



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1DZB
Title : CRYSTAL STRUCTURE OF PHAGE LIBRARY-DERIVED SINGLE-CHAIN FV FRAGMENT 1F9 IN COMPLEX WITH TURKEY EGG-WHITE LYSOZYME
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Deposited on : 2000-02-23
Resolution : 2.00 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

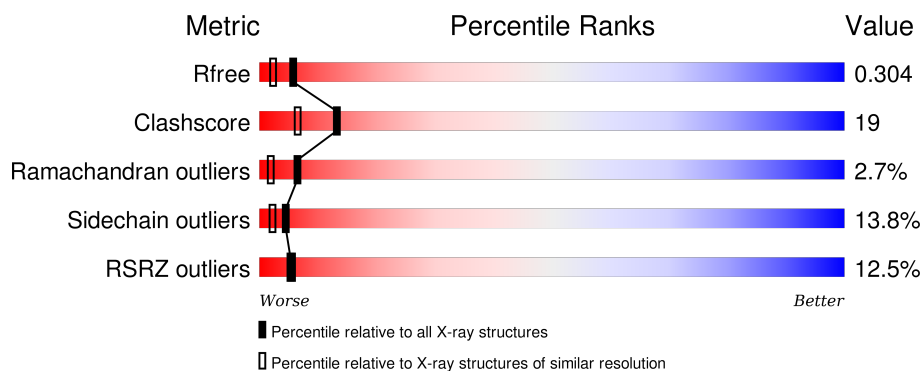
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	A	253	<div> <div>8%</div> <div>50%</div> <div>27%</div> <div>9%</div> <div>11%</div> </div>
1	B	253	<div> <div>9%</div> <div>47%</div> <div>29%</div> <div>10%</div> <div>11%</div> </div>
2	X	129	<div> <div>%</div> <div>68%</div> <div>28%</div> <div>•</div> </div>
2	Y	129	<div> <div>33%</div> <div>60%</div> <div>27%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5709 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 SCFV FRAGMENT 1F9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	2
			1727	1086	284	351	6			
1	B	224	Total	C	N	O	S	0	0	2
			1727	1086	284	351	6			

- Molecule 2 is a protein called TURKEY EGG-WHITE LYSOZYME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	129	Total	C	N	O	S	0	1	0
			1001	615	194	182	10			
2	Y	129	Total	C	N	O	S	0	0	0
			994	611	191	182	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	105	Total	O	0	0
			105	105		
3	X	53	Total	O	0	0
			53	53		
3	Y	28	Total	O	0	0
			28	28		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

8% 50% 27% 9% 11%

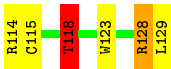
Q1 V2 K3 L4 Q5 Q6 S7 G8 V12 K13 V18 F27 N28 I29 K30 D31 T32 Y33 M34 H35 Q43 W47 R50 I51 D52 P53 K59 Y60 D61 P62 K63 T71 T74 S75 W76 N77 Y80 L81 S84 S85 L86 T87 S88 R98 W99 D100 Y101 Y102 F103 D104 V105 L106 G107 Q108 G109 T110 S116 G117 G1Y G1Y S1R G1Y G1Y G1Y G1Y G1Y G1Y S1R D201 T202 E203 L204 S207 P208 W211 V212 T213 S214 L215 G216 V219 S226 A227 A228 A229 G230 S231 T232 L233 R234 W235 T236 Q237 Q238 T239 P240 K245 T246 L247 I248 Y249 Y250 A251 G257 S260 S261 Q269 L273 S276 S277 L278 E279 S280 D281 L282 T283 T284 Y287 C288 L289 Q290 H291 G292 E293 S294 P295 Y296 T297 L304 E305 L306 K307 ARG ALA ALA ALA GLU GLU GLN LYS LEU LEU ILE R234 GLU GLU ASP LEU ASN K245 T246

Chain B:

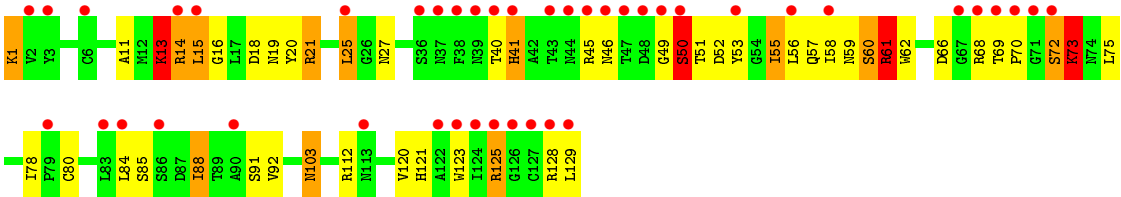
9% 47% 29% 10% 11%

Chain X:

Item	Category
K1	Green
E7	Green
A11	Green
R14	Green
D18	Green
N19	Green
Y20	Green
R21	Green
L25	Green
K33	Green
S36	Green
R45	Green
D49	Green
I55	Green
I58	Green
N59	Green
S60	Green
R61	Green
K62	Green
K63	Green
D66	Green
G67	Green
G67	Green
R68	Green
T69	Green
P70	Green
G71	Green
S72	Green
K73	Green
N74	Green
L75	Green
C76	Green
L83	Green
D87	Green
I98	Green
A99	Green
S100	Green
G101	Green
G102	Green
M103	Green
V109	Green
A110	Green
W111	Green
R112	Green
K113	Green



● Molecule 2: TURKEY EGG-WHITE LYSOZYME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.71Å 112.44Å 80.00Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.00) 87.9 (19.77-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.306 0.227 , 0.304	Depositor DCC
R_{free} test set	2011 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40208 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5709	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 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.14	3/1768 (0.2%)	1.84	48/2404 (2.0%)
1	B	1.17	2/1768 (0.1%)	1.99	50/2404 (2.1%)
2	X	1.22	2/1026 (0.2%)	1.81	26/1385 (1.9%)
2	Y	0.98	0/1015	1.79	13/1371 (0.9%)
All	All	1.14	7/5577 (0.1%)	1.88	137/7564 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	74	ASN	N-CA	6.42	1.59	1.46
1	A	231	SER	CA-CB	5.90	1.61	1.52
1	A	84	SER	CA-CB	5.70	1.61	1.52
1	A	208	PRO	N-CA	-5.53	1.37	1.47
1	B	98	ARG	NE-CZ	-5.46	1.25	1.33

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ARG	NE-CZ-NH1	26.30	133.45	120.30
2	Y	21	ARG	CD-NE-CZ	21.04	153.05	123.60
1	B	98	ARG	CD-NE-CZ	19.00	150.20	123.60
2	X	45	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	A	281	ASP	CA-CB-CG	13.57	143.26	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	SER	Mainchain,Peptide
1	A	294	SER	Mainchain,Peptide
1	B	207	SER	Mainchain,Peptide
1	B	294	SER	Mainchain,Peptide

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	1727	0	1646	69	0
1	B	1727	0	1646	89	0
2	X	1001	0	965	21	0
2	Y	994	0	956	34	0
3	A	74	0	0	6	0
3	B	105	0	0	4	0
3	X	53	0	0	3	0
3	Y	28	0	0	0	0
All	All	5709	0	5213	202	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 19.

The worst 5 of 202 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:30:LYS:HE3	1:A:74:THR:HB	1.43	1.01
1:A:71:THR:HG22	1:A:80:TYR:HB2	1.42	0.99
1:A:278:LEU:HD21	1:A:306:ILE:HD12	1.47	0.96
1:A:35:HIS:HD2	1:A:47:TRP:HE1	1.10	0.95
1:B:29:ILE:H	1:B:77:ASN:HD21	1.11	0.94

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	220/253 (87%)	200 (91%)	13 (6%)	7 (3%)	5	1
1	B	220/253 (87%)	202 (92%)	10 (4%)	8 (4%)	4	1
2	X	128/129 (99%)	123 (96%)	4 (3%)	1 (1%)	24	15
2	Y	127/129 (98%)	106 (84%)	18 (14%)	3 (2%)	7	2
All	All	695/764 (91%)	631 (91%)	45 (6%)	19 (3%)	6	2

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	LEU
1	A	229	ILE
1	A	276	SER
1	B	8	GLY
1	B	215	LEU

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	191/207 (92%)	161 (84%)	30 (16%)	3	1
1	B	191/207 (92%)	165 (86%)	26 (14%)	5	2
2	X	104/103 (101%)	97 (93%)	7 (7%)	20	14
2	Y	103/103 (100%)	85 (82%)	18 (18%)	2	1
All	All	589/620 (95%)	508 (86%)	81 (14%)	4	2

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	B	226	SER
2	Y	78	ILE
1	B	59	LYS
1	B	98	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	B	237	GLN
2	Y	59	ASN
1	B	108	GLN
1	B	290	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 ⓘ

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	A	224/253 (88%)	0.53	20 (8%) 12 13	15, 27, 70, 80	0
1	B	224/253 (88%)	0.47	24 (10%) 8 8	11, 24, 68, 79	0
2	X	129/129 (100%)	-0.20	1 (0%) 87 88	12, 20, 32, 51	0
2	Y	129/129 (100%)	1.56	43 (33%) 0 1	15, 43, 73, 80	0
All	All	706/764 (92%)	0.56	88 (12%) 5 5	11, 27, 69, 80	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	48	ASP	8.6
1	B	117	GLY	7.9
2	Y	129	LEU	6.9
1	B	229	ILE	6.7
1	A	215	LEU	6.2

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.