



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:18 am GMT

PDB ID : 3IY7
EMDB ID: : EMD-5112
Title : Variable domains of the computer generated model (WAM) of Fab F fitted into the cryoEM reconstruction of the virus-Fab F complex
Authors : Hafenstein, S.; Bowman, V.D.; Sun, T.; Nelson, C.D.; Palermo, L.M.; Chipman, P.R.; Battisti, A.J.; Parrish, C.R.; Rossmann, M.G.
Deposited on : 2009-04-09
Resolution : 14.00 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) : recalc29047

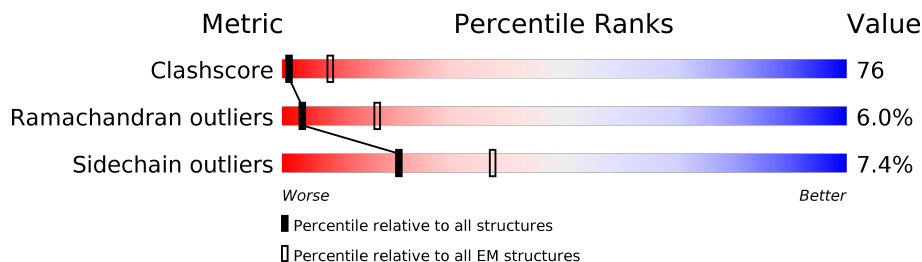
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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	A	106	
2	B	115	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1717 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 fragment from neutralizing antibody F (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			822	517	139	163	3		

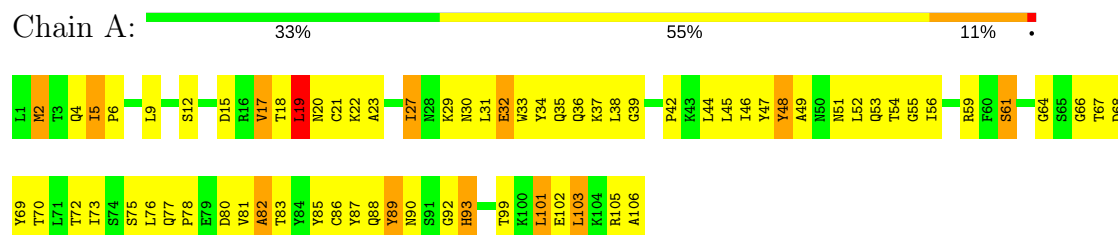
- Molecule 2 is a protein called fragment from neutralizing antibody F (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	S	0	0
			895	566	153	171	5		

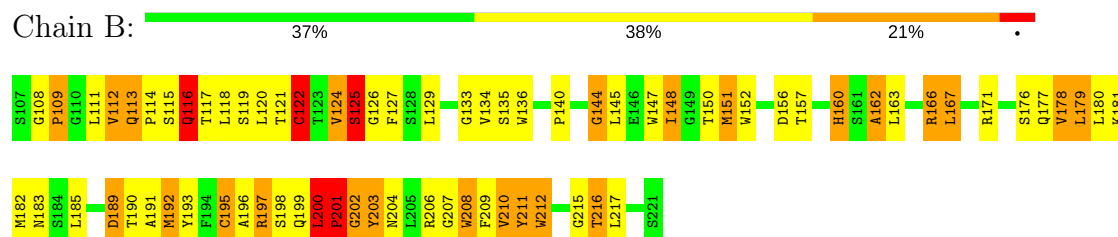
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: fragment from neutralizing antibody F (light chain)



- Molecule 2: fragment from neutralizing antibody F (heavy chain)



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	1769	Depositor
Resolution determination method	FSC at 0.5 cutoff	Depositor
CTF correction method	robem	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	1.0	Depositor
Maximum defocus (nm)	7.3	Depositor
Magnification	47190	Depositor
Image detector	Kodak SO-163 film	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.05	0/838	1.39	10/1134 (0.9%)
2	B	1.22	5/918 (0.5%)	1.74	27/1247 (2.2%)
All	All	1.14	5/1756 (0.3%)	1.58	37/2381 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	0	5
All	All	1	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	GLN	CD-NE2	-8.21	1.12	1.32
2	B	112	VAL	N-CA	-7.67	1.31	1.46
2	B	208	TRP	CD2-CE2	-5.80	1.34	1.41
2	B	208	TRP	CD2-CE3	-5.43	1.32	1.40
