



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 08:07 AM EDT

PDB ID : 1FQ9
Title : CRYSTAL STRUCTURE OF A TERNARY FGF2-FGFR1-HEPARIN COMPLEX
Authors : Schlessinger, J.; Plotnikov, A.N.; Ibrahimi, O.A.; Eliseenkova, A.V.; Yeh, B.K.; Yayon, A.; Linhardt, R.J.; Mohammadi, M.
Deposited on : 2000-09-04
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.23.2

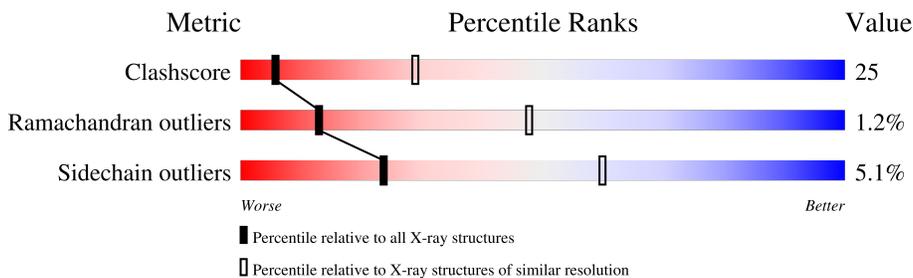
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	132	48% 46% ..
1	B	132	49% 46% ..
2	C	225	48% 43% • 6%
2	D	225	47% 37% • 13%
3	E	8	62% 38%
4	F	6	83% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SGN	E	3	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5496 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1040	660	190	186	4	0	0	0
1	B	129	1040	660	190	186	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	engineered mutation	UNP P09038
A	87	SER	CYS	engineered mutation	UNP P09038
B	69	SER	CYS	engineered mutation	UNP P09038
B	87	SER	CYS	engineered mutation	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	211	1638	1047	280	302	9	0	0	0
2	D	196	1533	980	263	281	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	engineered mutation	UNP P11362
D	185	GLN	ASN	engineered mutation	UNP P11362

- Molecule 3 is an oligosaccharide called 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoami

no)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	8	140	48	4	76	12	0	0	0

- Molecule 4 is an oligosaccharide called 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	6	105	36	3	57	9	0	0	0

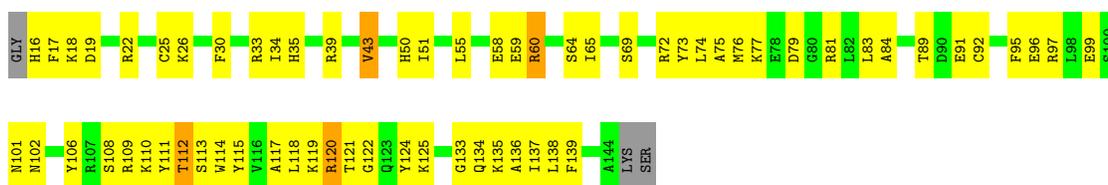
3 Residue-property plots

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.

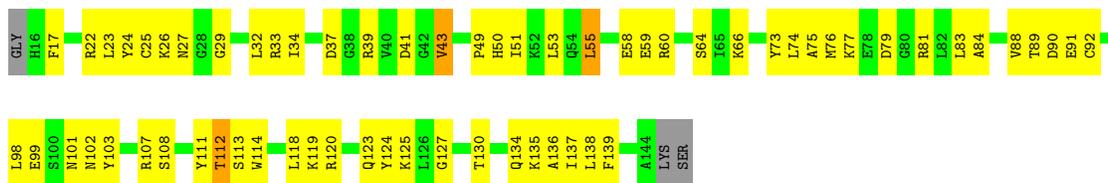
- Molecule 1: FIBROBLAST GROWTH FACTOR 2

Chain A: 



