

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 03:36 PM EDT

PDB ID	:	1A2Y
Title	:	HEN EGG WHITE LYSOZYME, D18A MUTANT, IN COMPLEX WITH
		MOUSE MONOCLONAL ANTIBODY D1.3
Authors	:	Tsuchiya, D.; Mariuzza, R.A.
Deposited on		
Resolution	:	1.50 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 following versions of software and data (see references (1)) were used in the production of this report:

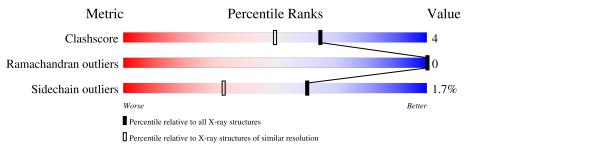
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.50 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)	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	А	107	93%	7% •
2	В	116	93%	7%
3	С	129	88%	11% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3244 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 IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	107	Total 843	C 533	N 139	O 169	${ m S} { m 2}$	0	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	3	VAL	GLU	conflict	UNP P01635
А	50	TYR	LYS	conflict	UNP P01635
А	51	THR	ALA	conflict	UNP P01635
А	52	THR	GLN	conflict	UNP P01635
А	?	-	PRO	deletion	UNP P01635
A	96	ARG	TRP	conflict	UNP P01635

• Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	116	Total 906	$\begin{array}{c} \mathrm{C} \\ 565 \end{array}$	N 157	0 180	S 4	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	5	GLN	LYS	conflict	UNP P01820
В	56	ASN	SER	conflict	UNP P01820
В	86	HIS	GLN	conflict	UNP P01820

• Molecule 3 is a protein called LYSOZYME.

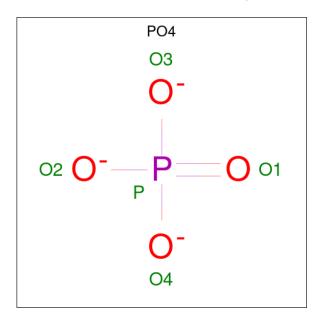
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	129	Total 1005	C 616	N 193	0 186	S 10	0	2	0



There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	ALA	ASP	engineered mutation	UNP P00698

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	С	1	Total 5	0 4	Р 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	166	Total O 166 166	0	0
5	В	168	Total O 168 168	0	0
5	С	151	Total O 151 151	0	0

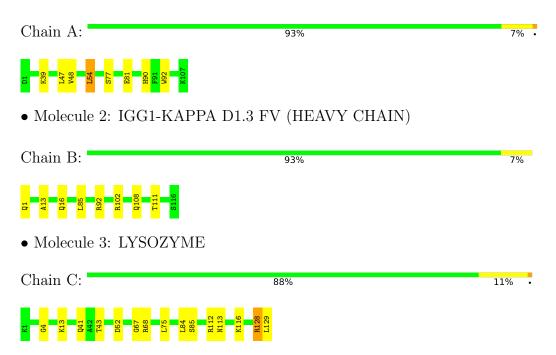


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	130.67Å 61.21 Å 57.42 Å	Depositor
a, b, c, α , β , γ	90.00° 119.14° 90.00°	Depositor
Resolution (Å)	7.00 - 1.50	Depositor
% Data completeness	90.4 (7.00-1.50)	Depositor
(in resolution range)	50.4 (1.00-1.50)	Depositor
R_{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3244	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP



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: PO4

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.68	0/892	0.70	1/1210~(0.1%)	
2	В	0.61	0/930	0.74	0/1260	
3	С	0.52	0/1033	0.67	1/1395~(0.1%)	
All	All	0.60	0/2855	0.70	2/3865~(0.1%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	А	47	LEU	CA-CB-CG	5.20	127.25	115.30
3	С	4	GLY	N-CA-C	-5.17	100.18	113.10

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	А	843	0	813	4	0
2	В	906	0	873	6	0
3	С	1005	0	963	12	0
4	С	5	0	0	1	0
5	А	166	0	0	2	0
5	В	168	0	0	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	151	0	0	4	0
All	All	3244	0	2649	22	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 4.

The worst 5 of 22 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)
3:C:116:LYS:HA	5:C:242:HOH:O	1.86	0.75
1:A:90:HIS:HD2	1:A:92:TRP:H	1.37	0.69
3:C:112:ARG:HD3	5:C:215:HOH:O	2.02	0.59
3:C:85:SER:HB3	5:C:154:HOH:O	2.04	0.57
2:B:13:ALA:O	2:B:16:GLN:HG2	2.05	0.57

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	Perce	ntiles
1	А	112/107~(105%)	109~(97%)	3~(3%)	0	100	100
2	В	115/116~(99%)	111 (96%)	4 (4%)	0	100	100
3	С	129/129~(100%)	124 (96%)	5 (4%)	0	100	100
All	All	356/352~(101%)	344 (97%)	12 (3%)	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	Percentil	es
1	А	98/91~(108%)	97~(99%)	1 (1%)	76 57	
2	В	101/100 (101%)	99~(98%)	2(2%)	55 25	
3	С	106/104 (102%)	104 (98%)	2(2%)	57 27	·
All	All	305/295~(103%)	300~(98%)	5(2%)	60 36	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	54	LEU
2	В	85	LEU
2	В	102	ARG
3	С	75	LEU
3	С	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	С	65	ASN
3	С	93	ASN
3	С	113	ASN
2	В	77	GLN
2	В	108	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	B	ond leng	gths	В	ond ang	gles
WIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	PO4	С	130	-	4,4,4	0.99	0	$6,\!6,\!6$	0.88	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	130	PO4	1	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

