34	0.57
1:B:345:HIS:HE1	1:B:391:LYS:O	1.87	0.57
1:B:535:ASP:HB3	1:B:538:LYS:HD2	1.87	0.56
1:B:516:PHE:CD2	1:B:523:LYS:HG3	2.40	0.56
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.87	0.56
1:A:542:LEU:C	1:A:542:LEU:HD23	2.31	0.56
1:A:415:LEU:HD23	1:A:415:LEU:C	2.30	0.56
1:B:501:ASP:O	1:B:505:GLN:HG2	2.06	0.56
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.06	0.55
1:B:107:ILE:HD12	1:B:107:ILE:H	1.72	0.55
1:A:502:LYS:HD3	1:A:502:LYS:C	2.31	0.55
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.89	0.55
1:B:60:LEU:HD12	1:B:60:LEU:C	2.32	0.54
1:A:109:PRO:HG2	1:A:158:SER:O	2.07	0.54
1:A:428:GLY:O	1:A:429:ARG:HD2	2.08	0.53
1:A:501:ASP:O	1:A:505:GLN:HG2	2.09	0.53
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.38	0.53
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.38	0.53
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.09	0.53
1:B:536:LYS:HG3	1:B:618:PHE:CD2	2.44	0.53
1:A:391:LYS:HE3	6:A:2069:HOH:O	2.08	0.53
1:B:176:ILE:HD13	1:B:183:TYR:CE1	2.44	0.53
1:A:741:GLY:O	1:A:742:ILE:C	2.52	0.52
1:B:472:CYS:O	1:B:478:PRO:HA	2.10	0.52
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.10	0.52
1:B:512:LYS:HD3	6:B:1883:HOH:O	2.09	0.52
1:B:388:GLN:HB2	1:B:391:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HG2	1:A:73:GLU:HG3	1.92	0.51
1:A:751:ILE:O	1:A:755:MET:HG3	2.10	0.51
1:A:600:THR:O	1:A:604:GLU:HG3	2.11	0.51
1:B:73:GLU:O	1:B:74:ASN:HB2	2.10	0.51
