



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 01:13 AM BST

PDB ID : 6GB6
Title : Structure of H-2Kb with dipeptide GL
Authors : Hafstrand, I.; Sandalova, T.; Achour, A.
Deposited on : 2018-04-13
Resolution : 1.78 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : **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) : 2.14.4.dev1

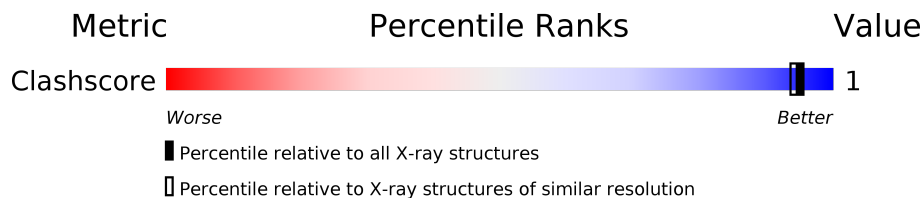
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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))
Clashscore	141614	10184 (1.80-1.76)

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 on 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	276	 94% 5%
1	D	276	 97%
2	B	100	 97%
2	E	100	 97%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6719 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2192	1391	377	414	10	0	3	0
1	D	276	2199	1390	381	418	10	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	100	821	523	138	153	7	0	0	0
2	B	100	821	523	138	153	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

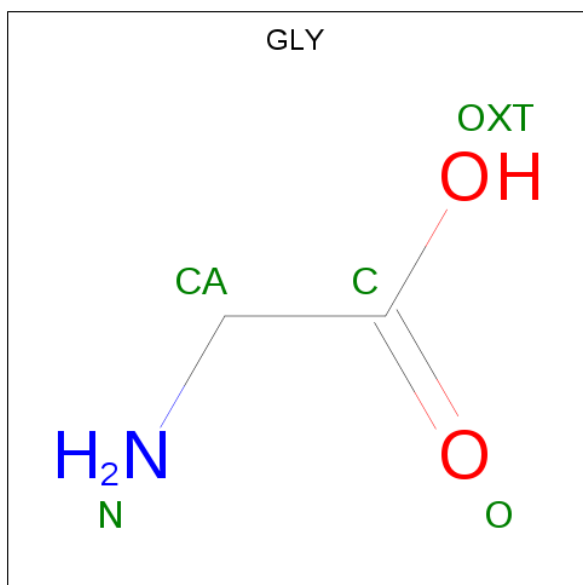
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	ALA	conflict	UNP P01887
E	85	ASP	ALA	variant	UNP P01887
B	0	GLY	ALA	conflict	UNP P01887
B	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



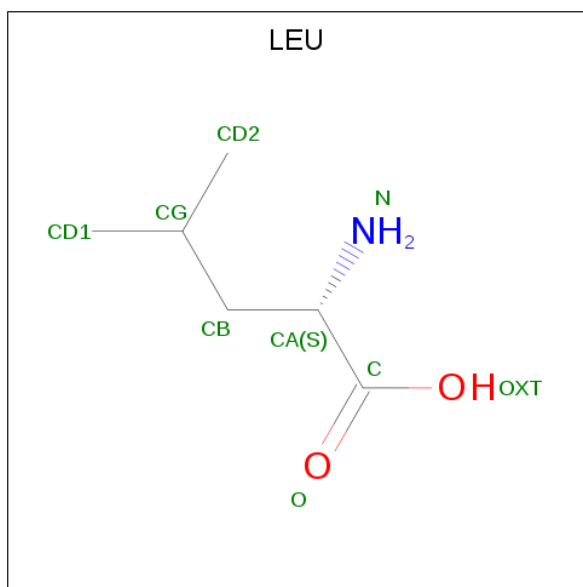
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			4	2	1	1		
4	D	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 5 is LEUCINE (three-letter code: LEU) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	6	1	2		
5	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	D	184	Total	O	0	0
			184	184		
6	E	134	Total	O	0	0
			134	134		
6	B	127	Total	O	0	0
			127	127		

