wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:50 PM BST

PDB ID	:	3JA9
EMDB ID:	:	EMD-6339
Title	:	Structure of native human PCNA
Authors	:	Lau, W.C.Y.; Li, Y.; Zhang, Q.; Huen, M.S.Y.
Deposited on	:	2015-05-19
Resolution	:	22.00 Å(reported)
Based on PDB ID	:	1VYM

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

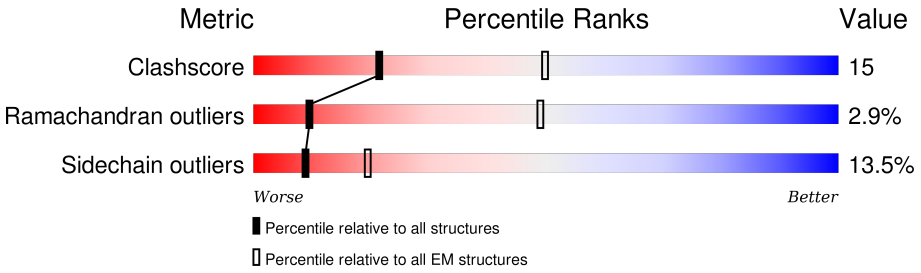
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 22.00 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	261	69% 22% 6%
1	B	261	63% 26% 7%
1	C	261	68% 24% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6033 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	256	Total	C	N	O	S	0	1
			1964	1233	323	392	16		
1	B	256	Total	C	N	O	S	0	1
			1964	1233	323	392	16		
1	C	256	Total	C	N	O	S	0	1
			1964	1233	323	392	16		

- Molecule 2 is water.

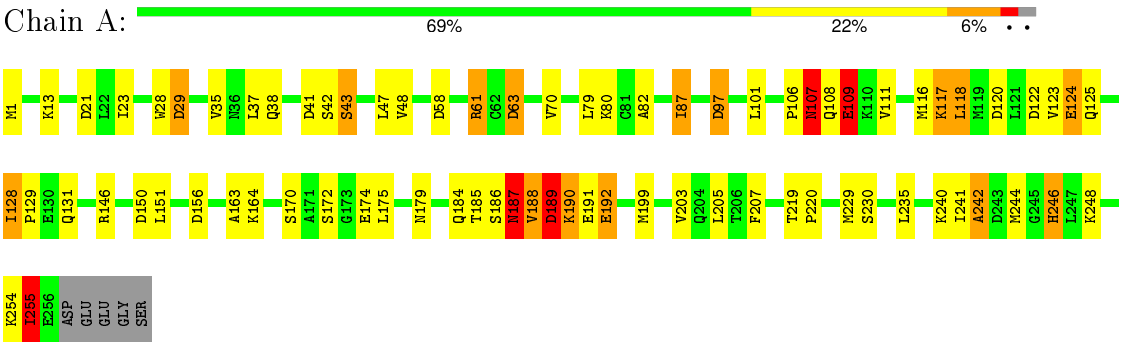
Mol	Chain	Residues	Atoms		AltConf
2	A	39	Total	O	0
			39	39	
2	B	44	Total	O	0
			44	44	
2	C	58	Total	O	0
			58	58	

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.

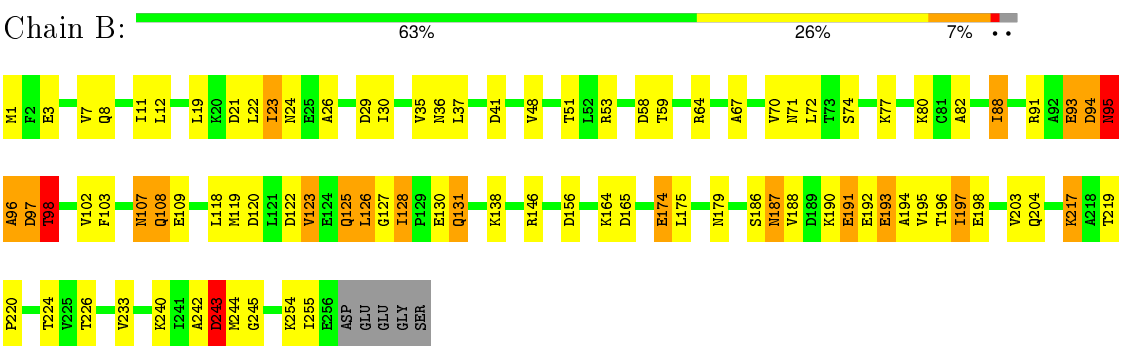
- Molecule 1: Proliferating cell nuclear antigen

