



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:49 PM GMT

PDB ID : 4JHA
Title : Crystal Structure of RSV-Neutralizing Human Antibody D25
Authors : Mclellan, J.S.; Chen, M.; Leung, S.; Graepel, K.W.; Du, X.; Yang, Y.; Zhou, T.; Baxa, U.; Yasuda, E.; Beaumont, T.; Kumar, A.; Modjarrad, K.; Zheng, Z.; Zhao, M.; Xia, N.; Kwong, P.D.; Graham, B.S.
Deposited on : 2013-03-04
Resolution : 1.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

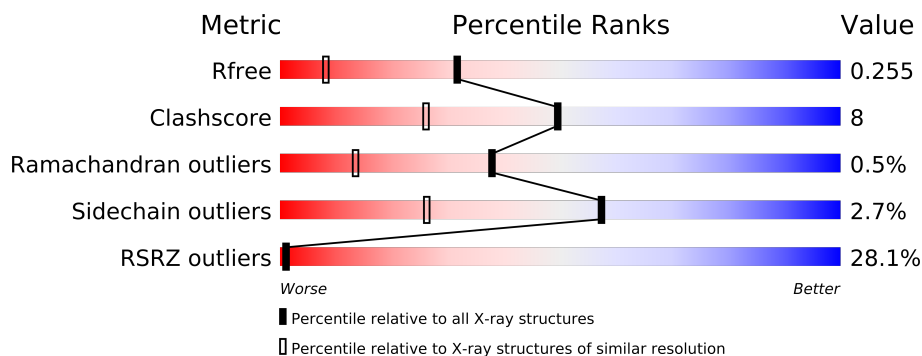
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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	H	231	
2	L	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3575 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 D25 antigen-binding fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	1	0
			1686	1069	279	330	8			

- Molecule 2 is a protein called D25 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1619	1014	269	331	5			

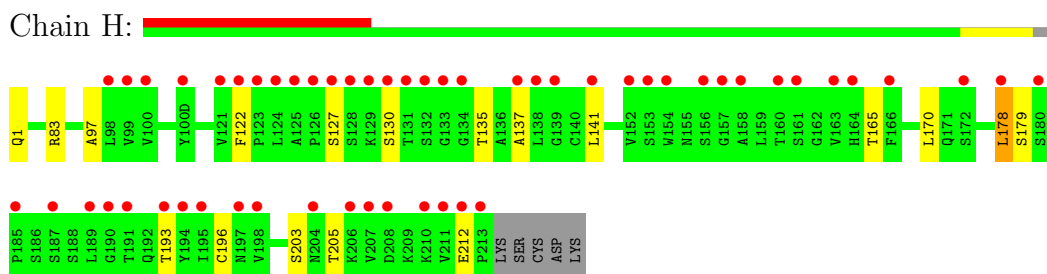
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	141	Total	O	0	0
			141	141		
3	L	129	Total	O	0	0
			129	129		

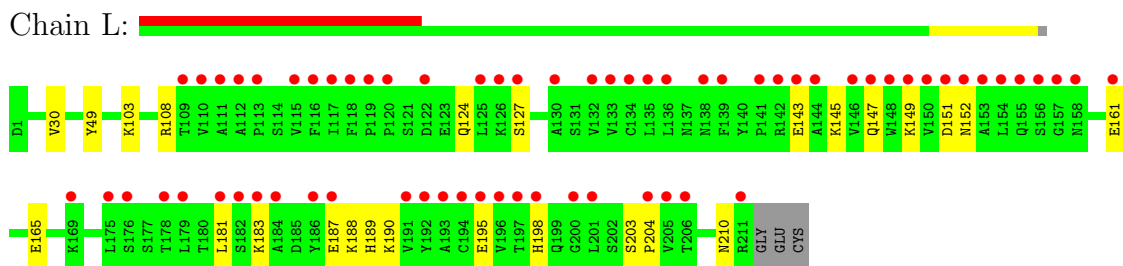
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: D25 antigen-binding fragment heavy chain



