



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:32 PM UTC

PDB ID : 1F6A / pdb_00001f6a
Title : Structure of the human ige-fc bound to its high affinity receptor
fc(epsilon)ri(alpha)
Authors : Garman, S.C.; Wurzburg, B.A.; Tarchevskaya, S.S.; Kinet, J.P.; Jardetzky,
T.S.
Deposited on : 2000-06-20
Resolution : 3.50 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 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

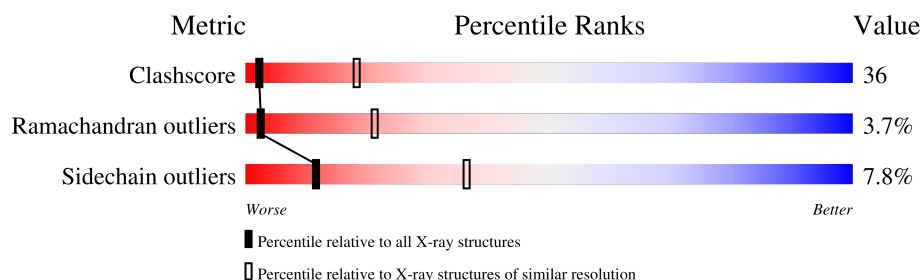
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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	176	51% 42% . . .
2	B	222	45% 42% 8% . .
2	D	222	48% 41% 8% . .
3	C	4	75% 25%
4	E	5	20% 40% 40%
5	F	3	67% 33%
6	G	6	17% 50% 33%
7	H	3	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	3	X	-	-	-
4	MAN	E	3	X	-	-	-
6	MAN	G	3	X	-	X	-
6	MAN	G	4	-	-	X	-
7	MAN	H	3	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5251 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1406	902	229	270	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ASN	engineered mutation	UNP P12319
A	135	ALA	ASN	engineered mutation	UNP P12319
A	142	ALA	THR	engineered mutation	UNP P12319
A	143	ALA	VAL	cloning artifact	UNP P12319

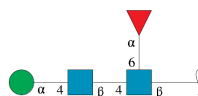
- Molecule 2 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1711	1067	317	320	7			
2	D	216	Total	C	N	O	S	0	0	0
			1704	1062	316	319	7			

There are 8 discrepancies between the modelled and reference sequences:

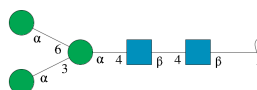
Chain	Residue	Modelled	Actual	Comment	Reference
B	326	ALA	-	cloning artifact	UNP P01854
B	327	ASP	-	cloning artifact	UNP P01854
B	328	PRO	-	cloning artifact	UNP P01854
B	329	CYS	-	cloning artifact	UNP P01854
D	326	ALA	-	cloning artifact	UNP P01854
D	327	ASP	-	cloning artifact	UNP P01854
D	328	PRO	-	cloning artifact	UNP P01854
D	329	CYS	-	cloning artifact	UNP P01854

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



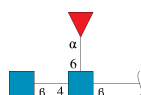
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



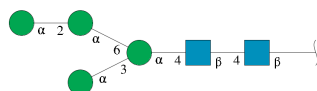
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



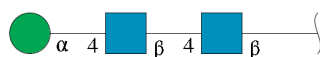
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



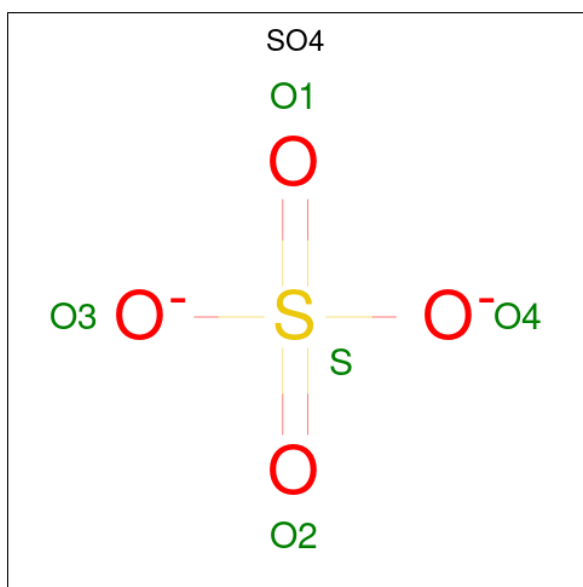
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



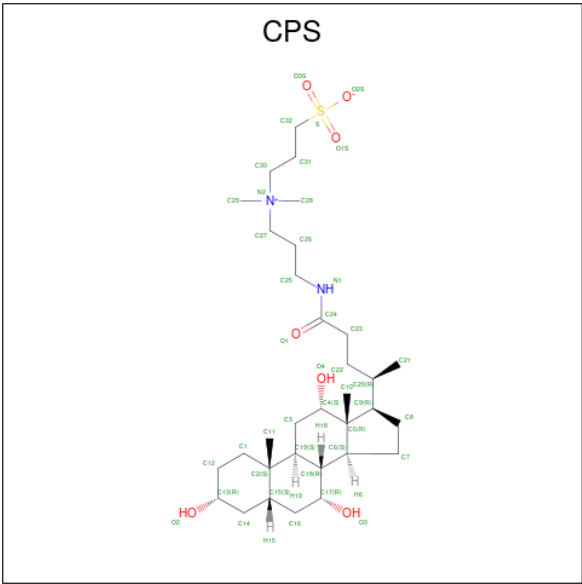
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O		0	0
			26	23	3			
9	A	1	Total	C	N	O	0	0
			42	32	2	7		
9	D	1	Total	C	O		0	0
			26	23	3			
9	D	1	Total	C	O		0	0
			26	23	3			
9	D	1	Total	C	O		0	0
			26	23	3			

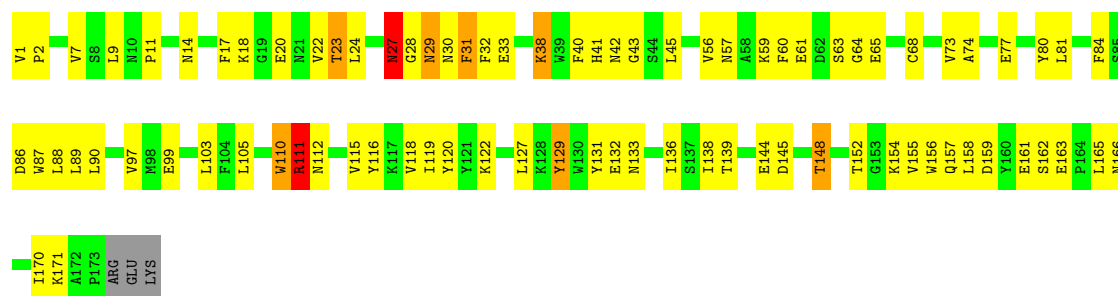
3 Residue-property plots [i](#)

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.

