wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:38 PM BST

PDB ID	:	3IY1
EMDB ID:	:	EMD-5106
Title	:	Variable domains of the WAM of Fab B fitted into the cryoEM reconstruction of the virus-Fab B complex
Authors	:	Hafenstein, S.; Bowman, V.D.; Sun, T.; Nelson, C.D.; Palermo, L.M.; Battisti, A.J.; Parrish, C.R.; Rossmann, M.G.
Deposited on	:	2009-04-09
Resolution	:	18.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

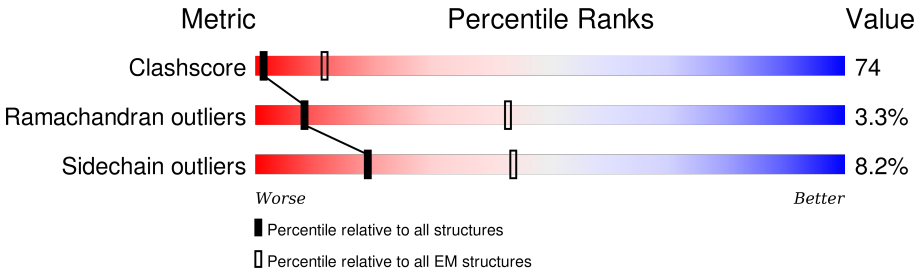
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 18.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	107	43% 42% 13% .
2	B	109	45% 34% 15% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1648 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 Fab B, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	107	819	517	137	162	3	0	0

- Molecule 2 is a protein called Fab B, heavy chain.

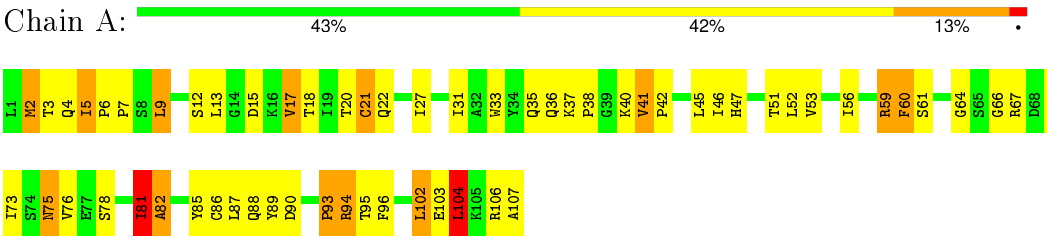
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	109	829	526	130	169	4	0	0

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. 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.

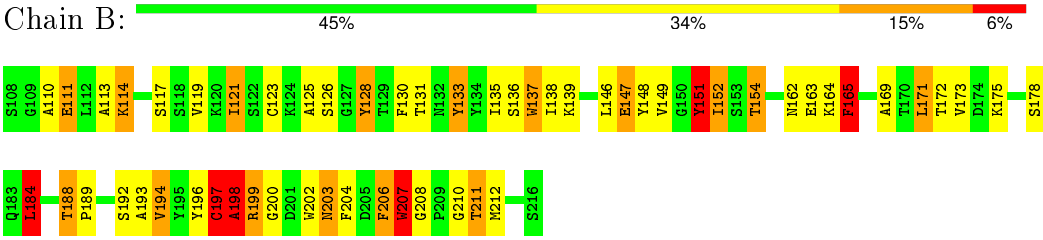
- Molecule 1: Fab B, light chain

Chain A:



- Molecule 2: Fab B, heavy chain

Chain B:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	1126	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 ($e^-/Å^2$)	28.4	Depositor
Minimum defocus (nm)	1.7	Depositor
Maximum defocus (nm)	3.7	Depositor
Magnification	45000	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	1.04	2/837 (0.2%)	1.47	16/1132 (1.4%)
2	B	1.47	6/850 (0.7%)	2.52	48/1151 (4.2%)
All	All	1.28	8/1687 (0.5%)	2.07	64/2283 (2.8%)

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	4
All	All	1	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	207	TRP	CD2-CE2	-19.02	1.18	1.41
2	B	207	TRP	NE1-CE2	9.69	1.50	1.37
2	B	207	TRP	CZ3-CH2	-6.09	1.30	1.40
1	A	60	PHE	CG-CD2	-5.66	1.30	1.38
2	B	165	PHE	CE2-CZ	-5.47	1.26	1.37
2	B	165	PHE	CD2-CE2	-5.24	1.28	1.39
2	B	207	TRP	CG-CD1	-5.11	1.29	1.36
