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

Sep 2, 2019 – 11:31 AM EDT

PDB ID	:	6KL9
EMDB ID:	:	EMD-0704
Title	:	Structure of LbCas12a-crRNA complex bound to AcrVA4 (form A complex)
Authors	:	Peng, R.; Li, Z.; Xu, Y.; He, S.; Peng, Q.; Shi, Y.; Gao, G.F.
Deposited on	:	2019-07-30
Resolution	:	3.25 Å(reported)
Based on PDB ID	:	5ID6

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.

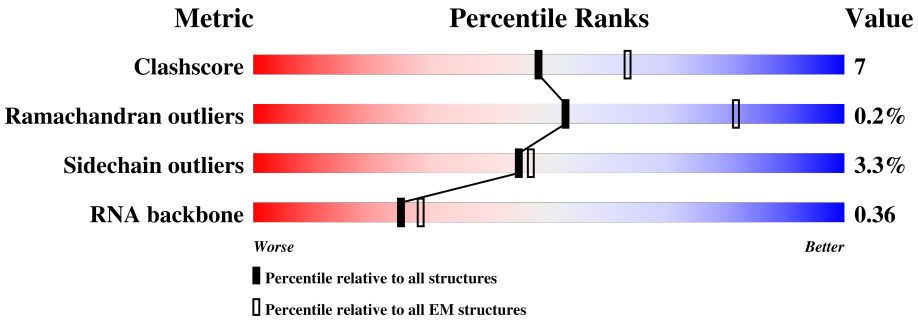
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 3.25 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	1228	83% 12%
2	B	234	33% 15% 50%
2	C	234	42% 8% 50%
3	G	42	31% 26% 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12191 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 LbCas12a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1180	9720	6259	1589	1845	27	1	0

- Molecule 2 is a protein called AcrVA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	117	967	613	163	185	6	0	0
2	C	117	Total	C	N	O	S	0	0
			967	613	163	185	6		

- Molecule 3 is a RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	G	25	529	237	90	177	25	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	G	1	1	1	0
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is water.

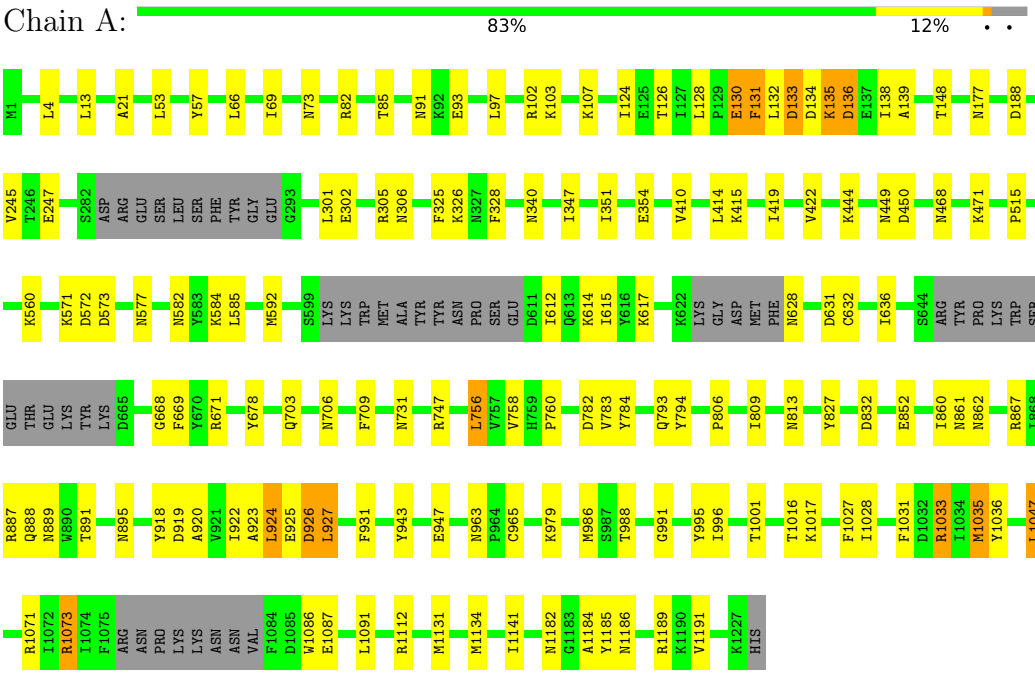
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	G	6	6	6	0

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 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.