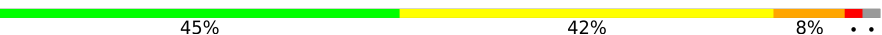
Note EDS was not executed.

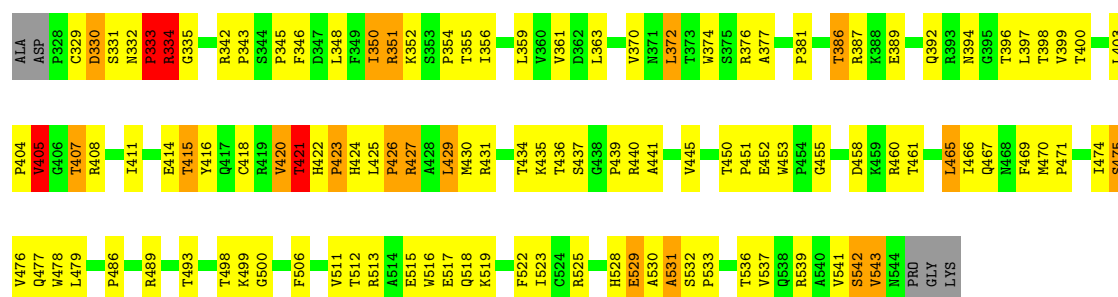
• Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT

Chain A: 



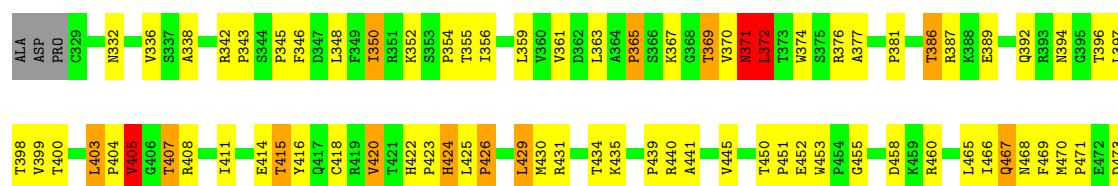
• Molecule 2: IG EPSILON CHAIN C REGION

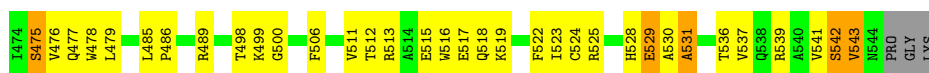
Chain B: 



• Molecule 2: IG EPSILON CHAIN C REGION

Chain D: 

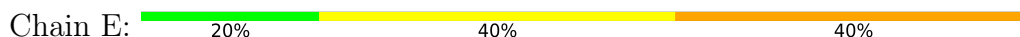




- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



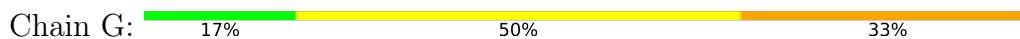
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.80 Å 192.80 Å 302.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.87 – 3.50	Depositor
% Data completeness (in resolution range)	99.6 (36.87-3.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	89.0	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: CPS, MAN, FUC, NAG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/1448 (0.1%)	1.10	12/1974 (0.6%)
2	B	0.53	0/1755	1.07	12/2389 (0.5%)
2	D	0.53	0/1747	1.03	10/2378 (0.4%)
All	All	0.55	1/4950 (0.0%)	1.06	34/6741 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	C-N	-5.55	1.26	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	PRO	CA-C-N	9.69	131.96	119.84
1	A	11	PRO	C-N-CA	9.69	131.96	119.84
2	B	529	GLU	OE1-CD-OE2	-8.32	102.93	122.90
2	D	529	GLU	OE1-CD-OE2	-8.20	103.23	122.90
2	B	330	ASP	N-CA-C	-8.19	102.06	113.20

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	1406	0	1322	83	0
2	B	1711	0	1687	138	1
2	D	1704	0	1679	135	1
3	C	49	0	43	0	0
4	E	61	0	52	4	0
5	F	38	0	34	0	0
6	G	72	0	61	9	0
7	H	39	0	34	0	0
8	A	5	0	0	1	0
8	B	15	0	0	2	0
8	D	5	0	0	0	0
9	A	68	0	91	13	0
9	D	78	0	105	12	0
All	All	5251	0	5108	377	2

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 36.

The worst 5 of 377 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)
9:A:371:CPS:C5	9:A:371:CPS:C10	1.75	1.65
9:D:105:CPS:C5	9:D:105:CPS:C10	1.75	1.58
9:A:371:CPS:N1	9:A:371:CPS:C25	1.67	1.50
6:G:3:MAN:H61	6:G:4:MAN:H3	1.41	1.00
1:A:115:VAL:HG22	1:A:155:VAL:HG22	1.49	0.92

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:GLN:OE1	2:D:518:GLN:OE1[11_566]	1.79	0.41
2:B:351:ARG:NH2	2:B:351:ARG:NH2[4_556]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	171/176 (97%)	147 (86%)	20 (12%)	4 (2%)	5	30
2	B	215/222 (97%)	177 (82%)	29 (14%)	9 (4%)	2	19
2	D	214/222 (96%)	175 (82%)	30 (14%)	9 (4%)	2	19
All	All	600/620 (97%)	499 (83%)	79 (13%)	22 (4%)	2	21

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
2	B	334	ARG
2	B	531	ALA
2	D	426	PRO
2	D	531	ALA

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	A	154/157 (98%)	146 (95%)	8 (5%)	21	47
2	B	192/195 (98%)	173 (90%)	19 (10%)	7	29
2	D	191/195 (98%)	176 (92%)	15 (8%)	11	36
All	All	537/547 (98%)	495 (92%)	42 (8%)	11	36