1	A	60	PHE	CG-CD1	-5.00	1.31	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	165	PHE	CD1-CE1-CZ	-30.00	84.10	120.10
2	B	165	PHE	CZ-CE2-CD2	-24.60	90.58	120.10
2	B	207	TRP	NE1-CE2-CZ2	-19.87	108.54	130.40
2	B	154	THR	CA-CB-CG2	17.62	137.06	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	207	TRP	CD2-CE2-CZ2	17.41	143.19	122.30
2	B	207	TRP	CE2-CD2-CG	14.84	119.17	107.30
2	B	207	TRP	CD1-NE1-CE2	-14.04	96.36	109.00
2	B	207	TRP	CH2-CZ2-CE2	-13.68	103.72	117.40
2	B	121	ILE	CA-CB-CG2	13.03	136.95	110.90
2	B	206	PHE	CB-CA-C	10.59	131.57	110.40
2	B	147	GLU	CG-CD-OE1	-10.11	98.09	118.30
2	B	121	ILE	CB-CA-C	10.07	131.75	111.60
1	A	93	PRO	N-CA-CB	-9.98	91.32	103.30
2	B	171	LEU	N-CA-CB	-9.98	90.44	110.40
1	A	17	VAL	CA-CB-CG2	-9.34	96.89	110.90
2	B	154	THR	CB-CA-C	9.31	136.74	111.60
2	B	165	PHE	CG-CD2-CE2	-9.28	110.59	120.80
1	A	60	PHE	CB-CG-CD2	9.15	127.21	120.80
1	A	60	PHE	CG-CD1-CE1	9.03	130.73	120.80
2	B	171	LEU	CB-CG-CD2	-8.85	95.95	111.00
2	B	151	TYR	CB-CA-C	-8.79	92.82	110.40
2	B	207	TRP	CD1-CG-CD2	-8.69	99.35	106.30
2	B	165	PHE	CB-CG-CD2	-8.26	115.02	120.80
2	B	207	TRP	CG-CD2-CE3	-8.07	126.64	133.90
2	B	147	GLU	CG-CD-OE2	7.81	133.93	118.30
1	A	104	LEU	N-CA-CB	-7.56	95.28	110.40
1	A	81	ILE	CB-CA-C	-7.55	96.50	111.60
2	B	207	TRP	CB-CG-CD2	7.46	136.30	126.60
2	B	197	CYS	O-C-N	-7.41	110.84	122.70
2	B	154	THR	N-CA-CB	-7.33	96.37	110.30
1	A	81	ILE	CA-CB-CG2	7.04	124.98	110.90
2	B	188	THR	CA-CB-CG2	7.04	122.25	112.40
2	B	165	PHE	CB-CG-CD1	-6.88	115.99	120.80
2	B	165	PHE	CG-CD1-CE1	-6.87	113.25	120.80
1	A	104	LEU	CA-CB-CG	-6.85	99.54	115.30
2	B	179	THR	CA-CB-CG2	-6.84	102.82	112.40
2	B	165	PHE	CD1-CG-CD2	6.79	127.12	118.30
2	B	207	TRP	CG-CD1-NE1	6.71	116.81	110.10
2	B	171	LEU	CB-CA-C	-6.64	97.58	110.20
2	B	206	PHE	N-CA-CB	-6.44	99.01	110.60
2	B	207	TRP	CE3-CZ3-CH2	6.44	128.28	121.20
2	B	165	PHE	CE1-CZ-CE2	6.16	131.09	120.00
1	A	81	ILE	CA-CB-CG1	6.16	122.69	111.00
2	B	206	PHE	CA-C-N	6.04	130.49	117.20
2	B	199	ARG	N-CA-C	-6.02	94.75	111.00
