

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 03:53 AM EDT

PDB ID : 6V80

Title: Crystal structure of human CD1d presenting alpha-Galactosylceramide in

complex with NKT12 TCR and VHH nanobody 1D12

Authors : Shahine, A.; Rossjohn, J.

Deposited on : 2019-12-10

Resolution : 3.53 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 (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 : FAILED

Mogul : 1.8.5 (274361), CSD as 541 be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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 3.53 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 8 unique types of molecules in this entry. The entry contains 14208 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	274	Total 2130	C 1362	11	O 389	S 7	0	0	0
1	F	270		C 1327		O 376	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
F	4	MET	-	initiating methionine	UNP P15813

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	B	98	Total	С	N	О	S	0	0	0
	Б	90	743	477	116	148	2	0	U	0
2	С	94	Total	С	N	О	S	0	0	0
	G	94	745	473	126	144	2	0	0	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called T cell receptor alpha variable 10, nkt tcr alpha chain fusion.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	C	198	Total	С	N	О	S	0	0	0
3		196	1514	937	256	312	9	0	U	U
2	П	181	Total	С	N	О	S	0	0	0
3	11	101	1376	844	237	287	8	0		U



Thorn one 1	disarananaias	hotrmon	the modelled	and	reference sequences:
There are 4	discrepancies	perween	me modened	and	reference sequences.

Chain	Residue	Modelled	Actual	Comment	Reference
С	1	HIS	-	expression tag	UNP A0A0B4J240
С	2	MET	-	expression tag	UNP A0A0B4J240
Н	1	HIS	-	expression tag	UNP A0A0B4J240
Н	2	MET	-	expression tag	UNP A0A0B4J240

• Molecule 4 is a protein called nkt tcr beta chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
4	D	240	Total	С	N	О	S	0	0	0
4	Ъ	240	1848	1166	317	357	8	0	0	U
4	т	237	Total	С	N	О	S	0	0	0
4	1	231	1888	1190	327	363	8	0	U	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	92	THR	SER	linker	UNP K7N5M4
D	93	SER	GLU	linker	UNP K7N5M4
D	94	ARG	ASN	linker	UNP K7N5M4
D	95	ARG	SER	linker	UNP K7N5M4
D	97	SER	THR	linker	UNP K7N5M4
D	?	-	GLY	deletion	UNP K7N5M4
D	?	-	ARG	deletion	UNP K7N5M4
D	?	-	ILE	deletion	UNP K7N5M4
I	92	THR	SER	linker	UNP K7N5M4
I	93	SER	GLU	linker	UNP K7N5M4
I	94	ARG	ASN	linker	UNP K7N5M4
I	95	ARG	SER	linker	UNP K7N5M4
I	97	SER	THR	linker	UNP K7N5M4
I	?	-	GLY	deletion	UNP K7N5M4
I	?	-	ARG	deletion	UNP K7N5M4
I	?	-	ILE	deletion	UNP K7N5M4

• Molecule 5 is a protein called Nanobody VHH ID12.

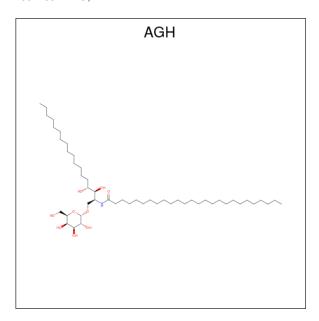
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	E	117	Total 851	C 529		O 174	S 4	0	0	0
5	J	118	Total 834	C 522		O 168	S 4	0	1	0



• Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	K	2	Total C N O 28 16 2 10	0	0	0
6	L	2	Total C N O 28 16 2 10	0	0	0

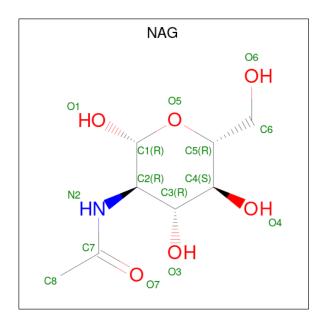
• Molecule 7 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (three-letter code: AGH) (formula: $C_{50}H_{99}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 60				7	0
7	F	1	Total 60	C 50		O 9	16	0

• Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total 14				0	0
8	F	1	Total 14	C 8		O 5	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	C 1 2 1	Depositor
Cell constants	210.67Å 165.25Å 84.50Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.63 - 3.53	Depositor
% Data completeness	100.0 (82.63-3.53)	Depositor
(in resolution range)		_
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.76 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.254	Depositor
Wilson B-factor (Å ²)	104.5	Xtriage
Anisotropy	0.327	Xtriage
L-test for twinning ²	$< L >=0.36, < L^2>=0.19$	Xtriage
Estimated twinning fraction	0.297 for -h,-k,l	Xtriage
Reported twinning fraction	0.390 for -h,-k,l	Depositor
Outliers	0 of 35558 reflections	Xtriage
Total number of atoms	14208	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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)

4 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	Tuno	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	K	1	6,1	14,14,15	0.47	0	17,19,21	0.69	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.28	0
6	NAG	L	1	6,1	14,14,15	1.48	4 (28%)	17,19,21	3.88	8 (47%)
6	NAG	L	2	6	14,14,15	0.69	0	17,19,21	1.99	6 (35%)

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	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
6	L	1	NAG	O5-C1	-2.64	1.39	1.43
6	L	1	NAG	C2-N2	-2.35	1.42	1.46
6	L	1	NAG	C4-C5	-2.04	1.48	1.53
6	L	1	NAG	C1-C2	-2.02	1.49	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	L	1	NAG	C2-N2-C7	-11.12	107.06	122.90
6	L	1	NAG	C6-C5-C4	-6.43	97.95	113.00
6	L	1	NAG	O3-C3-C4	-5.10	98.56	110.35
6	L	2	NAG	O5-C5-C6	4.86	114.83	107.20
6	L	1	NAG	O4-C4-C3	4.19	120.05	110.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C3-C2-N2-C7
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2

Continued on next page...



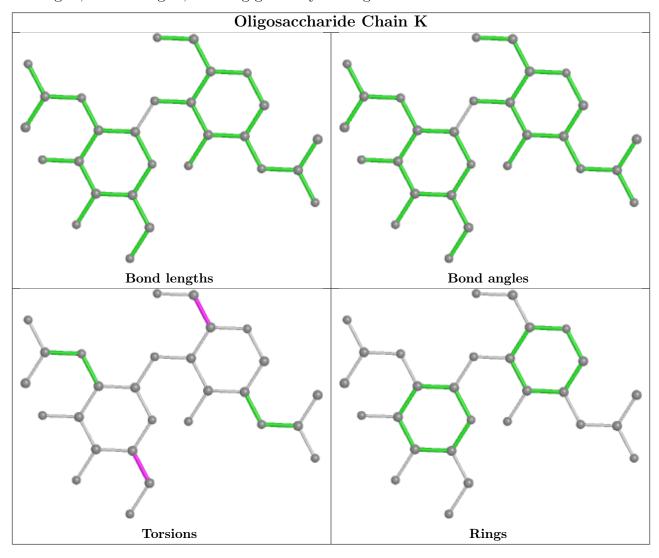
Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	2	NAG	C8-C7-N2-C2
6	K	1	NAG	O5-C5-C6-O6

