



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2021 – 08:04 AM EST

PDB ID : 7SI0
Title : IgE-Fc in complex with 813
Authors : Pennington, L.F.; Jardetzky, T.J.; Kleinboelting, S.
Deposited on : 2021-10-12
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)
Xtriage (Phenix) : 1.13
EDS : 2.24
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

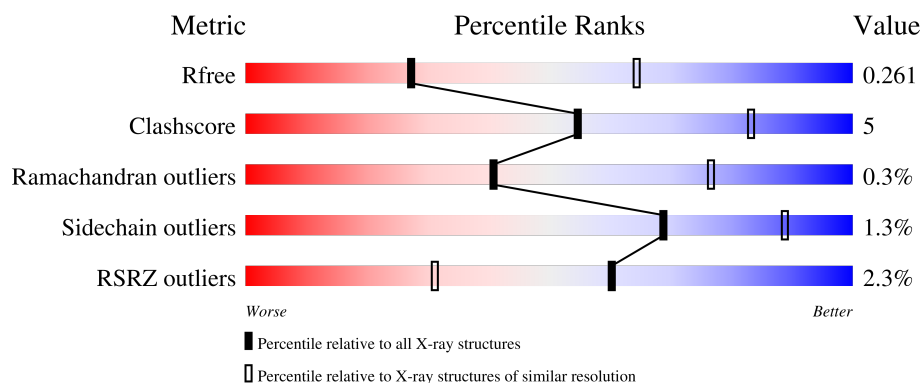
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	
1	G	247	
1	H	247	
2	C	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	123	
2	I	123	
2	K	123	
3	D	134	
3	F	134	
3	J	134	
3	L	134	
4	M	4	
4	O	4	
4	P	4	
5	N	2	
5	Q	2	
6	R	5	

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	NAG	O	2	-	-	-	X
4	MAN	O	4	-	-	-	X
4	NAG	P	1	-	-	-	X
4	MAN	P	4	-	-	-	X
5	MAN	N	2	-	-	-	X
5	MAN	Q	2	-	-	-	X
6	NAG	R	1	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14043 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 IgE Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	209	Total	C	N	O	S	0	0	0
			1648	1032	302	308	6			
1	G	209	Total	C	N	O	S	0	0	0
			1639	1027	301	305	6			
1	H	209	Total	C	N	O	S	0	0	0
			1643	1027	302	308	6			
1	A	209	Total	C	N	O	S	0	0	0
			1631	1021	298	306	6			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	299	ALA	-	expression tag	UNP P01854
B	300	PRO	-	expression tag	UNP P01854
B	301	MET	-	expression tag	UNP P01854
B	302	ALA	-	expression tag	UNP P01854
B	303	GLU	-	expression tag	UNP P01854
B	304	GLY	-	expression tag	UNP P01854
B	305	GLY	-	expression tag	UNP P01854
B	306	GLY	-	expression tag	UNP P01854
B	307	GLN	-	expression tag	UNP P01854
B	308	ASN	-	expression tag	UNP P01854
B	309	HIS	-	expression tag	UNP P01854
B	310	HIS	-	expression tag	UNP P01854
B	311	HIS	-	expression tag	UNP P01854
B	312	HIS	-	expression tag	UNP P01854
B	313	HIS	-	expression tag	UNP P01854
B	314	HIS	-	expression tag	UNP P01854
B	315	HIS	-	expression tag	UNP P01854
B	316	HIS	-	expression tag	UNP P01854
B	317	GLY	-	expression tag	UNP P01854
B	318	GLY	-	expression tag	UNP P01854
B	319	GLU	-	expression tag	UNP P01854

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	320	ASN	-	expression tag	UNP P01854
B	321	LEU	-	expression tag	UNP P01854
B	322	TYR	-	expression tag	UNP P01854
B	323	PHE	-	expression tag	UNP P01854
B	324	GLN	-	expression tag	UNP P01854
B	325	GLY	-	expression tag	UNP P01854
B	326	GLY	-	expression tag	UNP P01854
B	327	SER	-	expression tag	UNP P01854
G	299	ALA	-	expression tag	UNP P01854
G	300	PRO	-	expression tag	UNP P01854
G	301	MET	-	expression tag	UNP P01854
G	302	ALA	-	expression tag	UNP P01854
G	303	GLU	-	expression tag	UNP P01854
G	304	GLY	-	expression tag	UNP P01854
G	305	GLY	-	expression tag	UNP P01854
G	306	GLY	-	expression tag	UNP P01854
G	307	GLN	-	expression tag	UNP P01854
G	308	ASN	-	expression tag	UNP P01854
G	309	HIS	-	expression tag	UNP P01854
G	310	HIS	-	expression tag	UNP P01854
G	311	HIS	-	expression tag	UNP P01854
G	312	HIS	-	expression tag	UNP P01854
G	313	HIS	-	expression tag	UNP P01854
G	314	HIS	-	expression tag	UNP P01854
G	315	HIS	-	expression tag	UNP P01854
G	316	HIS	-	expression tag	UNP P01854
G	317	GLY	-	expression tag	UNP P01854
G	318	GLY	-	expression tag	UNP P01854
G	319	GLU	-	expression tag	UNP P01854
G	320	ASN	-	expression tag	UNP P01854
G	321	LEU	-	expression tag	UNP P01854
G	322	TYR	-	expression tag	UNP P01854
G	323	PHE	-	expression tag	UNP P01854
G	324	GLN	-	expression tag	UNP P01854
G	325	GLY	-	expression tag	UNP P01854
G	326	GLY	-	expression tag	UNP P01854
G	327	SER	-	expression tag	UNP P01854
H	299	ALA	-	expression tag	UNP P01854
H	300	PRO	-	expression tag	UNP P01854
H	301	MET	-	expression tag	UNP P01854
H	302	ALA	-	expression tag	UNP P01854
H	303	GLU	-	expression tag	UNP P01854

