



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 02:55 pm GMT

PDB ID : 3HFM
Title : STRUCTURE OF AN ANTIBODY-ANTIGEN COMPLEX. CRYSTAL
STRUCTURE OF THE HY/HEL-10 FAB-LYSOZYME COMPLEX
Authors : Padlan, E.A.; Davies, D.R.
Deposited on : 1988-08-11
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

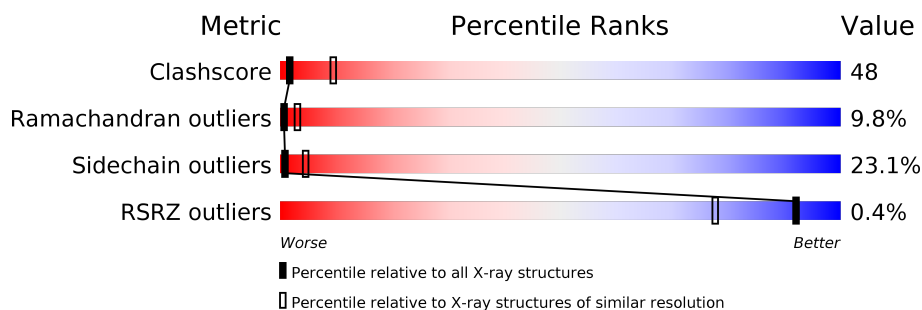
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 $\leq 5\%$. 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	L	214	<div> <div>27%</div> <div>52%</div> <div>19%</div> <div>.</div> </div>
2	H	215	<div> <div>%</div> <div>30%</div> <div>45%</div> <div>19%</div> <div>6%</div> </div>
3	Y	129	<div> <div>22%</div> <div>56%</div> <div>19%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4297 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 HYHEL-10 IGG1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1655	1026	281	341	7			

- Molecule 2 is a protein called HYHEL-10 IGG1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1640	1032	266	335	7			

- Molecule 3 is a protein called HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

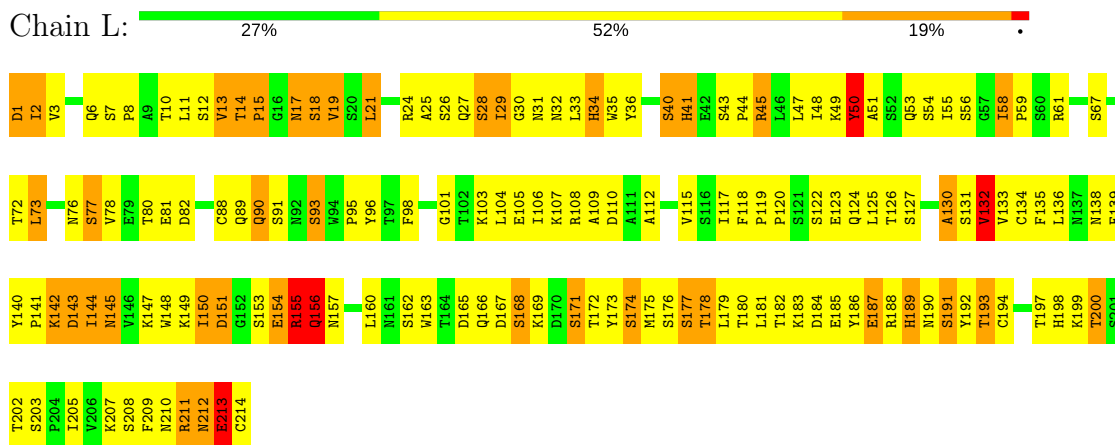
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total	O	0
			1	1	

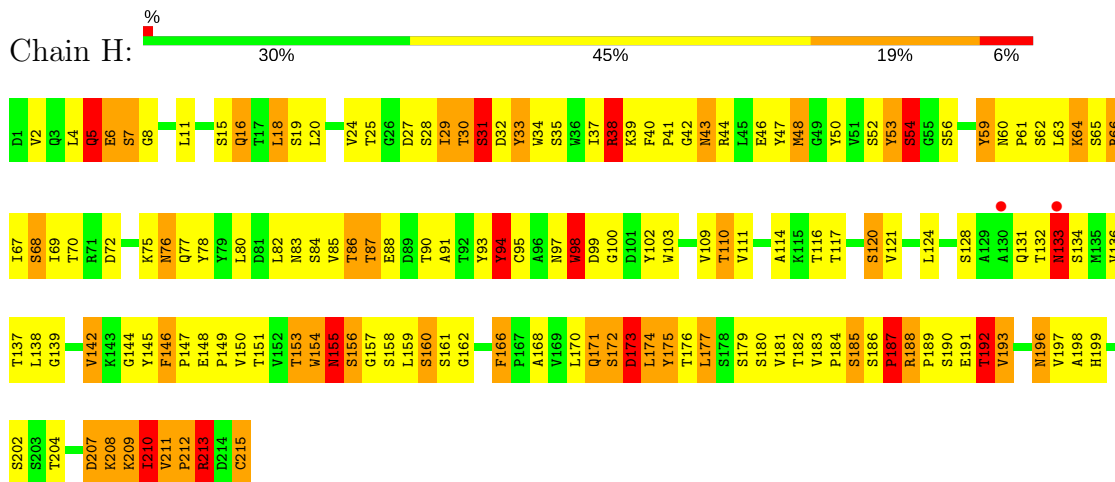
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

