wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:41 PM BST

PDB ID	:	3J2J
EMDB ID:	:	EMD-5514
Title	:	Empty coxsackievirus A9 capsid
Authors	:	Shakeel, S.; Seitsonen, J.J.T.; Kajander, T.; Laurinmaki, P.; Hyypia, T.; Susi, P.; Butcher, S.J.
Deposited on	:	2012-10-04
Resolution	:	9.54 Å(reported)
Based on PDB ID	:	1D4M

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

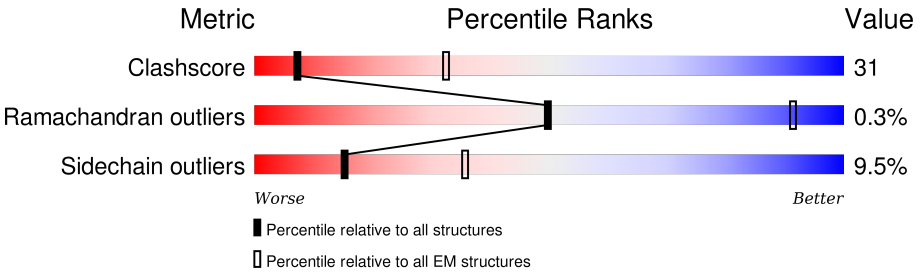
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 9.54 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	222	66% 26% 8%
2	B	238	73% 22% 5%
3	C	252	83% 15% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5601 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 Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	222	Total	C	N	O	S	0	0
			1799	1152	308	329	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ASN	LYS	CONFLICT	UNP P21404
A	23	ASP	HIS	CONFLICT	UNP P21404
A	80	HIS	ARG	CONFLICT	UNP P21404

- Molecule 2 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	238	Total	C	N	O	S	0	0
			1843	1173	302	350	18		

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	252	Total	C	N	O	S	0	0
			1959	1239	332	372	16		

There is a discrepancy between the modelled and reference sequences:

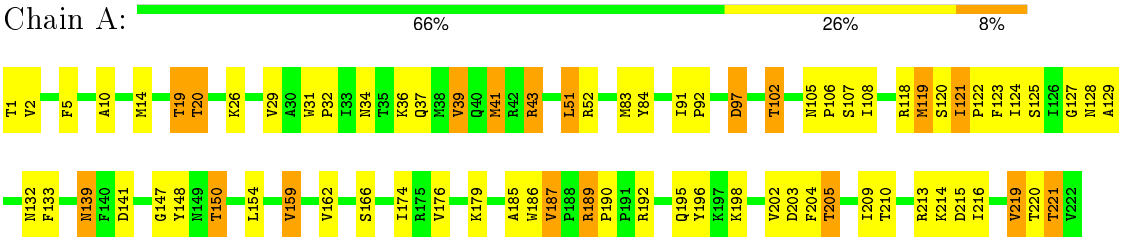
Chain	Residue	Modelled	Actual	Comment	Reference
C	101	VAL	LEU	CONFLICT	UNP P21404

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.

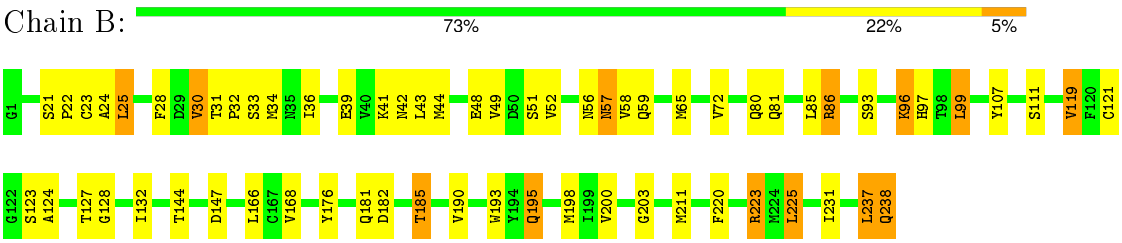
- Molecule 1: Protein VP1

Chain A:



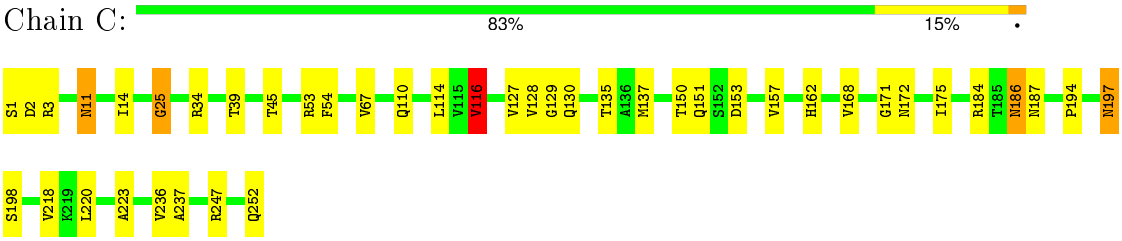
- Molecule 2: Protein VP3

Chain B:



- Molecule 3: Protein VP2

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	1200	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	whole micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	830	Depositor
Maximum defocus (nm)	4120	Depositor
Magnification	62000	Depositor
Image detector	Not provided	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	0/1855	0.81	0/2531
2	B	0.55	0/1892	0.80	0/2581
3	C	0.55	0/2009	0.81	2/2740 (0.1%)
All	All	0.56	0/5756	0.81	2/7852 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	116	VAL	CB-CA-C	-5.86	100.27	111.40
3	C	186	ASN	CB-CA-C	-5.80	98.80	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	186	ASN	Mainchain

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	1799	0	1754	272	0
2	B	1843	0	1799	269	0
3	C	1959	0	1881	64	0
All	All	5601	0	5434	338	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 31.

All (338) 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:119:MET:CE	2:B:24:ALA:CB	1.81	1.59
1:A:118:ARG:CD	2:B:21:SER:CB	1.79	1.57
1:A:118:ARG:CG	2:B:21:SER:CB	1.81	1.56
1:A:216:ILE:HB	2:B:58:VAL:CG1	1.38	1.54
1:A:118:ARG:CD	2:B:21:SER:HB3	1.30	1.51
1:A:198:LYS:CD	2:B:238:GLN:HE22	1.22	1.51
1:A:124:ILE:CG2	2:B:28:PHE:CE2	1.92	1.49
1:A:216:ILE:CD1	2:B:56:ASN:HD22	1.24	1.49
1:A:124:ILE:HG22	2:B:28:PHE:CE2	0.98	1.48
1:A:119:MET:CE	2:B:24:ALA:HB3	1.35	1.47
1:A:119:MET:HE3	2:B:24:ALA:CB	1.40	1.46
1:A:214:LYS:O	2:B:59:GLN:CB	1.64	1.46
2:B:124:ALA:CA	3:C:184:ARG:NH1	1.74	1.46
2:B:124:ALA:CA	3:C:184:ARG:HH11	1.21	1.44
1:A:124:ILE:HG22	2:B:28:PHE:CZ	1.53	1.43
1:A:118:ARG:HG2	2:B:21:SER:CB	1.36	1.42
1:A:204:PHE:O	3:C:128:VAL:CG1	1.64	1.42
1:A:216:ILE:N	2:B:58:VAL:HG12	1.11	1.41
1:A:216:ILE:CA	2:B:58:VAL:HG12	1.51	1.38
1:A:216:ILE:CD1	2:B:56:ASN:ND2	1.82	1.37
1:A:119:MET:HE3	2:B:24:ALA:CA	1.55	1.36
1:A:216:ILE:CB	2:B:58:VAL:CG1	2.03	1.35
1:A:118:ARG:CG	2:B:21:SER:OG	1.72	1.33
1:A:119:MET:HE3	2:B:24:ALA:N	1.41	1.32
1:A:122:PRO:HB2	2:B:30:VAL:CG2	1.58	1.32
1:A:198:LYS:HD3	2:B:238:GLN:NE2	1.40	1.31
1:A:198:LYS:CD	2:B:238:GLN:NE2	1.91	1.31
2:B:124:ALA:HA	3:C:184:ARG:NH1	1.00	1.30
1:A:216:ILE:N	2:B:58:VAL:CG1	1.93	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:NH1	2:B:33:SER:HA	1.46	1.28
1:A:124:ILE:CG2	2:B:28:PHE:CZ	2.13	1.25
1:A:214:LYS:C	2:B:59:GLN:HB2	1.57	1.24
1:A:52:ARG:CZ	2:B:33:SER:HA	1.66	1.24
1:A:216:ILE:CA	2:B:58:VAL:CG1	2.15	1.24
1:A:119:MET:CE	2:B:24:ALA:H	1.51	1.22
1:A:124:ILE:HG22	2:B:28:PHE:CD2	1.77	1.20
1:A:216:ILE:HD12	2:B:56:ASN:ND2	0.85	1.18
1:A:123:PHE:N	2:B:30:VAL:HG22	1.60	1.16
1:A:52:ARG:CZ	2:B:33:SER:CA	2.22	1.16