1	A	71	PHE	CE1-CZ-CE2	5.99	130.77	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	137	TRP	CD1-NE1-CE2	-5.77	103.80	109.00
2	B	121	ILE	N-CA-CB	-5.66	97.78	110.80
2	B	126	SER	CA-C-N	-5.55	105.11	116.20
2	B	206	PHE	N-CA-C	-5.46	96.25	111.00
2	B	126	SER	O-C-N	5.39	132.36	123.20
2	B	202	TRP	CD1-NE1-CE2	-5.38	104.16	109.00
1	A	9	LEU	CB-CG-CD2	-5.37	101.86	111.00
2	B	128	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	59	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	B	152	ILE	CB-CA-C	-5.32	100.97	111.60
2	B	152	ILE	CA-CB-CG2	5.30	121.50	110.90
2	B	206	PHE	O-C-N	-5.28	114.25	122.70
2	B	184	LEU	CB-CG-CD1	5.27	119.96	111.00
1	A	21	CYS	CA-CB-SG	-5.22	104.60	114.00
1	A	94	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	17	VAL	CA-CB-CG1	5.15	118.62	110.90
1	A	94	ARG	N-CA-CB	-5.09	101.43	110.60
2	B	207	TRP	CD2-CE3-CZ3	-5.06	112.22	118.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	81	ILE	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	TYR	Sidechain
2	B	165	PHE	Sidechain
2	B	197	CYS	Mainchain
2	B	198	ALA	Mainchain

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	A	819	0	812	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	829	0	786	160	0
All	All	1648	0	1598	237	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 74.

All (237) 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)
2:B:198:ALA:HB1	2:B:204:PHE:HB3	1.28	1.16
1:A:9:LEU:HD21	1:A:17:VAL:HG21	1.35	1.07
1:A:9:LEU:HD21	1:A:17:VAL:CG2	1.86	1.04
2:B:206:PHE:CB	2:B:207:TRP:HB3	1.91	1.01
1:A:60:PHE:HD1	1:A:71:PHE:CZ	1.77	1.01
1:A:60:PHE:CD1	1:A:71:PHE:HZ	1.79	1.00
1:A:87:LEU:HD21	1:A:94:ARG:HG2	1.44	0.98
2:B:154:THR:HG23	2:B:173:VAL:CB	1.94	0.98
1:A:60:PHE:HD1	1:A:71:PHE:HZ	1.04	0.96
2:B:179:THR:HG21	2:B:181:PHE:CZ	2.01	0.96
2:B:123:CYS:HB3	2:B:180:THR:CG2	1.98	0.94
2:B:154:THR:CB	2:B:173:VAL:HG21	1.97	0.94
2:B:206:PHE:HB3	2:B:207:TRP:HB3	1.46	0.94
2:B:154:THR:HG23	2:B:173:VAL:HB	1.50	0.92
2:B:152:ILE:HB	2:B:171:LEU:CD2	2.02	0.89
2:B:154:THR:HA	2:B:173:VAL:HG21	1.54	0.89
2:B:123:CYS:HB3	2:B:180:THR:HG23	1.54	0.88