- Molecule 2: D25 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.72Å 108.72Å 139.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.40 – 1.60 35.40 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.40-1.60) 98.1 (35.40-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.60Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.255 0.242 , 0.255	Depositor DCC
R_{free} test set	3212 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 63432 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3575	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	H	0.38	0/1732	0.61	1/2371 (0.0%)
2	L	0.35	0/1652	0.57	0/2247
All	All	0.37	0/3384	0.59	1/4618 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	178	LEU	CA-CB-CG	5.50	127.96	115.30

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	H	1686	0	0	9	0
2	L	1619	0	0	16	1
3	H	141	0	0	5	0
3	L	129	0	0	10	0
All	All	3575	0	0	25	1

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 8.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:147:GLN:O	3:L:418:HOH:O	1.82	0.97
2:L:161:GLU:O	3:L:408:HOH:O	1.89	0.90
1:H:165:THR:N	3:H:434:HOH:O	2.03	0.89
1:H:179:SER:OG	3:H:412:HOH:O	1.91	0.87
2:L:203:SER:OG	3:L:420:HOH:O	1.96	0.82
2:L:183:LYS:NZ	3:L:378:HOH:O	2.15	0.79
2:L:187:GLU:OE1	3:L:427:HOH:O	2.05	0.74
2:L:149:LYS:NZ	2:L:152:ASN:O	2.22	0.73
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.33	0.61
2:L:147:GLN:CG	3:L:418:HOH:O	2.56	0.53
1:H:127:SER:N	1:H:130:SER:OG	2.42	0.53
2:L:198:HIS:CD2	3:L:415:HOH:O	2.61	0.53
1:H:137:ALA:N	3:H:433:HOH:O	2.44	0.51
1:H:196:CYS:N	3:H:431:HOH:O	2.45	0.49
1:H:170:LEU:N	3:H:364:HOH:O	2.46	0.49
2:L:124:GLN:O	2:L:127:SER:OG	2.31	0.48
2:L:143:GLU:OE1	2:L:143:GLU:N	2.49	0.46
2:L:161:GLU:N	3:L:329:HOH:O	2.49	0.45
2:L:103:LYS:NZ	3:L:382:HOH:O	2.50	0.43
1:H:203:SER:OG	1:H:205:THR:OG1	2.36	0.43
1:H:122:PHE:O	1:H:141:LEU:N	2.52	0.42
2:L:165:GLU:OE1	3:L:395:HOH:O	2.21	0.42
2:L:190:LYS:NZ	2:L:210:ASN:CG	2.73	0.42
2:L:188:LYS:NZ	2:L:189:HIS:NE2	2.69	0.41
1:H:1:GLN:OE1	1:H:1:GLN:N	2.55	0.40

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	Distance(Å)	Clash(Å)
2:L:49:TYR:OH	2:L:204:PRO:O[8_565]	2.01	0.19

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	H	225/231 (97%)	217 (96%)	7 (3%)	1 (0%)	43	18
2	L	209/214 (98%)	202 (97%)	6 (3%)	1 (0%)	38	13
All	All	434/445 (98%)	419 (96%)	13 (3%)	2 (0%)	38	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	ALA
2	L	30	VAL

