Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 03:25 PM EDT

PDB ID	:	6WOL
Title	:	Next generation monomeric IgG4 Fc bound to neonatal Fc receptor
Authors	:	Oganesyan, V.Y.; Shan, L.; van Dyk, N.; Dall'Acqua, W.F.
Deposited on	:	2020-04-24
Resolution	:	2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

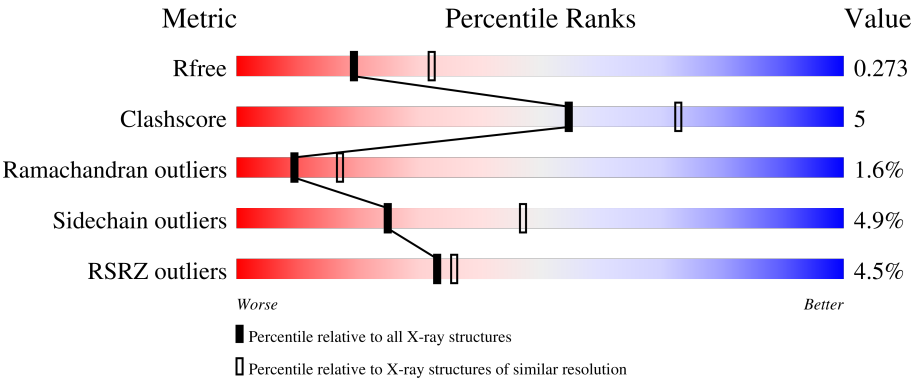
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	H	209	9% 82% 17%
2	A	267	2% 82% 15%
3	B	99	2% 85% 15%
4	C	8	12% 88%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4708 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 Immunoglobulin heavy constant gamma 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	0
			1667	1052	282	324	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	351	PHE	LEU	engineered mutation	UNP P01861
H	354	GLU	SER	engineered mutation	UNP P01861
H	366	ARG	THR	engineered mutation	UNP P01861
H	395	LYS	PRO	engineered mutation	UNP P01861
H	405	ARG	PHE	engineered mutation	UNP P01861
H	407	GLU	TYR	engineered mutation	UNP P01861
H	432	CYS	LEU	engineered mutation	UNP P01861
H	433	SER	HIS	engineered mutation	UNP P01861
H	434	TYR	ASN	engineered mutation	UNP P01861
H	436	LEU	TYR	engineered mutation	UNP P01861
H	437	CYS	THR	engineered mutation	UNP P01861
H	?	-	GLN	deletion	UNP P01861

- Molecule 2 is a protein called IgG receptor FcRn large subunit p51.

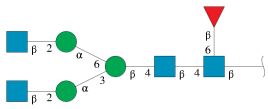
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	264	Total	C	N	O	S	0	0	0
			2080	1330	360	382	8			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp

ha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
4	C	8	Total C N O 99 56 4 39	0	0	0

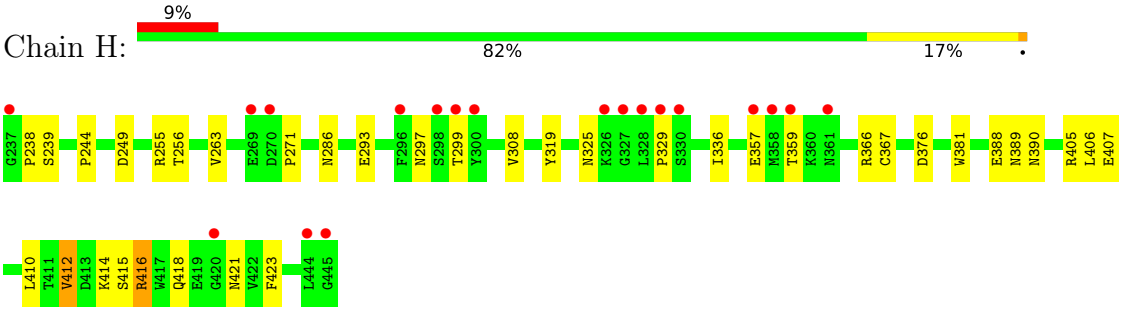
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	9	Total O 9 9	0	0
5	A	19	Total O 19 19	0	0
5	B	5	Total O 5 5	0	0

