wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 02:41 am GMT

PDB ID	:	1E4K
Title	:	CRYSTAL STRUCTURE OF SOLUBLE HUMAN IGG1 FC FRAGMENT-FC-GAMMA RECEPTOR III COMPLEX
Authors	:	Sondermann, P.; Huber, R.; Oosthuizen, V.; Jacob, U.
Deposited on	:	2000-07-07
Resolution	:	3.20 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:

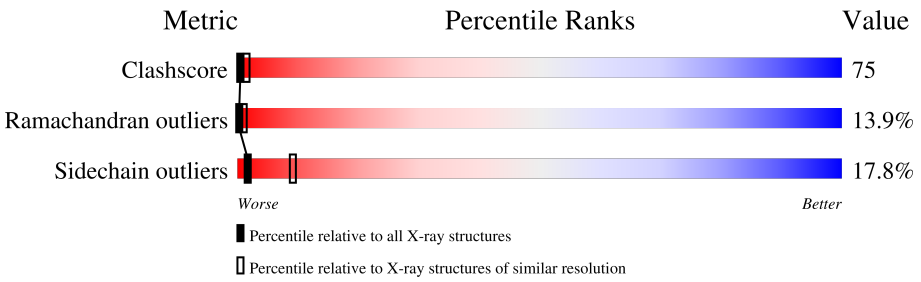
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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	225	16% 56% 20% • •
1	B	225	20% 52% 21% • •
2	C	176	19% 57% 18% • •
3	D	9	56% 44%
4	E	9	33% 67%

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
4	GAL	E	6	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5042 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.

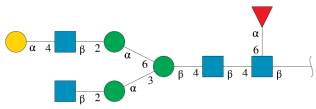
- Molecule 1 is a protein called FC FRAGMENT OF HUMAN IGG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1719	1094	291	326	8	0	0	0
1	B	216	1719	1094	291	326	8	0	0	0

- Molecule 2 is a protein called LOW AFFINITY IMMUNOGLOBULIN GAMMA FC RECEPTOR III.

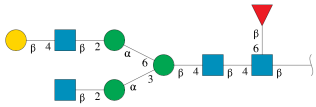
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	172	1384	877	237	266	4	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-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
			Total	C	N	O			
3	D	9	110	62	4	44	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	9	110	62	4	44	0	0	0

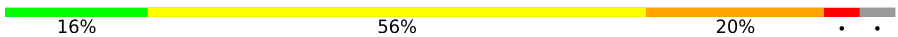
3 Residue-property plots (i)

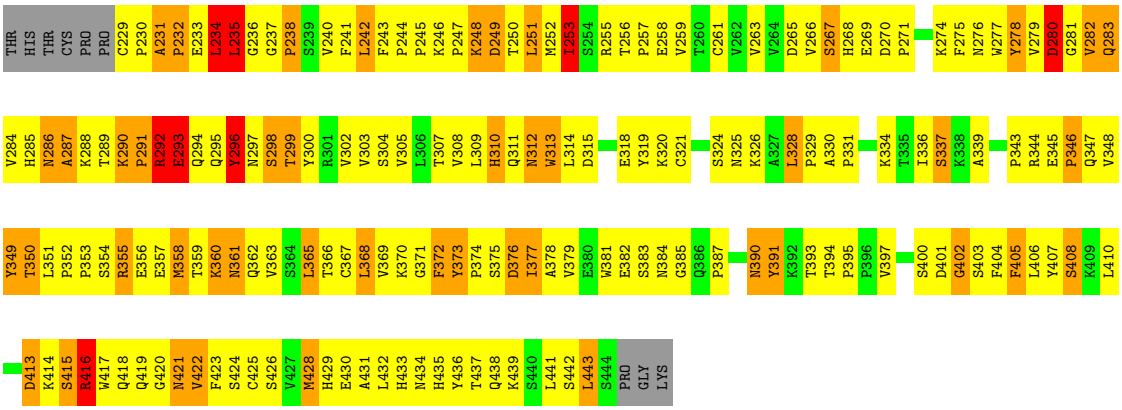
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: FC FRAGMENT OF HUMAN IGG1