1:A:122:PRO:CB	2:B:30:VAL:HG23	1.74	1.16
1:A:118:ARG:HD3	2:B:21:SER:OG	1.44	1.15
1:A:186:TRP:CD1	2:B:36:ILE:O	2.00	1.15
1:A:118:ARG:HG2	2:B:21:SER:OG	1.36	1.13
1:A:118:ARG:CG	2:B:21:SER:HB2	1.60	1.11
1:A:213:ARG:HH21	2:B:57:ASN:ND2	1.47	1.11
1:A:52:ARG:NH2	2:B:33:SER:N	1.99	1.11
2:B:123:SER:HB3	3:C:110:GLN:NE2	1.66	1.10
1:A:216:ILE:CB	2:B:58:VAL:HG11	1.75	1.10
1:A:118:ARG:CD	2:B:21:SER:OG	1.86	1.09
1:A:127:GLY:O	2:B:31:THR:HG21	1.53	1.09
1:A:204:PHE:O	3:C:128:VAL:HG11	1.36	1.08
1:A:1:THR:HA	2:B:41:LYS:O	1.53	1.07
1:A:119:MET:CE	2:B:24:ALA:HB2	1.83	1.06
1:A:122:PRO:HG2	2:B:28:PHE:CD2	1.90	1.05
1:A:204:PHE:O	3:C:128:VAL:HG12	1.53	1.05
2:B:124:ALA:HB2	3:C:184:ARG:HG3	1.33	1.05
1:A:213:ARG:CZ	2:B:57:ASN:HD21	1.70	1.05
1:A:198:LYS:HD2	2:B:238:GLN:NE2	1.69	1.04
1:A:216:ILE:HB	2:B:58:VAL:HG13	1.37	1.03
1:A:213:ARG:NH2	2:B:57:ASN:ND2	2.07	1.02
1:A:216:ILE:HD12	2:B:56:ASN:CG	1.79	1.02
1:A:118:ARG:O	2:B:22:PRO:HG2	1.60	1.02
1:A:213:ARG:NH2	2:B:57:ASN:HD21	1.57	1.02
1:A:213:ARG:HE	2:B:57:ASN:ND2	1.56	1.01
1:A:122:PRO:HG2	2:B:28:PHE:HD2	1.18	1.01
1:A:52:ARG:NH1	2:B:33:SER:CA	2.22	1.01
1:A:123:PHE:N	2:B:30:VAL:CG2	2.23	1.01
1:A:118:ARG:HG2	2:B:21:SER:HB2	1.06	1.00
2:B:123:SER:CB	3:C:110:GLN:HE21	1.73	1.00
1:A:216:ILE:H	2:B:58:VAL:CG1	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:SER:HB3	3:C:110:GLN:HE21	0.85	0.98
1:A:186:TRP:CD2	2:B:36:ILE:HB	1.99	0.98
1:A:119:MET:HE1	2:B:24:ALA:CB	1.64	0.98
1:A:216:ILE:HG13	2:B:56:ASN:HA	1.46	0.98
1:A:120:SER:H	2:B:23:CYS:HA	1.26	0.97
1:A:214:LYS:O	2:B:59:GLN:HB2	0.79	0.97
2:B:121:CYS:HB3	3:C:218:VAL:HG21	1.44	0.97
1:A:118:ARG:HD3	2:B:21:SER:CB	1.80	0.97
1:A:124:ILE:CB	2:B:28:PHE:CZ	2.48	0.96
1:A:186:TRP:CG	2:B:36:ILE:HB	2.00	0.96
1:A:216:ILE:CG1	2:B:56:ASN:HD22	1.80	0.95
1:A:216:ILE:HB	2:B:58:VAL:HG11	0.98	0.94
1:A:119:MET:HB2	2:B:24:ALA:N	1.83	0.94
1:A:195:GLN:HE22	2:B:231:ILE:HD12	1.30	0.94
1:A:120:SER:N	2:B:23:CYS:HA	1.84	0.93
1:A:213:ARG:NE	2:B:57:ASN:ND2	2.16	0.93
1:A:118:ARG:HG2	2:B:21:SER:HG	1.29	0.93
1:A:190:PRO:HB2	3:C:168:VAL:CG1	1.99	0.92
1:A:216:ILE:CB	2:B:58:VAL:HG13	1.96	0.91
1:A:1:THR:CA	2:B:41:LYS:O	2.19	0.91
1:A:190:PRO:HB2	3:C:168:VAL:HG12	1.49	0.91
1:A:119:MET:CE	2:B:24:ALA:N	2.15	0.90
1:A:52:ARG:NH1	2:B:32:PRO:O	2.04	0.90
1:A:52:ARG:HH12	2:B:32:PRO:C	1.74	0.90
1:A:186:TRP:CE2	2:B:36:ILE:HB	2.08	0.89
1:A:52:ARG:HH22	2:B:33:SER:N	1.66	0.89
1:A:186:TRP:CE3	2:B:36:ILE:HD12	2.08	0.89
1:A:186:TRP:CD1	2:B:36:ILE:HB	2.07	0.88
1:A:204:PHE:C	3:C:128:VAL:HG11	1.94	0.88
1:A:118:ARG:HD2	2:B:21:SER:CB	1.70	0.88
1:A:186:TRP:NE1	2:B:36:ILE:O	2.07	0.88