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	304	GLY	-	expression tag	UNP P01854
H	305	GLY	-	expression tag	UNP P01854
H	306	GLY	-	expression tag	UNP P01854
H	307	GLN	-	expression tag	UNP P01854
H	308	ASN	-	expression tag	UNP P01854
H	309	HIS	-	expression tag	UNP P01854
H	310	HIS	-	expression tag	UNP P01854
H	311	HIS	-	expression tag	UNP P01854
H	312	HIS	-	expression tag	UNP P01854
H	313	HIS	-	expression tag	UNP P01854
H	314	HIS	-	expression tag	UNP P01854
H	315	HIS	-	expression tag	UNP P01854
H	316	HIS	-	expression tag	UNP P01854
H	317	GLY	-	expression tag	UNP P01854
H	318	GLY	-	expression tag	UNP P01854
H	319	GLU	-	expression tag	UNP P01854
H	320	ASN	-	expression tag	UNP P01854
H	321	LEU	-	expression tag	UNP P01854
H	322	TYR	-	expression tag	UNP P01854
H	323	PHE	-	expression tag	UNP P01854
H	324	GLN	-	expression tag	UNP P01854
H	325	GLY	-	expression tag	UNP P01854
H	326	GLY	-	expression tag	UNP P01854
H	327	SER	-	expression tag	UNP P01854
A	299	ALA	-	expression tag	UNP P01854
A	300	PRO	-	expression tag	UNP P01854
A	301	MET	-	expression tag	UNP P01854
A	302	ALA	-	expression tag	UNP P01854
A	303	GLU	-	expression tag	UNP P01854
A	304	GLY	-	expression tag	UNP P01854
A	305	GLY	-	expression tag	UNP P01854
A	306	GLY	-	expression tag	UNP P01854
A	307	GLN	-	expression tag	UNP P01854
A	308	ASN	-	expression tag	UNP P01854
A	309	HIS	-	expression tag	UNP P01854
A	310	HIS	-	expression tag	UNP P01854
A	311	HIS	-	expression tag	UNP P01854
A	312	HIS	-	expression tag	UNP P01854
A	313	HIS	-	expression tag	UNP P01854
A	314	HIS	-	expression tag	UNP P01854
A	315	HIS	-	expression tag	UNP P01854
A	316	HIS	-	expression tag	UNP P01854

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	GLY	-	expression tag	UNP P01854
A	318	GLY	-	expression tag	UNP P01854
A	319	GLU	-	expression tag	UNP P01854
A	320	ASN	-	expression tag	UNP P01854
A	321	LEU	-	expression tag	UNP P01854
A	322	TYR	-	expression tag	UNP P01854
A	323	PHE	-	expression tag	UNP P01854
A	324	GLN	-	expression tag	UNP P01854
A	325	GLY	-	expression tag	UNP P01854
A	326	GLY	-	expression tag	UNP P01854
A	327	SER	-	expression tag	UNP P01854

- Molecule 2 is a protein called 813 Variable fragment Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	122	Total	C	N	O	S	0	0	0
			944	595	164	182	3			
2	E	123	Total	C	N	O	S	0	0	0
			949	598	165	183	3			
2	C	121	Total	C	N	O	S	0	0	0
			940	593	163	181	3			
2	K	121	Total	C	N	O	S	0	0	0
			940	593	163	181	3			

- Molecule 3 is a protein called 813 Variable fragment Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	112	Total	C	N	O	S	0	0	0
			851	529	138	181	3			
3	F	114	Total	C	N	O	S	0	0	0
			862	536	141	182	3			
3	D	114	Total	C	N	O	S	0	0	0
			863	536	141	183	3			
3	L	114	Total	C	N	O	S	0	0	0
			863	536	141	183	3			

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



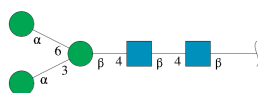
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	N	2	Total	C	O	0	0	0
			22	12	10			
5	Q	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-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	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total 1	Na 1	0	0
7	K	1	Total 1	Na 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	4	Total 4	O 4	0	0
8	J	1	Total 1	O 1	0	0
8	F	1	Total 1	O 1	0	0
8	G	1	Total 1	O 1	0	0
8	H	2	Total 2	O 2	0	0
8	D	1	Total 1	O 1	0	0
8	K	1	Total 1	O 1	0	0
8	L	1	Total 1	O 1	0	0

- MAN1
MAN2

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

Chain R:



MAG1
MAG2
BMJ3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.96Å 132.00Å 177.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 3.00 39.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.59-3.00) 99.6 (39.59-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.210 , 0.261 0.211 , 0.261	Depositor DCC
R_{free} test set	2291 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14043	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, NA

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	0.30	0/1673	0.49	0/2282
1	B	0.31	0/1690	0.49	0/2302
1	G	0.30	0/1680	0.47	0/2289
1	H	0.31	0/1684	0.50	0/2294
2	C	0.32	0/966	0.54	1/1315 (0.1%)
2	E	0.38	0/975	0.53	0/1327
2	I	0.38	0/970	0.54	0/1320
2	K	0.34	0/966	0.52	0/1315
3	D	0.33	0/882	0.50	0/1196
3	F	0.33	0/881	0.51	0/1195
3	J	0.32	0/870	0.51	0/1182
3	L	0.34	0/882	0.50	0/1196
All	All	0.33	0/14119	0.51	1/19213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	98	ARG	NE-CZ-NH1	-5.69	117.46	120.30

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	1631	0	1591	21	0
1	B	1648	0	1626	17	0
1	G	1639	0	1615	26	0
1	H	1643	0	1615	18	0
2	C	940	0	885	12	0
2	E	949	0	890	14	0
2	I	944	0	888	6	0
2	K	940	0	885	8	0
3	D	863	0	813	4	0
3	F	862	0	810	5	0
3	J	851	0	796	2	0
3	L	863	0	813	8	0
4	M	50	0	43	3	0
4	O	50	0	43	1	0
4	P	50	0	43	4	0
5	N	22	0	19	1	0
5	Q	22	0	19	2	0
6	R	61	0	52	5	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	K	1	0	0	0	0
8	B	4	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	2	0	0	0	0
8	J	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
All	All	14043	0	13446	144	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 5.

The worst 5 of 144 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:31:SER:HB3	3:D:36:TYR:HE2	1.60	0.67
1:G:494:GLN:OE1	1:G:496:ARG:NH2	2.29	0.65
1:G:342:ARG:NH2	1:G:473:ASP:OD1	2.31	0.63
1:G:365:PRO:HG3	1:G:397:LEU:HB2	1.81	0.62
1:A:422:HIS:CE1	1:A:424:HIS:HB2	2.35	0.62

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	207/247 (84%)	199 (96%)	7 (3%)	1 (0%)	29	68
1	B	207/247 (84%)	200 (97%)	7 (3%)	0	100	100
1	G	207/247 (84%)	197 (95%)	10 (5%)	0	100	100
1	H	207/247 (84%)	196 (95%)	11 (5%)	0	100	100
2	C	119/123 (97%)	112 (94%)	7 (6%)	0	100	100
2	E	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	19	57
2	I	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	9	39
2	K	119/123 (97%)	113 (95%)	5 (4%)	1 (1%)	19	57
3	D	112/134 (84%)	108 (96%)	4 (4%)	0	100	100
3	F	112/134 (84%)	106 (95%)	6 (5%)	0	100	100
3	J	110/134 (82%)	105 (96%)	5 (4%)	0	100	100
3	L	112/134 (84%)	108 (96%)	4 (4%)	0	100	100
All	All	1753/2016 (87%)	1667 (95%)	81 (5%)	5 (0%)	41	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	32	GLY
2	K	32	GLY
2	E	33	TYR
2	I	33	TYR
1	A	366	SER

