wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 02:03 PM EDT

PDB ID	:	1QSW
Title	:	CRYSTAL STRUCTURE ANALYSIS OF A HUMAN LYSOZYME MUTANT W64C C65A
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Deposited on	:	1999-06-24
Resolution	:	1.85 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:

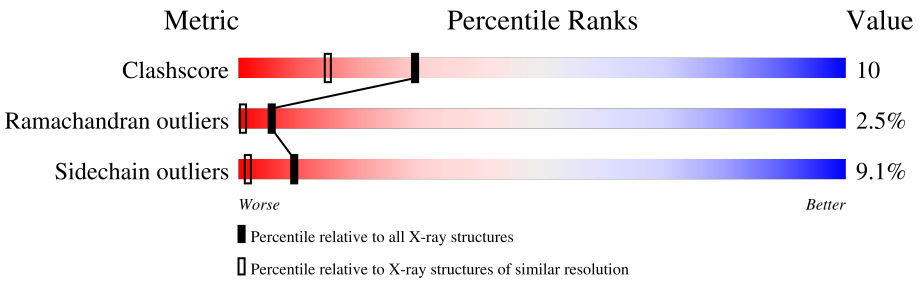
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.85 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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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	A	130	67% 25% 5% •
1	B	130	77% 22% •
1	C	130	70% 21% 8% •
1	D	130	69% 20% 7% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4312 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 HUMAN LYSOZYME MUTANT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	130	1020	625	199	186	10	0	0	0
1	B	130	1020	625	199	186	10	0	0	0
1	C	130	1020	625	199	186	10	0	0	0
1	D	130	1020	625	199	186	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	CYS	TRP	engineered mutation	UNP P61626
A	65	ALA	CYS	engineered mutation	UNP P61626
B	64	CYS	TRP	engineered mutation	UNP P61626
B	65	ALA	CYS	engineered mutation	UNP P61626
C	64	CYS	TRP	engineered mutation	UNP P61626
C	65	ALA	CYS	engineered mutation	UNP P61626
D	64	CYS	TRP	engineered mutation	UNP P61626
D	65	ALA	CYS	engineered mutation	UNP P61626

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	50	50	50	0	0
2	B	60	60	60	0	0
2	C	48	48	48	0	0
2	D	74	74	74	0	0

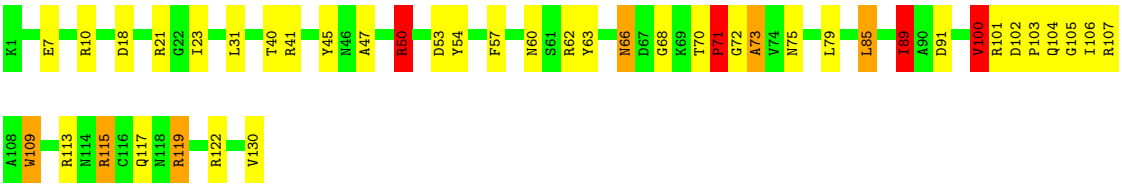
3 Residue-property plots (i)

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: HUMAN LYSOZYME MUTANT

Chain A:

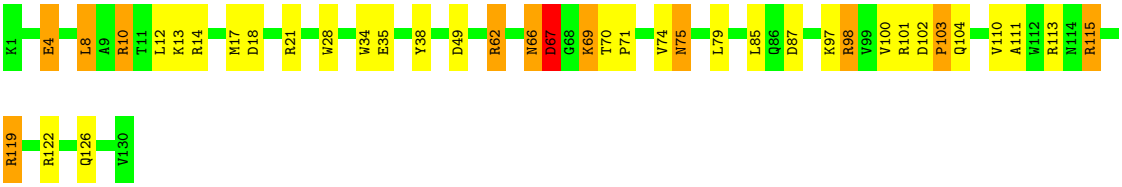


• Molecule 1: HUMAN LYSOZYME MUTANT

Chain B:

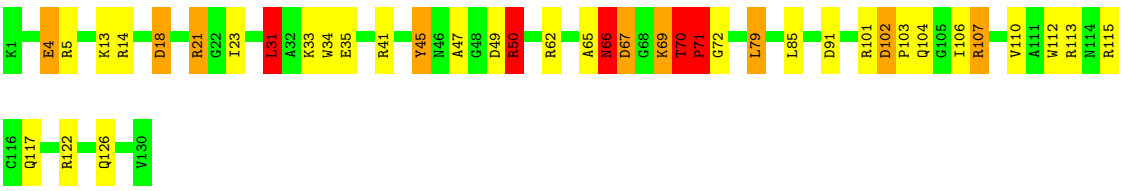
• Molecule 1: HUMAN LYSOZYME MUTANT

Chain C:



• Molecule 1: HUMAN LYSOZYME MUTANT

Chain D:



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	Depositor
Cell constants a, b, c, α, β, γ	45.92Å 107.24Å 32.08Å 98.59° 110.45° 78.04°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.85)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4312	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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	A	0.81	0/1038	1.67	19/1400 (1.4%)
1	B	0.86	0/1038	1.78	23/1400 (1.6%)
1	C	0.82	0/1038	1.64	13/1400 (0.9%)
1	D	1.03	1/1038 (0.1%)	1.95	27/1400 (1.9%)
All	All	0.89	1/4152 (0.0%)	1.77	82/5600 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	PRO	N-CD	16.45	1.70	1.47

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	71	PRO	CA-N-CD	-22.40	80.14	111.50
1	D	70	THR	O-C-N	17.39	154.13	121.10
1	B	119	ARG	NE-CZ-NH2	16.77	128.69	120.30
1	D	70	THR	C-N-CD	-15.57	86.35	120.60
1	C	62	ARG	NE-CZ-NH1	13.03	126.81	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	A	1020	0	987	30	1
1	B	1020	0	987	8	0
1	C	1020	0	987	14	0
1	D	1020	0	987	26	0
2	A	50	0	0	4	0
2	B	60	0	0	2	0
2	C	48	0	0	2	0
2	D	74	0	0	2	1
All	All	4312	0	3948	77	1

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 10.

The worst 5 of 77 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:D:71:PRO:N	1:D:71:PRO:CD	1.70	1.32
1:D:70:THR:C	1:D:71:PRO:CD	2.09	1.21
1:A:122:ARG:HH11	1:C:119:ARG:HG2	1.40	0.86
1:D:70:THR:C	1:D:71:PRO:HD3	2.04	0.78
1:A:70:THR:N	1:A:71:PRO:HD3	2.03	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:O	2:D:200:HOH:O[1_444]	2.04	0.16

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	128/130 (98%)	119 (93%)	5 (4%)	4 (3%)	4 0
1	B	128/130 (98%)	122 (95%)	5 (4%)	1 (1%)	19 7
1	C	128/130 (98%)	118 (92%)	7 (6%)	3 (2%)	6 1
1	D	128/130 (98%)	119 (93%)	4 (3%)	5 (4%)	3 0
All	All	512/520 (98%)	478 (93%)	21 (4%)	13 (2%)	5 1

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ALA
1	C	103	PRO
1	D	66	ASN
1	D	67	ASP
1	D	71	PRO

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	104/104 (100%)	96 (92%)	8 (8%)	13 2
1	B	104/104 (100%)	99 (95%)	5 (5%)	25 10
1	C	104/104 (100%)	88 (85%)	16 (15%)	2 0
1	D	104/104 (100%)	95 (91%)	9 (9%)	10 2
All	All	416/416 (100%)	378 (91%)	38 (9%)	9 1

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	126	GLN
1	D	79	LEU
1	D	4	GLU
1	D	50	ARG
1	D	107	ARG

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

Mol	Chain	Res	Type
1	B	86	GLN
1	C	126	GLN
1	C	44	ASN
1	D	117	GLN
1	C	118	ASN

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)

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.