

wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 04:59 AM EDT

PDB ID : 6MP0

Title : Crystal structures of the murine class I major histocompatibility complex H-

2Db in complex with the TRP1-M9 peptide

Authors: Clancy-Thompson, E.; Devlin, C.A.; Birnbaum, M.E.; Dougan, S.K.

Deposited on : 2018-10-05

Resolution : 2.00 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 (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 2.00 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 3580 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-M9 peptide, Beta-2-microglobulin, H-2 class I histocompatibility antigen, D-B alpha chain, chimeric construct.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1	Λ	388	Total	С	N	О	S	0	9	0
1	A	300	3171	2006	555	593	17	0	2	

There are 65 discrepancies between the modelled and reference sequences:

A 10 GLY - linker UNP P07147 A 11 GLY - linker UNP P07147 A 12 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 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 1988 GLY -	Chain	Residue	Modelled	Actual	Comment	Reference
A 11 GLY - linker UNP P07147 A 12 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 1999 GLY - linker UNP P07147 A 1981 GLY <td< td=""><td>A</td><td>9</td><td>MET</td><td>ALA</td><td>engineered mutation</td><td>UNP P07147</td></td<>	A	9	MET	ALA	engineered mutation	UNP P07147
A 12 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 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P07147 A 1982 GLY <	A	10	GLY	-		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 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P01487 A 1982 GLY	A	11	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 998 GLY - linker UNP P07147 A 999 GLY - linker UNP P07147 A 1981 GLY - linker UNP P01887 A 1982 GLY	A	12	GLY	-	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 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P01487 A 1981 GLY - linker UNP P01887 A 1983 GLY - linker UNP P01887 A 1985 SER	A	989	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 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P01887 A 1982 GLY - linker UNP P01887 A 1983 GLY - linker UNP P01887 A 1985 SER	A	990	SER	-	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 1981 GLY - linker UNP P01887 A 1982 GLY - linker UNP P01887 A 1984 GLY - linker UNP P01887 A 1985 SER	A	991	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 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P07147 A 1981 GLY - linker UNP P01487 A 1981 GLY - linker UNP P01887 A 1983 GLY - linker UNP P01887 A 1985 SER - linker UNP P01887 A 1986 GLY - linker UNP P01887 A 1988 GLY	A	992	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 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 1988 GLY	A	993	GLY	-	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 P07147 A 1981 GLY - linker UNP P07147 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 1988 GLY - linker UNP P01887 A A 1989	A	994	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	A	995	SER	-	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	A	996	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 1989 GLY - linker UNP P01887	A	997	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 1989 GLY - linker UNP P01887 A 1989 GLY - linker UNP P01887	A	998	GLY	-	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 1989 GLY - linker UNP P01887	A	999	GLY	-	linker	UNP P07147
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	A	1000	SER	-	linker	UNP P07147
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	A	1981	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	A	1982	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	A	1983	GLY	-	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	A	1984	GLY	-	linker	UNP P01887
A 1987 GLY - linker UNP P01887 A 1988 GLY - linker UNP P01887 A 1989 GLY - linker UNP P01887	A	1985	SER	-	linker	UNP P01887
A 1988 GLY - linker UNP P01887 A 1989 GLY - linker UNP P01887	A	1986	GLY	-	linker	UNP P01887
A 1989 GLY - linker UNP P01887	A	1987	GLY	-	linker	UNP P01887
	A	1988	GLY	-	linker	UNP P01887
A 1990 SER - linker UNP P01887	A	1989	GLY	-	linker	UNP P01887
	A	1990	SER	-	linker	UNP P01887

Continued on next page...

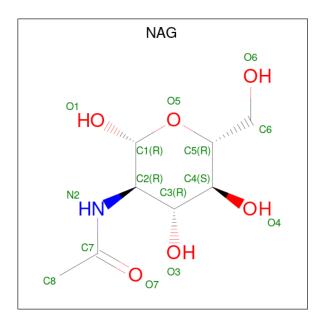


 $Continued\ from\ previous\ page...$

Chain	Residue	Modelled Modelled	Actual	Comment	Reference
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

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14				0	0
2	A	1	Total 14	C 8		O 5	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	381	Total O 381 381	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 2 21 21	Depositor
Cell constants	50.06Å 98.44Å 121.77Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.68 - 2.00	Depositor
% Data completeness	97.5 (31.68-2.00)	Depositor
(in resolution range)	,	-
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.195 , 0.228	Depositor
Wilson B-factor (\mathring{A}^2)	30.0	Xtriage
Anisotropy	0.182	Xtriage
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3580	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.54% 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)

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 Re			Link	Bond lengths				Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	NAG	A	2902	1	14,14,15	0.86	1 (7%)	17,19,21	0.62	0	
2	NAG	A	2901	1	14,14,15	1.08	2 (14%)	17,19,21	0.72	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	2902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2901	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	A	2901	NAG	O5-C1	2.98	1.48	1.43
2	A	2901	NAG	C1-C2	2.55	1.56	1.52
2	A	2902	NAG	C1-C2	2.32	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	2901	NAG	C1-O5-C5	2.07	115.00	112.19

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.