Chain A:



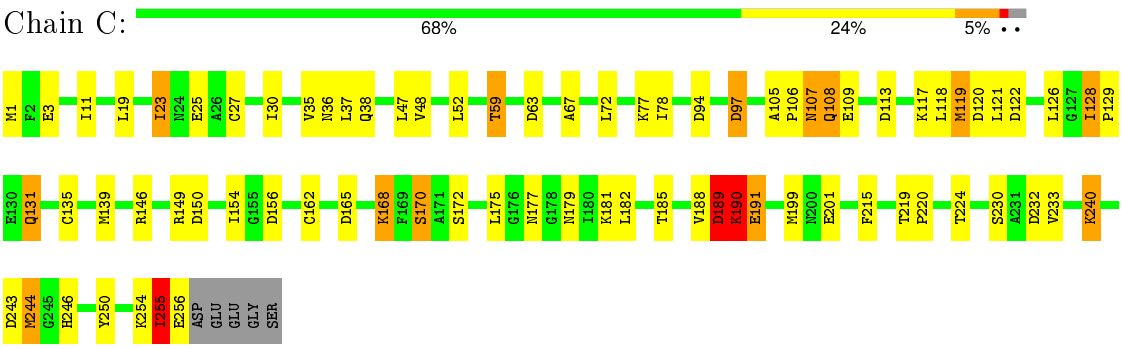
- Molecule 1: Proliferating cell nuclear antigen

Chain B:



- Molecule 1: Proliferating cell nuclear antigen

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	7330	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Particles	Depositor
Microscope	JEOL 2010	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (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	0.57	0/1990	0.95	10/2689 (0.4%)
1	B	0.61	0/1990	1.00	10/2689 (0.4%)
1	C	0.67	0/1990	1.01	12/2689 (0.4%)
All	All	0.62	0/5970	0.99	32/8067 (0.4%)

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	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	ASP	CB-CG-OD2	8.31	125.78	118.30
1	B	243	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	150	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	156	ASP	CB-CG-OD2	6.96	124.57	118.30
1	B	156	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	41	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	97	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	63	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	29	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	97	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	120	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	94	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	120	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	MET	CG-SD-CE	-6.01	90.59	100.20
1	A	122	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	150	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	21	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	120	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	113	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	58	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	217	LYS	CG-CD-CE	5.40	128.09	111.90
1	B	122	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	217	LYS	CD-CE-NZ	5.37	124.04	111.70
1	A	189	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	189	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	165	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	97	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	156	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	243	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	122	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	70	VAL	CB-CA-C	-5.04	101.83	111.40
1	C	232	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASN	Peptide
1	A	109	GLU	Peptide
1	A	192	GLU	Peptide
1	B	95	ASN	Mainchain
1	B	98	THR	Peptide

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	1964	0	1973	57	0
1	B	1964	0	1973	67	0
1	C	1964	0	1973	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	39	0	0	3	0
2	B	44	0	0	11	0
2	C	58	0	0	7	0
All	All	6033	0	5919	181	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 15.

