Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 05:17 AM EDT

PDB ID	:	6MP1
Title	:	Crystal structures of the murine class I major histocompatibility complex H-2Db in complex with the mutant TRP1-K8 peptide
Authors	:	Clancy-Thompson, E.; Devlin, C.A.; Birnbaum, M.E.; Dougan, S.K.
Deposited on	:	2018-10-05
Resolution	:	2.21 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 2.21 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 3 unique types of molecules in this entry. The entry contains 3225 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 TRP1-K8 peptide, Beta-2-microglobulin,H-2 class I histocompatibility antigen, D-B alpha chain, chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3139	1985	550	588	16	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	LYS	TYR	engineered mutation	UNP P07147
A	9	MET	ALA	engineered mutation	UNP P07147
A	10	GLY	-	linker	UNP P07147
A	987	GLY	-	linker	UNP P07147
A	988	GLY	-	linker	UNP P07147
A	989	GLY	-	linker	UNP P07147
A	990	SER	-	linker	UNP P07147
A	991	GLY	-	linker	UNP P07147
A	992	GLY	-	linker	UNP P07147
A	993	GLY	-	linker	UNP P07147
A	994	GLY	-	linker	UNP P07147
A	995	SER	-	linker	UNP P07147
A	996	GLY	-	linker	UNP P07147
A	997	GLY	-	linker	UNP P07147
A	998	GLY	-	linker	UNP P07147
A	999	GLY	-	linker	UNP P07147
A	1000	SER	-	linker	UNP P07147
A	1981	GLY	-	linker	UNP P01887
A	1982	GLY	-	linker	UNP P01887
A	1983	GLY	-	linker	UNP P01887
A	1984	GLY	-	linker	UNP P01887
A	1985	SER	-	linker	UNP P01887
A	1986	GLY	-	linker	UNP P01887
A	1987	GLY	-	linker	UNP P01887
A	1988	GLY	-	linker	UNP P01887
A	1989	GLY	-	linker	UNP P01887

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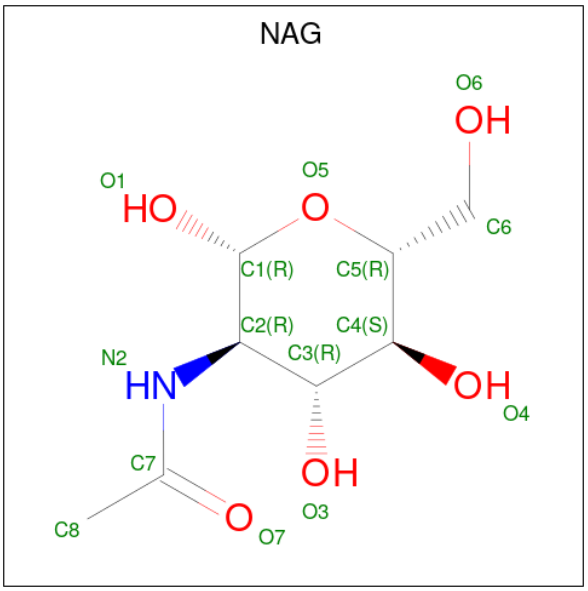
Chain	Residue	Modelled	Actual	Comment	Reference
A	1990	SER	-	linker	UNP P01887
A	1991	GLY	-	linker	UNP P01887
A	1992	GLY	-	linker	UNP P01887
A	1993	GLY	-	linker	UNP P01887
A	1994	GLY	-	linker	UNP P01887
A	1995	SER	-	linker	UNP P01887
A	1996	GLY	-	linker	UNP P01887
A	1997	GLY	-	linker	UNP P01887
A	1998	GLY	-	linker	UNP P01887
A	1999	GLY	-	linker	UNP P01887
A	2000	SER	-	linker	UNP P01887
A	2084	ALA	TYR	engineered mutation	UNP P01899
A	2277	ALA	-	expression tag	UNP P01899
A	2278	ALA	-	expression tag	UNP P01899
A	2279	ALA	-	expression tag	UNP P01899
A	2280	GLY	-	expression tag	UNP P01899
A	2281	GLY	-	expression tag	UNP P01899
A	2282	GLY	-	expression tag	UNP P01899
A	2283	LEU	-	expression tag	UNP P01899
A	2284	ASN	-	expression tag	UNP P01899
A	2285	ASP	-	expression tag	UNP P01899
A	2286	ILE	-	expression tag	UNP P01899
A	2287	PHE	-	expression tag	UNP P01899
A	2288	GLU	-	expression tag	UNP P01899
A	2289	ALA	-	expression tag	UNP P01899
A	2290	GLN	-	expression tag	UNP P01899
A	2291	LYS	-	expression tag	UNP P01899
A	2292	ILE	-	expression tag	UNP P01899
A	2293	GLU	-	expression tag	UNP P01899
A	2294	TRP	-	expression tag	UNP P01899
A	2295	HIS	-	expression tag	UNP P01899
A	2296	GLU	-	expression tag	UNP P01899
A	2297	HIS	-	expression tag	UNP P01899
A	2298	HIS	-	expression tag	UNP P01899
A	2299	HIS	-	expression tag	UNP P01899
A	2300	HIS	-	expression tag	UNP P01899
A	2301	HIS	-	expression tag	UNP P01899
A	2302	HIS	-	expression tag	UNP P01899
A	2303	HIS	-	expression tag	UNP P01899
A	2304	HIS	-	expression tag	UNP P01899

- Molecule 2 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		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.57Å 68.33Å 117.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 2.21	Depositor
% Data completeness (in resolution range)	99.3 (48.01-2.21)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.209 , 0.244	Depositor
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.282	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3225	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	NAG	A	2901	1	14,14,15	0.55	0	17,19,21	0.70	1 (5%)
2	NAG	A	2902	1	14,14,15	0.37	0	17,19,21	1.06	1 (5%)

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	A	2901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	2902	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2902	NAG	C1-O5-C5	3.09	116.38	112.19
2	A	2901	NAG	C1-O5-C5	2.47	115.53	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2901	NAG	O5-C5-C6-O6
2	A	2901	NAG	C4-C5-C6-O6
2	A	2902	NAG	C3-C2-N2-C7

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.