



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 04:37 AM EDT

PDB ID : 7SHU
Title : IgE-Fc in complex with omalizumab variant C02
Authors : Pennington, L.F.; Jardetzky, T.J.; Kleinboelting, S.
Deposited on : 2021-10-11
Resolution : 2.75 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 : 4.02b-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

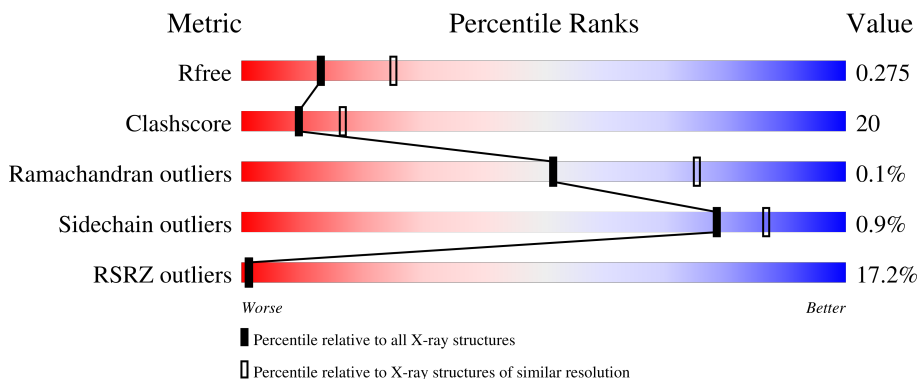
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	C	123	 4% 63% 36% ..
1	E	123	 3% 76% 22% .
2	D	134	 7% 57% 29% 14%
2	F	134	 2% 61% 22% 16%
3	A	220	 46% 37% 37% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	220	
4	G	4	
5	H	3	

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	G	1	-	-	X	-
4	NAG	G	2	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6555 atoms, of which 6 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 omalizumab variant C02 VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	120	Total	C	N	O	S	0	0	0
			932	589	161	179	3			
1	C	122	Total	C	N	O	S	0	0	0
			938	592	163	180	3			

- Molecule 2 is a protein called omalizumab variant C02 VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	112	Total	C	N	O	S	0	0	0
			846	523	140	180	3			
2	D	115	Total	C	N	O	S	0	0	0
			862	533	143	183	3			

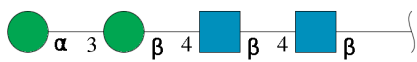
- Molecule 3 is a protein called Immunoglobulin heavy constant epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	203	Total	C	N	O	S	0	0	0
			1578	986	289	297	6			
3	A	166	Total	C	N	O	S	0	0	0
			1271	799	225	241	6			

There are 4 discrepancies between the modelled and reference sequences:

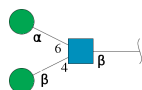
Chain	Residue	Modelled	Actual	Comment	Reference
B	326	GLY	-	expression tag	UNP P01854
B	327	SER	-	expression tag	UNP P01854
A	326	GLY	-	expression tag	UNP P01854
A	327	SER	-	expression tag	UNP P01854

- 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.



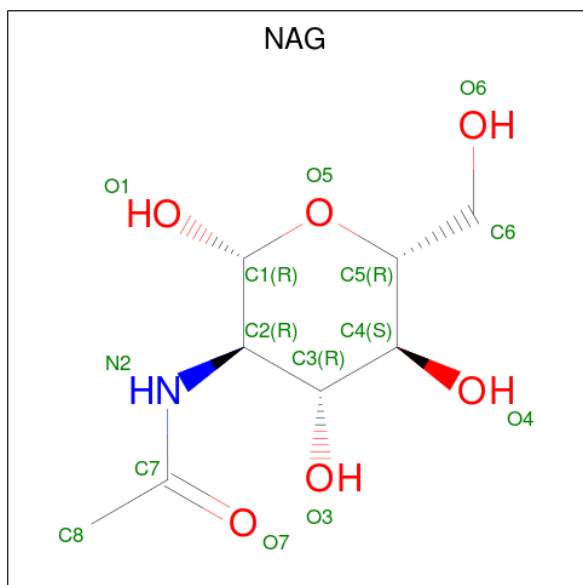
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
4	G	4	50	28	2	20	0	0	0