All (181) 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:C:254:LYS:O	1:C:255:ILE:HB	1.28	1.07
1:C:128:ILE:HD13	1:C:129:PRO:HD2	1.36	1.02
1:B:187:ASN:ND2	1:B:188:VAL:HG23	1.75	1.00
1:B:187:ASN:HD22	1:B:188:VAL:HG23	1.28	0.98
1:A:187:ASN:HB3	1:A:190:LYS:NZ	1.81	0.96
1:A:37:LEU:HD23	1:A:38:GLN:N	1.80	0.96
1:C:128:ILE:CD1	1:C:129:PRO:HD2	2.00	0.91
1:A:254:LYS:O	1:A:255:ILE:O	1.88	0.90
1:A:188:VAL:O	1:A:189:ASP:HB2	1.70	0.89
1:B:226:THR:HB	2:B:2039:HOH:O	1.72	0.88
1:A:107:ASN:O	1:A:109:GLU:HG3	1.73	0.88
1:A:37:LEU:C	1:A:37:LEU:HD23	1.95	0.86
1:C:185:THR:HB	1:C:188:VAL:HG22	1.62	0.82
1:B:29:ASP:OD1	1:B:123:VAL:HG22	1.79	0.82
1:C:189:ASP:OD2	1:C:189:ASP:O	1.99	0.80
1:A:174:GLU:HG2	2:A:2029:HOH:O	1.82	0.79
1:B:29:ASP:OD1	1:B:123:VAL:CG2	2.30	0.79
1:C:254:LYS:O	1:C:255:ILE:CB	2.19	0.75
1:C:117:LYS:HA	2:C:2030:HOH:O	1.86	0.75
1:B:36:ASN:HB3	2:B:2008:HOH:O	1.87	0.73
1:B:125:GLN:O	1:B:126:LEU:HB2	1.86	0.73
1:A:106:PRO:HA	2:A:2017:HOH:O	1.87	0.73
1:C:128:ILE:CG1	1:C:129:PRO:HD2	2.19	0.72
1:A:117:LYS:O	1:A:118:LEU:HB2	1.88	0.71
1:A:187:ASN:HB3	1:A:190:LYS:HZ1	1.55	0.71
1:C:25:GLU:HG2	1:C:119:MET:SD	2.31	0.69
1:B:97:ASP:OD2	1:B:98:THR:HG23	1.93	0.69
1:C:52:LEU:HD22	1:C:244:MET:HE3	1.75	0.68
1:C:128:ILE:HD13	1:C:129:PRO:CD	2.20	0.68
1:C:126:LEU:HG	1:C:128:ILE:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HG12	1:B:188:VAL:O	1.94	0.68
1:C:106:PRO:HD2	2:C:2024:HOH:O	1.92	0.68
1:A:246:HIS:CE1	1:A:248:LYS:HE3	2.30	0.67
1:C:59:THR:HG22	2:C:2001:HOH:O	1.95	0.67
1:B:174:GLU:CD	1:B:174:GLU:H	1.99	0.66
1:A:186:SER:O	1:A:188:VAL:HG23	1.96	0.66
1:C:190:LYS:O	1:C:191:GLU:HB3	1.96	0.65
1:A:123:VAL:HG13	1:A:124:GLU:N	2.11	0.65
1:C:255:ILE:HG23	1:C:256:GLU:N	2.12	0.64
1:C:59:THR:CG2	2:C:2001:HOH:O	2.46	0.63
1:A:187:ASN:HB3	1:A:190:LYS:HZ2	1.60	0.63
1:B:226:THR:CB	2:B:2039:HOH:O	2.38	0.63
1:B:67:ALA:HB1	1:B:123:VAL:HG23	1.79	0.62
1:B:93:GLU:O	1:B:94:ASP:CB	2.47	0.62
1:B:59:THR:HG22	2:B:2001:HOH:O	1.99	0.62
1:C:154:ILE:HD13	1:C:175:LEU:HD11	1.82	0.62
1:B:23:ILE:HD11	1:B:26:ALA:HB2	1.82	0.61
1:A:1:MET:SD	1:A:61:ARG:NH1	2.73	0.61
1:C:255:ILE:CG2	1:C:256:GLU:N	2.64	0.61
1:B:107:ASN:C	1:B:108:GLN:HG2	2.20	0.61
1:A:203:VAL:HG11	1:A:205:LEU:HD11	1.83	0.61
1:C:107:ASN:C	1:C:107:ASN:HD22	2.03	0.60
1:A:117:LYS:O	1:A:118:LEU:CB	2.49	0.60
1:B:94:ASP:O	1:B:95:ASN:HB2	2.02	0.59
1:B:21:ASP:OD2	1:B:217:LYS:CE	2.51	0.59
1:B:191:GLU:HG2	1:B:191:GLU:O	2.03	0.58
1:B:71:ASN:HB3	1:B:74:SER:OG	2.03	0.58
1:C:11:ILE:HG21	1:C:244:MET:HE2	1.86	0.58
1:C:189:ASP:O	1:C:189:ASP:CG	2.42	0.57
1:B:21:ASP:OD2	1:B:217:LYS:NZ	2.37	0.57
1:A:87:ILE:HD13	1:A:87:ILE:N	2.20	0.57
1:B:21:ASP:OD2	1:B:217:LYS:HE2	2.05	0.57
