Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Feb 18, 2018 – 05:19 am GMT

PDB ID	:	5OQV
EMDB ID:	:	EMD-3851
Title	:	Near-atomic resolution fibril structure of complete amyloid-beta(1-42) by cryo-EM
Authors	:	Gremer, L.; Schoelzel, D.; Schenk, C.; Reinartz, E.; Labahn, J.; Ravelli, R.; Tusche, M.; Lopez-Iglesias, C.; Hoyer, W.; Heise, H.; Willbold, D.; Schroeder, G.F.
Deposited on	:	2017-08-14
Resolution	:	4.00 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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

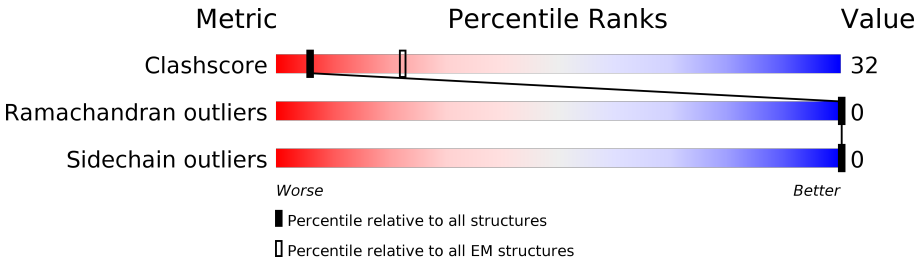
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

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 4.00 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	42	57% 43%
1	B	42	60% 40%
1	C	42	55% 45%
1	D	42	62% 38%
1	E	42	62% 38%
1	F	42	62% 38%
1	G	42	62% 38%
1	H	42	60% 40%
1	I	42	60% 40%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5805 atoms, of which 2835 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 Amyloid beta A4 protein.

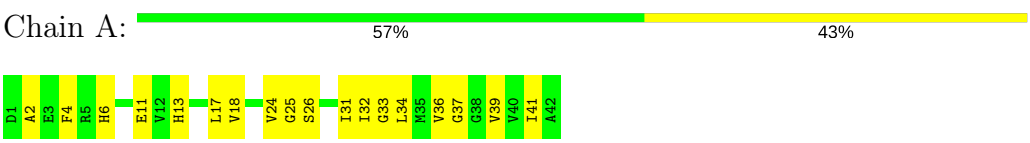
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	B	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	C	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	D	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	E	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	F	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	G	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	H	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		
1	I	42	Total	C	H	N	O	S	2	0
			645	212	315	56	61	1		

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.

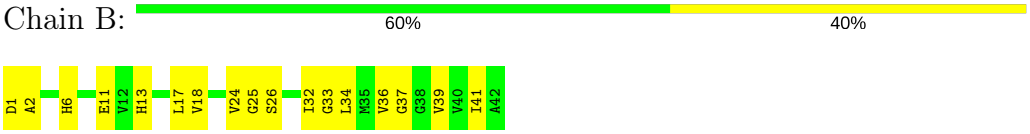
- Molecule 1: Amyloid beta A4 protein

Chain A:



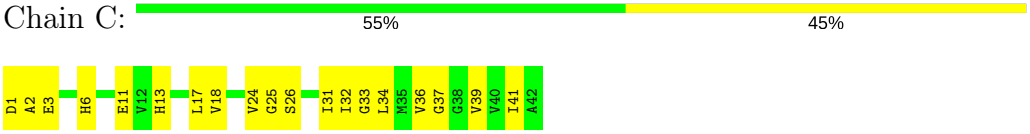
- Molecule 1: Amyloid beta A4 protein

Chain B:



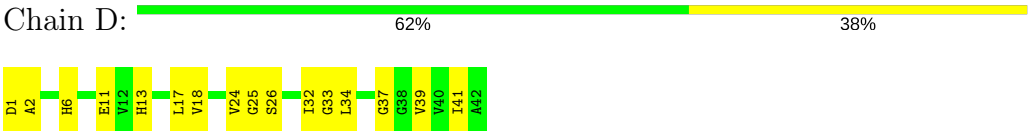
- Molecule 1: Amyloid beta A4 protein

Chain C:



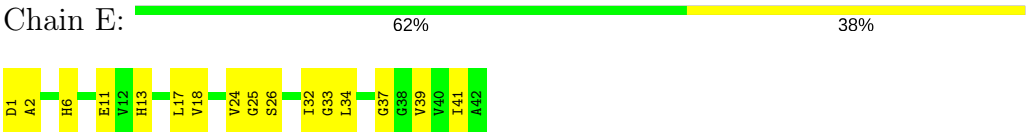
- Molecule 1: Amyloid beta A4 protein

Chain D:



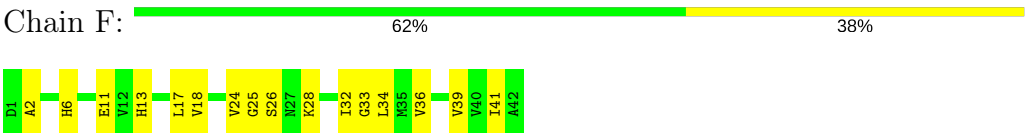
- Molecule 1: Amyloid beta A4 protein

Chain E:



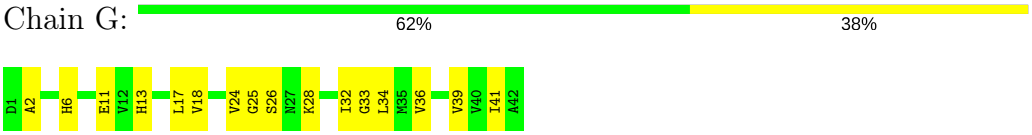
- Molecule 1: Amyloid beta A4 protein

Chain F:



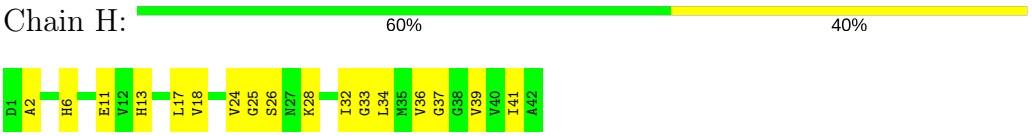
• Molecule 1: Amyloid beta A4 protein

Chain G:



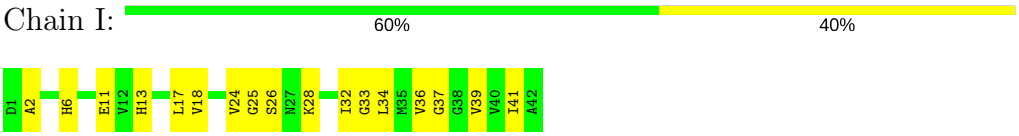
• Molecule 1: Amyloid beta A4 protein

Chain H:



• Molecule 1: Amyloid beta A4 protein

Chain I:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-179.275°, rise=2.335 Å, axial sym=C1	Depositor
Number of segments used	127765	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	24	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	110000	Depositor
Image detector	FEI FALCON III (4k x 4k)	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	0.58	0/342	0.80	0/458
1	B	0.58	0/342	0.80	0/458
1	C	0.59	0/342	0.80	0/458
1	D	0.58	0/342	0.80	0/458
1	E	0.58	0/342	0.80	0/458
1	F	0.58	0/342	0.80	0/458
1	G	0.58	0/342	0.80	0/458
1	H	0.59	0/342	0.80	0/458
1	I	0.58	0/342	0.80	0/458
All	All	0.58	0/3078	0.80	0/4122

There are no bond length outliers.

There are no bond angle outliers.

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	330	315	312	45	0
1	B	330	315	312	44	0
1	C	330	315	312	43	0
1	D	330	315	312	25	0
1	E	330	315	312	23	0
1	F	330	315	312	24	0
1	G	330	315	312	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	330	315	312	43	0
1	I	330	315	312	44	0
All	All	2970	2835	2808	185	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 32.

