

wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 10:08 AM EDT

PDB ID : 1WCY

Title : Crystal Structure Of Human Dipeptidyl Peptidase IV (DPPIV) Complex With

Diprotin A

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Deposited on : 2004-05-07

Resolution : 2.20 Å(reported)

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

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

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

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

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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)

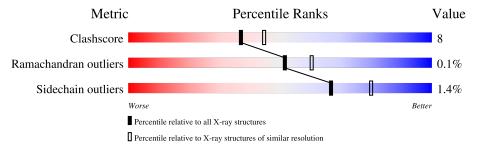
Validation Pipeline (wwPDB-VP) : 2.36

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 2.20 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.

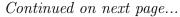


Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	740	81%	L7%	
1	В	740	80%	8%	
2	С	3	100%	0,0	
2	D	3	100%		
3	Е	2	100%		
3	I	2	100%		
4	F	2	100%		
4	G	2	50% 50%		





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Mol	Chain	Length	Quality	of chain
4	Н	2	10	00%
4	J	2	10	00%
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 5971	C 3831	N 983	O 1131	S 26	0	0	0
1	В	729	Total 5971	C 3831	N 983	O 1131	S 26	0	0	0

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	ı	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	ı	expression tag	UNP P27487
A	771	HIS	ı	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
В	767	HIS	ı	expression tag	UNP P27487
В	768	HIS	-	expression tag	UNP P27487
В	769	HIS	ı	expression tag	UNP P27487
В	770	HIS	-	expression tag	UNP P27487
В	771	HIS	-	expression tag	UNP P27487
В	772	HIS	-	expression tag	UNP P27487

• Molecule 2 is a protein called Diprotin A.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	С	ર	Total	С	N	О	0	0	0
		3	24	17	3	4	0	0	0
2	D	2	Total	С	N	О	0	0	0
	ט	3	24	17	3	4	U	0	U

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





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

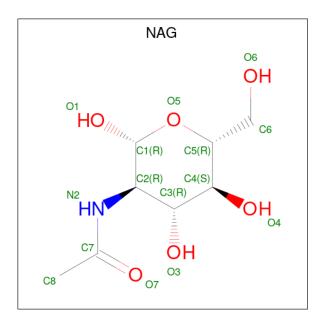
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	2	Total C N O 28 16 2 10	0	0	0
4	G	2	Total C N O 28 16 2 10	0	0	0
4	Н	2	Total C N O 28 16 2 10	0	0	0
4	J	2	Total C N O 28 16 2 10	0	0	0
4	К	2	Total C N O 28 16 2 10	0	0	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	602	Total O 602 602	0	0
6	В	631	Total O 631 631	0	0
6	С	2	Total O 2 2	0	0
6	D	2	Total O 2 2	0	0

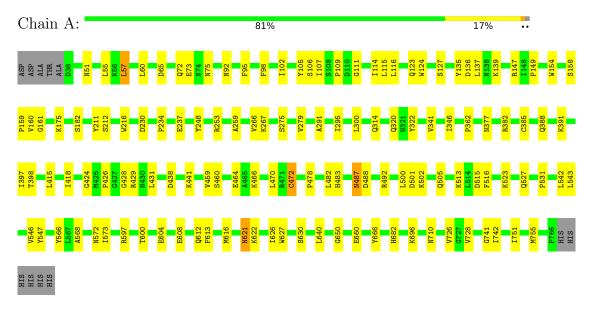


3 Residue-property plots (i)

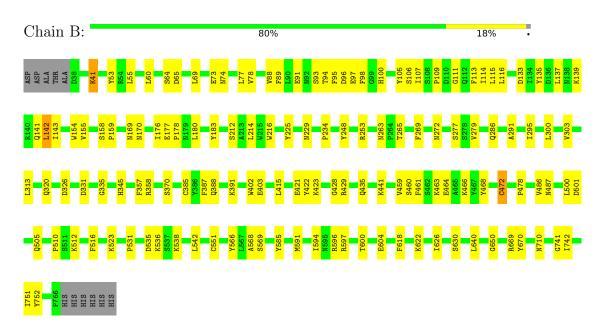
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: Dipeptidyl peptidase IV