1:C:190:LYS:O	1:C:191:GLU:CB	2.54	0.56
1:B:67:ALA:CB	1:B:123:VAL:HG23	2.36	0.56
1:B:242:ALA:O	1:B:244:MET:N	2.34	0.56
1:B:97:ASP:HA	1:B:118:LEU:H	1.71	0.56
1:B:77:LYS:O	1:B:80:LYS:HB2	2.06	0.55
1:A:187:ASN:CB	1:A:190:LYS:HZ2	2.19	0.55
1:A:37:LEU:CD2	1:A:37:LEU:C	2.68	0.55
1:A:123:VAL:HG22	1:A:124:GLU:H	1.71	0.55
1:B:93:GLU:O	1:B:94:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:C:78:ILE:HD11	2.37	0.54
1:C:189:ASP:O	1:C:190:LYS:HB2	2.08	0.54
1:B:187:ASN:HD22	1:B:188:VAL:CG2	2.12	0.54
1:C:185:THR:CB	1:C:188:VAL:HG22	2.37	0.54
1:C:240:LYS:NZ	2:C:2056:HOH:O	2.37	0.54
1:A:175:LEU:HD13	1:C:78:ILE:HD11	1.90	0.53
1:C:27:CYS:SG	1:C:67:ALA:HB1	2.49	0.53
1:C:105:ALA:HB1	1:C:106:PRO:CD	2.38	0.53
1:A:61:ARG:NE	1:A:63:ASP:OD1	2.42	0.52
1:A:23:ILE:HD11	1:A:48:VAL:CG2	2.39	0.52
1:B:26:ALA:HB1	1:B:37:LEU:HD11	1.91	0.52
1:B:226:THR:CG2	2:B:2038:HOH:O	2.58	0.52
1:B:108:GLN:HA	2:B:2018:HOH:O	2.10	0.51
1:B:197:ILE:HD12	1:B:198:GLU:N	2.25	0.51
1:B:59:THR:CG2	2:B:2001:HOH:O	2.57	0.51
1:C:240:LYS:HE2	1:C:246:HIS:HB3	1.92	0.51
1:C:185:THR:HB	1:C:188:VAL:CG2	2.38	0.51
1:B:41:ASP:C	1:B:41:ASP:OD1	2.49	0.51
1:A:37:LEU:CD2	1:A:38:GLN:N	2.67	0.51
1:C:118:LEU:HD23	2:C:2028:HOH:O	2.12	0.50
1:C:154:ILE:HG21	1:C:177:ASN:HA	1.92	0.49
1:C:219:THR:N	1:C:220:PRO:CD	2.74	0.49
1:A:13:LYS:NZ	1:A:82:ALA:O	2.38	0.49
1:A:185:THR:HG21	1:C:109:GLU:HG2	1.93	0.49
1:B:226:THR:C	2:B:2039:HOH:O	2.51	0.49
1:B:174:GLU:N	1:B:174:GLU:CD	2.65	0.49
1:A:87:ILE:N	1:A:87:ILE:CD1	2.76	0.49
1:B:82:ALA:HB2	1:B:103:PHE:CG	2.48	0.48
1:B:88:ILE:HD13	1:B:103:PHE:CE1	2.48	0.48
1:A:187:ASN:CG	1:A:190:LYS:HZ2	2.17	0.48
1:B:30:ILE:HD13	1:B:35:VAL:HG22	1.94	0.48
1:C:19:LEU:HD21	1:C:48:VAL:HG11	1.96	0.48
1:B:187:ASN:ND2	1:B:188:VAL:CG2	2.64	0.47
1:B:123:VAL:HG12	1:B:123:VAL:O	2.13	0.47
1:C:52:LEU:HD22	1:C:244:MET:CE	2.45	0.47
1:A:109:GLU:OE1	1:B:193:GLU:OE2	2.32	0.47
1:B:29:ASP:OD1	1:B:123:VAL:HG21	2.11	0.47
1:C:107:ASN:O	1:C:108:GLN:HG2	2.14	0.47
1:A:254:LYS:O	1:A:255:ILE:C	2.53	0.47
1:A:123:VAL:HG13	1:A:124:GLU:H	1.79	0.47
1:A:101:LEU:HD12	1:A:101:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD12	1:A:175:LEU:C	2.35	0.47
1:C:185:THR:CB	1:C:188:VAL:CG2	2.93	0.46
1:A:241:ILE:HG22	1:A:241:ILE:O	2.14	0.46
1:C:128:ILE:HG12	1:C:129:PRO:HD2	1.98	0.46
1:C:25:GLU:OE2	1:C:119:MET:SD	2.74	0.46
1:B:82:ALA:HB2	1:B:103:PHE:CD2	2.51	0.46
1:A:219:THR:HB	1:A:220:PRO:HD3	1.97	0.46
1:B:8:GLN:HA	2:B:2002:HOH:O	2.16	0.46
1:A:229:MET:HG3	1:A:235:LEU:HD13	1.98	0.46
1:B:19:LEU:CD2	1:B:48:VAL:HG11	2.46	0.46
1:B:125:GLN:O	1:B:126:LEU:CB	2.58	0.46
1:A:205:LEU:HB2	1:A:207:PHE:CE2	2.50	0.45
1:A:246:HIS:HD2	1:A:246:HIS:O	1.99	0.45