2:B:164:LYS:HG2	2:B:165:PHE:HZ	1.36	0.87
2:B:182:MET:HG3	2:B:184:LEU:HD11	1.55	0.87
2:B:154:THR:HB	2:B:175:LYS:HZ3	1.40	0.86
2:B:188:THR:HG23	2:B:189:PRO:HD2	1.55	0.86
1:A:93:PRO:HB2	2:B:148:TYR:CE2	2.10	0.86
1:A:41:VAL:HG13	2:B:196:TYR:CE1	2.12	0.85
2:B:114:LYS:HE2	2:B:117:SER:HB3	1.57	0.84
2:B:198:ALA:HA	2:B:207:TRP:CD1	2.13	0.84
2:B:182:MET:HG3	2:B:184:LEU:CD1	2.06	0.84
1:A:9:LEU:CD2	1:A:17:VAL:HG21	2.07	0.84
2:B:179:THR:HG21	2:B:181:PHE:CE2	2.13	0.84
1:A:93:PRO:HB2	2:B:148:TYR:CD2	2.13	0.84
2:B:149:VAL:HG12	2:B:182:MET:HE1	1.60	0.83
2:B:119:VAL:HG12	2:B:184:LEU:HB2	1.61	0.83
2:B:119:VAL:CG1	2:B:184:LEU:HD22	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:CG2	2:B:189:PRO:HD2	2.07	0.83
1:A:89:TYR:HB2	1:A:94:ARG:HH12	1.44	0.81
1:A:5:ILE:HD12	1:A:6:PRO:HA	1.63	0.80
1:A:87:LEU:HD11	1:A:94:ARG:HD3	1.63	0.80
1:A:36:GLN:O	1:A:82:ALA:HB1	1.82	0.80
1:A:87:LEU:HD11	1:A:94:ARG:CG	2.12	0.79
2:B:121:ILE:HD12	2:B:184:LEU:HD22	1.65	0.79
2:B:154:THR:HG23	2:B:173:VAL:CG2	2.12	0.79
2:B:154:THR:HG22	2:B:175:LYS:HD3	1.63	0.79
2:B:198:ALA:CB	2:B:204:PHE:HB3	2.10	0.79
1:A:53:VAL:O	1:A:56:ILE:HG22	1.81	0.78
2:B:121:ILE:HD12	2:B:184:LEU:CD2	2.14	0.78
2:B:154:THR:HB	2:B:175:LYS:HE2	1.66	0.77
2:B:198:ALA:C	2:B:207:TRP:HE1	1.88	0.77
2:B:169:ALA:HB1	2:B:182:MET:HE3	1.65	0.76
2:B:137:TRP:HD1	2:B:171:LEU:CD1	1.99	0.76
2:B:154:THR:CA	2:B:173:VAL:HG21	2.16	0.76
2:B:164:LYS:HE2	2:B:165:PHE:CZ	2.20	0.75
1:A:37:LYS:HB2	1:A:40:LYS:HE2	1.68	0.74
1:A:87:LEU:HD11	1:A:94:ARG:CD	2.17	0.74
1:A:96:PHE:CE2	2:B:138:ILE:HD12	2.21	0.74
2:B:154:THR:HB	2:B:175:LYS:CE	2.19	0.72
2:B:154:THR:HB	2:B:175:LYS:NZ	2.04	0.72
2:B:154:THR:CG2	2:B:173:VAL:HG21	2.20	0.72
2:B:110:ALA:O	2:B:111:GLU:HG2	1.89	0.71
1:A:87:LEU:HD11	1:A:94:ARG:HG3	1.72	0.71
2:B:114:LYS:HE2	2:B:117:SER:CB	2.21	0.70
1:A:37:LYS:HA	1:A:82:ALA:CB	2.22	0.70
1:A:87:LEU:HD23	1:A:96:PHE:CG	2.26	0.69
2:B:136:SER:HB3	2:B:204:PHE:CZ	2.27	0.69
2:B:169:ALA:HB1	2:B:182:MET:CE	2.23	0.69
1:A:9:LEU:HD21	1:A:17:VAL:HG22	1.74	0.69
2:B:152:ILE:CD1	2:B:172:THR:HA	2.22	0.69