1:A:516:PHE:CD2	1:A:523:LYS:HD2	2.46	0.51
1:B:111:GLY:O	1:B:137:LEU:HD12	2.10	0.51
1:B:429:ARG:HG3	1:B:429:ARG:NH1	2.19	0.51
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.93	0.51
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.93	0.51
1:A:630:SER:OG	2:C:2:PRO:C	2.54	0.50
1:A:418:ILE:HD13	1:A:431:LEU:HA	1.93	0.50
1:A:482:LEU:HD23	1:A:492:ARG:NH1	2.27	0.50
1:B:93:SER:HB2	1:B:96:ASP:OD2	2.12	0.50
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.94	0.49
1:B:415:LEU:C	1:B:415:LEU:HD23	2.37	0.49
1:B:542:LEU:C	1:B:542:LEU:HD23	2.37	0.49
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.37	0.49
1:B:143:ILE:HD12	1:B:178:PRO:HB2	1.94	0.49
1:A:95:PHE:CE2	1:A:116:LEU:HD11	2.47	0.49
1:A:438:ASP:CG	1:A:441:LYS:HD3	2.37	0.49
1:A:60:LEU:HD12	1:A:60:LEU:C	2.36	0.49
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.47	0.49
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.27	0.49
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.28	0.49
1:B:596:ARG:O	1:B:597:ARG:HD2	2.12	0.49
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.95	0.48
1:B:60:LEU:HD12	1:B:60:LEU:O	2.13	0.48
4:F:1:NAG:C6	4:F:2:NAG:H82	2.39	0.48
1:B:428:GLY:O	1:B:429:ARG:HG3	2.13	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.49	0.48
1:A:531:PRO:HB3	1:A:568:ALA:O	2.14	0.47
1:B:486:VAL:HG13	1:B:487:ASN:N	2.29	0.47
1:A:102:ILE:HG21	1:A:105:TYR:CE1	2.48	0.47
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.47
