



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 23, 2017 – 07:49 PM EDT

PDB ID : 5LJO
EMDB ID: : EMD-4061
Title : E. coli BAM complex (BamABCDE) by cryoEM
Authors : Iadanza, M.G.; Ranson, N.A.; Radford, S.E.; Higgins, A.J.; Schffrin, B.; Calabrese, A.N.; Ashcroft, A.E.; Brockwell, D.J.
Deposited on : unknown
Resolution : 4.90 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

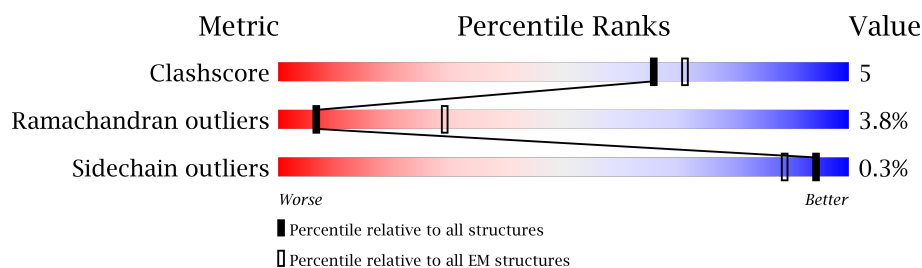
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	371	
2	C	165	
3	D	218	
4	E	87	
5	A	783	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24947 atoms, of which 12255 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 Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	371	Total	C	H	N	O	S	0	0
			5534	1754	2739	478	557	6		

- Molecule 2 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	165	Total	C	H	N	O	S	0	0
			2498	784	1241	223	248	2		

- Molecule 3 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	218	Total	C	H	N	O	S	0	0
			3461	1109	1700	309	336	7		

- Molecule 4 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	87	Total	C	H	N	O	S	0	0
			1352	432	667	119	132	2		

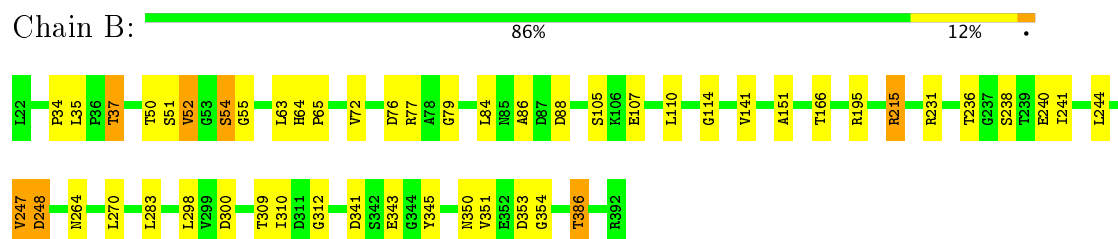
- Molecule 5 is a protein called Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	783	Total	C	H	N	O	S	0	0
			12102	3907	5908	1043	1228	16		

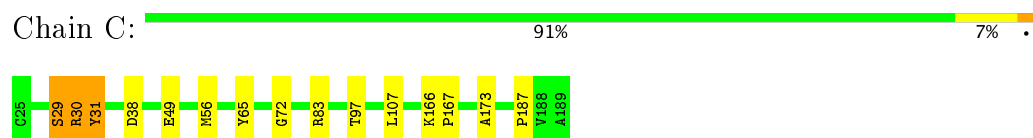
3 Residue-property plots

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.

