



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:34 AM UTC

PDB ID : 1OH2 / pdb_00001oh2
Title : Sucrose-Specific Porin, with Bound Sucrose Molecules
Authors : Diederichs, K.; Welte, W.
Deposited on : 2003-05-21
Resolution : 2.40 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

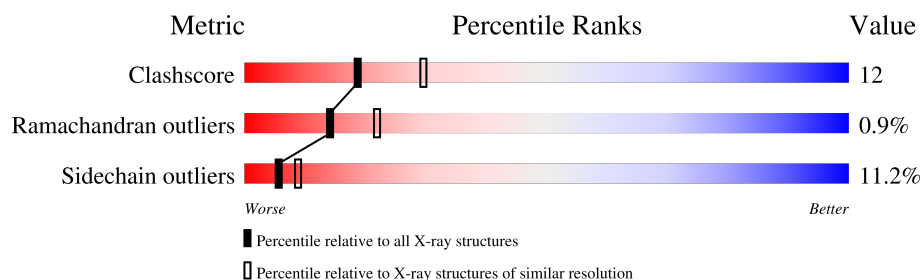
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	P	413	72% 23% 5%
1	R	413	72% 22% 6%
2	Q	413	71% 23% 5%
3	A	2	50% 50%
3	B	2	100%
3	C	2	100%
3	D	2	100%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9717 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 Sucrose porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	413	Total	C	N	O	S	0	0	0
			3202	2011	553	628	10			
1	R	413	Total	C	N	O	S	0	0	0
			3202	2011	553	628	10			

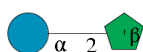
- Molecule 2 is a protein called Sucrose porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	413	Total	C	N	O	S	0	0	0
			3172	2000	542	619	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	80	PRO	ARG	conflict	UNP P22340
Q	110	PRO	ARG	engineered mutation	UNP P22340
Q	114	ALA	GLN	engineered mutation	UNP P22340
Q	120	ILE	GLU	engineered mutation	UNP P22340
Q	161	LEU	ARG	engineered mutation	UNP P22340
Q	194	ALA	ASP	engineered mutation	UNP P22340
Q	199	LEU	ASP	engineered mutation	UNP P22340
Q	201	CYS	ASP	conflict	UNP P22340
Q	482	ALA	TRP	engineered mutation	UNP P22340

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	A	2	Total	C	O	0	0	0
			23	12	11			
3	B	2	Total	C	O	0	0	0
			23	12	11			
3	C	2	Total	C	O	0	0	0
			23	12	11			
3	D	2	Total	C	O	0	0	0
			23	12	11			
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

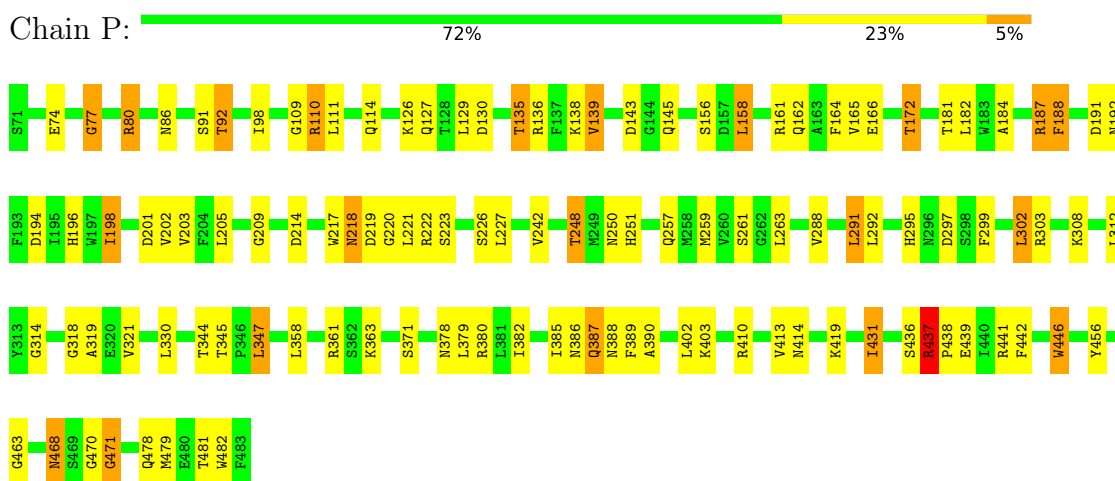
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Ca	0	0
			1	1		
4	Q	1	Total	Ca	0	0
			1	1		
4	R	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

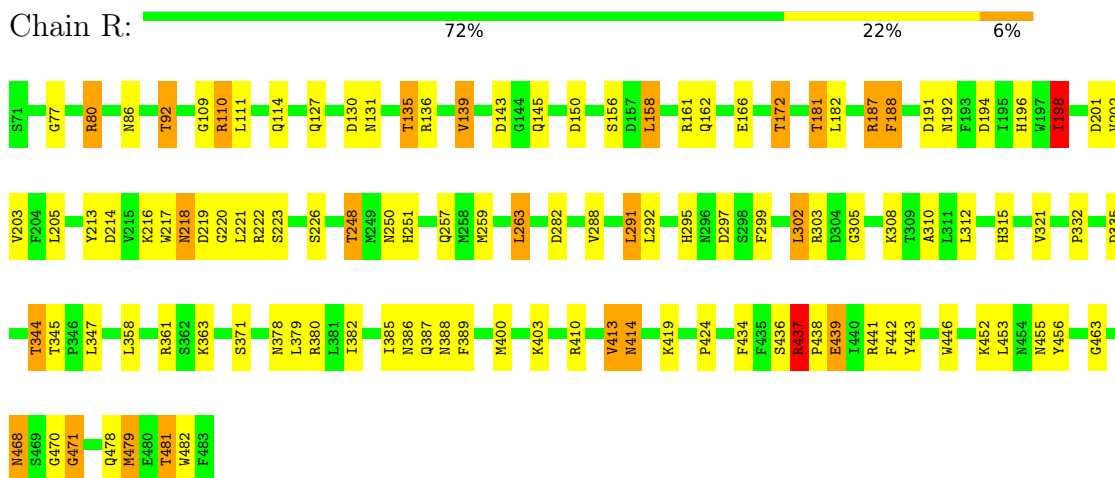
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

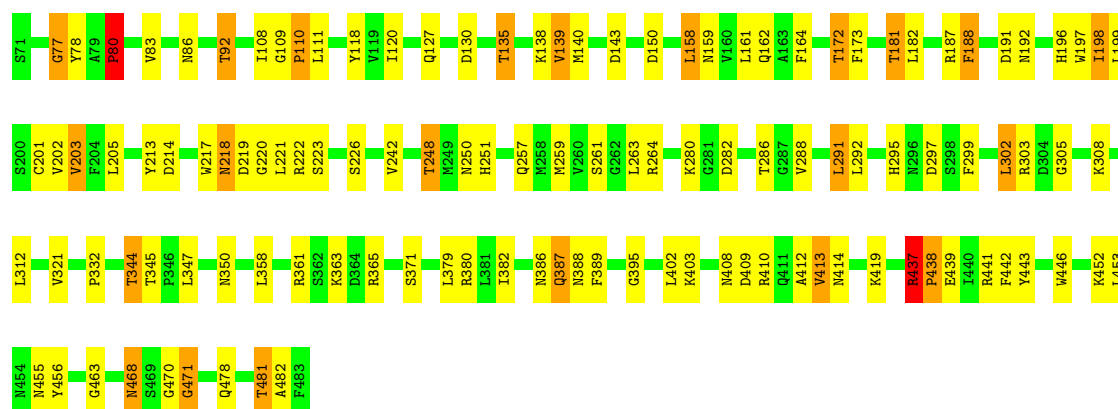


- Molecule 1: Sucrose porin



- Molecule 2: Sucrose porin





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain A: 50% 50%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain B: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain C: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E: 50% 50%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F: 100%

CLC1
FR02

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	111.80Å 111.80Å 147.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	67.4 (100.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: GLC, FRU, CA