1:A:459:VAL:HG22	1:A:460:SER:N	2.29	0.47
1:A:487:ASN:HD22	1:A:487:ASN:H	1.63	0.47
1:A:111:GLY:O	1:A:137:LEU:HD12	2.15	0.47
1:A:513:LYS:O	1:A:527:GLN:HA	2.15	0.47
1:B:142:LEU:HD23	1:B:142:LEU:N	2.21	0.47
1:B:169:ASN:O	1:B:170:ASN:HB2	2.15	0.46
1:B:630:SER:OG	2:D:2:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.50	0.46
1:B:594:ILE:HD12	1:B:594:ILE:C	2.39	0.46
1:A:147:ARG:NH2	5:A:1201:NAG:HN2	2.14	0.46
1:B:459:VAL:HG22	1:B:460:SER:N	2.30	0.46
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.46
1:B:370:SER:HB2	1:B:387:PHE:O	2.15	0.46
2:C:1:ILE:HG22	2:C:3:ILE:HG22	1.98	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.51	0.46
1:A:149:PRO:HA	5:A:1201:NAG:H81	1.97	0.46
1:A:542:LEU:HD23	1:A:543:LEU:N	2.31	0.46
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.46
1:A:314:GLN:NE2	1:A:362:PRO:HD3	2.31	0.46
1:A:568:ALA:HA	1:A:573:ILE:O	2.15	0.45
1:A:472:CYS:O	1:A:478:PRO:HA	2.16	0.45
1:A:696:LYS:CG	1:A:728:VAL:HG22	2.46	0.45
1:B:97:GLU:N	1:B:97:GLU:OE2	2.50	0.45
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.42	0.45
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1.98	0.45
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.47	0.45
1:A:123:GLN:HG2	1:A:124:TRP:CD2	2.51	0.45
1:A:377:ASN:HB2	6:A:2001:HOH:O	2.16	0.45
1:A:621:ASN:N	1:A:621:ASN:ND2	2.64	0.45
1:B:303:VAL:HG22	1:B:313:LEU:HD22	1.96	0.45
1:A:487:ASN:HD22	1:A:487:ASN:C	2.24	0.45