1:A:119:MET:HE3	2:B:24:ALA:HB2	1.43	0.88
1:A:123:PHE:H	2:B:30:VAL:CG2	1.83	0.87
2:B:124:ALA:CA	3:C:184:ARG:HH12	1.81	0.87
2:B:124:ALA:CB	3:C:184:ARG:NH1	2.39	0.86
1:A:124:ILE:HB	2:B:28:PHE:CZ	2.09	0.85
1:A:119:MET:HE2	2:B:24:ALA:H	1.38	0.85
1:A:213:ARG:HH21	2:B:57:ASN:HD22	1.24	0.85
1:A:195:GLN:NE2	2:B:231:ILE:HD12	1.91	0.85
1:A:119:MET:SD	2:B:24:ALA:HB2	2.16	0.84
1:A:106:PRO:HG3	2:B:25:LEU:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:CG1	2:B:56:ASN:HA	2.07	0.84
1:A:121:ILE:HG12	2:B:25:LEU:HD22	1.59	0.84
1:A:213:ARG:NE	2:B:57:ASN:HD21	1.71	0.84
1:A:122:PRO:HB2	2:B:30:VAL:HG23	0.84	0.84
1:A:121:ILE:CG1	2:B:25:LEU:HD22	2.09	0.83
2:B:124:ALA:C	3:C:184:ARG:HH12	1.82	0.83
1:A:185:ALA:O	2:B:39:GLU:HA	1.78	0.83
1:A:34:ASN:HD21	1:A:37:GLN:HE21	1.27	0.82
1:A:106:PRO:HB2	2:B:24:ALA:O	1.79	0.82
1:A:204:PHE:O	3:C:128:VAL:CB	2.26	0.82
1:A:83:MET:SD	1:A:102:THR:HG23	2.20	0.81
1:A:52:ARG:CZ	2:B:33:SER:N	2.41	0.81
2:B:124:ALA:CB	3:C:184:ARG:HG3	2.10	0.81
1:A:198:LYS:HD3	2:B:238:GLN:HE22	0.64	0.80
1:A:118:ARG:CB	2:B:21:SER:HB2	2.12	0.80
1:A:147:GLY:O	1:A:150:THR:HG23	1.81	0.80
1:A:213:ARG:HE	2:B:57:ASN:CG	1.84	0.80
1:A:118:ARG:HD2	2:B:21:SER:HB3	0.80	0.79
1:A:52:ARG:HH22	2:B:32:PRO:C	1.85	0.79
2:B:195:GLN:HA	2:B:195:GLN:HE21	1.47	0.79
1:A:186:TRP:CD1	2:B:36:ILE:C	2.56	0.79
1:A:216:ILE:CD1	2:B:56:ASN:HA	2.12	0.79
1:A:214:LYS:HA	2:B:59:GLN:CG	2.05	0.79
1:A:123:PHE:CE2	2:B:31:THR:HB	2.19	0.78
1:A:124:ILE:CB	2:B:28:PHE:CE2	2.67	0.78
2:B:42:ASN:HD22	2:B:44:MET:H	1.31	0.76
1:A:118:ARG:CG	2:B:21:SER:HG	1.90	0.76
2:B:65:MET:SD	3:C:162:HIS:HB3	2.26	0.76
1:A:215:ASP:C	2:B:58:VAL:HG12	2.04	0.75
1:A:119:MET:HE1	2:B:24:ALA:HB3	0.75	0.75
2:B:124:ALA:C	3:C:184:ARG:NH1	2.38	0.75
2:B:121:CYS:CB	3:C:218:VAL:HG21	2.17	0.74
1:A:216:ILE:HA	2:B:58:VAL:HG12	1.64	0.74
1:A:124:ILE:HB	2:B:28:PHE:HZ	1.51	0.73
1:A:119:MET:HB2	2:B:24:ALA:H	1.48	0.73
1:A:123:PHE:CA	2:B:30:VAL:HG22	2.18	0.73
1:A:120:SER:H	2:B:23:CYS:CA	2.01	0.73
1:A:119:MET:HG2	2:B:24:ALA:HB2	1.70	0.72
1:A:123:PHE:H	2:B:30:VAL:HG21	1.53	0.72
2:B:51:SER:CB	3:C:172:ASN:OD1	2.37	0.72
1:A:186:TRP:HD1	2:B:36:ILE:O	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:NH1	2:B:32:PRO:C	2.41	0.71
1:A:34:ASN:HD21	1:A:37:GLN:NE2	1.88	0.71
1:A:128:ASN:HB3	2:B:34:MET:CB	2.19	0.71
2:B:107:TYR:CE2	2:B:225:LEU:HD13	2.26	0.70
1:A:210:THR:OG1	2:B:97:HIS:HD2	1.74	0.70
1:A:198:LYS:HD2	2:B:238:GLN:HE21	1.54	0.70
1:A:123:PHE:O	2:B:30:VAL:HA	1.91	0.70
1:A:214:LYS:CA	2:B:59:GLN:HB2	2.21	0.70
1:A:186:TRP:CZ3	2:B:36:ILE:HD12	2.26	0.70
1:A:119:MET:CG	2:B:24:ALA:HB2	2.22	0.69