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



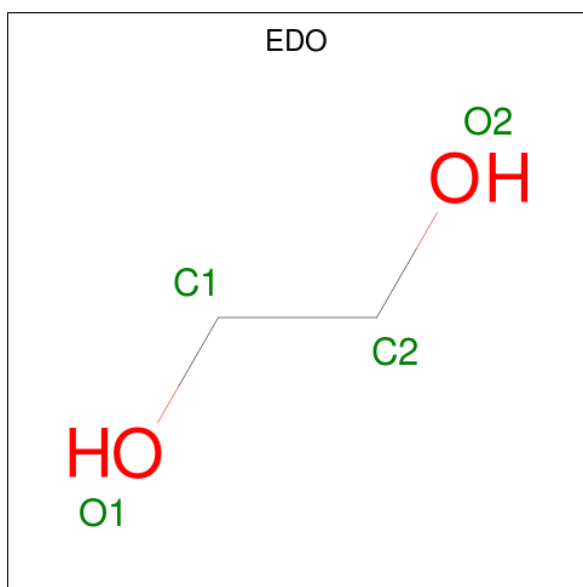
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
5	H	3	36	20	1	15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



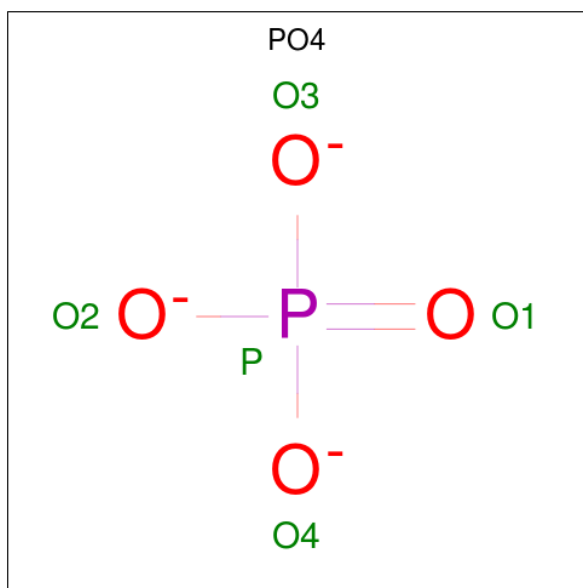
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
6	E	1	14	8	1	5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	E	1	10	2	6	2	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