1:B:139:LYS:HB2	1:B:141:GLN:HG2	1.98	0.45
1:A:502:LYS:HD3	1:A:502:LYS:O	2.17	0.45
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.51	0.45
1:A:621:ASN:HD22	1:A:622:LYS:N	2.15	0.45
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.98	0.45
1:B:176:ILE:HD12	1:B:176:ILE:N	2.32	0.45
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.98	0.45
1:A:75:ASN:ND2	1:A:92:ASN:HD22	2.11	0.45
1:A:175:LYS:HG2	1:A:182:SER:OG	2.16	0.45
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.90	0.45
1:A:291:ALA:O	1:A:295:ILE:HG23	2.17	0.45
1:A:487:ASN:HD22	1:A:488:ASP:N	2.15	0.45
1:B:422:TYR:CZ	1:B:423:LYS:HE3	2.52	0.44
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.52	0.44
1:B:622:LYS:NZ	1:B:622:LYS:HB2	2.32	0.44
1:B:671:MET:HE1	1:B:682:HIS:CD2	2.52	0.44
1:A:531:PRO:HB3	1:A:572:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:NH2	6:A:1700:HOH:O	2.49	0.44
1:A:666:TYR:CE1	2:C:2:PRO:HD2	2.53	0.44
1:A:74:ASN:C	1:A:92:ASN:HB3	2.42	0.44
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.53	0.44
1:A:75:ASN:HB3	1:A:92:ASN:H	1.83	0.44
1:B:113:PHE:CE2	1:B:178:PRO:HG3	2.53	0.43
1:B:143:ILE:CD1	1:B:178:PRO:HB2	2.47	0.43
1:B:531:PRO:HB3	1:B:568:ALA:O	2.18	0.43
1:B:358:ARG:NE	6:B:2229:HOH:O	2.50	0.43
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.18	0.43
2:D:1:ILE:HG22	2:D:3:ILE:HG22	2.01	0.43
1:B:88:VAL:HG11	1:B:91:GLU:OE2	2.18	0.43
1:B:91:GLU:HB2	1:B:94:THR:OG1	2.19	0.43
1:A:139:LYS:O	1:A:140:ARG:C	2.62	0.43