1:A:203:VAL:CG1	1:A:205:LEU:HD11	2.46	0.45
1:C:107:ASN:ND2	1:C:109:GLU:H	2.15	0.45
1:C:219:THR:HB	1:C:220:PRO:HD3	1.98	0.45
1:A:255:ILE:HG22	1:A:255:ILE:O	2.15	0.45
1:C:37:LEU:HD23	1:C:38:GLN:N	2.32	0.45
1:B:53:ARG:NH1	1:B:243:ASP:O	2.50	0.45
1:B:11:ILE:HD13	1:B:244:MET:CE	2.46	0.45
1:A:128:ILE:HG13	1:A:129:PRO:HD2	2.00	0.45
1:A:174:GLU:O	1:C:117:LYS:HD2	2.17	0.44
1:A:246:HIS:CD2	1:A:246:HIS:C	2.90	0.44
1:C:25:GLU:CG	1:C:119:MET:SD	3.04	0.44
1:C:131:GLN:HE22	1:C:233:VAL:HG21	1.83	0.44
1:A:70:VAL:HG13	1:A:116:MET:CE	2.47	0.44
1:C:126:LEU:HG	1:C:128:ILE:N	2.30	0.44
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.48	0.44
1:A:111:VAL:HG22	2:A:2018:HOH:O	2.16	0.44
1:A:37:LEU:HD23	1:A:38:GLN:CA	2.45	0.44
1:C:47:LEU:HB3	1:C:250:TYR:HB2	2.00	0.44
1:B:226:THR:HG23	2:B:2038:HOH:O	2.17	0.44
1:A:203:VAL:HG12	1:A:205:LEU:HG	1.98	0.44
1:A:241:ILE:O	1:A:242:ALA:C	2.55	0.44
1:B:88:ILE:HD13	1:B:103:PHE:CD1	2.53	0.43
1:C:105:ALA:HB1	1:C:106:PRO:HD2	2.00	0.43
1:C:135:CYS:SG	1:C:162:CYS:HB2	2.58	0.43
1:C:215:PHE:N	1:C:215:PHE:CD1	2.83	0.43
1:A:61:ARG:NH2	1:A:63:ASP:OD2	2.51	0.43
1:C:37:LEU:HD23	1:C:37:LEU:C	2.38	0.43
1:B:244:MET:N	2:B:2044:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:THR:HB	1:B:220:PRO:HD3	2.00	0.43
1:A:97:ASP:O	1:A:117:LYS:O	2.37	0.43
1:B:51:THR:O	1:B:245:GLY:HA3	2.18	0.43
1:A:255:ILE:CG2	1:A:255:ILE:O	2.65	0.43
1:B:3:GLU:OE2	1:B:91:ARG:NH1	2.51	0.43
1:A:28:TRP:CZ3	1:A:35:VAL:HG11	2.54	0.42
1:B:127:GLY:O	1:B:128:ILE:C	2.58	0.42
1:B:23:ILE:HG13	1:B:24:ASN:N	2.35	0.42
1:A:185:THR:CG2	1:C:109:GLU:HG2	2.48	0.42
1:B:88:ILE:HA	1:B:102:VAL:O	2.19	0.42
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.84	0.42
1:B:95:ASN:O	1:B:96:ALA:C	2.57	0.42
1:C:131:GLN:HE22	1:C:233:VAL:HG11	1.85	0.42
1:B:93:GLU:O	1:B:94:ASP:CG	2.59	0.41
1:C:1:MET:SD	1:C:3:GLU:HB2	2.60	0.41
1:A:163:ALA:HA	1:A:199:MET:HE2	2.01	0.41
1:B:130:GLU:C	1:B:131:GLN:HG2	2.41	0.41
1:C:23:ILE:HG12	1:C:72:LEU:HD12	2.03	0.41
1:B:23:ILE:HG12	1:B:72:LEU:HD12	2.02	0.41
1:B:53:ARG:NH2	1:B:243:ASP:O	2.54	0.41
1:C:168:LYS:CE	1:C:170:SER:OG	2.69	0.41
1:B:194:ALA:O	1:B:196:THR:CG2	2.68	0.41
1:B:194:ALA:O	1:B:196:THR:HG23	2.21	0.41
1:C:224:THR:HG22	2:C:2044:HOH:O	2.21	0.41
1:C:30:ILE:HD13	1:C:35:VAL:HG13	2.02	0.41
1:C:11:ILE:HG21	1:C:244:MET:CE	2.49	0.40
1:B:93:GLU:O	1:B:94:ASP:OD2	2.39	0.40
1:A:151:LEU:HA	1:A:151:LEU:HD23	1.94	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	254/261 (97%)	223 (88%)	20 (8%)	11 (4%)	3 34
1	B	254/261 (97%)	229 (90%)	17 (7%)	8 (3%)	5 42
1	C	254/261 (97%)	238 (94%)	13 (5%)	3 (1%)	16 61
All	All	762/783 (97%)	690 (91%)	50 (7%)	22 (3%)	9 43

