wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	3J9O
EMDB ID:	:	EMD-6266
Title	:	CryoEM structure of a type VI secretion system
Authors	:	Clemens, D.L.; Ge, P.; Lee, B.-Y.; Horwitz, M.A.; Zhou, Z.H.
Deposited on	:	2015-02-11
Resolution	:	3.70 Å(reported)

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

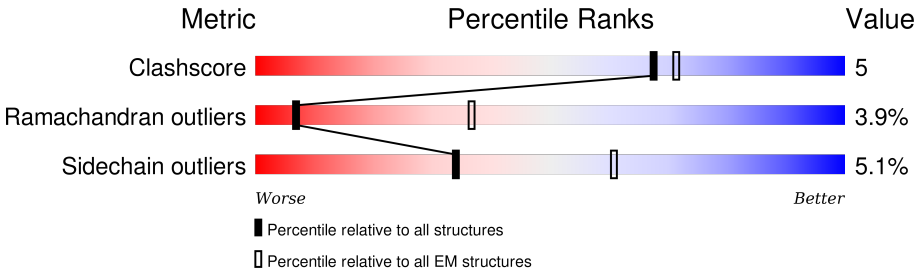
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.70 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	184	58% 14% • 27%
1	C	184	57% 15% • 27%
1	E	184	57% 15% • 27%
1	G	184	57% 15% • 27%
1	I	184	58% 14% • 27%
1	K	184	55% 16% • 27%
2	B	506	68% 15% • 16%
2	D	506	69% 15% • 16%
2	F	506	69% 15% • 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	506	69% 15% • 16%
2	J	506	67% 16% • 16%
2	L	506	69% 15% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27264 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 Intracellular growth locus protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	C	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	E	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	G	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	I	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	K	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		

- Molecule 2 is a protein called Intracellular growth locus protein B.

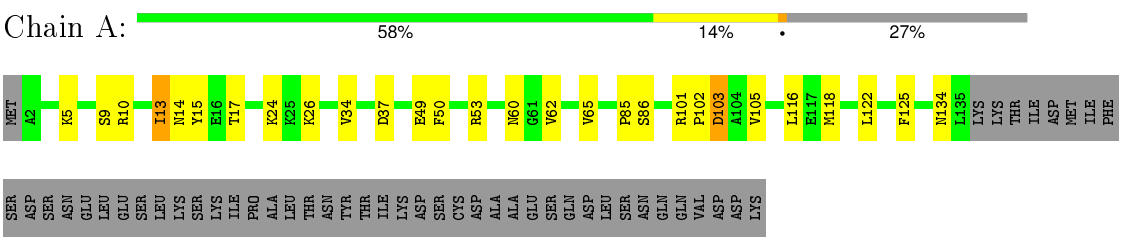
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	D	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	F	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	H	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	J	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	L	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		

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.

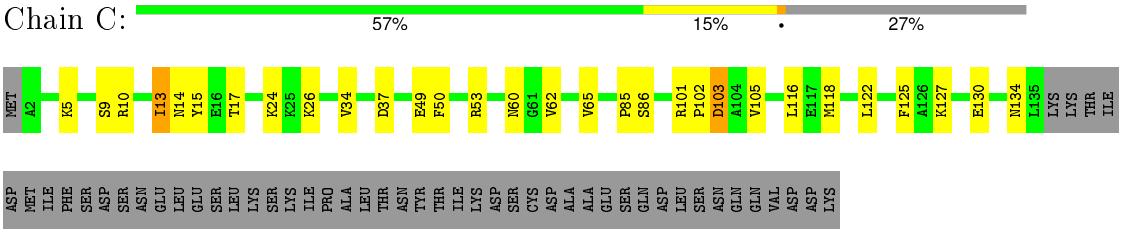
- Molecule 1: Intracellular growth locus protein A

Chain A:



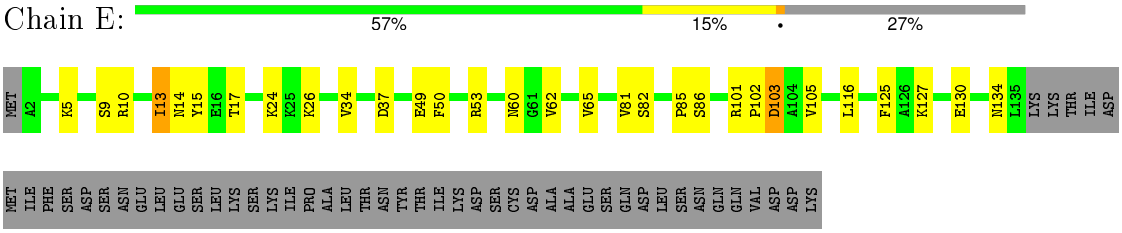
- Molecule 1: Intracellular growth locus protein A

Chain C:



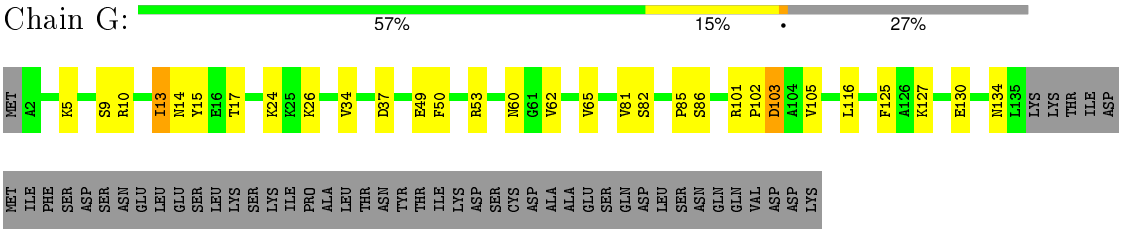
- Molecule 1: Intracellular growth locus protein A

Chain E:



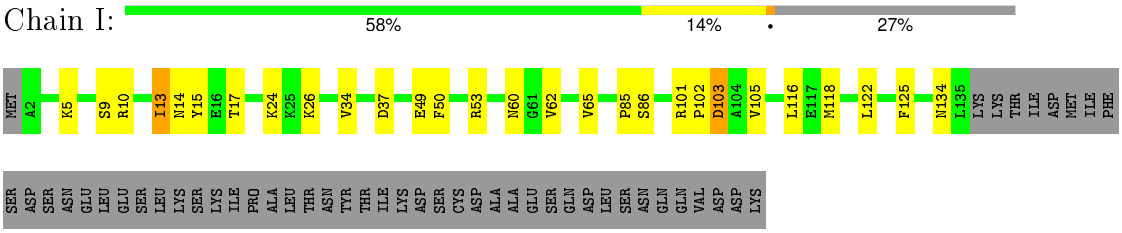
- Molecule 1: Intracellular growth locus protein A

Chain G:



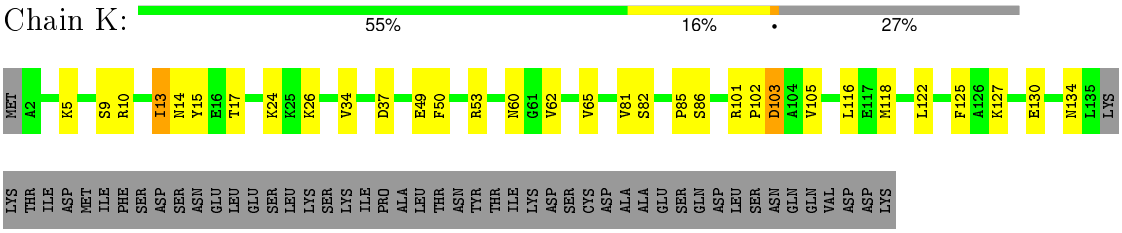
- Molecule 1: Intracellular growth locus protein A

Chain I:



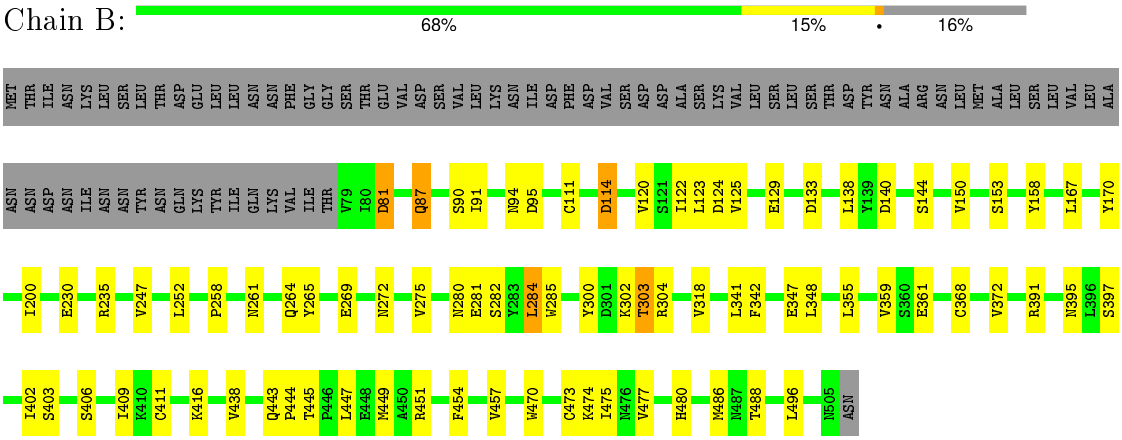
• Molecule 1: Intracellular growth locus protein A

Chain K:



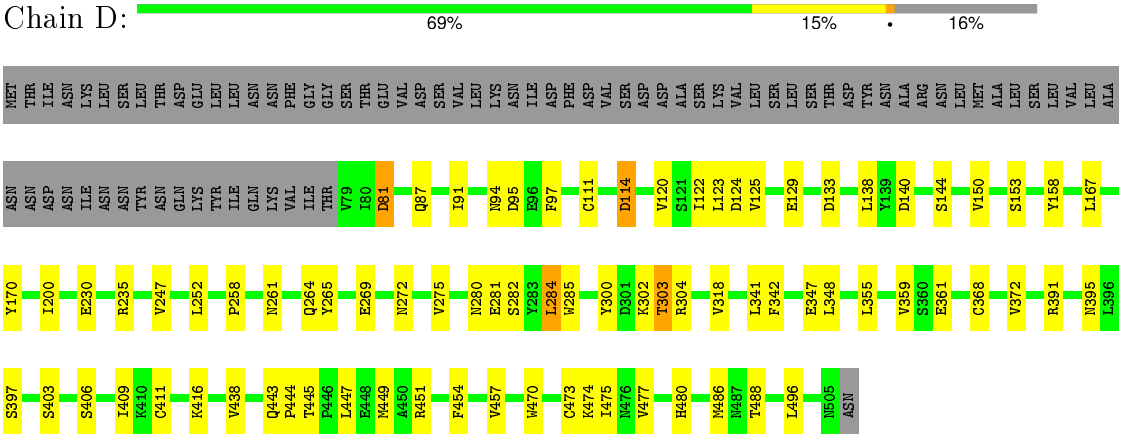
• Molecule 2: Intracellular growth locus protein B

Chain B:



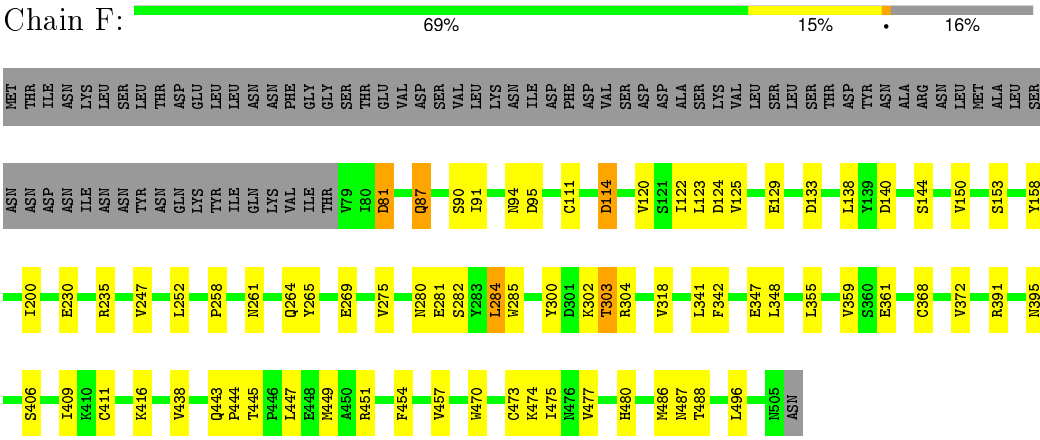
• Molecule 2: Intracellular growth locus protein B

