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wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 14, 2017 – 01:09 am GMT

PDB ID : 1FFP

Title : CRYSTAL STRUCTURE OF MURINE CLASS I H-2DB COMPLEXED WITH PEPTIDE GP33 (C9M/K1S)

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Deposited on : 2000-07-25

Resolution : 2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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		0.299
Clashscore		27
Ramachandran outliers		3.5%
Sidechain outliers		4.3%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
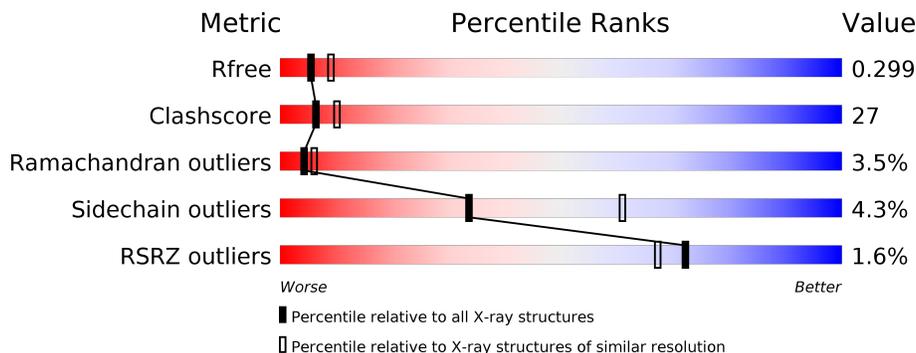
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	273	% 59% 36% · ·
1	D	273	% 58% 37% · ·
2	B	100	3% 36% 56% 8%
2	E	100	3% 37% 55% 8%
3	C	9	67% 33%
3	F	9	56% 44%

WORLDWIDE PDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6302 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, D-B, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2245	1418	397	421	9			
1	D	273	Total	C	N	O	S	0	0	0
			2245	1418	397	421	9			

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			829	529	139	153	8			
2	E	100	Total	C	N	O	S	0	0	0
			829	529	139	153	8			

- Molecule 3 is a protein called SYNTHETIC PEPTIDE WITH SEQUENCE SER-ALA-VAL-TYR-ASN-PHE-ALA-THR-MET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			70	45	10	14	1			
3	F	9	Total	C	N	O	S	0	0	0
			70	45	10	14	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	3	Total	O	0	0
			3	3		
4	D	6	Total	O	1	0
			6	6		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B, ALPHA CHAIN
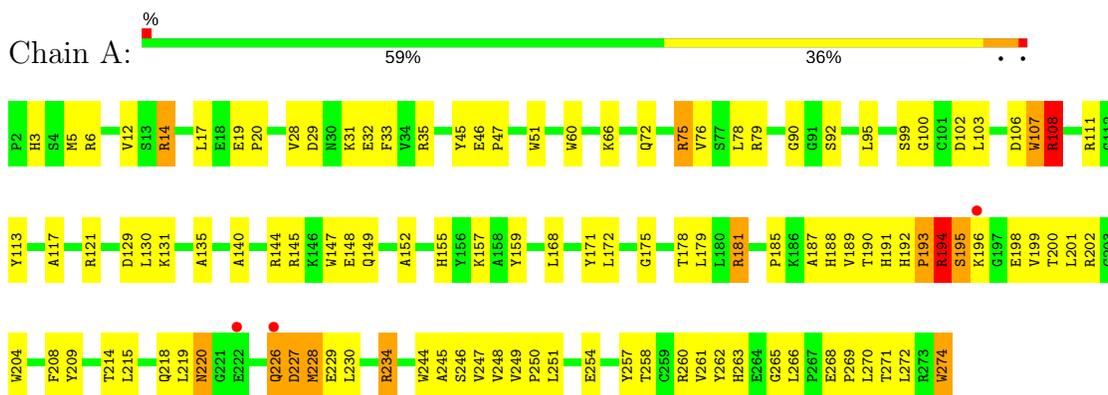

- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B, ALPHA CHAIN
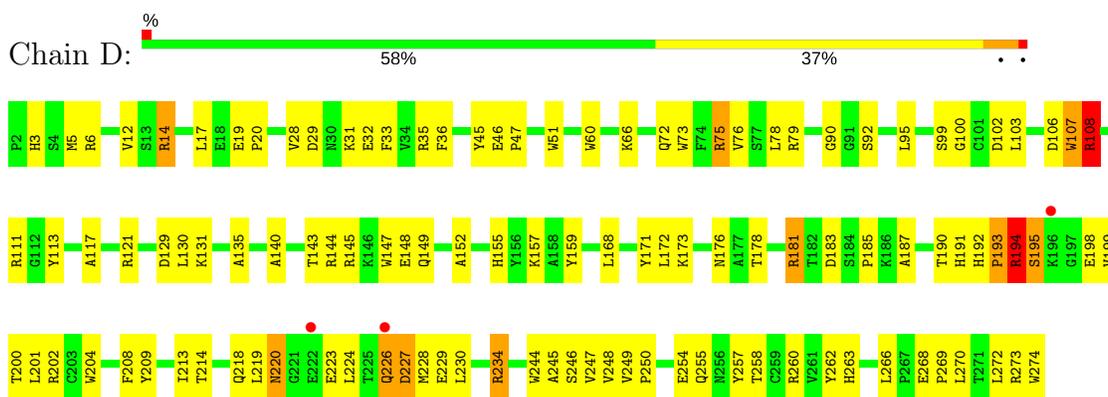
- Molecule 2: BETA-2 MICROGLOBULIN BETA CHAIN
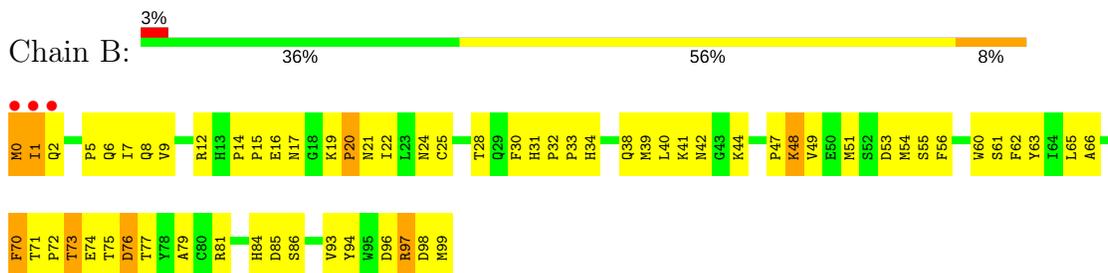
- Molecule 2: BETA-2 MICROGLOBULIN BETA CHAIN
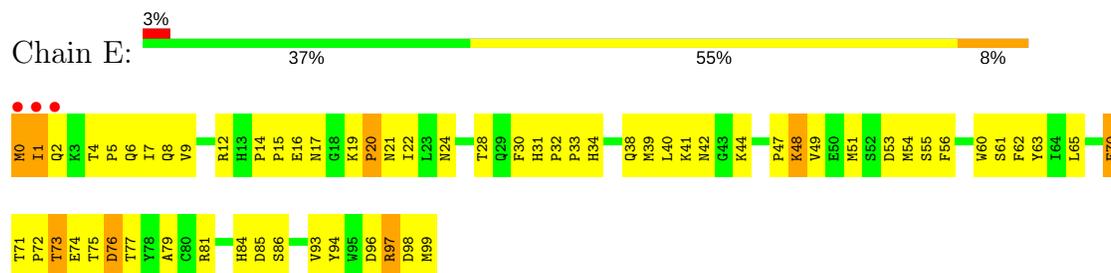
Chain E:

● Molecule 3: SYNTHETIC PEPTIDE WITH SEQUENCE SER-ALA-VAL-TYR-ASN-PHE-ALA-THR-MET

Chain C:

● Molecule 3: SYNTHETIC PEPTIDE WITH SEQUENCE SER-ALA-VAL-TYR-ASN-PHE-ALA-THR-MET

Chain F:
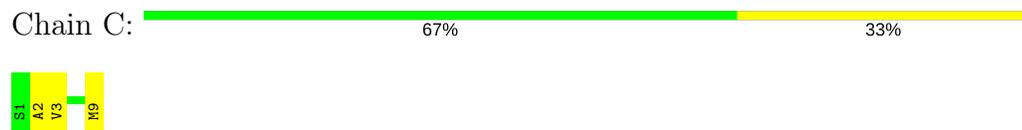
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.01Å 66.90Å 80.41Å 75.10° 72.90° 69.28°	Depositor
Resolution (Å)	50.00 – 2.60 41.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.60) 90.5 (41.50-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.61Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.250 , 0.303 0.247 , 0.299	Depositor DCC
R_{free} test set	1304 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 22.1	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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 ⓘ

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	0.44	0/2311	0.78	5/3136 (0.2%)
1	D	0.45	0/2311	0.75	4/3136 (0.1%)
2	B	0.41	0/855	0.69	0/1158
2	E	0.41	0/855	0.69	0/1158
3	C	0.65	0/71	0.76	0/94
3	F	0.62	0/71	0.71	0/94
All	All	0.44	0/6474	0.75	9/8776 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH1	-15.36	112.62	120.30
1	A	108	ARG	NE-CZ-NH2	14.32	127.46	120.30
1	D	108	ARG	NE-CZ-NH2	-13.49	113.55	120.30
1	D	108	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	108	ARG	CD-NE-CZ	7.85	134.59	123.60

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	2245	0	2118	110	0
1	D	2245	0	2118	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	829	0	805	64	0
2	E	829	0	805	66	0
3	C	70	0	66	6	0
3	F	70	0	66	9	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	6	0	0	0	0
4	E	2	0	0	0	0
All	All	6302	0	5978	327	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 27.

The worst 5 of 327 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:95:LEU:HD21	3:C:9:MET:HE1	1.36	1.08
1:D:95:LEU:HD21	3:F:9:MET:HE3	1.45	0.99
2:E:72:PRO:O	2:E:73:THR:HG23	1.76	0.86
2:B:72:PRO:O	2:B:73:THR:HG23	1.77	0.85
1:D:218:GLN:HA	1:D:224:LEU:HD23	1.63	0.80

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	271/273 (99%)	253 (93%)	12 (4%)	6 (2%)	8	14
1	D	271/273 (99%)	250 (92%)	15 (6%)	6 (2%)	8	14
2	B	98/100 (98%)	80 (82%)	11 (11%)	7 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	98/100 (98%)	80 (82%)	11 (11%)	7 (7%)	1	1
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	F	7/9 (78%)	4 (57%)	3 (43%)	0	100	100
All	All	752/764 (98%)	672 (89%)	54 (7%)	26 (4%)	4	6

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	195	SER
1	A	220	ASN
1	A	227	ASP
2	B	74	GLU

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	232/232 (100%)	221 (95%)	11 (5%)	30	57
1	D	232/232 (100%)	222 (96%)	10 (4%)	33	61
2	B	95/95 (100%)	91 (96%)	4 (4%)	34	62
2	E	95/95 (100%)	91 (96%)	4 (4%)	34	62
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	668/668 (100%)	639 (96%)	29 (4%)	33	61

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	ASP
1	D	17	LEU
2	E	70	PHE
2	B	77	THR

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Mol	Chain	Res	Type
1	D	45	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	GLN
2	B	84	HIS
2	E	8	GLN
2	B	8	GLN
2	B	17	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

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	273/273 (100%)	-0.28	3 (1%)	80	77	11, 24, 45, 51	0
1	D	273/273 (100%)	-0.25	3 (1%)	80	77	10, 25, 45, 52	0
2	B	100/100 (100%)	-0.11	3 (3%)	51	43	17, 35, 45, 53	0
2	E	100/100 (100%)	-0.06	3 (3%)	51	43	16, 35, 45, 53	0
3	C	9/9 (100%)	-0.27	0	100	100	16, 19, 21, 23	0
3	F	9/9 (100%)	-0.41	0	100	100	14, 16, 18, 20	0
All	All	764/764 (100%)	-0.22	12 (1%)	72	67	10, 27, 45, 53	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	GLN	3.8
2	E	1	ILE	3.6
1	D	226	GLN	3.3
2	B	1	ILE	3.1
2	B	2	GLN	2.9

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

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6.5 Other polymers (i)

There are no such residues in this entry.