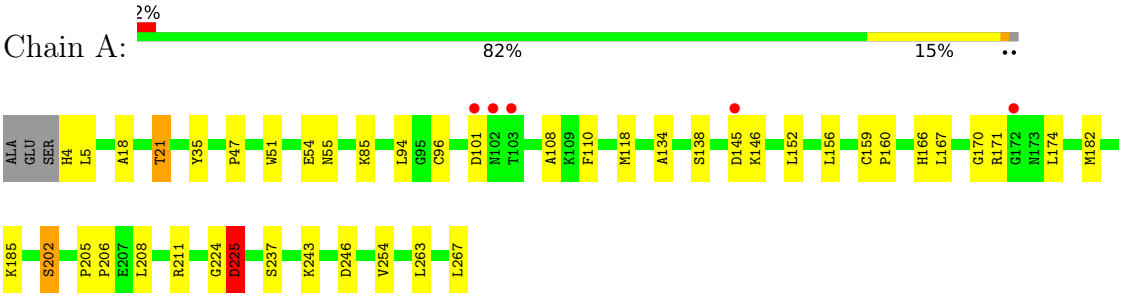
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

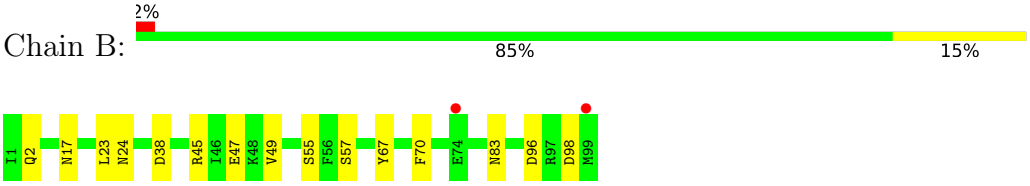
• Molecule 1: Immunoglobulin heavy constant gamma 4



• Molecule 2: IgG receptor FcRn large subunit p51



• Molecule 3: Beta-2-microglobulin



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	68.28Å 122.60Å 178.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.10 – 2.49 36.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.10-2.49) 99.2 (36.07-2.49)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.270 0.239 , 0.273	Depositor DCC
R_{free} test set	1032 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.056 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.077 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4708	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NAG, FUL, BMA

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	H	0.66	0/1708	0.80	0/2318
2	A	0.66	0/2146	0.79	0/2915
3	B	0.65	0/852	0.83	0/1152
All	All	0.66	0/4706	0.80	0/6385

There are no bond length outliers.

There are no bond angle outliers.

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	H	1667	0	1626	19	0
2	A	2080	0	1990	25	0
3	B	829	0	794	5	0
4	C	99	0	85	0	0
5	A	19	0	0	0	0
5	B	5	0	0	0	0
5	H	9	0	0	0	0
All	All	4708	0	4495	48	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.

