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

Sep 3, 2019 – 11:42 AM EDT

PDB ID	:	6P7V
EMDB ID:	:	EMD-20270
Title	:	Structure of the K. lactis CBF3 core
Authors	:	Lee, P.D.; Wei, H.; Tan, D.; Harrison, S.C.
Deposited on	:	2019-06-06
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.

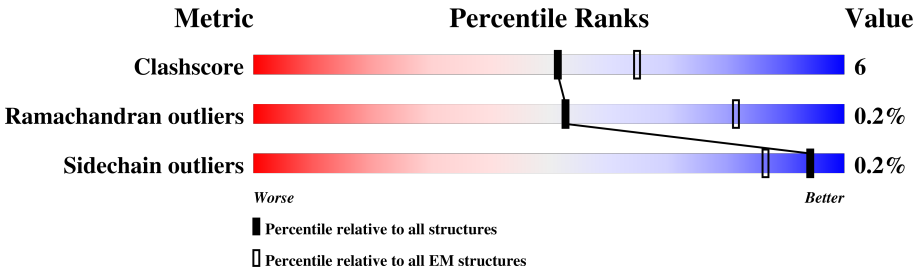
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	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	C	389	64% 19% • 16%
2	D	182	58% 12% 31%
3	A	634	60% 12% 28%
3	B	634	64% 11% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23152 atoms, of which 11620 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 Ctf13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	325	5437	1753	2726	449	497	12	0	0

- Molecule 2 is a protein called Skp1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	126	2059	648	1036	180	191	4	0	0

- Molecule 3 is a protein called Cep3.

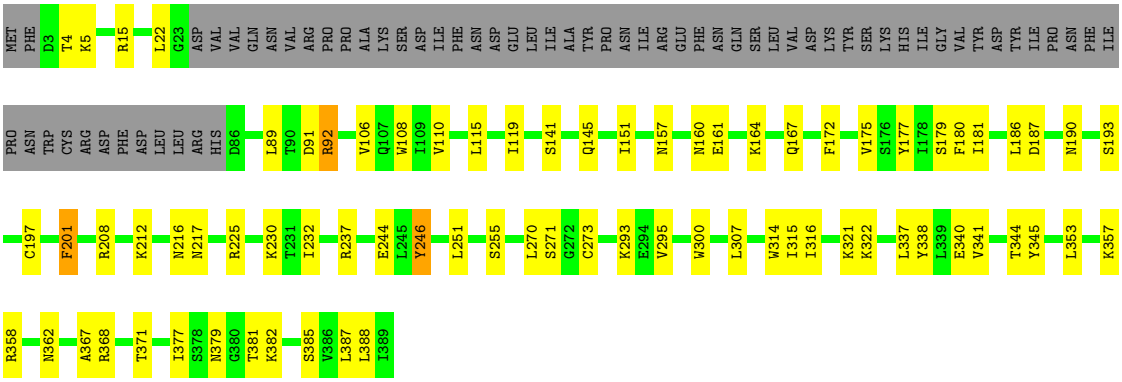
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	B	476	7977	2596	4004	650	707	20	0	0
3	A	457	7679	2504	3854	627	674	20	0	0

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 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.

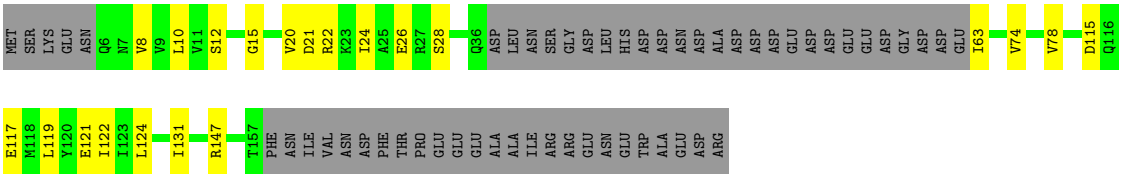
- Molecule 1: Ctf13

Chain C:



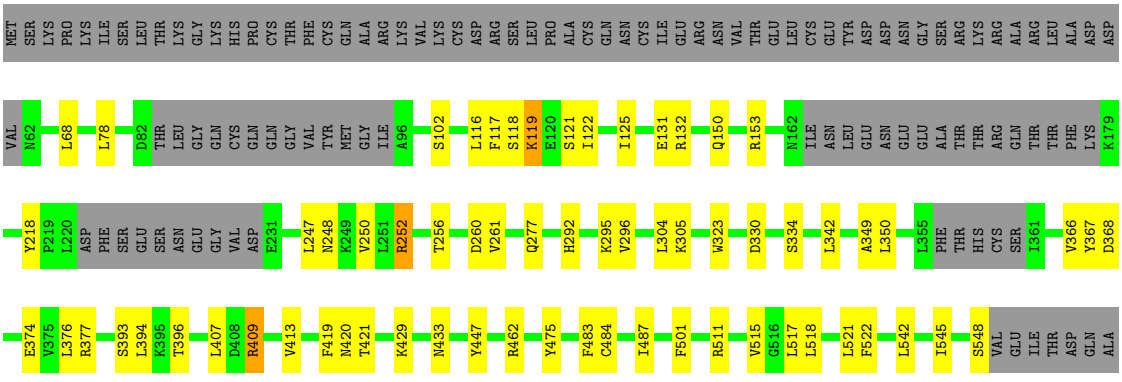
- Molecule 2: Skp1

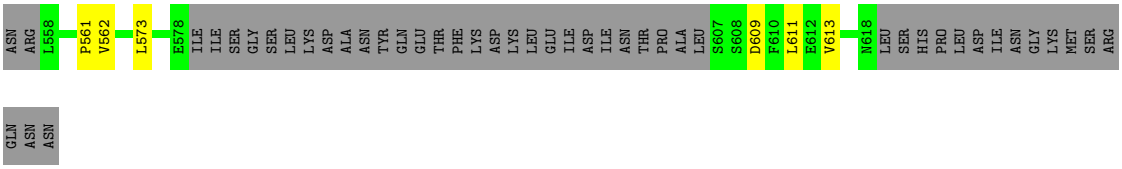
Chain D:



- Molecule 3: Cep3

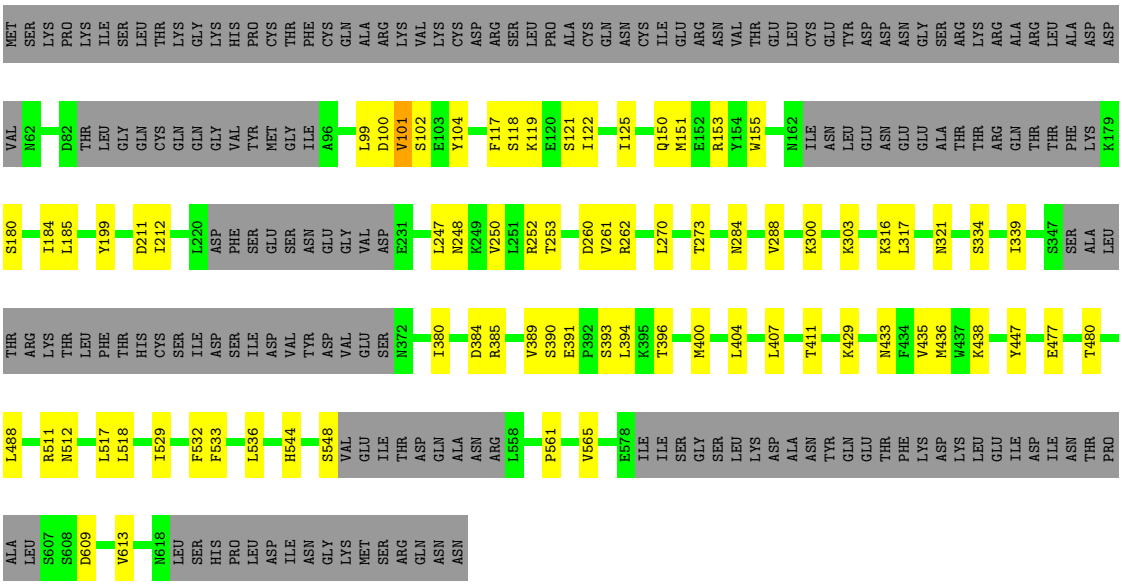
Chain B:





• Molecule 3: Cep3

Chain A:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130143	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	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

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	C	0.45	0/2768	0.74	1/3754 (0.0%)
2	D	0.37	0/1040	0.73	1/1408 (0.1%)
3	A	0.49	0/3916	0.77	1/5289 (0.0%)
3	B	0.58	0/4065	0.73	2/5492 (0.0%)
All	All	0.50	0/11789	0.74	5/15943 (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
1	C	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	252	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	92	ARG	NE-CZ-NH2	5.64	123.12	120.30
3	B	409	ARG	NE-CZ-NH2	5.61	123.11	120.30
3	A	517	LEU	CA-CB-CG	5.46	127.86	115.30
2	D	147	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	201	PHE	Peptide
1	C	246	TYR	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	C	2711	2726	2725	45	0
2	D	1023	1036	1036	11	0
3	A	3825	3854	3852	43	0
3	B	3973	4004	4001	50	0
All	All	11532	11620	11614	145	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 6.