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	H	192/196 (98%)	186 (97%)	6 (3%)	52	21
2	L	186/188 (99%)	182 (98%)	4 (2%)	64	34
All	All	378/384 (98%)	368 (97%)	10 (3%)	57	28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	83	ARG
1	H	135	THR
1	H	178	LEU
1	H	184	VAL
1	H	193	THR
1	H	212	GLU
2	L	108	ARG
2	L	145	LYS
2	L	181	LEU
2	L	195	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	H	226/231 (97%)	1.11	57 (25%) 1 1	17, 32, 135, 157	0
2	L	211/214 (98%)	1.38	66 (31%) 1 1	18, 50, 94, 102	0
All	All	437/445 (98%)	1.24	123 (28%) 1 1	17, 42, 115, 157	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	100	VAL	8.9
2	L	196	VAL	8.3
1	H	138	LEU	8.2
2	L	116	PHE	8.0
1	H	191	THR	7.9
2	L	153	ALA	7.7
2	L	193	ALA	7.5
1	H	132	SER	7.3
2	L	142	ARG	7.0
1	H	158	ALA	7.0
2	L	186	TYR	6.9
1	H	128	SER	6.6
1	H	190	GLY	6.6
1	H	181	VAL	6.5
1	H	161	SER	6.5
1	H	126	PRO	6.3
2	L	197	THR	6.3
1	H	131	THR	6.2
2	L	146	VAL	6.0
1	H	195	ILE	6.0
1	H	99	VAL	6.0
1	H	134	GLY	5.9
2	L	117	ILE	5.9
1	H	211	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	206	LYS	5.7
1	H	127	SER	5.6
2	L	181	LEU	5.4
1	H	124	LEU	5.4
1	H	157	GLY	5.3
2	L	200	GLY	5.2
1	H	152	VAL	5.2
1	H	163	VAL	5.1
2	L	152	ASN	5.0
2	L	184	ALA	5.0
2	L	134	CYS	5.0
1	H	197	ASN	4.9
2	L	144	ALA	4.7
2	L	127	SER	4.7
1	H	187	SER	4.6
2	L	147	GLN	4.5
1	H	133	GLY	4.5
2	L	175	LEU	4.3
2	L	192	TYR	4.3
1	H	137	ALA	4.3
2	L	198	HIS	4.3
1	H	129	LYS	4.2
2	L	118	PHE	4.1
1	H	178	LEU	4.1
1	H	125	ALA	4.1
2	L	119	PRO	4.1
1	H	160	THR	4.0
2	L	136	LEU	4.0
2	L	133	VAL	3.9
1	H	98	LEU	3.8
1	H	166	PHE	3.8
2	L	126	LYS	3.8
2	L	182	SER	3.8
2	L	179	LEU	3.8
2	L	111	ALA	3.7
2	L	120	PRO	3.7
2	L	157	GLY	3.7
2	L	138	ASN	3.6
2	L	143	GLU	3.6
1	H	153	SER	3.5
1	H	172	SER	3.5
2	L	135	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	194	CYS	3.5
1	H	198	VAL	3.4
2	L	155	GLN	3.4
1	H	122	PHE	3.4
2	L	191	VAL	3.4
1	H	204	ASN	3.3
2	L	132	VAL	3.3
2	L	158	ASN	3.3
2	L	151	ASP	3.3
1	H	130	SER	3.2
1	H	182	VAL	3.2
1	H	193	THR	3.1
1	H	154	TRP	3.1
2	L	112	ALA	3.1
1	H	189	LEU	3.0
1	H	156	SER	3.0
1	H	184	VAL	3.0
2	L	109	THR	3.0
1	H	212	GLU	3.0
1	H	210	LYS	3.0
2	L	205	VAL	3.0
2	L	141	PRO	2.9
2	L	125	LEU	2.9
1	H	207	VAL	2.9
2	L	139	PHE	2.9
2	L	148	TRP	2.9
2	L	150	VAL	2.9
1	H	123	PRO	2.9
2	L	183	LYS	2.8
1	H	213	PRO	2.8
2	L	201	LEU	2.8
2	L	122	ASP	2.8
1	H	208	ASP	2.7
2	L	110	VAL	2.7
2	L	115	VAL	2.7
2	L	206	THR	2.7
1	H	139	GLY	2.6
2	L	176	SER	2.6
1	H	185	PRO	2.6
2	L	195	GLU	2.5
2	L	113	PRO	2.5
2	L	178	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	211	ARG	2.5
1	H	194	TYR	2.4
2	L	149	LYS	2.4
2	L	204	PRO	2.4
1	H	141	LEU	2.3
2	L	169	LYS	2.3
1	H	100(D)	TYR	2.3
2	L	156	SER	2.2
2	L	187	GLU	2.2
2	L	154	LEU	2.2
1	H	164	HIS	2.2
2	L	130	ALA	2.1
1	H	180	SER	2.1
2	L	161	GLU	2.1
1	H	121	VAL	2.0

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.