



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:10 PM GMT

PDB ID : 4NYL
Title : Crystal structure of adalimumab FAB fragment
Authors : Fan, L.J.; Lv, L.L.; Zhang, Q.J.; Chen, C.L.
Deposited on : 2013-12-10
Resolution : 2.80 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

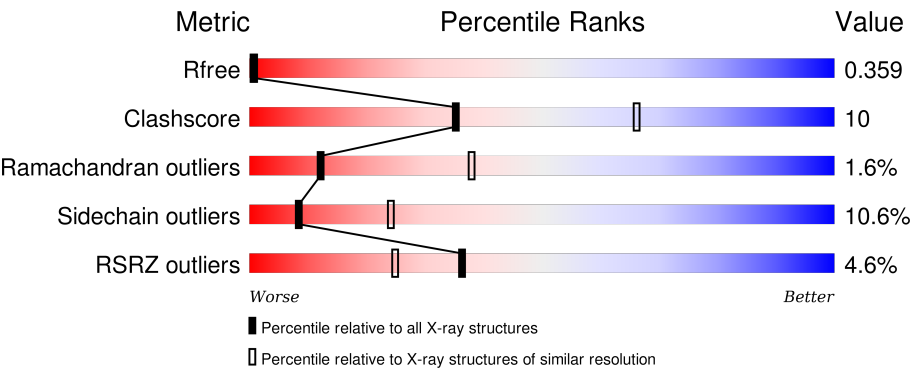
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	B	214	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>41%11%•45%</div></div>
1	D	214	<div><div></div><div><div></div><div></div></div><div>77%19%••</div></div>
1	F	214	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>46%9%•42%</div></div>
1	L	214	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>78%19%••</div></div>
2	A	230	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>68%16%•13%</div></div>

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Mol	Chain	Length	Quality of chain
2	C	230	<div><div></div><div>73%</div><div>15%</div><div>•</div><div>7%</div></div>
2	E	230	<div><div>3%</div><div></div><div>54%</div><div>14%</div><div>•</div><div>30%</div></div>
2	H	230	<div><div></div><div>66%</div><div>22%</div><div>••</div><div>8%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10495 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 Adalimumab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1546	966	262	313	5			
1	B	117	Total	C	N	O	S	0	0	0
			829	518	144	164	3			
1	D	211	Total	C	N	O	S	0	0	0
			1557	972	261	319	5			
1	F	124	Total	C	N	O	S	0	0	0
			876	543	149	181	3			

- Molecule 2 is a protein called Adalimumab Heavy Chain.

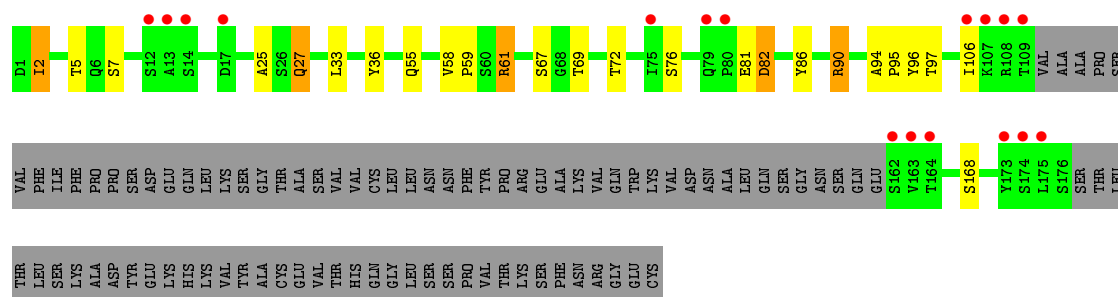
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1564	991	263	304	6			
2	A	199	Total	C	N	O	S	0	0	0
			1405	879	239	281	6			
2	C	213	Total	C	N	O	S	0	0	0
			1561	987	263	305	6			
2	E	162	Total	C	N	O	S	0	1	0
			1155	723	200	228	4			

- Molecule 3 is water.