All (185) 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:E:11:GLU:OE2	1:E:13:HIS:NE2	2.24	0.71
1:C:11:GLU:OE2	1:C:13:HIS:NE2	2.24	0.71
1:A:11:GLU:OE2	1:A:13:HIS:NE2	2.24	0.70
1:B:11:GLU:OE2	1:B:13:HIS:NE2	2.24	0.70
1:I:11:GLU:OE2	1:I:13:HIS:NE2	2.24	0.70
1:D:11:GLU:OE2	1:D:13:HIS:NE2	2.24	0.70
1:F:11:GLU:OE2	1:F:13:HIS:NE2	2.24	0.70
1:G:11:GLU:OE2	1:G:13:HIS:NE2	2.24	0.70
1:H:11:GLU:OE2	1:H:13:HIS:NE2	2.24	0.70
1:B:37:GLY:HA2	1:I:36:VAL:O	1.93	0.68
1:A:36:VAL:O	1:C:37:GLY:HA2	1.93	0.68
1:A:37:GLY:HA2	1:H:36:VAL:O	1.95	0.67
1:C:1:ASP:OD2	1:G:28:LYS:NZ	2.28	0.66
1:B:1:ASP:OD2	1:F:28:LYS:NZ	2.28	0.66
1:F:36:VAL:O	1:H:37:GLY:HA2	1.96	0.65
1:G:36:VAL:O	1:I:37:GLY:HA2	1.96	0.65
1:E:1:ASP:OD2	1:I:28:LYS:NZ	2.30	0.65
1:B:36:VAL:O	1:D:37:GLY:HA2	1.96	0.65
1:C:36:VAL:O	1:E:37:GLY:HA2	1.96	0.65
1:D:1:ASP:OD2	1:H:28:LYS:NZ	2.29	0.64
1:A:41:ILE:HA	1:H:41:ILE:HG23	1.79	0.64
1:B:41:ILE:HA	1:I:41:ILE:HG23	1.80	0.62
1:A:41:ILE:HG23	1:C:41:ILE:HA	1.82	0.61
1:D:24:VAL:HG22	1:D:25:GLY:N	2.15	0.61
1:C:41:ILE:HG23	1:E:41:ILE:HA	1.82	0.61
1:G:24:VAL:HG22	1:G:25:GLY:N	2.16	0.60
1:G:41:ILE:HG23	1:I:41:ILE:HA	1.82	0.60
1:F:41:ILE:HG23	1:H:41:ILE:HA	1.82	0.60
1:B:24:VAL:HG22	1:B:25:GLY:N	2.16	0.60
1:I:24:VAL:HG22	1:I:25:GLY:N	2.16	0.60
1:B:41:ILE:HG23	1:D:41:ILE:HA	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:VAL:HG22	1:H:25:GLY:N	2.16	0.60
1:A:24:VAL:HG22	1:A:25:GLY:N	2.16	0.60
1:C:24:VAL:HG22	1:C:25:GLY:N	2.16	0.59
1:F:24:VAL:HG22	1:F:25:GLY:N	2.16	0.59
1:E:24:VAL:HG22	1:E:25:GLY:N	2.16	0.59
1:A:18:VAL:HG22	1:H:18:VAL:CG1	2.35	0.57
1:A:32:ILE:H	1:H:32:ILE:HG12	1.68	0.57
1:B:39:VAL:CG1	1:I:39:VAL:HG22	2.34	0.57
1:A:39:VAL:CG1	1:H:39:VAL:HG22	2.34	0.57
1:A:39:VAL:HG22	1:C:39:VAL:CG1	2.35	0.56
1:G:39:VAL:HG22	1:I:39:VAL:CG1	2.36	0.56
1:F:39:VAL:HG22	1:H:39:VAL:CG1	2.36	0.56
1:B:39:VAL:HG22	1:D:39:VAL:CG1	2.36	0.56
1:A:18:VAL:HG22	1:H:18:VAL:HG12	1.89	0.55
1:A:18:VAL:CG1	1:C:18:VAL:HG22	2.37	0.55
1:B:32:ILE:H	1:I:32:ILE:HG12	1.71	0.55
1:C:39:VAL:HG22	1:E:39:VAL:CG1	2.36	0.55
1:B:18:VAL:HG22	1:I:18:VAL:CG1	2.36	0.55
1:C:32:ILE:HG12	1:E:32:ILE:H	1.72	0.54
1:C:18:VAL:CG1	1:E:18:VAL:HG22	2.38	0.54
1:B:32:ILE:HG12	1:D:32:ILE:H	1.72	0.54
