wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 02:15 pm BST

PDB ID	:	1FDL
Title	:	CRYSTALLOGRAPHIC REFINEMENT OF THE THREE-DIMENSIONAL STRUCTURE OF THE FAB D1.3-LYSOZYME COMPLEX AT 2.5-ANGSTROMS RESOLUTION
Authors	:	Fischmann, T.O.; Poljak, R.J.
Deposited on	:	1990-08-27
Resolution	:	2.50 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 (i)) were used in the production of this report:

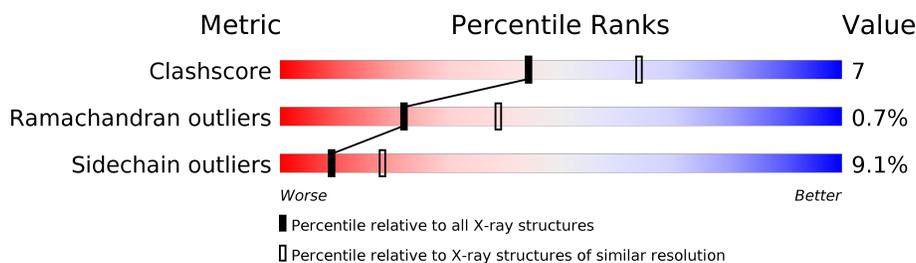|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		9.1%

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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	L	214	72% 24% •
2	H	218	67% 29% •
3	Y	129	72% 26% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4309 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 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1665	1037	282	339	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	50	TYR	ASN	CONFLICT	GB 2072141
L	51	THR	ALA	CONFLICT	GB 2072141
L	52	THR	LYS	CONFLICT	GB 2072141
L	85	SER	THR	CONFLICT	GB 2072141
L	89	GLN	HIS	CONFLICT	GB 2072141
L	96	ARG	TRP	CONFLICT	GB 2072141
L	106	ILE	VAL	CONFLICT	GB 2072141
L	118	PHE	LEU	CONFLICT	GB 2072141

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1643	1030	279	326	8			

- 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			

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. 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.
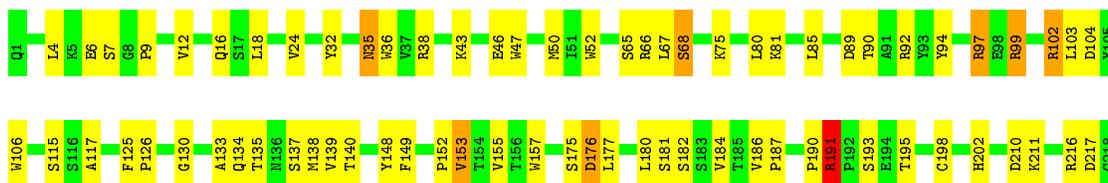
Note EDS was not executed.

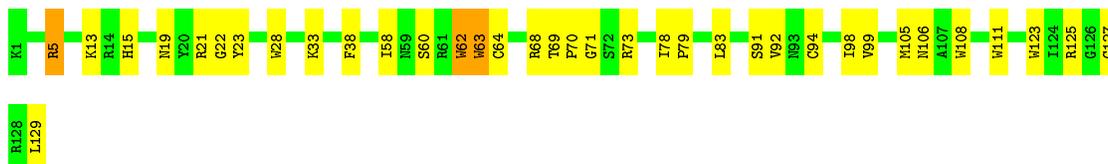• Molecule 1: IGG1-KAPPA D1.3 FAB (LIGHT CHAIN)

Chain L:
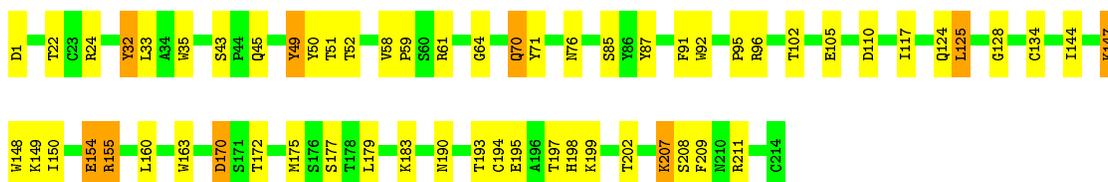
• Molecule 2: IGG1-KAPPA D1.3 FAB (HEAVY CHAIN)

Chain H:

• Molecule 3: HEN EGG WHITE LYSOZYME

Chain Y:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.00Å 143.50Å 49.30Å 90.00° 120.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4309	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

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	0.80	0/1705	1.54	26/2315 (1.1%)
2	H	0.88	0/1684	1.83	34/2300 (1.5%)
3	Y	0.91	0/1021	1.77	25/1379 (1.8%)
All	All	0.85	0/4410	1.71	85/5994 (1.4%)

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	66	ARG	NE-CZ-NH2	-19.60	110.50	120.30
2	H	191	ARG	NE-CZ-NH1	13.71	127.16	120.30
2	H	97	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	L	163	TRP	CD1-CG-CD2	10.21	114.47	106.30
2	H	52	TRP	CD1-CG-CD2	9.68	114.04	106.30

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	1665	0	1583	20	0
2	H	1643	0	1611	24	0
3	Y	1001	0	959	15	0
All	All	4309	0	4153	56	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 7.

The worst 5 of 56 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)
2:H:191:ARG:HG2	2:H:191:ARG:HH11	1.31	0.94
2:H:191:ARG:HG2	2:H:191:ARG:NH1	1.97	0.75
1:L:61:ARG:HB2	1:L:76:ASN:O	1.95	0.67
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.78	0.66
1:L:155:ARG:HH11	1:L:179:LEU:HD11	1.62	0.63

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%)	199 (94%)	11 (5%)	2 (1%)	17	31
2	H	216/218 (99%)	201 (93%)	13 (6%)	2 (1%)	17	31
3	Y	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
All	All	555/561 (99%)	515 (93%)	36 (6%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	170	ASP
1	L	199	LYS
2	H	133	ALA
2	H	137	SER

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	189/189 (100%)	168 (89%)	21 (11%)	6	11
2	H	190/190 (100%)	169 (89%)	21 (11%)	6	11
3	Y	105/105 (100%)	103 (98%)	2 (2%)	57	80
All	All	484/484 (100%)	440 (91%)	44 (9%)	9	18

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	208	SER
2	H	16	GLN
2	H	195	THR
1	L	209	PHE
2	H	9	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
3	Y	106	ASN
1	L	189	HIS
1	L	76	ASN
1	L	90	HIS

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)

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.