All (145) 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)
3:B:330:ASP:O	3:B:334:SER:OG	2.08	0.72
3:B:117:PHE:O	3:B:121:SER:OG	2.08	0.72
1:C:22:LEU:O	1:C:92:ARG:NH1	2.24	0.71
1:C:295:VAL:O	1:C:357:LYS:NZ	2.24	0.70
3:A:270:LEU:O	3:A:273:THR:OG1	2.10	0.70
3:B:248:ASN:OD1	3:B:252:ARG:NE	2.25	0.69
3:A:317:LEU:O	3:A:321:ASN:ND2	2.26	0.69
1:C:367:ALA:O	1:C:371:THR:OG1	2.12	0.67
3:B:150:GLN:OE1	3:B:153:ARG:NH2	2.27	0.67
3:B:429:LYS:O	3:B:433:ASN:ND2	2.27	0.67
1:C:362:ASN:OD1	1:C:385:SER:OG	2.13	0.67
3:A:117:PHE:O	3:A:121:SER:OG	2.13	0.67
1:C:141:SER:O	1:C:145:GLN:NE2	2.29	0.66
1:C:321:LYS:NZ	1:C:322:LYS:O	2.27	0.66
3:A:150:GLN:OE1	3:A:153:ARG:NH2	2.29	0.65
1:C:358:ARG:NH2	1:C:382:LYS:O	2.31	0.64
2:D:10:LEU:HD11	2:D:20:VAL:HG22	1.80	0.64
3:B:374:GLU:OE1	3:B:377:ARG:NH2	2.31	0.64
1:C:187:ASP:OD1	1:C:230:LYS:NZ	2.27	0.64
3:B:131:GLU:OE1	3:B:132:ARG:NH2	2.31	0.63
3:A:429:LYS:O	3:A:433:ASN:ND2	2.33	0.62
1:C:208:ARG:NH2	1:C:246:TYR:OH	2.32	0.62
1:C:177:TYR:OH	1:C:244:GLU:OE1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:O	3:A:184:ILE:HD12	2.01	0.61
3:B:393:SER:OG	3:B:394:LEU:N	2.33	0.60
1:C:186:LEU:O	1:C:230:LYS:NZ	2.24	0.59
2:D:28:SER:HB2	2:D:131:ILE:HD11	1.84	0.59
1:C:212:LYS:O	1:C:216:ASN:ND2	2.36	0.59
1:C:273:CYS:H	1:C:295:VAL:HG12	1.66	0.59
3:B:252:ARG:NH1	3:A:101:VAL:O	2.35	0.59
3:B:122:ILE:HA	3:B:125:ILE:HD12	1.86	0.57
1:C:164:LYS:NZ	1:C:197:CYS:O	2.29	0.57
3:A:488:LEU:HB3	3:A:518:LEU:HD11	1.87	0.57
3:A:252:ARG:HG3	3:A:253:THR:HG23	1.85	0.56
2:D:22:ARG:NE	2:D:26:GLU:OE2	2.35	0.56
1:C:251:LEU:O	1:C:255:SER:OG	2.10	0.56
3:A:122:ILE:HA	3:A:125:ILE:HD12	1.87	0.55
3:B:68:LEU:HD22	3:B:501:PHE:HE2	1.72	0.55
3:B:256:THR:OG1	3:A:99:LEU:O	2.22	0.55
3:A:303:LYS:O	3:A:316:LYS:NZ	2.39	0.55
3:A:396:THR:HG22	3:A:400:MET:SD	2.47	0.54
2:D:119:LEU:HA	2:D:122:ILE:HD12	1.87	0.54
3:A:407:LEU:O	3:A:411:THR:OG1	2.14	0.54
1:C:108:TRP:HE3	1:C:115:LEU:HD21	1.72	0.54
2:D:21:ASP:HB3	2:D:24:ILE:HD12	1.88	0.54
3:B:376:LEU:CD1	3:B:407:LEU:HD22	2.38	0.53
3:A:118:SER:OG	3:A:118:SER:O	2.25	0.53
1:C:167:GLN:NE2	1:C:172:PHE:O	2.41	0.53
1:C:89:LEU:HD12	1:C:92:ARG:HD3	1.90	0.53
3:B:409:ARG:O	3:B:413:VAL:HG23	2.09	0.53
3:B:542:LEU:HD11	3:B:562:VAL:HG13	1.91	0.53
3:B:394:LEU:HD21	3:B:447:TYR:CD2	2.44	0.52
1:C:175:VAL:HG13	1:C:201:PHE:CE1	2.45	0.52
3:B:330:ASP:OD2	3:B:342:LEU:N	2.41	0.52