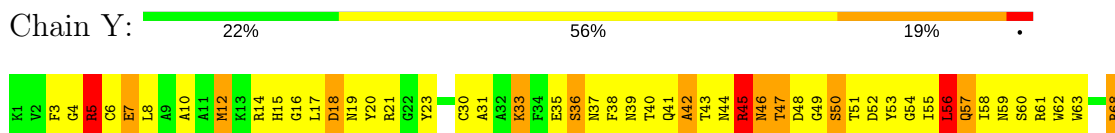
• Molecule 1: HYHEL-10 IGG1 FAB (LIGHT CHAIN)



• Molecule 2: HYHEL-10 IGG1 FAB (HEAVY CHAIN)



• Molecule 3: HEN EGG WHITE LYSOZYME



T69	P70	G71	R73	N74	L75	C76	N77	L78	P79	C80	S81	A82	L83	L84	S85	S86	D87	T88	T89	Y92	N93	C94	A95	R96	K97	I98	V99	S100	D101	G102	N103	G104	M105	N106	V109	A110	W111	R112	N113	R114	C115	K116	G117	T118	D119	V120	Q121	A122	W123	I124	R125	R128	L129
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.47Å 118.73Å 137.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 9.99 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 65.0 (9.99-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.246 , (Not available) 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 38.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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](#)

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	L	0.81	0/1693	1.72	21/2297 (0.9%)
2	H	0.83	0/1684	1.70	29/2310 (1.3%)
3	Y	0.79	0/1021	1.62	16/1379 (1.2%)
All	All	0.81	0/4398	1.69	66/5986 (1.1%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	45	ARG	CD-NE-CZ	20.15	151.81	123.60
1	L	155	ARG	NE-CZ-NH1	13.40	127.00	120.30
2	H	162	GLY	N-CA-C	10.52	139.39	113.10
2	H	44	ARG	NE-CZ-NH2	-9.41	115.59	120.30
3	Y	45	ARG	NE-CZ-NH1	8.92	124.76	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	L	1655	0	1572	138	0
2	H	1640	0	1582	176	0
3	Y	1001	0	959	102	0
4	Y	1	0	0	0	0
All	All	4297	0	4113	401	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 48.

The worst 5 of 401 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:L:214:CYS:HA	2:H:215:CYS:CB	1.80	1.11
1:L:214:CYS:CA	2:H:215:CYS:HB3	1.79	1.10
2:H:183:VAL:HB	2:H:184:PRO:HD2	1.27	1.08
2:H:53:TYR:O	2:H:54:SER:HB3	1.35	1.08
1:L:156:GLN:HG3	1:L:157:ASN:H	1.17	1.07

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	L	212/214 (99%)	162 (76%)	33 (16%)	17 (8%)	1	5
2	H	213/215 (99%)	155 (73%)	38 (18%)	20 (9%)	1	3
3	Y	127/129 (98%)	86 (68%)	24 (19%)	17 (13%)	0	1
All	All	552/558 (99%)	403 (73%)	95 (17%)	54 (10%)	1	3

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	ILE
1	L	50	TYR
1	L	130	ALA
1	L	144	ILE
1	L	154	GLU

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	L	192/192 (100%)	144 (75%)	48 (25%)	1	3
2	H	192/192 (100%)	140 (73%)	52 (27%)	0	2
3	Y	105/105 (100%)	92 (88%)	13 (12%)	5	23
All	All	489/489 (100%)	376 (77%)	113 (23%)	1	4

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	11	LEU
2	H	54	SER
3	Y	68	ARG
2	H	15	SER
2	H	29	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	16	GLN
2	H	43	ASN
3	Y	59	ASN
2	H	5	GLN
3	Y	57	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	214/214 (100%)	-0.72	0 100 100	11, 16, 20, 26	0
2	H	215/215 (100%)	-0.50	2 (0%) 84 61	14, 18, 23, 26	0
3	Y	129/129 (100%)	-0.75	0 100 100	11, 16, 20, 21	0
All	All	558/558 (100%)	-0.64	2 (0%) 92 77	11, 17, 22, 26	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	ASN	2.6
2	H	130	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.