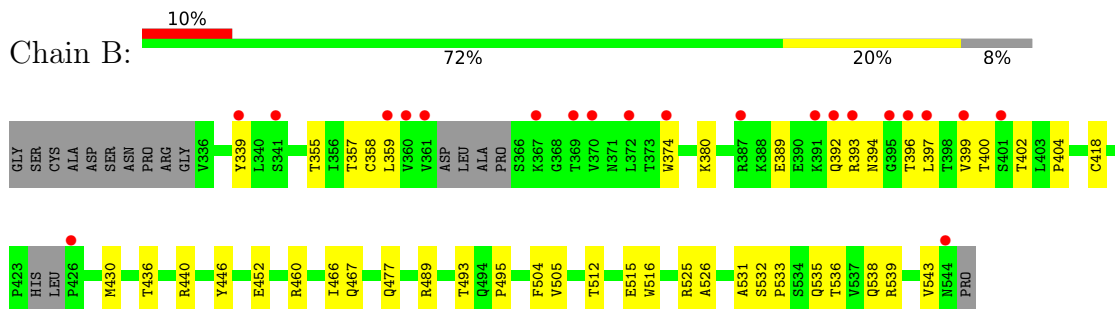


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
8	E	1	5	4	1	0	0

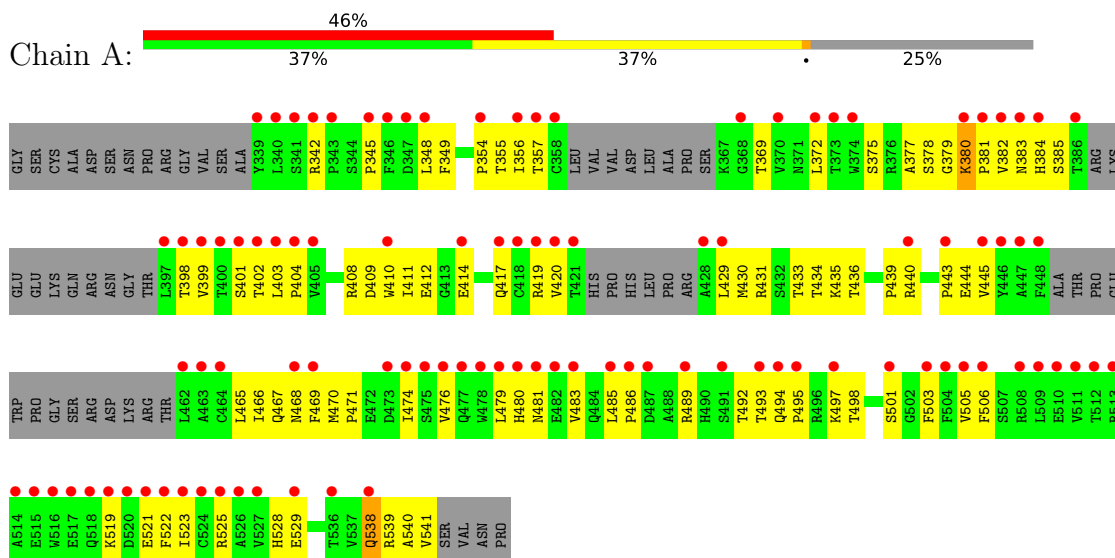
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total O 1 1	0	0
9	F	1	Total O 1 1	0	0
9	B	5	Total O 5 5	0	0
9	C	5	Total O 5 5	0	0
9	A	1	Total O 1 1	0	0

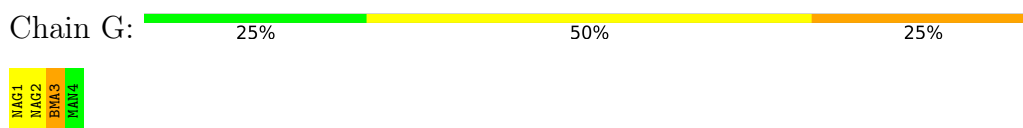
- Molecule 3: Immunoglobulin heavy constant epsilon



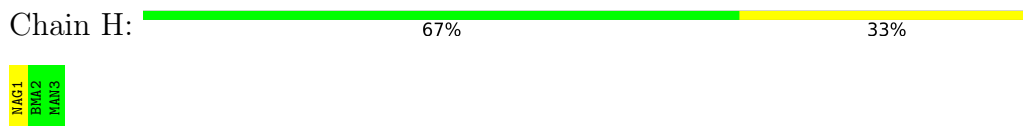
- Molecule 3: Immunoglobulin heavy constant epsilon



- Molecule 4: 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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	90.07Å 176.12Å 142.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.75 49.18 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.19-2.75) 99.9 (49.18-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.220 , 0.275 0.222 , 0.275	Depositor DCC
R_{free} test set	1494 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtrriage
Anisotropy	0.522	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6555	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, EDO, NAG, PO4, MAN

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	C	0.27	0/963	0.45	0/1311
1	E	0.27	0/957	0.46	0/1303
2	D	0.27	0/881	0.46	0/1195
2	F	0.27	0/864	0.46	0/1173
3	A	0.25	0/1296	0.45	0/1761
3	B	0.26	0/1616	0.46	0/2198
All	All	0.26	0/6577	0.46	0/8941

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 [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	C	938	0	885	43	1
1	E	932	0	881	25	0
2	D	862	0	801	34	1
2	F	846	0	795	24	0
3	A	1271	0	1227	101	0
3	B	1578	0	1527	37	0
4	G	50	0	42	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	36	0	31	0	0
6	E	14	0	13	0	0
7	E	4	6	6	0	0
8	E	5	0	0	0	0
9	A	1	0	0	0	0
9	B	5	0	0	0	0
9	C	5	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	6549	6	6208	250	1

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 20.