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	365	PRO
2	D	420	VAL
2	D	371	ASN
2	D	405	VAL
2	D	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	477	GLN
2	D	528	HIS
2	D	538	GLN
2	D	518	GLN
2	B	518	GLN

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 ⓘ

21 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	C	1	3,1	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	0.78	0
3	MAN	C	3	3	11,11,12	0.47	0	15,15,17	0.22	0
3	FUC	C	4	3	10,10,11	0.53	0	14,14,16	0.39	0
4	NAG	E	1	4,1	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
4	MAN	E	3	4	11,11,12	0.70	0	15,15,17	0.36	0
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	0.61	0
4	MAN	E	5	4	11,11,12	0.52	0	15,15,17	0.59	0
5	NAG	F	1	5,1	14,14,15	0.62	0	17,19,21	0.85	1 (5%)
5	NAG	F	2	5	14,14,15	0.49	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	F	3	5	10,10,11	0.48	0	14,14,16	0.41	0
6	NAG	G	1	2,6	14,14,15	0.40	0	17,19,21	0.80	0
6	NAG	G	2	6	14,14,15	0.72	0	17,19,21	0.71	1 (5%)
6	MAN	G	3	6	11,11,12	0.63	0	15,15,17	0.76	0
6	MAN	G	4	6	11,11,12	0.73	0	15,15,17	1.12	0
6	MAN	G	5	6	11,11,12	1.07	1 (9%)	15,15,17	0.83	1 (6%)
6	MAN	G	6	6	11,11,12	0.59	0	15,15,17	0.55	0
7	NAG	H	1	2,7	14,14,15	0.66	0	17,19,21	0.71	0
7	NAG	H	2	7	14,14,15	0.74	0	17,19,21	0.80	1 (5%)
7	MAN	H	3	7	11,11,12	0.56	0	15,15,17	0.27	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	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
6	NAG	G	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
6	MAN	G	3	6	1/1/4/5	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
6	MAN	G	6	6	-	2/2/19/22	0/1/1/1
7	NAG	H	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	MAN	H	3	7	1/1/4/5	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5	MAN	O5-C5	2.20	1.47	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C2-N2-C7	-2.84	119.10	122.90
4	E	1	NAG	C2-N2-C7	-2.71	119.27	122.90
6	G	5	MAN	C1-O5-C5	2.64	115.73	112.19
5	F	1	NAG	C2-N2-C7	-2.53	119.51	122.90
4	E	2	NAG	C2-N2-C7	-2.51	119.53	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	MAN	C1
4	E	3	MAN	C1
6	G	3	MAN	C1
7	H	3	MAN	C1

5 of 40 torsion outliers are listed below:

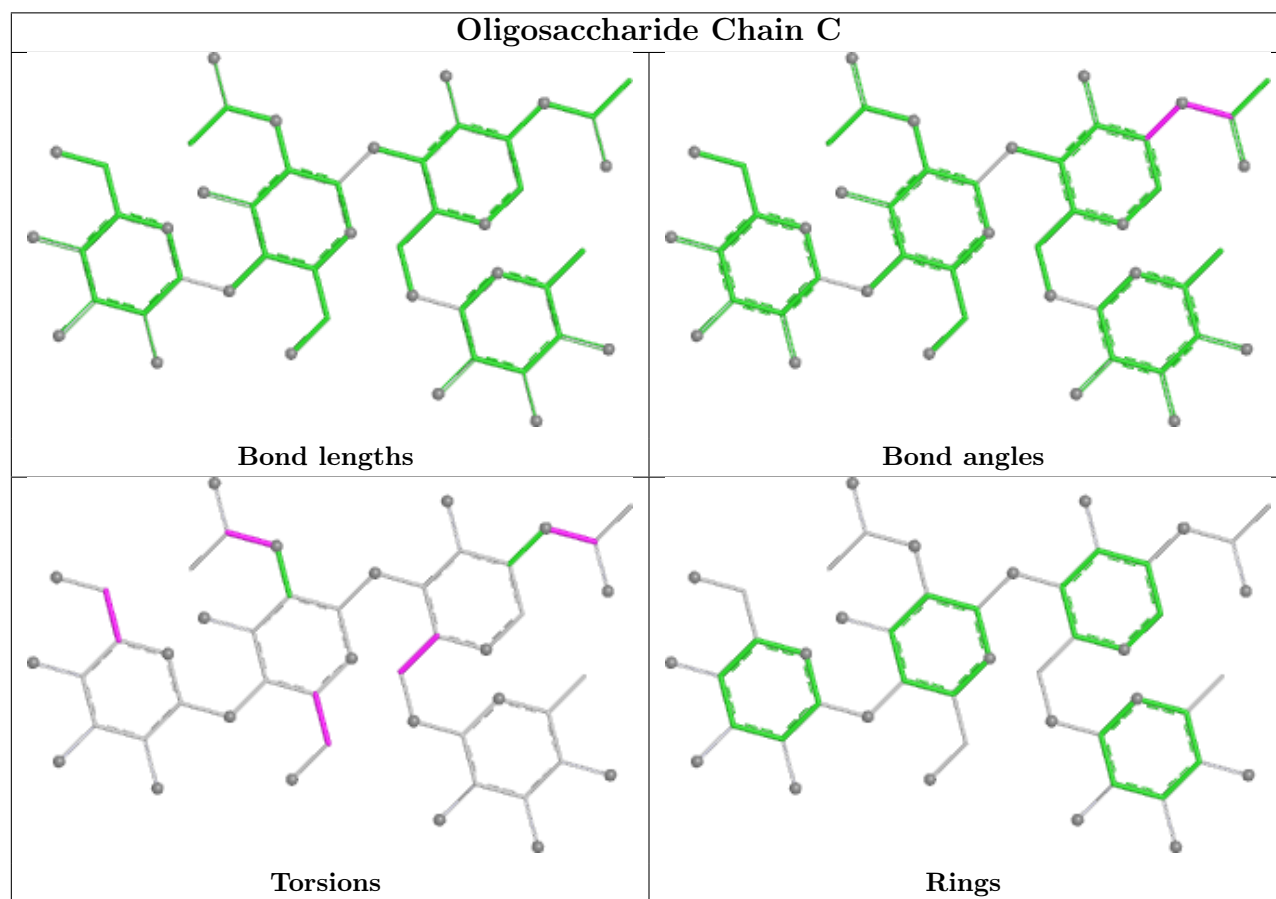
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2

