



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 5, 2017 – 01:11 AM EST

PDB ID : 5MBV
EMDB ID: : EMD-3460
Title : Cryo-EM structure of Lambda Phage protein GamS bound to RecBCD
Authors : Wilkinson, M.; Chaban, Y.; Wigley, D.B.
Deposited on : 2016-11-08
Resolution : 3.80 Å(reported)
Based on PDB ID : 5LD2, 2UUZ

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
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) : rb-20028442

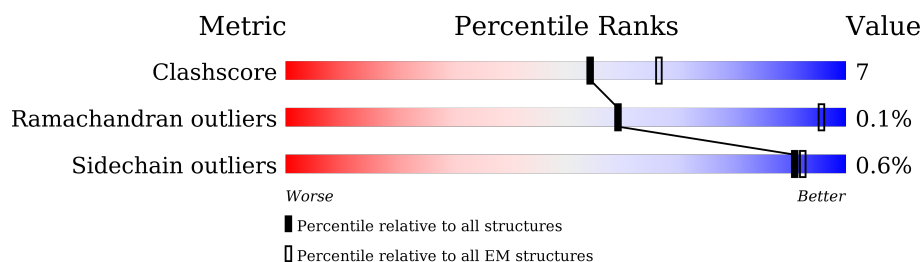
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	1181	
2	C	1122	
3	D	609	
4	A	98	
4	E	98	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24118 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 RecBCD enzyme subunit RecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1127	Total	C	N	O	S	0	0
			9037	5704	1601	1694	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P08394

- Molecule 2 is a protein called RecBCD enzyme subunit RecC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0
			9078	5783	1568	1684	43		

- Molecule 3 is a protein called RecBCD enzyme subunit RecD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	593	Total	C	N	O	S	0	0
			4570	2854	840	856	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P04993
D	1	GLY	-	expression tag	UNP P04993

- Molecule 4 is a protein called Host-nuclease inhibitor protein gam.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	98	Total	C	N	O	S	0	0
			817	505	147	160	5		
4	E	75	Total	C	N	O	S	0	0
			616	379	111	122	4		

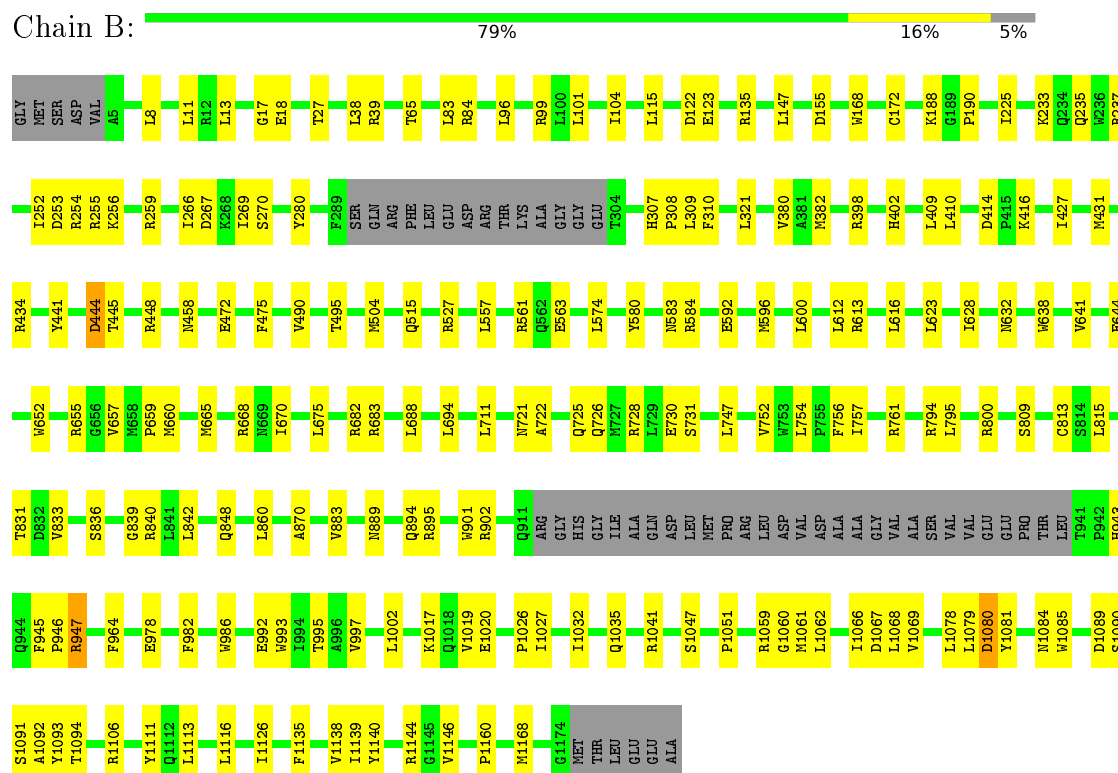
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ILE	LEU	engineered mutation	UNP P03702
E	79	ILE	LEU	engineered mutation	UNP P03702