1:B:331:ASP:O	1:B:335:GLY:N	2.48	0.43
4:G:1:NAG:O6	4:G:2:NAG:H82	2.19	0.43
1:A:341:VAL:HG23	6:A:2014:HOH:O	2.18	0.42
1:B:422:TYR:CE2	1:B:423:LYS:HE3	2.54	0.42
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.42
1:B:710:ASN:C	1:B:710:ASN:HD22	2.26	0.42
1:A:275:SER:O	1:A:279:VAL:HG22	2.19	0.42
1:B:64:SER:HA	1:B:463:LYS:HG3	2.01	0.42
1:A:60:LEU:HD12	1:A:60:LEU:O	2.19	0.42
1:A:710:ASN:C	1:A:710:ASN:HD22	2.27	0.42
1:A:64:SER:C	1:A:463:LYS:HB2	2.45	0.42
1:A:237:GLU:HG2	1:A:253:ARG:HG2	2.01	0.42
1:B:626:ILE:O	1:B:650:GLY:HA2	2.19	0.42
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.55	0.42
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.45	0.42
1:A:266:VAL:HG22	1:A:267:LYS:N	2.34	0.41
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:322:TYR:OH	1:A:346:ILE:HD13	2.20	0.41
1:B:109:PRO:HG2	1:B:158:SER:O	2.21	0.41
1:B:206:GLU:CD	2:D:1:ILE:H1	2.28	0.41
1:A:613:PHE:HA	1:A:616:MET:HG3	2.01	0.41
1:A:626:ILE:O	1:A:650:GLY:HA2	2.19	0.41
1:A:314:GLN:HG3	6:A:1702:HOH:O	2.19	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.50	0.41
4:K:1:NAG:H62	4:K:2:NAG:HN2	1.84	0.41
1:A:136:ASP:OD1	1:A:139:LYS:HD3	2.20	0.41
1:A:127:SER:HB3	1:A:211:TYR:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG12	1:A:161:GLY:N	2.36	0.41
1:A:546:VAL:HG22	1:A:547:TYR:N	2.35	0.41
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.56	0.41
1:B:538:LYS:O	1:B:618:PHE:HA	2.21	0.41