2	B	152	TRP	CD2-CE2	-5.05	1.35	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	ALA	N-CA-CB	12.45	127.54	110.10
2	B	112	VAL	CG1-CB-CG2	-11.36	92.73	110.90
2	B	112	VAL	CA-CB-CG1	10.71	126.97	110.90
2	B	144	GLY	O-C-N	-10.07	106.59	122.70
1	A	17	VAL	CA-CB-CG2	-9.11	97.24	110.90
1	A	19	LEU	N-CA-CB	8.98	128.36	110.40
2	B	140	PRO	CA-N-CD	-8.35	99.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	178	VAL	CG1-CB-CG2	-8.31	97.60	110.90
2	B	162	ALA	CB-CA-C	-7.79	98.41	110.10
2	B	210	VAL	CA-CB-CG2	7.73	122.50	110.90
1	A	32	GLU	CB-CA-C	-7.70	95.00	110.40
2	B	112	VAL	CA-C-O	-7.67	103.99	120.10
1	A	103	LEU	N-CA-CB	-7.67	95.06	110.40
2	B	112	VAL	CA-C-N	7.59	133.91	117.20
2	B	211	TYR	CB-CA-C	-7.52	95.35	110.40
2	B	151	MET	CB-CA-C	-7.30	95.81	110.40
1	A	103	LEU	CA-CB-CG	-7.18	98.79	115.30
1	A	48	TYR	CB-CA-C	6.92	124.24	110.40
2	B	116	GLN	OE1-CD-NE2	-6.70	106.49	121.90
2	B	112	VAL	N-CA-C	6.68	129.04	111.00
2	B	122	CYS	CB-CA-C	6.54	123.48	110.40
1	A	27	ILE	CG1-CB-CG2	6.41	125.49	111.40
2	B	124	VAL	CA-CB-CG1	6.36	120.44	110.90
2	B	148	ILE	CG1-CB-CG2	-6.16	97.85	111.40
2	B	208	TRP	CD1-NE1-CE2	-6.14	103.48	109.00
2	B	116	GLN	N-CA-CB	6.06	121.51	110.60
1	A	48	TYR	N-CA-CB	6.04	121.47	110.60
2	B	125	SER	O-C-N	-5.95	113.09	123.20
2	B	208	TRP	CG-CD2-CE3	-5.72	128.76	133.90
2	B	140	PRO	CB-CG-CD	-5.61	84.64	106.50
2	B	166	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	210	VAL	CG1-CB-CG2	-5.49	102.11	110.90
2	B	178	VAL	CA-CB-CG2	5.43	119.05	110.90
1	A	89	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	19	LEU	CB-CG-CD1	5.30	120.02	111.00
2	B	152	TRP	CD1-NE1-CE2	-5.22	104.30	109.00
2	B	189	ASP	CB-CG-OD2	-5.21	113.61	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	19	LEU	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	116	GLN	Sidechain
2	B	125	SER	Mainchain,Peptide
2	B	144	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	B	160	HIS	Sidechain

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	822	0	809	105	0
2	B	895	0	870	160	0
All	All	1717	0	1679	255	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 76.