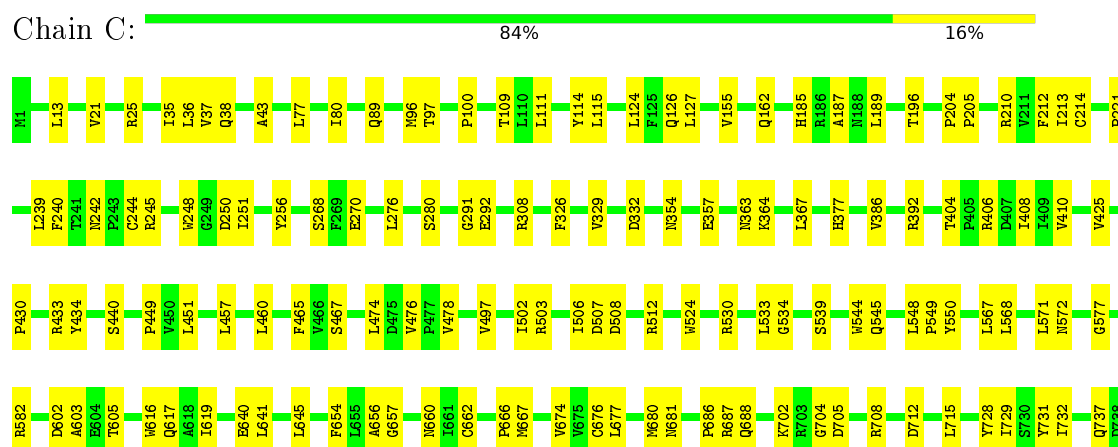
3 Residue-property plots

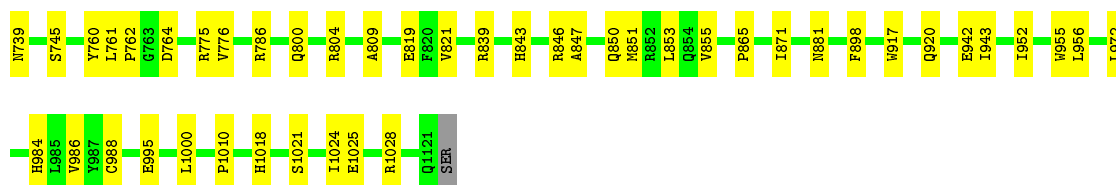
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: RecBCD enzyme subunit RecB