The worst 5 of 250 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:A:403:LEU:HD12	3:A:404:PRO:HD2	1.24	1.18
3:A:525:ARG:HG2	3:A:538:GLN:HB3	1.28	1.10
3:A:355:THR:HG22	3:A:404:PRO:HA	1.39	1.02
3:A:348:LEU:HD12	3:A:354:PRO:HG3	1.46	0.97
3:A:523:ILE:HA	3:A:540:ALA:HB2	1.45	0.96

All (1) 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)
1:C:44:LYS:NZ	2:D:112:GLY:O[3_455]	2.07	0.13

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	C	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
1	E	118/123 (96%)	114 (97%)	4 (3%)	0	100	100
2	D	113/134 (84%)	108 (96%)	5 (4%)	0	100	100
2	F	110/134 (82%)	106 (96%)	4 (4%)	0	100	100
3	A	156/220 (71%)	141 (90%)	14 (9%)	1 (1%)	25	42
3	B	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
All	All	814/954 (85%)	774 (95%)	39 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	380	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	C	99/101 (98%)	98 (99%)	1 (1%)	76	85
1	E	99/101 (98%)	98 (99%)	1 (1%)	76	85
2	D	95/113 (84%)	95 (100%)	0	100	100
2	F	95/113 (84%)	94 (99%)	1 (1%)	73	84
3	A	138/193 (72%)	135 (98%)	3 (2%)	52	70
3	B	172/193 (89%)	172 (100%)	0	100	100
All	All	698/814 (86%)	692 (99%)	6 (1%)	78	87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	382	VAL
3	A	467	GLN
3	A	538	GLN
2	F	34	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	477	GLN
1	C	82	GLN
3	A	417	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

7 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	G	1	4	14,14,15	0.44	0	17,19,21	0.63	0
4	NAG	G	2	4	14,14,15	0.50	0	17,19,21	0.56	0
4	BMA	G	3	4	11,11,12	0.84	1 (9%)	15,15,17	0.93	0
4	MAN	G	4	4	11,11,12	0.77	0	15,15,17	0.88	0
5	NAG	H	1	5,1	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
5	BMA	H	2	5	11,11,12	0.71	0	15,15,17	0.79	0
5	MAN	H	3	5	11,11,12	0.79	0	15,15,17	0.92	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
4	NAG	G	1	4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	BMA	H	2	5	-	0/2/19/22	0/1/1/1
5	MAN	H	3	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)
4	G	3	BMA	C1-C2	2.50	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