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	P	0.65	0/3283	1.07	25/4443 (0.6%)
1	R	0.65	0/3283	1.07	24/4443 (0.5%)
2	Q	0.69	4/3253 (0.1%)	1.09	23/4407 (0.5%)
All	All	0.66	4/9819 (0.0%)	1.08	72/13293 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	110	PRO	N-CD	7.61	1.58	1.47
2	Q	80	PRO	N-CD	7.16	1.57	1.47
2	Q	80	PRO	CG-CD	-6.68	1.28	1.50
2	Q	110	PRO	CG-CD	-6.67	1.28	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	437	ARG	N-CA-C	10.63	133.31	109.81
2	Q	437	ARG	N-CA-C	10.63	133.29	109.81
1	R	202	VAL	N-CA-C	-10.60	100.53	110.82
1	P	437	ARG	N-CA-C	10.59	133.22	109.81
1	P	202	VAL	N-CA-C	-9.26	101.84	110.82
2	Q	202	VAL	N-CA-C	-8.94	102.15	110.82
1	R	196	HIS	N-CA-C	8.69	121.84	111.33
2	Q	196	HIS	N-CA-C	8.57	121.40	111.11
1	R	437	ARG	CA-C-N	-8.07	109.75	119.84
1	R	437	ARG	C-N-CA	-8.07	109.75	119.84
1	P	196	HIS	N-CA-C	8.01	120.73	111.11
1	P	387	GLN	N-CA-C	-7.90	103.78	113.50
1	P	385	ILE	N-CA-C	-7.44	105.87	112.12
1	R	192	ASN	N-CA-C	-7.40	100.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	403	LYS	CA-C-N	7.29	127.45	119.87
1	P	403	LYS	C-N-CA	7.29	127.45	119.87
1	R	214	ASP	N-CA-C	7.24	121.06	111.28
1	R	188	PHE	N-CA-C	-7.05	98.20	109.76
1	P	437	ARG	CA-C-N	-7.02	111.07	119.84
1	P	437	ARG	C-N-CA	-7.02	111.07	119.84
1	R	226	SER	N-CA-C	6.95	119.42	108.79
1	P	188	PHE	N-CA-C	-6.91	98.43	109.76
2	Q	192	ASN	N-CA-C	-6.90	101.42	110.53
1	R	403	LYS	CA-C-N	6.84	126.99	119.87
1	R	403	LYS	C-N-CA	6.84	126.99	119.87
1	P	139	VAL	CB-CA-C	-6.79	100.05	110.50
2	Q	191	ASP	N-CA-C	6.78	120.52	112.93
1	P	214	ASP	N-CA-C	6.77	121.00	111.52
2	Q	443	TYR	N-CA-C	6.69	118.37	108.60
1	R	321	VAL	N-CA-C	6.68	121.69	113.00
2	Q	214	ASP	N-CA-C	6.66	120.27	111.28
2	Q	188	PHE	N-CA-C	-6.62	98.90	109.76
1	R	191	ASP	N-CA-C	6.54	120.73	113.21
2	Q	139	VAL	CB-CA-C	-6.37	100.69	110.50
2	Q	387	GLN	N-CA-C	-6.29	105.42	113.23
1	R	80	ARG	N-CA-C	-6.21	99.69	109.50
1	R	387	GLN	N-CA-C	-6.19	105.56	113.23
1	P	226	SER	N-CA-C	6.16	117.90	108.42
1	P	321	VAL	N-CA-C	6.15	120.65	112.04
2	Q	403	LYS	CA-C-N	6.13	125.75	119.56
2	Q	403	LYS	C-N-CA	6.13	125.75	119.56
1	P	442	PHE	N-CA-C	-6.09	100.26	109.95
1	R	443	TYR	N-CA-C	6.08	117.47	108.60
1	P	436	SER	N-CA-C	-6.02	100.93	109.96
2	Q	437	ARG	CA-C-N	-5.98	112.37	119.84
2	Q	437	ARG	C-N-CA	-5.98	112.37	119.84
1	P	192	ASN	N-CA-C	-5.94	102.69	110.53
1	R	455	ASN	N-CA-C	5.94	120.39	113.20
1	P	98	ILE	N-CA-C	5.86	118.41	111.09
2	Q	321	VAL	N-CA-C	5.83	121.01	113.07
1	R	139	VAL	CB-CA-C	-5.80	101.57	110.50
1	P	471	GLY	N-CA-C	5.80	119.14	111.03
1	P	80	ARG	N-CA-C	-5.75	100.41	109.50
2	Q	80	PRO	N-CA-C	-5.72	100.69	112.47
2	Q	455	ASN	N-CA-C	5.60	119.98	113.20
2	Q	109	GLY	C-N-CD	-5.54	102.27	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	226	SER	N-CA-C	5.48	117.18	108.79
2	Q	365	ARG	N-CA-C	5.39	117.01	111.03
1	P	191	ASP	N-CA-C	5.37	118.94	112.93
2	Q	442	PHE	N-CA-C	-5.28	101.27	109.72
1	P	431	ILE	N-CA-C	5.27	115.99	110.62
1	R	471	GLY	N-CA-C	5.25	118.39	111.03
1	R	436	SER	N-CA-C	-5.22	101.91	109.59
1	P	77	GLY	N-CA-C	5.17	117.57	110.69
1	R	187	ARG	N-CA-C	5.16	116.13	108.60
1	R	198	ILE	N-CA-CB	-5.14	105.48	112.16
1	R	385	ILE	N-CA-C	-5.14	107.74	111.90
1	P	187	ARG	N-CA-C	5.14	116.10	108.60
1	R	442	PHE	N-CA-C	-5.11	101.82	109.95
1	P	91	SER	N-CA-C	5.09	117.28	110.35
2	Q	77	GLY	N-CA-C	5.03	117.38	110.69
2	Q	471	GLY	N-CA-C	5.01	118.04	111.03

