wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2026 – 02:16 PM EST

PDB ID	:	9OJF / pdb_00009ojf
Title	:	X-ray Structure of MHC-IGRP228 in Complex with FAb 3
Authors	:	Fischmann, T.; Jaremko, M.J.
Deposited on	:	2025-05-07
Resolution	:	1.61 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 (1)) were used in the production of this report:

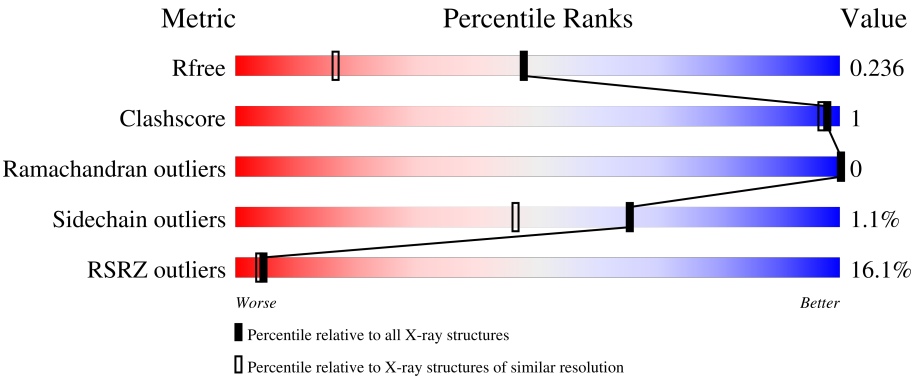
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.61 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 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	278	7% 97% .
2	B	100	6% 97% .
3	C	9	89% 11%
4	D	214	15% 95% 5%
5	E	227	33% 93% . .

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13182 atoms, of which 6199 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 MHC class I antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	277	4369	1412	2108	412	428	9	2108	2	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP Q8WLS4
A	301	GLY	-	expression tag	UNP Q8WLS4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	100	1657	538	813	142	160	4	813	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Glucose-6-phosphatase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	C	9	156	51	80	11	14	80	0	0

- Molecule 4 is a protein called FAb 3 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	214	3245	1029	1598	280	333	5	1598	0	0

- Molecule 5 is a protein called FAb 3 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	220	Total	C	H	N	O	S	1600	0	1
			3240	1035	1600	272	325	8			

- Molecule 6 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Br	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	207	Total	O	0	0
			207	207		
7	B	86	Total	O	0	0
			86	86		
7	C	4	Total	O	0	0
			4	4		
7	D	108	Total	O	0	0
			108	108		
7	E	109	Total	O	0	0
			109	109		

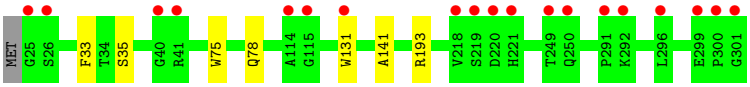
3 Residue-property plots (i)

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: MHC class I antigen

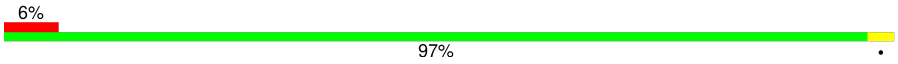
Chain A:





• Molecule 2: Beta-2-microglobulin

Chain B:





• Molecule 3: Glucose-6-phosphatase 2

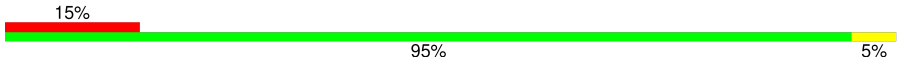
Chain C:

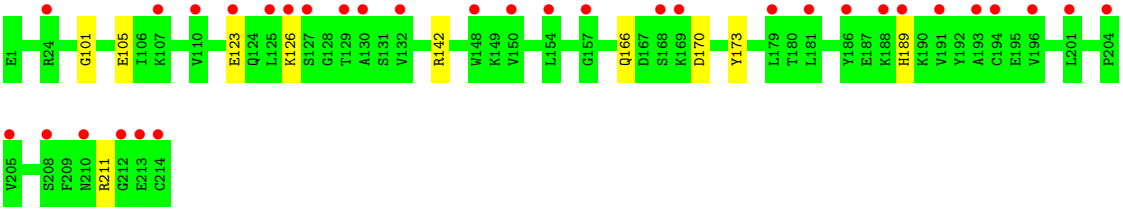




• Molecule 4: FAb 3 Light Chain

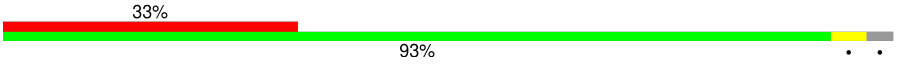
Chain D:

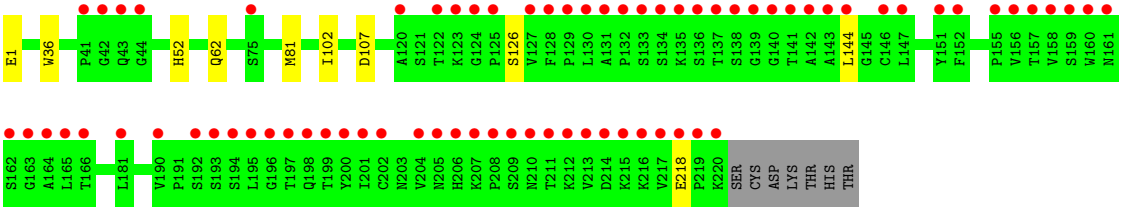




• Molecule 5: FAb 3 Heavy Chain

Chain E:




E1
W36
P41
G42
Q43
G44
H52
Q62
S75
M81
I102
D107
A120
S121
T122
K123
G124
P125
S126
V127
F128
P129
L130
A131
P132
S133
S134
K135
S136
T137
S138
G139
G140
T141
A142
A143
L144
G145
C146
L147
Y151
F152
P155
V156
T157
V158
S159
W160
N161
S162
G163
A164
L165
T166
L181
V190
P191
S192
S193
S194
L195
G196
T197
Q198
T199
Y200
I201
C202
N203
V204
N205
H206
K207
P208
S209
N210
T211
K212
V213
D214
K215
K216
V217
E218
P219
K220
SER
CYS
ASP
LYS
THR
HIS
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.63Å 92.63Å 207.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.61 – 1.61 84.61 – 1.61	Depositor EDS
% Data completeness (in resolution range)	61.8 (84.61-1.61) 61.8 (84.61-1.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.61Å)	Xtriage
Refinement program	BUSTER 2.11.8 (3-JUN-2022)	Depositor
R, R_{free}	0.204 , 0.238 0.198 , 0.236	Depositor DCC
R_{free} test set	3622 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

5.1 Standard geometry

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

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	0.83	0/2335	1.00	1/3170 (0.0%)
2	B	0.81	0/873	0.97	1/1180 (0.1%)
3	C	0.82	0/77	0.70	0/104
4	D	0.82	0/1684	0.94	2/2289 (0.1%)
5	E	0.79	0/1681	0.94	2/2290 (0.1%)
All	All	0.82	0/6650	0.96	6/9033 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	107	ASP	CA-CB-CG	6.94	119.54	112.60
5	E	102	ILE	N-CA-C	-6.16	98.25	107.37
4	D	170	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	26	LYS	N-CA-C	-5.31	101.04	109.96
4	D	101	GLY	N-CA-C	5.27	118.85	112.48

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	2261	2108	2097	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	844	813	804	2	0
3	C	76	80	77	1	0
4	D	1647	1598	1598	3	0
5	E	1640	1600	1599	2	0
6	B	1	0	0	0	0
7	A	207	0	0	0	0
7	B	86	0	0	1	0
7	C	4	0	0	0	0
7	D	108	0	0	0	0
7	E	109	0	0	0	0
All	All	6983	6199	6175	9	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.

The worst 5 of 9 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:75:TRP:O	1:A:78:GLN:HG2	2.02	0.59
4:D:189:HIS:O	4:D:211:ARG:HD3	2.08	0.52
2:B:107:LEU:O	7:B:301:HOH:O	2.19	0.49
1:A:131:TRP:O	1:A:193:ARG:HD3	2.15	0.47
1:A:141:ALA:HB2	2:B:80:TRP:CE2	2.49	0.46

There are no symmetry-related clashes.

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	277/278 (100%)	273 (99%)	4 (1%)	0	100	100
2	B	100/100 (100%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
5	E	218/227 (96%)	218 (100%)	0	0	100	100
All	All	814/828 (98%)	806 (99%)	8 (1%)	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	234/233 (100%)	233 (100%)	1 (0%)	84	75
2	B	97/95 (102%)	97 (100%)	0	100	100
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	186/186 (100%)	184 (99%)	2 (1%)	65	46
5	E	184/192 (96%)	179 (97%)	5 (3%)	39	16
All	All	710/715 (99%)	702 (99%)	8 (1%)	65	46

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	218	GLU
5	E	144	LEU
5	E	62	GLN
5	E	1	GLU
5	E	126	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	38	GLN
4	D	160	GLN

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Mol	Chain	Res	Type
5	E	39	GLN
4	D	189	HIS
1	A	175	HIS

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

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, 95^{th} 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	277/278 (99%)	0.18	19 (6%) 23 23	5, 12, 22, 41	1 (0%)
2	B	100/100 (100%)	0.26	6 (6%) 27 28	4, 13, 24, 30	1 (1%)
3	C	9/9 (100%)	-0.28	0 100 100	7, 8, 11, 12	0
4	D	214/214 (100%)	0.74	33 (15%) 5 4	7, 16, 30, 46	0
5	E	220/227 (96%)	1.36	74 (33%) 1 1	6, 19, 37, 45	0
All	All	820/828 (99%)	0.64	132 (16%) 4 4	4, 14, 31, 46	2 (0%)

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	220	LYS	8.1
1	A	300	PRO	8.0
1	A	301	GLY	7.8
1	A	25	GLY	7.3
1	A	218	VAL	6.2

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 oligosaccharides 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, 95^{th} 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
6	BR	B	201	1/1	0.95	0.06	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.