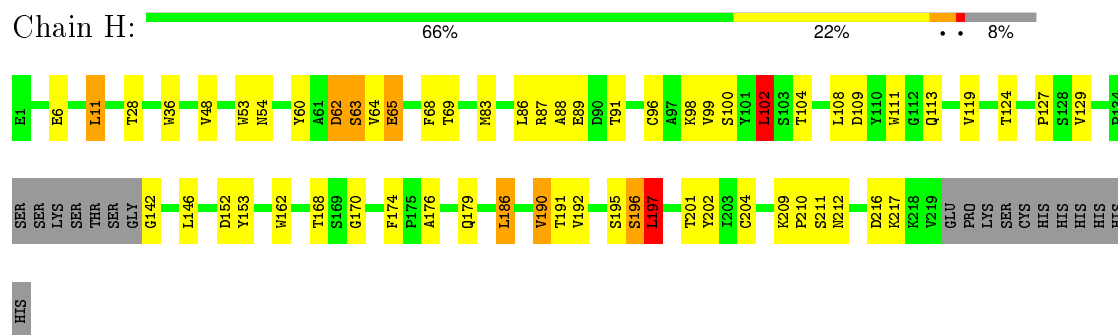
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		

- Molecule 1: Adalimumab Light Chain

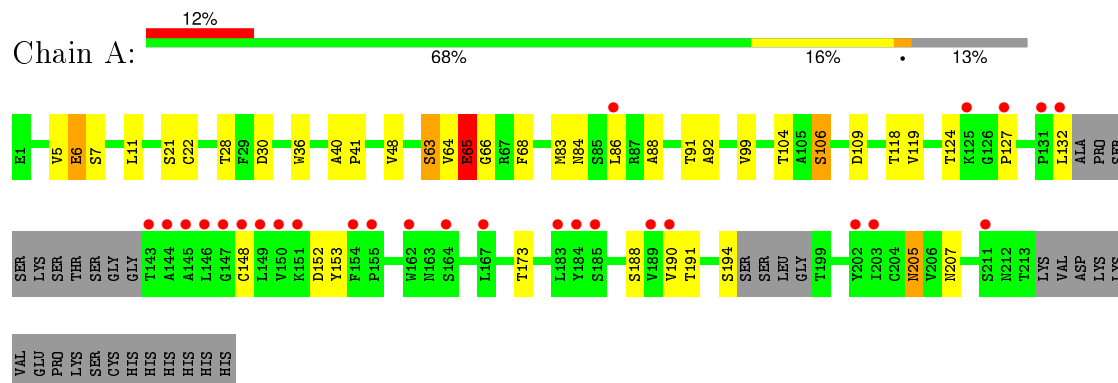




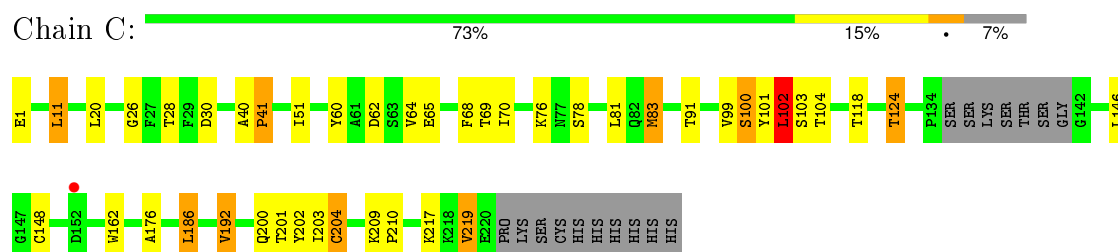
• Molecule 2: Adalimumab Heavy Chain



• Molecule 2: Adalimumab Heavy Chain



• Molecule 2: Adalimumab Heavy Chain



• Molecule 2: Adalimumab Heavy Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.42Å 47.05Å 168.51Å 90.00° 101.33° 90.00°	Depositor
Resolution (Å)	42.03 – 2.80 40.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.1 (42.03-2.80) 87.1 (40.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.275 , 0.358 0.273 , 0.359	Depositor DCC
R_{free} test set	2249 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 44308 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 [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	B	0.53	0/848	0.73	0/1161
1	D	0.55	0/1591	0.74	1/2177 (0.0%)
1	F	0.49	0/892	0.69	0/1221
1	L	0.53	0/1580	0.75	0/2162
2	A	0.50	0/1438	0.68	0/1974
2	C	0.57	0/1599	0.77	3/2189 (0.1%)
2	E	0.54	0/1186	0.72	0/1623
2	H	0.62	1/1602 (0.1%)	0.80	0/2189
All	All	0.55	1/10736 (0.0%)	0.74	4/14696 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	142	GLY	N-CA	-5.14	1.38	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	103	SER	N-CA-C	-5.74	95.49	111.00
1	D	93	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	C	102	LEU	CA-CB-CG	5.54	128.05	115.30
2	C	30	ASP	CB-CG-OD2	5.00	122.80	118.30

