



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jul 31, 2017 – 06:05 PM EDT

PDB ID : 5W3E
EMDB ID: : EMD-8754
Title : CryoEM structure of rhinovirus B14 in complex with C5 Fab (33 degrees Celsius, molar ratio 1:3, full particle)
Authors : Liu, Y.; Dong, Y.; Rossmann, M.G.
Deposited on : unknown
Resolution : 2.53 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

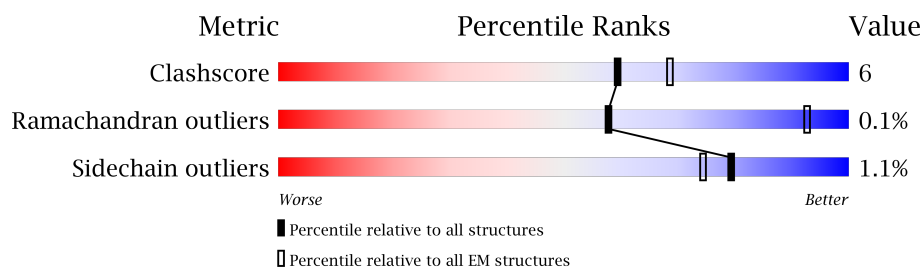
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	116	84% 16%
2	G	107	85% 14% .
3	A	289	83% 11% . 5%
4	B	236	81% 18%
5	C	262	84% 13% .
6	D	68	53% 6% 41%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8107 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 C5 antibody variable heavy domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	116	Total	C	N	O	S	0	0
			845	538	140	164	3		

- Molecule 2 is a protein called C5 antibody variable light domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	107	Total	C	N	O	S	0	0
			769	490	131	146	2		

- Molecule 3 is a protein called viral protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	274	Total	C	N	O	S	0	0
			2179	1378	377	416	8		

- Molecule 4 is a protein called viral protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	236	Total	C	N	O	S	0	0
			1849	1184	305	353	7		

- Molecule 5 is a protein called viral protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	255	Total	C	N	O	S	0	0
			1952	1238	330	372	12		

- Molecule 6 is a protein called viral protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	40	Total	C	N	O	S	0	0
			297	186	47	62	2		

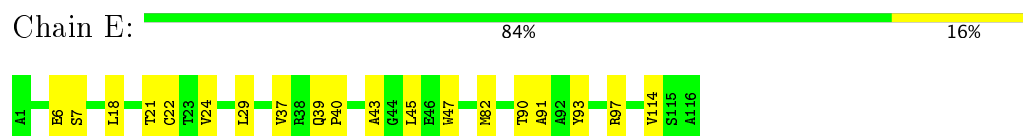
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	E	10	Total 10	O 10	0
7	G	8	Total 8	O 8	0
7	A	69	Total 69	O 69	0
7	B	58	Total 58	O 58	0
7	C	62	Total 62	O 62	0
7	D	9	Total 9	O 9	0

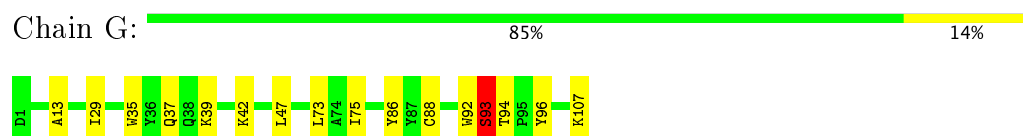
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

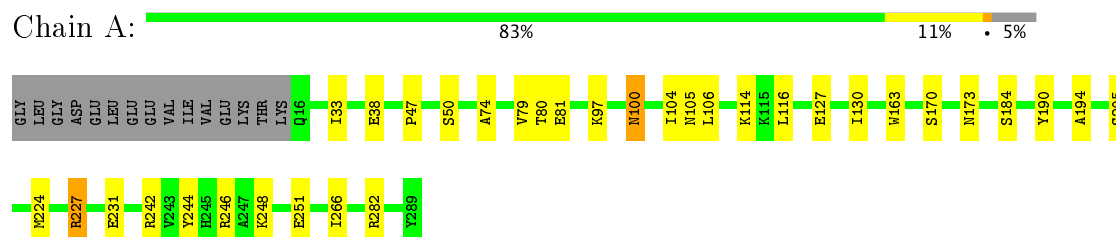
- Molecule 1: C5 antibody variable heavy domain