All (255) 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:A:9:LEU:HD21	1:A:17:VAL:HG21	1.29	1.11
1:A:9:LEU:HD21	1:A:17:VAL:CG2	1.81	1.09
1:A:77:GLN:HB3	1:A:78:PRO:HD2	1.40	1.01
2:B:119:SER:HB2	2:B:181:LYS:NZ	1.77	1.00
2:B:200:LEU:H	2:B:201:PRO:HD2	1.28	0.99
2:B:148:ILE:CD1	2:B:180:LEU:HD21	1.91	0.98
2:B:112:VAL:HG21	2:B:118:LEU:HD22	1.43	0.97
1:A:81:VAL:HG11	1:A:103:LEU:HD12	1.48	0.95
2:B:148:ILE:HD11	2:B:167:LEU:HD12	1.47	0.94
2:B:112:VAL:HG13	2:B:116:GLN:HG3	1.49	0.94
2:B:200:LEU:HB3	2:B:206:ARG:HA	1.51	0.93
1:A:27:ILE:HD13	1:A:88:GLN:HG3	1.48	0.93
2:B:124:VAL:HG21	2:B:127:PHE:CZ	2.04	0.92
2:B:112:VAL:HG11	2:B:185:LEU:CD1	2.00	0.91
1:A:42:PRO:HB2	2:B:211:TYR:CZ	2.07	0.89
1:A:9:LEU:CD2	1:A:17:VAL:HG21	2.03	0.88
2:B:121:THR:HG21	2:B:177:GLN:HE22	1.40	0.87
2:B:121:THR:HG23	2:B:177:GLN:OE1	1.74	0.86
1:A:81:VAL:CG1	1:A:103:LEU:HD12	2.07	0.85
2:B:148:ILE:HG13	2:B:163:LEU:HD22	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:LEU:HD12	2:B:206:ARG:HB3	1.57	0.85
1:A:18:THR:HG23	1:A:70:THR:CG2	2.08	0.83
2:B:147:TRP:HZ2	2:B:150:THR:HG22	1.43	0.82
2:B:124:VAL:HB	2:B:212:TRP:CH2	2.13	0.82
2:B:148:ILE:HD11	2:B:180:LEU:HD21	1.59	0.82
2:B:148:ILE:HD13	2:B:180:LEU:HD21	1.61	0.81
1:A:5:ILE:HD12	1:A:6:PRO:HA	1.64	0.80
1:A:36:GLN:O	1:A:82:ALA:HB1	1.81	0.79
2:B:119:SER:HB2	2:B:181:LYS:HZ3	1.47	0.78
1:A:27:ILE:HA	1:A:90:ASN:OD1	1.86	0.76
1:A:27:ILE:HG21	1:A:88:GLN:HE21	1.50	0.76
2:B:127:PHE:CZ	2:B:197:ARG:HG2	2.20	0.75
2:B:136:TRP:O	2:B:148:ILE:HG22	1.86	0.75
2:B:162:ALA:HB3	2:B:163:LEU:HD12	1.68	0.74
2:B:163:LEU:HD23	2:B:167:LEU:HG	1.70	0.74
2:B:112:VAL:HG11	2:B:185:LEU:HD12	1.68	0.74
2:B:119:SER:HB2	2:B:181:LYS:HZ1	1.52	0.74
1:A:52:LEU:HD22	1:A:56:ILE:HG23	1.68	0.73
2:B:133:GLY:HA2	2:B:171:ARG:HH22	1.55	0.72
2:B:112:VAL:CG2	2:B:118:LEU:HD22	2.18	0.71
2:B:136:TRP:HB3	2:B:148:ILE:CG2	2.20	0.71
1:A:27:ILE:HG21	1:A:88:GLN:NE2	2.06	0.70
2:B:136:TRP:C	2:B:148:ILE:HG22	2.11	0.70
1:A:42:PRO:HB2	2:B:211:TYR:OH	1.91	0.70
2:B:121:THR:CG2	2:B:177:GLN:HE22	2.04	0.70