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	P	3202	0	2985	63	0
1	R	3202	0	2985	69	0
2	Q	3172	0	2977	98	0
3	A	23	0	21	3	0
3	B	23	0	21	0	0
3	C	23	0	21	3	0
3	D	23	0	21	0	0
3	E	23	0	21	2	0
3	F	23	0	21	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
All	All	9717	0	9073	223	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 12.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:110:PRO:CG	2:Q:199:LEU:HD13	1.59	1.32
2:Q:80:PRO:HD2	2:Q:118:TYR:O	1.28	1.31
2:Q:110:PRO:CD	2:Q:197:TRP:O	1.85	1.24
2:Q:110:PRO:HD2	2:Q:197:TRP:O	1.02	1.19
2:Q:78:TYR:CE1	2:Q:80:PRO:HD3	1.84	1.13
2:Q:120:ILE:HG21	2:Q:140:MET:HE2	1.22	1.13
2:Q:120:ILE:CG2	2:Q:140:MET:HE2	1.87	1.03
2:Q:110:PRO:CG	2:Q:199:LEU:CD1	2.40	1.00
2:Q:110:PRO:HG2	2:Q:199:LEU:CD1	1.92	0.99
2:Q:201:CYS:SG	2:Q:203:VAL:O	2.22	0.97
2:Q:110:PRO:HG2	2:Q:199:LEU:HD13	1.42	0.95
2:Q:110:PRO:HG3	2:Q:199:LEU:HD13	1.49	0.94
1:P:110:ARG:HH11	1:P:114:GLN:HE22	1.15	0.93
2:Q:110:PRO:CB	2:Q:199:LEU:HD13	2.01	0.89
2:Q:250:ASN:HD21	2:Q:257:GLN:HE21	1.21	0.88
1:R:110:ARG:HH11	1:R:114:GLN:HE22	1.21	0.88
2:Q:78:TYR:HE1	2:Q:80:PRO:HG3	1.43	0.83
2:Q:110:PRO:CB	2:Q:199:LEU:CD1	2.57	0.82
1:P:188:PHE:HE2	3:A:2:FRU:H61	1.45	0.80
2:Q:110:PRO:CG	2:Q:197:TRP:O	2.29	0.80
1:P:161:ARG:HD2	1:R:150:ASP:O	1.83	0.79
2:Q:78:TYR:CE1	2:Q:80:PRO:CD	2.64	0.79
2:Q:159:ASN:O	2:Q:161:LEU:CD1	2.32	0.78
1:P:143:ASP:HB2	1:P:158:LEU:HD13	1.67	0.77
1:P:188:PHE:CE2	3:A:2:FRU:H61	2.19	0.77
2:Q:80:PRO:CD	2:Q:118:TYR:O	2.23	0.76
1:P:217:TRP:HD1	1:P:221:LEU:HD12	1.50	0.75
1:P:250:ASN:HD21	1:P:257:GLN:HE21	1.33	0.73
1:R:143:ASP:HB2	1:R:158:LEU:HD13	1.70	0.73
2:Q:78:TYR:CE1	2:Q:80:PRO:HG3	2.23	0.72
1:R:217:TRP:HD1	1:R:221:LEU:HD12	1.54	0.71
1:R:303:ARG:HH11	1:R:303:ARG:HB2	1.55	0.71
2:Q:78:TYR:CD1	2:Q:80:PRO:HD3	2.24	0.71
1:P:217:TRP:CD1	1:P:221:LEU:HD12	2.26	0.71
2:Q:199:LEU:HD12	2:Q:199:LEU:N	2.05	0.71
1:P:86:ASN:HB3	1:P:92:THR:HG23	1.73	0.70
2:Q:150:ASP:O	1:R:161:ARG:HD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:295:HIS:HD2	1:R:308:LYS:NZ	1.89	0.70
2:Q:161:LEU:HD12	2:Q:161:LEU:N	2.05	0.69
2:Q:78:TYR:HE1	2:Q:80:PRO:HD3	1.51	0.69
2:Q:143:ASP:HB2	2:Q:158:LEU:HD13	1.74	0.69
1:R:437:ARG:HG3	1:R:482:TRP:CE3	2.28	0.68
1:R:217:TRP:CD1	1:R:221:LEU:HD12	2.28	0.68
2:Q:110:PRO:HG2	2:Q:197:TRP:O	1.93	0.68
1:P:303:ARG:HB2	1:P:303:ARG:NH1	2.09	0.68
2:Q:78:TYR:HE1	2:Q:80:PRO:CG	2.08	0.67
1:R:162:GLN:NE2	1:R:188:PHE:H	1.93	0.67
2:Q:303:ARG:NH1	2:Q:303:ARG:HB2	2.10	0.67
1:R:250:ASN:HD21	1:R:257:GLN:HE21	1.41	0.66
1:P:437:ARG:HG3	1:P:482:TRP:CE3	2.30	0.66
2:Q:259:MET:HB3	2:Q:291:LEU:HB3	1.78	0.66
2:Q:78:TYR:HE1	2:Q:80:PRO:CD	2.07	0.66
2:Q:223:SER:OG	2:Q:251:HIS:HD2	1.80	0.65
2:Q:86:ASN:HB3	2:Q:92:THR:HG23	1.78	0.65
2:Q:388:ASN:OD1	1:R:172:THR:HB	1.97	0.65
1:R:223:SER:OG	1:R:251:HIS:HD2	1.79	0.65
2:Q:217:TRP:CD1	2:Q:221:LEU:HD12	2.32	0.64
1:P:223:SER:OG	1:P:251:HIS:HD2	1.81	0.64
1:P:172:THR:HB	1:R:388:ASN:OD1	1.96	0.64
2:Q:217:TRP:HD1	2:Q:221:LEU:HD12	1.63	0.64
2:Q:438:PRO:HA	2:Q:481:THR:CG2	2.29	0.63
1:P:110:ARG:HH11	1:P:114:GLN:NE2	1.93	0.63
1:R:303:ARG:HB2	1:R:303:ARG:NH1	2.13	0.62
1:P:259:MET:HB3	1:P:291:LEU:HB3	1.81	0.62
1:P:110:ARG:HD3	1:P:114:GLN:NE2	2.14	0.62
1:R:295:HIS:HD2	1:R:308:LYS:HZ2	1.47	0.62
1:R:437:ARG:O	1:R:437:ARG:HD3	2.00	0.62
2:Q:303:ARG:HB2	2:Q:303:ARG:HH11	1.65	0.62
2:Q:217:TRP:O	2:Q:219:ASP:N	2.34	0.61
1:P:86:ASN:HB3	1:P:92:THR:CG2	2.31	0.61
2:Q:110:PRO:HB3	2:Q:199:LEU:CD1	2.31	0.61
2:Q:110:PRO:HD3	2:Q:198:ILE:HA	1.82	0.61
1:R:479:MET:SD	1:R:479:MET:C	2.84	0.61
2:Q:159:ASN:O	2:Q:161:LEU:HD12	2.01	0.61
2:Q:78:TYR:CE1	2:Q:80:PRO:CG	2.83	0.60
1:R:86:ASN:HB3	1:R:92:THR:HG23	1.83	0.60
2:Q:188:PHE:CE2	3:E:2:FRU:H61	2.36	0.60
1:R:188:PHE:HE2	3:C:2:FRU:H61	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:201:CYS:SG	2:Q:203:VAL:C	2.85	0.60
1:R:259:MET:HB3	1:R:291:LEU:HB3	1.82	0.60
1:P:295:HIS:HD2	1:P:308:LYS:NZ	2.00	0.60
2:Q:110:PRO:CD	2:Q:198:ILE:HA	2.31	0.60
1:P:303:ARG:HB2	1:P:303:ARG:HH11	1.66	0.59
1:R:217:TRP:O	1:R:219:ASP:N	2.35	0.59
1:P:438:PRO:HA	1:P:481:THR:CG2	2.32	0.59
2:Q:110:PRO:CB	2:Q:199:LEU:HD11	2.32	0.58
1:P:217:TRP:O	1:P:219:ASP:N	2.36	0.58
2:Q:161:LEU:CD1	2:Q:161:LEU:N	2.67	0.58
2:Q:199:LEU:CD1	2:Q:199:LEU:N	2.67	0.58
1:P:162:GLN:NE2	1:P:188:PHE:H	2.02	0.57
1:P:437:ARG:HG3	1:P:482:TRP:CD2	2.39	0.57
2:Q:438:PRO:HA	2:Q:481:THR:HG23	1.86	0.57
2:Q:110:PRO:HB3	2:Q:199:LEU:HD13	1.84	0.56
2:Q:386:ASN:HB2	2:Q:389:PHE:H	1.69	0.56
1:R:437:ARG:HG3	1:R:482:TRP:CD2	2.40	0.56
1:P:205:LEU:HD21	1:P:248:THR:HG21	1.89	0.56
2:Q:437:ARG:O	2:Q:438:PRO:C	2.44	0.56
1:R:386:ASN:HB2	1:R:389:PHE:H	1.70	0.56
2:Q:188:PHE:HE2	3:E:2:FRU:H61	1.71	0.55
2:Q:295:HIS:HD2	2:Q:308:LYS:NZ	2.03	0.55
2:Q:299:PHE:O	2:Q:302:LEU:HD12	2.06	0.55
1:R:438:PRO:HA	1:R:481:THR:CG2	2.35	0.55
1:R:188:PHE:CE2	3:C:2:FRU:H61	2.41	0.55
1:R:446:TRP:CZ3	1:R:471:GLY:HA3	2.42	0.55
1:P:437:ARG:O	1:P:438:PRO:C	2.48	0.55
2:Q:205:LEU:HD21	2:Q:248:THR:HG21	1.89	0.55
2:Q:108:ILE:O	2:Q:110:PRO:HD3	2.06	0.54
1:R:299:PHE:O	1:R:302:LEU:HD12	2.06	0.54
1:P:77:GLY:O	1:P:482:TRP:HA	2.07	0.54
1:P:248:THR:HB	1:P:261:SER:OG	2.07	0.54
1:R:437:ARG:O	1:R:438:PRO:C	2.47	0.54
2:Q:80:PRO:HG2	2:Q:118:TYR:HB3	1.89	0.54
1:R:77:GLY:O	1:R:482:TRP:HA	2.08	0.54