2:B:57:ASN:HD22	2:B:57:ASN:H	1.39	0.69
1:A:52:ARG:NH2	2:B:33:SER:CA	2.49	0.69
1:A:119:MET:HB2	2:B:23:CYS:CA	2.22	0.69
1:A:102:THR:HG21	1:A:107:SER:OG	1.93	0.68
1:A:122:PRO:CB	2:B:30:VAL:CG2	2.50	0.68
1:A:122:PRO:CG	2:B:28:PHE:HB3	2.23	0.68
1:A:119:MET:HB2	2:B:23:CYS:HA	1.75	0.68
1:A:209:ILE:HD11	3:C:162:HIS:HD2	1.59	0.68
1:A:19:THR:HG21	1:A:166:SER:OG	1.93	0.68
2:B:51:SER:HB2	3:C:172:ASN:OD1	1.94	0.67
1:A:128:ASN:HB3	2:B:34:MET:HB2	1.75	0.67
1:A:196:TYR:HB2	2:B:237:LEU:HD21	1.77	0.67
3:C:151:GLN:HE21	3:C:153:ASP:H	1.42	0.67
1:A:118:ARG:O	2:B:22:PRO:CG	2.41	0.67
1:A:213:ARG:CZ	2:B:57:ASN:ND2	2.40	0.67
1:A:119:MET:SD	2:B:24:ALA:CB	2.74	0.66
1:A:123:PHE:HB3	2:B:30:VAL:HG13	1.76	0.66
1:A:106:PRO:CB	2:B:24:ALA:O	2.42	0.66
1:A:124:ILE:HA	2:B:28:PHE:HE2	1.61	0.66
1:A:1:THR:HA	2:B:42:ASN:HA	1.77	0.66
2:B:144:THR:HG23	2:B:147:ASP:H	1.60	0.66
3:C:114:LEU:HG	3:C:116:VAL:HG22	1.79	0.65
1:A:122:PRO:HG3	2:B:28:PHE:HB3	1.79	0.64
1:A:186:TRP:CG	2:B:36:ILE:CB	2.79	0.64
1:A:203:ASP:OD2	3:C:129:GLY:HA2	1.97	0.64
1:A:52:ARG:CZ	2:B:33:SER:CB	2.76	0.64
1:A:186:TRP:CD1	2:B:36:ILE:CB	2.80	0.63
1:A:122:PRO:CG	2:B:28:PHE:CD2	2.76	0.63
1:A:214:LYS:O	2:B:59:GLN:HB3	1.89	0.63
2:B:124:ALA:CB	3:C:184:ARG:HH11	2.00	0.63
1:A:119:MET:HB2	2:B:23:CYS:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TRP:NE1	2:B:36:ILE:HB	2.12	0.62
1:A:204:PHE:O	3:C:128:VAL:HB	1.99	0.62
1:A:190:PRO:CB	3:C:168:VAL:CG1	2.75	0.62
1:A:19:THR:CG2	1:A:20:THR:HG22	2.29	0.62
1:A:52:ARG:NH1	2:B:33:SER:N	2.48	0.61
1:A:119:MET:CE	2:B:24:ALA:CA	2.39	0.61
1:A:190:PRO:HG2	3:C:168:VAL:CB	2.31	0.61
1:A:2:VAL:N	2:B:41:LYS:O	2.33	0.61
3:C:11:ASN:HD21	3:C:53:ARG:HE	1.49	0.60
1:A:121:ILE:HG13	2:B:25:LEU:HD22	1.81	0.60
1:A:19:THR:HG22	1:A:20:THR:HG22	1.83	0.60
1:A:102:THR:HG22	1:A:105:ASN:HB2	1.82	0.60
2:B:132:ILE:HG22	2:B:166:LEU:HD22	1.84	0.60
1:A:119:MET:CB	2:B:24:ALA:N	2.62	0.59
1:A:190:PRO:CG	3:C:168:VAL:HG11	2.32	0.59
1:A:216:ILE:H	2:B:58:VAL:HG11	1.62	0.59
1:A:219:VAL:HG22	2:B:86:ARG:HG2	1.84	0.59
1:A:122:PRO:CG	2:B:28:PHE:HD2	2.03	0.59
1:A:139:ASN:N	1:A:139:ASN:HD22	2.01	0.59
1:A:214:LYS:HA	2:B:59:GLN:CB	2.33	0.58
2:B:51:SER:HB3	3:C:172:ASN:OD1	2.02	0.58
2:B:81:GLN:HB2	2:B:193:TRP:CZ3	2.39	0.58
1:A:52:ARG:NH2	2:B:32:PRO:C	2.50	0.58
1:A:10:ALA:HB3	1:A:41:MET:HG2	1.85	0.58
1:A:128:ASN:HB3	2:B:34:MET:HB3	1.84	0.57
1:A:39:VAL:HG22	1:A:196:TYR:HD2	1.68	0.57
1:A:186:TRP:CG	2:B:36:ILE:CG2	2.87	0.57
2:B:121:CYS:HB3	3:C:218:VAL:CG2	2.26	0.57
1:A:216:ILE:CD1	2:B:56:ASN:CB	2.83	0.56
1:A:31:TRP:HE1	1:A:37:GLN:HE22	1.53	0.56
2:B:237:LEU:O	2:B:238:GLN:HB2	2.03	0.56