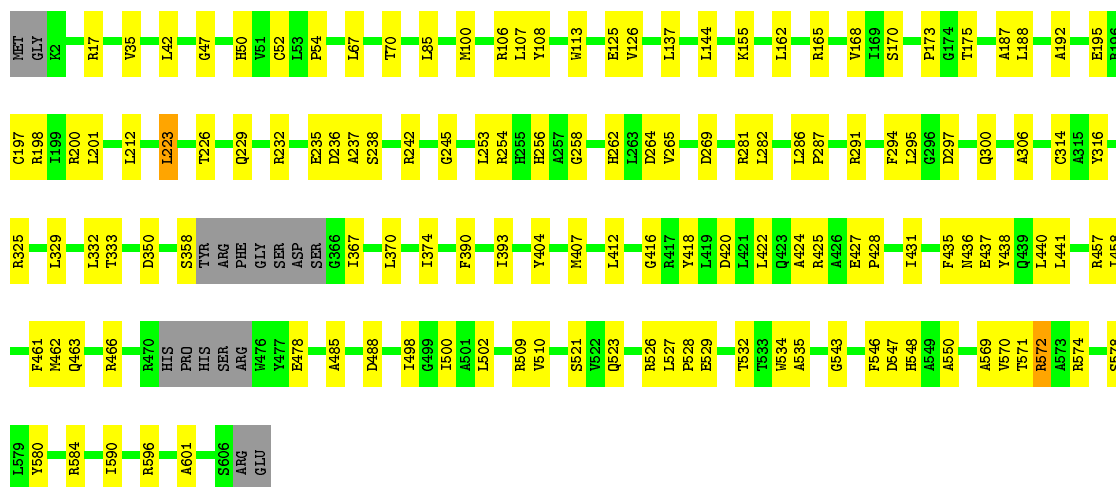
• Molecule 2: RecBCD enzyme subunit RecC





• Molecule 3: RecBCD enzyme subunit RecD

Chain D: 76% 22%



• Molecule 4: Host-nuclease inhibitor protein gam

Chain A: 89% 11%



• Molecule 4: Host-nuclease inhibitor protein gam

Chain E: 70% 6% 23%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	122796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	37313	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.23	0/9231	0.39	1/12521 (0.0%)
2	C	0.23	0/9305	0.39	0/12644
3	D	0.24	0/4643	0.41	0/6287
4	A	0.22	0/833	0.32	0/1120
4	E	0.22	0/626	0.33	0/839
All	All	0.23	0/24638	0.39	1/33411 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1080	ASP	CB-CG-OD2	5.14	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

