



wwPDB X-ray Structure Validation Summary Report

Oct 4, 2023 – 10:00 PM EDT

PDB ID : 6UQR
Title : Complex of IgE and Ligelizumab
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Deposited on : 2019-10-21
Resolution : 3.65 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 3.65 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6822 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 Ligelizumab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	Total 1738	C 1102	N 284	O 344	S 8	0	0	0
1	C	221	Total 1691	C 1075	N 276	O 333	S 7	0	0	0

- Molecule 2 is a protein called IgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	Total 1643	C 1027	N 299	O 311	S 6	0	0	0
2	D	212	Total 1639	C 1025	N 299	O 309	S 6	0	0	0

There are 58 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

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

- Molecule 3 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
			Total	C	N	O			
3	E	5	61	34	2	25	0	0	0

- 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	F	4	50	28	2	20	0	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.96Å 103.18Å 124.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.65	Depositor
% Data completeness (in resolution range)	99.9 (19.95-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.290 , 0.295	Depositor
Wilson B-factor (Å ²)	112.2	Xtrriage
Anisotropy	0.313	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

9 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	E	1	3,2	14,14,15	0.57	0	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.33	1 (5%)
3	BMA	E	3	3	11,11,12	1.33	1 (9%)	15,15,17	1.46	2 (13%)
3	MAN	E	4	3	11,11,12	1.40	2 (18%)	15,15,17	1.29	2 (13%)
3	MAN	E	5	3	11,11,12	1.37	2 (18%)	15,15,17	1.31	2 (13%)
4	NAG	F	1	4,2	14,14,15	1.20	1 (7%)	17,19,21	1.53	2 (11%)
4	NAG	F	2	4	14,14,15	0.14	0	17,19,21	0.50	0
4	BMA	F	3	4	11,11,12	1.51	3 (27%)	15,15,17	1.49	4 (26%)
4	MAN	F	4	4	11,11,12	1.53	3 (27%)	15,15,17	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	1/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	4.36	1.50	1.43
3	E	4	MAN	C1-C2	3.15	1.59	1.52
3	E	3	BMA	O5-C1	-3.10	1.38	1.43
4	F	3	BMA	O5-C5	-2.96	1.37	1.43
3	E	2	NAG	O5-C1	2.79	1.48	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	4.94	118.88	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	4.81	118.72	112.19
3	E	3	BMA	C1-O5-C5	3.07	116.35	112.19
4	F	1	NAG	C2-N2-C7	2.74	126.81	122.90
3	E	4	MAN	C1-C2-C3	2.69	112.97	109.67

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

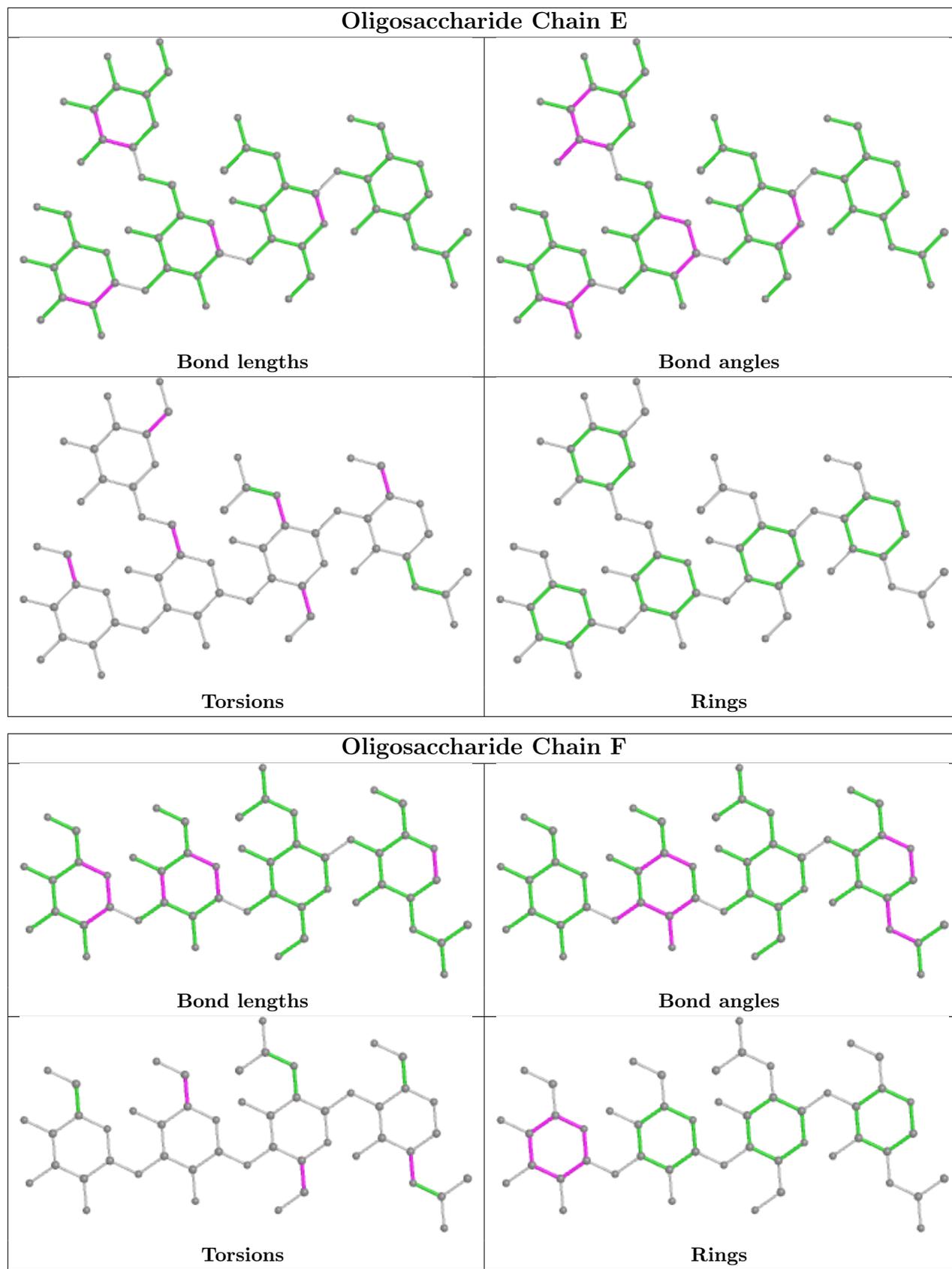
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C3-C2-N2-C7
3	E	3	BMA	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	4	MAN	C1-C2-C3-C4-C5-O5

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.



4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.