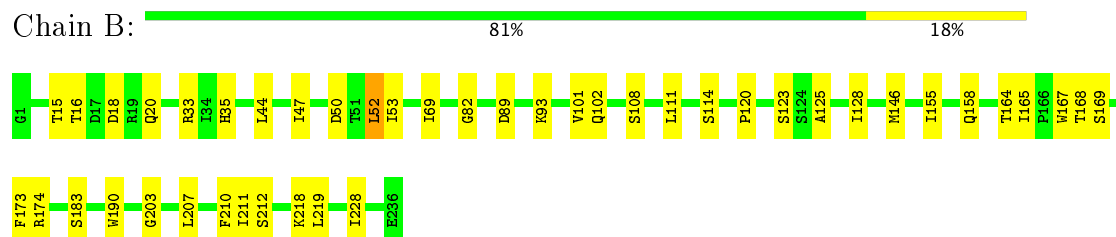
- Molecule 2: C5 antibody variable light domain



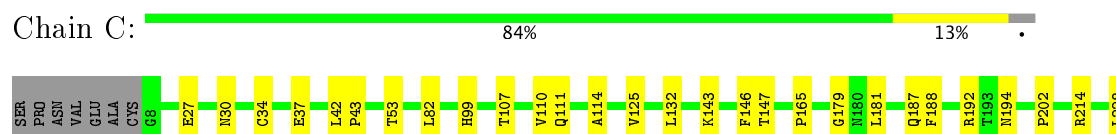
- Molecule 3: viral protein 1



- Molecule 4: viral protein 3

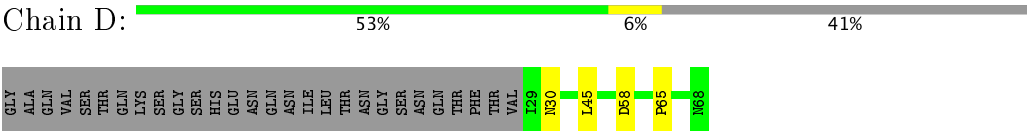


- Molecule 5: viral protein 2





● Molecule 6: viral protein 4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of particles used	23242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On-the-fly CTF correction during 2D alignment and 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	E	0.41	0/866	0.60	0/1188
2	G	0.46	1/788 (0.1%)	0.57	0/1075
3	A	0.50	0/2237	0.58	0/3043
4	B	0.52	0/1898	0.67	1/2597 (0.0%)
5	C	0.50	0/2001	0.62	0/2735
6	D	0.37	0/302	0.61	1/406 (0.2%)
All	All	0.49	1/8092 (0.0%)	0.61	2/11044 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	88	CYS	CB-SG	-6.52	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	45	LEU	CA-CB-CG	6.56	130.38	115.30
4	B	52	LEU	CA-CB-CG	5.15	127.14	115.30

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	E	845	0	814	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	769	0	747	14	0
3	A	2179	0	2115	23	0
4	B	1849	0	1833	33	0
5	C	1952	0	1927	21	0
6	D	297	0	294	3	0
7	A	69	0	0	1	0
7	B	58	0	0	0	0
7	C	62	0	0	0	0
7	D	9	0	0	0	0
7	E	10	0	0	0	0
7	G	8	0	0	0	0
All	All	8107	0	7730	86	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 6.