2:B:178:VAL:C	2:B:179:LEU:HD13	2.12	0.70
1:A:9:LEU:HD21	1:A:17:VAL:HG22	1.72	0.69
2:B:147:TRP:HE1	2:B:150:THR:HB	1.57	0.68
2:B:112:VAL:CG1	2:B:185:LEU:HD12	2.23	0.68
2:B:113:GLN:O	2:B:116:GLN:HG2	1.93	0.68
1:A:37:LYS:HA	1:A:82:ALA:CB	2.23	0.68
1:A:22:LYS:HA	1:A:67:THR:O	1.94	0.68
1:A:27:ILE:HD11	1:A:69:TYR:CE1	2.29	0.68
1:A:30:ASN:HB2	1:A:90:ASN:HB2	1.76	0.67
1:A:2:MET:HG2	1:A:86:CYS:SG	2.35	0.67
2:B:167:LEU:CD1	2:B:182:MET:HG2	2.24	0.67
2:B:112:VAL:HA	2:B:116:GLN:HE21	1.60	0.66
2:B:112:VAL:CA	2:B:116:GLN:HE21	2.08	0.66
2:B:122:CYS:HB3	2:B:178:VAL:HG13	1.78	0.66
2:B:135:SER:O	2:B:195:CYS:HA	1.94	0.66
1:A:17:VAL:HG22	1:A:18:THR:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:O	1:A:56:ILE:HG22	1.96	0.65
2:B:122:CYS:HB3	2:B:178:VAL:CG1	2.26	0.65
2:B:112:VAL:HG11	2:B:185:LEU:HD13	1.74	0.65
1:A:32:GLU:OE1	1:A:44:LEU:HD11	1.96	0.65
1:A:18:THR:HG23	1:A:70:THR:HG21	1.79	0.65
1:A:46:ILE:HG23	1:A:51:ASN:H	1.60	0.65
2:B:133:GLY:O	2:B:197:ARG:HA	1.97	0.65
1:A:53:GLN:HG2	1:A:54:THR:H	1.62	0.65
2:B:148:ILE:HG13	2:B:163:LEU:CD2	2.25	0.65
1:A:27:ILE:HD13	1:A:88:GLN:CG	2.26	0.64
2:B:109:PRO:HD3	2:B:216:THR:OG1	1.97	0.64
1:A:61:SER:OG	1:A:72:THR:HG23	1.97	0.63
1:A:2:MET:SD	1:A:88:GLN:HB2	2.38	0.63
2:B:112:VAL:HG22	2:B:116:GLN:NE2	2.13	0.63
2:B:112:VAL:CG1	2:B:185:LEU:CD1	2.74	0.63
2:B:197:ARG:HD2	2:B:210:VAL:HG23	1.81	0.63
2:B:162:ALA:CB	2:B:163:LEU:HD12	2.29	0.63
2:B:148:ILE:HD13	2:B:180:LEU:CD2	2.28	0.63
1:A:2:MET:SD	1:A:88:GLN:OE1	2.56	0.63
2:B:136:TRP:CB	2:B:148:ILE:CG2	2.77	0.62
2:B:197:ARG:O	2:B:210:VAL:HG22	1.99	0.62
2:B:122:CYS:HG	2:B:195:CYS:CB	2.13	0.62
2:B:215:GLY:O	2:B:216:THR:HB	1.98	0.62
1:A:29:LYS:HB3	1:A:49:ALA:HB2	1.83	0.61
2:B:178:VAL:O	2:B:179:LEU:HD13	1.99	0.61
1:A:37:LYS:HA	1:A:82:ALA:HB2	1.81	0.61
2:B:160:HIS:CD2	2:B:162:ALA:H	2.19	0.61
2:B:120:LEU:HD12	2:B:180:LEU:HD23	1.84	0.60
2:B:147:TRP:CZ2	2:B:150:THR:HG22	2.31	0.60
1:A:105:ARG:HG2	1:A:106:ALA:N	2.15	0.60
2:B:167:LEU:HD13	2:B:182:MET:HG2	1.83	0.60