3:C:127:VAL:HG22	3:C:130:GLN:HB2	1.86	0.56
2:B:85:LEU:CD1	2:B:190:VAL:HB	2.35	0.56
1:A:190:PRO:HG2	3:C:168:VAL:HB	1.87	0.56
2:B:182:ASP:OD2	2:B:185:THR:HB	2.05	0.56
2:B:93:SER:HA	2:B:96:LYS:HG2	1.88	0.56
1:A:124:ILE:HA	2:B:28:PHE:CE2	2.41	0.55
2:B:123:SER:CB	3:C:110:GLN:NE2	2.49	0.55
1:A:43:ARG:NH1	1:A:192:ARG:O	2.39	0.55
1:A:123:PHE:C	2:B:30:VAL:HG22	2.27	0.55
1:A:108:ILE:HD11	1:A:119:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:CA	2:B:28:PHE:CE2	2.90	0.55
2:B:49:VAL:HG11	3:C:175:ILE:HG23	1.89	0.55
1:A:51:LEU:HD22	1:A:132:ASN:HD21	1.71	0.55
1:A:216:ILE:HD11	2:B:56:ASN:CB	2.37	0.54
1:A:124:ILE:CG2	2:B:28:PHE:CD2	2.61	0.54
1:A:36:LYS:HE3	1:A:148:TYR:CE2	2.42	0.54
2:B:85:LEU:HD11	2:B:190:VAL:HB	1.90	0.54
1:A:124:ILE:HG21	2:B:28:PHE:CZ	2.34	0.54
1:A:29:VAL:HG13	1:A:159:VAL:HG13	1.87	0.54
1:A:205:THR:HA	3:C:128:VAL:HG11	1.90	0.53
1:A:39:VAL:HG23	2:B:237:LEU:CD2	2.38	0.53
1:A:198:LYS:HA	2:B:238:GLN:OE1	2.07	0.53
1:A:5:PHE:CD1	2:B:43:LEU:HD11	2.43	0.53
2:B:195:GLN:HA	2:B:195:GLN:NE2	2.20	0.53
1:A:106:PRO:CG	2:B:25:LEU:HD12	2.35	0.53
1:A:216:ILE:CD1	2:B:56:ASN:CA	2.84	0.53
1:A:123:PHE:CZ	1:A:125:SER:HB3	2.45	0.52
1:A:216:ILE:HD11	2:B:56:ASN:HA	1.89	0.52
1:A:39:VAL:HG22	1:A:196:TYR:CD2	2.44	0.52
1:A:119:MET:CE	1:A:121:ILE:HD11	2.40	0.52
2:B:51:SER:HB3	2:B:99:LEU:HD22	1.90	0.52
1:A:190:PRO:HG2	3:C:168:VAL:HG11	1.92	0.51
1:A:123:PHE:O	2:B:30:VAL:HG22	2.10	0.51
1:A:205:THR:CA	3:C:128:VAL:HG11	2.40	0.51
1:A:196:TYR:HB2	2:B:237:LEU:CD2	2.41	0.51
1:A:118:ARG:HG3	2:B:21:SER:OG	1.97	0.51
1:A:10:ALA:CB	1:A:41:MET:HG2	2.41	0.50
1:A:122:PRO:CD	2:B:28:PHE:HB3	2.42	0.49
1:A:106:PRO:HG3	2:B:25:LEU:CD1	2.35	0.49
1:A:127:GLY:O	2:B:31:THR:CG2	2.42	0.49
1:A:186:TRP:CB	2:B:36:ILE:CG2	2.91	0.49
1:A:214:LYS:HA	2:B:59:GLN:HB2	1.90	0.49
3:C:197:ASN:ND2	3:C:198:SER:H	2.10	0.49
1:A:119:MET:HE1	1:A:121:ILE:HD11	1.93	0.48
1:A:190:PRO:CG	3:C:168:VAL:CG1	2.91	0.48
1:A:84:TYR:CD2	2:B:25:LEU:HD11	2.48	0.48
1:A:214:LYS:O	2:B:59:GLN:N	2.46	0.48
2:B:123:SER:N	3:C:110:GLN:NE2	2.62	0.48
1:A:122:PRO:HB2	2:B:30:VAL:HG21	1.74	0.48
1:A:124:ILE:CG2	2:B:28:PHE:CE1	2.90	0.48
1:A:186:TRP:CD2	2:B:36:ILE:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:CB	3:C:168:VAL:HB	2.43	0.48
1:A:119:MET:CB	2:B:23:CYS:CA	2.92	0.47
1:A:52:ARG:NH2	2:B:33:SER:HB2	2.29	0.47
1:A:203:ASP:OD2	3:C:129:GLY:CA	2.61	0.47
2:B:182:ASP:H	2:B:185:THR:HG22	1.79	0.47
1:A:190:PRO:HG2	3:C:168:VAL:CG1	2.44	0.47
1:A:31:TRP:HE1	1:A:37:GLN:NE2	2.11	0.47
1:A:19:THR:CG2	1:A:166:SER:OG	2.60	0.47
1:A:129:ALA:HB2	2:B:36:ILE:HD11	1.96	0.47
3:C:1:SER:HB3	3:C:3:ARG:HG2	1.97	0.47