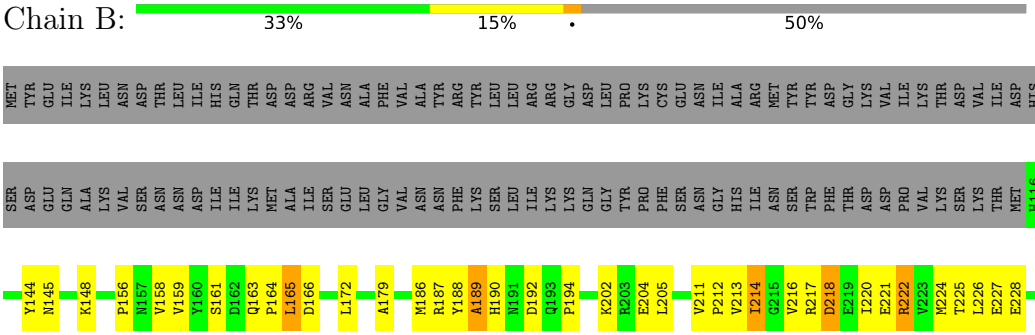
- Molecule 1: LbCas12a

Chain A:



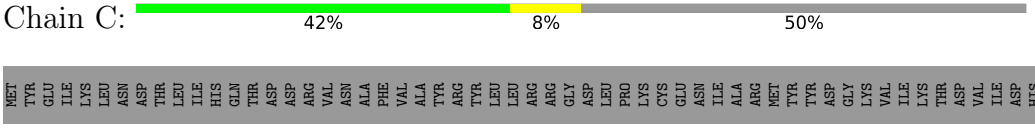
- Molecule 2: AcrVA4

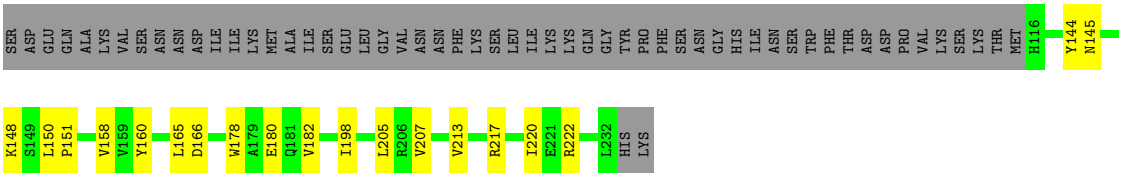
Chain B:



- Molecule 2: AcrVA4

Chain C:





• Molecule 3: RNA (42-MER)

Chain G:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	508000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.29	0/9914	0.56	0/13312
2	B	0.31	0/986	0.57	0/1341
2	C	0.28	0/986	0.60	0/1341
3	G	0.43	0/590	0.94	0/916
All	All	0.30	0/12476	0.59	0/16910

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	9720	0	9662	118	0
2	B	967	0	953	33	0
2	C	967	0	953	11	0
3	G	529	0	267	6	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
5	G	6	0	0	0	0
All	All	12191	0	11835	163	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 7.