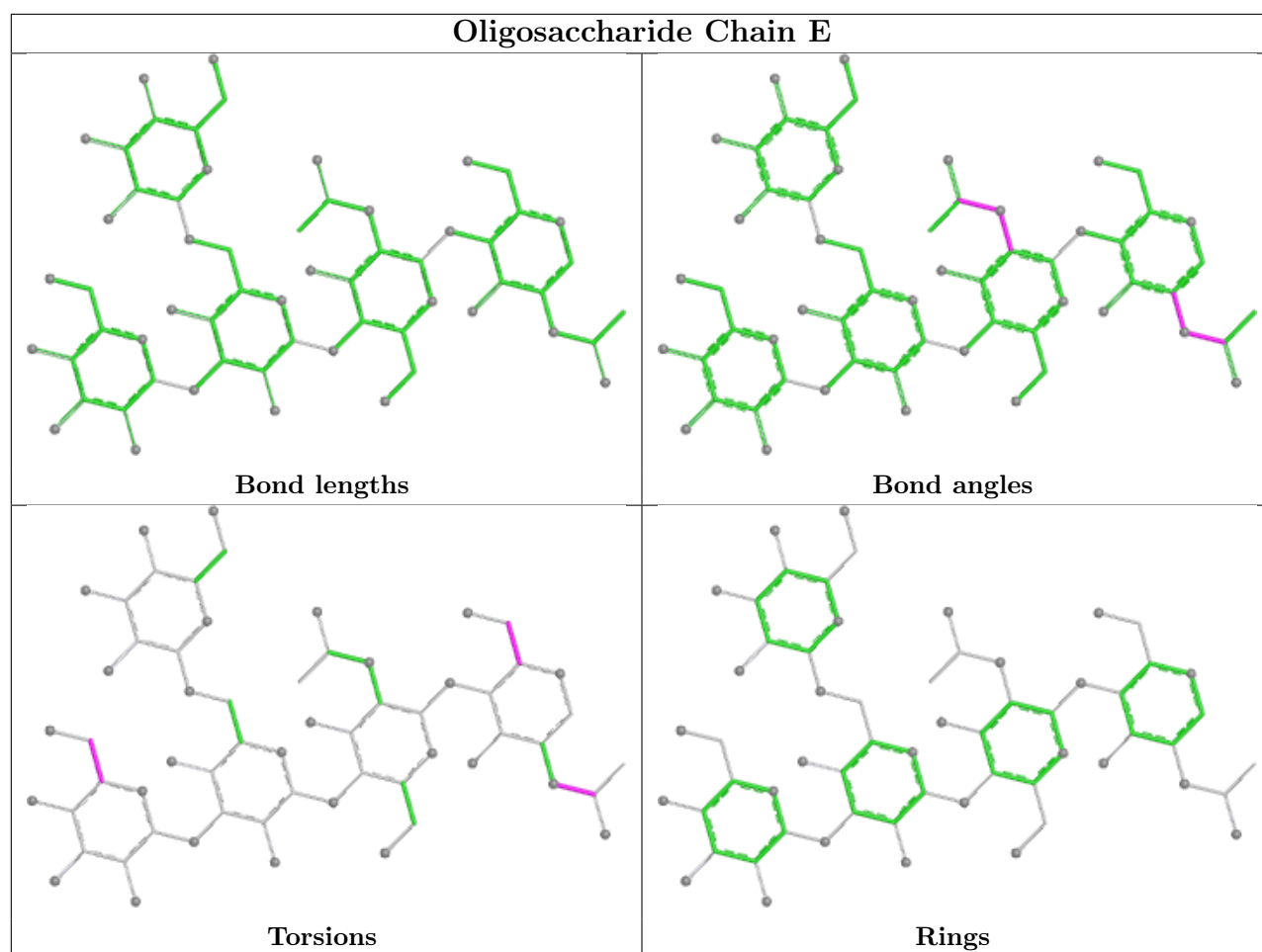
There are no ring outliers.

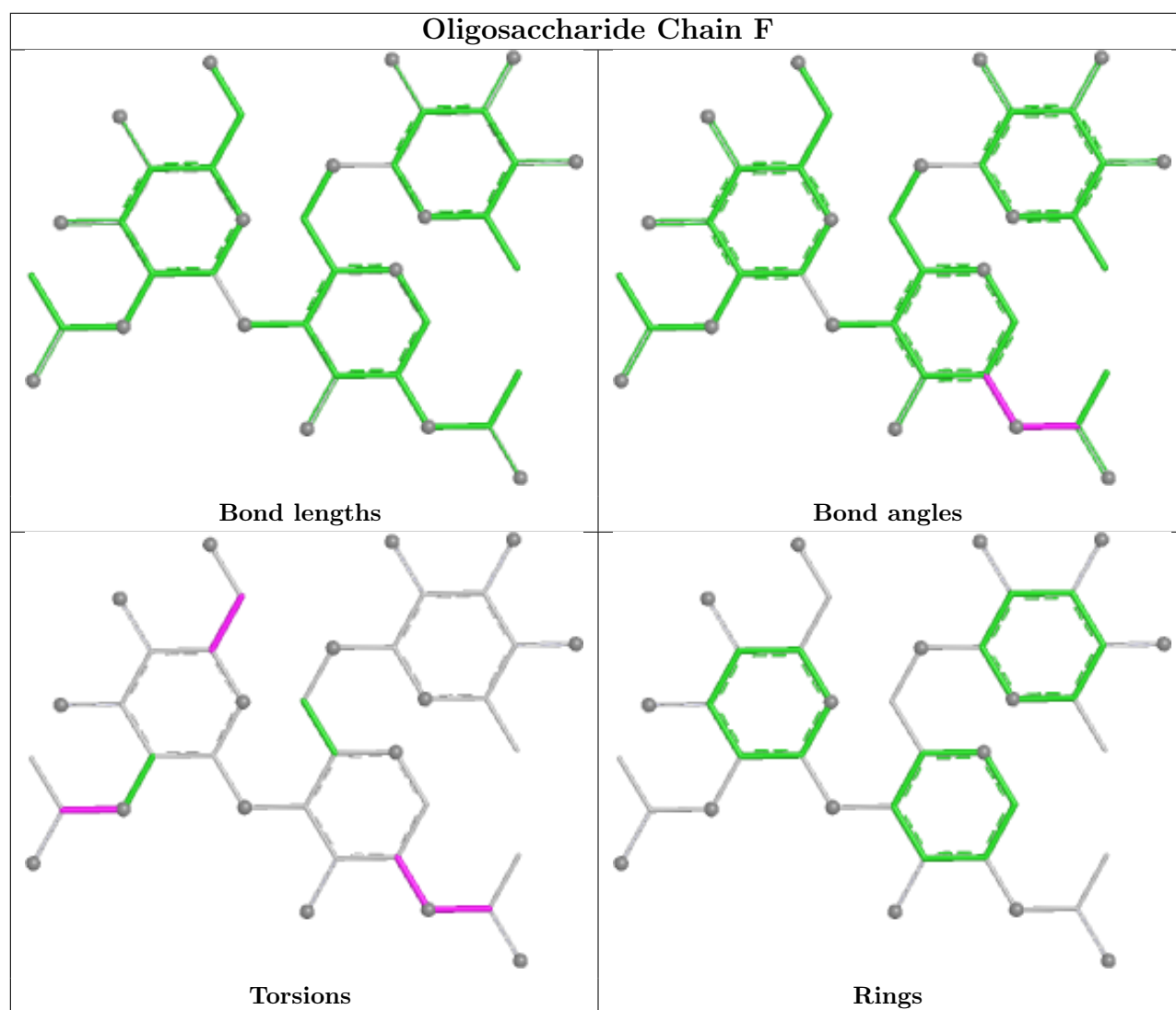
9 monomers are involved in 13 short contacts:

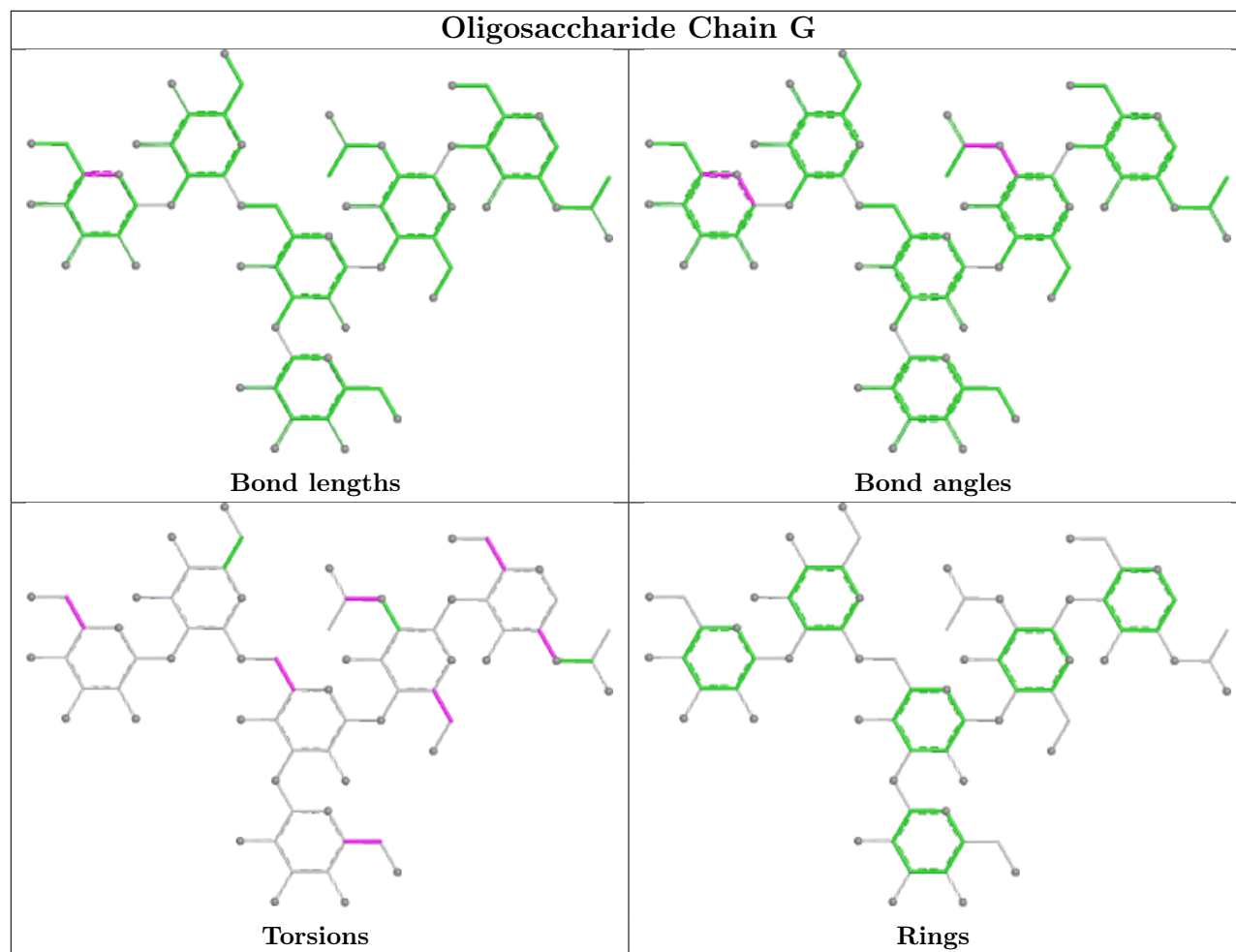
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0
6	G	2	NAG	1	0
4	E	4	MAN	1	0
6	G	4	MAN	8	0
6	G	3	MAN	7	0
4	E	2	NAG	3	0
6	G	5	MAN	1	0
6	G	1	NAG	1	0
4	E	3	MAN	1	0