Chain D:



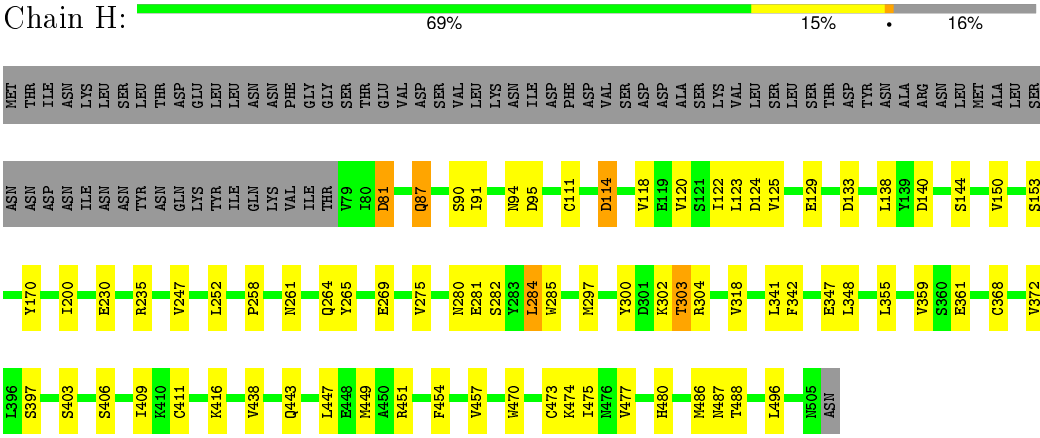
• Molecule 2: Intracellular growth locus protein B

Chain F:



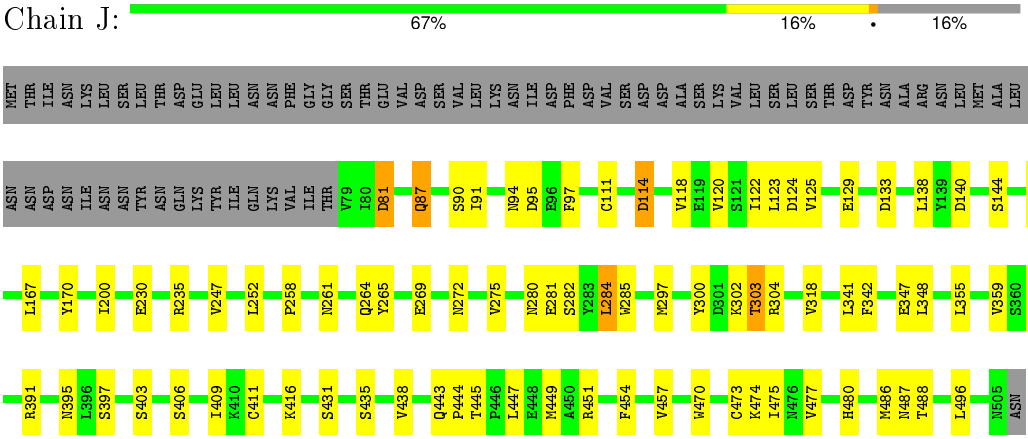
- Molecule 2: Intracellular growth locus protein B

Chain H:



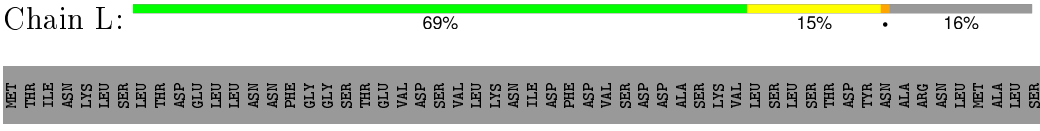
- Molecule 2: Intracellular growth locus protein B

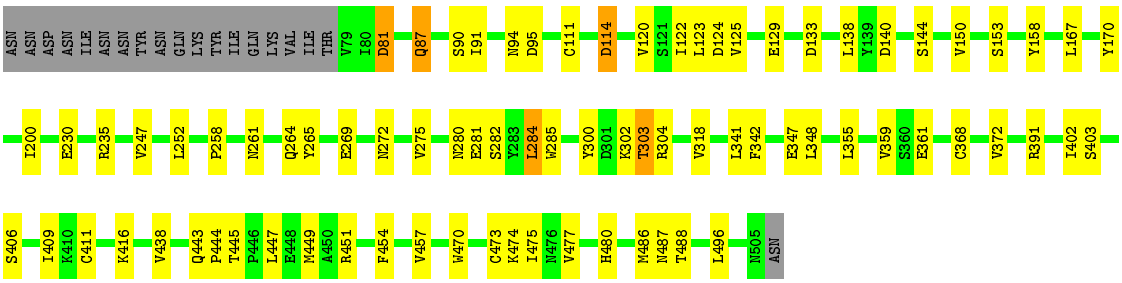
Chain J:



- Molecule 2: Intracellular growth locus protein B

Chain L:




ASN ASN ASP ASN ILE ASN ASN TYR ASN GLN LYS TYR ILE GLN LYS VAL ILE THR V79 I80 D81 Q87 S90 I91 N94 D95 C111 D114 V120 S121 I122 L123 D124 V125 E129 D133 L138 Y139 D140 S144 V150 S153 Y158 L167 Y170
I200 E230 R235 V247 L252 P258 N261 Q264 Y265 E269 N272 V275 N280 E281 S282 Y283 L284 W285 Y300 D301 K302 T303 R304 V318 L341 F342 E347 L348 L355 V359 S360 E361 C368 V372 R391 I402 S403
S406 I409 K410 C411 K416 V438 Q443 P444 T445 P446 L447 E448 M449 A450 R451 F454 V457 W470 C473 K474 I475 H476 V477 H480 M486 N487 T488 L496 N505 ASN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 (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	0.23	0/1095	0.39	0/1470
1	C	0.23	0/1095	0.38	0/1470
1	E	0.23	0/1095	0.39	0/1470
1	G	0.23	0/1095	0.38	0/1470
1	I	0.23	0/1095	0.38	0/1470
1	K	0.23	0/1095	0.38	0/1470
2	B	0.26	0/3546	0.39	0/4806
2	D	0.26	0/3546	0.39	0/4806
2	F	0.26	0/3546	0.39	0/4806
2	H	0.26	0/3546	0.39	0/4806
2	J	0.26	0/3546	0.39	0/4806
2	L	0.26	0/3546	0.39	0/4806
All	All	0.25	0/27846	0.39	0/37656