2:Q:199:LEU:HD12	2:Q:199:LEU:H	1.71	0.54
1:R:162:GLN:HE21	1:R:187:ARG:HA	1.72	0.54
2:Q:162:GLN:HE21	2:Q:187:ARG:HA	1.74	0.53
1:P:184:ALA:HB3	1:R:479:MET:HB3	1.89	0.53
1:P:437:ARG:O	1:P:437:ARG:HD3	2.08	0.53
2:Q:162:GLN:NE2	2:Q:188:PHE:H	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:143:ASP:HB2	1:P:158:LEU:CD1	2.38	0.53
2:Q:446:TRP:CZ3	2:Q:471:GLY:HA3	2.44	0.53
1:P:363:LYS:HD3	1:P:371:SER:HB2	1.91	0.53
1:P:386:ASN:HB2	1:P:389:PHE:H	1.72	0.53
1:R:438:PRO:HA	1:R:481:THR:HG23	1.91	0.52
1:P:388:ASN:OD1	2:Q:172:THR:HB	2.10	0.52
2:Q:361:ARG:HG2	2:Q:361:ARG:HH11	1.73	0.52
2:Q:120:ILE:HG23	2:Q:140:MET:HG3	1.90	0.51
1:R:110:ARG:HD3	1:R:114:GLN:NE2	2.25	0.51
1:R:181:THR:HG23	1:R:213:TYR:HB2	1.91	0.51
1:P:291:LEU:HD23	1:P:312:LEU:HG	1.93	0.51
1:R:303:ARG:HG2	1:R:345:THR:OG1	2.11	0.51
1:R:437:ARG:O	1:R:439:GLU:N	2.44	0.51
2:Q:264:ARG:HG3	2:Q:286:THR:HG22	1.93	0.51
1:R:205:LEU:HD21	1:R:248:THR:HG21	1.91	0.51
1:P:299:PHE:O	1:P:302:LEU:HD12	2.11	0.50
1:P:303:ARG:HG2	1:P:345:THR:OG1	2.11	0.50
1:P:314:GLY:HA3	1:P:318:GLY:O	2.11	0.50
1:R:217:TRP:HD1	1:R:221:LEU:CD1	2.22	0.49
2:Q:77:GLY:O	2:Q:482:ALA:HA	2.12	0.49
1:P:162:GLN:HE21	1:P:187:ARG:HA	1.77	0.49
2:Q:181:THR:HG23	2:Q:213:TYR:HB2	1.94	0.49
1:R:136:ARG:HD3	1:R:166:GLU:OE1	2.12	0.49
1:P:479:MET:SD	1:P:479:MET:C	2.95	0.49
1:R:86:ASN:HB3	1:R:92:THR:CG2	2.43	0.49
1:P:446:TRP:CZ3	1:P:471:GLY:HA3	2.47	0.49
1:P:198:ILE:HD11	1:P:378:ASN:HB2	1.95	0.49
2:Q:282:ASP:O	2:Q:332:PRO:HD3	2.13	0.48
1:R:110:ARG:NH1	1:R:114:GLN:HE22	2.02	0.48
1:P:80:ARG:NH2	3:A:1:GLC:O3	2.44	0.48
2:Q:248:THR:HB	2:Q:261:SER:OG	2.13	0.48
2:Q:437:ARG:O	2:Q:437:ARG:HD3	2.13	0.48
2:Q:86:ASN:HB3	2:Q:92:THR:CG2	2.42	0.48
2:Q:110:PRO:HG2	2:Q:199:LEU:HD12	1.91	0.48
2:Q:291:LEU:HD23	2:Q:312:LEU:HG	1.95	0.48
1:P:437:ARG:O	1:P:439:GLU:N	2.47	0.48
1:P:145:GLN:NE2	1:P:156:SER:HA	2.29	0.48
2:Q:408:ASN:O	2:Q:409:ASP:HB2	2.14	0.47
2:Q:217:TRP:HD1	2:Q:221:LEU:CD1	2.26	0.47
2:Q:437:ARG:O	2:Q:439:GLU:N	2.47	0.47
1:P:295:HIS:HD2	1:P:308:LYS:HZ2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:295:HIS:HD2	2:Q:308:LYS:HZ2	1.63	0.47
1:P:361:ARG:HG2	1:P:361:ARG:HH11	1.80	0.47
1:P:438:PRO:HA	1:P:481:THR:HG23	1.96	0.47
1:R:361:ARG:HH11	1:R:361:ARG:HG2	1.80	0.47
1:R:143:ASP:HB2	1:R:158:LEU:CD1	2.44	0.47
1:R:145:GLN:NE2	1:R:156:SER:HA	2.29	0.47
2:Q:410:ARG:HA	2:Q:456:TYR:O	2.16	0.46
1:R:127:GLN:OE1	1:R:135:THR:HG21	2.15	0.46
1:R:291:LEU:HD23	1:R:312:LEU:HG	1.97	0.46
1:P:74:GLU:OE2	1:P:126:LYS:HD2	2.16	0.46
1:R:363:LYS:HD3	1:R:371:SER:HB2	1.98	0.46
1:R:198:ILE:HD11	1:R:378:ASN:HB2	1.97	0.46
1:P:127:GLN:OE1	1:P:135:THR:HG21	2.16	0.45
1:R:410:ARG:HA	1:R:456:TYR:O	2.16	0.45
2:Q:127:GLN:OE1	2:Q:135:THR:HG21	2.16	0.45
1:P:136:ARG:HD3	1:P:166:GLU:OE1	2.17	0.45
1:P:319:ALA:HB3	1:P:330:LEU:HD13	1.98	0.45
1:P:463:GLY:HA2	1:P:468:ASN:HB3	1.99	0.45
2:Q:363:LYS:HD3	2:Q:371:SER:HB2	1.97	0.45
2:Q:303:ARG:HG2	2:Q:345:THR:OG1	2.16	0.44
1:R:257:GLN:OE1	1:R:295:HIS:HE1	2.00	0.44
1:R:305:GLY:HA3	1:R:344:THR:O	2.17	0.44
1:R:463:GLY:HA2	1:R:468:ASN:HB3	1.99	0.44
1:R:413:VAL:HG21	1:R:453:LEU:HA	2.00	0.44
2:Q:387:GLN:HE22	1:R:131:ASN:ND2	2.15	0.44
2:Q:110:PRO:HG2	2:Q:197:TRP:C	2.43	0.44
2:Q:386:ASN:HB3	2:Q:387:GLN:H	1.64	0.43
1:R:109:GLY:O	1:R:419:LYS:HE2	2.17	0.43
1:P:194:ASP:CB	1:P:201:ASP:HA	2.48	0.43
1:R:282:ASP:O	1:R:332:PRO:HD3	2.18	0.43
1:R:216:LYS:HE2	1:R:216:LYS:HB2	1.88	0.43
2:Q:143:ASP:HB2	2:Q:158:LEU:CD1	2.45	0.43
1:P:386:ASN:HB3	1:P:387:GLN:H	1.61	0.43
1:P:410:ARG:HA	1:P:456:TYR:O	2.18	0.43
2:Q:172:THR:HG22	2:Q:173:PHE:HD1	1.84	0.43
1:P:109:GLY:O	1:P:419:LYS:HE2	2.18	0.43
1:R:80:ARG:NH2	3:C:1:GLC:C2	2.82	0.43
2:Q:395:GLY:HA2	2:Q:419:LYS:O	2.19	0.42
1:P:390:ALA:HB2	1:P:431:ILE:HD13	2.02	0.42
2:Q:413:VAL:CG2	2:Q:452:LYS:HG2	2.48	0.42
1:R:194:ASP:CB	1:R:201:ASP:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:463:GLY:HA2	2:Q:468:ASN:HB3	2.01	0.42
1:R:434:PHE:O	1:R:437:ARG:NH2	2.53	0.42
1:P:347:LEU:HD12	1:P:347:LEU:HA	1.95	0.42
1:R:162:GLN:HE21	1:R:187:ARG:CA	2.33	0.42
1:R:263:LEU:N	1:R:263:LEU:HD23	2.35	0.41
1:P:138:LYS:HD3	1:P:164:PHE:CE1	2.55	0.41
2:Q:413:VAL:HG21	2:Q:453:LEU:HA	2.02	0.41
1:R:110:ARG:HH11	1:R:114:GLN:NE2	2.01	0.41
1:R:413:VAL:HG23	1:R:452:LYS:HG2	2.03	0.41
2:Q:120:ILE:HG23	2:Q:140:MET:CG	2.51	0.41
1:P:209:GLY:HA3	1:P:227:LEU:O	2.21	0.41
2:Q:402:LEU:O	2:Q:412:ALA:HA	2.21	0.41
1:P:217:TRP:HD1	1:P:221:LEU:CD1	2.24	0.41
1:R:315:HIS:HD2	1:R:335:ASP:OD1	2.04	0.41
1:R:291:LEU:HD21	1:R:310:ALA:HB1	2.02	0.40
1:P:129:LEU:HD12	1:P:129:LEU:N	2.35	0.40
2:Q:305:GLY:HA3	2:Q:344:THR:O	2.22	0.40
1:R:400:MET:O	1:R:414:ASN:HA	2.21	0.40
1:P:136:ARG:O	1:P:165:VAL:HA	2.21	0.40
2:Q:138:LYS:HD3	2:Q:164:PHE:CE1	2.56	0.40
2:Q:162:GLN:HE21	2:Q:187:ARG:CA	2.35	0.40
1:R:361:ARG:HH11	1:R:361:ARG:CG	2.33	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	P	411/413 (100%)	387 (94%)	21 (5%)	3 (1%)	18	28
1	R	411/413 (100%)	390 (95%)	18 (4%)	3 (1%)	18	28
2	Q	411/413 (100%)	386 (94%)	20 (5%)	5 (1%)	10	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1233/1239 (100%)	1163 (94%)	59 (5%)	11 (1%)	14	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	218	ASN
2	Q	218	ASN
1	R	218	ASN
2	Q	80	PRO
2	Q	220	GLY
1	R	220	GLY
1	P	220	GLY
1	P	470	GLY
2	Q	438	PRO
2	Q	470	GLY
1	R	470	GLY