1:A:85:TYR:CD1	2:B:145:LEU:HD12	2.36	0.60
2:B:136:TRP:CB	2:B:148:ILE:HG23	2.32	0.59
2:B:197:ARG:CD	2:B:210:VAL:HG23	2.32	0.59
1:A:12:SER:O	1:A:15:ASP:HB2	2.03	0.59
1:A:27:ILE:CB	1:A:90:ASN:HB3	2.33	0.59
1:A:45:LEU:HB3	1:A:56:ILE:HD12	1.84	0.58
2:B:163:LEU:N	2:B:163:LEU:HD12	2.17	0.58
2:B:198:SER:HA	2:B:208:TRP:O	2.04	0.58
2:B:151:MET:HG2	2:B:157:THR:HG22	1.85	0.58
1:A:44:LEU:HB3	1:A:53:GLN:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:CA	1:A:56:ILE:HD12	2.34	0.57
2:B:117:THR:HG22	2:B:183:ASN:HA	1.85	0.57
1:A:42:PRO:HB2	2:B:211:TYR:CE1	2.39	0.57
2:B:136:TRP:HB3	2:B:148:ILE:HG21	1.84	0.57
2:B:133:GLY:HA2	2:B:171:ARG:NH2	2.18	0.57
2:B:109:PRO:HG3	2:B:216:THR:OG1	2.05	0.57
1:A:27:ILE:HG22	1:A:90:ASN:HB3	1.87	0.57
1:A:27:ILE:HB	1:A:90:ASN:HB3	1.86	0.57
2:B:148:ILE:HD11	2:B:167:LEU:CD1	2.28	0.57
1:A:23:ALA:HB1	1:A:88:GLN:HE22	1.70	0.57
1:A:81:VAL:CG1	1:A:103:LEU:CD1	2.82	0.56
1:A:18:THR:CG2	1:A:70:THR:CG2	2.82	0.56
1:A:18:THR:HG23	1:A:70:THR:HG23	1.86	0.56
1:A:27:ILE:CG2	1:A:88:GLN:HE21	2.19	0.56
2:B:160:HIS:CE1	2:B:163:LEU:CD1	2.88	0.56
2:B:124:VAL:HG23	2:B:212:TRP:CZ3	2.39	0.56
2:B:109:PRO:HB2	2:B:217:LEU:O	2.06	0.56
1:A:45:LEU:HB3	1:A:56:ILE:CD1	2.36	0.56
2:B:124:VAL:HG22	2:B:125:SER:N	2.20	0.56
1:A:5:ILE:HD12	1:A:6:PRO:CA	2.34	0.56
2:B:200:LEU:HD12	2:B:206:ARG:CB	2.32	0.56
2:B:112:VAL:HA	2:B:116:GLN:NE2	2.21	0.56
2:B:122:CYS:CB	2:B:195:CYS:HG	2.18	0.56
2:B:112:VAL:HG21	2:B:118:LEU:CD2	2.27	0.56
2:B:162:ALA:C	2:B:163:LEU:HD12	2.26	0.55
2:B:136:TRP:HB2	2:B:148:ILE:HG23	1.87	0.55
2:B:160:HIS:NE2	2:B:162:ALA:HB3	2.21	0.55
1:A:27:ILE:CG2	1:A:90:ASN:HB3	2.37	0.55
2:B:112:VAL:HG22	2:B:116:GLN:HE22	1.72	0.55
2:B:121:THR:CG2	2:B:177:GLN:NE2	2.70	0.55
2:B:167:LEU:HD11	2:B:182:MET:HG2	1.88	0.54
1:A:77:GLN:HB3	1:A:78:PRO:CD	2.25	0.54
2:B:109:PRO:CG	2:B:216:THR:OG1	2.55	0.54
1:A:45:LEU:CB	1:A:56:ILE:HD12	2.38	0.54
1:A:78:PRO:HA	1:A:103:LEU:HD11	1.90	0.54
1:A:32:GLU:HG2	1:A:89:TYR:CE1	2.43	0.54
2:B:134:VAL:HA	2:B:196:ALA:O	2.08	0.54