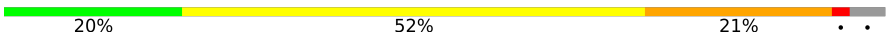
Chain A:

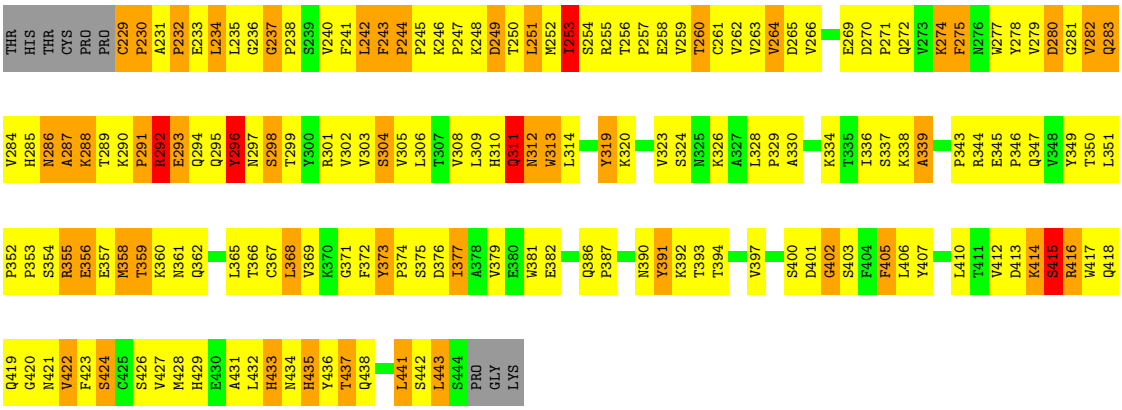




• Molecule 1: FC FRAGMENT OF HUMAN IGG1

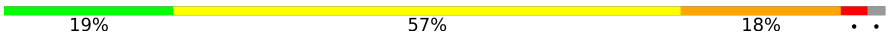
Chain B:

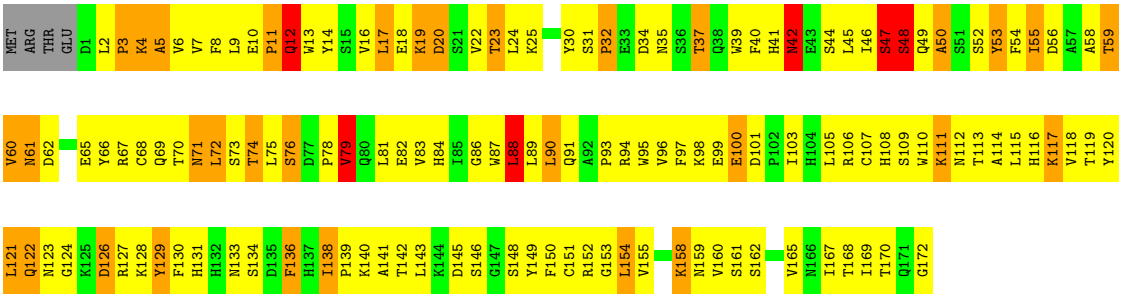




• Molecule 2: LOW AFFINITY IMMUNOGLOBULIN GAMMA FC RECEPTOR III

Chain C:





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

Chain D: 56% 44%

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

Chain E: 33% 67%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.32Å 115.32Å 299.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.20	Depositor
% Data completeness (in resolution range)	94.9 (100.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.271 , 0.357	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5042	wwPDB-VP
Average B, all atoms (Å^2)	95.0	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: GAL, BMA, MAN, FUL, GLA, NAG, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.66	0/1767	0.99	7/2408 (0.3%)
1	B	0.88	3/1767 (0.2%)	1.00	1/2408 (0.0%)
2	C	0.77	0/1422	1.03	4/1933 (0.2%)
All	All	0.77	3/4956 (0.1%)	1.00	12/6749 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	CG-CD	7.51	1.63	1.51
1	B	292	ARG	N-CA	6.11	1.58	1.46
1	B	293	GLU	CB-CG	5.44	1.62	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	425	CYS	CA-CB-SG	7.16	126.89	114.00
1	A	234	LEU	C-N-CA	6.88	138.91	121.70
2	C	42	ASN	N-CA-C	-6.46	93.56	111.00
2	C	88	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	328	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	TYR	Sidechain
1	B	319	TYR	Sidechain
1	B	373	TYR	Sidechain

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	1719	0	1689	297	0
1	B	1719	0	1690	256	0
2	C	1384	0	1324	208	0
3	D	110	0	94	9	0
4	E	110	0	94	19	0
All	All	5042	0	4891	748	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 75.

