WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 09:17 pm GMT

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PDB ID	:	5AAW
Title	:	Structure of a redesigned cross-reactive antibody to dengue virus with increased in vivo potency
Authors	:	Wong, Y.; Robinson, L.; Lescar, J.; Sasisekharan, R.
Deposited on	:	2015-07-30
Resolution	:	3.27 Å(reported)

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 3.27 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.
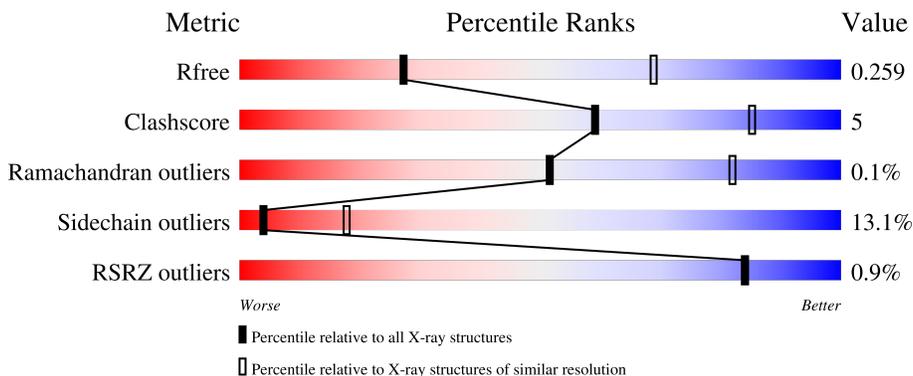
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	252	73% 14% • 10%
1	B	252	.% 72% 17% • 9%
1	D	252	75% 13% • 10%
1	F	252	69% 15% 6% 10%
1	H	252	73% 15% • 10%

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Mol	Chain	Length	Quality of chain
1	K	252	71% 17% 10%
2	C	115	2% 62% 19% 17%
2	E	115	71% 12% 17%
2	G	115	9% 65% 15% 19%
2	I	115	% 70% 13% 17%
2	J	115	72% 10% 17%
2	L	115	% 71% 11% 17%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 15132 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 SCFV513.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			
1	B	229	Total	C	N	O	S	0	0	0
			1788	1121	309	348	10			
1	D	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			
1	F	227	Total	C	N	O	S	0	0	0
			1773	1113	306	344	10			
1	H	228	Total	C	N	O	S	0	1	0
			1787	1122	308	347	10			
1	K	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			

- Molecule 2 is a protein called DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	S	0	1	0
			745	471	126	144	4			
2	E	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	G	93	Total	C	N	O	S	0	0	0
			706	446	117	139	4			
2	I	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	J	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	L	96	Total	C	N	O	S	0	1	0
			745	471	126	144	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	6	Total 6	O 6	0	0
3	C	2	Total 2	O 2	0	0
3	D	4	Total 4	O 4	0	0
3	E	5	Total 5	O 5	0	0
3	F	5	Total 5	O 5	0	0
3	G	4	Total 4	O 4	0	0
3	H	3	Total 3	O 3	0	0
3	J	3	Total 3	O 3	0	0
3	K	1	Total 1	O 1	0	0
3	L	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: SCFV513

Chain A:

• Molecule 1: SCFV513

Chain B:

• Molecule 1: SCFV513

Chain D:

• Molecule 1: SCFV513

Chain F:

GLY GLY GLY **S132 D133 I134** T137 Q138 L147 G148 Q149 T152 C155 E159 N166 K175 L190 R197 S212 S213 L214 E217 Y222 Y223 C224 Q225 R226 E229 Q236 L240 K243 R244 THR VAL ALA HIS HIS HIS HIS HIS HIS

- Molecule 1: SCFV513

Chain H: 73%   15%   •   10%

GLN Q2 V3 E11 K20 K24 N28 V32 R38 E42 R50 P62 K63 L64 Q65 G66 R67 V68 T69 M81 E82 L83 R84 T91 C96 A97 R98 W106 T113 S116 GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY S132

D133 I134 T137 Q138 L147 G148 Q149 T152 C155 K175 K181 L182 R186 L190 Q191 L214 E217 Y222 Y223 C224 Q225 R226 E229 Q236 L240 K243 R244 THR VAL ALA HIS HIS HIS HIS HIS