1:A:32:ILE:HG12	1:C:32:ILE:H	1.73	0.53
1:B:18:VAL:CG1	1:D:18:VAL:HG22	2.38	0.53
1:F:18:VAL:CG1	1:H:18:VAL:HG22	2.39	0.53
1:G:32:ILE:HG12	1:I:32:ILE:H	1.74	0.53
1:G:18:VAL:CG1	1:I:18:VAL:HG22	2.39	0.52
1:B:2:ALA:HA	1:I:2:ALA:O	2.10	0.52
1:B:18:VAL:HG22	1:I:18:VAL:HG12	1.91	0.52
1:A:32:ILE:O	1:H:32:ILE:HA	2.10	0.52
1:B:32:ILE:O	1:I:32:ILE:HA	2.10	0.52
1:A:32:ILE:HA	1:C:32:ILE:O	2.10	0.51
1:F:32:ILE:HG12	1:H:32:ILE:H	1.74	0.51
1:H:24:VAL:CG2	1:H:25:GLY:N	2.74	0.51
1:A:24:VAL:CG2	1:A:25:GLY:N	2.74	0.51
1:A:2:ALA:HA	1:H:2:ALA:O	2.10	0.51
1:A:18:VAL:HG12	1:C:18:VAL:HG22	1.93	0.51
1:F:24:VAL:CG2	1:F:25:GLY:N	2.74	0.51
1:C:18:VAL:HG12	1:E:18:VAL:HG22	1.93	0.51
1:C:24:VAL:CG2	1:C:25:GLY:N	2.74	0.51
1:B:18:VAL:HG12	1:D:18:VAL:HG22	1.93	0.51
1:I:24:VAL:CG2	1:I:25:GLY:N	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:CG2	1:B:25:GLY:N	2.73	0.51
1:G:24:VAL:CG2	1:G:25:GLY:N	2.74	0.50
1:A:2:ALA:O	1:C:2:ALA:HA	2.10	0.50
1:F:32:ILE:HA	1:H:32:ILE:O	2.12	0.50
1:B:39:VAL:HA	1:I:39:VAL:O	2.12	0.50
1:A:39:VAL:O	1:C:39:VAL:HA	2.11	0.50
1:E:24:VAL:CG2	1:E:25:GLY:N	2.74	0.50
1:G:32:ILE:HA	1:I:32:ILE:O	2.11	0.50
1:B:34:LEU:HG	1:I:34:LEU:HD22	1.94	0.50
1:D:24:VAL:CG2	1:D:25:GLY:N	2.73	0.50
1:A:32:ILE:N	1:H:32:ILE:HG12	2.26	0.50
1:F:18:VAL:HG12	1:H:18:VAL:HG22	1.94	0.50
1:B:32:ILE:HA	1:D:32:ILE:O	2.12	0.50
1:G:39:VAL:O	1:I:39:VAL:HA	2.12	0.49
1:C:32:ILE:HA	1:E:32:ILE:O	2.12	0.49
1:B:39:VAL:O	1:D:39:VAL:HA	2.12	0.49
1:F:39:VAL:O	1:H:39:VAL:HA	2.12	0.49
1:G:18:VAL:HG12	1:I:18:VAL:HG22	1.94	0.49
1:A:34:LEU:HD22	1:C:34:LEU:HG	1.93	0.49
1:C:39:VAL:O	1:E:39:VAL:HA	2.12	0.49
1:A:39:VAL:HA	1:H:39:VAL:O	2.12	0.49
1:A:34:LEU:HG	1:H:34:LEU:HD22	1.94	0.49
1:A:39:VAL:HG12	1:H:39:VAL:HG22	1.94	0.48
1:B:2:ALA:O	1:D:2:ALA:HA	2.13	0.48
1:B:32:ILE:N	1:I:32:ILE:HG12	2.28	0.48
1:G:2:ALA:O	1:I:2:ALA:HA	2.14	0.48
1:B:34:LEU:HD22	1:D:34:LEU:HG	1.96	0.48
1:A:36:VAL:O	1:C:37:GLY:CA	2.60	0.48
1:C:6:HIS:NE2	1:C:11:GLU:OE1	2.47	0.48
1:C:2:ALA:O	1:E:2:ALA:HA	2.13	0.48
1:E:6:HIS:NE2	1:E:11:GLU:OE1	2.47	0.47
1:F:39:VAL:HG22	1:H:39:VAL:HG12	1.96	0.47
1:F:2:ALA:O	1:H:2:ALA:HA	2.14	0.47
1:G:34:LEU:HD22	1:I:34:LEU:HG	1.97	0.47
1:B:39:VAL:HG12	1:I:39:VAL:HG22	1.95	0.47