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	180/212 (85%)	180 (100%)	0	100	100
1	B	184/212 (87%)	183 (100%)	1 (0%)	88	96
1	G	181/212 (85%)	179 (99%)	2 (1%)	73	90
1	H	182/212 (86%)	179 (98%)	3 (2%)	62	86
2	C	100/101 (99%)	97 (97%)	3 (3%)	41	75
2	E	100/101 (99%)	98 (98%)	2 (2%)	55	83
2	I	100/101 (99%)	98 (98%)	2 (2%)	55	83
2	K	100/101 (99%)	97 (97%)	3 (3%)	41	75
3	D	97/113 (86%)	96 (99%)	1 (1%)	76	91
3	F	96/113 (85%)	95 (99%)	1 (1%)	76	91
3	J	96/113 (85%)	95 (99%)	1 (1%)	76	91
3	L	97/113 (86%)	97 (100%)	0	100	100
All	All	1513/1704 (89%)	1494 (99%)	19 (1%)	69	89

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

Mol	Chain	Res	Type
2	C	82	GLN
2	K	52	VAL
2	K	71	SER
2	K	34	SER
1	G	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	477	GLN
1	A	422	HIS

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	$\# Z > 2$
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	1.52	3 (17%)
4	NAG	M	2	4	14,14,15	0.30	0	17,19,21	0.58	0
4	BMA	M	3	4	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
4	MAN	M	4	4	11,11,12	0.95	0	15,15,17	0.90	1 (6%)
5	MAN	N	1	5	11,11,12	1.13	0	15,15,17	1.68	3 (20%)
5	MAN	N	2	5	11,11,12	1.36	1 (9%)	15,15,17	1.47	4 (26%)
4	NAG	O	1	1,4	14,14,15	0.33	0	17,19,21	1.47	2 (11%)
4	NAG	O	2	4	14,14,15	0.22	0	17,19,21	0.50	0
4	BMA	O	3	4	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
4	MAN	O	4	4	11,11,12	0.86	0	15,15,17	0.99	1 (6%)
4	NAG	P	1	4	14,14,15	0.30	0	17,19,21	1.44	3 (17%)
4	NAG	P	2	4	14,14,15	0.28	0	17,19,21	0.57	0
4	BMA	P	3	4	11,11,12	0.80	0	15,15,17	1.01	1 (6%)
4	MAN	P	4	4	11,11,12	1.02	0	15,15,17	1.03	1 (6%)
5	MAN	Q	1	5	11,11,12	1.14	1 (9%)	15,15,17	1.50	2 (13%)
5	MAN	Q	2	5	11,11,12	1.07	0	15,15,17	1.18	1 (6%)
6	NAG	R	1	1,6	14,14,15	0.29	0	17,19,21	1.54	3 (17%)
6	NAG	R	2	6	14,14,15	0.20	0	17,19,21	0.55	0
6	BMA	R	3	6	11,11,12	0.76	0	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	R	4	6	11,11,12	1.10	0	15,15,17	1.09	1 (6%)
6	MAN	R	5	6	11,11,12	1.46	2 (18%)	15,15,17	1.20	1 (6%)

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
4	NAG	M	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	2/2/19/22	0/1/1/1
5	MAN	N	1	5	-	1/2/19/22	1/1/1/1
5	MAN	N	2	5	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	1/2/19/22	0/1/1/1
4	NAG	P	1	4	-	5/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	1/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
5	MAN	Q	1	5	-	0/2/19/22	1/1/1/1
5	MAN	Q	2	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
6	MAN	R	5	6	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	2	MAN	C4-C3	2.55	1.58	1.52
5	Q	1	MAN	O5-C5	2.46	1.48	1.43
6	R	5	MAN	O5-C5	2.14	1.47	1.43
6	R	5	MAN	C4-C3	2.07	1.57	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	NAG	C2-N2-C7	4.44	129.22	122.90
5	N	1	MAN	C1-O5-C5	4.43	118.20	112.19
4	M	1	NAG	C2-N2-C7	4.41	129.18	122.90
4	O	1	NAG	C2-N2-C7	4.40	129.16	122.90
6	R	1	NAG	C2-N2-C7	4.33	129.07	122.90

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	3	BMA	C4-C5-C6-O6
5	Q	2	MAN	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6

All (2) ring outliers are listed below:

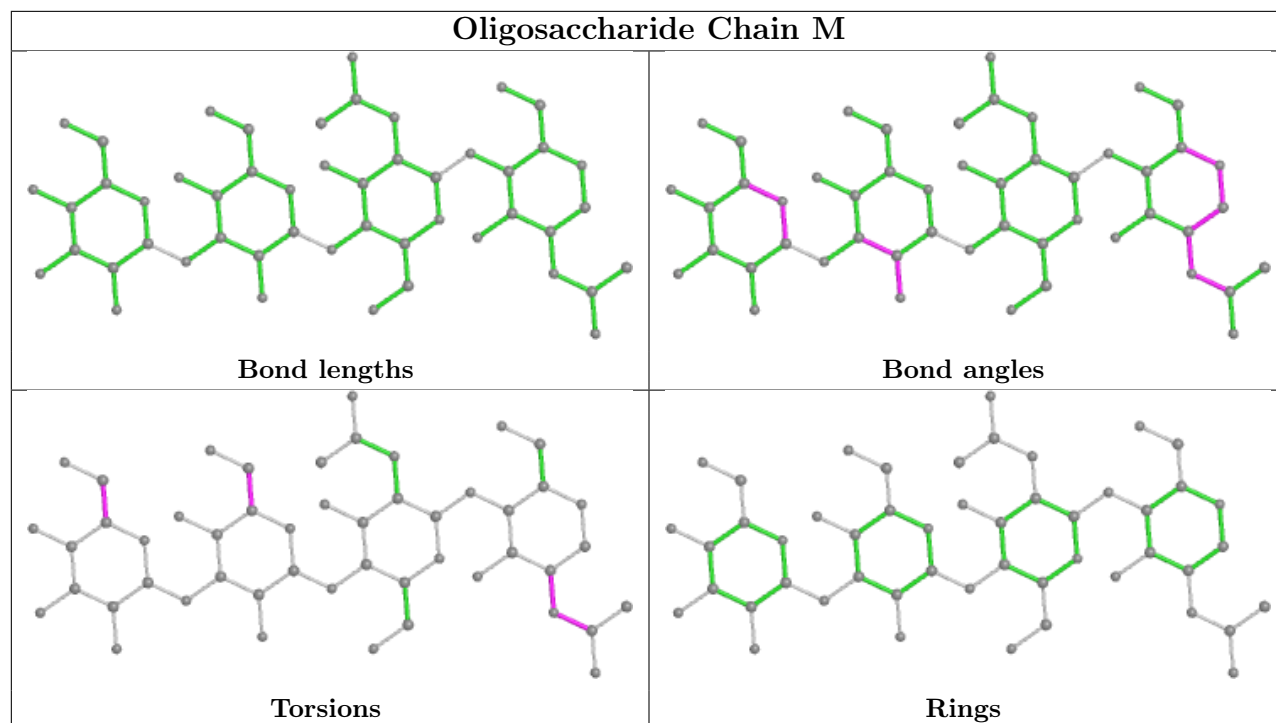
Mol	Chain	Res	Type	Atoms
5	N	1	MAN	C1-C2-C3-C4-C5-O5
5	Q	1	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 14 short contacts:

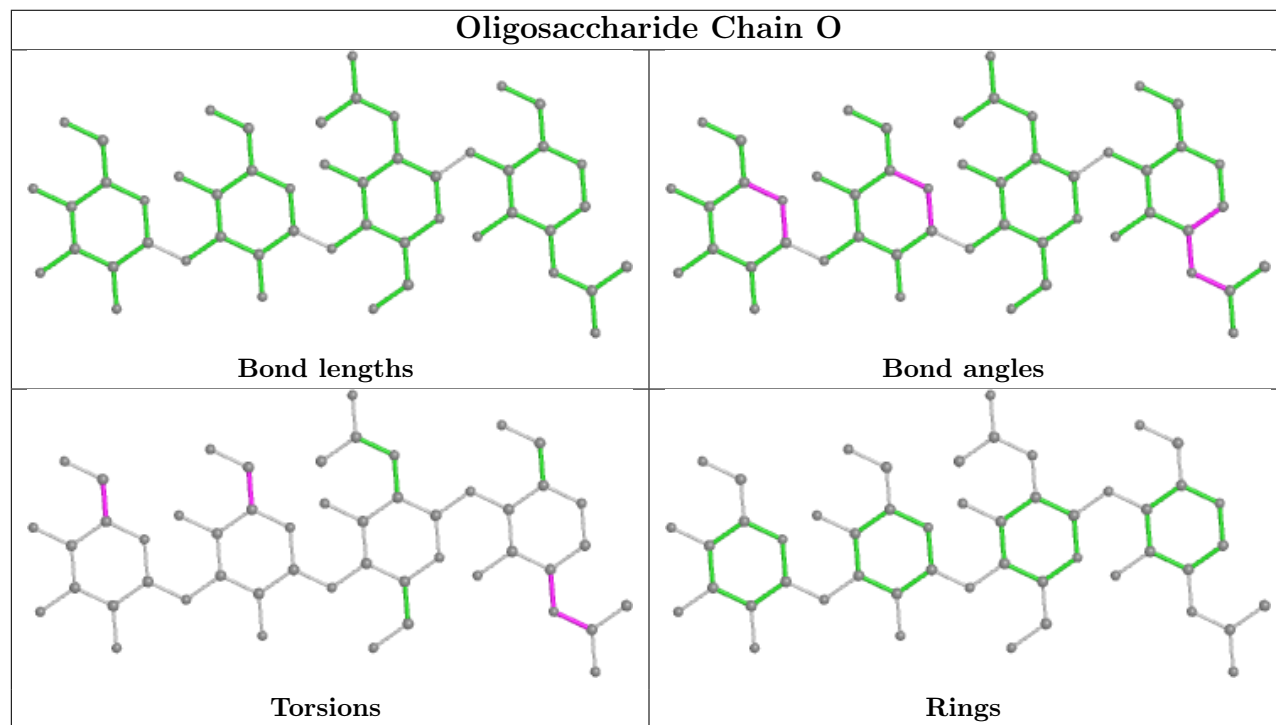
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	2	0
4	M	3	BMA	1	0
4	P	1	NAG	2	0
4	P	3	BMA	2	0
5	Q	1	MAN	1	0
4	P	2	NAG	2	0
4	O	1	NAG	1	0
6	R	3	BMA	1	0
6	R	1	NAG	4	0
5	Q	2	MAN	1	0
6	R	2	NAG	2	0
5	N	1	MAN	1	0