All (48) 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)
1:H:390:ASN:O	1:H:410:LEU:HD12	1.89	0.72
3:B:24:ASN:HD22	3:B:67:TYR:HB3	1.59	0.67
1:H:238:PRO:HG3	1:H:325:ASN:HD22	1.60	0.66
2:A:182:MET:HE2	2:A:254:VAL:HG11	1.85	0.58
1:H:308:VAL:HG12	1:H:319:TYR:CE2	2.42	0.55
2:A:254:VAL:HG13	2:A:263:LEU:HB3	1.89	0.54
2:A:182:MET:CE	2:A:254:VAL:HG11	2.38	0.53
1:H:416:ARG:CG	1:H:421:ASN:HD22	2.22	0.52
2:A:205:PRO:HB2	2:A:206:PRO:HD2	1.92	0.52
3:B:45:ARG:NH1	3:B:47:GLU:OE1	2.43	0.51
2:A:254:VAL:CG1	2:A:263:LEU:HB3	2.41	0.51
2:A:182:MET:HE3	2:A:254:VAL:HB	1.93	0.50
2:A:134:ALA:O	2:A:138:SER:HB3	2.12	0.49
2:A:243:LYS:HB2	2:A:246:ASP:HB2	1.95	0.49
1:H:414:LYS:HE2	1:H:418:GLN:HE21	1.78	0.49
2:A:159:CYS:HB3	2:A:160:PRO:HD3	1.95	0.48
1:H:297:ASN:OD1	1:H:299:THR:HG22	2.13	0.48
2:A:182:MET:CE	2:A:254:VAL:HB	2.44	0.47
2:A:54:GLU:OE2	2:A:166:HIS:ND1	2.39	0.47
1:H:406:LEU:C	1:H:406:LEU:HD12	2.34	0.47
2:A:94:LEU:HD23	2:A:108:ALA:HA	1.97	0.47
2:A:35:TYR:O	2:A:47:PRO:HA	2.15	0.46
2:A:110:PHE:HB2	2:A:118:MET:HB3	1.97	0.46
1:H:367:CYS:HB2	1:H:381:TRP:CH2	2.51	0.46
1:H:416:ARG:O	1:H:421:ASN:HB2	2.15	0.45
2:A:182:MET:CE	2:A:254:VAL:CB	2.95	0.44
3:B:23:LEU:O	3:B:67:TYR:HA	2.17	0.44
1:H:416:ARG:HG2	1:H:421:ASN:HD22	1.82	0.44
1:H:366:ARG:NH2	1:H:407:GLU:OE1	2.50	0.44
2:A:185:LYS:HE3	3:B:98:ASP:HA	2.00	0.44
2:A:208:LEU:HD11	2:A:254:VAL:CG2	2.47	0.44
2:A:5:LEU:HD12	2:A:5:LEU:HA	1.88	0.43
1:H:412:VAL:HG11	1:H:423:PHE:CE1	2.54	0.43
1:H:286:ASN:OD1	1:H:286:ASN:N	2.51	0.42
1:H:239:SER:O	1:H:263:VAL:HA	2.20	0.42
1:H:416:ARG:HG3	1:H:421:ASN:HD22	1.85	0.42
2:A:51:TRP:CZ3	2:A:170:GLY:HA3	2.54	0.42
3:B:96:ASP:OD1	3:B:98:ASP:HB2	2.19	0.42
1:H:244:PRO:HD3	1:H:336:ILE:HD11	2.02	0.41
2:A:152:LEU:HD23	2:A:156:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:367:CYS:HB2	1:H:381:TRP:CZ2	2.56	0.41
2:A:5:LEU:HD21	2:A:174:LEU:HD22	2.01	0.41
2:A:224:GLY:O	2:A:225:ASP:HB2	2.20	0.41
2:A:18:ALA:O	2:A:21:THR:HG22	2.21	0.40
1:H:249:ASP:OD1	1:H:255:ARG:HD3	2.21	0.40
1:H:388:GLU:OE2	1:H:416:ARG:NH2	2.53	0.40
2:A:167:LEU:O	2:A:171:ARG:HB2	2.22	0.40
2:A:96:CYS:N	2:A:159:CYS:SG	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	207/209 (99%)	194 (94%)	10 (5%)	3 (1%)	11 20
2	A	262/267 (98%)	244 (93%)	12 (5%)	6 (2%)	6 10
3	B	97/99 (98%)	94 (97%)	3 (3%)	0	100 100
All	All	566/575 (98%)	532 (94%)	25 (4%)	9 (2%)	9 17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	271	PRO
1	H	357	GLU
2	A	101	ASP
2	A	55	ASN
2	A	145	ASP
2	A	202	SER
2	A	225	ASP
1	H	329	PRO
2	A	85	LYS

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	H	195/195 (100%)	186 (95%)	9 (5%)	27 50
2	A	218/220 (99%)	210 (96%)	8 (4%)	34 60
3	B	94/94 (100%)	86 (92%)	8 (8%)	10 21
All	All	507/509 (100%)	482 (95%)	25 (5%)	25 47

