Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:37 PM EDT

PDB ID	:	6OEL
Title	:	Engineered Fab bound to IL-4 receptor
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Deposited on	:	2019-03-27
Resolution	:	3.10 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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 9 unique types of molecules in this entry. The entry contains 7209 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 engineered Interleukin-4, RGA variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	988	621	180	180	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	LYS	engineered mutation	UNP P05112
A	118	VAL	THR	engineered mutation	UNP P05112
A	121	GLN	ARG	engineered mutation	UNP P05112
A	122	SER	GLU	engineered mutation	UNP P05112
A	124	TRP	TYR	engineered mutation	UNP P05112
A	125	PHE	SER	engineered mutation	UNP P05112
A	128	GLY	SER	engineered mutation	UNP P05112
A	129	ALA	SER	engineered mutation	UNP P05112

- Molecule 2 is a protein called Interleukin-4 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	199	1581	1009	263	299	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP P24394
B	-1	ASP	-	expression tag	UNP P24394
B	0	PRO	-	expression tag	UNP P24394
B	1	PHE	-	expression tag	UNP P24394

- Molecule 3 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	160	1285	824	227	226	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	53	GLN	ASN	engineered mutation	UNP P31785

- Molecule 4 is a protein called engineered Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	223	1643	1031	278	328	6	0	0	0

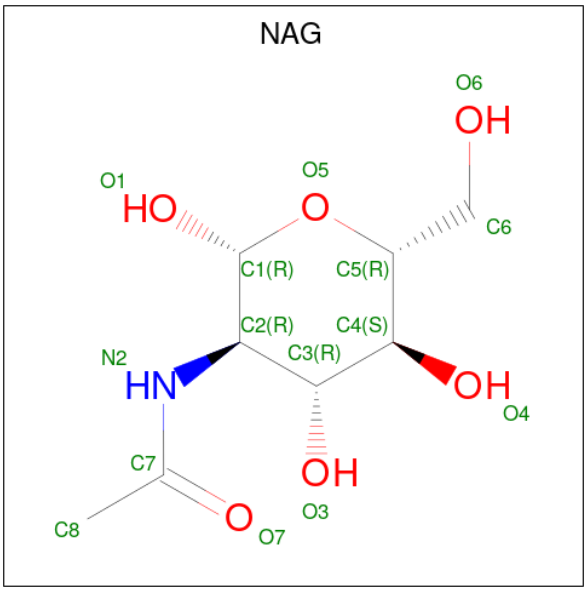
- Molecule 5 is a protein called engineered Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	213	1594	999	266	325	4	0	0	0

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

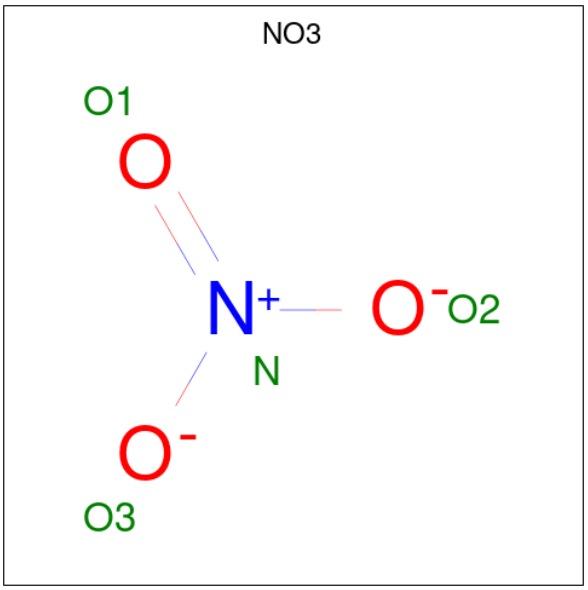
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	D	2	24	14	1	9	0	0	0

- Molecule 7 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		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0

- Molecule 8 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
8	H	1	4	1	3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	B	6	6	6	0	0
			Total	O		
9	C	1	1	1	0	0
			Total	O		
9	H	9	9	9	0	0
			Total	O		
9	L	4	4	4	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	328.10Å 328.10Å 328.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.14 – 3.10	Depositor
% Data completeness (in resolution range)	95.1 (63.14-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.199 , 0.256	Depositor
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7209	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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.