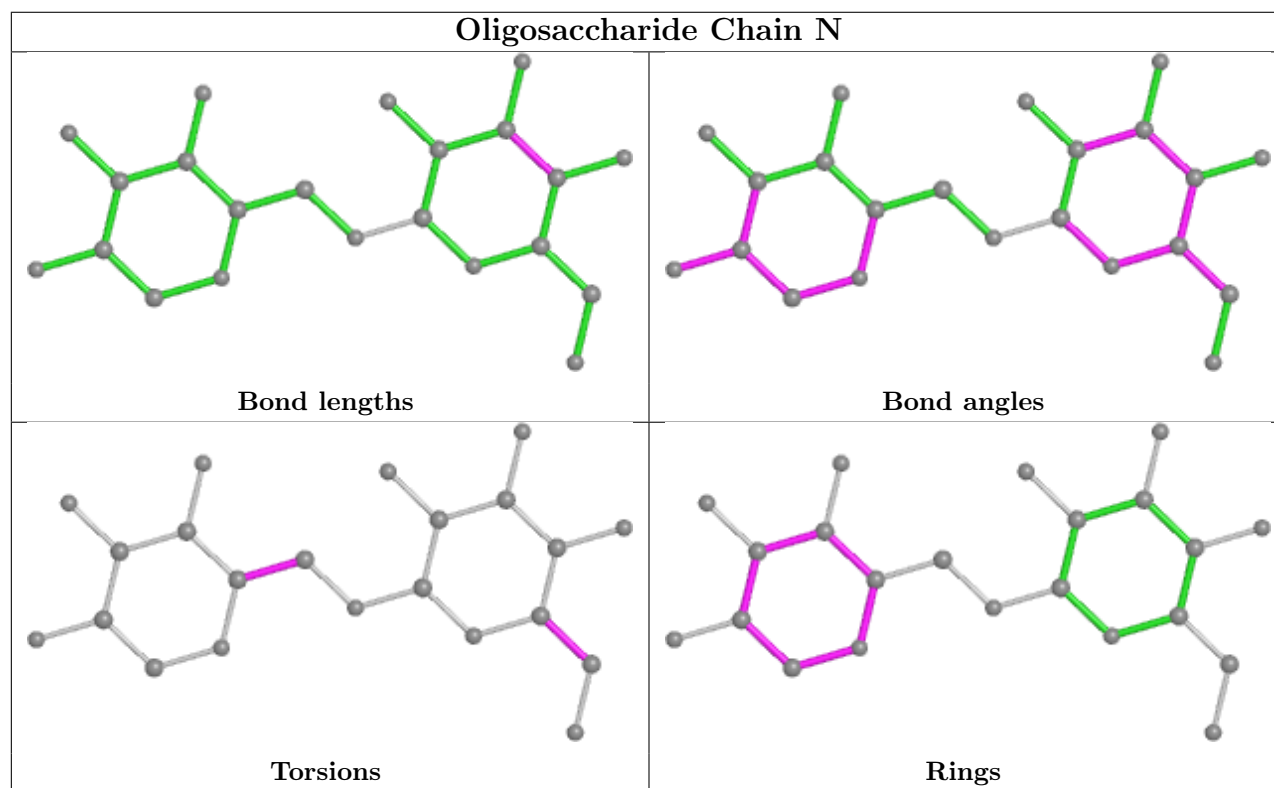
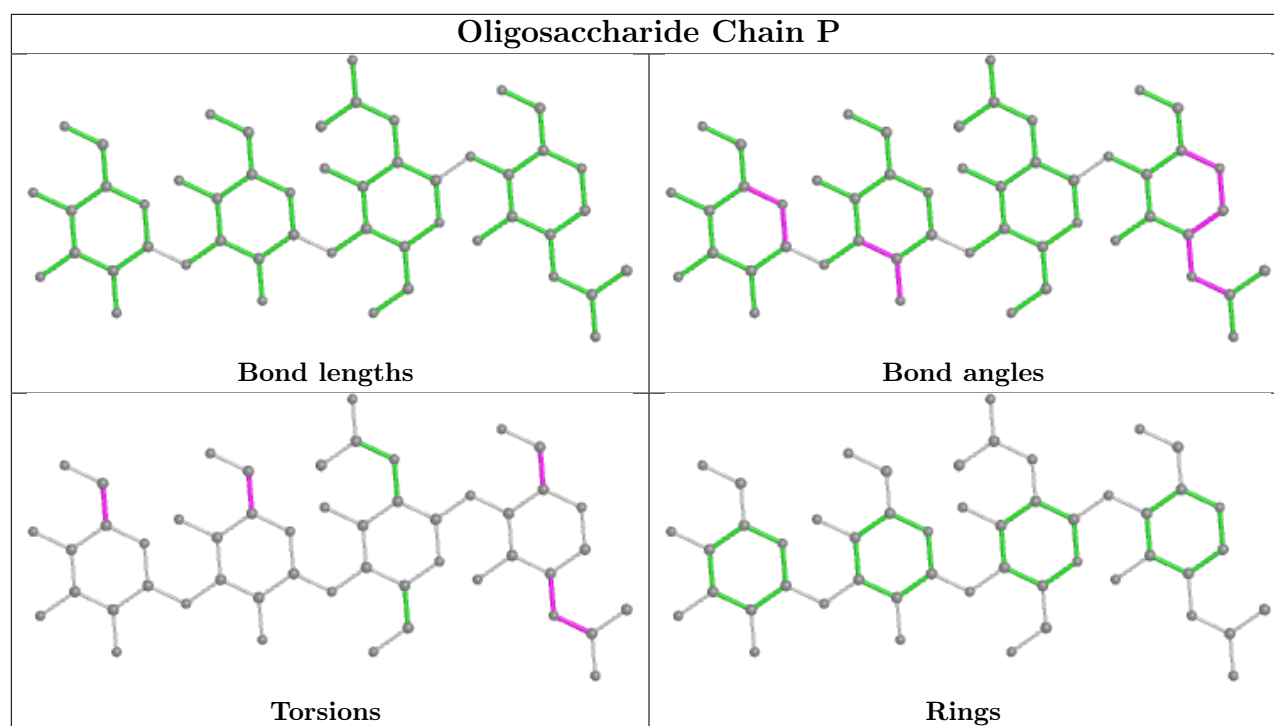
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