2:B:154:THR:HA	2:B:173:VAL:CG2	2.24	0.68
2:B:164:LYS:HG2	2:B:165:PHE:CZ	2.23	0.67
2:B:113:ALA:HB1	2:B:117:SER:OG	1.93	0.67
1:A:87:LEU:HD11	1:A:94:ARG:HH11	1.60	0.67
1:A:22:GLN:HA	1:A:67:ARG:O	1.94	0.66
2:B:149:VAL:CG1	2:B:182:MET:HE1	2.23	0.66
1:A:2:MET:HG2	1:A:86:CYS:SG	2.35	0.66
2:B:136:SER:HB3	2:B:204:PHE:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:CYS:CB	2:B:180:THR:CG2	2.72	0.66
1:A:60:PHE:CD1	1:A:71:PHE:CZ	2.64	0.65
2:B:152:ILE:HB	2:B:171:LEU:HD21	1.77	0.65
2:B:128:TYR:CE1	2:B:130:PHE:HA	2.32	0.64
1:A:13:LEU:CD2	1:A:104:LEU:HD21	2.26	0.64
1:A:27:ILE:HB	1:A:90:ASP:HB2	1.79	0.64
2:B:152:ILE:HB	2:B:171:LEU:HD23	1.80	0.64
2:B:198:ALA:CA	2:B:207:TRP:NE1	2.60	0.64
1:A:85:TYR:CD1	2:B:146:LEU:HD12	2.33	0.64
1:A:37:LYS:HA	1:A:82:ALA:HB2	1.80	0.64
1:A:41:VAL:HG11	2:B:208:GLY:O	1.98	0.63
2:B:128:TYR:CE1	2:B:199:ARG:HD2	2.33	0.63
2:B:154:THR:HG22	2:B:175:LYS:CD	2.29	0.62
2:B:182:MET:CG	2:B:184:LEU:HD11	2.29	0.62
1:A:17:VAL:HG22	1:A:18:THR:N	2.14	0.62
2:B:206:PHE:CA	2:B:207:TRP:HB3	2.30	0.62
2:B:123:CYS:HG	2:B:197:CYS:CB	2.13	0.62
2:B:130:PHE:CE1	2:B:135:ILE:HD11	2.35	0.62
2:B:154:THR:HG23	2:B:173:VAL:HG21	1.75	0.61
1:A:13:LEU:HD21	1:A:104:LEU:HD21	1.80	0.61
2:B:199:ARG:O	2:B:204:PHE:HA	2.01	0.61
2:B:130:PHE:CE2	2:B:175:LYS:HA	2.35	0.61
1:A:27:ILE:HA	1:A:90:ASP:OD2	2.01	0.60
1:A:106:ARG:HG2	1:A:107:ALA:N	2.17	0.60
1:A:87:LEU:CD1	1:A:94:ARG:HH11	2.13	0.60
2:B:138:ILE:HG23	2:B:196:TYR:HB2	1.82	0.59
2:B:114:LYS:HD3	2:B:114:LYS:H	1.67	0.59
2:B:152:ILE:N	2:B:171:LEU:HD21	2.18	0.59
2:B:139:LYS:CE	2:B:164:LYS:HZ3	2.14	0.59
1:A:12:SER:O	1:A:15:ASP:HB2	2.03	0.58
2:B:139:LYS:CE	2:B:164:LYS:NZ	2.66	0.58
2:B:154:THR:CB	2:B:175:LYS:HZ3	2.14	0.58
2:B:198:ALA:HA	2:B:207:TRP:NE1	2.18	0.58
2:B:154:THR:HG22	2:B:175:LYS:CE	2.33	0.57
1:A:45:LEU:CA	1:A:56:ILE:HD12	2.34	0.57
2:B:123:CYS:CB	2:B:197:CYS:HG	2.17	0.57
1:A:45:LEU:HB3	1:A:56:ILE:HD12	1.86	0.57
1:A:5:ILE:HD12	1:A:6:PRO:CA	2.33	0.57
1:A:87:LEU:CD1	1:A:94:ARG:HD3	2.34	0.56
1:A:41:VAL:HG12	1:A:42:PRO:HD2	1.86	0.56