All (163) 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:53:LEU:HD22	1:A:132:LEU:HD13	1.36	1.05
1:A:924:LEU:CD1	1:A:947:GLU:HG2	1.94	0.97
1:A:827:TYR:O	1:A:920:ALA:HB1	1.64	0.96
2:B:161:SER:HB3	2:B:165:LEU:HD22	1.46	0.94
1:A:53:LEU:HD22	1:A:132:LEU:CD1	2.00	0.90
1:A:126:THR:O	1:A:130:GLU:HG3	1.72	0.89
2:B:225:THR:O	2:B:227:GLU:HG3	1.74	0.87
2:B:222:ARG:HH11	2:B:222:ARG:HG3	1.42	0.84
1:A:57:TYR:HD1	1:A:131:PHE:CE2	1.96	0.83
1:A:57:TYR:HD1	1:A:131:PHE:CD2	2.00	0.80
1:A:827:TYR:HB2	1:A:920:ALA:HB2	1.63	0.80
1:A:21:ALA:O	1:A:794:TYR:HB2	1.82	0.79
1:A:924:LEU:HD11	1:A:947:GLU:HG2	1.66	0.76
2:B:214:ILE:HG22	2:B:221:GLU:HB2	1.67	0.76
3:G:1:A:OP2	3:G:1:A:H3'	1.86	0.76
1:A:1033:ARG:HG3	1:A:1033:ARG:HH11	1.51	0.76
1:A:1033:ARG:NH1	1:A:1033:ARG:HG3	2.02	0.74
1:A:131:PHE:CD1	1:A:131:PHE:C	2.61	0.71
1:A:923:ALA:HB2	1:A:1191:VAL:HG21	1.72	0.71
1:A:134:ASP:H	1:A:138:ILE:CD1	2.03	0.71
1:A:924:LEU:HD11	1:A:947:GLU:CG	2.21	0.70
2:B:163:GLN:HB3	2:B:164:PRO:HD2	1.71	0.69
1:A:924:LEU:HD11	1:A:947:GLU:CD	2.12	0.69
1:A:57:TYR:CD1	1:A:131:PHE:CD2	2.82	0.68
2:B:222:ARG:NH1	2:B:222:ARG:HG3	2.06	0.67
1:A:131:PHE:HD1	1:A:131:PHE:O	1.78	0.67
1:A:924:LEU:CD1	1:A:947:GLU:CG	2.70	0.65
1:A:131:PHE:HD1	1:A:131:PHE:C	2.00	0.64
1:A:132:LEU:O	1:A:138:ILE:HD11	1.97	0.64
2:B:217:ARG:HG2	2:B:217:ARG:HH21	1.63	0.63
1:A:102:ARG:NH2	1:A:177:ASN:OD1	2.33	0.62
1:A:103:LYS:O	1:A:107:LYS:HB2	2.00	0.61
1:A:1016:THR:HG22	1:A:1027:PHE:CZ	2.36	0.61
1:A:124:ILE:HD11	1:A:148:THR:HG22	1.82	0.61
2:B:224:MET:HG2	2:B:227:GLU:HB2	1.82	0.60
1:A:126:THR:O	1:A:130:GLU:CG	2.48	0.60
1:A:21:ALA:HA	1:A:703:GLN:O	2.01	0.59
1:A:1033:ARG:CG	1:A:1033:ARG:HH11	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:OE2	1:A:306:ASN:ND2	2.35	0.59
1:A:758:VAL:HG12	2:B:189:ALA:HB2	1.86	0.58
1:A:1031:PHE:CE1	1:A:1047:LEU:HD13	2.39	0.58
1:A:543:ARG:HH12	1:A:560:LYS:HB3	1.69	0.58
1:A:136:ASP:N	1:A:136:ASP:OD1	2.31	0.57
1:A:747:ARG:NH2	1:A:793:GLN:OE1	2.37	0.57
1:A:924:LEU:HD13	1:A:947:GLU:HG2	1.82	0.57
1:A:827:TYR:C	1:A:920:ALA:HB1	2.23	0.56
1:A:206:LYS:O	1:A:210:LEU:HB2	2.05	0.56
1:A:133:ASP:HA	1:A:138:ILE:HD11	1.88	0.55
1:A:852:GLU:OE1	1:A:918:TYR:OH	2.24	0.55
2:B:156:PRO:O	2:B:158:VAL:HG23	2.08	0.54
1:A:128:LEU:HD11	1:A:132:LEU:CD1	2.38	0.53
3:G:1:A:H2'	3:G:1:A:P	2.48	0.53
1:A:57:TYR:CD1	1:A:131:PHE:HD2	2.27	0.53
1:A:134:ASP:H	1:A:138:ILE:HD12	1.73	0.52
1:A:1131:MET:HE1	1:A:1134:MET:HE1	1.90	0.52
1:A:668:GLY:HA2	1:A:671:ARG:HD3	1.91	0.52