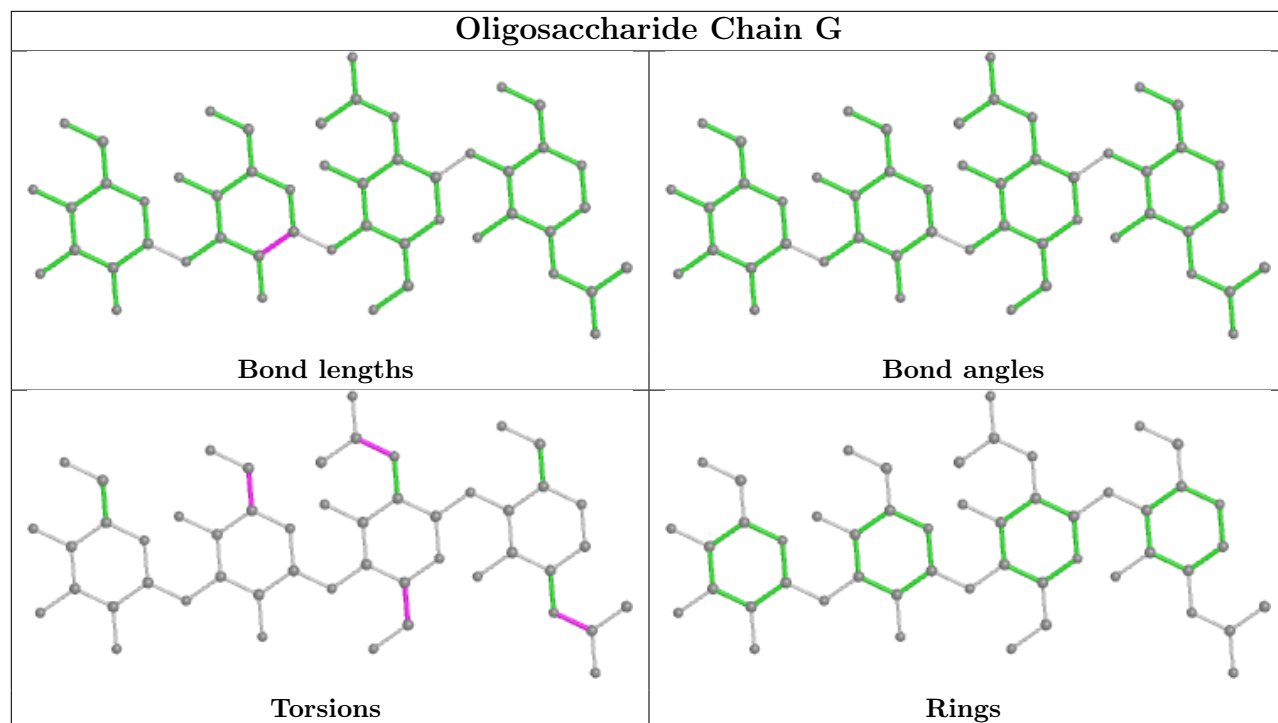
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
5	H	3	MAN	O5-C5-C6-O6