2:B:182:MET:HG3	2:B:184:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:TRP:HD1	2:B:171:LEU:HD12	1.70	0.56
1:A:89:TYR:HB2	1:A:94:ARG:NH1	2.19	0.56
1:A:96:PHE:CZ	2:B:138:ILE:HD12	2.40	0.56
2:B:162:ASN:OD1	2:B:164:LYS:HB3	2.05	0.56
1:A:87:LEU:HD13	1:A:87:LEU:C	2.25	0.55
2:B:139:LYS:HE2	2:B:164:LYS:HZ3	1.72	0.55
2:B:123:CYS:SG	2:B:180:THR:CG2	2.95	0.55
2:B:194:VAL:HG11	2:B:196:TYR:CZ	2.41	0.55
2:B:154:THR:CB	2:B:175:LYS:HE2	2.34	0.55
1:A:87:LEU:HD22	1:A:95:THR:O	2.06	0.54
1:A:45:LEU:HA	1:A:56:ILE:HD12	1.89	0.54
2:B:137:TRP:CD1	2:B:171:LEU:HD12	2.43	0.54
2:B:123:CYS:HB3	2:B:180:THR:HG22	1.87	0.54
2:B:198:ALA:CA	2:B:207:TRP:HE1	2.19	0.54
1:A:45:LEU:HB3	1:A:56:ILE:CD1	2.38	0.54
1:A:87:LEU:HD23	1:A:96:PHE:CD2	2.42	0.54
2:B:119:VAL:HG11	2:B:184:LEU:HD22	1.89	0.54
2:B:154:THR:CA	2:B:175:LYS:HE2	2.39	0.53
2:B:135:ILE:HD13	2:B:180:THR:HB	1.90	0.53
2:B:114:LYS:CD	2:B:114:LYS:H	2.22	0.53
2:B:130:PHE:CD2	2:B:175:LYS:HA	2.43	0.53
2:B:121:ILE:HD12	2:B:184:LEU:HD21	1.89	0.53
1:A:93:PRO:CB	2:B:148:TYR:CE2	2.88	0.53
2:B:130:PHE:CE2	2:B:178:SER:HA	2.43	0.53
2:B:137:TRP:CD1	2:B:171:LEU:CD1	2.86	0.53
2:B:133:TYR:HB3	2:B:199:ARG:HG2	1.91	0.53
2:B:125:ALA:HA	2:B:207:TRP:CZ3	2.44	0.53
1:A:9:LEU:CG	1:A:17:VAL:HG21	2.39	0.53
2:B:211:THR:HG23	2:B:211:THR:O	2.09	0.53
2:B:130:PHE:HE1	2:B:135:ILE:HD11	1.74	0.53
2:B:154:THR:CG2	2:B:175:LYS:HZ3	2.21	0.52
2:B:198:ALA:C	2:B:207:TRP:NE1	2.59	0.52
1:A:71:PHE:HE2	1:A:73:ILE:HD11	1.73	0.52
2:B:137:TRP:HD1	2:B:171:LEU:HD11	1.73	0.52
2:B:169:ALA:CB	2:B:182:MET:HE3	2.37	0.52
1:A:45:LEU:CB	1:A:56:ILE:HD12	2.39	0.52
1:A:60:PHE:CE1	1:A:71:PHE:HZ	2.24	0.52
2:B:123:CYS:CB	2:B:180:THR:HG22	2.39	0.52
1:A:38:PRO:HD3	1:A:82:ALA:HB2	1.90	0.51
2:B:164:LYS:HD3	2:B:165:PHE:CE1	2.46	0.51
2:B:154:THR:CG2	2:B:175:LYS:NZ	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PHE:CE2	2:B:138:ILE:CD1	2.94	0.51
2:B:110:ALA:HB1	2:B:212:MET:O	2.10	0.51
1:A:3:THR:HB	1:A:22:GLN:HG2	1.92	0.50
2:B:152:ILE:HD13	2:B:172:THR:HA	1.93	0.50
2:B:154:THR:HG23	2:B:173:VAL:CG1	2.42	0.49
2:B:192:SER:O	2:B:193:ALA:HB2	2.11	0.49
