Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:05 PM GMT

PDB ID	:	4KHX
Title	:	Crystal structure of gp41 helix complexed with antibody 8062
Authors	:	Li, M.; Gustchina, A,; Wlodawer, A.
Deposited on	:	2013-05-01
Resolution	:	2.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

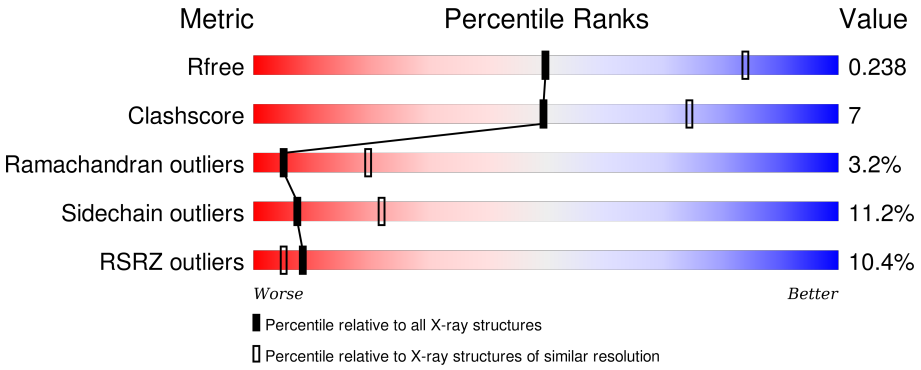
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	67	7%, 76%, 21%
2	H	245	8%, 63%, 19%, 15%
3	L	213	12%, 68%, 27%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3625 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 gp41 helix.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			525	333	95	95	2			

- Molecule 2 is a protein called 8062 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1566	999	256	305	6			

- Molecule 3 is a protein called 8062 light chain.

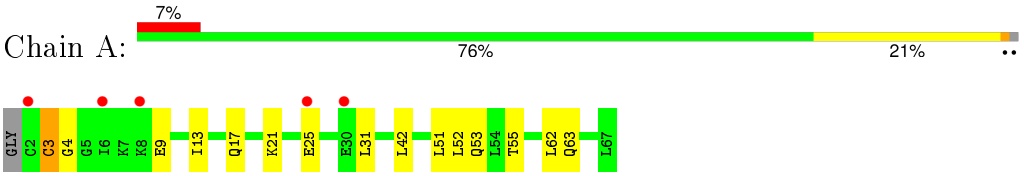
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	205	Total	C	N	O	S	0	0	0
			1534	961	251	317	5			

3 Residue-property plots (i)

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 (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.

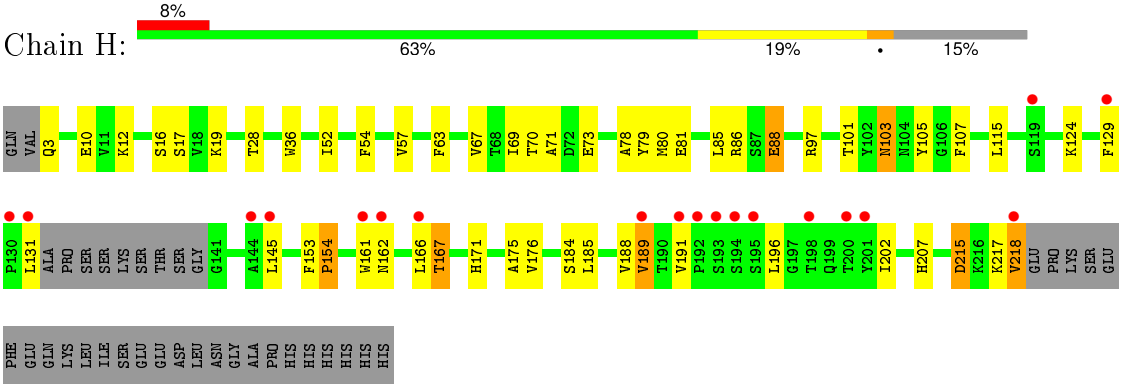
- Molecule 1: gp41 helix

Chain A:



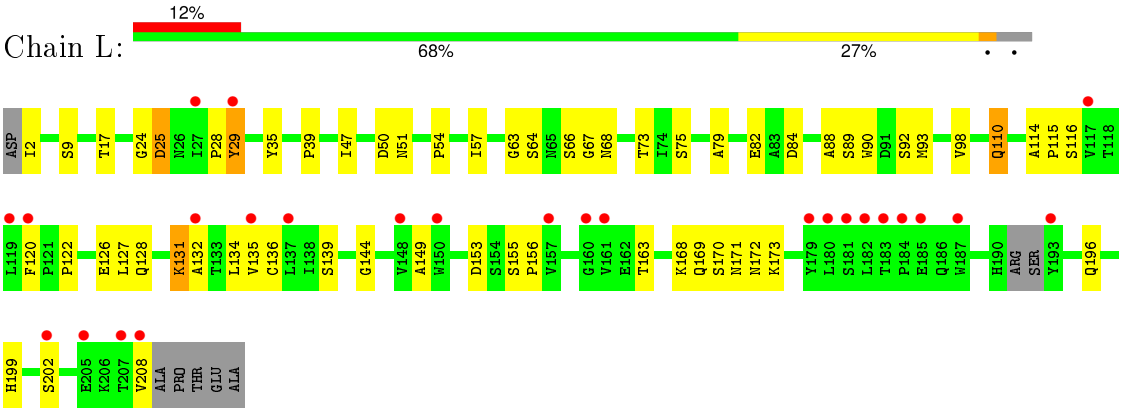
- Molecule 2: 8062 heavy chain

Chain H:



- Molecule 3: 8062 light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.81Å 106.81Å 98.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.95 – 2.92 41.87 – 2.92	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.95-2.92) 86.7 (41.87-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.237 , 0.289 0.226 , 0.238	Depositor DCC
R_{free} test set	621 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.3	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 13239 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3625	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.29	0/527	0.44	0/702
2	H	0.26	0/1605	0.44	0/2186
3	L	0.25	0/1572	0.46	0/2151
All	All	0.26	0/3704	0.45	0/5039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	525	0	571	5	0
2	H	1566	0	1524	28	0
3	L	1534	0	1465	23	0
All	All	3625	0	3560	51	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 7.

All (51) 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)
3:L:131:LYS:HA	3:L:132:ALA:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:CYS:SG	1:A:4:GLY:N	2.63	0.70
3:L:17:THR:HG22	3:L:75:SER:HA	1.79	0.64
3:L:116:SER:OG	3:L:139:SER:OG	2.16	0.63
1:A:53:GLN:NE2	2:H:105:TYR:OH	2.32	0.63
2:H:175:ALA:HB2	2:H:185:LEU:HD12	1.83	0.60
3:L:2:ILE:HD11	3:L:25:ASP:HB3	1.83	0.60
2:H:202:ILE:HG23	2:H:215:ASP:HB3	1.86	0.58
2:H:171:HIS:CE1	3:L:169:GLN:HE21	2.22	0.56
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.41	0.55
2:H:103:ASN:HD22	2:H:103:ASN:H	1.54	0.55
3:L:122:PRO:HD3	3:L:134:LEU:HD23	1.88	0.55
3:L:82:GLU:HB3	3:L:172:ASN:HD21	1.72	0.54
3:L:149:ALA:HB3	3:L:196:GLN:HB2	1.91	0.53
3:L:24:GLY:O	3:L:68:ASN:HB3	2.10	0.51
2:H:176:VAL:HG12	2:H:184:SER:HB2	1.93	0.51
3:L:51:ASN:ND2	3:L:63:GLY:H	2.09	0.50
2:H:215:ASP:OD1	2:H:215:ASP:N	2.44	0.50
2:H:145:LEU:HD12	2:H:218:VAL:HG21	1.94	0.50
2:H:131:LEU:HD22	3:L:120:PHE:HB3	1.95	0.49
3:L:54:PRO:HD2	3:L:57:ILE:HG13	1.94	0.48
1:A:55:THR:HG22	2:H:54:PHE:HZ	1.78	0.48
2:H:63:PHE:O	2:H:67:VAL:HG12	2.14	0.48
2:H:71:ALA:HA	2:H:78:ALA:HA	1.96	0.48
2:H:103:ASN:HD22	2:H:103:ASN:N	2.12	0.47
2:H:162:ASN:HB2	2:H:166:LEU:HD13	1.96	0.47
2:H:145:LEU:HD23	2:H:145:LEU:H	1.79	0.46
2:H:154:PRO:O	2:H:207:HIS:NE2	2.40	0.46
2:H:70:THR:O	2:H:79:TYR:N	2.37	0.46
2:H:57:VAL:HG11	2:H:69:ILE:HB	1.97	0.46
3:L:66:SER:OG	3:L:67:GLY:N	2.47	0.45
2:H:86:ARG:HG3	2:H:88:GLU:HG2	1.97	0.45
3:L:79:ALA:O	3:L:172:ASN:ND2	2.50	0.45
2:H:36:TRP:CD2	2:H:80:MET:HB2	2.51	0.45
3:L:89:SER:OG	3:L:90:TRP:N	2.50	0.45
2:H:217:LYS:HG2	2:H:218:VAL:H	1.81	0.44
1:A:9:GLU:O	1:A:13:ILE:HG13	2.17	0.44
2:H:107:PHE:HD2	3:L:35:TYR:HH	1.66	0.44
2:H:153:PHE:HA	2:H:154:PRO:HA	1.77	0.44
3:L:126:GLU:O	3:L:128:GLN:N	2.51	0.43
2:H:161:TRP:HB3	2:H:166:LEU:HD22	2.01	0.43
3:L:116:SER:O	3:L:116:SER:OG	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:114:ALA:HA	3:L:115:PRO:HD3	1.92	0.43
3:L:35:TYR:HE2	3:L:88:ALA:HB3	1.84	0.42
3:L:168:LYS:HE2	3:L:168:LYS:HB3	1.90	0.42
2:H:16:SER:OG	2:H:17:SER:N	2.53	0.42
2:H:19:LYS:HG3	2:H:81:GLU:HB2	2.02	0.42
2:H:217:LYS:HG2	2:H:218:VAL:N	2.34	0.42
1:A:21:LYS:O	1:A:25:GLU:HG2	2.19	0.42
3:L:110:GLN:HE21	3:L:110:GLN:HB3	1.71	0.41
3:L:155:SER:HA	3:L:156:PRO:HD3	1.78	0.40