opyranose

• Molecule 2:	Diprotin A	
Chain C:	100%	
• Molecule 2:	Diprotin A	
Chain D:	100%	
• Molecule 3:	alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-gluco	opyranose
Chain E:	100%	
• Molecule 3:	alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-gluco	opyranose
Chain I:	100%	
• Molecule 4: opyranose	$2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-(1-4)-2\hbox{-}acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-$	o-2-deoxy-beta-D-gluc
Chain F:	100%	
• Molecule 4: opyranose	$2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-} (1\hbox{-}4)-2\hbox{-}acetamido-2-deoxy-beta-D-glucopyranose-} (1\hbox{-}4)-2\hbox{-}a$	o-2-deoxy-beta-D-gluc
Chain G:	50%	
• Molecule 4: opyranose	$2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-} (1\hbox{-}4)-2\hbox{-}acetamido-2-deoxy-beta-D-glucopyranose-} (1\hbox{-}4)-2\hbox{-}a$	o-2-deoxy-beta-D-gluc
Chain H:	100%	
	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido	o-2-deoxy-beta-D-gluc



Chain J:	100)%	_
NAG1 NAG2			
• Molecule 4: opyranose	2-acetamido-2-deoxy-beta-D	0-glucopyranose-(1-4)-2-acetam	ido-2-deoxy-beta-D-gluc
Chain K:	50%	50%	_
NAG1			



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	118.02Å 126.06Å 136.67Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 2.20	Depositor	
% Data completeness	99.8 (20.00-2.20)	Depositor	
(in resolution range)	33.0 (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: FUC, 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	0.27	0/6143	0.60	2/8355~(0.0%)	
1	В	0.27	0/6143	0.60	1/8355 (0.0%)	
2	С	0.47	0/24	0.71	0/31	
2	D	0.48	0/24	0.72	0/31	
All	All	0.27	0/12334	0.60	3/16772 (0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	388	GLN	N-CA-C	-5.45	96.30	111.00
1	A	300	LEU	N-CA-C	-5.31	96.67	111.00
1	В	300	LEU	N-CA-C	-5.11	97.21	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5971	0	5683	88	0
1	В	5971	0	5683	96	0
2	С	24	0	31	3	0
2	D	24	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Е	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	Н	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	В	42	0	39	0	0
6	A	602	0	0	5	0
6	В	631	0	0	2	0
6	С	2	0	0	0	0
6	D	2	0	0	0	0
All	All	13485	0	11662	186	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.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1100111 1	1100111 =	${ m distance} ({ m \AA})$	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

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	Perce	$_{ m ntiles}$
1	A	727/740 (98%)	695 (96%)	31 (4%)	1 (0%)	51	60
1	В	727/740 (98%)	703 (97%)	23 (3%)	1 (0%)	51	60
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1456/1486 (98%)	1400 (96%)	54 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	В	320	GLN

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%)	644 (98%)	10 (2%)	65 78		
1	В	654/663 (99%)	645 (99%)	9 (1%)	67 80		
2	С	3/3 (100%)	3 (100%)	0	100 100		
2	D	3/3 (100%)	3 (100%)	0	100 100		
All	All	1314/1332 (99%)	1295 (99%)	19 (1%)	67 80		

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	326	ASP
1	В	566	TYR
1	В	710	ASN
1	В	472	CYS
1	A	627	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:



Mol	Chain	Res	Type
1	A	710	ASN
1	В	138	ASN
1	В	112	GLN
1	В	169	ASN
1	A	169	ASN

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)