1:A:17:VAL:HG22	1:A:18:THR:H	1.72	0.53
2:B:206:ARG:O	2:B:206:ARG:HG3	2.09	0.53
1:A:45:LEU:HA	1:A:56:ILE:HD12	1.89	0.53
2:B:129:LEU:HD12	2:B:176:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:CD1	1:A:80:ASP:HB2	2.39	0.53
2:B:160:HIS:CE1	2:B:163:LEU:HD13	2.44	0.52
2:B:190:THR:O	2:B:191:ALA:HB2	2.09	0.52
2:B:121:THR:HG23	2:B:177:GLN:CD	2.29	0.52
2:B:108:GLY:N	2:B:109:PRO:CD	2.73	0.52
2:B:121:THR:HG22	2:B:122:CYS:N	2.24	0.52
2:B:124:VAL:HB	2:B:212:TRP:HH2	1.73	0.52
2:B:196:ALA:HA	2:B:212:TRP:CD1	2.45	0.52
2:B:134:VAL:CG1	2:B:178:VAL:HG21	2.40	0.51
2:B:197:ARG:HD3	2:B:210:VAL:CG2	2.39	0.51
1:A:9:LEU:CG	1:A:17:VAL:HG21	2.39	0.51
2:B:216:THR:HG23	2:B:216:THR:O	2.11	0.51
1:A:31:LEU:HD22	1:A:87:TYR:O	2.09	0.51
2:B:109:PRO:CD	2:B:216:THR:OG1	2.59	0.51
2:B:111:LEU:HD12	2:B:112:VAL:H	1.77	0.50
2:B:121:THR:CG2	2:B:122:CYS:N	2.73	0.50
1:A:6:PRO:HD2	1:A:19:LEU:HB3	1.94	0.50
1:A:32:GLU:OE2	1:A:47:TYR:HB2	2.10	0.50
2:B:122:CYS:SG	2:B:178:VAL:CG1	2.99	0.50
2:B:163:LEU:HB3	2:B:167:LEU:HG	1.94	0.50
2:B:112:VAL:HG13	2:B:116:GLN:CG	2.32	0.50
1:A:18:THR:HG22	1:A:20:ASN:OD1	2.11	0.50
1:A:101:LEU:HD12	1:A:102:GLU:N	2.27	0.50
2:B:196:ALA:HA	2:B:212:TRP:NE1	2.26	0.49
2:B:202:GLY:O	2:B:203:TYR:HB2	2.13	0.49
1:A:18:THR:CG2	1:A:70:THR:HG23	2.42	0.49
2:B:122:CYS:CB	2:B:178:VAL:CG1	2.90	0.49
1:A:59:ARG:HD3	1:A:75:SER:O	2.13	0.49
1:A:89:TYR:CD2	2:B:207:GLY:HA3	2.48	0.49
2:B:134:VAL:HG11	2:B:178:VAL:HG11	1.95	0.49
1:A:38:LEU:HD12	1:A:39:GLY:H	1.78	0.48
2:B:112:VAL:CG1	2:B:185:LEU:HD13	2.43	0.48
1:A:34:TYR:CD1	2:B:211:TYR:HE2	2.31	0.48
2:B:124:VAL:HG21	2:B:127:PHE:CE2	2.48	0.48
1:A:33:TRP:CZ3	1:A:86:CYS:HB3	2.49	0.48
1:A:32:GLU:HB2	1:A:87:TYR:HB3	1.95	0.48
2:B:192:MET:HG2	2:B:217:LEU:HD13	1.96	0.48
1:A:22:LYS:HG3	1:A:68:ASP:OD1	2.13	0.47
2:B:134:VAL:HG12	2:B:178:VAL:HG21	1.96	0.47
2:B:124:VAL:HG21	2:B:127:PHE:CE1	2.48	0.47
2:B:200:LEU:HA	2:B:208:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG2	1:A:106:ALA:H	1.79	0.47
1:A:29:LYS:HB3	1:A:49:ALA:CB	2.44	0.47