5.3.2 Protein sidechains ⓘ

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	P	327/327 (100%)	291 (89%)	36 (11%)	6	9
1	R	327/327 (100%)	290 (89%)	37 (11%)	5	8
2	Q	324/324 (100%)	287 (89%)	37 (11%)	5	8
All	All	978/978 (100%)	868 (89%)	110 (11%)	6	9

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	92	THR
1	P	110	ARG
1	P	111	LEU
1	P	130	ASP
1	P	135	THR

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Mol	Chain	Res	Type
1	P	139	VAL
1	P	158	LEU
1	P	172	THR
1	P	181	THR
1	P	182	LEU
1	P	198	ILE
1	P	203	VAL
1	P	218	ASN
1	P	222	ARG
1	P	242	VAL
1	P	248	THR
1	P	263	LEU
1	P	288	VAL
1	P	291	LEU
1	P	292	LEU
1	P	297	ASP
1	P	302	LEU
1	P	344	THR
1	P	347	LEU
1	P	358	LEU
1	P	379	LEU
1	P	380	ARG
1	P	382	ILE
1	P	402	LEU
1	P	413	VAL
1	P	414	ASN
1	P	437	ARG
1	P	441	ARG
1	P	446	TRP
1	P	468	ASN
1	P	478	GLN
2	Q	83	VAL
2	Q	92	THR
2	Q	111	LEU
2	Q	130	ASP
2	Q	135	THR
2	Q	139	VAL
2	Q	158	LEU
2	Q	172	THR
2	Q	181	THR
2	Q	182	LEU
2	Q	198	ILE

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Mol	Chain	Res	Type
2	Q	203	VAL
2	Q	218	ASN
2	Q	222	ARG
2	Q	242	VAL
2	Q	248	THR
2	Q	263	LEU
2	Q	280	LYS
2	Q	288	VAL
2	Q	291	LEU
2	Q	292	LEU
2	Q	297	ASP
2	Q	302	LEU
2	Q	344	THR
2	Q	347	LEU
2	Q	350	ASN
2	Q	358	LEU
2	Q	379	LEU
2	Q	380	ARG
2	Q	382	ILE
2	Q	413	VAL
2	Q	414	ASN
2	Q	437	ARG
2	Q	441	ARG
2	Q	468	ASN
2	Q	478	GLN
2	Q	481	THR
1	R	92	THR
1	R	110	ARG
1	R	111	LEU
1	R	130	ASP
1	R	135	THR
1	R	139	VAL
1	R	158	LEU
1	R	172	THR
1	R	181	THR
1	R	182	LEU
1	R	198	ILE
1	R	203	VAL
1	R	218	ASN
1	R	222	ARG
1	R	248	THR
1	R	263	LEU

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Mol	Chain	Res	Type
1	R	288	VAL
1	R	291	LEU
1	R	292	LEU
1	R	297	ASP
1	R	302	LEU
1	R	344	THR
1	R	347	LEU
1	R	358	LEU
1	R	379	LEU
1	R	380	ARG
1	R	382	ILE
1	R	413	VAL
1	R	414	ASN
1	R	424	PRO
1	R	437	ARG
1	R	439	GLU
1	R	441	ARG
1	R	468	ASN
1	R	478	GLN
1	R	479	MET
1	R	481	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	114	GLN
1	P	162	GLN
1	P	196	HIS
1	P	218	ASN
1	P	244	ASN
1	P	250	ASN
1	P	251	HIS
1	P	295	HIS
1	P	315	HIS
1	P	378	ASN
1	P	383	GLN
1	P	387	GLN
1	P	398	GLN
1	P	468	ASN
1	P	478	GLN
2	Q	162	GLN
2	Q	196	HIS

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Mol	Chain	Res	Type
2	Q	218	ASN
2	Q	244	ASN
2	Q	250	ASN
2	Q	251	HIS
2	Q	295	HIS
2	Q	315	HIS
2	Q	350	ASN
2	Q	383	GLN
2	Q	387	GLN
2	Q	468	ASN
1	R	114	GLN
1	R	145	GLN
1	R	162	GLN
1	R	196	HIS
1	R	218	ASN
1	R	244	ASN
1	R	250	ASN
1	R	251	HIS
1	R	295	HIS
1	R	315	HIS
1	R	350	ASN
1	R	378	ASN
1	R	383	GLN
1	R	387	GLN
1	R	468	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](#)

12 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	GLC	A	1	3	11,11,12	0.92	0	15,15,17	0.82	0
3	FRU	A	2	3	11,12,12	1.23	1 (9%)	10,18,18	0.77	0
3	GLC	B	1	3	11,11,12	0.69	0	15,15,17	0.74	0
3	FRU	B	2	3	11,12,12	0.63	0	10,18,18	0.54	0
3	GLC	C	1	3	11,11,12	1.05	1 (9%)	15,15,17	0.85	0
3	FRU	C	2	3	11,12,12	1.37	1 (9%)	10,18,18	0.91	0
3	GLC	D	1	3	11,11,12	0.56	0	15,15,17	0.99	1 (6%)
3	FRU	D	2	3	11,12,12	0.84	1 (9%)	10,18,18	0.57	0
3	GLC	E	1	3	11,11,12	0.97	0	15,15,17	0.86	0
3	FRU	E	2	3	11,12,12	1.28	1 (9%)	10,18,18	0.92	1 (10%)
3	GLC	F	1	3	11,11,12	0.69	0	15,15,17	0.71	0
3	FRU	F	2	3	11,12,12	0.59	0	10,18,18	0.55	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	GLC	A	1	3	-	2/2/19/22	0/1/1/1
3	FRU	A	2	3	-	3/5/24/24	0/1/1/1
3	GLC	B	1	3	-	2/2/19/22	0/1/1/1
3	FRU	B	2	3	-	0/5/24/24	0/1/1/1
3	GLC	C	1	3	-	2/2/19/22	0/1/1/1
3	FRU	C	2	3	-	5/5/24/24	0/1/1/1
3	GLC	D	1	3	-	0/2/19/22	0/1/1/1
3	FRU	D	2	3	-	0/5/24/24	0/1/1/1
3	GLC	E	1	3	-	2/2/19/22	0/1/1/1
3	FRU	E	2	3	-	2/5/24/24	0/1/1/1
3	GLC	F	1	3	-	2/2/19/22	0/1/1/1
3	FRU	F	2	3	-	2/5/24/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FRU	O2-C2	4.21	1.48	1.40
3	E	2	FRU	O2-C2	3.75	1.47	1.40
3	A	2	FRU	O2-C2	3.64	1.47	1.40
3	D	2	FRU	O2-C2	2.29	1.44	1.40
3	C	1	GLC	O5-C5	2.10	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLC	C1-O5-C5	2.18	115.11	112.19
3	E	2	FRU	O1-C1-C2	-2.11	107.02	111.67

There are no chirality outliers.