1:A:134:ASP:H	1:A:138:ILE:HD11	1.74	0.52
1:A:103:LYS:O	1:A:107:LYS:CB	2.58	0.51
2:B:161:SER:HB3	2:B:165:LEU:CD2	2.31	0.51
1:A:988:THR:H	1:A:995:TYR:HB2	1.75	0.51
2:B:228:GLU:OE1	2:B:228:GLU:HA	2.09	0.51
1:A:832:ASP:HB2	1:A:1184:ALA:HB2	1.91	0.51
1:A:135:LYS:O	1:A:139:ALA:N	2.38	0.51
1:A:468:ASN:HA	1:A:471:LYS:HG2	1.92	0.51
1:A:82:ARG:NH1	1:A:188:ASP:OD1	2.42	0.51
2:B:179:ALA:HB3	2:B:217:ARG:HA	1.93	0.51
2:C:160:TYR:HB3	2:C:198:ILE:HD13	1.93	0.51
1:A:1131:MET:HA	1:A:1131:MET:HE3	1.91	0.51
1:A:614:LYS:HA	1:A:617:LYS:HG2	1.94	0.50
1:A:1131:MET:CE	1:A:1134:MET:HE1	2.42	0.49
1:A:658:SER:H	1:A:669:PHE:HE1	1.58	0.49
1:A:612:ILE:HA	1:A:615:ILE:HD12	1.94	0.49
3:G:1:A:P	3:G:1:A:C3'	3.01	0.49
1:A:245:VAL:HG13	1:A:247:GLU:H	1.76	0.49
2:B:218:ASP:N	2:B:218:ASP:OD1	2.46	0.49
1:A:931:PHE:C	1:A:931:PHE:CD2	2.85	0.49
2:C:165:LEU:O	2:C:166:ASP:OD1	2.31	0.49
3:G:1:A:H3'	3:G:1:A:P	2.52	0.49
1:A:1016:THR:HG22	1:A:1027:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LEU:HD22	1:A:784:TYR:HD1	1.78	0.48
2:C:144:TYR:O	2:C:148:LYS:HB2	2.13	0.48
2:C:160:TYR:HB2	2:C:207:VAL:HG11	1.96	0.48
1:A:1031:PHE:HE1	1:A:1047:LEU:HD13	1.77	0.48
1:A:128:LEU:HD11	1:A:132:LEU:HD12	1.96	0.48
1:A:573:ASP:H	1:A:577:ASN:HD21	1.61	0.48
1:A:924:LEU:CD1	1:A:947:GLU:CD	2.83	0.47
2:C:158:VAL:HG11	2:C:182:VAL:HB	1.97	0.47
2:B:186:MET:HB2	2:B:186:MET:HE2	1.83	0.47
1:A:585:LEU:HD13	1:A:678:TYR:HD1	1.79	0.47
2:B:161:SER:CB	2:B:165:LEU:HD22	2.33	0.47
1:A:760:PRO:HG3	2:B:187:ARG:HG3	1.97	0.46
2:B:144:TYR:CE2	2:B:148:LYS:HD2	2.50	0.46
1:A:1035:MET:HG3	1:A:1036:TYR:N	2.30	0.46
1:A:347:ILE:HD11	1:A:414:LEU:HD13	1.96	0.46
1:A:73:ASN:HB3	1:A:97:LEU:HD11	1.98	0.46
2:B:120:MET:O	2:B:124:VAL:HB	2.16	0.46
1:A:1073:ARG:HB3	1:A:1087:GLU:O	2.16	0.46
1:A:57:TYR:CD1	1:A:131:PHE:CE2	2.89	0.46
1:A:135:LYS:HG2	1:A:135:LYS:H	1.42	0.46
2:B:225:THR:O	2:B:227:GLU:N	2.49	0.46
1:A:926:ASP:HB2	1:A:995:TYR:HB3	1.98	0.46
2:B:217:ARG:HG2	2:B:217:ARG:NH2	2.31	0.46
2:B:214:ILE:O	2:B:214:ILE:HG22	2.15	0.46
1:A:53:LEU:HD22	1:A:132:LEU:HD11	1.95	0.45
1:A:860:ILE:HG12	1:A:869:LYS:HG2	1.98	0.45
1:A:1131:MET:HE1	1:A:1134:MET:CE	2.46	0.45
2:C:178:TRP:CD1	2:C:180:GLU:HG3	2.52	0.45
1:A:326:LYS:HA	1:A:415:LYS:HE3	1.99	0.45
1:A:444:LYS:HB2	1:A:449:ASN:HB2	1.99	0.45
1:A:986:MET:HB3	1:A:995:TYR:CE1	2.50	0.45
1:A:1049:TYR:HA	1:A:1052:PHE:HD2	1.81	0.45
1:A:1131:MET:CE	1:A:1134:MET:CE	2.95	0.45
1:A:1131:MET:HE2	1:A:1131:MET:HB3	1.83	0.45
1:A:827:TYR:O	1:A:920:ALA:CB	2.52	0.45
