



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:23 PM GMT

PDB ID : 1KTR
Title : Crystal Structure of the Anti-His Tag Antibody 3D5 Single-Chain Fragment (scFv) in Complex with a Oligohistidine peptide
Authors : Kaufmann, M.; Lindner, P.; Honegger, A.; Blank, K.; Tschopp, M.; Capitani, G.; Plueckthun, A.; Gruetter, M.G.
Deposited on : 2002-01-17
Resolution : 2.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

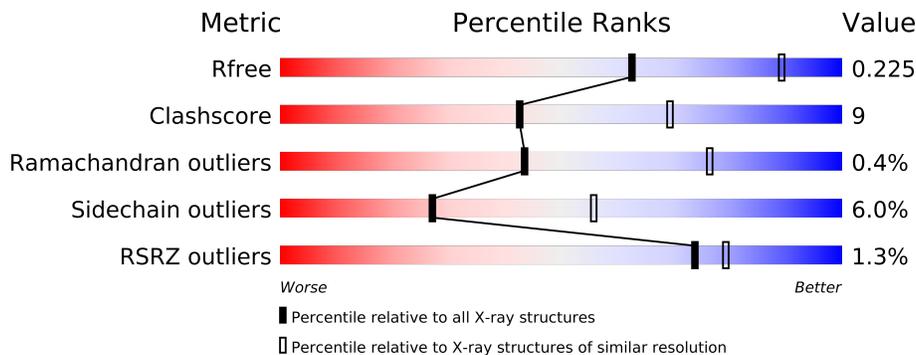
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	116	
2	M	20	
3	H	114	
4	P	6	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1945 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Anti-his tag antibody 3d5 variable light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	113	873	552	148	170	3	0	0	0

- Molecule 2 is a protein called Peptide linker.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	M	2	8	4	2	2	0	0	0

- Molecule 3 is a protein called Anti-his tag antibody 3d5 variable heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	114	872	542	144	182	4	0	0	0

- Molecule 4 is a protein called Oligohistidine peptide Antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	P	4	36	21	10	5	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	83	Total	O	0	0
			83	83		
5	L	66	Total	O	0	0
			66	66		
5	M	2	Total	O	0	0
			2	2		
5	P	5	Total	O	0	0
			5	5		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.51Å 106.51Å 92.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.70) 99.1 (29.33-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.222 0.194 , 0.225	Depositor DCC
R_{free} test set	996 reflections (5.88%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.5	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16996 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1945	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	L	0.34	0/893	0.64	0/1207
2	M	0.52	0/7	0.52	0/7
3	H	0.35	0/891	0.63	0/1206
4	P	0.40	0/38	0.35	0/49
All	All	0.35	0/1829	0.63	0/2469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	873	0	858	15	0
2	M	8	0	5	0	0
3	H	872	0	826	16	0
4	P	36	0	22	0	0
5	H	83	0	0	0	0
5	L	66	0	0	4	0
5	M	2	0	0	0	0
5	P	5	0	0	0	0
All	All	1945	0	1711	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:3:GLN:HE21	3:H:5:GLN:HG3	1.51	0.74
3:H:50:LYS:NZ	3:H:50:LYS:HB3	2.14	0.63
3:H:47:SER:HB3	3:H:102:SER:OG	2.00	0.62
1:L:101:LEU:HD12	1:L:145:LEU:CD1	2.33	0.58
3:H:107:GLU:CG	3:H:136:GLY:HA2	2.35	0.57

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	L	111/116 (96%)	105 (95%)	5 (4%)	1 (1%)	25	55
3	H	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
4	P	2/6 (33%)	2 (100%)	0	0	100	100
All	All	225/236 (95%)	218 (97%)	6 (3%)	1 (0%)	43	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	84	GLY

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	L	100/103 (97%)	95 (95%)	5 (5%)	34	66
3	H	96/96 (100%)	89 (93%)	7 (7%)	20	44
4	P	3/6 (50%)	3 (100%)	0	100	100
All	All	199/205 (97%)	187 (94%)	12 (6%)	27	56

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

Mol	Chain	Res	Type
3	H	2	VAL
3	H	24	LYS
3	H	93	LEU
1	L	101	LEU
3	H	82	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	3	GLN
3	H	109	GLN
3	H	5	GLN
1	L	111	HIS
3	H	46	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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

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	L	113/116 (97%)	-0.51	1 (0%) 81 85	20, 34, 48, 66	0
2	M	2/20 (10%)	-0.38	0 100 100	35, 35, 35, 42	0
3	H	114/114 (100%)	-0.47	2 (1%) 65 71	19, 26, 49, 70	0
4	P	4/6 (66%)	-0.73	0 100 100	21, 26, 27, 33	0
All	All	233/256 (91%)	-0.49	3 (1%) 74 79	19, 30, 49, 70	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	149	ALA	4.3
1	L	95	ARG	2.2
3	H	14	LYS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.