1:A:210:THR:OG1	2:B:97:HIS:CD2	2.60	0.47
2:B:144:THR:HG22	2:B:147:ASP:CG	2.34	0.47
2:B:44:MET:O	2:B:48:GLU:HG3	2.15	0.46
1:A:190:PRO:CG	3:C:168:VAL:HB	2.46	0.46
1:A:220:THR:HG22	1:A:221:THR:H	1.81	0.46
2:B:121:CYS:SG	3:C:218:VAL:HG21	2.56	0.45
1:A:190:PRO:HD2	3:C:168:VAL:HG11	1.99	0.45
1:A:216:ILE:HD11	2:B:56:ASN:CA	2.44	0.45
3:C:11:ASN:HD21	3:C:53:ARG:HH21	1.63	0.45
3:C:197:ASN:HD22	3:C:198:SER:H	1.64	0.45
1:A:186:TRP:HB3	2:B:36:ILE:HG22	1.98	0.45
2:B:181:GLN:HG2	2:B:185:THR:CG2	2.48	0.44
1:A:214:LYS:O	2:B:59:GLN:CA	2.55	0.44
3:C:11:ASN:N	3:C:11:ASN:HD22	2.15	0.44
2:B:176:TYR:CZ	2:B:223:ARG:HD3	2.52	0.44
1:A:128:ASN:CB	2:B:34:MET:HB2	2.46	0.44
3:C:25:GLY:HA3	3:C:194:PRO:HD3	2.00	0.44
1:A:84:TYR:HB3	1:A:106:PRO:HG2	1.99	0.44
2:B:119:VAL:HG13	2:B:211:MET:HB2	2.00	0.44
1:A:216:ILE:HD12	2:B:56:ASN:HD22	0.61	0.43
2:B:124:ALA:HB1	3:C:184:ARG:NH1	2.27	0.43
3:C:11:ASN:H	3:C:11:ASN:HD22	1.64	0.43
1:A:216:ILE:CG1	2:B:58:VAL:HG13	2.47	0.43
2:B:127:THR:HG22	2:B:128:GLY:N	2.34	0.43
1:A:216:ILE:HA	2:B:58:VAL:CG1	2.28	0.43
1:A:198:LYS:HA	2:B:238:GLN:NE2	2.34	0.43
2:B:107:TYR:CZ	2:B:225:LEU:HD13	2.54	0.43
2:B:203:GLY:O	3:C:223:ALA:HB2	2.19	0.42
3:C:11:ASN:HD21	3:C:53:ARG:NE	2.13	0.42
1:A:52:ARG:NH2	2:B:33:SER:CB	2.82	0.42
2:B:127:THR:O	2:B:198:MET:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:SER:O	2:B:220:PHE:HA	2.19	0.42
1:A:195:GLN:NE2	2:B:231:ILE:CD1	2.73	0.42
1:A:92:PRO:HA	1:A:97:ASP:OD1	2.20	0.42
1:A:31:TRP:HA	1:A:32:PRO:HD3	1.85	0.41
2:B:52:VAL:HG23	3:C:171:GLY:O	2.20	0.41
1:A:133:PHE:CE1	1:A:189:ARG:HD2	2.55	0.41
1:A:123:PHE:HE2	2:B:31:THR:HB	1.77	0.41
2:B:124:ALA:HA	3:C:184:ARG:HH11	0.39	0.41
1:A:129:ALA:CB	2:B:36:ILE:HD11	2.50	0.41
2:B:85:LEU:HD12	2:B:190:VAL:HB	2.01	0.41
1:A:219:VAL:O	2:B:86:ARG:CZ	2.68	0.41
1:A:119:MET:CB	2:B:23:CYS:HA	2.48	0.41
1:A:91:ILE:HA	1:A:92:PRO:HD3	1.95	0.41
1:A:118:ARG:HB3	2:B:21:SER:HB2	1.98	0.41
1:A:14:MET:HA	1:A:174:ILE:O	2.20	0.41
1:A:1:THR:CA	2:B:42:ASN:HA	2.49	0.41
1:A:122:PRO:C	2:B:30:VAL:CG2	2.86	0.40
1:A:52:ARG:NH2	2:B:33:SER:H	2.06	0.40
3:C:54:PHE:CD1	3:C:237:ALA:HB2	2.56	0.40
1:A:123:PHE:HB3	2:B:30:VAL:CG1	2.45	0.40
1:A:52:ARG:CZ	2:B:32:PRO:C	2.82	0.40
1:A:187:VAL:O	1:A:187:VAL:HG22	2.22	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	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	34 77
2	B	236/238 (99%)	228 (97%)	8 (3%)	0	100 100
3	C	250/252 (99%)	227 (91%)	22 (9%)	1 (0%)	39 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	706/712 (99%)	662 (94%)	42 (6%)	2 (0%)	50 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
3	C	25	GLY