- Molecule 1: SCFV513

Chain K: 71%   17%   •   10%

GLN Q2 V3 E11 K24 N28 I29 K30 D31 V32 W36 V37 R38 R50 D57 T58 K59 Y60 D61 L64 Q65 G66 R67 V68 T71 M81 E82 L83 D90 T91 C96 A97 R98 T113 S116 GLY GLY GLY SER GLY GLY GLY SER GLY GLY

GLY GLY **S132 D133 I134** T137 Q138 L147 G148 Q149 R150 A151 T152 C155 K175 P179 L190 S212 S213 L214 E217 Y222 Y223 C224 Q225 R226 S227 N228 E229 Q236 L240 K243 R244 THR VAL ALA HIS HIS HIS HIS HIS

- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain C: 2%
                    62%   19%   •   17%

MET ARG ILE LYS GLY MET SER Y299 T300 M301 C302 K305 D309 K310 E314 T315 Q316 H317 G318 T319 T320 V321 K325 R340 D341 V342 N343 K344 V347 I351 T355 P356 L357 L369 D375 S376 Y377 N384 S385 F392 R393 K394 GLY SER SER ILE GLY LYS

HIS HIS HIS HIS HIS

- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain E: 71%   12%   17%

MET ARG ILE LYS GLY MET SER Y299 T300 M301 C302 K305 D309 T315 T319 V348 G349 R350 T355 P356 L357 L369 P372 S376 S385 K394 GLY SER SER ILE GLY LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain G: 9%
                    65%   15%   •   19%

MET ARG ILE LYS GLY MET SER Y299 T300 M301 C302 K305 D309 A313 E314 T315 T320 V321 V342 G349 R350 I351 I352 S353 S354 T355 P356 L357 N362 S363 V364 I367 E368 L369 D375 S376 S385 T388 W391 PHE ARG LYS GLY SER SER ILE GLY LYS
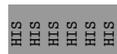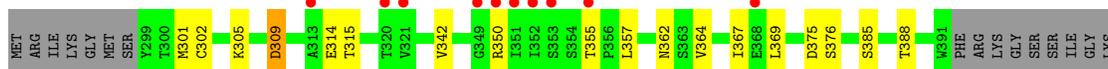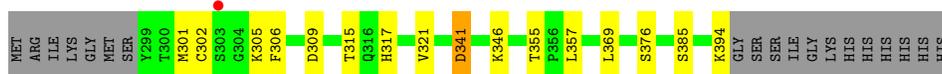
HIS HIS HIS HIS HIS HIS

• Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain I:

• Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain J:

• Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain L:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.11Å 131.67Å 176.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.27 45.71 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.75-3.27) 99.8 (45.71-3.27)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.227 , 0.263 0.225 , 0.259	Depositor DCC
R_{free} test set	1618 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 31.0	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15132	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 18.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.53	0/1819	0.74	1/2465 (0.0%)
1	B	0.49	0/1828	0.71	1/2477 (0.0%)
1	D	0.52	0/1819	0.74	1/2465 (0.0%)
1	F	0.59	0/1813	0.85	3/2457 (0.1%)
1	H	0.52	0/1827	0.74	0/2476
1	K	0.53	0/1819	0.77	2/2465 (0.1%)
2	C	0.54	0/759	0.80	1/1028 (0.1%)
2	E	0.51	0/751	0.74	0/1017
2	G	0.58	0/719	0.81	0/976
2	I	0.52	0/751	0.76	0/1017
2	J	0.51	0/751	0.75	0/1017
2	L	0.51	0/759	0.83	1/1028 (0.1%)
All	All	0.53	0/15415	0.77	10/20888 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	31	ASP	CB-CG-OD1	9.29	126.66	118.30
2	C	302	CYS	CA-CB-SG	7.82	128.07	114.00
1	K	227	SER	CB-CA-C	-7.60	95.65	110.10
1	F	31	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	D	133	ASP	CB-CG-OD1	5.55	123.29	118.30

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	1779	0	1718	18	0
1	B	1788	0	1729	19	0
1	D	1779	0	1718	12	0
1	F	1773	0	1713	25	0
1	H	1787	0	1728	28	0
1	K	1779	0	1718	13	0
2	C	745	0	746	22	0
2	E	737	0	741	4	0
2	G	706	0	706	5	0
2	I	737	0	741	5	0
2	J	737	0	741	3	0
2	L	745	0	746	11	0
3	A	3	0	0	0	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	4	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	4	0	0	0	0
3	H	3	0	0	0	0
3	J	3	0	0	1	0
3	K	1	0	0	0	0
3	L	4	0	0	0	0
All	All	15132	0	14745	140	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 5.