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	108	GLN
1	A	118	LEU
1	A	187	ASN
1	A	188	VAL
1	A	189	ASP
1	A	255	ILE
1	B	94	ASP
1	B	95	ASN
1	B	98	THR
1	B	243	ASP
1	C	190	LYS
1	C	255	ILE
1	B	126	LEU
1	B	186	SER
1	B	195	VAL
1	C	191	GLU
1	A	128	ILE
1	A	125	GLN
1	A	242	ALA
1	B	96	ALA
1	A	117	LYS

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	223/228 (98%)	195 (87%)	28 (13%)	5 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	223/228 (98%)	189 (85%)	34 (15%)	3 22
1	C	223/228 (98%)	195 (87%)	28 (13%)	5 29
All	All	669/684 (98%)	579 (86%)	90 (14%)	9 27

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	42	SER
1	A	43	SER
1	A	47	LEU
1	A	58	ASP
1	A	61	ARG
1	A	79	LEU
1	A	80	LYS
1	A	87	ILE
1	A	107	ASN
1	A	109	GLU
1	A	124	GLU
1	A	131	GLN
1	A	146	ARG
1	A	164	LYS
1	A	170	SER
1	A	172	SER
1	A	179	ASN
1	A	184	GLN
1	A	187	ASN
1	A	190	LYS
1	A	191	GLU
1	A	192	GLU
1	A	230	SER
1	A	240	LYS
1	A	244	MET
1	A	246	HIS
1	A	255	ILE
1	B	1	MET
1	B	7	VAL
1	B	22	LEU
1	B	23	ILE
1	B	64	ARG
1	B	88	ILE

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Mol	Chain	Res	Type
1	B	93	GLU
1	B	107	ASN
1	B	108	GLN
1	B	109	GLU
1	B	119	MET
1	B	123	VAL
1	B	125	GLN
1	B	128	ILE
1	B	131	GLN
1	B	138	LYS
1	B	146	ARG
1	B	164	LYS
1	B	174	GLU
1	B	175	LEU
1	B	179	ASN
1	B	187	ASN
1	B	190	LYS
1	B	191	GLU
1	B	192	GLU
1	B	193	GLU
1	B	197	ILE
1	B	203	VAL
1	B	204	GLN
1	B	224	THR
1	B	233	VAL
1	B	240	LYS
1	B	254	LYS
1	B	255	ILE
1	C	23	ILE
1	C	36	ASN
1	C	59	THR
1	C	77	LYS
1	C	97	ASP
1	C	107	ASN
1	C	108	GLN
1	C	119	MET
1	C	121	LEU
1	C	128	ILE
1	C	131	GLN
1	C	146	ARG
1	C	149	ARG
1	C	165	ASP

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Mol	Chain	Res	Type
1	C	168	LYS
1	C	170	SER
1	C	172	SER
1	C	179	ASN
1	C	181	LYS
1	C	182	LEU
1	C	189	ASP
1	C	190	LYS
1	C	199	MET
1	C	201	GLU
1	C	230	SER
1	C	240	LYS
1	C	244	MET
1	C	255	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	246	HIS
1	B	65	ASN
1	B	108	GLN
1	B	187	ASN
1	C	49	GLN
1	C	107	ASN
1	C	108	GLN
1	C	131	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

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.