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	Iol Type Chain Res Link				Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	NAG	Е	1	3,1	14,14,15	0.51	0	17,19,21	0.60	0	
3	FUC	Е	2	3	10,10,11	0.47	0	14,14,16	0.38	0	
4	NAG	F	1	4,1	14,14,15	0.48	0	17,19,21	0.66	0	
4	NAG	F	2	4	14,14,15	0.51	0	17,19,21	0.54	0	
4	NAG	G	1	4,1	14,14,15	0.50	0	17,19,21	0.72	1 (5%)	
4	NAG	G	2	4	14,14,15	0.47	0	17,19,21	0.65	0	
4	NAG	Н	1	4,1	14,14,15	0.51	0	17,19,21	0.82	1 (5%)	
4	NAG	Н	2	4	14,14,15	0.45	0	17,19,21	0.72	1 (5%)	
3	NAG	I	1	3,1	14,14,15	0.55	0	17,19,21	0.67	0	
3	FUC	I	2	3	10,10,11	0.49	0	14,14,16	0.36	0	
4	NAG	J	1	4,1	14,14,15	0.51	0	17,19,21	0.67	1 (5%)	
4	NAG	J	2	4	14,14,15	0.49	0	17,19,21	0.66	0	
4	NAG	K	1	4,1	14,14,15	0.50	0	17,19,21	0.67	1 (5%)	
4	NAG	K	2	4	14,14,15	0.46	0	17,19,21	0.66	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	Е	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	Е	2	3	-	-	0/1/1/1
4	NAG	F	1	4,1	-	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	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Н	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Н	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	4,1	-	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	4,1	-	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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
4	Н	1	NAG	C2-N2-C7	-2.25	119.70	122.90
4	Н	2	NAG	C2-N2-C7	-2.16	119.83	122.90
4	G	1	NAG	C2-N2-C7	-2.06	119.97	122.90
4	J	1	NAG	C2-N2-C7	-2.04	120.00	122.90
4	K	1	NAG	C2-N2-C7	-2.02	120.02	122.90

There are no chirality outliers.

5 of 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

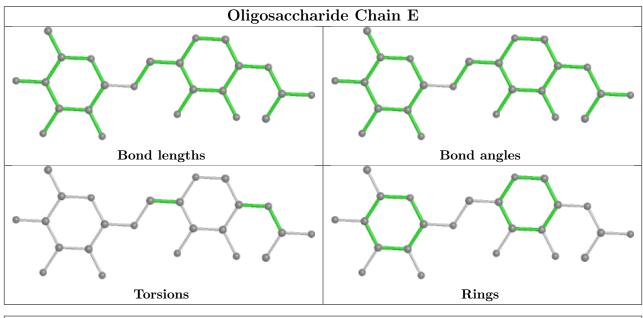
There are no ring outliers.

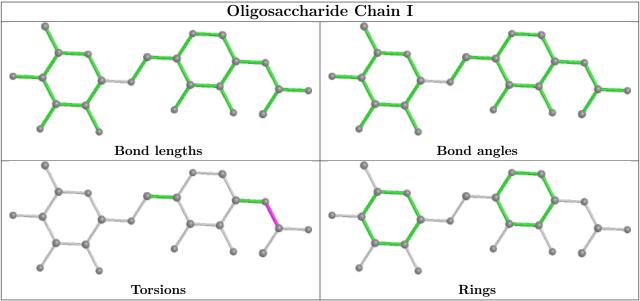


7 monomers are involved in 5 short contacts:

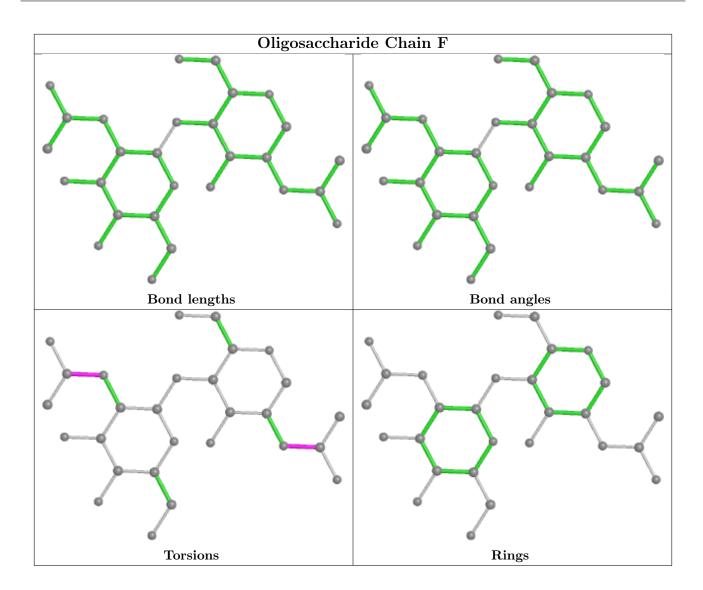
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	2	0
4	F	2	NAG	2	0
4	J	2	NAG	1	0
4	K	1	NAG	1	0
4	G	1	NAG	1	0
4	K	2	NAG	1	0
4	G	2	NAG	1	0