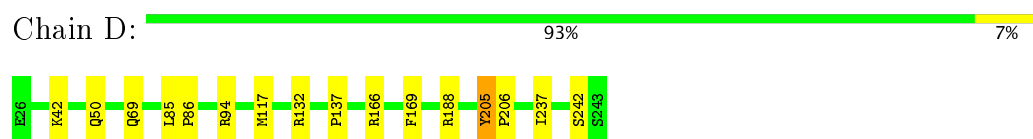
- Molecule 1: Outer membrane protein assembly factor BamB



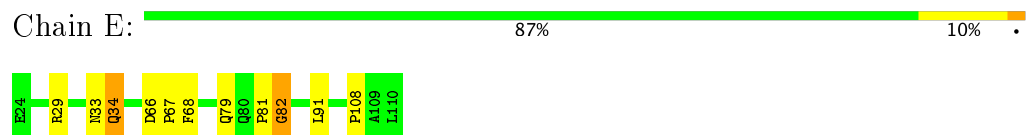
- Molecule 2: Outer membrane protein assembly factor BamC



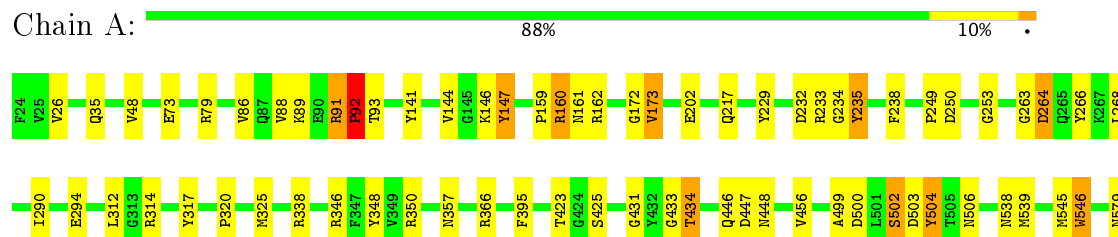
- Molecule 3: Outer membrane protein assembly factor BamD



- Molecule 4: Outer membrane protein assembly factor BamE



- Molecule 5: Outer membrane protein assembly factor BamA





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	95878	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	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	B	0.79	0/2846	0.82	3/3881 (0.1%)
2	C	0.69	0/1281	0.77	0/1748
3	D	0.78	0/1801	0.81	5/2447 (0.2%)
4	E	0.72	0/700	0.81	0/955
5	A	0.80	0/6337	0.83	9/8598 (0.1%)
All	All	0.78	0/12965	0.82	17/17629 (0.1%)

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	B	0	4
2	C	0	2
5	A	0	4
All	All	0	10

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	348	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	B	195	ARG	NE-CZ-NH2	-8.33	116.14	120.30
5	A	366	ARG	NE-CZ-NH2	-6.33	117.13	120.30
5	A	346	ARG	NE-CZ-NH1	6.03	123.32	120.30
3	D	166	ARG	NE-CZ-NH2	-5.64	117.48	120.30
5	A	235	TYR	CB-CG-CD2	-5.64	117.61	121.00
5	A	162	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	345	TYR	CB-CG-CD1	-5.49	117.70	121.00
5	A	637	TYR	CB-CG-CD1	-5.37	117.78	121.00
5	A	348	TYR	CB-CG-CD2	5.35	124.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	314	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	D	94	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	D	188	ARG	NE-CZ-NH2	-5.29	117.66	120.30
5	A	141	TYR	CB-CG-CD2	-5.21	117.87	121.00
3	D	205	TYR	CB-CG-CD1	-5.16	117.90	121.00
3	D	132	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	215	ARG	NE-CZ-NH2	-5.11	117.74	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	431	GLY	Mainchain,Peptide
5	A	92	PRO	Mainchain,Peptide
1	B	353	ASP	Mainchain,Peptide
1	B	54	SER	Mainchain,Peptide
2	C	72	GLY	Mainchain,Peptide