The worst 5 of 748 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)
3:D:4:MAN:O3	3:D:5:NAG:H2	1.34	1.25
1:A:232:PRO:O	1:A:233:GLU:HG2	1.43	1.17
1:B:245:PRO:HA	4:E:6:GAL:H61	1.18	1.13
1:B:258:GLU:O	4:E:6:GAL:H62	1.47	1.13
2:C:116:HIS:HB2	2:C:154:LEU:HB2	1.30	1.11

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	214/225 (95%)	147 (69%)	35 (16%)	32 (15%)	0 1
1	B	214/225 (95%)	154 (72%)	30 (14%)	30 (14%)	0 1
2	C	170/176 (97%)	131 (77%)	18 (11%)	21 (12%)	0 2
All	All	598/626 (96%)	432 (72%)	83 (14%)	83 (14%)	0 1

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	A	232	PRO
1	A	235	LEU
1	A	283	GLN
1	A	291	PRO

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	200/208 (96%)	163 (82%)	37 (18%)	1 8
1	B	200/208 (96%)	165 (82%)	35 (18%)	2 9
2	C	156/160 (98%)	129 (83%)	27 (17%)	2 10
All	All	556/576 (96%)	457 (82%)	99 (18%)	2 9

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	306	LEU
1	B	443	LEU
1	B	311	GLN
1	B	415	SER
2	C	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	325	ASN
1	B	438	GLN
2	C	137	HIS
2	C	108	HIS
1	B	435	HIS

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)

18 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	D	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.08	1 (5%)
3	NAG	D	2	3	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
3	BMA	D	3	3	11,11,12	0.91	0	15,15,17	1.00	1 (6%)
3	MAN	D	4	3	11,11,12	0.60	0	15,15,17	0.98	0
3	NAG	D	5	3	14,14,15	0.74	0	17,19,21	0.97	1 (5%)
3	GLA	D	6	3	11,11,12	0.83	1 (9%)	15,15,17	0.90	0
3	MAN	D	7	3	11,11,12	0.92	1 (9%)	15,15,17	1.31	1 (6%)
3	NAG	D	8	3	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
3	FUC	D	9	3	10,10,11	0.78	0	14,14,16	0.98	0
4	NAG	E	1	4,1	14,14,15	0.67	0	17,19,21	1.36	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	2	4	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
4	BMA	E	3	4	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
4	MAN	E	4	4	11,11,12	0.53	0	15,15,17	1.01	1 (6%)
4	NAG	E	5	4	14,14,15	0.64	0	17,19,21	0.98	1 (5%)
4	GAL	E	6	4	11,11,12	0.61	0	15,15,17	0.81	1 (6%)
4	MAN	E	7	4	11,11,12	0.59	0	15,15,17	0.87	0
4	NAG	E	8	4	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
4	FUL	E	9	4	10,10,11	0.80	0	14,14,16	1.52	2 (14%)

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	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	4/6/23/26	0/1/1/1
3	GLA	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	1/2/19/22	0/1/1/1
3	NAG	D	8	3	-	0/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	NAG	E	5	4	-	2/6/23/26	0/1/1/1
4	GAL	E	6	4	-	1/2/19/22	0/1/1/1
4	MAN	E	7	4	-	2/2/19/22	0/1/1/1
4	NAG	E	8	4	-	0/6/23/26	0/1/1/1
4	FUL	E	9	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7	MAN	C1-C2	2.22	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GLA	C1-C2	2.18	1.57	1.52
3	D	1	NAG	O5-C5	2.07	1.47	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	9	FUL	C1-C2-C3	4.49	115.18	109.67
3	D	7	MAN	C1-C2-C3	4.25	114.89	109.67
3	D	8	NAG	C2-N2-C7	-3.22	118.31	122.90
4	E	1	NAG	C3-C4-C5	-2.96	104.95	110.24
4	E	4	MAN	C1-O5-C5	2.95	116.19	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	5	NAG	C3-C2-N2-C7
3	D	5	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	D	6	GLA	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