1:B:357:PHE:O	1:B:358:ARG:HB3	2.21	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.40
1:B:78:VAL:CG2	1:B:89:PHE:HB2	2.44	0.40
1:A:424:GLY:O	1:A:426:PRO:HD3	2.21	0.40
1:B:77:LEU:HD23	1:B:88:VAL:HA	2.02	0.40
1:B:751:ILE:HG23	1:B:752:TYR:N	2.37	0.40
1:A:608:GLU:O	1:A:612:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	654/663 (99%)	649 (99%)	5 (1%)	73	85
1	B	654/663 (99%)	647 (99%)	7 (1%)	65	79
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1314/1332 (99%)	1302 (99%)	12 (1%)	70	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	263	ASN
1	A	487	ASN
1	A	621	ASN
1	A	627	TRP
1	B	41	LYS
1	B	133	ASP
1	B	142	LEU
1	B	263	ASN
1	B	326	ASP
1	B	472	CYS
1	B	489	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	66	HIS
1	A	92	ASN
1	A	112	GLN
1	A	119	ASN
1	A	123	GLN
1	A	141	GLN
1	A	169	ASN
1	A	227	GLN
1	A	263	ASN
1	A	286	GLN
1	A	388	GLN
1	A	435	GLN
1	A	487	ASN
1	A	606	GLN
1	A	621	ASN
1	A	694	ASN
1	A	697	GLN
1	A	710	ASN
1	B	66	HIS
1	B	123	GLN
1	B	151	ASN
1	B	169	ASN
1	B	227	GLN
1	B	263	ASN
1	B	286	GLN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	338	ASN
1	B	430	ASN
1	B	435	GLN
1	B	455	GLN
1	B	606	GLN
1	B	612	GLN
1	B	710	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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.53	0	17,19,21	0.63	0
3	FUC	E	2	3	10,10,11	0.46	0	14,14,16	0.34	0
4	NAG	F	1	1,4	14,14,15	0.48	0	17,19,21	0.69	1 (5%)
4	NAG	F	2	4	14,14,15	0.53	0	17,19,21	0.56	0
