



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:02 PM GMT

PDB ID : 1HQR
Title : CRYSTAL STRUCTURE OF A SUPERANTIGEN BOUND TO THE HIGH-AFFINITY, ZINC-DEPENDENT SITE ON MHC CLASS II
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Deposited on : 2000-12-19
Resolution : 3.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

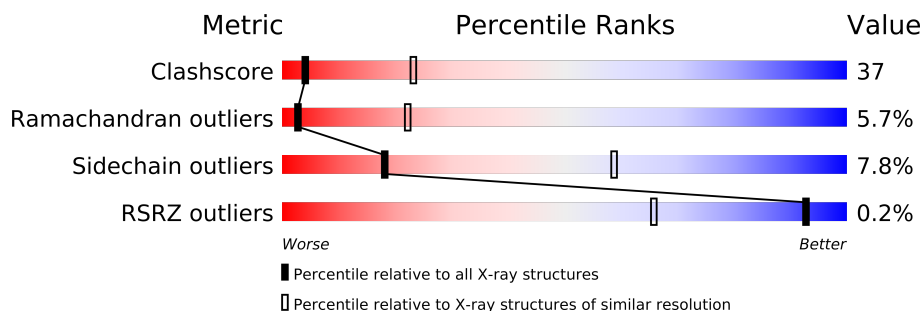
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	181	
2	B	190	
3	C	13	
4	D	208	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4539 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HLA-DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1411	920	228	258	5			

- Molecule 2 is a protein called HLA-DR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1398	887	247	259	5			

- Molecule 3 is a protein called MYELIN BASIC PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			85	59	14	12			

- Molecule 4 is a protein called STREPTOCOCCAL PYROGENIC EXOTOXIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	206	Total	C	N	O	S	0	0	1
			1644	1052	269	319	4			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

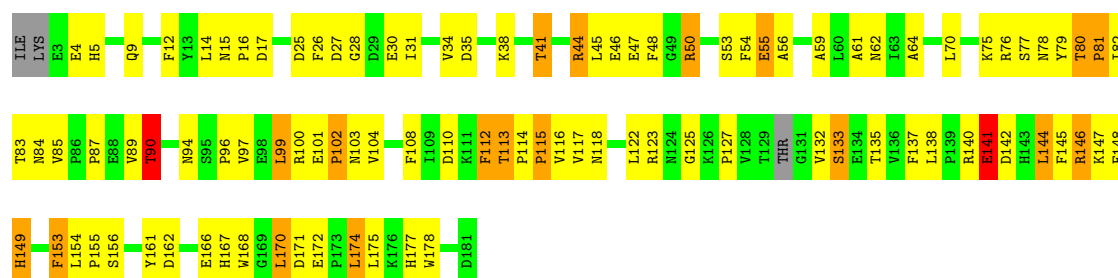
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Zn	0	0
			1	1		

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 errors 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.

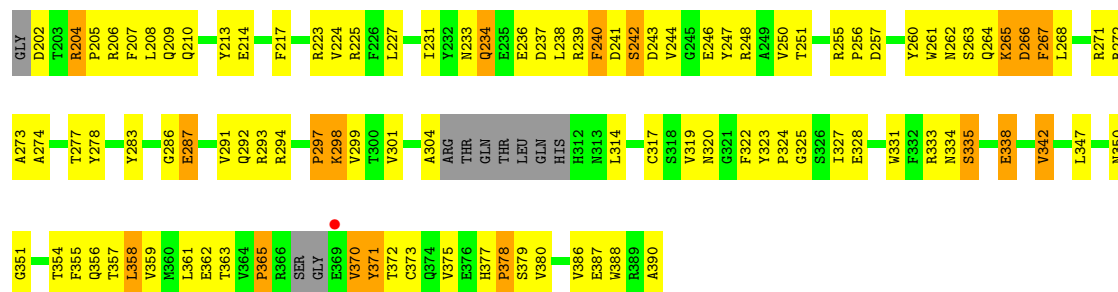
• Molecule 1: HLA-DR ALPHA CHAIN

Chain A: 