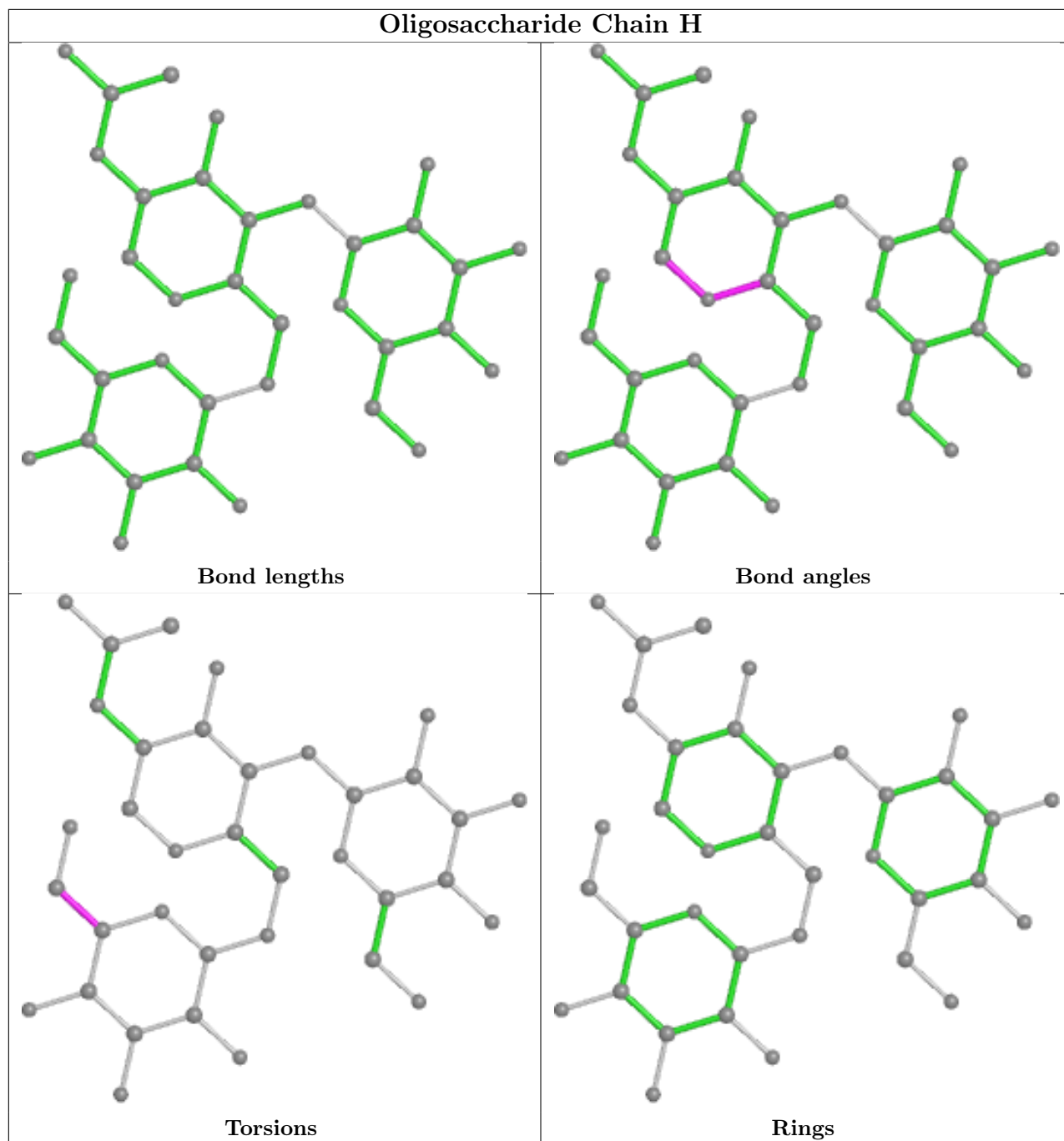
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	4	0
4	G	3	BMA	3	0
4	G	1	NAG	7	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](#)

3 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
6	NAG	E	201	1	14,14,15	0.46	0	17,19,21	0.52	0
7	EDO	E	202	-	3,3,3	0.48	0	2,2,2	0.31	0
8	PO4	E	203	-	4,4,4	1.03	0	6,6,6	0.57	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
6	NAG	E	201	1	-	0/6/23/26	0/1/1/1
7	EDO	E	202	-	-	0/1/1/1	-

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 [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](#)

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	C	122/123 (99%)	0.79	5 (4%) 37 44	57, 90, 134, 142	0
1	E	120/123 (97%)	0.77	4 (3%) 46 54	52, 80, 119, 170	0
2	D	115/134 (85%)	1.01	10 (8%) 10 12	59, 86, 126, 189	0
2	F	112/134 (83%)	0.54	3 (2%) 54 63	52, 73, 106, 123	0
3	A	166/220 (75%)	2.81	101 (60%) 0 0	89, 147, 198, 220	0
3	B	203/220 (92%)	1.00	21 (10%) 6 7	51, 80, 151, 212	0
All	All	838/954 (87%)	1.23	144 (17%) 1 1	51, 88, 170, 220	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	522	PHE	12.8
3	A	356	ILE	10.8
3	A	419	ARG	9.8
3	A	518	GLN	8.7
3	A	511	VAL	8.1