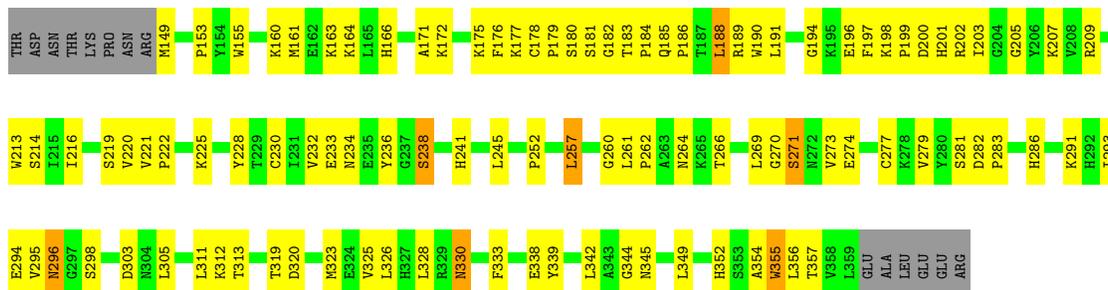
- Molecule 1: FIBROBLAST GROWTH FACTOR 2

Chain B: 



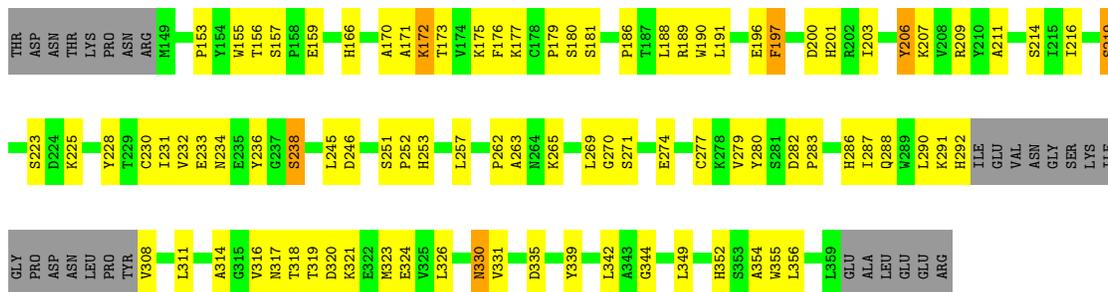
- Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1

Chain C: 



- Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1

Chain D: 



- Molecule 3: 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain E: 62% 38%



- Molecule 4: 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain F: 83% 17%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.89Å 98.89Å 196.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: SGN, IDS, IDU, UAP

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	0.44	0/1063	0.70	1/1425 (0.1%)
1	B	0.45	0/1063	0.68	1/1425 (0.1%)
2	C	0.44	0/1685	0.68	0/2299
2	D	0.42	0/1576	0.69	0/2146
All	All	0.44	0/5387	0.69	2/7295 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	SER	N-CA-C	-5.30	96.68	111.00
1	B	64	SER	N-CA-C	-5.16	97.08	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	1040	0	1040	59	0
1	B	1040	0	1040	61	0
2	C	1638	0	1603	92	0
2	D	1533	0	1506	82	0
3	E	140	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	105	0	34	1	0
All	All	5496	0	5267	273	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 25.

The worst 5 of 273 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:D:175:LYS:HG3	2:D:216:ILE:HG12	1.42	0.99
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.44	0.98
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.45	0.96
2:D:286:HIS:HD2	2:D:314:ALA:HB3	1.37	0.90
2:C:207:LYS:HE2	2:C:209:ARG:HE	1.35	0.89

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	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	19 57
1	B	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	19 57
2	C	209/225 (93%)	194 (93%)	11 (5%)	4 (2%)	8 36
2	D	192/225 (85%)	176 (92%)	14 (7%)	2 (1%)	15 53
All	All	655/714 (92%)	602 (92%)	45 (7%)	8 (1%)	13 48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR

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Mol	Chain	Res	Type
1	B	112	THR
2	C	271	SER
2	C	296	ASN
2	C	281	SER

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	110/113 (97%)	105 (96%)	5 (4%)	27	64
1	B	110/113 (97%)	106 (96%)	4 (4%)	35	70
2	C	180/198 (91%)	170 (94%)	10 (6%)	21	56
2	D	169/198 (85%)	159 (94%)	10 (6%)	19	54
All	All	569/622 (92%)	540 (95%)	29 (5%)	24	60