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	B	9037	0	8887	119	0
2	C	9078	0	8877	115	0
3	D	4570	0	4614	85	0
4	A	817	0	764	11	0
4	E	616	0	583	6	0
All	All	24118	0	23725	315	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 (315) 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:C:37:VAL:HG21	2:C:43:ALA:HB2	1.62	0.81
2:C:503:ARG:HE	2:C:865:PRO:HG2	1.48	0.77
1:B:252:ILE:HG23	1:B:254:ARG:H	1.52	0.75
3:D:144:LEU:HD22	3:D:223:LEU:HD11	1.70	0.72
2:C:539:SER:HA	2:C:549:PRO:HG2	1.72	0.72
1:B:580:TYR:O	1:B:583:ASN:ND2	2.22	0.71
1:B:8:LEU:HB2	1:B:441:TYR:HB3	1.74	0.70
1:B:1080:ASP:OD1	1:B:1081:TYR:N	2.26	0.68
3:D:509:ARG:HE	3:D:521:SER:HB2	1.59	0.68
1:B:978:GLU:O	2:C:617:GLN:NE2	2.26	0.67
3:D:428:PRO:HG3	3:D:502:LEU:HD11	1.76	0.67
1:B:1002:LEU:HD23	1:B:1139:ILE:HD13	1.76	0.67
2:C:955:TRP:HE1	3:D:262:HIS:HB3	1.59	0.67
1:B:616:LEU:HD11	1:B:641:VAL:HG11	1.76	0.66
2:C:676:CYS:HA	2:C:728:TYR:HB3	1.78	0.66
2:C:276:LEU:HB2	2:C:280:SER:HB3	1.78	0.65
3:D:52:CYS:HA	3:D:108:TYR:HB3	1.79	0.64
2:C:654:PHE:O	2:C:660:ASN:ND2	2.31	0.64
4:E:79:ILE:HG23	4:E:83:LEU:HD23	1.80	0.64
2:C:548:LEU:HD12	2:C:549:PRO:HD2	1.79	0.63
3:D:165:ARG:NH2	3:D:287:PRO:O	2.31	0.63
3:D:173:PRO:HG2	3:D:571:THR:HB	1.80	0.63
2:C:680:MET:HB2	2:C:731:TYR:HB3	1.80	0.63
2:C:533:LEU:HG	2:C:549:PRO:HB3	1.80	0.62
2:C:972:LEU:HA	2:C:1000:LEU:HD22	1.83	0.61
3:D:523:GLN:HB2	3:D:526:ARG:HG3	1.83	0.61
1:B:235:GLN:HB3	1:B:309:LEU:HD22	1.83	0.60
2:C:248:TRP:O	2:C:308:ARG:NH1	2.34	0.60
1:B:1032:ILE:HG22	1:B:1035:GLN:H	1.65	0.60
1:B:628:ILE:O	1:B:632:ASN:ND2	2.35	0.59
1:B:616:LEU:HB3	1:B:623:LEU:HD12	1.83	0.59
1:B:101:LEU:HD23	1:B:104:ILE:HD12	1.83	0.59
2:C:687:ARG:HD2	2:C:708:ARG:HH21	1.68	0.59
2:C:497:VAL:HG13	2:C:502:ILE:HB	1.85	0.59
2:C:13:LEU:HB3	2:C:239:LEU:HD22	1.85	0.57
1:B:307:HIS:HD2	1:B:309:LEU:HG	1.70	0.57
2:C:250:ASP:OD1	2:C:308:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:488:ASP:HB2	3:D:528:PRO:HG3	1.85	0.57
3:D:547:ASP:HA	3:D:574:ARG:HB2	1.87	0.57
1:B:17:GLY:O	1:B:409:LEU:N	2.36	0.57
1:B:237:ARG:HH11	1:B:267:ASP:HA	1.69	0.57
3:D:137:LEU:HD21	3:D:162:LEU:HD13	1.87	0.57
3:D:245:GLY:HA3	3:D:254:ARG:HG2	1.86	0.57
1:B:584:ARG:HH12	4:A:49:ARG:HA	1.70	0.57
1:B:515:GLN:HE22	4:A:59:TYR:HE1	1.53	0.57
1:B:1019:VAL:HG12	1:B:1020:GLU:HG2	1.86	0.57
1:B:255:ARG:O	1:B:280:TYR:OH	2.23	0.57
2:C:36:LEU:HD12	2:C:213:ILE:HG12	1.86	0.57