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	B	829	0	747	20	0
1	D	1557	0	1433	25	0
1	F	876	0	773	15	0
1	L	1546	0	1422	29	0
2	A	1405	0	1243	19	0
2	C	1561	0	1472	27	0
2	E	1155	0	1019	20	0
2	H	1564	0	1489	42	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	10495	0	9598	197	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 10.

The worst 5 of 197 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:196:SER:OG	2:H:197:LEU:HD23	1.51	1.10
2:A:40:ALA:HB1	2:A:41:PRO:HD2	1.42	1.01
1:L:107:LYS:CB	1:L:108:ARG:HA	1.92	1.00
2:H:88:ALA:O	2:H:91:THR:HG23	1.66	0.94
2:H:197:LEU:HD23	2:H:197:LEU:N	1.87	0.88

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	B	115/214 (54%)	97 (84%)	13 (11%)	5 (4%)	3 10
1	D	209/214 (98%)	183 (88%)	24 (12%)	2 (1%)	19 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	120/214 (56%)	108 (90%)	12 (10%)	0	100	100
1	L	209/214 (98%)	195 (93%)	10 (5%)	4 (2%)	10	32
2	A	193/230 (84%)	168 (87%)	22 (11%)	3 (2%)	12	38
2	C	209/230 (91%)	196 (94%)	12 (6%)	1 (0%)	34	69
2	E	159/230 (69%)	139 (87%)	17 (11%)	3 (2%)	10	32
2	H	208/230 (90%)	189 (91%)	14 (7%)	5 (2%)	7	25
All	All	1422/1776 (80%)	1275 (90%)	124 (9%)	23 (2%)	12	38

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	107	LYS
1	L	124	GLN
1	L	211	ARG
2	H	102	LEU
2	H	196	SER

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	B	80/186 (43%)	71 (89%)	9 (11%)	7	22
1	D	165/186 (89%)	147 (89%)	18 (11%)	8	23
1	F	85/186 (46%)	72 (85%)	13 (15%)	3	10
1	L	162/186 (87%)	152 (94%)	10 (6%)	23	54
2	A	138/194 (71%)	121 (88%)	17 (12%)	6	18
2	C	165/194 (85%)	147 (89%)	18 (11%)	8	23
2	E	110/194 (57%)	99 (90%)	11 (10%)	9	27
2	H	166/194 (86%)	149 (90%)	17 (10%)	9	26
All	All	1071/1520 (70%)	958 (89%)	113 (11%)	8	24

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	205	ASN
1	D	97	THR
2	E	28	THR
2	A	207	ASN
1	D	20	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	163	ASN
2	H	200	GLN
2	C	207	ASN
2	H	113	GLN
2	C	200	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 ⓘ

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	B	117/214 (54%)	0.20	7 (5%) 25 15	49, 83, 104, 140	0
1	D	211/214 (98%)	-0.20	1 (0%) 91 88	44, 63, 82, 93	0
1	F	124/214 (57%)	0.41	17 (13%) 4 2	54, 83, 103, 121	0
1	L	211/214 (98%)	-0.17	5 (2%) 62 50	46, 64, 85, 99	0
2	A	199/230 (86%)	0.35	27 (13%) 4 2	47, 75, 116, 126	0
2	C	213/230 (92%)	-0.26	1 (0%) 91 88	37, 64, 79, 98	0
2	E	162/230 (70%)	0.06	8 (4%) 33 22	45, 69, 122, 140	0
2	H	212/230 (92%)	-0.29	0 100 100	45, 61, 76, 101	0
All	All	1449/1776 (81%)	-0.03	66 (4%) 36 25	37, 66, 102, 140	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	ILE	7.1
2	A	150	VAL	5.6
2	E	166	ALA	5.5
1	F	174	SER	5.3
1	F	80	PRO	4.7

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.