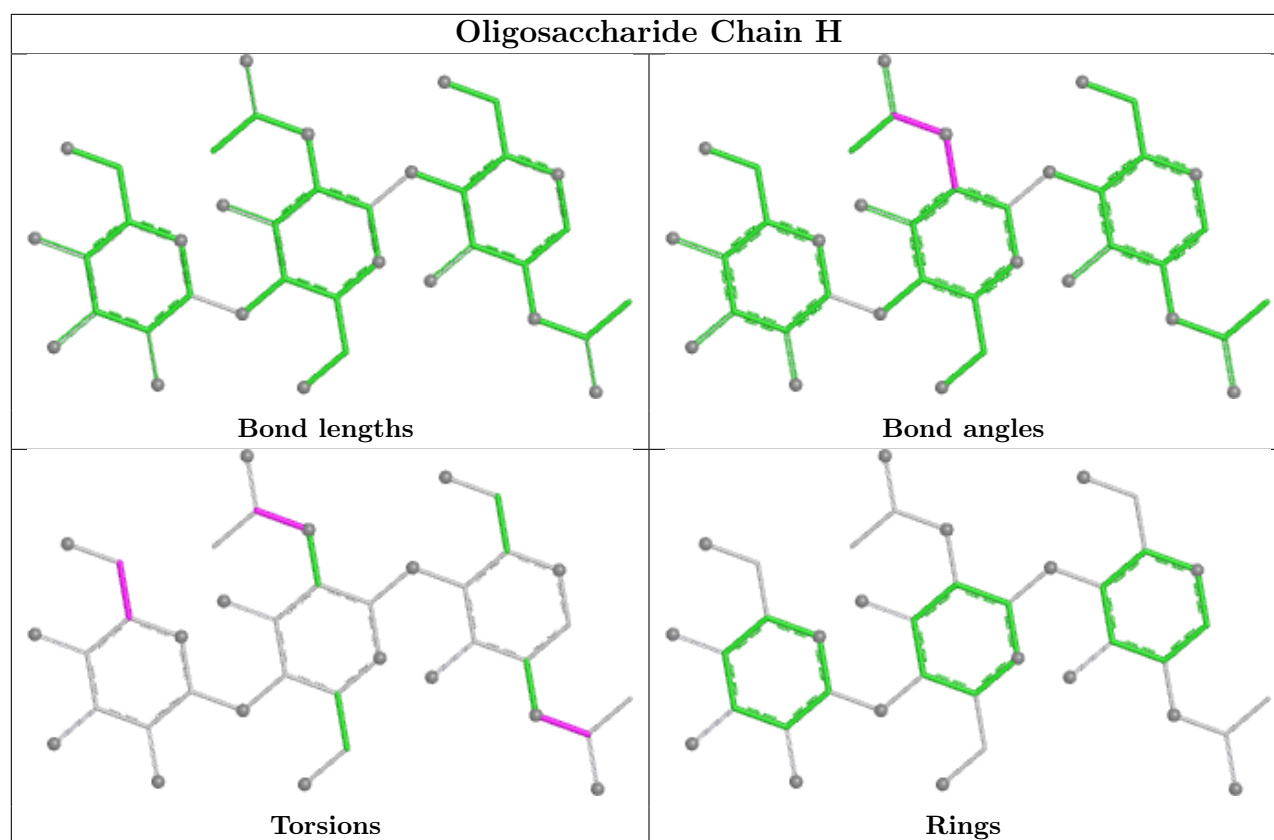
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
9	CPS	A	370	-	29,29,45	4.78	16 (55%)	47,47,70	4.07	29 (61%)
8	SO4	B	201	-	4,4,4	0.52	0	6,6,6	0.14	0
8	SO4	B	202	-	4,4,4	0.36	0	6,6,6	0.27	0
9	CPS	D	104	-	29,29,45	4.96	17 (58%)	47,47,70	3.92	28 (59%)
9	CPS	D	103	-	29,29,45	4.94	18 (62%)	47,47,70	3.91	28 (59%)
9	CPS	D	105	-	29,29,45	5.15	17 (58%)	47,47,70	3.83	28 (59%)
9	CPS	A	371	-	45,45,45	5.05	23 (51%)	70,70,70	3.33	31 (44%)
8	SO4	D	205	-	4,4,4	0.59	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	203	-	4,4,4	0.59	0	6,6,6	0.27	0
8	SO4	B	204	-	4,4,4	0.63	0	6,6,6	0.36	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
9	CPS	A	370	-	-	0/6/71/90	0/4/4/4
9	CPS	D	104	-	-	0/6/71/90	0/4/4/4
9	CPS	D	105	-	-	0/6/71/90	0/4/4/4
9	CPS	A	371	-	-	7/25/90/90	0/4/4/4
9	CPS	D	103	-	-	0/6/71/90	0/4/4/4

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	371	CPS	C32-S	-16.45	1.54	1.77
9	D	103	CPS	O4-C4	-13.76	1.21	1.43
9	A	370	CPS	O4-C4	-13.57	1.21	1.43
9	D	104	CPS	O4-C4	-13.42	1.21	1.43
9	D	105	CPS	O4-C4	-13.32	1.21	1.43

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	105	CPS	C6-C18-C17	11.12	126.61	111.85
9	A	370	CPS	C6-C18-C17	10.48	125.76	111.85
9	D	104	CPS	C6-C18-C17	10.41	125.66	111.85
9	D	103	CPS	C6-C18-C17	9.49	124.45	111.85
9	A	370	CPS	C19-C18-C17	-8.83	100.75	111.86

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	371	CPS	C20-C22-C23-C24
9	A	371	CPS	C25-C26-C27-N2
9	A	371	CPS	C30-C31-C32-S
9	A	371	CPS	C26-C25-N1-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	371	CPS	C26-C27-N2-C28