1:B:694:LEU:HD21	1:B:711:LEU:HD13	1.87	0.56
3:D:42:LEU:HD11	3:D:108:TYR:HA	1.87	0.56
2:C:357:GLU:OE2	2:C:363:ASN:ND2	2.38	0.56
2:C:881:ASN:OD1	2:C:920:GLN:NE2	2.38	0.56
2:C:80:ILE:HD13	2:C:189:LEU:HD21	1.88	0.56
1:B:557:LEU:HD13	1:B:752:VAL:HG13	1.86	0.56
2:C:508:ASP:OD2	2:C:512:ARG:NH1	2.38	0.56
2:C:524:TRP:HB3	2:C:568:LEU:HD13	1.88	0.56
1:B:1051:PRO:O	1:B:1106:ARG:NH1	2.39	0.56
3:D:550:ALA:HB1	3:D:580:TYR:HE2	1.71	0.56
3:D:316:TYR:OH	3:D:601:ALA:O	2.22	0.55
2:C:577:GLY:O	2:C:582:ARG:NH2	2.38	0.55
1:B:613:ARG:HB2	1:B:638:TRP:HH2	1.71	0.55
3:D:485:ALA:HB3	3:D:529:GLU:HB3	1.89	0.55
1:B:414:ASP:OD1	1:B:416:LYS:NZ	2.30	0.55
3:D:463:GLN:O	3:D:466:ARG:NH1	2.40	0.54
1:B:946:PRO:O	1:B:1144:ARG:NH2	2.41	0.54
1:B:1111:TYR:HB2	1:B:1138:VAL:HG11	1.90	0.54
2:C:478:VAL:HG21	2:C:605:THR:HG21	1.90	0.54
1:B:188:LYS:HB3	2:C:871:ILE:HG21	1.89	0.54
2:C:292:GLU:HB3	2:C:308:ARG:HH12	1.72	0.54
2:C:111:LEU:HD21	2:C:127:LEU:HD21	1.90	0.53
1:B:761:ARG:O	1:B:794:ARG:NE	2.27	0.53
2:C:332:ASP:N	2:C:332:ASP:OD1	2.41	0.53
3:D:188:LEU:HD11	3:D:265:VAL:HG11	1.89	0.53
3:D:256:HIS:CD2	3:D:258:GLY:H	2.26	0.53
3:D:510:VAL:HG11	3:D:527:LEU:HD11	1.89	0.53
1:B:135:ARG:NH1	2:C:688:GLN:OE1	2.42	0.53
1:B:945:PHE:O	1:B:947:ARG:NH1	2.41	0.53
3:D:297:ASP:HB3	3:D:300:GLN:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HG13	1:B:270:SER:H	1.74	0.53
1:B:561:ARG:HG3	1:B:580:TYR:HE2	1.74	0.53
2:C:677:LEU:HD12	2:C:729:ILE:HG12	1.89	0.53
3:D:269:ASP:HA	3:D:295:LEU:HB2	1.89	0.52
1:B:1135:PHE:HE2	1:B:1160:PRO:HD2	1.75	0.52
2:C:686:PRO:HB3	2:C:712:ASP:HB2	1.91	0.52
1:B:795:LEU:HD21	1:B:840:ARG:HD2	1.91	0.52
3:D:67:LEU:O	3:D:70:THR:OG1	2.17	0.52
3:D:197:CYS:HB2	3:D:232:ARG:HD3	1.90	0.52
3:D:175:THR:HA	3:D:358:SER:HA	1.92	0.52
3:D:144:LEU:HD11	3:D:187:ALA:HB2	1.91	0.52
4:A:79:ILE:HA	4:A:83:LEU:HD12	1.91	0.51
1:B:889:ASN:O	2:C:800:GLN:NE2	2.43	0.51
1:B:728:ARG:O	2:C:786:ARG:NH1	2.43	0.51
3:D:265:VAL:HG12	3:D:291:ARG:HB2	1.92	0.51
2:C:602:ASP:OD1	2:C:603:ALA:N	2.39	0.51
1:B:1066:ILE:HG21	1:B:1069:VAL:HG23	1.92	0.51
2:C:530:ARG:HG2	2:C:550:TYR:HB2	1.92	0.51
2:C:89:GLN:OE1	2:C:89:GLN:N	2.43	0.51
1:B:225:ILE:HG21	1:B:321:LEU:HB3	1.93	0.51
3:D:532:THR:HG23	3:D:534:TRP:HD1	1.75	0.51
1:B:527:ARG:HD3	1:B:574:LEU:HD13	1.93	0.51
1:B:382:MET:HG2	1:B:410:LEU:HD12	1.92	0.50
1:B:252:ILE:HG13	1:B:253:ASP:H	1.75	0.50