All (22) torsion outliers are listed below:

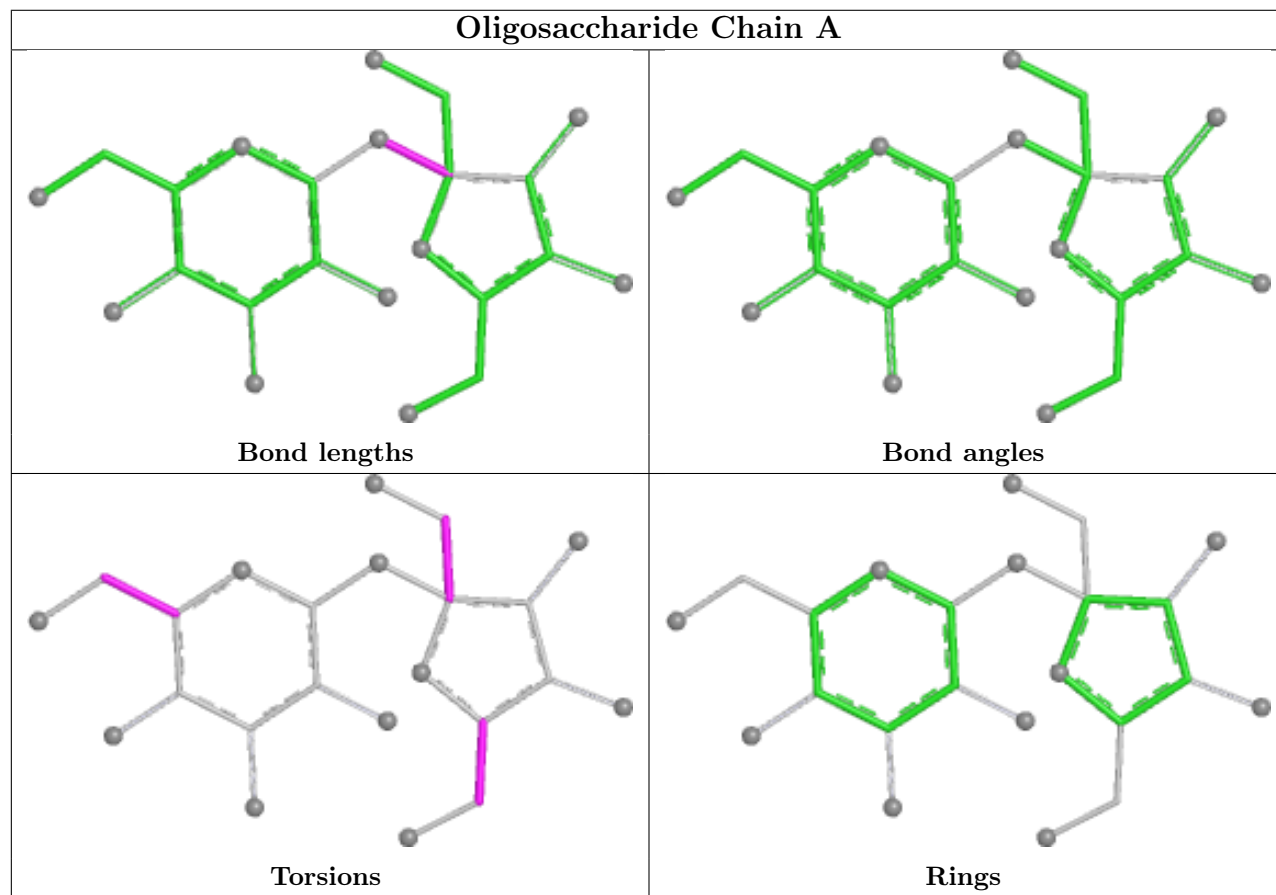
Mol	Chain	Res	Type	Atoms
3	C	2	FRU	O1-C1-C2-C3
3	C	2	FRU	O1-C1-C2-O2
3	E	2	FRU	C4-C5-C6-O6
3	A	2	FRU	C4-C5-C6-O6
3	A	2	FRU	O5-C5-C6-O6
3	C	2	FRU	O5-C5-C6-O6
3	E	2	FRU	O5-C5-C6-O6
3	C	2	FRU	C4-C5-C6-O6
3	C	1	GLC	O5-C5-C6-O6
3	A	1	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6
3	E	1	GLC	C4-C5-C6-O6
3	A	1	GLC	C4-C5-C6-O6
3	F	2	FRU	C4-C5-C6-O6
3	F	2	FRU	O5-C5-C6-O6
3	C	2	FRU	O1-C1-C2-O5
3	B	1	GLC	C4-C5-C6-O6
3	B	1	GLC	O5-C5-C6-O6
3	F	1	GLC	C4-C5-C6-O6
3	A	2	FRU	O1-C1-C2-C3
3	F	1	GLC	O5-C5-C6-O6