• Molecule 2: HLA-DR BETA CHAIN

Chain B: 



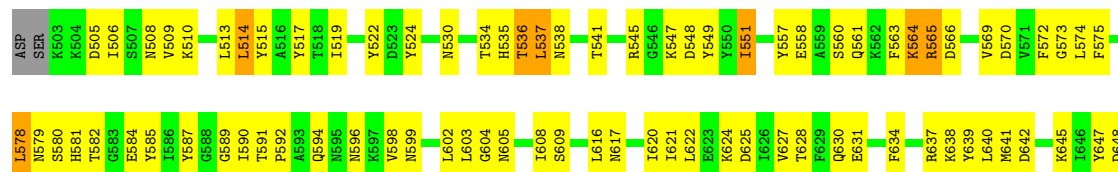
• Molecule 3: MYELIN BASIC PROTEIN

Chain C: 



• Molecule 4: STREPTOCOCCAL PYROGENIC EXOTOXIN C

Chain D: 



I649	I650	S651	F652	Y653	Y654	S655	E659	T662	K663	D664	F673	D674	N677	R681	I684	F685	A686	K687	Y688	K689	D690	N691	N692	I693	I694	N695	N696	K697	S700	D703	I704	Y705	L706	E707	K708
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	61.83Å 111.95Å 216.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.20 99.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (100.00-3.20) 90.6 (99.45-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.01Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.224 , 0.288 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14091 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: ZN

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	0.43	0/1455	0.66	0/1990
2	B	0.39	0/1433	0.65	1/1952 (0.1%)
3	C	0.46	0/88	0.64	0/119
4	D	0.42	0/1680	0.68	0/2275
All	All	0.42	0/4656	0.66	1/6336 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	PRO	N-CA-CB	5.30	109.67	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1411	0	1294	111	0
2	B	1398	0	1237	116	0
3	C	85	0	86	10	0
4	D	1644	0	1530	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	4539	0	4147	320	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 320 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:LEU:HD23	1:A:170:LEU:H	1.26	0.97
1:A:118:ASN:HB3	1:A:166:GLU:HB2	1.46	0.97
2:B:299:VAL:HG21	2:B:375:VAL:HG21	1.45	0.97
4:D:578:LEU:CD2	4:D:579:ASN:H	1.82	0.93
4:D:578:LEU:HD23	4:D:579:ASN:H	1.33	0.92

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	174/181 (96%)	142 (82%)	20 (12%)	12 (7%)	2	14
2	B	174/190 (92%)	141 (81%)	20 (12%)	13 (8%)	2	12
3	C	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
4	D	204/208 (98%)	157 (77%)	40 (20%)	7 (3%)	6	38
All	All	560/592 (95%)	447 (80%)	81 (14%)	32 (6%)	3	22

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	133	SER
2	B	266	ASP
2	B	297	PRO

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Mol	Chain	Res	Type
2	B	298	LYS

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	146/166 (88%)	130 (89%)	16 (11%)	9	36
2	B	135/171 (79%)	127 (94%)	8 (6%)	28	72
3	C	10/13 (77%)	10 (100%)	0	100	100
4	D	171/192 (89%)	159 (93%)	12 (7%)	21	64
All	All	462/542 (85%)	426 (92%)	36 (8%)	18	59

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	202	ASP
2	B	263	SER
4	D	650	THR
2	B	240	PHE
2	B	342	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	234	GLN
2	B	292	GLN
4	D	614	GLN
2	B	233	ASN
4	D	617	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.

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(Å ²)	Q<0.9
1	A	178/181 (98%)	-0.24	0 100 100	10, 37, 72, 89	0
2	B	180/190 (94%)	-0.13	1 (0%) 86 41	10, 44, 79, 89	0
3	C	10/13 (76%)	-0.04	0 100 100	23, 42, 80, 89	0
4	D	206/208 (99%)	-0.24	0 100 100	9, 36, 75, 89	0
All	All	574/592 (96%)	-0.20	1 (0%) 93 66	9, 39, 78, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	369	GLU	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	D	709	1/1	0.14	-1.65	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.