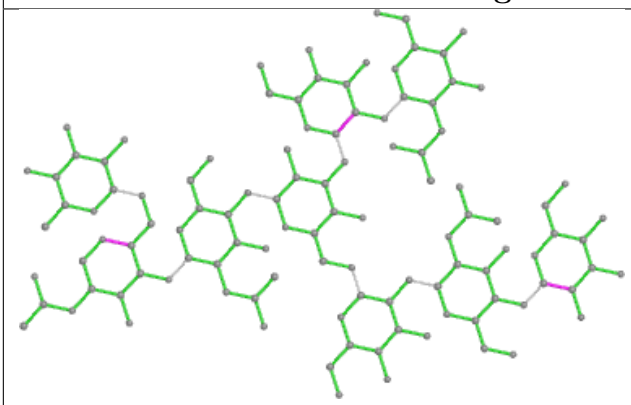
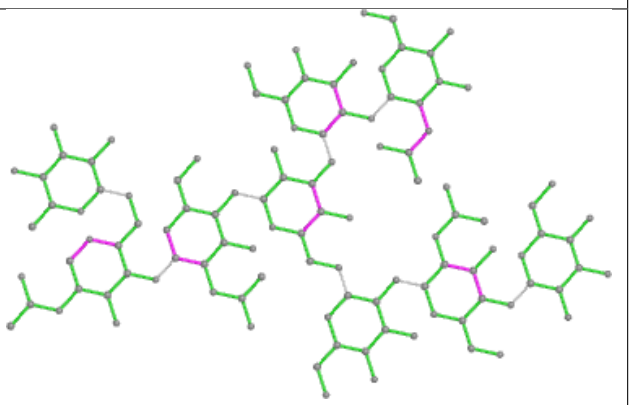
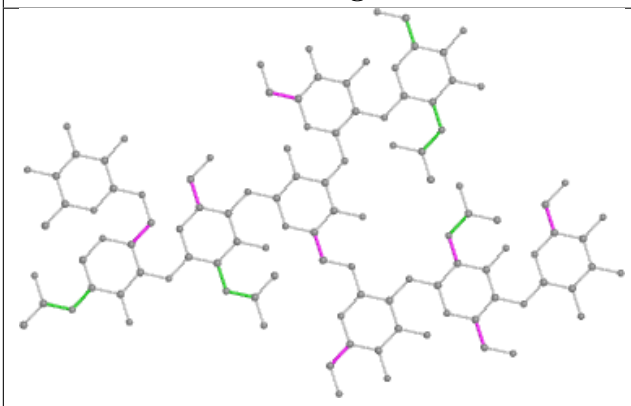
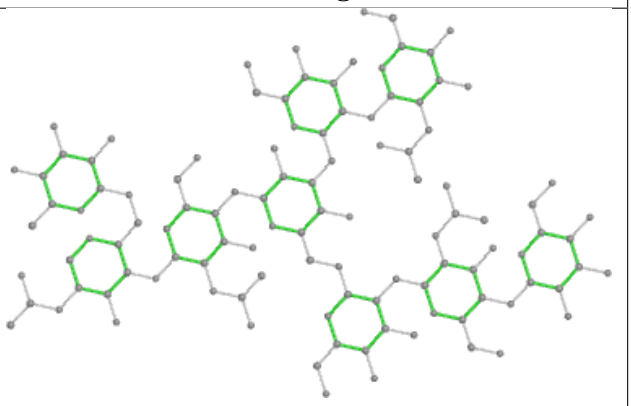
There are no ring outliers.