1:A:758:VAL:HG23	1:A:783:VAL:O	2.16	0.45
1:A:325:PHE:HA	1:A:328:PHE:HB2	1.99	0.44
1:A:66:LEU:HA	1:A:69:ILE:HD12	1.99	0.44
2:C:160:TYR:HE1	2:C:178:TRP:HB3	1.82	0.44
1:A:1028:ILE:HA	1:A:1031:PHE:HD2	1.82	0.44
2:B:218:ASP:O	2:B:220:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ILE:HA	1:A:422:VAL:HG22	1.99	0.44
1:A:515:PRO:HG3	2:B:204:GLU:HG2	2.00	0.44
1:A:628:ASN:ND2	1:A:631:ASP:OD2	2.51	0.44
1:A:571:LYS:HG2	1:A:572:ASP:H	1.83	0.43
1:A:706:ASN:H	1:A:709:PHE:HD2	1.66	0.43
1:A:354:GLU:OE2	1:A:1017:LYS:NZ	2.48	0.43
2:B:165:LEU:HD12	2:B:165:LEU:HA	1.75	0.43
2:B:211:VAL:HA	2:B:212:PRO:HD3	1.90	0.43
2:B:222:ARG:H	2:B:222:ARG:HG2	1.64	0.43
2:B:159:VAL:HG23	2:B:213:VAL:HG21	2.01	0.43
1:A:85:THR:OG1	1:A:91:ASN:ND2	2.52	0.43
1:A:731:ASN:ND2	1:A:965:CYS:SG	2.92	0.43
1:A:758:VAL:HG21	1:A:782:ASP:HB3	2.01	0.43
1:A:923:ALA:CB	1:A:1191:VAL:HG21	2.44	0.43
3:G:21:C:O2'	3:G:22:G:O4'	2.29	0.43
2:C:213:VAL:HG11	2:C:220:ILE:HD12	2.01	0.42
1:A:862:ASN:OD1	1:A:867:ARG:NH1	2.52	0.42
1:A:1182:ASN:OD1	1:A:1186:ASN:ND2	2.51	0.42
1:A:544:ALA:HA	1:A:556:ALA:O	2.19	0.42
2:C:150:LEU:HA	2:C:151:PRO:HD3	1.79	0.42
1:A:351:ILE:HD13	1:A:410:VAL:HG13	2.00	0.42
2:C:198:ILE:HG21	2:C:205:LEU:HD23	2.01	0.42
1:A:93:GLU:O	1:A:97:LEU:HB2	2.20	0.42
1:A:927:LEU:HD22	1:A:927:LEU:HA	1.82	0.42
1:A:806:PRO:HB2	1:A:809:ILE:HD11	2.02	0.42
1:A:4:LEU:HG	1:A:919:ASP:OD1	2.20	0.42
1:A:895:ASN:ND2	2:B:202:LYS:O	2.52	0.41
2:B:225:THR:O	2:B:227:GLU:CG	2.57	0.41
1:A:1071:ARG:HD3	1:A:1091:LEU:HD21	2.03	0.41
2:C:165:LEU:C	2:C:166:ASP:OD1	2.58	0.41
2:B:202:LYS:NZ	3:G:7:U:OP1	2.41	0.41
2:B:216:VAL:O	2:B:220:ILE:HG22	2.20	0.41
1:A:13:LEU:HD13	1:A:979:LYS:HE2	2.02	0.41
2:B:172:LEU:HD22	2:B:220:ILE:HD11	2.03	0.41
1:A:927:LEU:HG	1:A:943:TYR:HD2	1.86	0.41
1:A:861:ASN:O	1:A:867:ARG:HA	2.21	0.41
1:A:1185:TYR:CZ	1:A:1189:ARG:HD2	2.56	0.40
1:A:134:ASP:O	1:A:138:ILE:HG13	2.20	0.40
1:A:301:LEU:O	1:A:305:ARG:HG2	2.21	0.40
1:A:924:LEU:HG	1:A:924:LEU:O	2.20	0.40
1:A:1086:TRP:HE1	1:A:1141:ILE:HG12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:ASN:ND2	1:A:991:GLY:H	2.19	0.40
1:A:632:CYS:O	1:A:636:ILE:HG12	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	1167/1228 (95%)	1060 (91%)	106 (9%)	1 (0%)	53 85
2	B	115/234 (49%)	96 (84%)	17 (15%)	2 (2%)	10 41
2	C	115/234 (49%)	102 (89%)	13 (11%)	0	100 100
All	All	1397/1696 (82%)	1258 (90%)	136 (10%)	3 (0%)	53 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	226	LEU
2	B	189	ALA
1	A	133	ASP