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	B	2795	2739	2738	31	0
2	C	1257	1241	1240	13	0
3	D	1761	1700	1699	8	0
4	E	685	667	666	8	0
5	A	6194	5908	5907	57	0
All	All	12692	12255	12250	116	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 (116) 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:B:50:THR:O	1:B:50:THR:HG23	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:PHE:CD1	3:D:169:PHE:O	2.33	0.81
5:A:586:PHE:CD2	5:A:586:PHE:O	2.37	0.77
1:B:50:THR:O	1:B:50:THR:CG2	2.31	0.77
5:A:586:PHE:CD2	5:A:586:PHE:C	2.64	0.69
1:B:76:ASP:C	1:B:76:ASP:OD1	2.30	0.68
1:B:343:GLU:N	1:B:343:GLU:OE2	2.26	0.67
3:D:69:GLN:OE1	3:D:69:GLN:N	2.29	0.66
4:E:79:GLN:O	4:E:79:GLN:OE1	2.15	0.64
5:A:217:GLN:OE1	5:A:217:GLN:N	2.31	0.61
2:C:83:ARG:O	2:C:83:ARG:HG3	2.00	0.60
1:B:51:SER:O	1:B:386:THR:OG1	2.20	0.60
5:A:586:PHE:C	5:A:586:PHE:HD2	2.03	0.60
4:E:68:PHE:CD1	4:E:68:PHE:C	2.75	0.59
1:B:35:LEU:HD23	1:B:35:LEU:O	2.02	0.59
1:B:37:THR:O	1:B:37:THR:HG22	2.02	0.58
3:D:169:PHE:CD1	3:D:169:PHE:C	2.70	0.57
1:B:270:LEU:C	1:B:270:LEU:HD12	2.25	0.57
1:B:247:VAL:HG12	1:B:248:ASP:H	1.69	0.57
5:A:661:ARG:H	5:A:661:ARG:HD2	1.70	0.56
4:E:68:PHE:O	4:E:68:PHE:HD1	1.89	0.56
1:B:309:THR:OG1	1:B:312:GLY:O	2.25	0.54
1:B:76:ASP:O	1:B:76:ASP:OD1	2.26	0.54
4:E:68:PHE:O	4:E:68:PHE:CD1	2.60	0.54
5:A:91:ARG:N	5:A:92:PRO:CD	2.71	0.54
5:A:506:ASN:C	5:A:506:ASN:OD1	2.45	0.53
1:B:310:ILE:HD12	1:B:310:ILE:C	2.31	0.51
1:B:35:LEU:C	1:B:35:LEU:HD23	2.31	0.50
1:B:298:LEU:HD12	1:B:298:LEU:C	2.32	0.50
1:B:244:LEU:HD23	1:B:244:LEU:C	2.32	0.50
4:E:91:LEU:C	4:E:91:LEU:HD23	2.32	0.50
1:B:270:LEU:O	1:B:270:LEU:HD12	2.11	0.50
5:A:503:ASP:O	5:A:504:TYR:HB3	2.12	0.49
5:A:395:PHE:CD2	5:A:395:PHE:N	2.78	0.49
5:A:86:VAL:HG12	5:A:88:VAL:HG23	1.96	0.48
5:A:92:PRO:HB3	5:A:93:THR:HA	1.96	0.48
1:B:247:VAL:HG12	1:B:248:ASP:N	2.28	0.48
1:B:64:HIS:HB2	1:B:65:PRO:HD2	1.97	0.47
5:A:325:MET:N	5:A:338:ARG:O	2.47	0.47
5:A:704:ASP:O	5:A:706:VAL:N	2.47	0.47
1:B:350:ASN:HB3	1:B:354:GLY:H	1.79	0.47
1:B:244:LEU:HD23	1:B:244:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:TYR:O	3:D:205:TYR:CD2	2.68	0.47
5:A:546:TRP:CE3	5:A:546:TRP:HA	2.49	0.47
2:C:38:ASP:OD1	2:C:38:ASP:C	2.53	0.47
5:A:48:VAL:HG23	5:A:48:VAL:O	2.15	0.46
5:A:290:ILE:C	5:A:290:ILE:HD12	2.36	0.46
4:E:33:ASN:O	4:E:34:GLN:HB2	2.16	0.46
2:C:49:GLU:HG2	2:C:49:GLU:O	2.16	0.46
5:A:229:TYR:CD2	5:A:229:TYR:C	2.89	0.46
2:C:29:SER:O	2:C:30:ARG:HB2	2.15	0.46
5:A:232:ASP:OD1	5:A:232:ASP:C	2.54	0.46
5:A:446:GLN:HB2	5:A:456:VAL:HB	1.97	0.46
5:A:579:ASN:C	5:A:579:ASN:OD1	2.53	0.46
5:A:504:TYR:CD2	5:A:504:TYR:O	2.69	0.45
1:B:35:LEU:CD2	1:B:35:LEU:O	2.65	0.45
2:C:30:ARG:O	2:C:31:TYR:HB3	2.16	0.45
5:A:741:MET:SD	5:A:741:MET:N	2.89	0.45