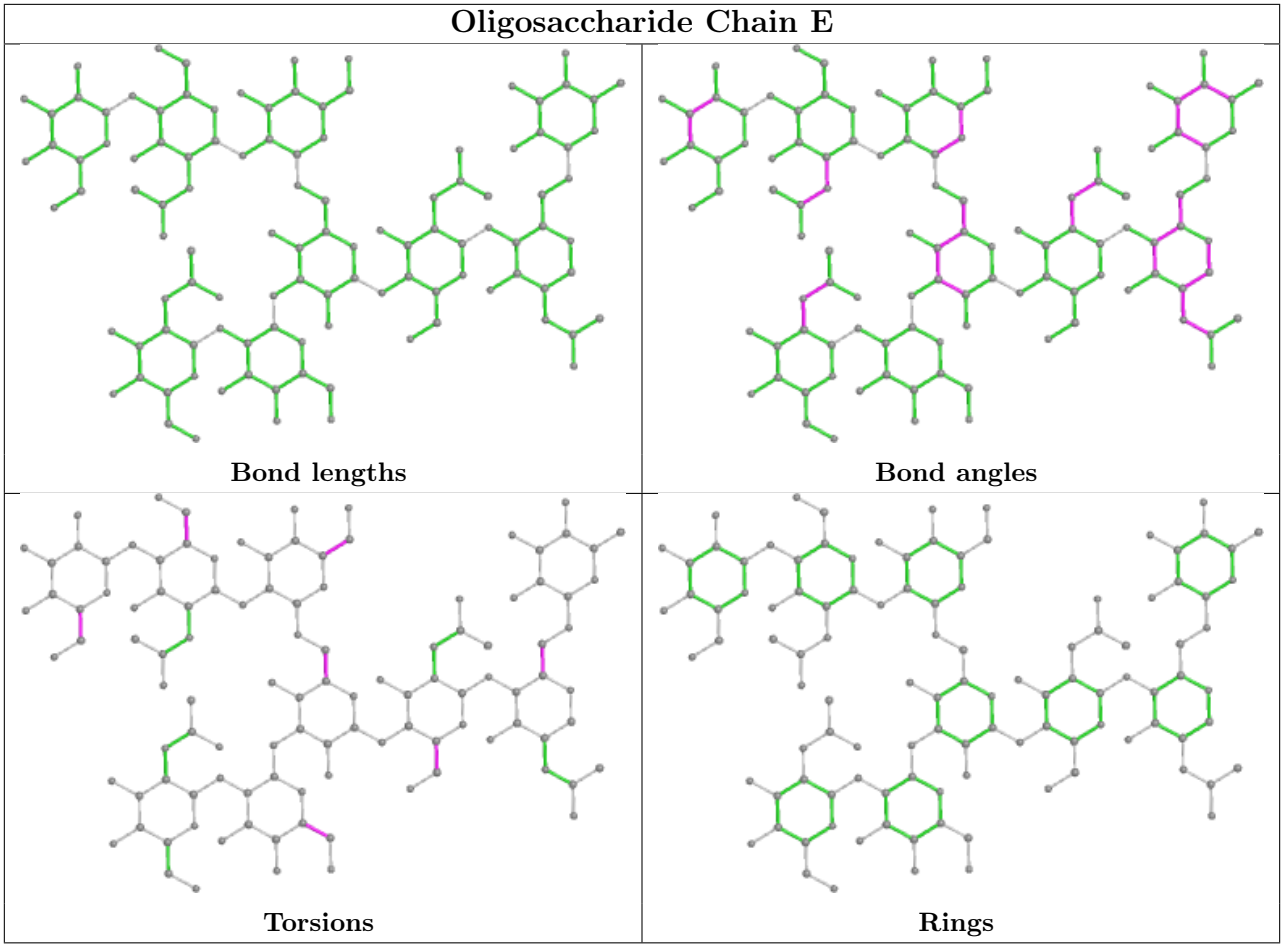
13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	4	0
4	E	5	NAG	3	0
3	D	9	FUC	2	0
3	D	6	GLA	1	0
3	D	4	MAN	4	0
4	E	7	MAN	1	0
3	D	5	NAG	4	0
3	D	2	NAG	2	0
3	D	1	NAG	1	0
4	E	1	NAG	1	0
4	E	3	BMA	3	0
4	E	4	MAN	3	0
4	E	6	GAL	9	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.

Oligosaccharide Chain D	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**



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.