All (86) 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:A:231:GLU:O	7:A:301:HOH:O	1.65	1.15
3:A:79:VAL:HG22	3:A:242:ARG:HG2	1.56	0.87
2:G:92:TRP:CE2	4:B:203:GLY:HA3	2.11	0.84
4:B:93:LYS:HG3	4:B:102:GLN:HE22	1.48	0.78
3:A:47:PRO:HA	4:B:164:THR:HG21	1.68	0.74
2:G:93:SER:O	2:G:94:THR:HG23	1.88	0.74
2:G:93:SER:HB2	4:B:203:GLY:HA2	1.74	0.70
2:G:92:TRP:NE1	4:B:203:GLY:HA3	2.06	0.69
4:B:114:SER:HB2	4:B:210:PHE:HB2	1.75	0.68
1:E:90:THR:HG22	1:E:114:VAL:H	1.58	0.68
5:C:30:ASN:O	5:C:187:GLN:NE2	2.29	0.65
1:E:40:PRO:HG2	1:E:43:ALA:HB3	1.80	0.62
4:B:168:THR:O	4:B:174:ARG:NH2	2.32	0.62
4:B:125:ALA:HB3	4:B:155:ILE:HD12	1.82	0.61
2:G:92:TRP:O	2:G:93:SER:CB	2.49	0.59
5:C:27:GLU:HG2	5:C:194:ASN:HA	1.83	0.59
4:B:50:ASP:HB2	4:B:210:PHE:HB3	1.84	0.58
2:G:93:SER:O	2:G:96:TYR:CE1	2.56	0.58
4:B:128:ILE:HG23	4:B:190:TRP:HB2	1.86	0.58
5:C:132:LEU:HD12	5:C:147:THR:HG22	1.86	0.57
1:E:24:VAL:HG21	1:E:29:LEU:HD21	1.86	0.57
2:G:92:TRP:O	2:G:93:SER:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:38:GLU:HA	5:C:188:PHE:HB2	1.87	0.57
4:B:89:ASP:HA	4:B:93:LYS:HE2	1.87	0.57
4:B:69:ILE:HB	4:B:207:LEU:HB2	1.88	0.56
3:A:251:GLU:OE2	4:B:33:ARG:NH1	2.40	0.55
3:A:114:LYS:HD2	4:B:228:ILE:HB	1.88	0.55
4:B:53:ILE:HD11	4:B:211:ILE:HB	1.88	0.55
3:A:104:ILE:HD11	3:A:224:MET:HG3	1.88	0.54
2:G:75:ILE:HD11	2:G:86:TYR:HE2	1.74	0.53
5:C:34:CYS:HB2	5:C:202:PRO:HD2	1.90	0.53
3:A:242:ARG:HB3	3:A:244:TYR:HE1	1.75	0.52
2:G:39:LYS:HB2	2:G:42:LYS:HD2	1.90	0.52
5:C:107:THR:OG1	5:C:247:MET:SD	2.64	0.52
1:E:7:SER:OG	1:E:21:THR:OG1	2.28	0.52
3:A:81:GLU:OE2	3:A:97:LYS:NZ	2.43	0.52
1:E:37:VAL:HG22	1:E:47:TRP:HA	1.92	0.51
3:A:246:ARG:NH1	4:B:18:ASP:OD1	2.43	0.51
3:A:282:ARG:NH1	4:B:82:GLY:O	2.43	0.51
4:B:167:TRP:CZ2	4:B:169:SER:HB3	2.46	0.50
3:A:80:THR:OG1	3:A:100:ASN:OD1	2.29	0.49
5:C:125:VAL:HG11	5:C:181:LEU:HD13	1.94	0.49
5:C:30:ASN:ND2	6:D:58:ASP:O	2.39	0.48
3:A:163:TRP:O	3:A:227:ARG:NH1	2.46	0.48
5:C:82:LEU:HD21	5:C:244:ILE:HD13	1.96	0.48
1:E:18:LEU:HD12	1:E:82:MET:HB2	1.95	0.47
3:A:130:ILE:HB	3:A:184:SER:HB3	1.96	0.47
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.97	0.47
4:B:120:PRO:O	5:C:192:ARG:NH2	2.48	0.47
1:E:91:ALA:HB3	1:E:93:TYR:HE1	1.80	0.46
3:A:127:GLU:HB2	3:A:248:LYS:HE2	1.98	0.46
5:C:53:THR:HG22	5:C:252:SER:HB2	1.98	0.45
4:B:120:PRO:HG2	4:B:123:SER:HB3	1.99	0.45
3:A:74:ALA:HB3	4:B:15:THR:HB	1.98	0.45
5:C:110:VAL:HG22	5:C:242:VAL:HG22	1.98	0.45
3:A:205:SER:O	5:C:214:ARG:NH1	2.50	0.45
5:C:99:HIS:CG	5:C:251:PHE:HB3	2.52	0.45
3:A:106:LEU:HD23	3:A:116:LEU:HD11	1.99	0.44
3:A:33:ILE:HG21	3:A:50:SER:HB3	1.98	0.44
5:C:146:PHE:HB3	5:C:165:PRO:HD3	1.99	0.44
4:B:108:SER:HB3	4:B:218:LYS:HB2	2.00	0.44
5:C:114:ALA:HB2	5:C:238:LEU:HD21	1.99	0.44
3:A:170:SER:OG	3:A:173:ASN:O	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:111:LEU:HB2	4:B:165:ILE:HB	1.99	0.44
4:B:44:LEU:HD23	4:B:47:ILE:HD11	2.00	0.44
5:C:42:LEU:HD12	5:C:43:PRO:HD2	1.99	0.44
4:B:52:LEU:HD12	5:C:179:GLY:HA2	1.99	0.43
5:C:143:LYS:HB2	5:C:146:PHE:HD2	1.84	0.43
4:B:158:GLN:HE22	6:D:65:PRO:HA	1.84	0.42
3:A:105:ASN:ND2	3:A:266:ILE:HD13	2.34	0.42
2:G:35:TRP:CE2	2:G:73:LEU:HB2	2.55	0.42
5:C:228:LEU:HD21	5:C:238:LEU:HD13	2.01	0.42
4:B:169:SER:HB2	4:B:174:ARG:CZ	2.50	0.42
2:G:93:SER:O	2:G:96:TYR:CZ	2.73	0.42
2:G:29:ILE:HD13	2:G:29:ILE:HG21	1.89	0.41
4:B:50:ASP:HA	4:B:212:SER:HB3	2.02	0.41
2:G:13:ALA:HA	2:G:107:LYS:HE3	2.01	0.41
4:B:20:GLN:HE22	6:D:30:ASN:HA	1.85	0.41
1:E:6:GLU:HG3	1:E:22:CYS:SG	2.61	0.41
3:A:105:ASN:HD21	3:A:266:ILE:HD13	1.85	0.41
3:A:190:TYR:OH	3:A:194:ALA:O	2.25	0.41
4:B:108:SER:HA	4:B:167:TRP:CH2	2.55	0.41
4:B:174:ARG:NH1	4:B:183:SER:O	2.54	0.41
4:B:35:HIS:HE2	5:C:37:GLU:CD	2.24	0.41
4:B:101:VAL:HG22	4:B:219:LEU:HD21	2.03	0.41
2:G:37:GLN:HB2	2:G:47:LEU:HD11	2.03	0.41