3:B:561:PRO:CB	3:B:611:LEU:HD13	2.39	0.51
3:A:185:LEU:HD23	3:A:262:ARG:HB2	1.92	0.51
3:A:248:ASN:OD1	3:A:252:ARG:NH2	2.43	0.51
2:D:28:SER:CB	2:D:131:ILE:HD11	2.41	0.50
1:C:293:LYS:O	1:C:295:VAL:HG13	2.11	0.50
3:A:384:ASP:OD1	3:A:438:LYS:NZ	2.34	0.49
1:C:108:TRP:CE3	1:C:115:LEU:HD21	2.47	0.49
3:A:334:SER:O	3:A:334:SER:OG	2.28	0.49
3:A:391:GLU:OE2	3:A:396:THR:HG21	2.13	0.49
1:C:4:THR:OG1	1:C:5:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:561:PRO:HB2	3:B:611:LEU:HD13	1.95	0.49
3:A:393:SER:OG	3:A:394:LEU:N	2.46	0.49
3:A:284:ASN:O	3:A:288:VAL:HG23	2.13	0.49
3:A:544:HIS:O	3:A:548:SER:N	2.46	0.49
3:B:295:LYS:HB3	3:A:339:ILE:HG21	1.94	0.49
3:B:609:ASP:O	3:B:613:VAL:HG23	2.13	0.49
3:A:394:LEU:HD21	3:A:447:TYR:CD2	2.48	0.48
1:C:232:ILE:HD11	1:C:237:ARG:HE	1.77	0.48
2:D:74:VAL:O	2:D:78:VAL:HG23	2.13	0.48
3:B:247:LEU:HA	3:B:250:VAL:HG12	1.95	0.48
3:B:349:ALA:HB1	3:B:367:TYR:OH	2.14	0.48
3:B:118:SER:OG	3:B:118:SER:O	2.21	0.48
2:D:121:GLU:HA	2:D:124:LEU:HD12	1.95	0.48
2:D:8:VAL:HG13	2:D:63:ILE:HG22	1.95	0.48
3:A:389:VAL:HG13	3:A:390:SER:HB3	1.95	0.47
3:B:376:LEU:HD13	3:B:407:LEU:HD22	1.96	0.47
1:C:232:ILE:HD11	1:C:237:ARG:NE	2.29	0.47
3:B:420:ASN:OD1	3:B:421:THR:N	2.47	0.47
3:B:518:LEU:HD12	3:B:522:PHE:CE2	2.50	0.47
3:B:368:ASP:N	3:B:368:ASP:OD2	2.44	0.47
3:B:511:ARG:O	3:B:515:VAL:HG22	2.13	0.47
1:C:300:TRP:HE1	1:C:345:TYR:HH	1.63	0.46
3:B:260:ASP:OD1	3:B:261:VAL:N	2.48	0.46
2:D:12:SER:O	2:D:15:GLY:N	2.45	0.46
1:C:157:ASN:O	1:C:161:GLU:N	2.44	0.46
1:C:179:SER:HB2	1:C:181:ILE:HD11	1.98	0.46
1:C:270:LEU:HD23	1:C:271:SER:N	2.31	0.45
1:C:338:TYR:OH	1:C:368:ARG:NE	2.49	0.45
1:C:177:TYR:OH	1:C:208:ARG:NE	2.49	0.45
3:A:385:ARG:O	3:A:389:VAL:HG12	2.17	0.45
3:B:116:LEU:HD13	3:B:218:TYR:CE2	2.52	0.45
3:B:483:PHE:CE2	3:B:487:ILE:HD11	2.51	0.45
3:B:68:LEU:HD22	3:B:501:PHE:CE2	2.51	0.45
1:C:387:LEU:O	1:C:388:LEU:HD23	2.17	0.45
1:C:106:VAL:HG13	1:C:119:ILE:HG22	1.99	0.45
3:B:542:LEU:HA	3:B:545:ILE:HD12	1.99	0.45
3:A:151:MET:SD	3:A:155:TRP:NE1	2.90	0.45
3:B:545:ILE:O	3:B:548:SER:OG	2.25	0.45
3:A:529:ILE:O	3:A:533:PHE:N	2.44	0.44
3:A:609:ASP:O	3:A:613:VAL:HG23	2.16	0.44
3:B:119:LYS:HA	3:B:122:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:VAL:HG22	1:C:115:LEU:HA	1.99	0.44
3:A:532:PHE:O	3:A:536:LEU:N	2.46	0.44
3:A:100:ASP:O	3:A:102:SER:N	2.51	0.44
1:C:106:VAL:HG22	1:C:119:ILE:HG22	1.99	0.44