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

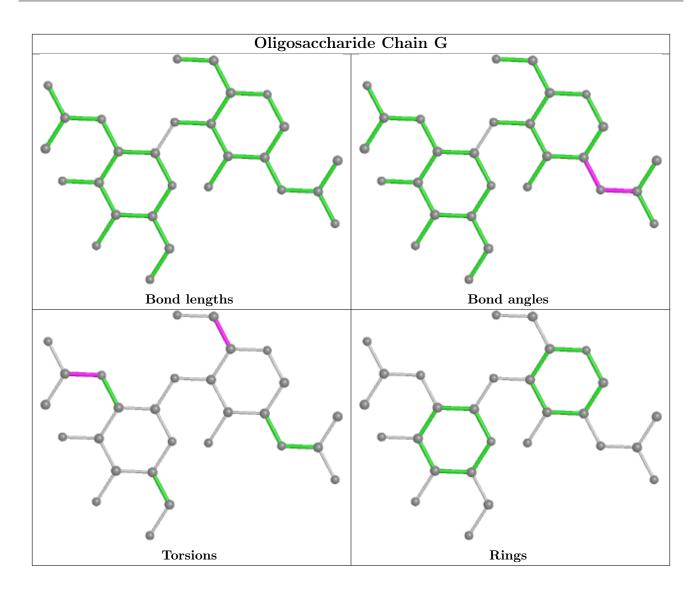




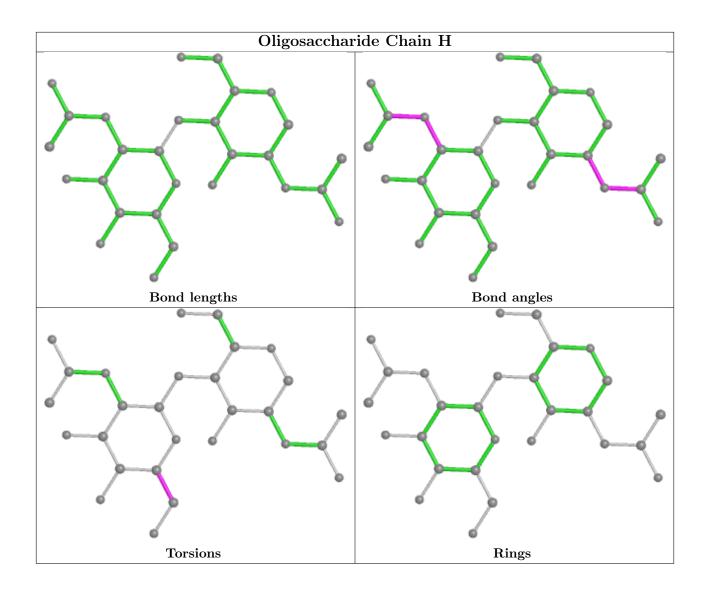




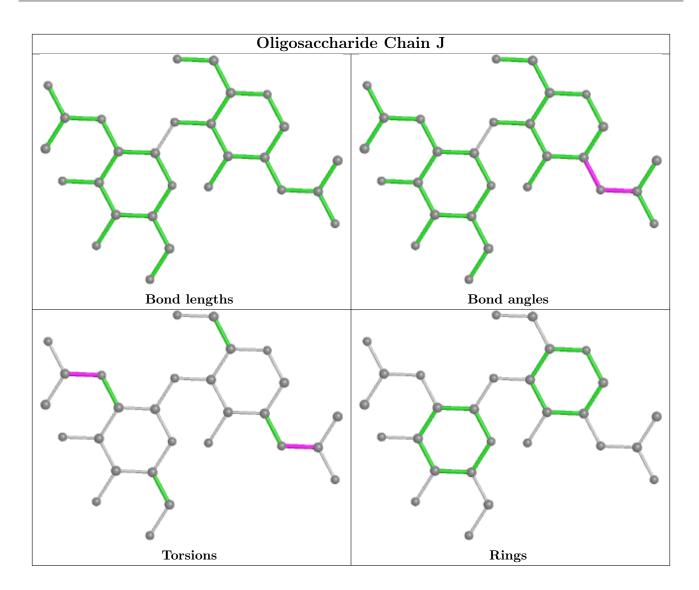




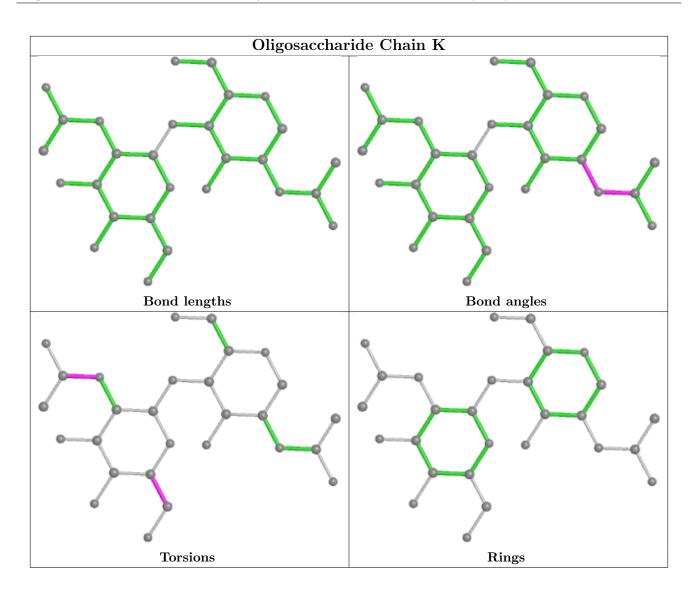












5.6 Ligand geometry (i)

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	Tuno	Chain	Chain Res		Во	ond leng	ths	В	ond ang	les
WIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	1201	1	14,14,15	0.49	0	17,19,21	0.68	1 (5%)
5	NAG	В	1601	1	14,14,15	0.53	0	17,19,21	0.67	0
5	NAG	A	1601	1	14,14,15	0.54	0	17,19,21	0.71	0



Mol	Trino	Chain	Dag	Link Bond lengths			Bond angles			
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	1501	1	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
5	NAG	A	1201	1	14,14,15	0.51	0	17,19,21	0.68	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	В	1201	1	-	0/6/23/26	0/1/1/1
5	NAG	В	1601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
5	NAG	В	1501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
5	В	1501	NAG	C2-N2-C7	-2.17	119.81	122.90
5	В	1201	NAG	C2-N2-C7	-2.07	119.95	122.90
5	A	1201	NAG	C2-N2-C7	-2.03	120.01	122.90

There are no chirality outliers.

5 of 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	В	1501	NAG	C8-C7-N2-C2

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