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	252	PRO
2	D	355	TRP
2	C	355	TRP
2	D	223	SER
2	C	313	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	317	ASN
2	C	330	ASN
2	D	317	ASN
2	D	292	HIS
2	C	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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	SGN	E	1	3	19,20,20	4.01	3 (15%)	24,31,31	1.39	3 (12%)
3	IDU	E	2	3	13,16,17	2.33	3 (23%)	15,24,26	1.51	1 (6%)
3	SGN	E	3	3	18,19,20	3.73	4 (22%)	22,29,31	1.64	3 (13%)
3	IDS	E	4	3	13,16,17	2.38	5 (38%)	15,24,26	1.74	4 (26%)
3	SGN	E	5	3	18,19,20	3.40	3 (16%)	22,29,31	1.56	5 (22%)
3	IDS	E	6	3	13,16,17	2.55	3 (23%)	15,24,26	2.09	5 (33%)
3	SGN	E	7	3	18,19,20	3.26	4 (22%)	22,29,31	2.14	6 (27%)
3	UAP	E	8	3	12,15,16	5.68	6 (50%)	13,22,24	3.38	4 (30%)
4	SGN	F	1	4	19,20,20	3.41	3 (15%)	24,31,31	1.31	2 (8%)
4	IDS	F	2	4	13,16,17	2.46	5 (38%)	15,24,26	2.88	4 (26%)
4	SGN	F	3	4	18,19,20	3.46	2 (11%)	22,29,31	1.58	3 (13%)
4	IDS	F	4	4	13,16,17	2.43	2 (15%)	15,24,26	1.75	4 (26%)
4	SGN	F	5	4	18,19,20	3.66	3 (16%)	22,29,31	1.63	5 (22%)
4	UAP	F	6	4	12,15,16	5.88	5 (41%)	13,22,24	3.51	5 (38%)

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	SGN	E	1	3	-	4/11/31/31	0/1/1/1
3	IDU	E	2	3	-	3/5/26/29	0/1/1/1
3	SGN	E	3	3	1/1/6/8	5/11/28/31	0/1/1/1
3	IDS	E	4	3	-	3/5/26/29	0/1/1/1
3	SGN	E	5	3	-	6/11/28/31	0/1/1/1
3	IDS	E	6	3	-	3/5/26/29	0/1/1/1
3	SGN	E	7	3	-	2/11/28/31	0/1/1/1
3	UAP	E	8	3	-	0/5/22/25	0/1/1/1
4	SGN	F	1	4	-	3/11/31/31	0/1/1/1
4	IDS	F	2	4	-	1/5/26/29	0/1/1/1
4	SGN	F	3	4	-	0/11/28/31	0/1/1/1
4	IDS	F	4	4	-	0/5/26/29	0/1/1/1
4	SGN	F	5	4	-	8/11/28/31	0/1/1/1
4	UAP	F	6	4	-	3/5/22/25	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6	UAP	C4-C5	17.72	1.53	1.32
3	E	8	UAP	C4-C5	17.07	1.52	1.32
3	E	1	SGN	S1-N2	14.64	1.79	1.59
4	F	5	SGN	S1-N2	13.17	1.77	1.59
3	E	3	SGN	S1-N2	12.90	1.76	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6	UAP	C1-C2-C3	10.40	118.60	108.98
3	E	8	UAP	C1-C2-C3	9.79	118.04	108.98
4	F	2	IDS	C1-C2-C3	8.23	121.70	109.40
3	E	7	SGN	C3-C2-N2	-6.83	101.35	110.32
3	E	6	IDS	C1-C2-C3	5.17	117.12	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	3	SGN	C1

5 of 41 torsion outliers are listed below:

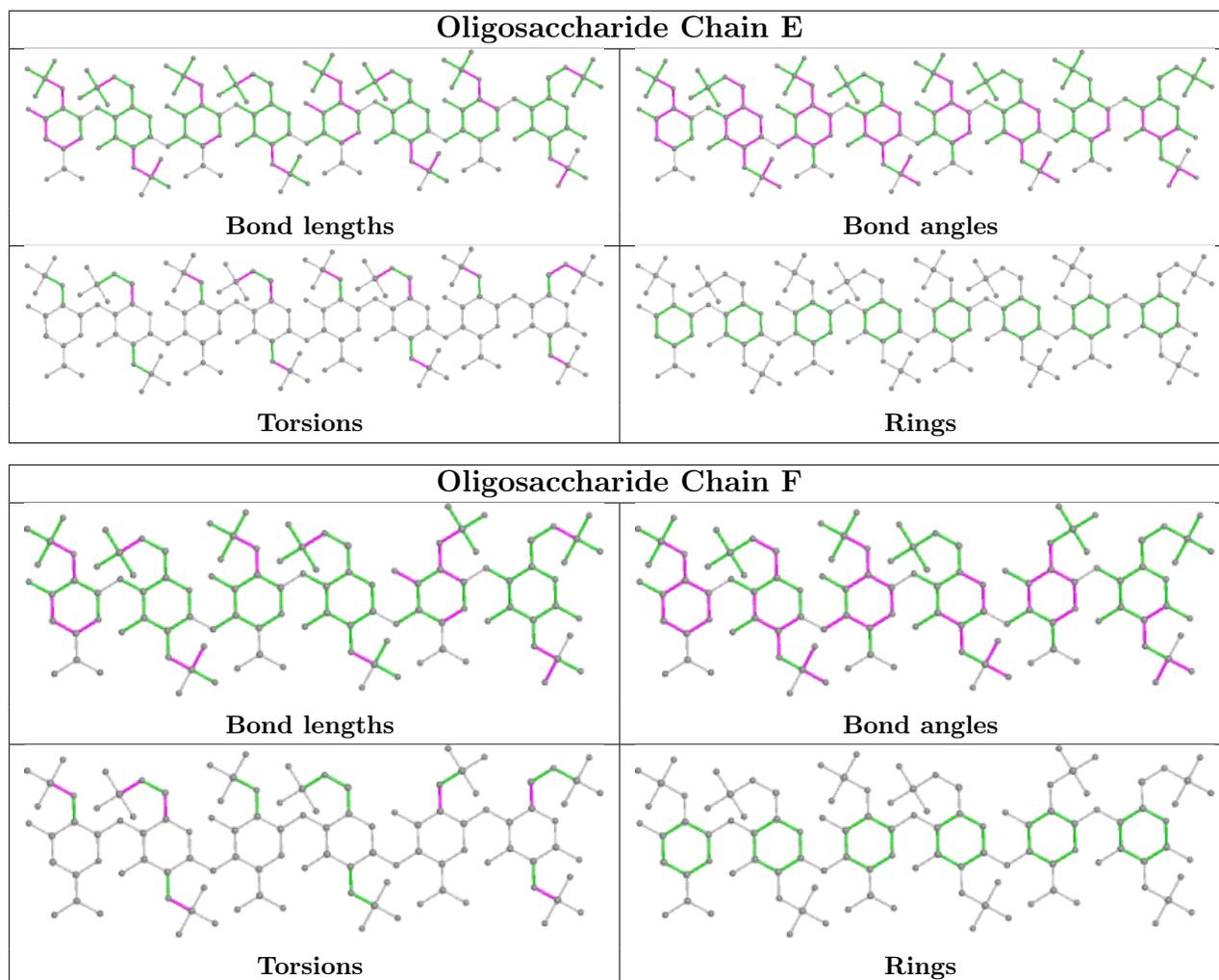
Mol	Chain	Res	Type	Atoms
3	E	2	IDU	C2-O2-S-O1S
3	E	2	IDU	C2-O2-S-O2S
3	E	2	IDU	C2-O2-S-O3S
3	E	3	SGN	O5-C5-C6-O6
3	E	3	SGN	C2-N2-S1-O3S

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	SGN	1	0
3	E	4	IDS	1	0
4	F	2	IDS	1	0
3	E	8	UAP	2	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](#)

There are no ligands in this entry.

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.