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	201/201 (100%)	177 (88%)	24 (12%)	6 31
2	B	211/211 (100%)	194 (92%)	17 (8%)	15 50
3	C	209/209 (100%)	191 (91%)	18 (9%)	13 47
All	All	621/621 (100%)	562 (90%)	59 (10%)	15 41

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	20	THR
1	A	26	LYS
1	A	39	VAL
1	A	41	MET
1	A	43	ARG
1	A	51	LEU
1	A	97	ASP
1	A	102	THR
1	A	119	MET
1	A	121	ILE
1	A	139	ASN
1	A	141	ASP
1	A	150	THR

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Mol	Chain	Res	Type
1	A	154	LEU
1	A	159	VAL
1	A	176	VAL
1	A	179	LYS
1	A	187	VAL
1	A	189	ARG
1	A	202	VAL
1	A	205	THR
1	A	219	VAL
1	A	221	THR
2	B	25	LEU
2	B	30	VAL
2	B	57	ASN
2	B	72	VAL
2	B	80	GLN
2	B	86	ARG
2	B	96	LYS
2	B	99	LEU
2	B	119	VAL
2	B	168	VAL
2	B	185	THR
2	B	195	GLN
2	B	200	VAL
2	B	223	ARG
2	B	225	LEU
2	B	237	LEU
2	B	238	GLN
3	C	2	ASP
3	C	11	ASN
3	C	14	ILE
3	C	34	ARG
3	C	39	THR
3	C	45	THR
3	C	67	VAL
3	C	116	VAL
3	C	135	THR
3	C	137	MET
3	C	150	THR
3	C	157	VAL
3	C	187	ASN
3	C	197	ASN
3	C	220	LEU

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Mol	Chain	Res	Type
3	C	236	VAL
3	C	247	ARG
3	C	252	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	132	ASN
1	A	139	ASN
1	A	142	GLN
1	A	152	ASN
1	A	195	GLN
2	B	12	GLN
2	B	35	ASN
2	B	42	ASN
2	B	56	ASN
2	B	57	ASN
2	B	97	HIS
2	B	195	GLN
2	B	206	ASN
2	B	238	GLN
3	C	11	ASN
3	C	43	GLN
3	C	110	GLN
3	C	151	GLN
3	C	154	GLN
3	C	162	HIS
3	C	163	ASN
3	C	197	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

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.