Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 12:57 PM EDT

PDB ID	:	6NG3
Title	:	Crystal structure of human CD160 and HVEM complex
Authors	:	Liu, W.; Bonanno, J.; Almo, S.C.
Deposited on	:	2018-12-21
Resolution	:	2.88 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 2.88 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 1616 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 CD160 antigen,Tumor necrosis factor receptor superfamily member 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	1537	945	274	294	24	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1019	GLY	-	linker	UNP O95971
A	1020	GLY	-	linker	UNP O95971
A	1021	GLY	-	linker	UNP O95971
A	1022	GLY	-	linker	UNP O95971
A	1023	SER	-	linker	UNP O95971
A	1024	GLY	-	linker	UNP O95971
A	1025	GLY	-	linker	UNP O95971
A	1026	GLY	-	linker	UNP O95971
A	1027	GLY	-	linker	UNP O95971
A	1028	SER	-	linker	UNP O95971
A	1029	GLY	-	linker	UNP O95971
A	1030	GLY	-	linker	UNP O95971
A	1031	GLY	-	linker	UNP O95971
A	1032	GLY	-	linker	UNP O95971
A	1033	SER	-	linker	UNP O95971
A	1034	GLY	-	linker	UNP O95971
A	1035	GLY	-	linker	UNP O95971
A	1036	GLY	-	linker	UNP O95971
A	1037	GLY	-	linker	UNP O95971
A	1038	SER	-	linker	UNP O95971
A	1144	GLY	-	expression tag	UNP Q92956
A	1145	HIS	-	expression tag	UNP Q92956
A	1146	HIS	-	expression tag	UNP Q92956
A	1147	HIS	-	expression tag	UNP Q92956
A	1148	HIS	-	expression tag	UNP Q92956
A	1149	HIS	-	expression tag	UNP Q92956

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1150	HIS	-	expression tag	UNP Q92956

- Molecule 2 is an oligosaccharide called beta-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			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is an oligosaccharide called 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	C	2	28	16	2	10	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	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	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.93Å 87.93Å 157.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.88	Depositor
% Data completeness (in resolution range)	99.5 (20.00-2.88)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.234 , 0.274	Depositor
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.081	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1616	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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.

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)

6 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	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.64	0	17,19,21	1.66	3 (17%)
2	NAG	B	2	2	14,14,15	0.45	0	17,19,21	1.04	2 (11%)
2	BMA	B	3	2	11,11,12	0.42	0	15,15,17	1.69	3 (20%)
2	BMA	B	4	2	11,11,12	0.71	0	15,15,17	1.66	6 (40%)
3	NAG	C	1	3,1	14,14,15	0.67	0	17,19,21	2.37	6 (35%)
3	NAG	C	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.49	3 (17%)

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
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	BMA	B	4	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.10	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-C2-N2	5.38	119.67	110.49
3	C	1	NAG	O5-C1-C2	-4.44	104.27	111.29
2	B	3	BMA	C1-O5-C5	4.24	117.93	112.19
2	B	1	NAG	O5-C1-C2	-3.98	105.00	111.29
3	C	2	NAG	C4-C3-C2	3.81	116.60	111.02
3	C	1	NAG	C4-C3-C2	-3.77	105.50	111.02
3	C	1	NAG	C1-O5-C5	3.27	116.63	112.19
2	B	1	NAG	C1-O5-C5	3.12	116.42	112.19
2	B	4	BMA	O3-C3-C2	2.87	115.48	109.99
3	C	2	NAG	C1-O5-C5	2.80	115.98	112.19
3	C	1	NAG	C3-C4-C5	-2.62	105.56	110.24
2	B	4	BMA	O5-C1-C2	-2.47	106.95	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C2-N2-C7	2.39	126.31	122.90
2	B	1	NAG	C3-C4-C5	-2.37	106.02	110.24
2	B	3	BMA	O3-C3-C2	-2.37	105.47	109.99
3	C	1	NAG	O3-C3-C4	2.27	115.60	110.35
2	B	3	BMA	C3-C4-C5	2.27	114.28	110.24
2	B	4	BMA	C1-O5-C5	2.21	115.19	112.19
2	B	4	BMA	O2-C2-C3	2.15	114.44	110.14
2	B	2	NAG	C4-C3-C2	2.13	114.14	111.02
2	B	4	BMA	O3-C3-C4	-2.03	105.66	110.35
2	B	4	BMA	C6-C5-C4	-2.02	108.27	113.00
2	B	2	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

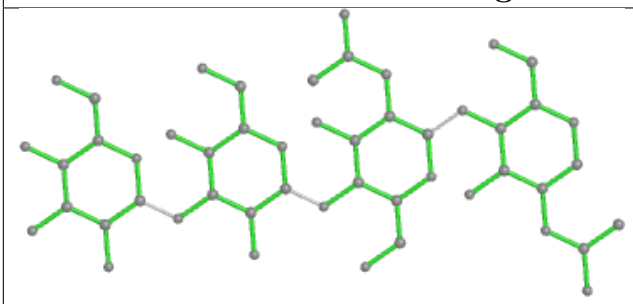
There are no ring outliers.