1:B:37:GLY:CA	1:I:36:VAL:O	2.60	0.47
1:B:39:VAL:HG22	1:D:39:VAL:HG12	1.96	0.47
1:G:39:VAL:HG22	1:I:39:VAL:HG12	1.96	0.47
1:A:39:VAL:HG22	1:C:39:VAL:HG12	1.96	0.47
1:C:34:LEU:HD22	1:E:34:LEU:HG	1.96	0.47
1:A:32:ILE:HG12	1:C:32:ILE:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ILE:HG12	1:E:32:ILE:N	2.30	0.46
1:C:39:VAL:HG22	1:E:39:VAL:HG12	1.96	0.46
1:F:34:LEU:HD22	1:H:34:LEU:HG	1.96	0.46
1:B:32:ILE:HG12	1:D:32:ILE:N	2.30	0.46
1:F:6:HIS:NE2	1:F:11:GLU:OE1	2.47	0.46
1:G:32:ILE:HG12	1:I:32:ILE:N	2.31	0.46
1:A:39:VAL:H	1:C:39:VAL:HG12	1.80	0.45
1:A:37:GLY:CA	1:H:36:VAL:O	2.62	0.45
1:B:39:VAL:HG12	1:I:39:VAL:H	1.81	0.45
1:F:32:ILE:HG12	1:H:32:ILE:N	2.31	0.45
1:G:6:HIS:NE2	1:G:11:GLU:OE1	2.47	0.45
1:H:6:HIS:NE2	1:H:11:GLU:OE1	2.47	0.45
1:D:6:HIS:NE2	1:D:11:GLU:OE1	2.47	0.45
1:A:17:LEU:HG	1:H:17:LEU:HB2	1.98	0.45
1:B:6:HIS:NE2	1:B:11:GLU:OE1	2.47	0.45
1:C:36:VAL:O	1:E:37:GLY:CA	2.63	0.45
1:B:39:VAL:HG11	1:I:39:VAL:HG22	1.98	0.45
1:I:6:HIS:NE2	1:I:11:GLU:OE1	2.47	0.44
1:A:6:HIS:NE2	1:A:11:GLU:OE1	2.47	0.44
1:A:39:VAL:HG22	1:C:39:VAL:HG11	1.97	0.44
1:B:36:VAL:O	1:D:37:GLY:CA	2.63	0.44
1:G:39:VAL:H	1:I:39:VAL:HG12	1.83	0.44
1:F:36:VAL:O	1:H:37:GLY:CA	2.64	0.44
1:A:17:LEU:HB2	1:C:17:LEU:HG	1.99	0.44
1:A:39:VAL:HG11	1:H:39:VAL:HG22	1.99	0.43
1:B:17:LEU:HG	1:I:17:LEU:HB2	1.99	0.43
1:D:24:VAL:HG22	1:D:26:SER:N	2.34	0.43
1:F:32:ILE:HG22	1:F:33:GLY:N	2.34	0.43
1:G:39:VAL:HG22	1:I:39:VAL:HG11	2.00	0.43
1:H:32:ILE:HG22	1:H:33:GLY:N	2.34	0.43
1:B:39:VAL:HG22	1:D:39:VAL:HG11	2.00	0.43
1:B:39:VAL:H	1:D:39:VAL:HG12	1.83	0.43
1:G:32:ILE:HG22	1:G:33:GLY:N	2.33	0.43
1:B:24:VAL:HG22	1:B:26:SER:N	2.34	0.43
1:B:41:ILE:HA	1:I:41:ILE:CG2	2.47	0.43
1:C:39:VAL:H	1:E:39:VAL:HG12	1.83	0.43
1:D:32:ILE:HG22	1:D:33:GLY:N	2.33	0.43
1:A:32:ILE:HG22	1:A:33:GLY:N	2.34	0.43
1:H:24:VAL:HG22	1:H:26:SER:N	2.34	0.43
1:F:39:VAL:H	1:H:39:VAL:HG12	1.83	0.43
1:I:32:ILE:HG22	1:I:33:GLY:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ILE:HG22	1:E:33:GLY:N	2.33	0.42
1:F:24:VAL:HG22	1:F:26:SER:N	2.34	0.42
1:I:24:VAL:HG22	1:I:26:SER:N	2.34	0.42
1:A:24:VAL:HG22	1:A:26:SER:N	2.34	0.42
1:C:24:VAL:HG22	1:C:26:SER:N	2.34	0.42
1:C:32:ILE:HG22	1:C:33:GLY:N	2.34	0.42