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	1081	0	1114	11	0
1	C	1081	0	1114	12	0
1	E	1081	0	1114	12	0
1	G	1081	0	1114	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1081	0	1114	11	0
1	K	1081	0	1114	14	0
2	B	3463	0	3372	35	0
2	D	3463	0	3372	34	0
2	F	3463	0	3372	34	0
2	H	3463	0	3372	34	0
2	J	3463	0	3372	38	0
2	L	3463	0	3372	35	0
All	All	27264	0	26916	258	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 5.

All (258) 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)
2:L:347:GLU:HG2	2:L:359:VAL:HG11	1.73	0.70
2:H:347:GLU:HG2	2:H:359:VAL:HG11	1.73	0.69
2:F:347:GLU:HG2	2:F:359:VAL:HG11	1.73	0.68
2:F:473:CYS:SG	2:F:474:LYS:N	2.68	0.67
2:J:473:CYS:SG	2:J:474:LYS:N	2.68	0.67
2:H:473:CYS:SG	2:H:474:LYS:N	2.68	0.67
2:L:473:CYS:SG	2:L:474:LYS:N	2.68	0.67
2:D:473:CYS:SG	2:D:474:LYS:N	2.67	0.66
2:B:473:CYS:SG	2:B:474:LYS:N	2.68	0.66
2:B:347:GLU:HG2	2:B:359:VAL:HG11	1.78	0.65
2:J:347:GLU:HG2	2:J:359:VAL:HG11	1.78	0.65
2:D:347:GLU:HG2	2:D:359:VAL:HG11	1.79	0.64
2:B:443:GLN:OE1	2:B:443:GLN:N	2.32	0.63
2:D:443:GLN:OE1	2:D:443:GLN:N	2.32	0.63
2:H:443:GLN:N	2:H:443:GLN:OE1	2.32	0.63
2:J:443:GLN:N	2:J:443:GLN:OE1	2.32	0.63
2:F:443:GLN:N	2:F:443:GLN:OE1	2.32	0.62
2:L:443:GLN:N	2:L:443:GLN:OE1	2.32	0.62
1:G:53:ARG:NH2	2:H:129:GLU:OE1	2.34	0.60
1:A:53:ARG:NH2	2:B:129:GLU:OE1	2.35	0.59
1:A:105:VAL:HG11	2:B:91:ILE:HD11	1.84	0.59
1:E:101:ARG:O	1:E:103:ASP:N	2.36	0.59
1:I:101:ARG:O	1:I:103:ASP:N	2.36	0.59
1:K:53:ARG:NH2	2:L:129:GLU:OE1	2.36	0.58
1:K:101:ARG:O	1:K:103:ASP:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:VAL:HG11	2:L:91:ILE:HD11	1.84	0.58
1:G:101:ARG:O	1:G:103:ASP:N	2.36	0.58
1:I:53:ARG:NH2	2:J:129:GLU:OE1	2.37	0.58
1:A:101:ARG:O	1:A:103:ASP:N	2.36	0.57
1:C:101:ARG:O	1:C:103:ASP:N	2.36	0.57
1:I:105:VAL:HG11	2:J:91:ILE:HD11	1.86	0.57
1:E:53:ARG:NH2	2:F:129:GLU:OE1	2.38	0.57
2:D:133:ASP:OD1	2:D:144:SER:OG	2.23	0.57
1:C:53:ARG:NH2	2:D:129:GLU:OE1	2.38	0.57
1:C:105:VAL:HG11	2:D:91:ILE:HD11	1.88	0.55
1:E:105:VAL:HG11	2:F:91:ILE:HD11	1.89	0.55
2:F:133:ASP:OD1	2:F:144:SER:OG	2.24	0.55
2:J:133:ASP:OD1	2:J:144:SER:OG	2.24	0.54
2:L:133:ASP:OD1	2:L:144:SER:OG	2.24	0.54
1:G:105:VAL:HG11	2:H:91:ILE:HD11	1.89	0.54
2:J:444:PRO:O	2:J:445:THR:OG1	2.24	0.53
2:J:264:GLN:OE1	2:J:264:GLN:N	2.43	0.52
2:L:264:GLN:OE1	2:L:264:GLN:N	2.43	0.51
2:B:264:GLN:OE1	2:B:264:GLN:N	2.43	0.51
2:H:133:ASP:OD1	2:H:144:SER:OG	2.23	0.51
2:L:122:ILE:HG22	2:L:123:LEU:N	2.26	0.51
2:D:264:GLN:N	2:D:264:GLN:OE1	2.43	0.51
2:B:122:ILE:HG22	2:B:123:LEU:N	2.26	0.51
1:G:62:VAL:HA	1:G:65:VAL:HG12	1.92	0.51
2:J:122:ILE:HG22	2:J:123:LEU:N	2.26	0.51
2:F:342:PHE:HB2	2:F:359:VAL:HG12	1.93	0.50
2:H:122:ILE:HG22	2:H:123:LEU:N	2.25	0.50
1:C:62:VAL:HA	1:C:65:VAL:HG12	1.94	0.50
2:D:403:SER:O	2:D:406:SER:OG	2.25	0.50
2:J:111:CYS:SG	2:J:120:VAL:HG21	2.51	0.50
2:L:457:VAL:HG22	2:L:477:VAL:HG12	1.93	0.50
2:F:403:SER:O	2:F:406:SER:OG	2.25	0.50
2:H:342:PHE:HB2	2:H:359:VAL:HG12	1.93	0.50
1:K:62:VAL:HA	1:K:65:VAL:HG12	1.94	0.50
1:A:62:VAL:HA	1:A:65:VAL:HG12	1.94	0.50
2:B:133:ASP:OD1	2:B:144:SER:OG	2.25	0.50
2:D:122:ILE:HG22	2:D:123:LEU:N	2.26	0.50
2:F:444:PRO:O	2:F:445:THR:OG1	2.24	0.50
2:H:281:GLU:OE2	2:H:285:TRP:NE1	2.45	0.50
2:F:122:ILE:HG22	2:F:123:LEU:N	2.26	0.50
2:F:200:ILE:HD13	2:F:355:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:ASN:OD1	2:B:397:SER:OG	2.26	0.49
1:E:62:VAL:HA	1:E:65:VAL:HG12	1.94	0.49
2:F:200:ILE:HD11	2:F:247:VAL:HG22	1.93	0.49
2:J:200:ILE:HD11	2:J:247:VAL:HG22	1.94	0.49
2:H:200:ILE:HD13	2:H:355:LEU:HD22	1.95	0.49
2:B:125:VAL:O	2:B:170:TYR:OH	2.30	0.49
1:I:62:VAL:HA	1:I:65:VAL:HG12	1.94	0.49
2:L:281:GLU:OE2	2:L:285:TRP:NE1	2.46	0.49
2:L:342:PHE:HB2	2:L:359:VAL:HG12	1.94	0.49
2:H:200:ILE:HD11	2:H:247:VAL:HG22	1.94	0.49
2:B:200:ILE:HD13	2:B:355:LEU:HD22	1.94	0.49
2:B:200:ILE:HD11	2:B:247:VAL:HG22	1.94	0.49
2:F:264:GLN:N	2:F:264:GLN:OE1	2.43	0.49
2:D:342:PHE:HB2	2:D:359:VAL:HG12	1.96	0.48
2:J:281:GLU:OE2	2:J:285:TRP:NE1	2.45	0.48
2:F:125:VAL:O	2:F:170:TYR:OH	2.31	0.48
2:B:403:SER:O	2:B:406:SER:OG	2.24	0.48
2:J:125:VAL:O	2:J:170:TYR:OH	2.30	0.48