1 monomer is involved in 1 short contact:

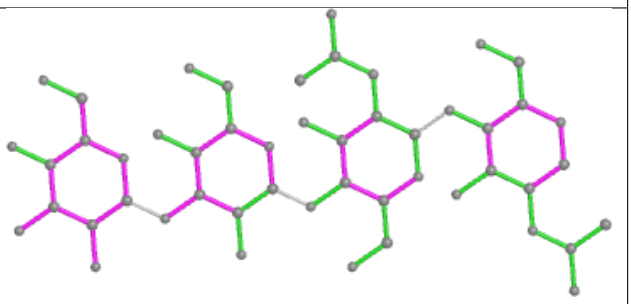
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BMA	0	1

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

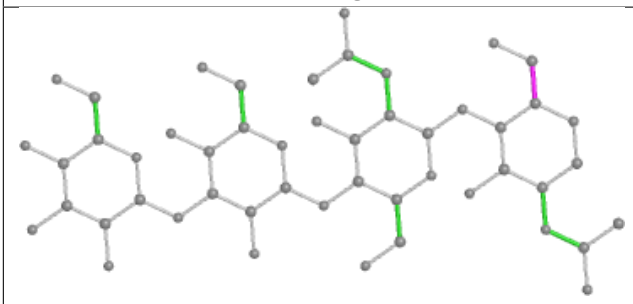
Oligosaccharide Chain B



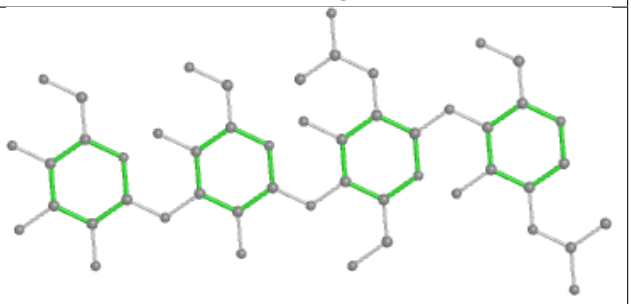
Bond lengths



Bond angles

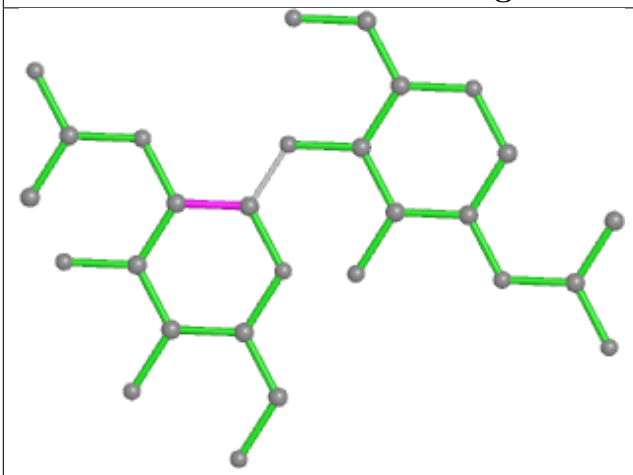


Torsions

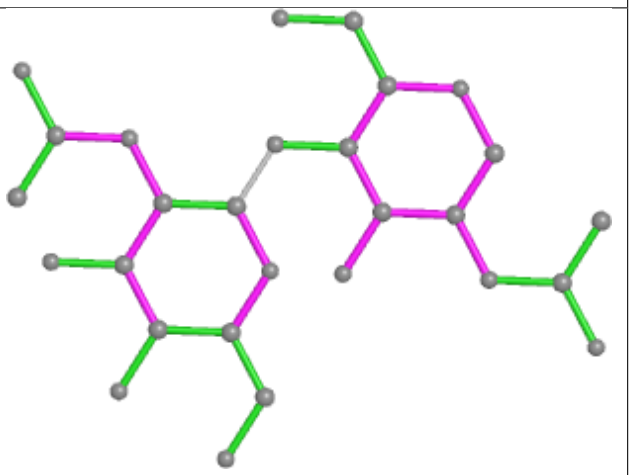


Rings

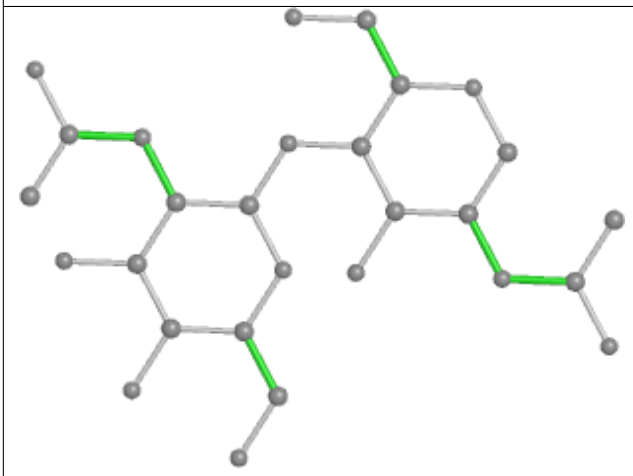
Oligosaccharide Chain C



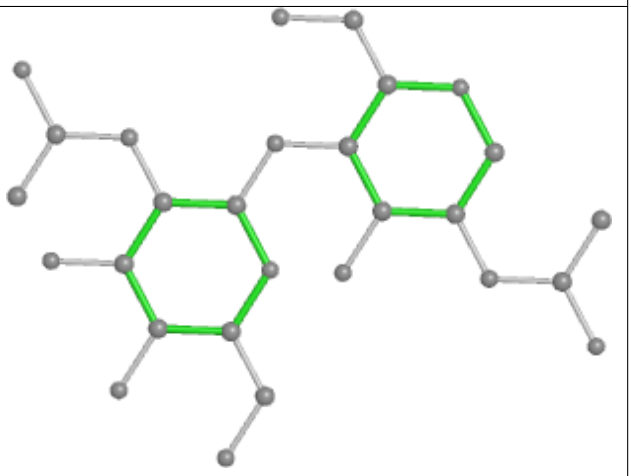
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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.

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.