2:C:952:ILE:HD11	2:C:1024:ILE:HD11	1.92	0.50
1:B:11:LEU:HD13	1:B:99:ARG:HH12	1.77	0.50
2:C:440:SER:HB2	2:C:662:CYS:HB3	1.93	0.50
2:C:819:GLU:HG3	2:C:821:VAL:HG22	1.93	0.50
1:B:682:ARG:NH1	1:B:726:GLN:OE1	2.45	0.50
2:C:430:PRO:O	2:C:434:TYR:N	2.44	0.50
2:C:449:PRO:HB2	2:C:476:VAL:HG22	1.93	0.50
2:C:942:GLU:OE2	3:D:198:ARG:NH2	2.45	0.50
1:B:434:ARG:NH2	1:B:472:GLU:OE1	2.45	0.49
2:C:21:VAL:HG22	2:C:210:ARG:HH12	1.78	0.49
3:D:253:LEU:HD21	3:D:281:ARG:HH11	1.77	0.49
2:C:616:TRP:HE3	2:C:641:LEU:HD11	1.76	0.49
1:B:754:LEU:HB2	1:B:815:LEU:HB3	1.94	0.49
3:D:404:TYR:HE2	3:D:457:ARG:HG2	1.77	0.49
2:C:433:ARG:NH1	2:C:804:ARG:H	2.10	0.49
3:D:235:GLU:HG2	3:D:236:ASP:H	1.77	0.49
3:D:229:GLN:OE1	3:D:229:GLN:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:O	1:B:402:HIS:HB2	2.13	0.49
2:C:1018:HIS:O	2:C:1021:SER:OG	2.29	0.49
2:C:943:ILE:HG21	2:C:986:VAL:HG22	1.94	0.49
3:D:238:SER:HB2	3:D:242:ARG:HD3	1.95	0.49
1:B:1111:TYR:HB3	1:B:1140:TYR:HE2	1.78	0.48
3:D:50:HIS:HA	3:D:306:ALA:HB1	1.95	0.48
1:B:233:LYS:HB3	1:B:266:ILE:HG23	1.95	0.48
2:C:666:PRO:HA	2:C:715:LEU:HD21	1.93	0.48
1:B:583:ASN:O	1:B:725:GLN:NE2	2.43	0.48
2:C:35:ILE:HG12	2:C:212:PHE:HB2	1.95	0.48
4:A:123:MET:HA	4:E:112:PHE:HE1	1.77	0.48
2:C:568:LEU:HD23	2:C:571:LEU:HD12	1.94	0.48
1:B:901:TRP:HA	1:B:1059:ARG:O	2.14	0.48
1:B:1116:LEU:HD22	1:B:1168:MET:HG2	1.96	0.48
2:C:507:ASP:OD2	2:C:572:ASN:ND2	2.47	0.48
2:C:460:LEU:HG	2:C:465:PHE:HZ	1.80	0.47
1:B:992:GLU:O	1:B:995:THR:OG1	2.28	0.47
1:B:1078:LEU:HD23	1:B:1138:VAL:HG13	1.96	0.47
3:D:192:ALA:HB1	3:D:195:GLU:HB2	1.95	0.47
1:B:444:ASP:N	1:B:444:ASP:OD1	2.48	0.47
2:C:457:LEU:HA	2:C:460:LEU:HD13	1.96	0.47
2:C:839:ARG:NH1	2:C:851:MET:SD	2.87	0.47
3:D:100:MET:HB3	3:D:107:LEU:HD11	1.96	0.47
1:B:600:LEU:HD11	1:B:694:LEU:HD13	1.97	0.47
4:A:122:TYR:CZ	4:E:115:ARG:HD3	2.50	0.47
1:B:1027:ILE:HG12	1:B:1060:GLY:O	2.14	0.47
1:B:833:VAL:HG12	1:B:839:GLY:HA3	1.97	0.47
2:C:404:THR:HG22	2:C:406:ARG:H	1.80	0.47
1:B:1067:ASP:OD2	1:B:1081:TYR:N	2.39	0.46
3:D:201:LEU:HB2	3:D:237:ALA:HB2	1.97	0.46
3:D:253:LEU:HD11	3:D:281:ARG:HE	1.80	0.46
3:D:425:ARG:NH1	3:D:478:GLU:OE2	2.48	0.46
2:C:846:ARG:O	2:C:850:GLN:HG2	2.16	0.46
1:B:8:LEU:HD11	1:B:13:LEU:HB2	1.97	0.46
3:D:407:MET:HG3	3:D:580:TYR:CG	2.51	0.46
4:A:92:LEU:HD21	4:E:79:ILE:HD11	1.97	0.46
3:D:200:ARG:NH2	3:D:238:SER:OG	2.48	0.46