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	1067/1115 (96%)	1039 (97%)	28 (3%)	49 75
2	B	110/217 (51%)	99 (90%)	11 (10%)	8 30
2	C	110/217 (51%)	107 (97%)	3 (3%)	48 74
All	All	1287/1549 (83%)	1245 (97%)	42 (3%)	45 70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	131	PHE
1	A	135	LYS
1	A	136	ASP
1	A	340	ASN
1	A	450	ASP
1	A	582	ASN
1	A	584	LYS
1	A	592	MET
1	A	756	LEU
1	A	875	LEU
1	A	887	ARG
1	A	888	GLN
1	A	889	ASN
1	A	891	THR
1	A	922	ILE
1	A	924	LEU
1	A	925	GLU
1	A	926	ASP
1	A	927	LEU
1	A	963	ASN
1	A	996	ILE
1	A	1001	THR
1	A	1033	ARG
1	A	1035	MET
1	A	1047	LEU
1	A	1073	ARG
1	A	1112	ARG
2	B	145	ASN
2	B	165	LEU
2	B	166	ASP
2	B	188	TYR
2	B	190	HIS
2	B	192	ASP

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Mol	Chain	Res	Type
2	B	194	PRO
2	B	205	LEU
2	B	214	ILE
2	B	218	ASP
2	B	222	ARG
2	C	145	ASN
2	C	217	ARG
2	C	222	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	340	ASN
1	A	582	ASN
1	A	731	ASN
1	A	803	ASN
1	A	813	ASN
1	A	963	ASN
1	A	989	GLN
2	B	145	ASN
2	C	145	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	24/42 (57%)	8 (33%)	1 (4%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	8	A
3	G	11	A
3	G	12	A
3	G	14	U
3	G	15	G
3	G	21	C
3	G	24	U
3	G	25	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	G	23	G

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.