The worst 5 of 140 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)
1:H:68:VAL:HG12	1:H:81:MET:CE	1.85	1.05
1:H:182[B]:LEU:H	1:H:182[B]:LEU:HD23	1.14	1.05
2:C:316:GLN:HB2	2:L:316:GLN:HB3	1.43	0.97
1:H:138:GLN:H	1:H:236:GLN:HE22	1.15	0.93
1:F:138:GLN:H	1:F:236:GLN:HE22	1.16	0.92

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	224/252 (89%)	217 (97%)	7 (3%)	0	100	100
1	B	225/252 (89%)	217 (96%)	8 (4%)	0	100	100
1	D	224/252 (89%)	216 (96%)	8 (4%)	0	100	100
1	F	223/252 (88%)	216 (97%)	7 (3%)	0	100	100
1	H	225/252 (89%)	215 (96%)	10 (4%)	0	100	100
1	K	224/252 (89%)	216 (96%)	8 (4%)	0	100	100
2	C	95/115 (83%)	92 (97%)	3 (3%)	0	100	100
2	E	94/115 (82%)	91 (97%)	3 (3%)	0	100	100
2	G	91/115 (79%)	87 (96%)	4 (4%)	0	100	100
2	I	94/115 (82%)	90 (96%)	4 (4%)	0	100	100
2	J	94/115 (82%)	90 (96%)	3 (3%)	1 (1%)	14	46
2	L	95/115 (83%)	87 (92%)	8 (8%)	0	100	100
All	All	1908/2202 (87%)	1834 (96%)	73 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	316	GLN

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	192/203 (95%)	164 (85%)	28 (15%)	3	14
1	B	193/203 (95%)	169 (88%)	24 (12%)	4	20
1	D	192/203 (95%)	168 (88%)	24 (12%)	4	19
1	F	191/203 (94%)	160 (84%)	31 (16%)	2	10
1	H	193/203 (95%)	168 (87%)	25 (13%)	4	18
1	K	192/203 (95%)	161 (84%)	31 (16%)	2	11
2	C	84/99 (85%)	75 (89%)	9 (11%)	6	25
2	E	83/99 (84%)	76 (92%)	7 (8%)	11	35
2	G	80/99 (81%)	68 (85%)	12 (15%)	3	13
2	I	83/99 (84%)	74 (89%)	9 (11%)	6	25
2	J	83/99 (84%)	74 (89%)	9 (11%)	6	25
2	L	84/99 (85%)	77 (92%)	7 (8%)	11	35
All	All	1650/1812 (91%)	1434 (87%)	216 (13%)	4	18

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	212	SER
1	H	81	MET
1	K	155	CYS
1	F	226	ARG
2	G	357	LEU

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

Mol	Chain	Res	Type
1	F	236	GLN
1	H	236	GLN
1	K	236	GLN
2	J	390	HIS
1	K	65	GLN

5.3.3   RNA (i)

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 monosaccharides 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	A	228/252 (90%)	-0.25	0	100	100	21, 39, 64, 83	1 (0%)
1	B	229/252 (90%)	-0.24	2 (0%)	84	84	22, 39, 74, 105	1 (0%)
1	D	228/252 (90%)	-0.18	1 (0%)	92	93	24, 41, 63, 92	1 (0%)
1	F	227/252 (90%)	-0.06	0	100	100	26, 47, 73, 95	1 (0%)
1	H	228/252 (90%)	-0.25	0	100	100	22, 40, 60, 81	1 (0%)
1	K	228/252 (90%)	-0.23	1 (0%)	92	93	22, 39, 64, 100	1 (0%)
2	C	96/115 (83%)	0.31	2 (2%)	63	61	38, 78, 107, 129	0
2	E	96/115 (83%)	0.03	0	100	100	37, 58, 81, 93	0
2	G	93/115 (80%)	0.88	10 (10%)	5	5	63, 91, 124, 141	0
2	I	96/115 (83%)	0.22	1 (1%)	82	82	36, 73, 108, 119	0
2	J	96/115 (83%)	0.05	0	100	100	34, 61, 102, 122	0
2	L	96/115 (83%)	0.10	1 (1%)	82	82	38, 70, 93, 108	0
All	All	1941/2202 (88%)	-0.06	18 (0%)	84	84	21, 46, 95, 141	6 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	353	SER	5.6
2	G	349	GLY	4.4
2	G	313	ALA	3.7
1	B	132	SER	3.2
2	C	384	ASN	3.0

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 monosaccharides 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.