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 PDB entries followed by that with respect to all EM entries.

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	E	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
2	G	105/107 (98%)	99 (94%)	5 (5%)	1 (1%)	18	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	272/289 (94%)	264 (97%)	8 (3%)	0	100	100
4	B	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
5	C	253/262 (97%)	242 (96%)	11 (4%)	0	100	100
6	D	38/68 (56%)	35 (92%)	3 (8%)	0	100	100
All	All	1016/1078 (94%)	973 (96%)	42 (4%)	1 (0%)	58	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	93	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 PDB entries followed by that with respect to all EM entries.

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	E	80/80 (100%)	79 (99%)	1 (1%)	73	90
2	G	72/72 (100%)	71 (99%)	1 (1%)	71	89
3	A	240/253 (95%)	238 (99%)	2 (1%)	85	94
4	B	209/209 (100%)	206 (99%)	3 (1%)	71	89
5	C	223/229 (97%)	221 (99%)	2 (1%)	82	93
6	D	33/57 (58%)	33 (100%)	0	100	100
All	All	857/900 (95%)	848 (99%)	9 (1%)	79	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	97	ARG
2	G	93	SER
3	A	100	ASN
3	A	227	ARG
4	B	16	THR
4	B	146	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	173	PHE
5	C	111	GLN
5	C	255	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	105	ASN
4	B	102	GLN
4	B	192	GLN
6	D	30	ASN

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 [i](#)

There are no chain breaks in this entry.