1:B:894:GLN:HG3	1:B:895:ARG:H	1.81	0.46
3:D:367:ILE:HG23	3:D:570:VAL:HG12	1.97	0.46
1:B:38:LEU:HD13	1:B:83:LEU:HD22	1.98	0.46
1:B:655:ARG:HB3	1:B:659:PRO:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:ASN:OD1	1:B:722:ALA:N	2.49	0.46
1:B:427:ILE:HB	1:B:800:ARG:HH12	1.80	0.46
1:B:945:PHE:HD2	1:B:1144:ARG:HH21	1.64	0.46
3:D:437:GLU:HA	3:D:547:ASP:HB3	1.96	0.46
3:D:390:PHE:HB2	3:D:393:ILE:HG22	1.98	0.45
1:B:722:ALA:O	2:C:737:GLN:NE2	2.50	0.45
1:B:490:VAL:HG12	1:B:495:THR:HG22	1.99	0.45
1:B:84:ARG:HE	1:B:115:LEU:HB2	1.81	0.45
2:C:214:CYS:HA	2:C:239:LEU:HB2	1.97	0.45
3:D:155:LYS:HE2	3:D:333:THR:HA	1.98	0.45
1:B:307:HIS:CG	1:B:308:PRO:HD2	2.52	0.45
1:B:504:MET:HA	1:B:870:ALA:HB3	1.99	0.45
2:C:410:VAL:HG22	2:C:676:CYS:HB2	1.99	0.45
3:D:85:LEU:HD13	3:D:107:LEU:HD22	1.98	0.45
3:D:418:TYR:CE2	3:D:422:LEU:HD11	2.50	0.45
3:D:431:ILE:HG22	3:D:500:ILE:HG12	1.98	0.45
1:B:754:LEU:HB3	1:B:757:ILE:HB	1.98	0.45
1:B:147:LEU:HD22	2:C:126:GLN:HG3	1.99	0.45
3:D:458:ILE:O	3:D:462:MET:HG2	2.17	0.45
3:D:35:VAL:HG22	3:D:85:LEU:HD23	1.99	0.45
1:B:992:GLU:HG3	1:B:993:TRP:H	1.82	0.45
2:C:995:GLU:HG2	2:C:1010:PRO:HD3	1.97	0.45
2:C:155:VAL:H	2:C:162:GLN:HE22	1.63	0.45
2:C:364:LYS:HB2	2:C:760:TYR:HD2	1.81	0.45
1:B:652:TRP:HB2	1:B:660:MET:SD	2.57	0.45
2:C:534:GLY:HA3	2:C:550:TYR:O	2.17	0.45
3:D:235:GLU:HG2	3:D:236:ASP:N	2.32	0.45
1:B:168:TRP:CD2	1:B:190:PRO:HD3	2.52	0.45
2:C:96:MET:HG3	2:C:124:LEU:HG	1.99	0.45
3:D:436:ASN:O	3:D:546:PHE:HA	2.16	0.45
3:D:374:ILE:HG23	3:D:590:ILE:HG23	1.99	0.45
1:B:1068:LEU:HD23	1:B:1079:LEU:HD23	1.99	0.44
1:B:1126:ILE:O	2:C:25:ARG:NH2	2.50	0.44
1:B:902:ARG:HA	2:C:656:ALA:O	2.16	0.44
2:C:956:LEU:HD11	2:C:986:VAL:HG13	1.99	0.44
1:B:1041:ARG:HA	1:B:1047:SER:HB3	1.97	0.44
1:B:233:LYS:HG2	1:B:266:ILE:HG12	2.00	0.44
2:C:77:LEU:HD21	2:C:196:THR:HG21	2.00	0.44
2:C:506:ILE:HA	2:C:524:TRP:HB2	2.00	0.44
2:C:761:LEU:HD12	2:C:775:ARG:HG2	2.00	0.44
1:B:964:PHE:HD2	1:B:1017:LYS:HZ3	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:THR:O	2:C:100:PRO:HD2	2.18	0.44
2:C:377:HIS:HE1	2:C:392:ARG:NH2	2.16	0.44
3:D:262:HIS:O	3:D:262:HIS:ND1	2.50	0.44
3:D:550:ALA:HB1	3:D:580:TYR:CE2	2.50	0.44
2:C:430:PRO:HD2	2:C:433:ARG:HB3	2.00	0.44
1:B:1084:ASN:O	1:B:1144:ARG:NH1	2.50	0.43
1:B:946:PRO:HD3	1:B:986:TRP:CH2	2.53	0.43
2:C:702:LYS:N	2:C:705:ASP:OD2	2.38	0.43
2:C:761:LEU:HG	2:C:776:VAL:HG22	1.99	0.43
