wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 04:16 PM 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:

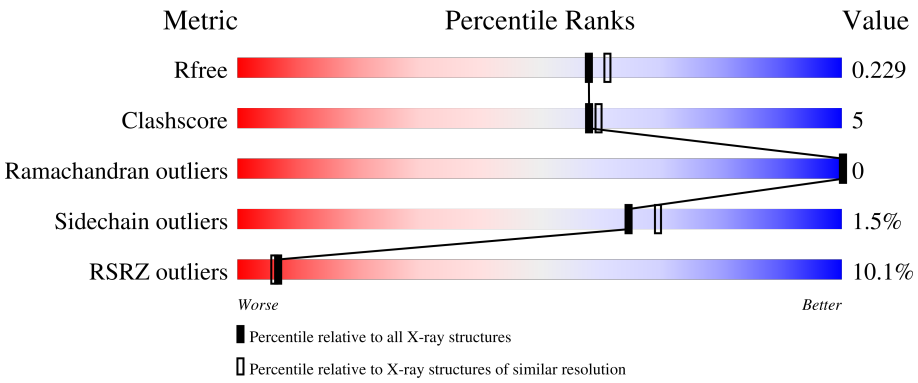
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	9% 77% 9% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2902	-	-	-	X

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	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3171	2006	555	593	17	0	2	0

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	ALA	engineered mutation	UNP P07147
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	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
A	1990	SER	-	linker	UNP P01887

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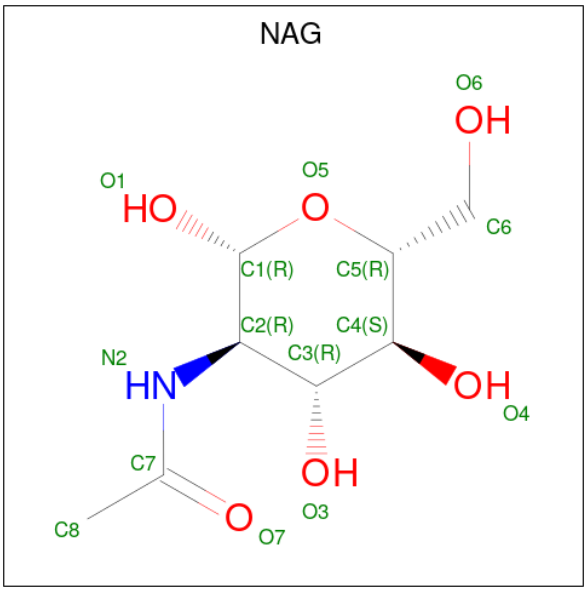
Chain	Residue	Modelled	Actual	Comment	Reference
A	1991	GLY	-	linker	UNP P01887
A	1992	GLY	-	linker	UNP P01887
A	1993	GLY	-	linker	UNP P01887
A	1994	GLY	-	linker	UNP P01887
A	1995	SER	-	linker	UNP P01887
A	1996	GLY	-	linker	UNP P01887
A	1997	GLY	-	linker	UNP P01887
A	1998	GLY	-	linker	UNP P01887
A	1999	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

- 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.

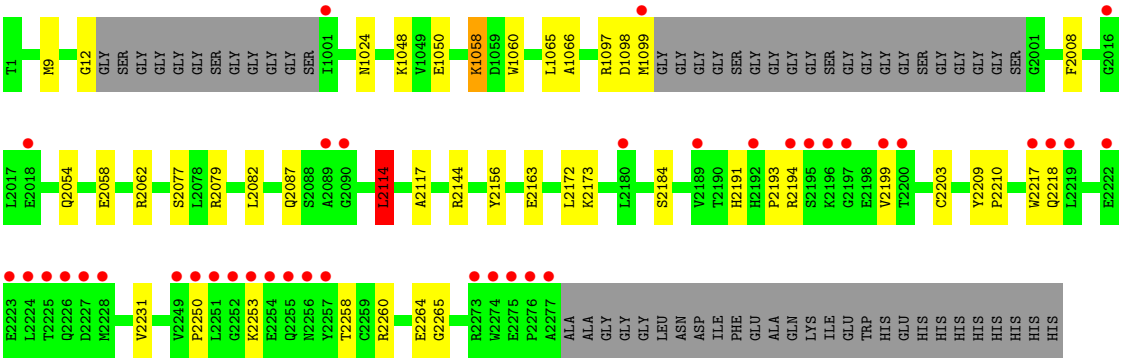
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	381	381	381	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TRP1-M9 peptide, Beta-2-microglobulin,H-2 class I histocompatibility antigen, D-B alpha chain, chimeric construct

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.06Å 98.44Å 121.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.68 – 2.00 51.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (31.68-2.00) 97.6 (51.78-2.00)	Depositor EDS
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 0.196 , 0.229	Depositor DCC
R_{free} test set	1996 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3580	wwPDB-VP
Average B, all atoms (Å^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.*

[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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.81	0/3268	0.83	4/4437 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2114	LEU	CB-CG-CD2	-8.94	95.81	111.00
1	A	2062	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	2114	LEU	CB-CG-CD1	5.20	119.83	111.00
1	A	2062	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3171	0	3010	29	1
2	A	28	0	26	1	0
3	A	381	0	0	13	2
All	All	3580	0	3036	30	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 30 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2218:GLN:HE22	1:A:2260:ARG:HG3	1.57	0.69
2:A:2901:NAG:O6	3:A:3001:HOH:O	2.11	0.68
1:A:2054:GLN:OE1	3:A:3002:HOH:O	2.15	0.64
1:A:2082:LEU:HD12	1:A:2087:GLN:HB2	1.81	0.61
1:A:2114:LEU:HD21	1:A:2156:TYR:CD1	2.35	0.61

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3211:HOH:O	3:A:3325:HOH:O[3_555]	1.89	0.31
1:A:2079:ARG:NH2	3:A:3005:HOH:O[3_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	384/447 (86%)	373 (97%)	11 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	335/361 (93%)	330 (98%)	5 (2%)	65 69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	LYS
1	A	1058	LYS
1	A	2114	LEU
1	A	2194	ARG
1	A	2231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2218	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 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	1.08	2 (14%)	17,19,21	0.72	1 (5%)
2	NAG	A	2902	1	14,14,15	0.86	1 (7%)	17,19,21	0.62	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
2	NAG	A	2901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2902	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	Observed(^{o})	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2901	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	388/447 (86%)	0.52	39 (10%) 7 6	18, 35, 79, 99	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2226	GLN	8.1
1	A	2277	ALA	7.6
1	A	2225	THR	7.3
1	A	2274	TRP	5.5
1	A	2089	ALA	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	2902	14/15	0.40	0.79	86,99,103,104	0
2	NAG	A	2901	14/15	0.43	0.25	80,87,93,94	0

6.5 Other polymers (i)

There are no such residues in this entry.