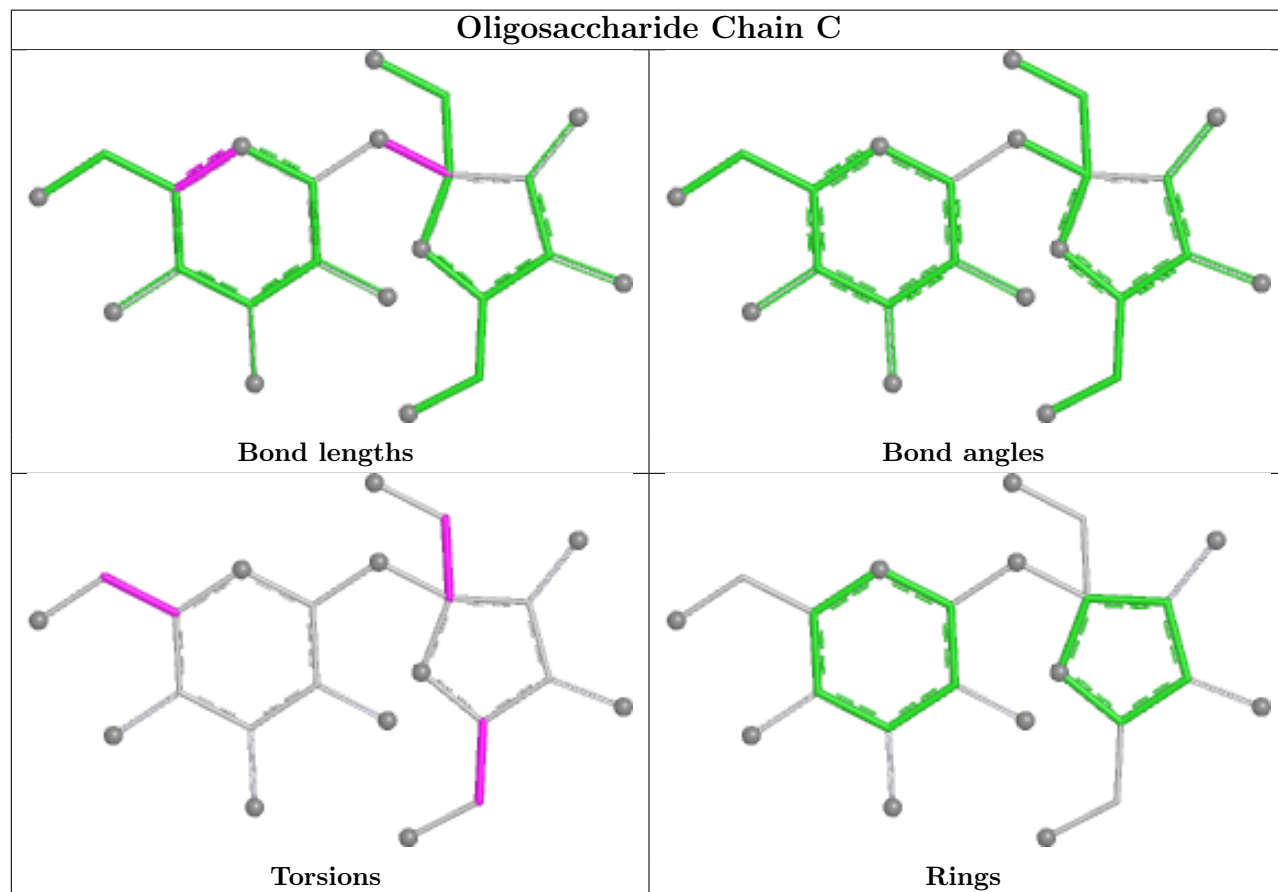
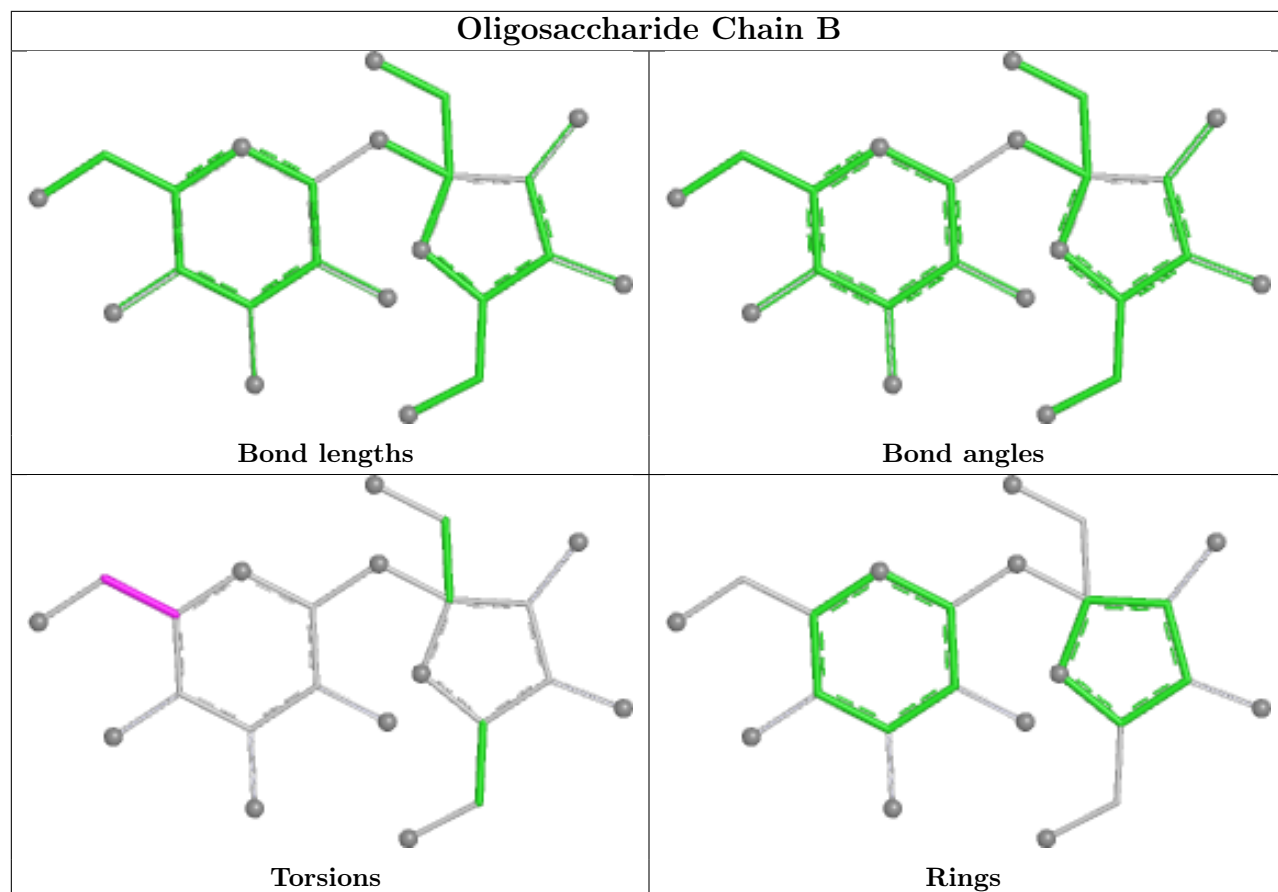
There are no ring outliers.