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	256	THR
1	H	293	GLU
1	H	359	THR
1	H	376	ASP
1	H	389	ASN
1	H	405	ARG
1	H	412	VAL
1	H	415	SER
1	H	416	ARG
2	A	4	HIS
2	A	21	THR
2	A	146	LYS
2	A	202	SER
2	A	211	ARG
2	A	225	ASP
2	A	237	SER
2	A	267	LEU
3	B	2	GLN
3	B	17	ASN
3	B	38	ASP
3	B	49	VAL
3	B	55	SER
3	B	57	SER
3	B	70	PHE
3	B	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	295	GLN
1	H	310	HIS
1	H	325	ASN
1	H	389	ASN
1	H	418	GLN
2	A	173	ASN
2	A	229	ASN
3	B	24	ASN
3	B	83	ASN

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

8 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	C	1	4,1	14,14,15	0.42	0	17,19,21	1.21	3 (17%)
4	NAG	C	2	4	14,14,15	0.43	0	17,19,21	1.01	0
4	BMA	C	3	4	11,11,12	0.39	0	15,15,17	1.14	1 (6%)
4	MAN	C	4	4	11,11,12	0.38	0	15,15,17	1.43	2 (13%)
4	NAG	C	5	4	14,14,15	0.32	0	17,19,21	1.28	2 (11%)
4	MAN	C	6	4	11,11,12	0.42	0	15,15,17	1.44	2 (13%)
4	NAG	C	7	4	14,14,15	0.36	0	17,19,21	1.48	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUL	C	8	4	10,10,11	0.67	0	14,14,16	1.66	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
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	NAG	C	5	4	-	2/6/23/26	0/1/1/1
4	MAN	C	6	4	-	0/2/19/22	0/1/1/1
4	NAG	C	7	4	-	2/6/23/26	0/1/1/1
4	FUL	C	8	4	-	-	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	8	FUL	C1-C2-C3	4.44	115.13	109.67
4	C	5	NAG	C1-O5-C5	4.29	118.01	112.19
4	C	7	NAG	O5-C5-C6	3.81	113.18	107.20
4	C	4	MAN	O5-C1-C2	-3.71	105.05	110.77
4	C	6	MAN	C1-O5-C5	3.60	117.06	112.19
4	C	3	BMA	C1-O5-C5	3.29	116.65	112.19
4	C	7	NAG	C1-O5-C5	3.28	116.64	112.19
4	C	1	NAG	C1-O5-C5	3.00	116.26	112.19
4	C	8	FUL	C2-C3-C4	2.66	115.50	110.89
4	C	4	MAN	C3-C4-C5	2.48	114.66	110.24
4	C	1	NAG	O5-C1-C2	-2.47	107.38	111.29
4	C	5	NAG	C4-C3-C2	-2.28	107.67	111.02
4	C	1	NAG	C4-C3-C2	-2.21	107.78	111.02
4	C	6	MAN	O2-C2-C1	2.01	113.27	109.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