3:A:404:LEU:HD22	3:A:436:MET:CG	2.48	0.43
3:A:511:ARG:NH1	3:A:512:ASN:OD1	2.49	0.43
3:B:102:SER:OG	3:A:252:ARG:NH1	2.49	0.43
3:B:277:GLN:OE1	3:B:277:GLN:N	2.51	0.43
3:B:292:HIS:O	3:B:296:VAL:HG23	2.17	0.43
3:A:104:TYR:O	3:A:248:ASN:ND2	2.51	0.43
2:D:115:ASP:OD2	2:D:117:GLU:N	2.51	0.43
1:C:160:ASN:ND2	1:C:193:SER:OG	2.52	0.43
3:B:518:LEU:HD12	3:B:522:PHE:CD2	2.54	0.43
1:C:151:ILE:HD11	1:C:180:PHE:CD2	2.54	0.43
1:C:187:ASP:O	1:C:190:ASN:ND2	2.52	0.43
3:A:561:PRO:O	3:A:565:VAL:HG23	2.19	0.42
3:B:304:LEU:HD12	3:B:305:LYS:H	1.85	0.42
3:B:78:LEU:HD12	3:B:573:LEU:HB3	2.01	0.42
3:A:477:GLU:OE1	3:A:477:GLU:N	2.47	0.42
3:B:433:ASN:OD1	3:B:462:ARG:NH2	2.53	0.42
3:B:517:LEU:O	3:B:521:LEU:HD13	2.18	0.42
3:A:380:ILE:CG2	3:A:435:VAL:HG21	2.49	0.42
3:A:199:TYR:OH	3:A:480:THR:O	2.29	0.42
1:C:337:LEU:O	1:C:341:VAL:HG23	2.20	0.42
1:C:353:LEU:HD12	1:C:377:ILE:HG22	2.02	0.42
1:C:15:ARG:NH1	1:C:91:ASP:OD2	2.53	0.42
1:C:340:GLU:O	1:C:344:THR:HG23	2.19	0.42
3:B:323:TRP:CH2	3:B:342:LEU:HD11	2.55	0.42
3:A:247:LEU:HA	3:A:250:VAL:HG12	2.01	0.41
3:B:78:LEU:HB3	3:B:573:LEU:HD13	2.00	0.41
1:C:217:ASN:O	1:C:225:ARG:NH1	2.53	0.41
1:C:307:LEU:HD22	1:C:362:ASN:ND2	2.35	0.41
1:C:379:ASN:C	1:C:381:THR:HG23	2.40	0.41
3:B:419:PHE:HE1	3:B:475:TYR:HH	1.68	0.41
3:A:260:ASP:OD1	3:A:261:VAL:N	2.53	0.41
3:B:366:VAL:HG12	3:B:367:TYR:H	1.86	0.41
3:B:484:CYS:HA	3:B:487:ILE:HD12	2.03	0.41
3:B:350:LEU:HD21	3:B:396:THR:HG23	2.02	0.40
1:C:315:ILE:O	1:C:316:ILE:HD13	2.20	0.40
3:A:211:ASP:OD1	3:A:212:ILE:N	2.50	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	C	321/389 (82%)	270 (84%)	51 (16%)	0	100 100
2	D	122/182 (67%)	112 (92%)	10 (8%)	0	100 100
3	A	443/634 (70%)	409 (92%)	32 (7%)	2 (0%)	31 72
3	B	462/634 (73%)	422 (91%)	39 (8%)	1 (0%)	49 84
All	All	1348/1839 (73%)	1213 (90%)	132 (10%)	3 (0%)	53 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	119	LYS
3	A	119	LYS
3	A	101	VAL

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	C	311/372 (84%)	310 (100%)	1 (0%)	93 96
2	D	115/165 (70%)	115 (100%)	0	100 100
3	A	432/592 (73%)	431 (100%)	1 (0%)	94 97
3	B	450/592 (76%)	450 (100%)	0	100 100
All	All	1308/1721 (76%)	1306 (100%)	2 (0%)	94 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	314	TRP
3	A	300	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	ASN
3	B	346	ASN
3	A	346	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.