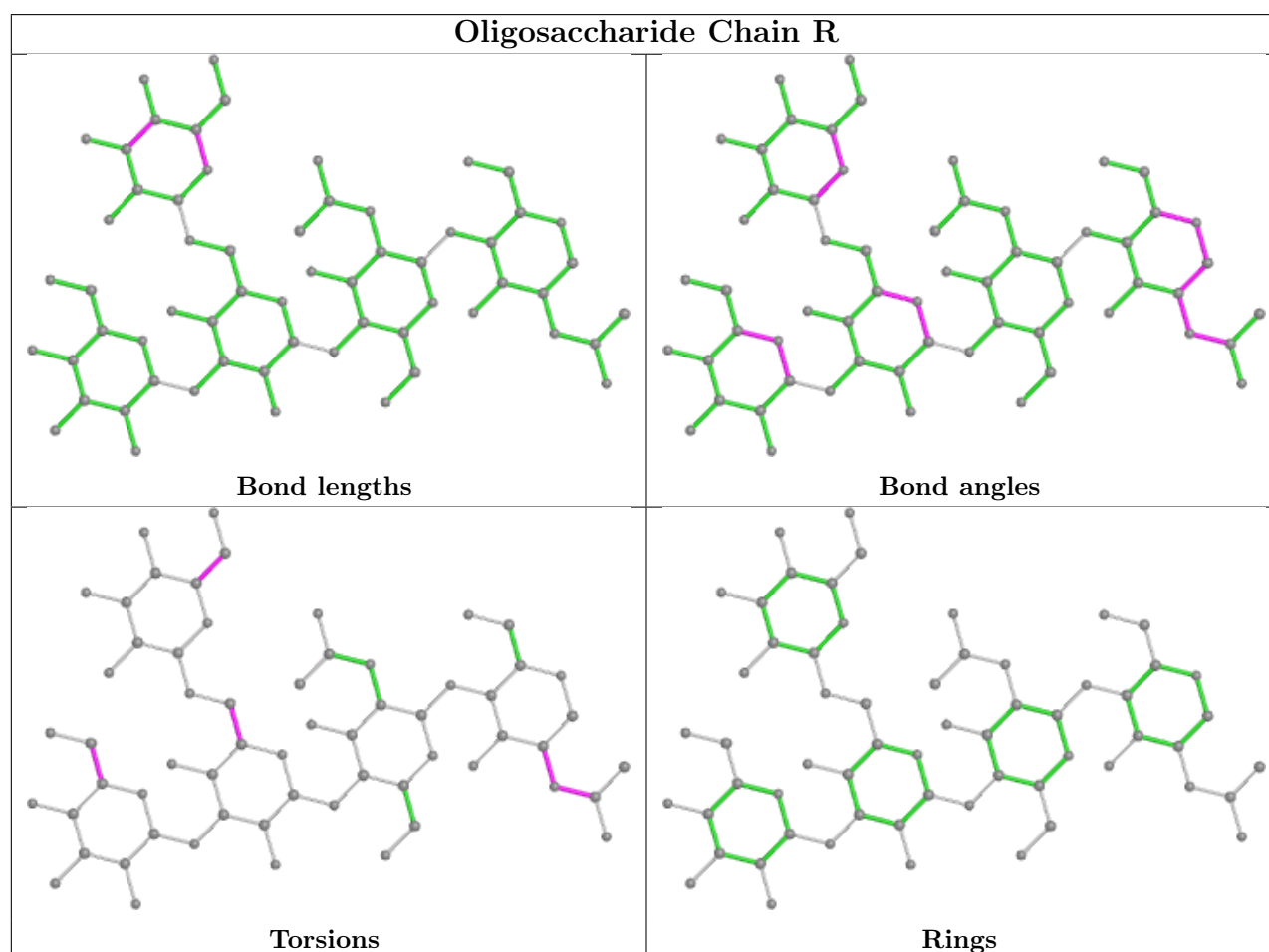
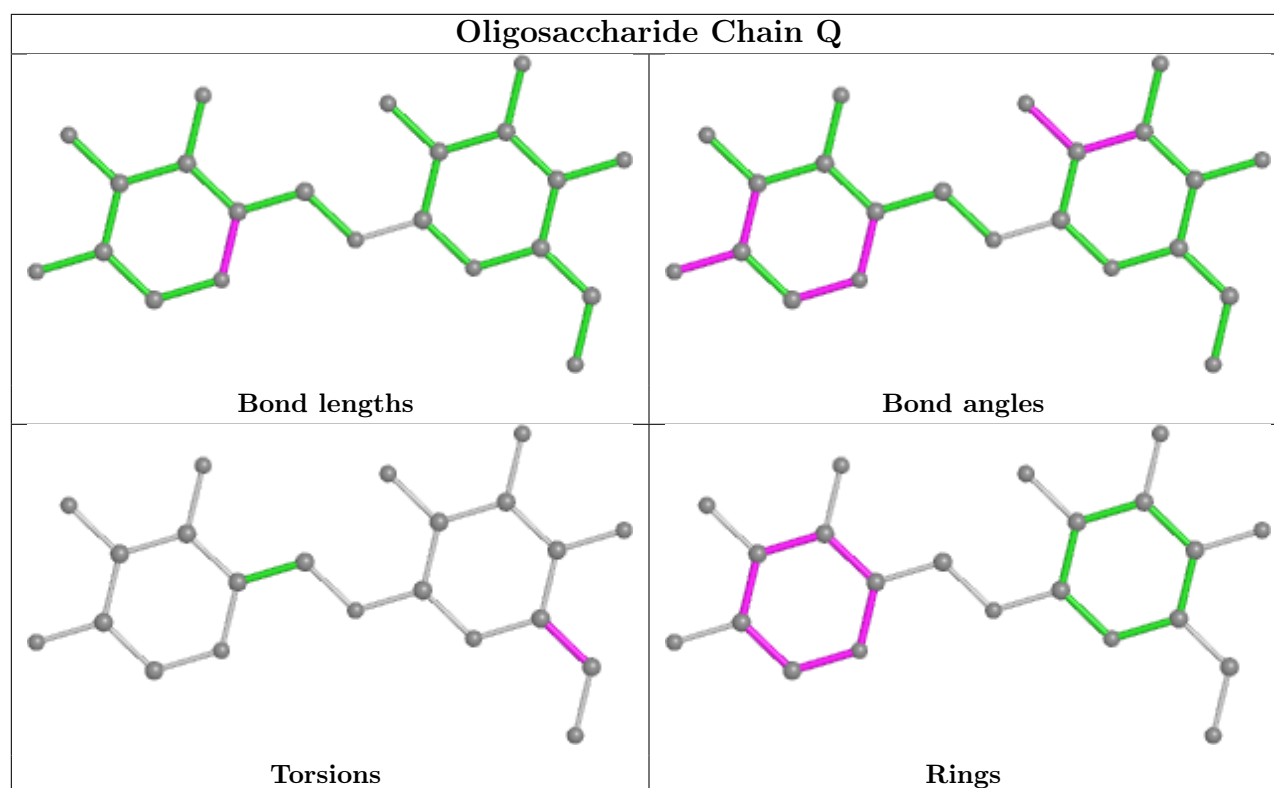
Oligosaccharide Chain M



Oligosaccharide Chain O







5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/247 (84%)	0.27	16 (7%) 13 4	48, 68, 110, 134	0
1	B	209/247 (84%)	0.04	3 (1%) 75 49	42, 60, 97, 115	0
1	G	209/247 (84%)	0.18	9 (4%) 35 13	54, 76, 119, 150	0
1	H	209/247 (84%)	0.34	10 (4%) 30 11	45, 71, 119, 167	0
2	C	121/123 (98%)	-0.11	1 (0%) 86 65	44, 62, 84, 92	0
2	E	123/123 (100%)	-0.02	0 100 100	51, 71, 94, 104	0
2	I	122/123 (99%)	-0.18	0 100 100	35, 50, 75, 85	0
2	K	121/123 (98%)	-0.12	0 100 100	38, 50, 71, 75	0
3	D	114/134 (85%)	-0.24	0 100 100	34, 51, 68, 86	0
3	F	114/134 (85%)	-0.12	1 (0%) 84 63	43, 57, 77, 84	0
3	J	112/134 (83%)	-0.27	0 100 100	41, 58, 73, 90	0
3	L	114/134 (85%)	-0.16	0 100 100	43, 52, 65, 74	0
All	All	1777/2016 (88%)	0.02	40 (2%) 60 31	34, 61, 99, 167	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	361	VAL	5.1
1	A	364	ALA	4.6
1	A	366	SER	3.8
1	A	370	VAL	3.4
1	H	369	THR	3.3

