WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2024 – 12:41 PM EDT

PDB ID	:	9C6V
Title	:	Crystal Structure of a single chain trimer composed of HLA-B*39:06 Y84C variant, beta-2microglobulin, and NRVMLPKAA peptide from NLRP2 (1 molecule/asymmetric unit)
Authors	:	Sharma, R.; Amdare, N.P.; Celikgil, A.; Garforth, S.J.; DiLorenzo, T.P.; Almo, S.C.; Ghosh, A.
Deposited on	:	2024-06-09
Resolution	:	1.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

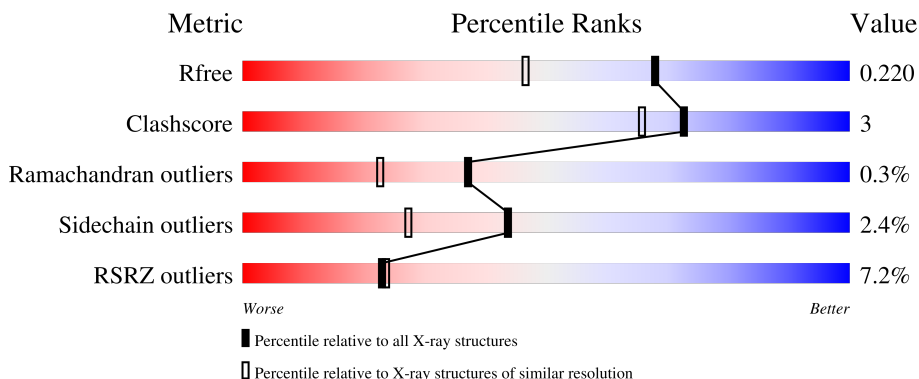|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 1.70 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.4%
RSRZ outliers		7.2%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	419	7% · 84% · 8% · 7%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3365 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 NACHT, LRR and PYD domains-containing protein 2,Beta-2 -microglobulin,MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total 3195	C 1997	N 572	O 612	S 14	0	5	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	GLY	-	linker	UNP Q9NX02
A	333	CYS	-	linker	UNP Q9NX02
A	988	GLY	-	linker	UNP Q9NX02
A	989	ALA	-	linker	UNP Q9NX02
A	990	SER	-	linker	UNP Q9NX02
A	991	GLY	-	linker	UNP Q9NX02
A	992	GLY	-	linker	UNP Q9NX02
A	993	GLY	-	linker	UNP Q9NX02
A	994	GLY	-	linker	UNP Q9NX02
A	995	SER	-	linker	UNP Q9NX02
A	996	GLY	-	linker	UNP Q9NX02
A	997	GLY	-	linker	UNP Q9NX02
A	998	GLY	-	linker	UNP Q9NX02
A	999	GLY	-	linker	UNP Q9NX02
A	1000	SER	-	linker	UNP Q9NX02
A	1001	MET	-	linker	UNP Q9NX02
A	1981	GLY	-	linker	UNP P61769
A	1982	GLY	-	linker	UNP P61769
A	1983	GLY	-	linker	UNP P61769
A	1984	GLY	-	linker	UNP P61769
A	1985	SER	-	linker	UNP P61769
A	1986	GLY	-	linker	UNP P61769
A	1987	GLY	-	linker	UNP P61769
A	1988	GLY	-	linker	UNP P61769
A	1989	GLY	-	linker	UNP P61769
A	1990	SER	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1991	GLY	-	linker	UNP P61769
A	1992	GLY	-	linker	UNP P61769
A	1993	GLY	-	linker	UNP P61769
A	1994	GLY	-	linker	UNP P61769
A	1995	SER	-	linker	UNP P61769
A	1996	GLY	-	linker	UNP P61769
A	1997	GLY	-	linker	UNP P61769
A	1998	GLY	-	linker	UNP P61769
A	1999	GLY	-	linker	UNP P61769
A	2000	SER	-	linker	UNP P61769
A	2084	CYS	TYR	variant	UNP I3ZN83

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
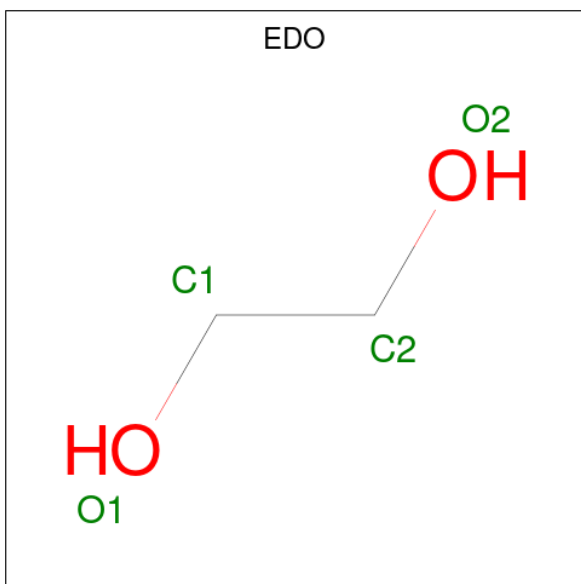
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO OH