2:B:342:PHE:HB2	2:B:359:VAL:HG12	1.95	0.48
2:D:281:GLU:OE2	2:D:285:TRP:NE1	2.45	0.48
2:J:87:GLN:O	2:J:90:SER:OG	2.19	0.48
2:H:264:GLN:N	2:H:264:GLN:OE1	2.43	0.48
2:F:281:GLU:OE2	2:F:285:TRP:NE1	2.45	0.48
2:J:342:PHE:HB2	2:J:359:VAL:HG12	1.96	0.47
2:F:111:CYS:SG	2:F:120:VAL:HG21	2.54	0.47
2:J:200:ILE:HD13	2:J:355:LEU:HD22	1.96	0.47
2:B:281:GLU:OE2	2:B:285:TRP:NE1	2.45	0.47
2:L:111:CYS:SG	2:L:120:VAL:HG21	2.55	0.47
2:H:111:CYS:SG	2:H:120:VAL:HG21	2.55	0.47
2:L:200:ILE:HD13	2:L:355:LEU:HD22	1.96	0.47
2:H:230:GLU:OE2	2:H:230:GLU:N	2.46	0.47
2:L:403:SER:O	2:L:406:SER:OG	2.25	0.47
2:D:230:GLU:N	2:D:230:GLU:OE2	2.46	0.47
2:F:87:GLN:O	2:F:90:SER:OG	2.19	0.47
2:D:444:PRO:O	2:D:445:THR:OG1	2.24	0.47
1:C:116:LEU:HD12	2:D:269:GLU:HB3	1.96	0.47
2:H:438:VAL:HG12	2:H:454:PHE:HB2	1.97	0.47
2:B:111:CYS:SG	2:B:120:VAL:HG21	2.55	0.47
2:D:200:ILE:HD13	2:D:355:LEU:HD22	1.97	0.47
2:H:125:VAL:O	2:H:170:TYR:OH	2.31	0.46
1:E:116:LEU:HD12	2:F:269:GLU:HB3	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:VAL:HG12	2:J:167:LEU:HB3	1.97	0.46
2:D:125:VAL:O	2:D:170:TYR:OH	2.31	0.46
2:J:438:VAL:HG12	2:J:454:PHE:HB2	1.96	0.46
2:H:94:ASN:OD1	2:H:95:ASP:N	2.49	0.46
2:J:258:PRO:HD3	2:J:275:VAL:HG12	1.97	0.46
1:A:34:VAL:HG12	2:B:167:LEU:HB3	1.97	0.46
2:F:230:GLU:N	2:F:230:GLU:OE2	2.46	0.46
2:H:403:SER:O	2:H:406:SER:OG	2.26	0.46
2:D:111:CYS:SG	2:D:120:VAL:HG21	2.55	0.46
1:A:9:SER:OG	1:A:10:ARG:N	2.48	0.46
2:L:87:GLN:O	2:L:90:SER:OG	2.19	0.46
2:D:438:VAL:HG12	2:D:454:PHE:HB2	1.98	0.46
2:F:438:VAL:HG12	2:F:454:PHE:HB2	1.98	0.46
2:H:347:GLU:CG	2:H:359:VAL:HG11	2.44	0.46
1:G:116:LEU:HD12	2:H:269:GLU:HB3	1.96	0.46
1:K:81:VAL:O	1:K:82:SER:OG	2.32	0.46
1:G:37:ASP:N	1:G:37:ASP:OD1	2.49	0.46
1:I:37:ASP:OD1	1:I:37:ASP:N	2.49	0.46
2:J:347:GLU:CG	2:J:359:VAL:HG11	2.45	0.46
1:I:116:LEU:HD12	2:J:269:GLU:HB3	1.97	0.46
2:D:395:ASN:OD1	2:D:397:SER:OG	2.26	0.46
2:J:94:ASN:OD1	2:J:95:ASP:N	2.49	0.46
2:D:200:ILE:HD11	2:D:247:VAL:HG22	1.98	0.46
2:J:403:SER:O	2:J:406:SER:OG	2.25	0.46
1:G:9:SER:OG	1:G:10:ARG:N	2.48	0.46
2:D:94:ASN:OD1	2:D:95:ASP:N	2.49	0.45
1:A:116:LEU:HD12	2:B:269:GLU:HB3	1.98	0.45
1:A:37:ASP:OD1	1:A:37:ASP:N	2.49	0.45
2:H:261:ASN:O	2:H:261:ASN:ND2	2.50	0.45
2:B:230:GLU:OE2	2:B:230:GLU:N	2.46	0.45
2:B:94:ASN:OD1	2:B:95:ASP:N	2.49	0.45
1:E:9:SER:OG	1:E:10:ARG:N	2.48	0.45
2:D:347:GLU:CG	2:D:359:VAL:HG11	2.46	0.45
2:L:94:ASN:OD1	2:L:95:ASP:N	2.49	0.45
2:D:261:ASN:ND2	2:D:261:ASN:O	2.50	0.45
2:F:261:ASN:ND2	2:F:261:ASN:O	2.50	0.45
1:C:37:ASP:OD1	1:C:37:ASP:N	2.49	0.45
2:F:94:ASN:OD1	2:F:95:ASP:N	2.49	0.45
1:K:116:LEU:HD12	2:L:269:GLU:HB3	1.98	0.45
2:J:230:GLU:OE2	2:J:230:GLU:N	2.46	0.45
2:L:124:ASP:OD2	2:L:124:ASP:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:NZ	1:C:130:GLU:OE2	2.37	0.45
2:B:438:VAL:HG12	2:B:454:PHE:HB2	1.98	0.45
2:B:261:ASN:O	2:B:261:ASN:ND2	2.50	0.45
1:E:34:VAL:HG12	2:F:167:LEU:HB3	1.99	0.45
2:L:125:VAL:O	2:L:170:TYR:OH	2.30	0.45
2:L:347:GLU:CG	2:L:359:VAL:HG11	2.44	0.45
2:B:473:CYS:SG	2:B:475:ILE:HG23	2.57	0.45
2:B:347:GLU:CG	2:B:359:VAL:HG11	2.45	0.45
2:B:258:PRO:HD3	2:B:275:VAL:HG12	1.98	0.45
1:I:9:SER:OG	1:I:10:ARG:N	2.49	0.45
1:K:49:GLU:N	1:K:49:GLU:OE2	2.48	0.45
2:L:258:PRO:HD3	2:L:275:VAL:HG12	1.99	0.45
2:F:303:THR:OG1	2:F:304:ARG:N	2.49	0.45
2:B:124:ASP:OD2	2:B:124:ASP:N	2.50	0.45
1:K:37:ASP:OD1	1:K:37:ASP:N	2.49	0.45
2:H:303:THR:OG1	2:H:304:ARG:N	2.50	0.45
2:F:124:ASP:OD2	2:F:124:ASP:N	2.50	0.45
2:J:261:ASN:O	2:J:261:ASN:ND2	2.50	0.45
2:H:87:GLN:O	2:H:90:SER:OG	2.20	0.45
2:L:473:CYS:SG	2:L:475:ILE:HG23	2.57	0.45
2:D:473:CYS:SG	2:D:475:ILE:HG23	2.57	0.45
1:K:34:VAL:HG12	2:L:167:LEU:HB3	1.98	0.45
1:C:118:MET:O	1:C:122:LEU:N	2.45	0.45
2:J:473:CYS:SG	2:J:475:ILE:HG23	2.57	0.44
2:H:258:PRO:HD3	2:H:275:VAL:HG12	1.97	0.44
2:L:261:ASN:O	2:L:261:ASN:ND2	2.50	0.44
2:H:473:CYS:SG	2:H:475:ILE:HG23	2.57	0.44
1:E:37:ASP:OD1	1:E:37:ASP:N	2.49	0.44
1:I:118:MET:O	1:I:122:LEU:N	2.45	0.44
2:J:124:ASP:N	2:J:124:ASP:OD2	2.50	0.44
2:J:303:THR:OG1	2:J:304:ARG:N	2.50	0.44
2:F:473:CYS:SG	2:F:475:ILE:HG23	2.57	0.44