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

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

6.3 Carbohydrates ⓘ

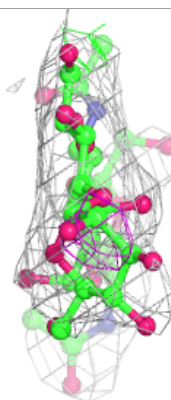
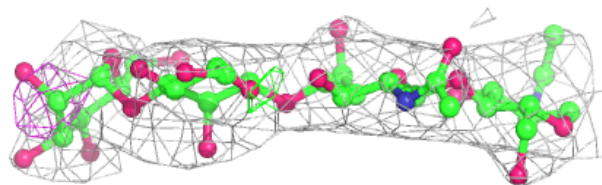
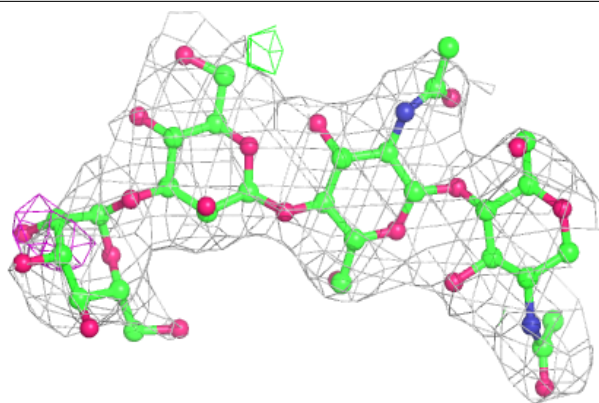
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	P	1	14/15	0.43	0.52	106,106,106,106	0
4	MAN	O	4	11/12	0.63	0.44	100,100,100,100	0
5	MAN	N	2	11/12	0.63	0.44	45,45,45,45	11
5	MAN	Q	1	11/12	0.65	0.34	72,72,72,72	0
4	MAN	P	4	11/12	0.67	0.60	94,94,94,94	0
6	MAN	R	4	11/12	0.73	0.33	85,85,85,85	0
6	NAG	R	1	14/15	0.75	0.47	99,99,99,99	0
5	MAN	Q	2	11/12	0.75	0.47	60,60,60,60	11
6	MAN	R	5	11/12	0.75	0.24	82,82,82,82	0
4	NAG	P	2	14/15	0.76	0.31	98,98,98,98	0
4	BMA	P	3	11/12	0.77	0.21	90,90,90,90	0
4	BMA	O	3	11/12	0.77	0.23	98,98,98,98	0
4	NAG	O	2	14/15	0.79	0.41	103,103,103,103	0
6	NAG	R	2	14/15	0.80	0.34	90,90,90,90	0
5	MAN	N	1	11/12	0.83	0.25	51,51,51,51	0
4	NAG	O	1	14/15	0.83	0.42	111,111,111,111	0
4	MAN	M	4	11/12	0.85	0.40	61,61,61,61	0
6	BMA	R	3	11/12	0.85	0.18	84,84,84,84	0
4	NAG	M	1	14/15	0.91	0.26	71,71,71,71	0
4	NAG	M	2	14/15	0.93	0.26	63,63,63,63	0
4	BMA	M	3	11/12	0.93	0.17	58,58,58,58	0

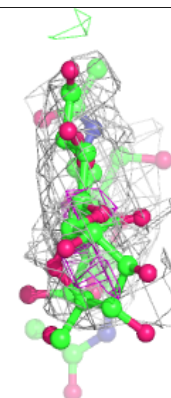
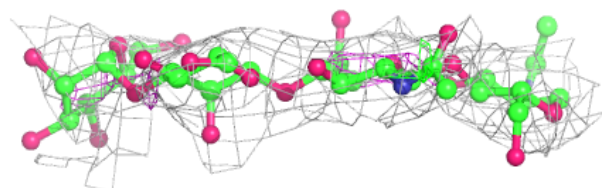
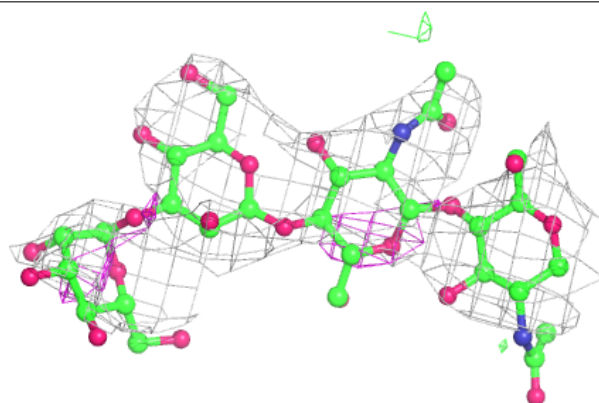
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

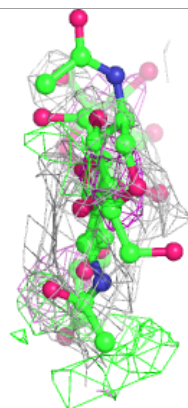
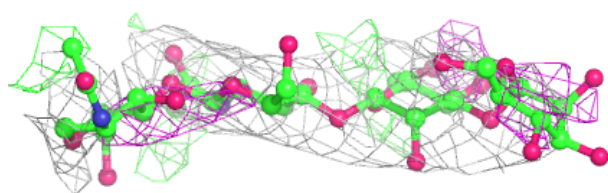
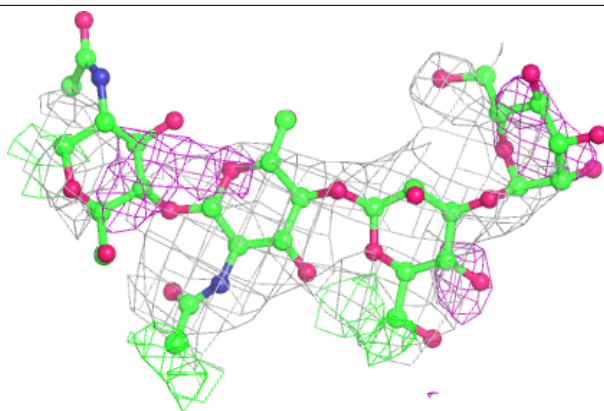
**Electron density around Chain O:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

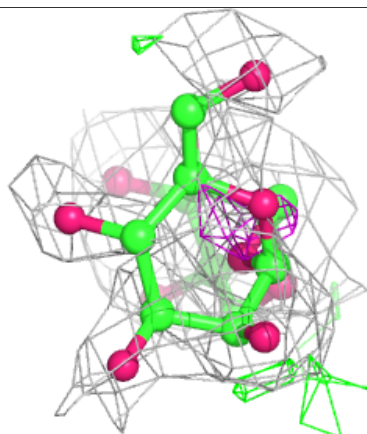
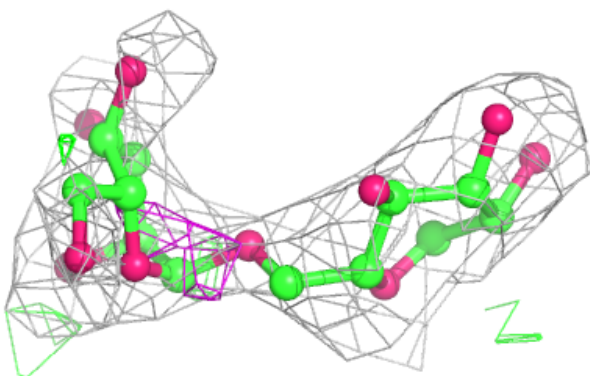
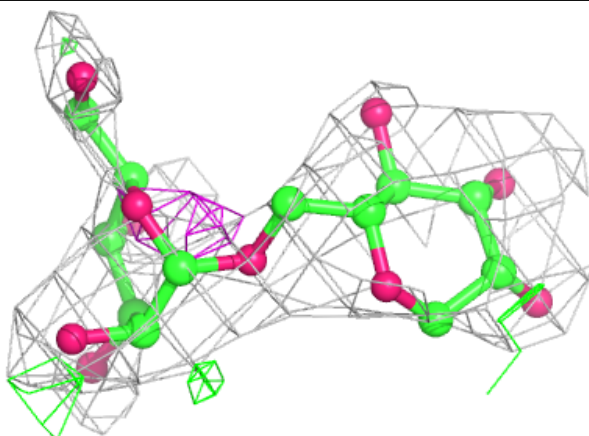