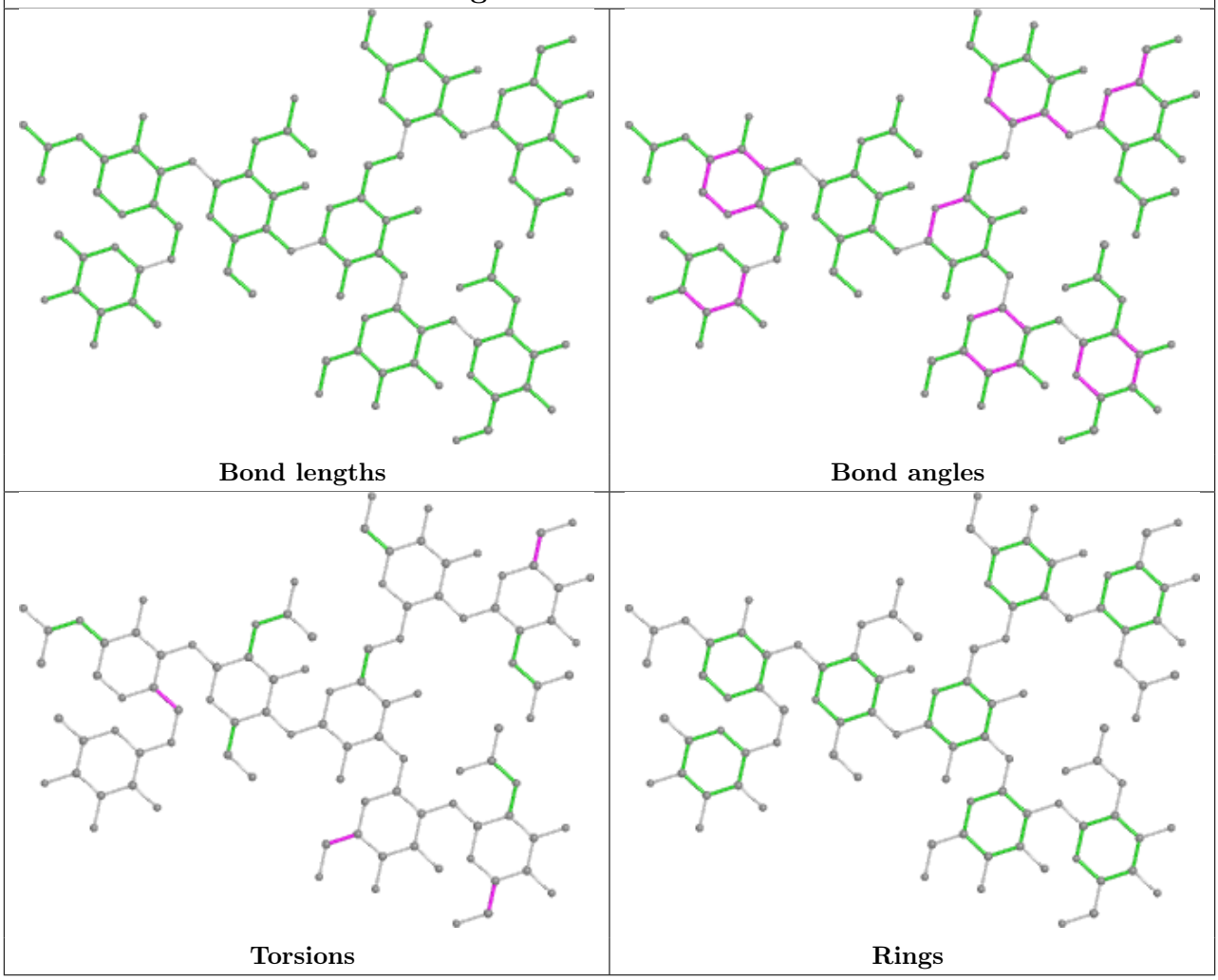
Mol	Chain	Res	Type	Atoms
4	C	5	NAG	O5-C5-C6-O6
4	C	7	NAG	O5-C5-C6-O6
4	C	5	NAG	C4-C5-C6-O6
4	C	7	NAG	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 C



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	H	209/209 (100%)	0.51	19 (9%) 9 9	28, 50, 94, 112	0
2	A	264/267 (98%)	0.27	5 (1%) 66 69	23, 40, 71, 97	0
3	B	99/99 (100%)	0.23	2 (2%) 65 68	25, 45, 77, 90	0
All	All	572/575 (99%)	0.35	26 (4%) 33 36	23, 44, 86, 112	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	296	PHE	9.2
1	H	359	THR	5.0
1	H	420	GLY	4.5
2	A	103	THR	4.0
1	H	361	ASN	4.0
1	H	329	PRO	3.8
1	H	358	MET	3.7
1	H	298	SER	3.6
1	H	327	GLY	3.6
1	H	269	GLU	3.2
1	H	330	SER	3.1
1	H	444	LEU	3.1
1	H	445	GLY	3.1
1	H	299	THR	3.0
3	B	99	MET	3.0
1	H	357	GLU	2.9
3	B	74	GLU	2.8
2	A	102	ASN	2.7
1	H	237	GLY	2.6
1	H	326	LYS	2.6
2	A	145	ASP	2.5
2	A	101	ASP	2.5
1	H	328	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	300	TYR	2.5
1	H	270	ASP	2.2
2	A	172	GLY	2.1

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 (i)