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:  94% 5%



- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain D:  97%



- Molecule 2: Beta-2-microglobulin

Chain E:  97%



- Molecule 2: Beta-2-microglobulin

Chain B:  97%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.63Å 82.24Å 89.55Å 90.00° 111.29° 90.00°	Depositor
Resolution (Å)	83.44 – 1.78	Depositor
% Data completeness (in resolution range)	99.9 (83.44-1.78)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.207 , 0.232	Depositor
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.742	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Total number of atoms	6719	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0216e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL

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	0.46	0/2259	0.72	3/3074 (0.1%)
1	D	0.46	0/2264	0.69	0/3085
2	B	0.48	0/847	0.69	0/1149
2	E	0.47	0/847	0.66	0/1149
All	All	0.46	0/6217	0.70	3/8457 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	170	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	202	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	A	79	ARG	NE-CZ-NH1	5.05	122.83	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	2192	0	2043	8	0
1	D	2199	0	2037	4	0
2	B	821	0	788	2	0
2	E	821	0	788	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	8	0	0
3	D	12	0	16	0	0
3	E	6	0	8	0	0
4	A	4	0	2	0	0
4	D	4	0	2	0	0
5	A	9	0	11	0	0
5	D	9	0	11	0	0
6	A	191	0	0	1	0
6	B	127	0	0	0	0
6	D	184	0	0	0	0
6	E	134	0	0	0	0
All	All	6719	0	5714	14	0

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 1.

All (14) 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)
2:B:7:ILE:HD12	2:B:91:LYS:HE3	1.78	0.66
1:A:173:LYS:HG3	1:A:178:THR:HG22	1.84	0.60
1:A:171:TYR:O	1:A:173:LYS:HD2	2.07	0.54
1:D:127:ASN:OD1	1:D:132:THR:HG23	2.08	0.54
1:A:127:ASN:OD1	1:A:132:THR:HG23	2.07	0.53
1:A:72:GLN:HG3	6:A:546:HOH:O	2.10	0.52
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.46	0.50
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.95	0.48
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.98	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:D:260:HIS:CE1	1:D:271:THR:HG22	2.55	0.42
1:D:55:GLU:OE2	1:D:170:ARG:NH1	2.53	0.41
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.56	0.41
1:A:170:ARG:HH21	1:A:170:ARG:HG3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

8 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	$\# Z > 2$
5	LEU	A	303	-	5,8,8	0.24	0	6,10,10	0.78	0
4	GLY	A	302	-	3,3,4	0.73	0	0,2,4	0.00	-
5	LEU	D	304	-	5,8,8	0.21	0	6,10,10	0.76	0
3	GOL	D	302	-	5,5,5	0.37	0	5,5,5	0.65	0
3	GOL	A	301	-	5,5,5	0.39	0	5,5,5	0.48	0
3	GOL	D	301	-	5,5,5	0.22	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLY	D	303	-	3,3,4	0.73	0	0,2,4	0.00	-
3	GOL	E	101	-	5,5,5	0.36	0	5,5,5	0.21	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
5	LEU	A	303	-	-	0/4/8/8	-
4	GLY	A	302	-	-	0/0/1/2	-
5	LEU	D	304	-	-	0/4/8/8	-
3	GOL	D	302	-	-	2/4/4/4	-
3	GOL	A	301	-	-	4/4/4/4	-
3	GOL	D	301	-	-	2/4/4/4	-
4	GLY	D	303	-	-	0/0/1/2	-
3	GOL	E	101	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302	GOL	C1-C2-C3-O3
3	A	301	GOL	O1-C1-C2-C3
3	D	301	GOL	O1-C1-C2-O2
3	A	301	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	D	302	GOL	O2-C2-C3-O3
3	A	301	GOL	O1-C1-C2-O2
3	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.