1:B:32:ILE:HG22	1:B:33:GLY:N	2.33	0.42
1:A:18:VAL:HG12	1:C:18:VAL:H	1.84	0.42
1:C:17:LEU:HB2	1:E:17:LEU:HG	2.01	0.42
1:G:36:VAL:O	1:I:37:GLY:CA	2.64	0.42
1:G:24:VAL:HG22	1:G:26:SER:N	2.34	0.42
1:A:41:ILE:HA	1:H:41:ILE:CG2	2.45	0.42
1:F:39:VAL:HG22	1:H:39:VAL:HG11	2.00	0.42
1:G:17:LEU:HB2	1:I:17:LEU:HG	2.01	0.42
1:A:39:VAL:HG12	1:H:39:VAL:H	1.84	0.42
1:E:24:VAL:HG22	1:E:26:SER:N	2.34	0.42
1:C:39:VAL:HG22	1:E:39:VAL:HG11	2.00	0.42
1:A:17:LEU:HA	1:H:17:LEU:O	2.20	0.41
1:F:17:LEU:HB2	1:H:17:LEU:HG	2.01	0.41
1:B:17:LEU:HB2	1:D:17:LEU:HG	2.01	0.41
1:A:18:VAL:O	1:H:18:VAL:HA	2.20	0.41
1:B:18:VAL:H	1:I:18:VAL:HG12	1.86	0.41
1:A:17:LEU:O	1:C:17:LEU:HA	2.22	0.40
1:B:18:VAL:HG12	1:D:18:VAL:H	1.87	0.40
1:F:18:VAL:HG12	1:H:18:VAL:H	1.86	0.40
1:G:18:VAL:HG12	1:I:18:VAL:H	1.86	0.40
1:B:41:ILE:CG2	1:D:41:ILE:HA	2.49	0.40
1:G:41:ILE:CG2	1:I:41:ILE:HA	2.50	0.40
1:A:31:ILE:O	1:C:31:ILE:HA	2.21	0.40
1:A:4:PHE:HB3	1:C:3:GLU:O	2.22	0.40
1:B:17:LEU:HA	1:I:17:LEU:O	2.21	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	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	B	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	C	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	D	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	E	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	F	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	G	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	H	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
1	I	42/42 (100%)	35 (83%)	7 (17%)	0	100	100
All	All	378/378 (100%)	315 (83%)	63 (17%)	0	100	100

There are no Ramachandran outliers to report.

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	33/32 (103%)	33 (100%)	0	100	100
1	B	33/32 (103%)	33 (100%)	0	100	100
1	C	33/32 (103%)	33 (100%)	0	100	100
1	D	33/32 (103%)	33 (100%)	0	100	100
1	E	33/32 (103%)	33 (100%)	0	100	100
1	F	33/32 (103%)	33 (100%)	0	100	100
1	G	33/32 (103%)	33 (100%)	0	100	100
1	H	33/32 (103%)	33 (100%)	0	100	100
1	I	33/32 (103%)	33 (100%)	0	100	100
All	All	297/288 (103%)	297 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 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 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.