1:C:9:SER:OG	1:C:10:ARG:N	2.48	0.44
2:L:200:ILE:HD11	2:L:247:VAL:HG22	1.98	0.44
2:H:395:ASN:OD1	2:H:397:SER:OG	2.26	0.44
2:L:438:VAL:HG12	2:L:454:PHE:HB2	1.98	0.44
2:J:81:ASP:N	2:J:81:ASP:OD2	2.51	0.44
2:F:395:ASN:OD1	2:F:397:SER:OG	2.26	0.44
1:C:34:VAL:HG12	2:D:167:LEU:HB3	1.98	0.43
2:H:81:ASP:OD2	2:H:81:ASP:N	2.52	0.43
2:F:347:GLU:CG	2:F:359:VAL:HG11	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:ASP:N	2:D:124:ASP:OD2	2.50	0.43
2:F:81:ASP:N	2:F:81:ASP:OD2	2.51	0.43
2:F:258:PRO:HD3	2:F:275:VAL:HG12	1.99	0.43
2:L:303:THR:OG1	2:L:304:ARG:N	2.50	0.43
2:L:81:ASP:N	2:L:81:ASP:OD2	2.51	0.43
2:D:303:THR:OG1	2:D:304:ARG:N	2.50	0.43
2:L:230:GLU:OE2	2:L:230:GLU:N	2.46	0.43
1:G:127:LYS:NZ	1:G:130:GLU:OE2	2.37	0.43
2:H:124:ASP:OD2	2:H:124:ASP:N	2.50	0.43
2:B:81:ASP:N	2:B:81:ASP:OD2	2.51	0.43
2:D:457:VAL:HG22	2:D:477:VAL:HG12	2.01	0.43
2:D:258:PRO:HD3	2:D:275:VAL:HG12	1.99	0.43
2:D:81:ASP:N	2:D:81:ASP:OD2	2.51	0.43
1:K:9:SER:OG	1:K:10:ARG:N	2.49	0.43
2:J:457:VAL:HG22	2:J:477:VAL:HG12	2.01	0.43
1:A:49:GLU:OE2	1:A:49:GLU:N	2.48	0.43
2:D:341:LEU:HD12	2:D:341:LEU:N	2.34	0.43
2:B:303:THR:OG1	2:B:304:ARG:N	2.50	0.43
2:H:457:VAL:HG22	2:H:477:VAL:HG12	2.01	0.43
2:H:341:LEU:HD12	2:H:341:LEU:N	2.34	0.43
2:B:444:PRO:O	2:B:445:THR:OG1	2.24	0.42
1:A:118:MET:O	1:A:122:LEU:N	2.45	0.42
1:K:118:MET:O	1:K:122:LEU:N	2.45	0.42
2:B:457:VAL:HG22	2:B:477:VAL:HG12	2.01	0.42
2:F:341:LEU:N	2:F:341:LEU:HD12	2.35	0.42
2:B:341:LEU:N	2:B:341:LEU:HD12	2.35	0.42
2:D:302:LYS:O	2:D:451:ARG:NH1	2.53	0.42
1:G:49:GLU:OE2	1:G:49:GLU:N	2.48	0.42
2:F:302:LYS:O	2:F:451:ARG:NH1	2.53	0.42
2:B:402:ILE:HG12	2:B:477:VAL:HG21	2.02	0.42
2:J:341:LEU:HD12	2:J:341:LEU:N	2.35	0.42
1:G:81:VAL:O	1:G:82:SER:OG	2.32	0.42
2:B:87:GLN:O	2:B:90:SER:OG	2.20	0.42
1:E:127:LYS:NZ	1:E:130:GLU:OE2	2.38	0.41
1:K:13:ILE:HD12	1:K:14:ASN:N	2.35	0.41
2:H:118:VAL:HG11	2:H:297:MET:HG2	2.01	0.41
1:G:13:ILE:HD12	1:G:14:ASN:N	2.35	0.41
2:J:118:VAL:HG11	2:J:297:MET:HG2	2.01	0.41
2:L:444:PRO:O	2:L:445:THR:OG1	2.24	0.41
2:L:402:ILE:HG12	2:L:477:VAL:HG21	2.03	0.41
1:E:13:ILE:HD12	1:E:14:ASN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LYS:O	2:B:451:ARG:NH1	2.53	0.41
1:A:13:ILE:HD12	1:A:14:ASN:N	2.35	0.41
2:J:302:LYS:O	2:J:451:ARG:NH1	2.53	0.41
2:H:302:LYS:O	2:H:451:ARG:NH1	2.53	0.41
2:J:431:SER:O	2:J:435:SER:OG	2.36	0.41
1:K:127:LYS:NZ	1:K:130:GLU:OE2	2.38	0.41
2:L:302:LYS:O	2:L:451:ARG:NH1	2.53	0.41
1:C:13:ILE:HD12	1:C:14:ASN:N	2.35	0.41
2:F:457:VAL:HG22	2:F:477:VAL:HG12	2.03	0.41
1:K:81:VAL:HG12	1:K:82:SER:N	2.36	0.41
1:C:49:GLU:OE2	1:C:49:GLU:N	2.48	0.41
2:F:487:ASN:N	2:F:487:ASN:OD1	2.54	0.41
2:J:95:ASP:O	2:J:97:PHE:N	2.49	0.40
1:I:13:ILE:HD12	1:I:14:ASN:N	2.35	0.40
1:I:49:GLU:N	1:I:49:GLU:OE2	2.48	0.40
2:L:341:LEU:N	2:L:341:LEU:HD12	2.35	0.40
2:L:272:ASN:OD1	2:L:272:ASN:N	2.55	0.40
2:J:395:ASN:OD1	2:J:397:SER:OG	2.28	0.40
2:D:95:ASP:O	2:D:97:PHE:N	2.49	0.40
1:E:81:VAL:HG12	1:E:82:SER:N	2.36	0.40
2:L:487:ASN:OD1	2:L:487:ASN:N	2.54	0.40
2:B:272:ASN:N	2:B:272:ASN:OD1	2.55	0.40
2:J:487:ASN:N	2:J:487:ASN:OD1	2.55	0.40
2:H:487:ASN:N	2:H:487:ASN:OD1	2.54	0.40
1:G:34:VAL:HG12	2:H:167:LEU:HB3	2.04	0.40
2:J:272:ASN:N	2:J:272:ASN:OD1	2.55	0.40
2:D:272:ASN:N	2:D:272:ASN:OD1	2.55	0.40
1:E:49:GLU:OE2	1:E:49:GLU:N	2.49	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	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	C	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26
1	E	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26
1	G	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	I	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	K	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26
2	B	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	D	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	F	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	H	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	J	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	L	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
All	All	3342/4140 (81%)	2739 (82%)	471 (14%)	132 (4%)	7	38