1:A:81:VAL:O	1:A:82:ALA:HB2	2.15	0.47
1:A:64:GLY:HA3	1:A:69:TYR:HA	1.98	0.46
1:A:81:VAL:HG11	1:A:103:LEU:CD1	2.32	0.46
1:A:32:GLU:HG2	1:A:89:TYR:HE1	1.79	0.46
2:B:160:HIS:CE1	2:B:162:ALA:HB3	2.50	0.46
1:A:18:THR:CG2	1:A:70:THR:HG21	2.43	0.46
2:B:200:LEU:HD22	2:B:201:PRO:N	2.31	0.46
1:A:81:VAL:O	1:A:82:ALA:CB	2.64	0.45
2:B:162:ALA:HB3	2:B:163:LEU:CD1	2.42	0.45
1:A:76:LEU:HD11	1:A:80:ASP:HB2	1.99	0.45
2:B:122:CYS:CB	2:B:195:CYS:SG	3.05	0.45
2:B:122:CYS:SG	2:B:178:VAL:HG11	2.57	0.44
2:B:129:LEU:HB3	2:B:171:ARG:HH11	1.81	0.44
2:B:200:LEU:HB2	2:B:204:ASN:O	2.17	0.44
2:B:124:VAL:CB	2:B:212:TRP:CH2	2.92	0.44
2:B:129:LEU:HB3	2:B:171:ARG:NH1	2.32	0.44
2:B:200:LEU:N	2:B:201:PRO:HD2	2.09	0.44
2:B:122:CYS:SG	2:B:195:CYS:CB	3.03	0.44
2:B:193:TYR:O	2:B:216:THR:HG22	2.18	0.44
2:B:160:HIS:HD2	2:B:162:ALA:H	1.63	0.44
2:B:196:ALA:HB3	2:B:209:PHE:HB3	1.98	0.44
1:A:34:TYR:CD1	2:B:211:TYR:CE2	3.06	0.44
2:B:208:TRP:CD1	2:B:210:VAL:CG1	3.02	0.43
2:B:177:GLN:OE1	2:B:179:LEU:HD11	2.17	0.43
2:B:208:TRP:HD1	2:B:210:VAL:HG12	1.82	0.43
1:A:35:GLN:HB2	1:A:45:LEU:HD11	1.99	0.43
1:A:53:GLN:HG2	1:A:54:THR:N	2.31	0.43
1:A:52:LEU:CD2	1:A:56:ILE:HG23	2.45	0.43
2:B:129:LEU:HD21	2:B:134:VAL:HG21	1.99	0.43
2:B:199:GLN:HB2	2:B:208:TRP:CE2	2.54	0.43
2:B:112:VAL:HG13	2:B:116:GLN:NE2	2.34	0.43
2:B:148:ILE:HD13	2:B:148:ILE:HG21	1.66	0.43
2:B:166:ARG:NH2	2:B:189:ASP:OD2	2.52	0.43
2:B:163:LEU:CD1	2:B:163:LEU:N	2.83	0.42
2:B:200:LEU:H	2:B:201:PRO:CD	2.15	0.42
1:A:89:TYR:HB2	2:B:207:GLY:HA3	2.01	0.42
1:A:47:TYR:O	1:A:51:ASN:HB3	2.20	0.42
1:A:19:LEU:HG	1:A:99:THR:HG21	2.01	0.42
1:A:30:ASN:OD1	1:A:48:TYR:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LEU:HD12	2:B:112:VAL:N	2.34	0.42
2:B:200:LEU:HD22	2:B:201:PRO:CD	2.50	0.42
1:A:76:LEU:HD12	1:A:80:ASP:HB2	2.01	0.42
1:A:92:GLY:O	1:A:93:HIS:HB2	2.19	0.42
1:A:85:TYR:CE1	2:B:145:LEU:HD12	2.54	0.42
2:B:200:LEU:HD22	2:B:201:PRO:HD3	2.01	0.42
1:A:81:VAL:HG13	1:A:103:LEU:HD12	1.96	0.42
1:A:29:LYS:HB2	1:A:48:TYR:CZ	2.55	0.42