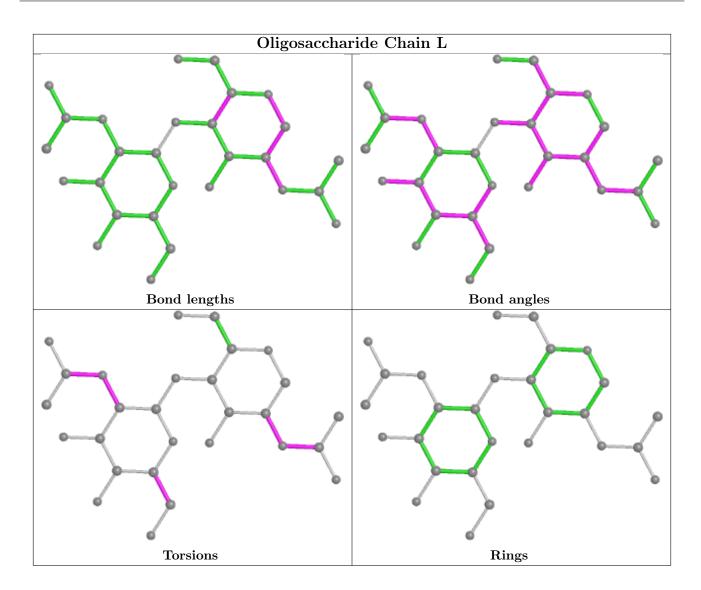
There are no ring outliers.

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.







4.6 Ligand geometry (i)

4 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	Mol Type Chain Res Link			Link	Bo	ond leng	$ ag{ths}$	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	AGH	A	401	-	60,60,60	1.40	5 (8%)	65,69,69	1.02	4 (6%)
8	NAG	F	404	1	14,14,15	0.76	0	17,19,21	1.55	4 (23%)
7	AGH	F	401	-	60,60,60	1.38	5 (8%)	65,69,69	1.15	4 (6%)



	Mol	Mol Type Chain Res		Res Link		Bo	ond leng	ths	Bond angles		
	MIOI	туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	8	NAG	F	405	1	14,14,15	1.10	2 (14%)	17,19,21	3.02	6 (35%)

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	AGH	A	401	-	-	15/58/78/78	0/1/1/1
8	NAG	F	404	1	-	4/6/23/26	0/1/1/1
7	AGH	F	401	-	-	22/58/78/78	0/1/1/1
8	NAG	F	405	1	-	5/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{A})$	Ideal(Å)
7	A	401	AGH	CAA-N2	7.02	1.49	1.34
7	F	401	AGH	CAA-N2	6.96	1.48	1.34
7	F	401	AGH	O1A-C1	-3.08	1.38	1.43
7	A	401	AGH	O1A-C1	-2.98	1.38	1.43
7	A	401	AGH	CAB-CAA	2.78	1.56	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
8	F	405	NAG	C1-O5-C5	7.61	122.50	112.19
8	F	405	NAG	O5-C1-C2	-6.09	101.66	111.29
8	F	405	NAG	C1-C2-N2	-4.26	103.20	110.49
8	F	405	NAG	C2-N2-C7	-3.98	117.23	122.90
7	F	401	AGH	C6-C5-C4	-3.67	108.15	114.18

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	AGH	O1A-C1-C2-C3
7	F	401	AGH	N2-C2-C3-O3
8	F	404	NAG	C8-C7-N2-C2
8	F	404	NAG	O7-C7-N2-C2
8	F	405	NAG	C3-C2-N2-C7

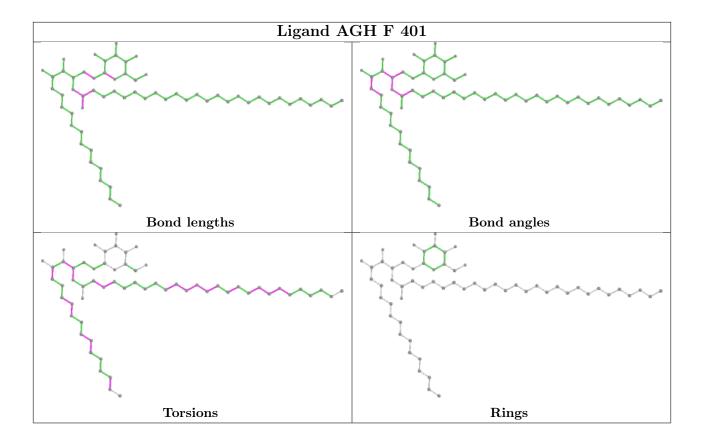


There are no ring outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

