W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 02:35 pm GMT

PDB ID	:	1NBY
Title	:	Crystal Structure of HyHEL-63 complexed with HEL mutant K96A
Authors	:	Mariuzza, R.A.; Li, Y.; Urrutia, M.; Smith-Gill, S.J.
Deposited on	:	2002-12-04
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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 1.80 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		14
Ramachandran outliers		0.9%
Sidechain outliers		2.5%

Worse   *Better*

▪ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
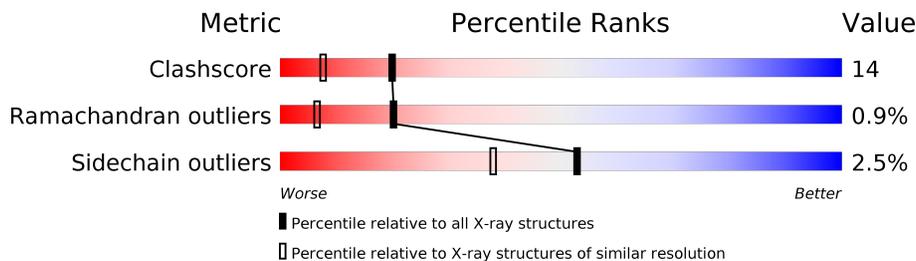
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	85% 13% •
2	B	210	80% 17% •
3	C	129	77% 22% •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4911 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 antibody kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total 1657	C 1027	N 280	O 343	S 7	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	GLU	CLONING ARTIFACT	UNP P01837
A	2	ILE	LEU	CLONING ARTIFACT	UNP P01837
A	4	LEU	MET	CLONING ARTIFACT	UNP P01837

- Molecule 2 is a protein called immunoglobulin gamma 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total 1587	C 1002	N 253	O 326	S 6	0	0	0

- Molecule 3 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total 997	C 610	N 192	O 185	S 10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	696	ALA	LYS	ENGINEERED	UNP P00698

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total 279	O 279	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	281	Total 281	O 281	0	0
4	C	110	Total 110	O 110	0	0

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.

Note EDS was not executed.

- Molecule 1: antibody kappa light chain
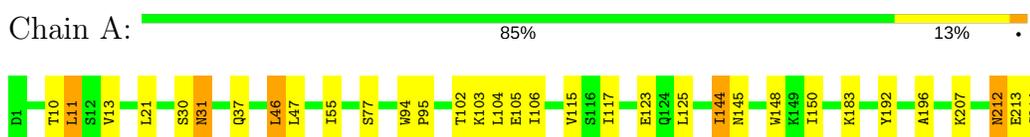
Chain A:

- Molecule 2: immunoglobulin gamma 1 chain

Chain B:
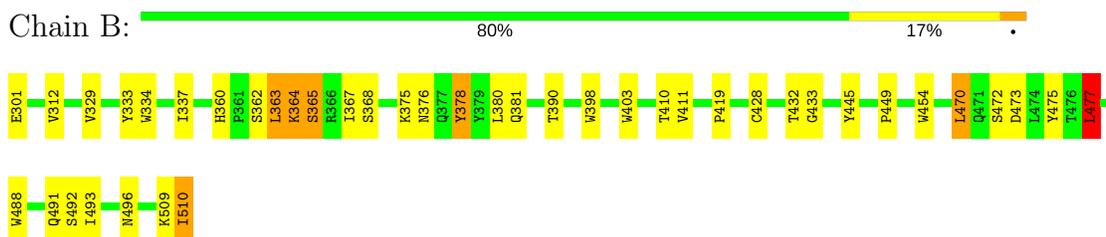
- Molecule 3: Lysozyme C

Chain C:
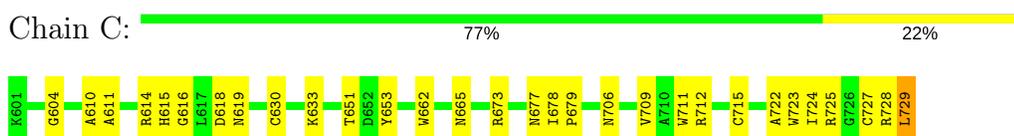
4　Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.87Å　　90.87Å　　151.94Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	19.89　–　1.80	Depositor
% Data completeness (in resolution range)	97.0 (19.89-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216　,　0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4911	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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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	0.40	0/1695	0.69	0/2300
2	B	0.44	0/1629	0.74	1/2233 (0.0%)
3	C	0.37	0/1017	0.65	1/1375 (0.1%)
All	All	0.41	0/4341	0.70	2/5908 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	477	LEU	CA-CB-CG	5.80	128.63	115.30
3	C	604	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	378	TYR	Sidechain

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	1657	0	1575	37	0
2	B	1587	0	1536	49	0
3	C	997	0	954	30	0
4	A	279	0	0	4	0
4	B	281	0	0	1	0
4	C	110	0	0	5	0
All	All	4911	0	4065	111	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 14.

The worst 5 of 111 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:B:488:TRP:HD1	2:B:493:ILE:HD13	1.24	1.01
2:B:367:ILE:HD11	2:B:380:LEU:HD12	1.44	0.97
2:B:329:VAL:H	2:B:376:ASN:HD21	1.12	0.92
2:B:493:ILE:O	2:B:510:ILE:HD13	1.74	0.88
2:B:367:ILE:HD11	2:B:380:LEU:CD1	2.05	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	32	17
2	B	208/210 (99%)	200 (96%)	4 (2%)	4 (2%)	9	2
3	C	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
All	All	547/553 (99%)	527 (96%)	15 (3%)	5 (1%)	20	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	365	SER
1	A	77	SER
2	B	364	LYS
2	B	433	GLY
2	B	432	THR

5.3.2 Protein sidechains ⓘ

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	193/193 (100%)	188 (97%)	5 (3%)	51	36
2	B	186/186 (100%)	180 (97%)	6 (3%)	44	28
3	C	104/104 (100%)	103 (99%)	1 (1%)	80	75
All	All	483/483 (100%)	471 (98%)	12 (2%)	53	38

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	363	LEU
2	B	449	PRO
2	B	496	ASN
1	A	212	ASN
2	B	477	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	376	ASN
2	B	381	GLN
3	C	693	ASN
2	B	360	HIS
3	C	641	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.