O1 O2

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total 159	O 159	0	1

3   Residue-property plots ⓘ

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: NACHT, LRR and PYD domains-containing protein 2,Beta-2-microglobulin,MHC class I antigen
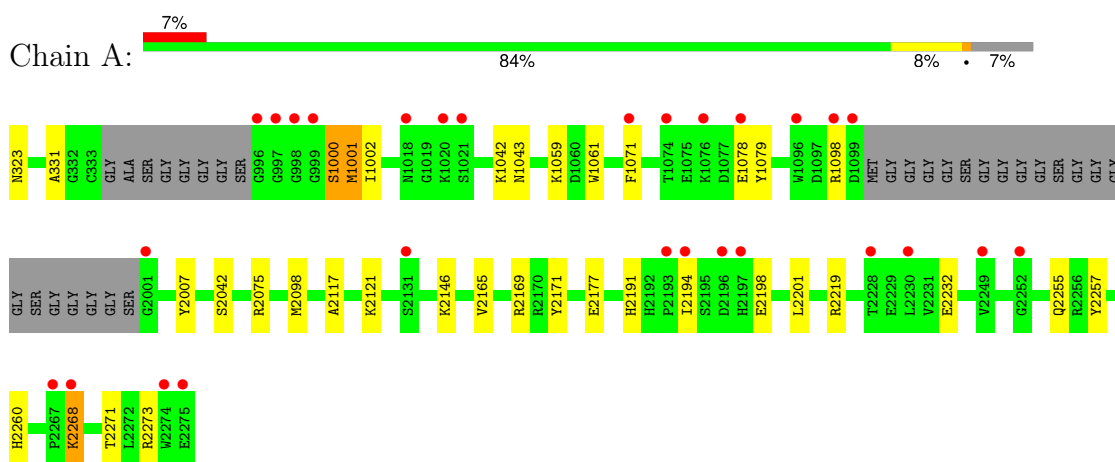
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	74.95Å 83.45Å 148.64Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	24.77 – 1.70	Depositor
	24.77 – 1.70	EDS
% Data completeness	97.3 (24.77-1.70)	Depositor
(in resolution range)	97.3 (24.77-1.70)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5156: ???)	Depositor
R, R_{free}	0.196 , 0.219	Depositor
	0.196 , 0.220	DCC
R_{free} test set	2642 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3365	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, EDO

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	0.41	2/3296 (0.1%)	0.64	2/4473 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1001[A]	MET	C-O	6.57	1.35	1.23
1	A	1001[B]	MET	C-O	6.57	1.35	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1001[A]	MET	CA-C-O	5.83	132.34	120.10
1	A	1001[B]	MET	CA-C-O	5.83	132.34	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	3195	0	3015	19	0
2	A	4	0	6	0	0
3	A	6	0	8	0	0
4	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	159	0	0	1	0
All	All	3365	0	3029	19	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 3.

The worst 5 of 19 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:2268:LYS:C	1:A:2268:LYS:HD3	2.12	0.69
1:A:323:ASN:N	1:A:2007:TYR:HH	2.00	0.58
1:A:2075:ARG:NH1	5:A:2403:HOH:O	2.38	0.57
1:A:2194:ILE:HD11	1:A:2198:GLU:HB3	1.87	0.56
1:A:323:ASN:N	1:A:2171:TYR:HH	2.03	0.55

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	389/419 (93%)	383 (98%)	5 (1%)	1 (0%)	37	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	SER

5.3.2 Protein sidechains ⓘ

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	344/346 (99%)	334 (97%)	10 (3%)	37	20

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2232[A]	GLU
1	A	2232[B]	GLU
1	A	2268	LYS
1	A	1071	PHE
1	A	2042	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2218	GLN
1	A	2255	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	EDO	A	2301	-	3,3,3	0.24	0	2,2,2	0.28	0
3	GOL	A	2302	-	5,5,5	0.32	0	5,5,5	0.37	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	EDO	A	2301	-	-	0/1/1/1	-
3	GOL	A	2302	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2302	GOL	O1-C1-C2-C3
3	A	2302	GOL	O2-C2-C3-O3
3	A	2302	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	390/419 (93%)	0.35	28 (7%)	23	23	17, 34, 78, 108	5 (1%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	996	GLY	4.1
1	A	1076	LYS	3.3
1	A	1021	SER	3.3
1	A	998	GLY	3.2
1	A	2197	HIS	3.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
2	EDO	A	2301	4/4	0.81	0.15	52,54,55,57	0
3	GOL	A	2302	6/6	0.84	0.11	47,50,58,60	0
4	CL	A	2303	1/1	0.91	0.14	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.