Electron density around Chain P:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

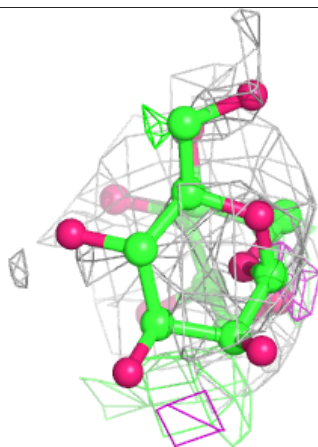
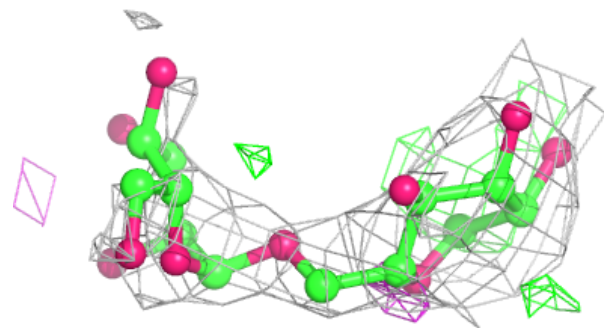
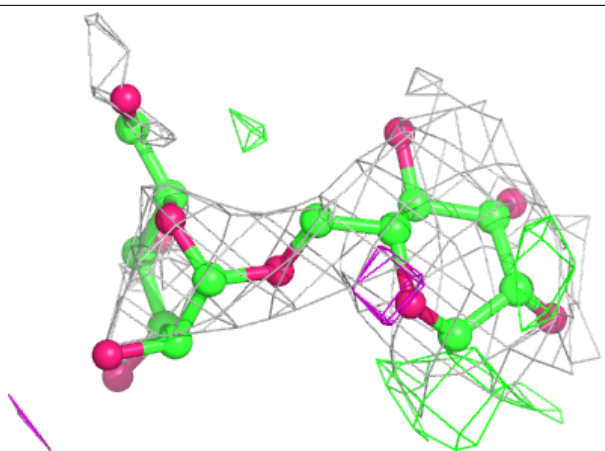
**Electron density around Chain N:**

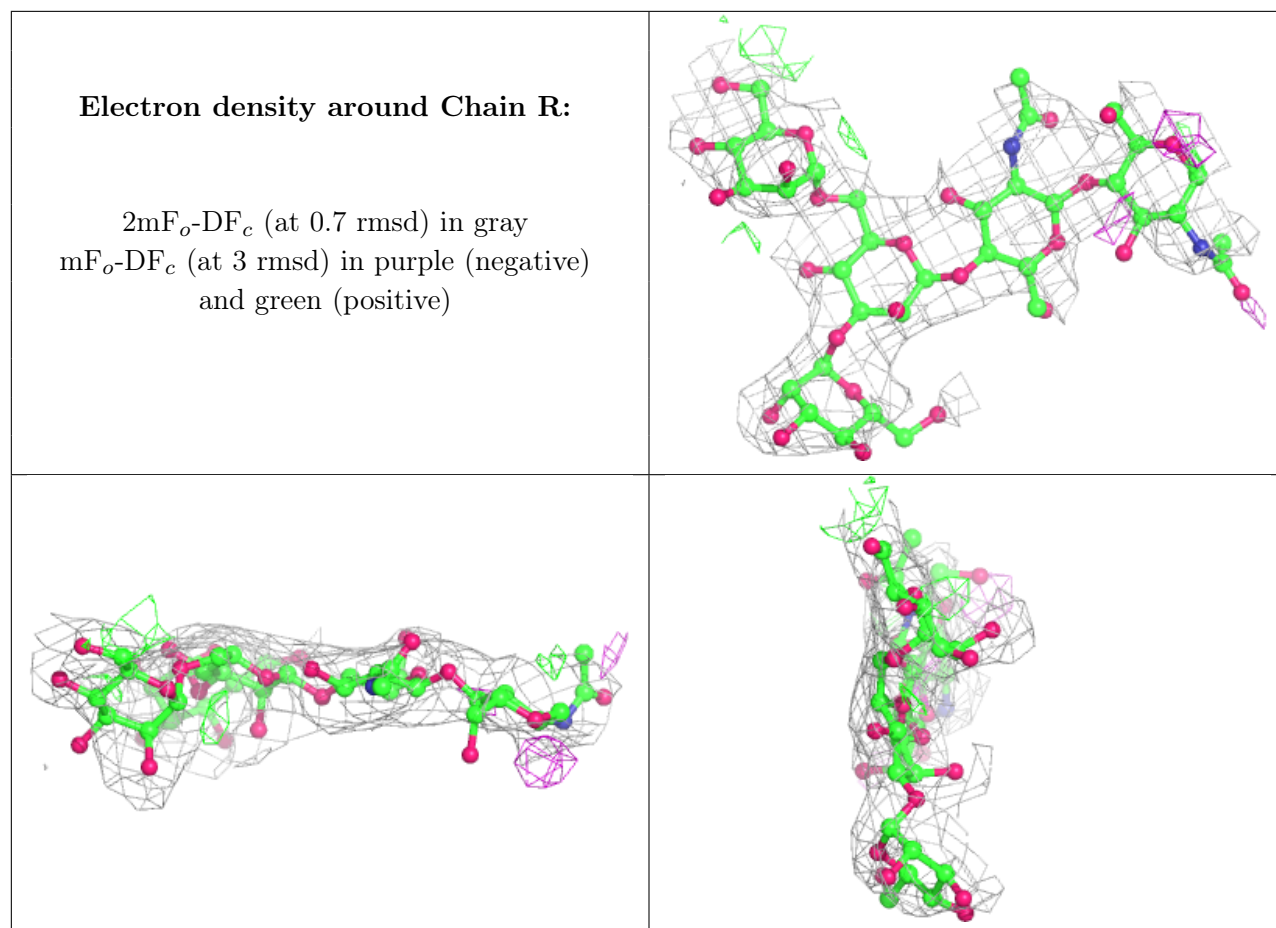
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NA	K	201	1/1	0.87	0.44	28,28,28,28	0
7	NA	E	201	1/1	0.92	0.57	38,38,38,38	0
7	NA	I	201	1/1	0.92	0.61	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.