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	103	ASP
2	B	150	VAL
2	B	153	SER
2	B	411	CYS
1	C	60	ASN
1	C	103	ASP
2	D	150	VAL
2	D	153	SER
2	D	411	CYS
1	E	60	ASN
1	E	103	ASP
2	F	150	VAL
2	F	153	SER
2	F	411	CYS
1	G	60	ASN
1	G	103	ASP
2	H	150	VAL
2	H	153	SER
2	H	411	CYS
1	I	60	ASN
1	I	103	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	150	VAL
2	J	153	SER
2	J	411	CYS
1	K	60	ASN
1	K	103	ASP
2	L	150	VAL
2	L	153	SER
2	L	411	CYS
2	B	158	TYR
2	B	284	LEU
2	B	303	THR
2	D	158	TYR
2	D	284	LEU
2	D	303	THR
2	F	158	TYR
2	F	284	LEU
2	F	303	THR
2	H	158	TYR
2	H	284	LEU
2	H	303	THR
2	J	158	TYR
2	J	284	LEU
2	J	303	THR
2	L	158	TYR
2	L	284	LEU
2	L	303	THR
1	A	85	PRO
1	A	134	ASN
2	B	114	ASP
2	B	140	ASP
1	C	85	PRO
1	C	134	ASN
2	D	114	ASP
2	D	140	ASP
1	E	85	PRO
1	E	134	ASN
2	F	114	ASP
2	F	140	ASP
1	G	85	PRO
1	G	134	ASN
2	H	114	ASP
2	H	140	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	85	PRO
1	I	134	ASN
2	J	114	ASP
2	J	140	ASP
1	K	85	PRO
1	K	134	ASN
2	L	114	ASP
2	L	140	ASP
1	A	5	LYS
1	A	15	TYR
1	A	86	SER
1	A	102	PRO
2	B	280	ASN
2	B	282	SER
2	B	300	TYR
2	B	368	CYS
2	B	409	ILE
1	C	5	LYS
1	C	15	TYR
1	C	86	SER
1	C	102	PRO
2	D	280	ASN
2	D	282	SER
2	D	300	TYR
2	D	368	CYS
1	E	5	LYS
1	E	15	TYR
1	E	86	SER
1	E	102	PRO
2	F	280	ASN
2	F	282	SER
2	F	300	TYR
2	F	368	CYS
2	F	409	ILE
1	G	5	LYS
1	G	15	TYR
1	G	86	SER
1	G	102	PRO
2	H	280	ASN
2	H	282	SER
2	H	300	TYR
2	H	368	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	409	ILE
1	I	5	LYS
1	I	15	TYR
1	I	86	SER
1	I	102	PRO
2	J	280	ASN
2	J	282	SER
2	J	300	TYR
2	J	368	CYS
1	K	5	LYS
1	K	15	TYR
1	K	86	SER
1	K	102	PRO
2	L	280	ASN
2	L	282	SER
2	L	300	TYR
2	L	368	CYS
2	B	318	VAL
2	D	318	VAL
2	D	409	ILE
2	H	318	VAL
2	J	318	VAL
2	J	409	ILE
2	L	409	ILE
2	F	318	VAL
2	L	318	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	A	121/168 (72%)	115 (95%)	6 (5%)	30 71
1	C	121/168 (72%)	115 (95%)	6 (5%)	30 71
1	E	121/168 (72%)	115 (95%)	6 (5%)	30 71
1	G	121/168 (72%)	115 (95%)	6 (5%)	30 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	K	121/168 (72%)	115 (95%)	6 (5%)	30	71
2	B	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	D	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	F	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	H	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	J	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	L	387/460 (84%)	367 (95%)	20 (5%)	29	70
All	All	3048/3768 (81%)	2892 (95%)	156 (5%)	34	70