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
4	NAG	G	2	4	14,14,15	0.48	0	17,19,21	0.68	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
4	NAG	H	2	4	14,14,15	0.46	0	17,19,21	0.76	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.57	0	17,19,21	0.70	1 (5%)
3	FUC	I	2	3	10,10,11	0.48	0	14,14,16	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	1,4	14,14,15	0.51	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.50	0	17,19,21	0.69	0
4	NAG	K	1	1,4	14,14,15	0.51	0	17,19,21	0.70	1 (5%)
4	NAG	K	2	4	14,14,15	0.47	0	17,19,21	0.69	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	E	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C2-N2-C7	-2.38	119.70	122.90
4	H	2	NAG	C2-N2-C7	-2.29	119.83	122.90
4	G	1	NAG	C2-N2-C7	-2.19	119.97	122.90
4	J	1	NAG	C2-N2-C7	-2.16	120.00	122.90
4	K	1	NAG	C2-N2-C7	-2.15	120.02	122.90
4	F	1	NAG	C2-N2-C7	-2.11	120.07	122.90
3	I	1	NAG	C2-N2-C7	-2.04	120.16	122.90
4	G	2	NAG	C2-N2-C7	-2.03	120.19	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

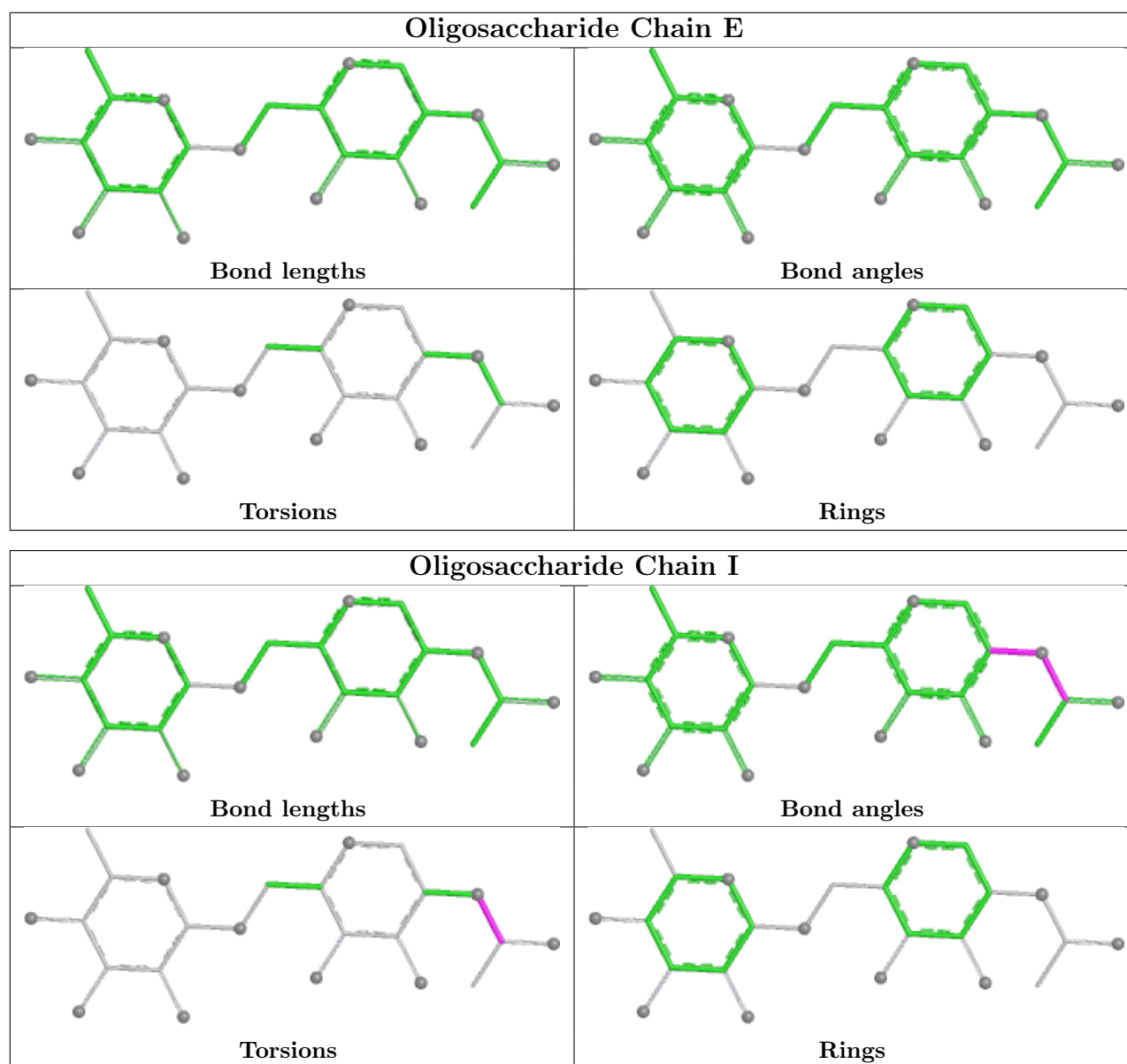
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2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

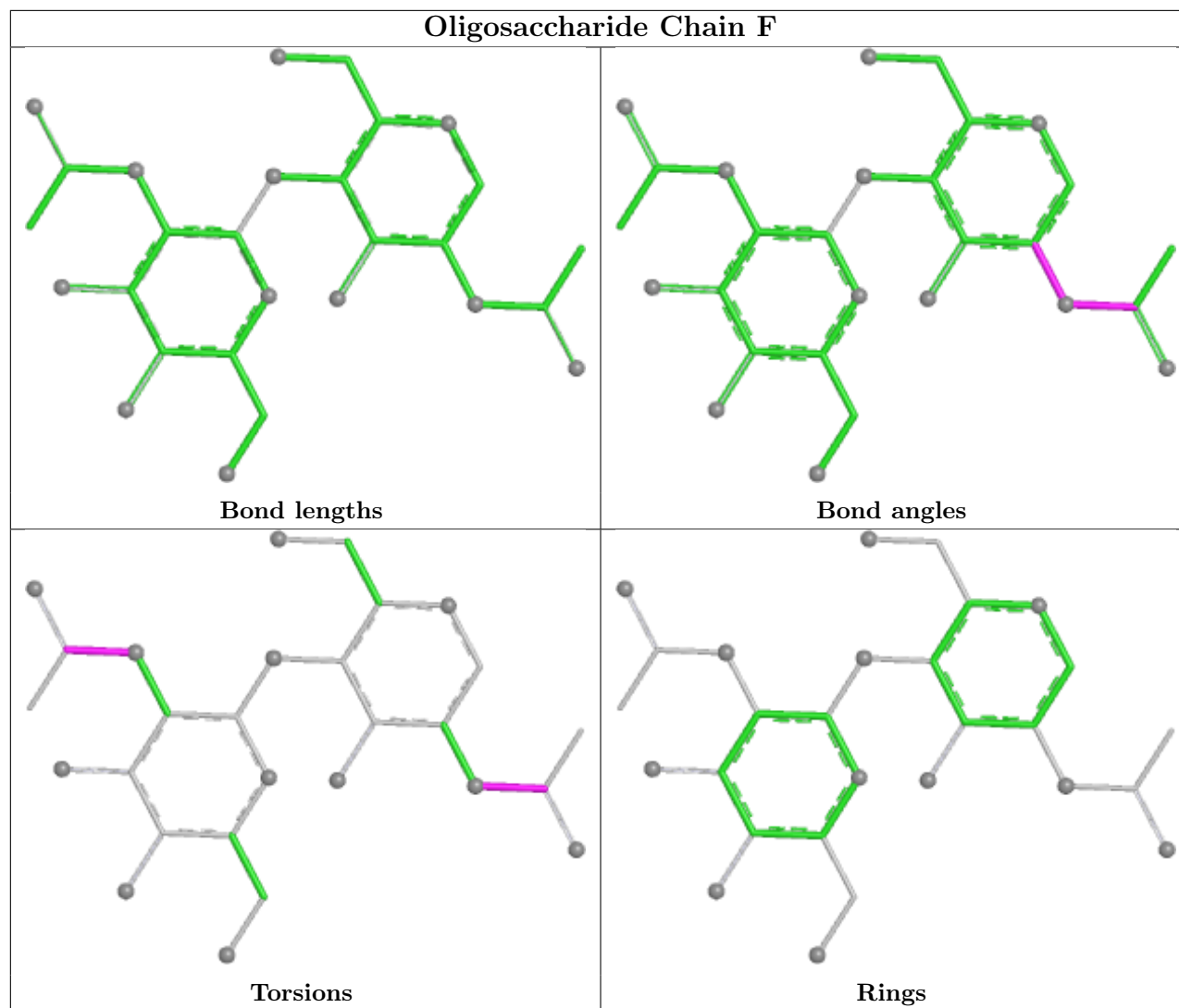
There are no ring outliers.

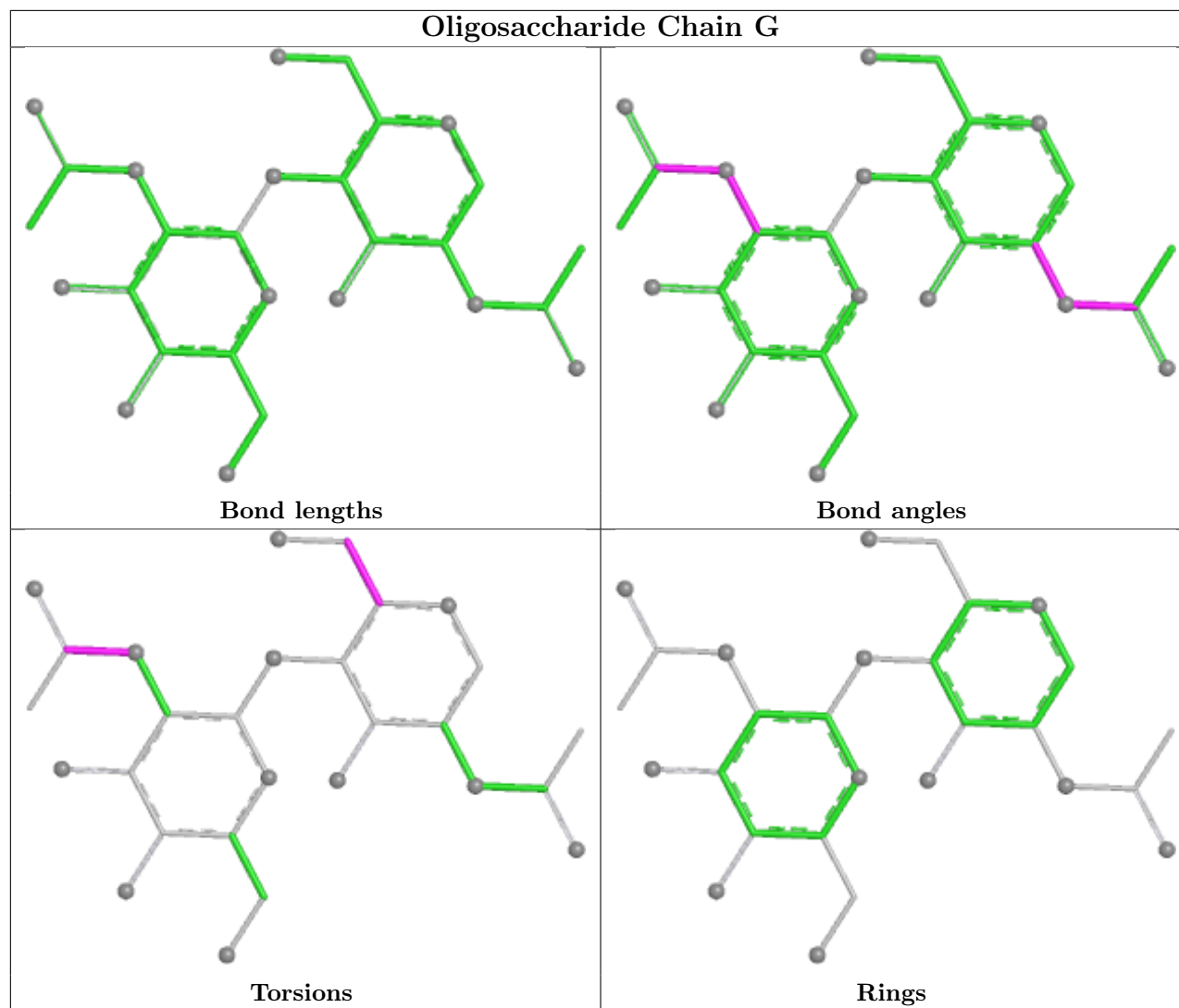
7 monomers are involved in 5 short contacts:

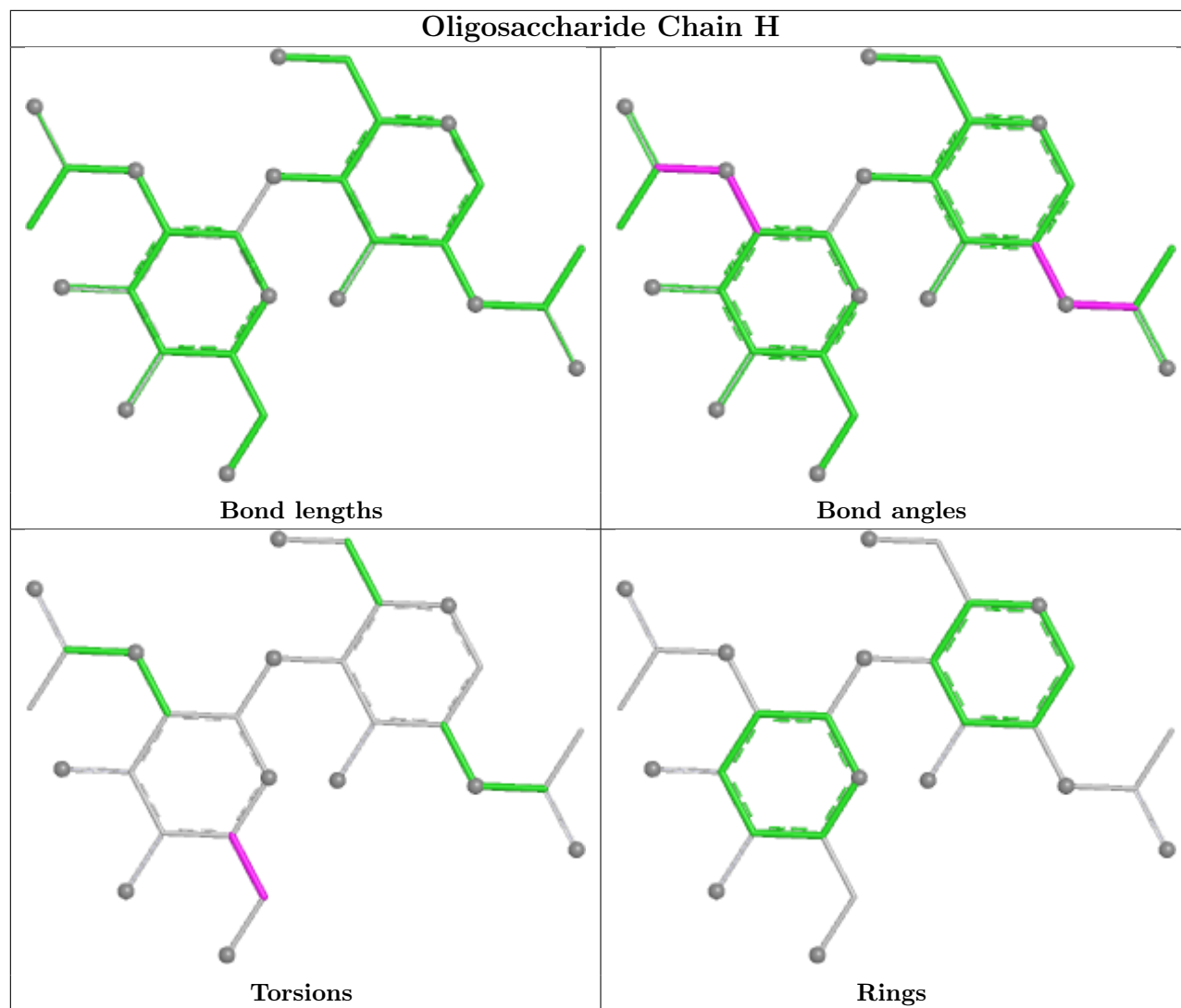
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	2	0