1:B:51:SER:O	1:B:52:VAL:HB	2.17	0.45
2:C:65:TYR:CD1	2:C:65:TYR:N	2.84	0.45
2:C:30:ARG:O	2:C:31:TYR:CB	2.65	0.45
5:A:235:TYR:HB3	5:A:238:PHE:HB2	1.98	0.45
5:A:433:GLY:O	5:A:434:THR:CB	2.65	0.45
1:B:72:VAL:HB	1:B:84:LEU:HB2	1.98	0.45
2:C:83:ARG:O	2:C:83:ARG:CG	2.66	0.44
4:E:66:ASP:OD1	4:E:66:ASP:C	2.56	0.44
5:A:144:VAL:O	5:A:144:VAL:HG12	2.17	0.44
5:A:263:GLY:O	5:A:264:ASP:CB	2.66	0.44
1:B:215:ARG:HG2	1:B:231:ARG:HA	1.99	0.44
1:B:54:SER:HA	1:B:55:GLY:HA3	1.79	0.44
5:A:268:LEU:N	5:A:294:GLU:O	2.48	0.44
1:B:264:ASN:OD1	1:B:264:ASN:C	2.57	0.44
4:E:29:ARG:HB3	4:E:82:GLY:HA2	1.99	0.44
5:A:92:PRO:CB	5:A:93:THR:HA	2.48	0.44
5:A:539:MET:HB3	5:A:545:MET:SD	2.58	0.43
5:A:229:TYR:O	5:A:233:ARG:HG2	2.18	0.43
5:A:586:PHE:CG	5:A:586:PHE:O	2.64	0.43
3:D:42:LYS:HD3	3:D:50:GLN:HB3	2.00	0.43
5:A:266:TYR:CD1	5:A:266:TYR:N	2.86	0.43
5:A:661:ARG:N	5:A:661:ARG:HD2	2.34	0.43
1:B:151:ALA:HA	1:B:166:THR:HA	2.01	0.43
3:D:117:MET:C	3:D:117:MET:SD	2.97	0.43
5:A:423:THR:HB	5:A:447:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:OD1	1:B:341:ASP:C	2.57	0.42
1:B:236:THR:HA	1:B:240:GLU:HA	2.01	0.42
5:A:675:PHE:HB3	5:A:676:PRO:HD2	2.01	0.42
5:A:447:ASP:O	5:A:448:ASN:HB3	2.19	0.42
5:A:73:GLU:N	5:A:89:LYS:O	2.52	0.42
2:C:107:LEU:HD12	2:C:107:LEU:N	2.35	0.42
3:D:85:LEU:HB2	3:D:86:PRO:HD3	2.02	0.42
5:A:312:LEU:HB3	5:A:317:TYR:HB2	2.02	0.42
5:A:144:VAL:O	5:A:144:VAL:CG1	2.68	0.42
5:A:546:TRP:HE3	5:A:546:TRP:HA	1.83	0.42
5:A:395:PHE:CD2	5:A:395:PHE:O	2.73	0.41
5:A:159:PRO:O	5:A:160:ARG:HB2	2.20	0.41
5:A:266:TYR:HD1	5:A:266:TYR:N	2.18	0.41
5:A:26:VAL:O	5:A:26:VAL:HG13	2.19	0.41
5:A:585:TYR:O	5:A:586:PHE:HB2	2.21	0.41
5:A:395:PHE:CG	5:A:395:PHE:O	2.67	0.41
5:A:697:LYS:O	5:A:698:ASP:HB2	2.19	0.41
2:C:166:LYS:HB2	2:C:173:ALA:HB3	2.03	0.41
5:A:172:GLY:O	5:A:173:VAL:HB	2.19	0.41
5:A:357:ASN:C	5:A:357:ASN:OD1	2.58	0.41
2:C:56:MET:SD	3:D:237:ILE:HG13	2.61	0.41
2:C:31:TYR:O	2:C:31:TYR:CG	2.73	0.41
5:A:502:SER:HA	5:A:538:ASN:HB3	2.03	0.41
5:A:757:TYR:HB3	5:A:758:PRO:HD2	2.01	0.41
5:A:759:ASP:C	5:A:759:ASP:OD1	2.59	0.41
1:B:63:LEU:HA	1:B:114:GLY:HA2	2.02	0.41
5:A:146:LYS:O	5:A:147:TYR:HB2	2.21	0.40
5:A:686:TYR:O	5:A:687:ASP:HB2	2.21	0.40
2:C:107:LEU:HG	2:C:173:ALA:HA	2.03	0.40
5:A:585:TYR:C	5:A:585:TYR:CD1	2.94	0.40
5:A:690:CYS:O	5:A:691:ALA:HB3	2.21	0.40
1:B:77:ARG:O	1:B:110:LEU:N	2.52	0.40
5:A:234:GLY:O	5:A:266:TYR:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	369/371 (100%)	313 (85%)	39 (11%)	17 (5%)	3	29
2	C	163/165 (99%)	138 (85%)	19 (12%)	6 (4%)	4	34
3	D	216/218 (99%)	208 (96%)	5 (2%)	3 (1%)	13	54
4	E	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	2	23
5	A	781/783 (100%)	674 (86%)	76 (10%)	31 (4%)	3	32
All	All	1614/1624 (99%)	1401 (87%)	151 (9%)	62 (4%)	7	33