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	17	THR
1	A	24	LYS
1	A	26	LYS
1	A	50	PHE
1	A	125	PHE
2	B	81	ASP
2	B	87	GLN
2	B	114	ASP
2	B	138	LEU
2	B	235	ARG
2	B	252	LEU
2	B	265	TYR
2	B	284	LEU
2	B	348	LEU
2	B	361	GLU
2	B	372	VAL
2	B	391	ARG
2	B	416	LYS
2	B	447	LEU
2	B	449	MET
2	B	470	TRP
2	B	480	HIS
2	B	486	MET
2	B	488	THR
2	B	496	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	13	ILE
1	C	17	THR
1	C	24	LYS
1	C	26	LYS
1	C	50	PHE
1	C	125	PHE
2	D	81	ASP
2	D	87	GLN
2	D	114	ASP
2	D	138	LEU
2	D	235	ARG
2	D	252	LEU
2	D	265	TYR
2	D	284	LEU
2	D	348	LEU
2	D	361	GLU
2	D	372	VAL
2	D	391	ARG
2	D	416	LYS
2	D	447	LEU
2	D	449	MET
2	D	470	TRP
2	D	480	HIS
2	D	486	MET
2	D	488	THR
2	D	496	LEU
1	E	13	ILE
1	E	17	THR
1	E	24	LYS
1	E	26	LYS
1	E	50	PHE
1	E	125	PHE
2	F	81	ASP
2	F	87	GLN
2	F	114	ASP
2	F	138	LEU
2	F	235	ARG
2	F	252	LEU
2	F	265	TYR
2	F	284	LEU
2	F	348	LEU
2	F	361	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	372	VAL
2	F	391	ARG
2	F	416	LYS
2	F	447	LEU
2	F	449	MET
2	F	470	TRP
2	F	480	HIS
2	F	486	MET
2	F	488	THR
2	F	496	LEU
1	G	13	ILE
1	G	17	THR
1	G	24	LYS
1	G	26	LYS
1	G	50	PHE
1	G	125	PHE
2	H	81	ASP
2	H	87	GLN
2	H	114	ASP
2	H	138	LEU
2	H	235	ARG
2	H	252	LEU
2	H	265	TYR
2	H	284	LEU
2	H	348	LEU
2	H	361	GLU
2	H	372	VAL
2	H	391	ARG
2	H	416	LYS
2	H	447	LEU
2	H	449	MET
2	H	470	TRP
2	H	480	HIS
2	H	486	MET
2	H	488	THR
2	H	496	LEU
1	I	13	ILE
1	I	17	THR
1	I	24	LYS
1	I	26	LYS
1	I	50	PHE
1	I	125	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	81	ASP
2	J	87	GLN
2	J	114	ASP
2	J	138	LEU
2	J	235	ARG
2	J	252	LEU
2	J	265	TYR
2	J	284	LEU
2	J	348	LEU
2	J	361	GLU
2	J	372	VAL
2	J	391	ARG
2	J	416	LYS
2	J	447	LEU
2	J	449	MET
2	J	470	TRP
2	J	480	HIS
2	J	486	MET
2	J	488	THR
2	J	496	LEU
1	K	13	ILE
1	K	17	THR
1	K	24	LYS
1	K	26	LYS
1	K	50	PHE
1	K	125	PHE
2	L	81	ASP
2	L	87	GLN
2	L	114	ASP
2	L	138	LEU
2	L	235	ARG
2	L	252	LEU
2	L	265	TYR
2	L	284	LEU
2	L	348	LEU
2	L	361	GLU
2	L	372	VAL
2	L	391	ARG
2	L	416	LYS
2	L	447	LEU
2	L	449	MET
2	L	470	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	480	HIS
2	L	486	MET
2	L	488	THR
2	L	496	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	291	HIS
2	D	291	HIS
2	F	291	HIS
2	H	291	HIS
2	J	291	HIS
2	L	291	HIS

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.