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

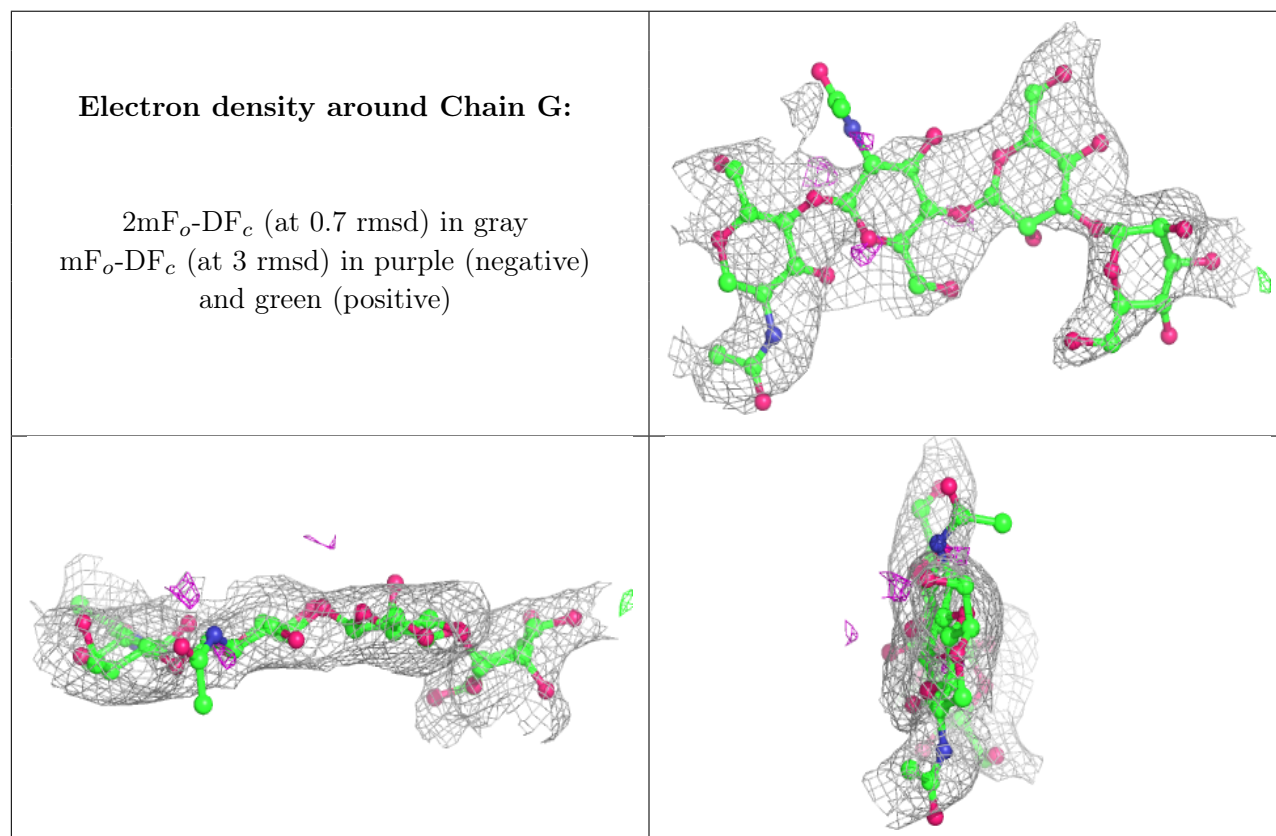
There are no non-standard protein/DNA/RNA residues in this entry.