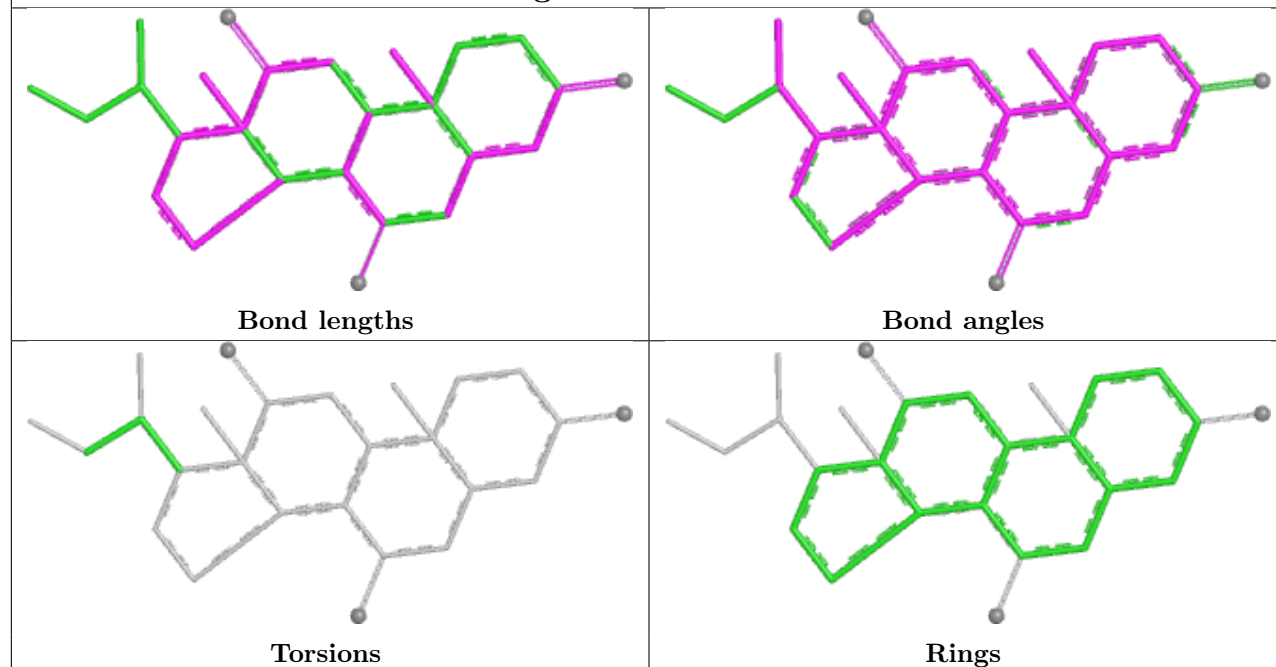
There are no ring outliers.

7 monomers are involved in 28 short contacts:

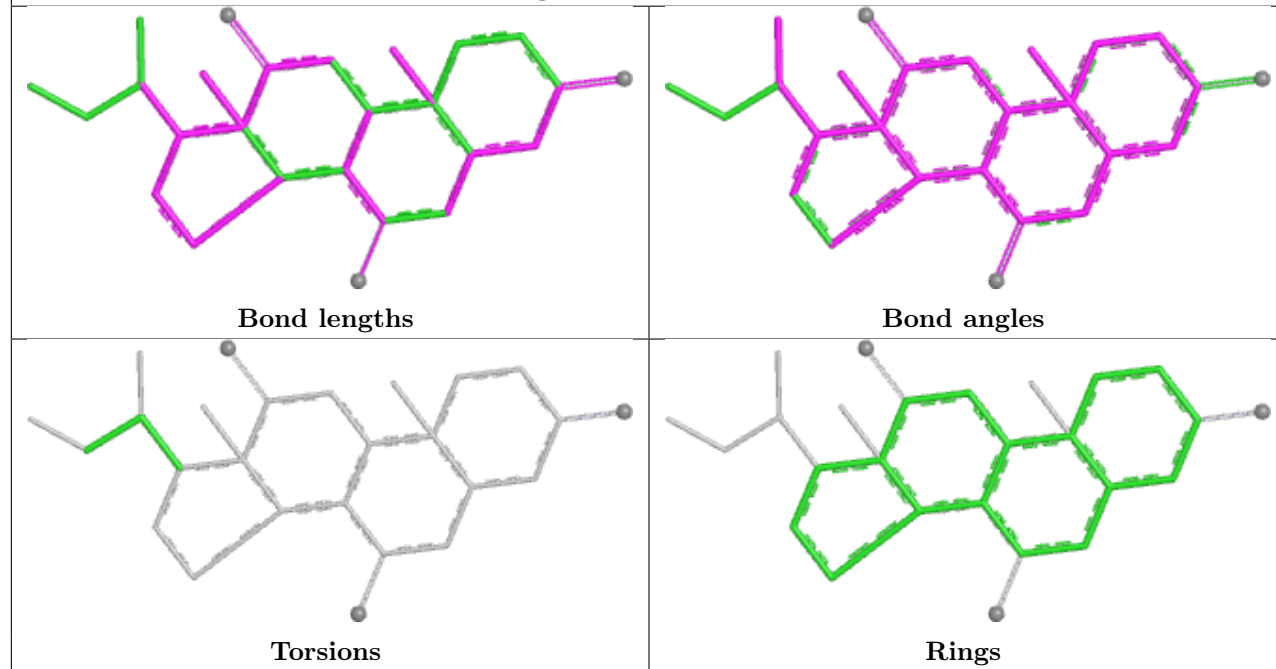
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	370	CPS	1	0
8	B	202	SO4	1	0
9	D	103	CPS	1	0
9	D	105	CPS	11	0
9	A	371	CPS	13	0
8	A	203	SO4	1	0
8	B	204	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