2:B:154:THR:HG22	2:B:175:LYS:NZ	2.27	0.49
2:B:154:THR:OG1	2:B:173:VAL:HG11	2.12	0.49
1:A:17:VAL:HG22	1:A:18:THR:H	1.75	0.49
2:B:179:THR:CG2	2:B:181:PHE:CE2	2.90	0.49
1:A:81:ILE:O	1:A:82:ALA:HB2	2.13	0.49
2:B:199:ARG:N	2:B:207:TRP:NE1	2.61	0.48
1:A:59:ARG:HD3	1:A:75:ASN:O	2.13	0.48
1:A:33:TRP:CZ3	1:A:86:CYS:HB3	2.49	0.48
2:B:125:ALA:HB2	2:B:207:TRP:CH2	2.49	0.48
2:B:151:TYR:C	2:B:171:LEU:HD21	2.34	0.47
2:B:131:THR:HA	2:B:175:LYS:HZ1	1.79	0.47
2:B:154:THR:C	2:B:175:LYS:HE2	2.35	0.47
1:A:85:TYR:CE1	2:B:146:LEU:HD12	2.49	0.47
2:B:125:ALA:HA	2:B:207:TRP:HZ3	1.80	0.47
1:A:102:LEU:HD12	1:A:103:GLU:N	2.29	0.47
2:B:163:GLU:HA	2:B:163:GLU:OE1	2.14	0.47
2:B:164:LYS:CE	2:B:165:PHE:CZ	2.96	0.47
2:B:130:PHE:HE2	2:B:175:LYS:HA	1.80	0.47
2:B:179:THR:HG22	2:B:179:THR:O	2.12	0.47
2:B:194:VAL:HG23	2:B:212:MET:SD	2.55	0.46
1:A:106:ARG:HG2	1:A:107:ALA:H	1.80	0.46
2:B:136:SER:O	2:B:197:CYS:HA	2.15	0.46
2:B:173:VAL:HG12	2:B:180:THR:HA	1.98	0.46
1:A:87:LEU:CD2	1:A:94:ARG:HG2	2.32	0.46
1:A:78:SER:HA	1:A:104:LEU:HD11	1.97	0.46
2:B:135:ILE:HG21	2:B:180:THR:HG21	1.98	0.46
1:A:46:ILE:CD1	1:A:52:LEU:HD23	2.45	0.46
1:A:2:MET:HE1	1:A:31:ILE:HD12	1.98	0.46
2:B:152:ILE:HG21	2:B:173:VAL:HG13	1.96	0.46
1:A:64:GLY:HA3	1:A:69:TYR:HA	1.96	0.46
2:B:147:GLU:CD	2:B:164:LYS:HZ2	2.18	0.46
2:B:123:CYS:SG	2:B:180:THR:HG21	2.56	0.45
2:B:128:TYR:CD1	2:B:199:ARG:HD2	2.51	0.45
2:B:199:ARG:N	2:B:207:TRP:HE1	2.13	0.45
1:A:45:LEU:O	1:A:53:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ILE:CD1	2:B:180:THR:HB	2.47	0.45
1:A:87:LEU:HD23	1:A:96:PHE:CD1	2.51	0.45
1:A:35:GLN:HB2	1:A:45:LEU:HD11	1.99	0.45
1:A:81:ILE:O	1:A:82:ALA:CB	2.64	0.45
2:B:198:ALA:HB1	2:B:204:PHE:CB	2.20	0.45
2:B:206:PHE:HB2	2:B:207:TRP:HB3	1.91	0.45
1:A:87:LEU:HD22	1:A:95:THR:C	2.38	0.44
1:A:15:ASP:O	1:A:76:VAL:HG23	2.16	0.44
2:B:121:ILE:HB	2:B:182:MET:HB3	2.00	0.44
2:B:200:GLY:HA2	2:B:203:ASN:O	2.17	0.44
2:B:137:TRP:CD1	2:B:171:LEU:HD11	2.53	0.44
2:B:110:ALA:C	2:B:111:GLU:HG2	2.39	0.44
2:B:119:VAL:HG13	2:B:184:LEU:HD22	1.97	0.44