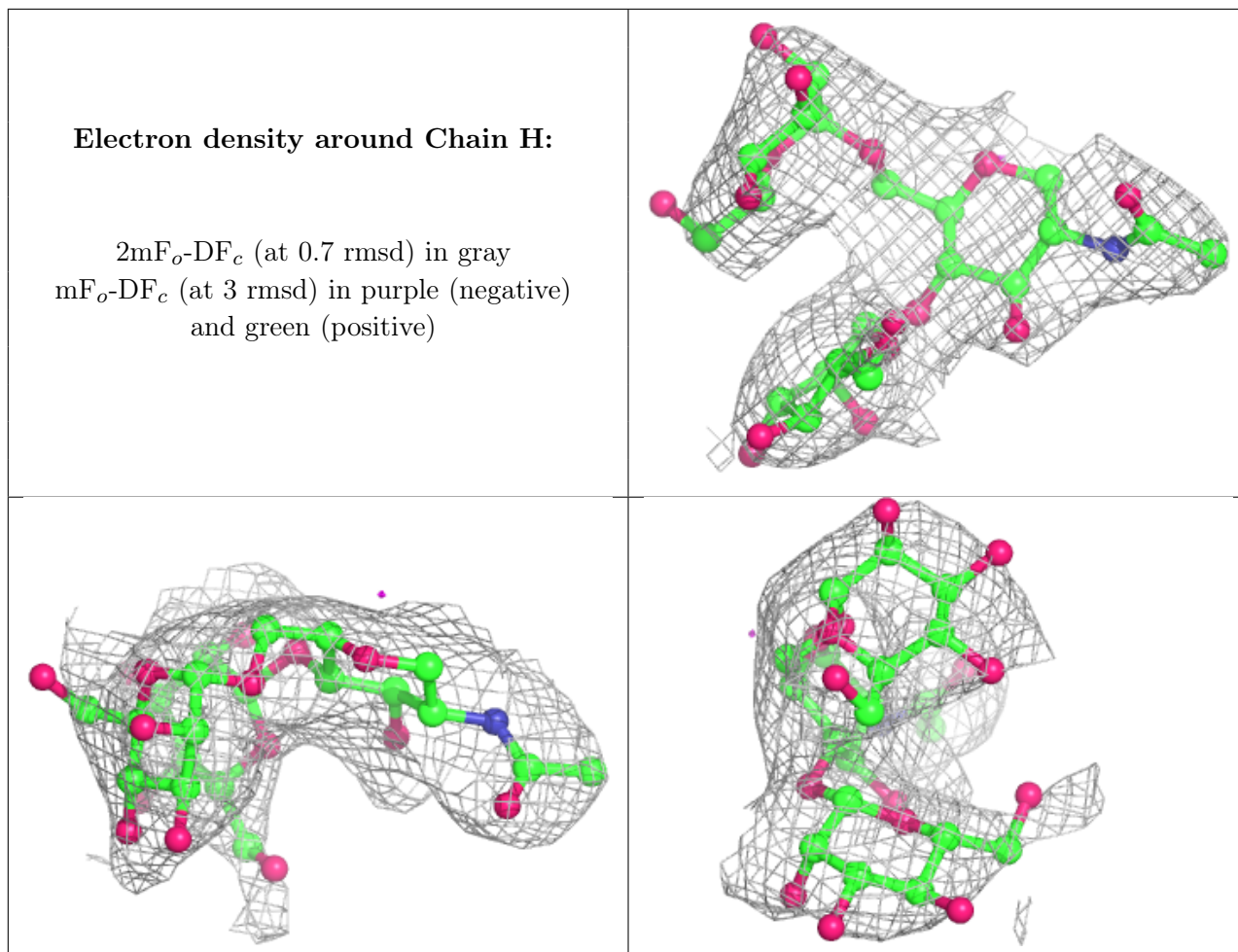
6.3 Carbohydrates [i](#)

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, 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
4	NAG	G	1	14/15	0.55	0.34	124,147,150,151	0
4	MAN	G	4	11/12	0.57	0.28	130,139,144,146	0
4	BMA	G	3	11/12	0.60	0.32	92,133,144,146	0
4	NAG	G	2	14/15	0.73	0.41	128,145,152,153	0
5	BMA	H	2	11/12	0.82	0.18	125,133,143,157	0
5	MAN	H	3	11/12	0.89	0.16	112,123,129,129	0
5	NAG	H	1	14/15	0.92	0.17	66,86,101,108	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.





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(Å ²)	Q<0.9
6	NAG	E	201	14/15	0.84	0.17	69,97,103,109	0
7	EDO	E	202	4/4	0.86	0.23	76,92,96,96	0
8	PO4	E	203	5/5	0.89	0.47	170,173,191,205	0

6.5 Other polymers [i](#)

There are no such residues in this entry.