1:A:29:LYS:HB2	1:A:48:TYR:CE2	2.55	0.41
2:B:200:LEU:HB3	2:B:206:ARG:CA	2.35	0.41
2:B:112:VAL:C	2:B:116:GLN:HE21	2.23	0.41
2:B:208:TRP:CD1	2:B:210:VAL:HG12	2.55	0.41
2:B:185:LEU:HD23	2:B:185:LEU:HA	1.87	0.41
1:A:17:VAL:CG2	1:A:18:THR:N	2.83	0.41
1:A:4:GLN:HG3	1:A:21:CYS:SG	2.61	0.41
2:B:108:GLY:N	2:B:109:PRO:HD2	2.35	0.41
2:B:151:MET:HA	2:B:156:ASP:O	2.20	0.41
1:A:19:LEU:CD1	1:A:19:LEU:N	2.84	0.41
1:A:36:GLN:HB3	1:A:83:THR:HG23	2.02	0.41
1:A:48:TYR:HB2	1:A:89:TYR:OH	2.21	0.41
1:A:59:ARG:O	1:A:73:ILE:HA	2.19	0.41
2:B:124:VAL:CB	2:B:212:TRP:CZ3	3.03	0.41
2:B:197:ARG:HH11	2:B:210:VAL:HG23	1.86	0.41
2:B:112:VAL:CA	2:B:116:GLN:NE2	2.78	0.40
2:B:151:MET:HG2	2:B:157:THR:CG2	2.49	0.40
1:A:2:MET:SD	1:A:88:GLN:CB	3.07	0.40
1:A:47:TYR:CD2	2:B:208:TRP:CZ2	3.09	0.40
2:B:136:TRP:C	2:B:148:ILE:CG2	2.87	0.40
1:A:20:ASN:OD1	1:A:70:THR:HG23	2.21	0.40
2:B:113:GLN:HA	2:B:114:PRO:HD3	1.95	0.40

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 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	A	104/106 (98%)	89 (86%)	11 (11%)	4 (4%)	4	32
2	B	113/115 (98%)	99 (88%)	5 (4%)	9 (8%)	1	17
All	All	217/221 (98%)	188 (87%)	16 (7%)	13 (6%)	3	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
2	B	201	PRO
2	B	212	TRP
2	B	216	THR
1	A	93	HIS
2	B	115	SER
2	B	126	GLY
2	B	200	LEU
2	B	202	GLY
2	B	203	TYR
1	A	55	GLY
1	A	66	GLY
2	B	109	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 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	A	90/90 (100%)	85 (94%)	5 (6%)	25	57
2	B	100/100 (100%)	91 (91%)	9 (9%)	11	38
All	All	190/190 (100%)	176 (93%)	14 (7%)	21	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	5	ILE
1	A	19	LEU
1	A	61	SER
1	A	101	LEU
2	B	113	GLN
2	B	122	CYS
2	B	167	LEU
2	B	179	LEU
2	B	192	MET
2	B	195	CYS
2	B	197	ARG
2	B	200	LEU
2	B	201	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	88	GLN
2	B	116	GLN
2	B	160	HIS
2	B	186	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 [i](#)

There are no chain breaks in this entry.