1:A:52:LEU:HD22	1:A:56:ILE:CG2	2.48	0.44
2:B:138:ILE:HD11	2:B:146:LEU:HD22	1.99	0.43
2:B:184:LEU:CD1	2:B:184:LEU:N	2.81	0.43
2:B:139:LYS:NZ	2:B:165:PHE:CE2	2.82	0.43
1:A:59:ARG:O	1:A:73:ILE:HA	2.19	0.43
1:A:52:LEU:HD22	1:A:56:ILE:HG23	2.00	0.43
2:B:198:ALA:HB3	2:B:204:PHE:CG	2.54	0.43
1:A:46:ILE:HD11	1:A:52:LEU:HD23	2.01	0.43
2:B:152:ILE:HD13	2:B:172:THR:CA	2.48	0.43
2:B:110:ALA:O	2:B:111:GLU:CG	2.62	0.43
2:B:194:VAL:CG1	2:B:196:TYR:CE2	3.01	0.43
2:B:188:THR:CG2	2:B:189:PRO:CD	2.87	0.43
1:A:4:GLN:HG3	1:A:21:CYS:SG	2.59	0.42
1:A:20:THR:HG23	1:A:69:TYR:O	2.20	0.42
1:A:87:LEU:HD21	1:A:94:ARG:CG	2.32	0.42
2:B:198:ALA:CB	2:B:204:PHE:CB	2.91	0.42
1:A:41:VAL:HG12	1:A:42:PRO:CD	2.49	0.42
1:A:87:LEU:HD13	1:A:88:GLN:N	2.35	0.42
2:B:121:ILE:CD1	2:B:184:LEU:CD2	2.93	0.41
2:B:123:CYS:SG	2:B:197:CYS:CB	3.06	0.41
2:B:164:LYS:CG	2:B:165:PHE:CZ	3.00	0.41
2:B:164:LYS:CD	2:B:165:PHE:CE1	3.03	0.41
1:A:46:ILE:HD11	1:A:52:LEU:CD2	2.50	0.40
2:B:133:TYR:CB	2:B:199:ARG:HG2	2.51	0.40
2:B:194:VAL:CG1	2:B:196:TYR:CZ	3.04	0.40
2:B:210:GLY:O	2:B:211:THR:HB	2.21	0.40
1:A:47:HIS:O	1:A:51:THR:HB	2.22	0.40
2:B:152:ILE:CB	2:B:171:LEU:HD21	2.49	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 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	105/107 (98%)	98 (93%)	4 (4%)	3 (3%)	6 43
2	B	107/109 (98%)	92 (86%)	11 (10%)	4 (4%)	4 38
All	All	212/216 (98%)	190 (90%)	15 (7%)	7 (3%)	8 40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
2	B	111	GLU
2	B	207	TRP
2	B	211	THR
2	B	198	ALA
1	A	66	GLY
1	A	7	PRO

5.3.2 Protein sidechains (i)

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	92/92 (100%)	84 (91%)	8 (9%)	13 45
2	B	90/90 (100%)	83 (92%)	7 (8%)	16 51
All	All	182/182 (100%)	167 (92%)	15 (8%)	19 49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	5	ILE
1	A	41	VAL
1	A	61	SER
1	A	75	ASN
1	A	81	ILE
1	A	102	LEU
1	A	104	LEU
2	B	114	LYS
2	B	151	TYR
2	B	179	THR
2	B	184	LEU
2	B	194	VAL
2	B	197	CYS
2	B	203	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
2	B	144	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.