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	PRO
1	B	247	VAL
1	B	386	THR
2	C	30	ARG
2	C	31	TYR
4	E	34	GLN
5	A	35	GLN
5	A	160	ARG
5	A	173	VAL
5	A	250	ASP
5	A	434	THR
5	A	500	ASP
5	A	582	ASP
5	A	586	PHE
5	A	682	TYR
5	A	698	ASP
5	A	705	ALA
1	B	37	THR
1	B	52	VAL
1	B	88	ASP
1	B	248	ASP

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Mol	Chain	Res	Type
1	B	351	VAL
2	C	97	THR
4	E	67	PRO
4	E	82	GLY
5	A	147	TYR
5	A	161	ASN
5	A	264	ASP
5	A	651	ASN
5	A	676	PRO
5	A	687	ASP
5	A	790	PRO
1	B	105	SER
2	C	167	PRO
3	D	206	PRO
5	A	249	PRO
5	A	253	GLY
5	A	502	SER
5	A	504	TYR
5	A	686	TYR
1	B	86	ALA
1	B	107	GLU
1	B	300	ASP
2	C	29	SER
2	C	187	PRO
4	E	81	PRO
4	E	108	PRO
5	A	202	GLU
5	A	320	PRO
5	A	350	ARG
5	A	499	ALA
5	A	585	TYR
1	B	238	SER
1	B	241	ILE
3	D	242	SER
5	A	425	SER
1	B	283	LEU
5	A	92	PRO
1	B	141	VAL
3	D	137	PRO
1	B	79	GLY
5	A	91	ARG

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	B	302/302 (100%)	302 (100%)	0	100	100
2	C	133/133 (100%)	133 (100%)	0	100	100
3	D	183/183 (100%)	183 (100%)	0	100	100
4	E	76/76 (100%)	76 (100%)	0	100	100
5	A	668/668 (100%)	664 (99%)	4 (1%)	89	94
All	All	1362/1362 (100%)	1358 (100%)	4 (0%)	94	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	79	ARG
5	A	546	TRP
5	A	586	PHE
5	A	661	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
4	E	89	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 [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.