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)

2 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	$\#\|Z\| > 2$
6	NAG	D	1	2,6	14,14,15	0.30	0	17,19,21	0.50	0
6	FUC	D	2	6	10,10,11	0.76	0	14,14,16	0.76	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	D	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	D	2	6	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

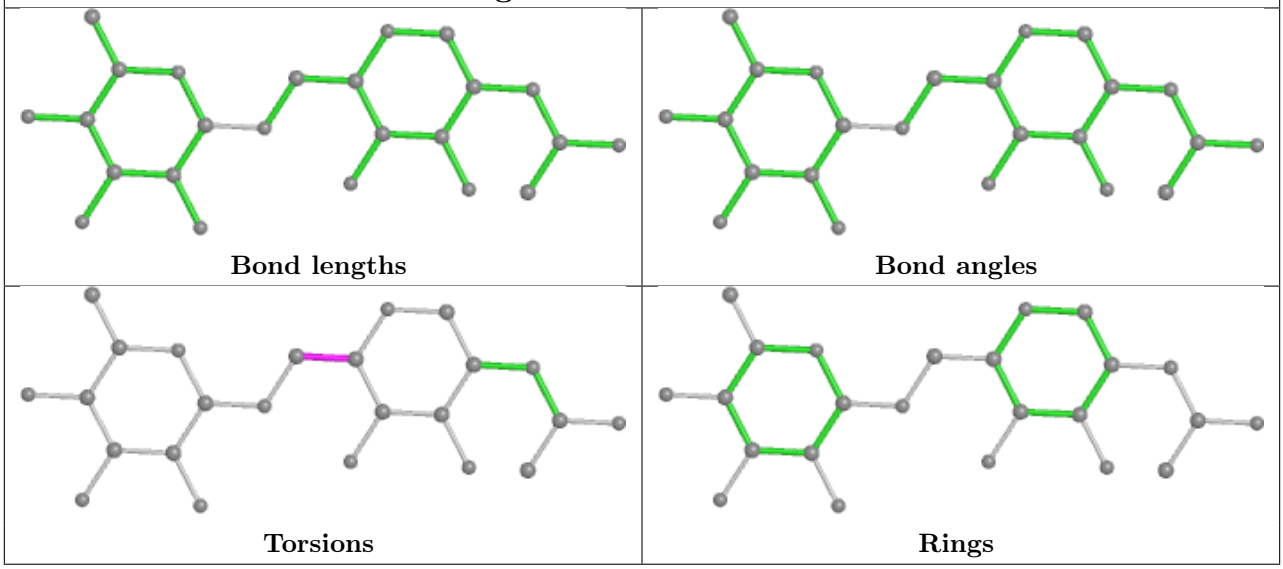
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6

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 D



4.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
8	NO3	H	301	-	1,3,3	0.62	0	0,3,3	-	-
7	NAG	B	201	2	14,14,15	0.38	0	17,19,21	0.51	0
7	NAG	C	301	3	14,14,15	0.29	0	17,19,21	0.48	0
7	NAG	B	206	2	14,14,15	0.23	0	17,19,21	0.38	0
7	NAG	B	204	2	14,14,15	0.29	0	17,19,21	0.40	0
7	NAG	B	205	2	14,14,15	0.31	0	17,19,21	0.47	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
7	NAG	B	201	2	-	2/6/23/26	0/1/1/1
7	NAG	C	301	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	206	2	-	0/6/23/26	0/1/1/1
7	NAG	B	204	2	-	2/6/23/26	0/1/1/1
7	NAG	B	205	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	204	NAG	O5-C5-C6-O6
7	B	204	NAG	C4-C5-C6-O6
7	B	201	NAG	O5-C5-C6-O6
7	B	201	NAG	C4-C5-C6-O6
7	C	301	NAG	O5-C5-C6-O6
7	C	301	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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