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	64/67 (96%)	61 (95%)	2 (3%)	1 (2%)	12 39
2	H	204/245 (83%)	184 (90%)	16 (8%)	4 (2%)	9 33
3	L	201/213 (94%)	172 (86%)	19 (10%)	10 (5%)	3 8
All	All	469/525 (89%)	417 (89%)	37 (8%)	15 (3%)	5 19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	25	ASP
3	L	28	PRO
3	L	39	PRO
3	L	50	ASP
3	L	29	TYR
3	L	127	LEU
3	L	171	ASN
3	L	202	SER

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Mol	Chain	Res	Type
2	H	167	THR
1	A	3	CYS
2	H	196	LEU
3	L	153	ASP
2	H	189	VAL
3	L	144	GLY
2	H	154	PRO

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	56/56 (100%)	49 (88%)	7 (12%)	6	16
2	H	174/207 (84%)	154 (88%)	20 (12%)	7	20
3	L	172/178 (97%)	154 (90%)	18 (10%)	8	25
All	All	402/441 (91%)	357 (89%)	45 (11%)	7	22

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	31	LEU
1	A	42	LEU
1	A	51	LEU
1	A	52	LEU
1	A	62	LEU
1	A	63	GLN
2	H	3	GLN
2	H	10	GLU
2	H	12	LYS
2	H	28	THR
2	H	52	ILE
2	H	73	GLU
2	H	85	LEU
2	H	88	GLU

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Mol	Chain	Res	Type
2	H	97	ARG
2	H	101	THR
2	H	103	ASN
2	H	115	LEU
2	H	124	LYS
2	H	129	PHE
2	H	167	THR
2	H	188	VAL
2	H	189	VAL
2	H	191	VAL
2	H	215	ASP
2	H	218	VAL
3	L	9	SER
3	L	29	TYR
3	L	47	ILE
3	L	64	SER
3	L	73	THR
3	L	84	ASP
3	L	92	SER
3	L	93	MET
3	L	98	VAL
3	L	110	GLN
3	L	131	LYS
3	L	135	VAL
3	L	136	CYS
3	L	163	THR
3	L	170	SER
3	L	173	LYS
3	L	199	HIS
3	L	208	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	39	ASN
1	A	40	ASN
1	A	53	GLN
1	A	63	GLN
2	H	3	GLN
2	H	103	ASN
2	H	109	ASN

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Mol	Chain	Res	Type
2	H	171	HIS
3	L	51	ASN
3	L	110	GLN
3	L	172	ASN

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

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, 95^{th} 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	66/67 (98%)	0.84	5 (7%) 17 11	51, 89, 181, 253	0
2	H	208/245 (84%)	0.37	19 (9%) 11 7	57, 108, 216, 275	1 (0%)
3	L	205/213 (96%)	0.60	26 (12%) 5 3	68, 136, 216, 254	0
All	All	479/525 (91%)	0.53	50 (10%) 8 5	51, 113, 216, 275	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	182	LEU	8.6
1	A	2	CYS	7.2
3	L	184	PRO	6.7
3	L	119	LEU	5.4
2	H	131	LEU	5.4
2	H	194	SER	4.7
3	L	185	GLU	4.4
3	L	183	THR	4.3
2	H	144	ALA	4.2
2	H	130	PRO	4.1
3	L	29	TYR	4.1
3	L	181	SER	4.0
2	H	145	LEU	3.9
3	L	180	LEU	3.9
3	L	132	ALA	3.8
2	H	193	SER	3.8
3	L	179	TYR	3.8
3	L	157	VAL	3.7
2	H	200	THR	3.7
2	H	119	SER	3.5
3	L	150	TRP	3.4
3	L	120	PHE	3.4
2	H	162	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	161	TRP	3.1
2	H	166	LEU	3.1
3	L	160	GLY	3.1
2	H	189	VAL	3.1
3	L	193	TYR	3.1
3	L	187	TRP	3.0
3	L	117	VAL	3.0
2	H	201	TYR	2.8
3	L	148	VAL	2.8
3	L	161	VAL	2.8
1	A	25	GLU	2.5
2	H	198	THR	2.5
3	L	202	SER	2.4
1	A	6	ILE	2.4
3	L	207	THR	2.4
2	H	129	PHE	2.4
2	H	195	SER	2.4
2	H	191	VAL	2.4
3	L	205	GLU	2.3
1	A	8	LYS	2.3
3	L	135	VAL	2.3
2	H	218	VAL	2.2
3	L	208	VAL	2.2
3	L	137	LEU	2.2
2	H	192	PRO	2.1
3	L	27	ILE	2.0
1	A	30	GLU	2.0

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.