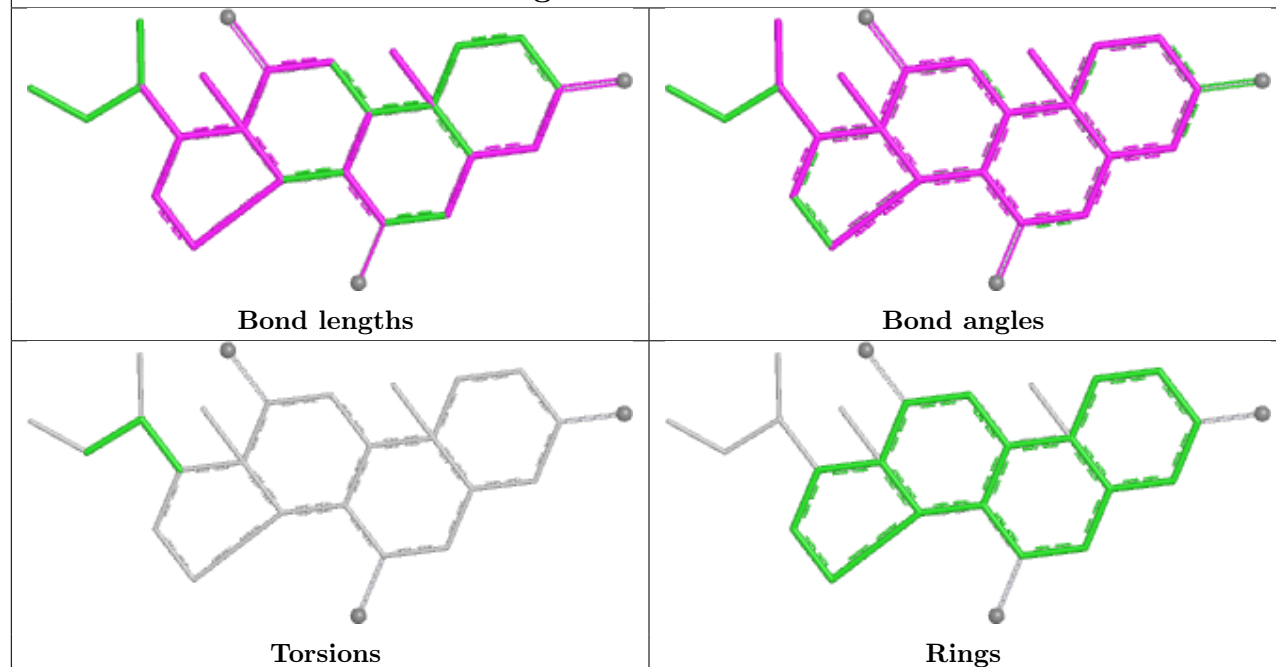
Ligand CPS A 370



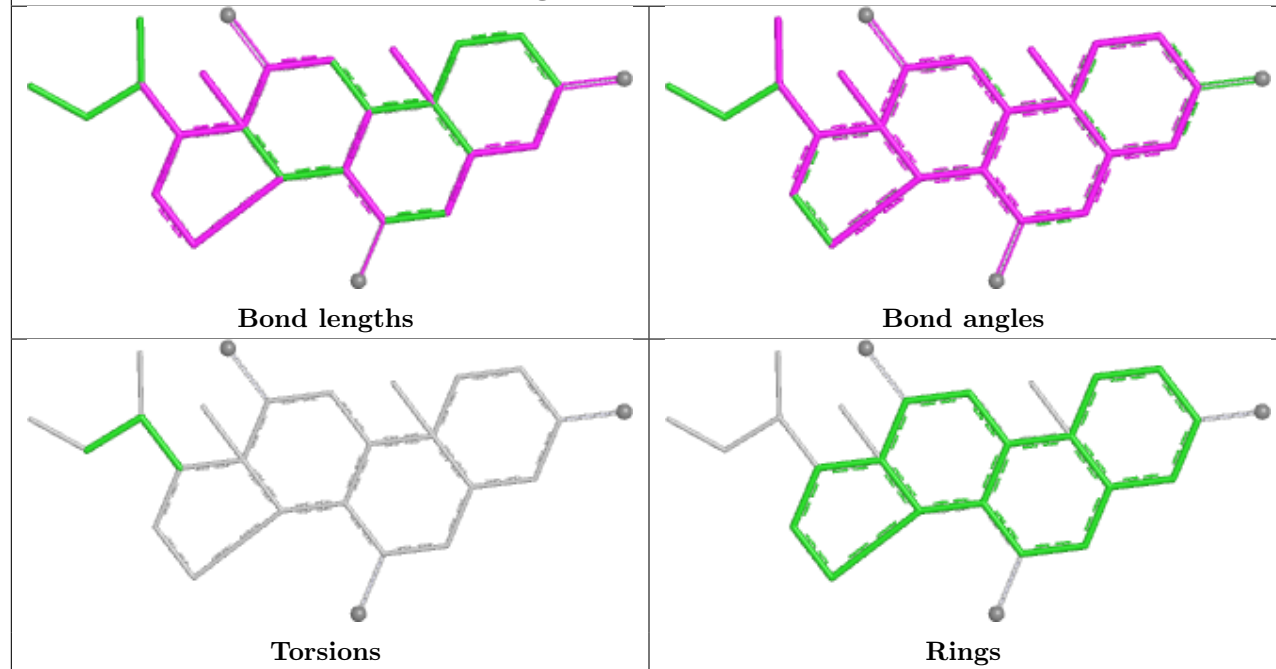
Ligand CPS D 104

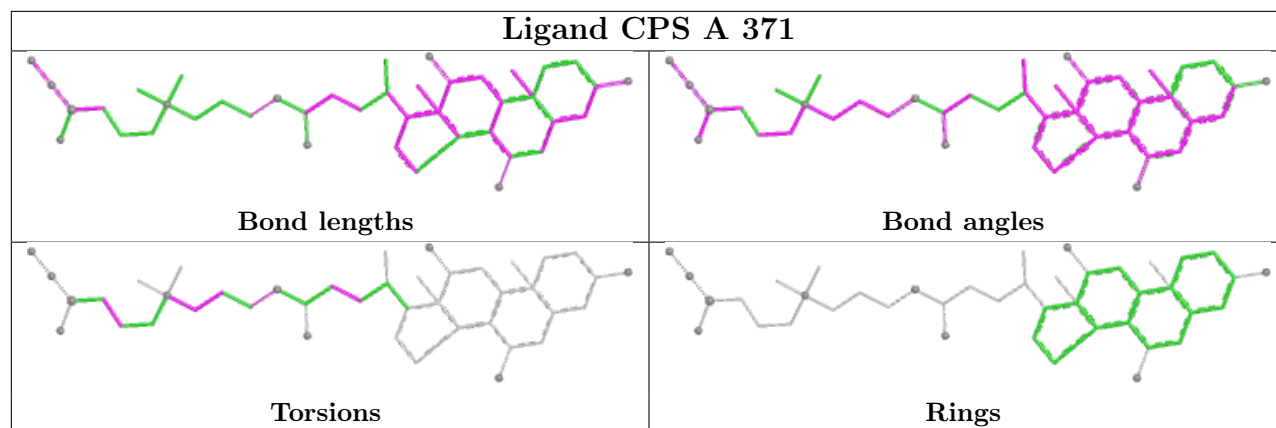


Ligand CPS D 103



Ligand CPS D 105





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.