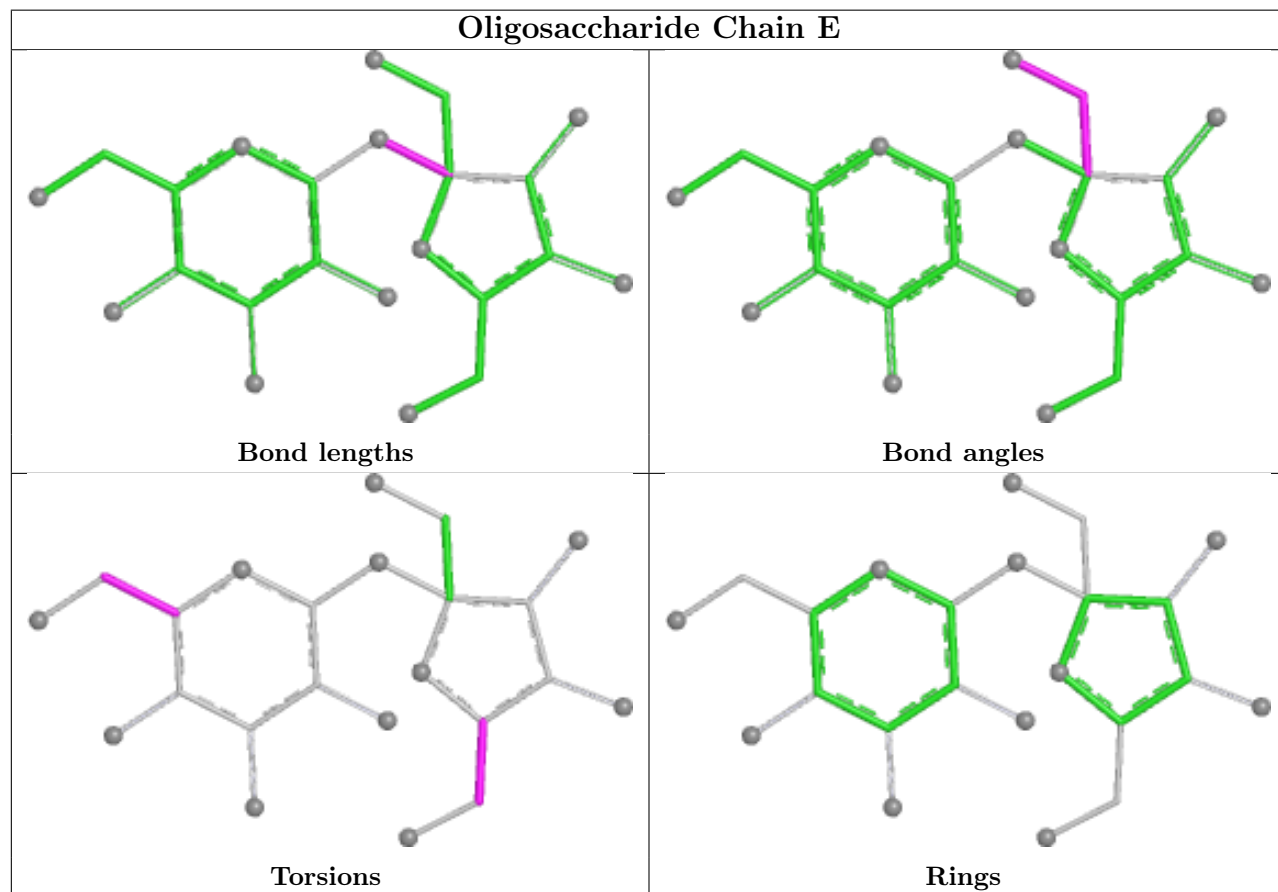
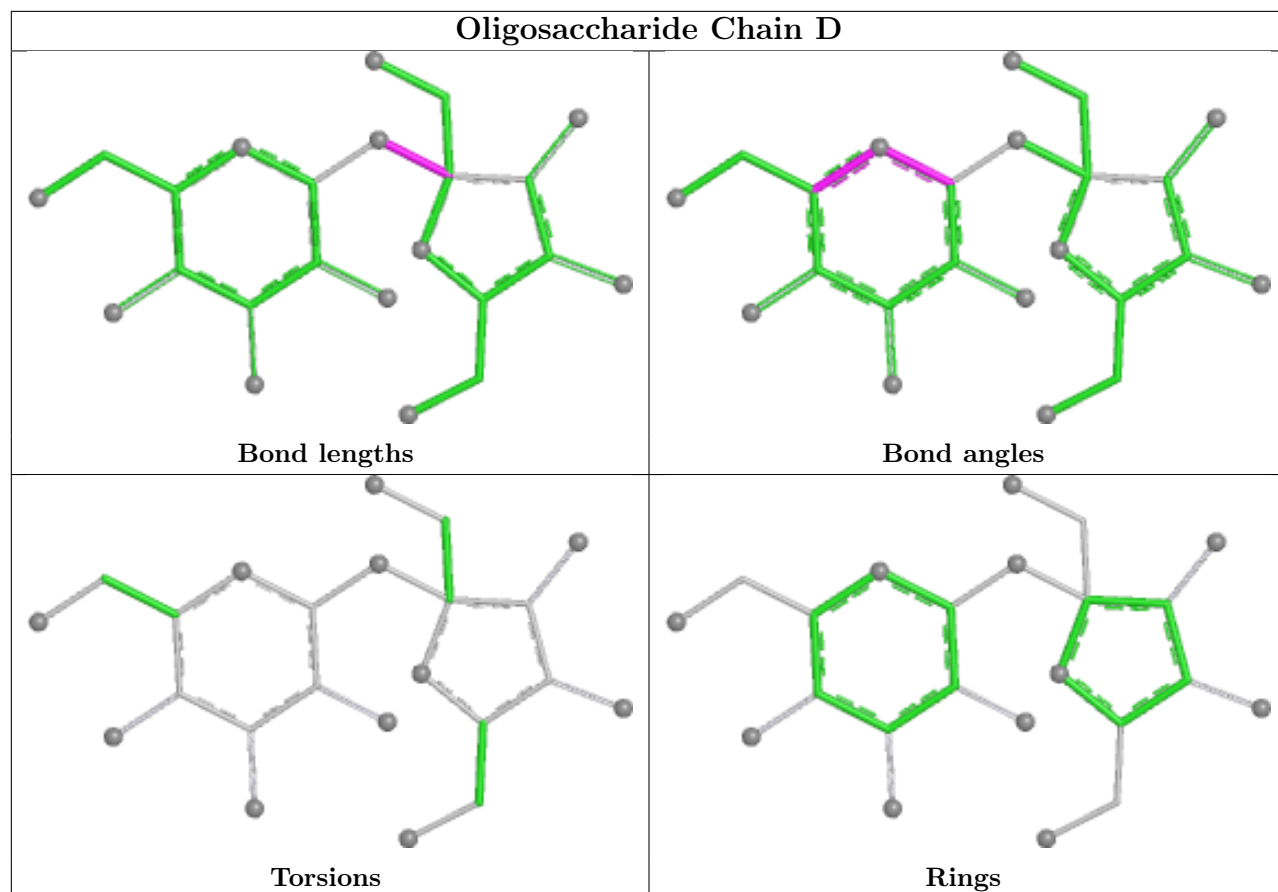
5 monomers are involved in 8 short contacts:

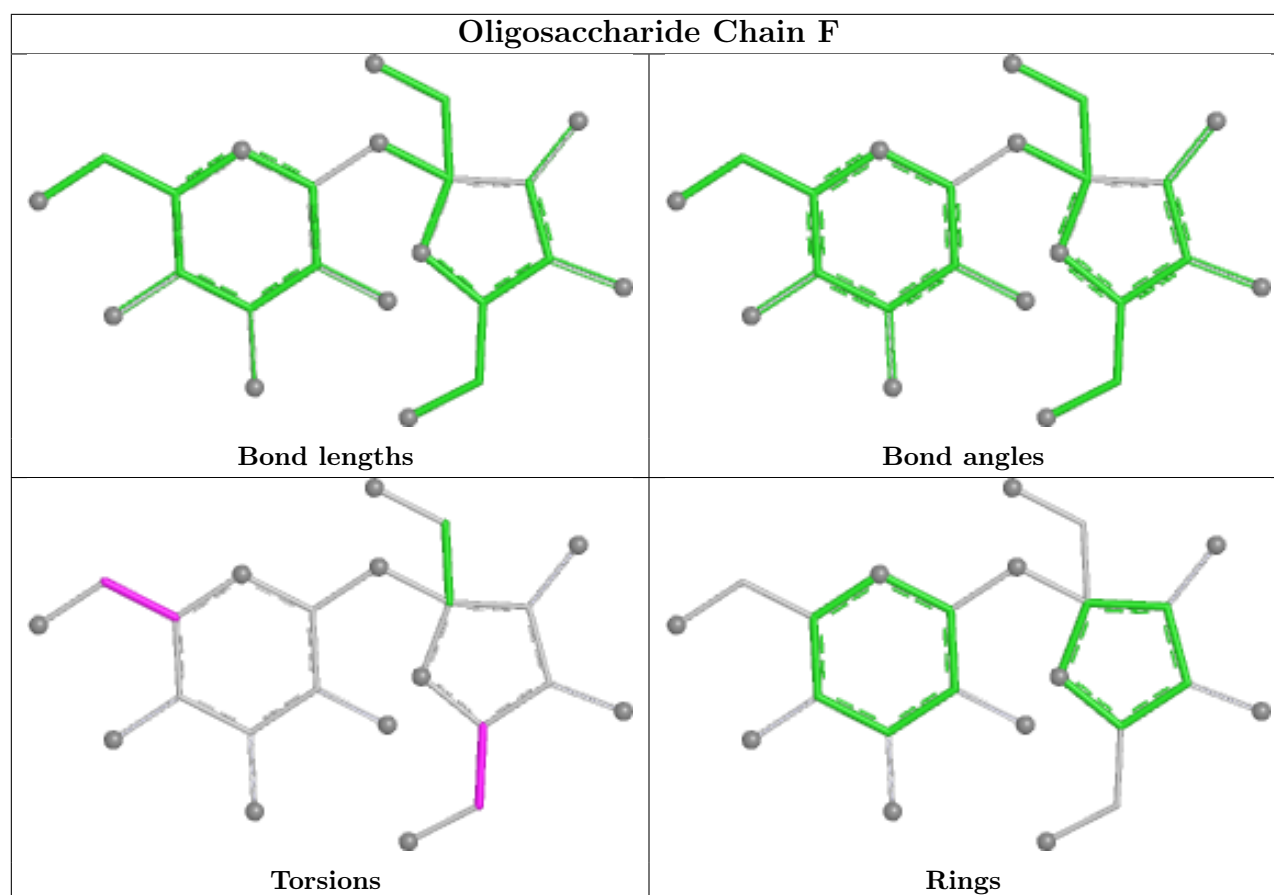
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	FRU	2	0
3	A	1	GLC	1	0
3	A	2	FRU	2	0
3	C	2	FRU	2	0
3	C	1	GLC	1	0

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.