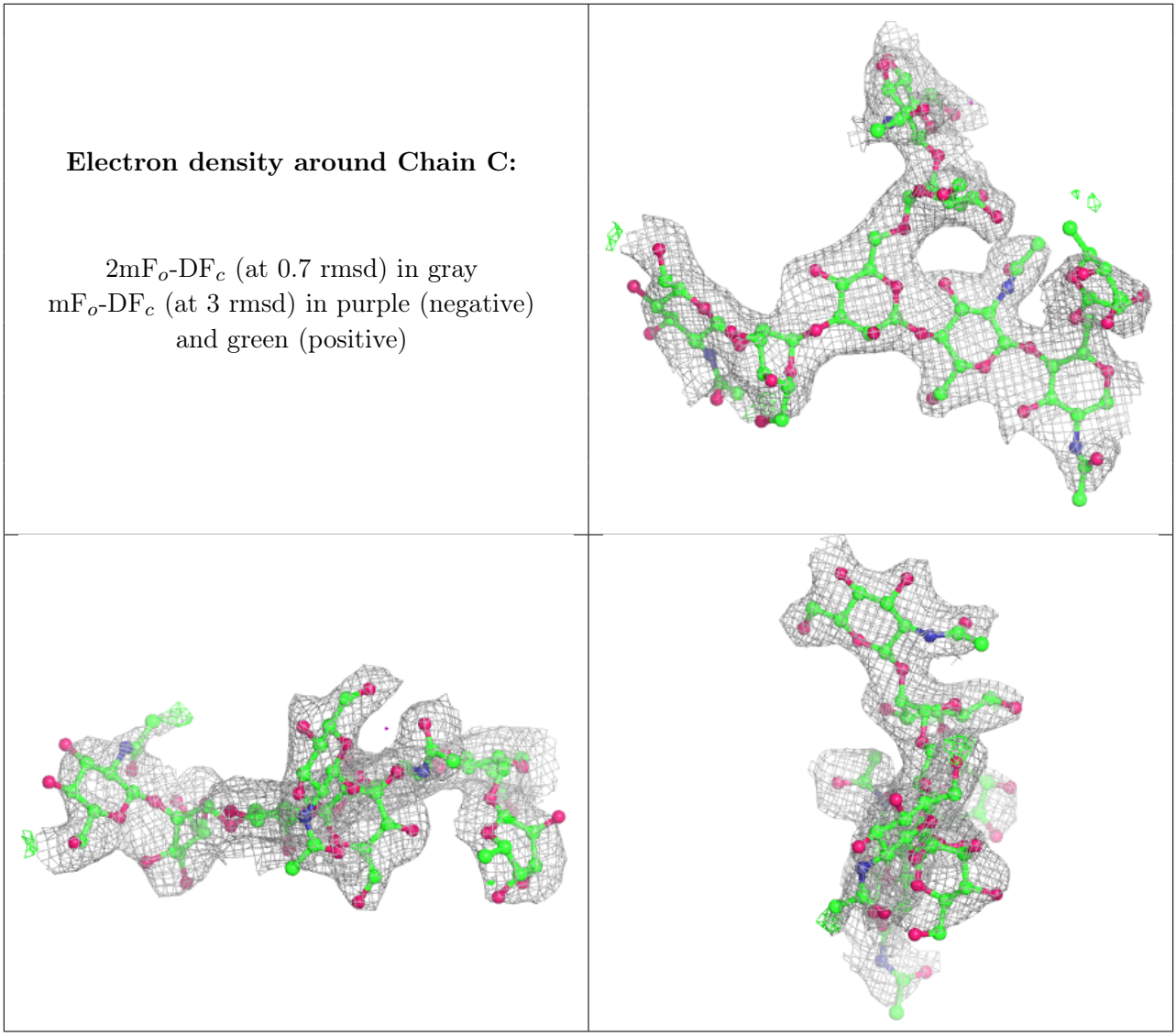
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C	5	14/15	0.72	0.25	67,99,106,111	0
4	NAG	C	1	14/15	0.83	0.29	91,99,102,103	0
4	BMA	C	3	11/12	0.85	0.13	63,71,76,82	0
4	FUL	C	8	10/11	0.87	0.44	58,62,65,65	0
4	NAG	C	7	14/15	0.89	0.15	54,68,74,74	0
4	NAG	C	2	14/15	0.90	0.26	59,71,78,80	0
4	MAN	C	4	11/12	0.93	0.21	83,89,95,96	0
4	MAN	C	6	11/12	0.93	0.16	63,65,68,69	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 C:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.