4	K	1	NAG	1	0
4	G	2	NAG	1	0
4	J	2	NAG	1	0
4	G	1	NAG	1	0
4	F	1	NAG	2	0
4	K	2	NAG	1	0

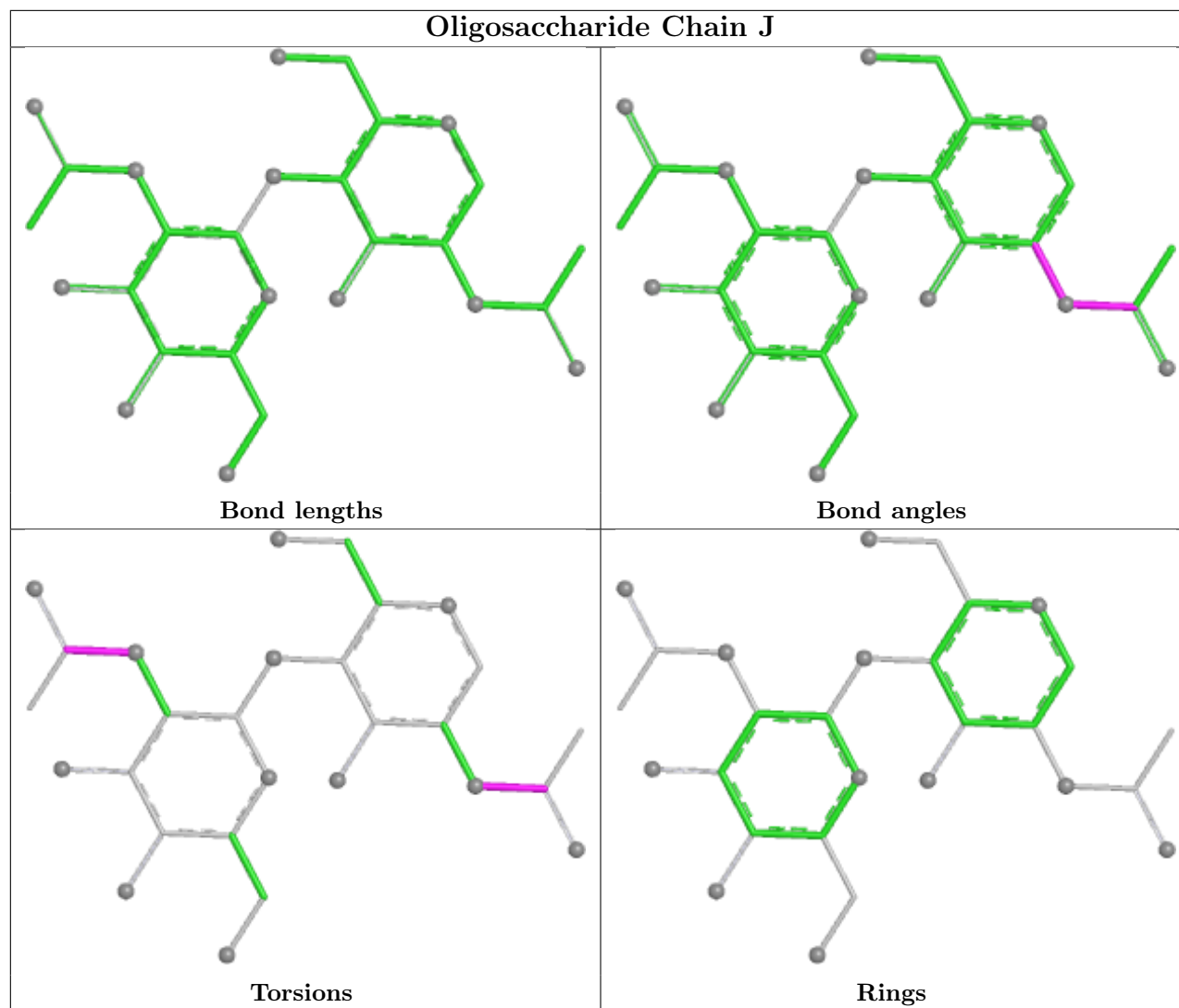
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

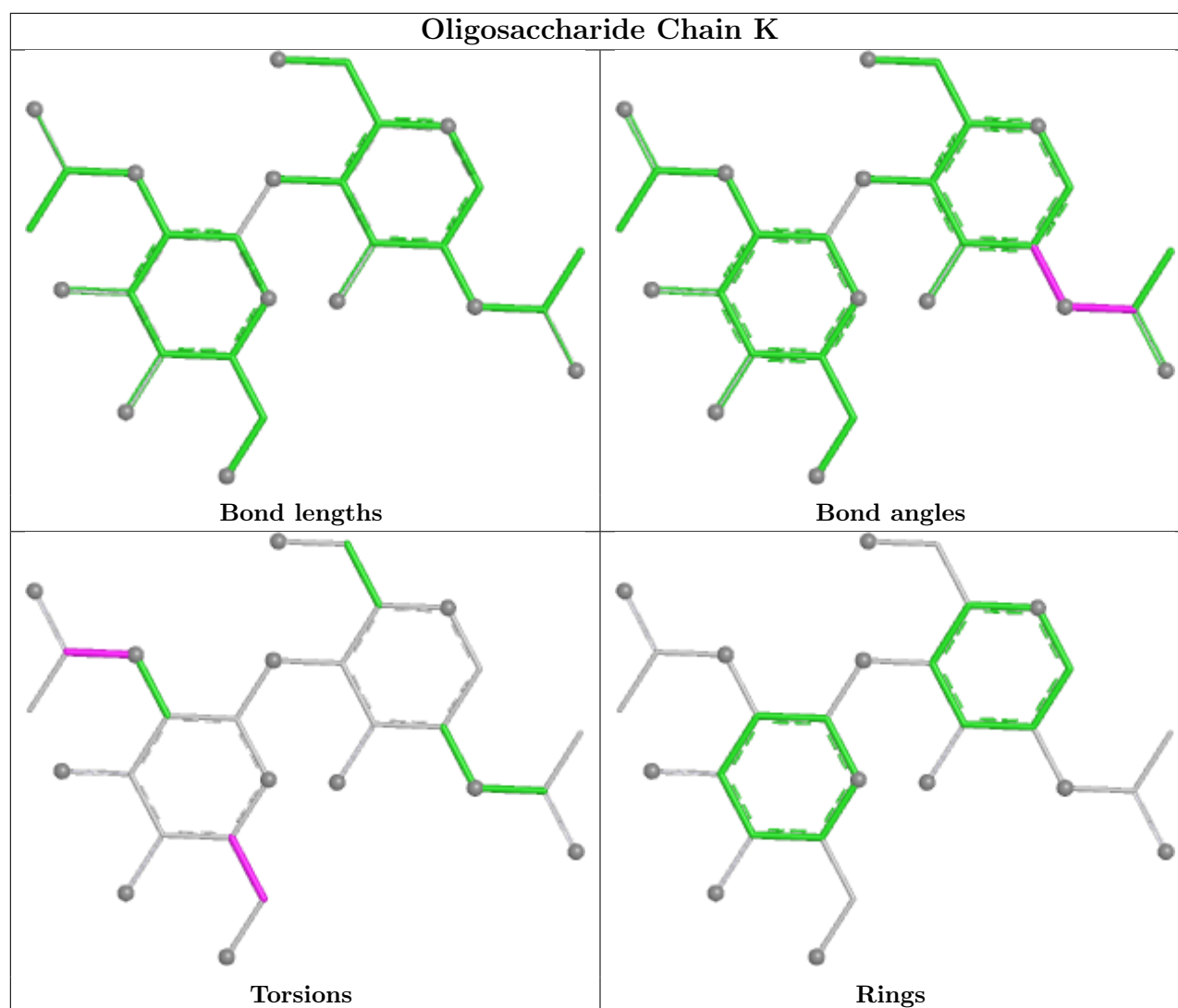












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
5	NAG	A	1601	1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
5	NAG	A	1201	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
5	NAG	B	1601	1	14,14,15	0.55	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1201	1	14,14,15	0.51	0	17,19,21	0.71	1 (5%)
5	NAG	B	1501	1	14,14,15	0.49	0	17,19,21	0.74	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
5	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1601	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1201	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1501	NAG	C2-N2-C7	-2.31	119.81	122.90
5	B	1201	NAG	C2-N2-C7	-2.20	119.95	122.90
5	A	1201	NAG	C2-N2-C7	-2.16	120.01	122.90
5	B	1601	NAG	C2-N2-C7	-2.03	120.18	122.90
5	A	1601	NAG	C2-N2-C7	-2.01	120.20	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	NAG	C8-C7-N2-C2
5	A	1201	NAG	O7-C7-N2-C2
5	A	1601	NAG	C8-C7-N2-C2
5	A	1601	NAG	O7-C7-N2-C2
5	B	1501	NAG	C8-C7-N2-C2
5	B	1501	NAG	O7-C7-N2-C2
5	B	1601	NAG	C8-C7-N2-C2
5	B	1601	NAG	O7-C7-N2-C2
5	A	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	NAG	2	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.