1:B:809:SER:HB3	1:B:813:CYS:HB3	2.00	0.43
2:C:898:PHE:HB2	2:C:917:TRP:CE2	2.53	0.43
3:D:168:VAL:HG22	3:D:294:PHE:HB2	2.00	0.43
1:B:168:TRP:O	1:B:172:CYS:HB2	2.18	0.43
2:C:619:ILE:HD13	2:C:640:GLU:HG3	2.00	0.43
4:A:88:CYS:HB3	4:A:92:LEU:HD12	2.00	0.43
1:B:307:HIS:HB3	1:B:310:PHE:HB2	2.00	0.43
1:B:652:TRP:HZ3	1:B:657:VAL:HG13	1.84	0.43
2:C:38:GLN:HG2	2:C:667:MET:HG3	2.00	0.43
3:D:52:CYS:HB2	3:D:108:TYR:CD2	2.53	0.43
3:D:572:ARG:HD3	3:D:572:ARG:HA	1.87	0.43
1:B:431:MET:HG3	1:B:472:GLU:HG3	2.01	0.43
1:B:254:ARG:HH22	4:E:80:PRO:HA	1.82	0.43
2:C:244:CYS:HB3	2:C:248:TRP:CD1	2.53	0.43
2:C:474:LEU:HD21	2:C:567:LEU:HD22	1.99	0.43
1:B:668:ARG:HB3	1:B:670:ILE:HG23	2.01	0.43
1:B:592:GLU:HG3	1:B:683:ARG:HG3	2.01	0.43
2:C:204:PRO:HA	2:C:205:PRO:HD3	1.88	0.43
2:C:843:HIS:HB3	2:C:846:ARG:HB3	2.00	0.43
1:B:1068:LEU:HB3	1:B:1079:LEU:HB3	2.01	0.43
1:B:842:LEU:HD22	1:B:860:LEU:HD21	2.01	0.43
2:C:240:PHE:CE2	2:C:242:ASN:HB3	2.54	0.43
2:C:530:ARG:HH22	2:C:548:LEU:HB3	1.83	0.43
3:D:212:LEU:HD22	3:D:269:ASP:HB2	2.01	0.43
3:D:412:LEU:O	3:D:416:GLY:N	2.52	0.43
3:D:420:ASP:O	3:D:424:ALA:N	2.46	0.42
1:B:1085:TRP:CG	1:B:1093:TYR:HE1	2.37	0.42
1:B:155:ASP:OD1	1:B:155:ASP:N	2.52	0.42
2:C:681:ASN:HD21	2:C:732:ILE:HD13	1.84	0.42
4:A:77:LYS:HD3	4:A:77:LYS:HA	1.88	0.42
3:D:370:LEU:O	3:D:374:ILE:HG12	2.19	0.42
1:B:18:GLU:HA	1:B:409:LEU:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:O	1:B:39:ARG:NH1	2.52	0.42
3:D:438:TYR:HA	3:D:548:HIS:O	2.19	0.42
2:C:251:ILE:HG22	2:C:291:GLY:HA2	2.00	0.42
2:C:764:ASP:N	2:C:764:ASP:OD1	2.51	0.42
3:D:170:SER:OG	3:D:314:CYS:SG	2.73	0.42
3:D:543:GLY:H	3:D:572:ARG:NH1	2.17	0.42
3:D:329:LEU:HD23	3:D:332:LEU:HD12	2.01	0.42
1:B:27:THR:HG23	1:B:445:THR:O	2.19	0.42
1:B:1062:LEU:HD11	1:B:1113:LEU:HD13	2.00	0.42
1:B:982:PHE:HB3	1:B:986:TRP:HD1	1.84	0.42
2:C:251:ILE:HD12	2:C:256:TYR:HD2	1.85	0.42
2:C:162:GLN:O	2:C:162:GLN:HG2	2.20	0.42
2:C:451:LEU:HD13	2:C:645:LEU:HD21	2.01	0.42
3:D:584:ARG:HD2	3:D:584:ARG:H	1.85	0.42
1:B:122:ASP:OD1	1:B:123:GLU:N	2.51	0.41
2:C:185:HIS:CD2	2:C:187:ALA:HB3	2.55	0.41
2:C:114:TYR:HD2	2:C:115:LEU:HD12	1.85	0.41
2:C:544:TRP:CD2	2:C:545:GLN:HG2	2.55	0.41
2:C:847:ALA:O	2:C:851:MET:N	2.52	0.41
3:D:325:ARG:HG3	3:D:350:ASP:CG	2.40	0.41
4:A:79:ILE:HD13	4:E:92:LEU:HD11	2.02	0.41
4:A:88:CYS:O	4:A:92:LEU:HB2	2.21	0.41
2:C:354:ASN:N	2:C:354:ASN:OD1	2.54	0.41
3:D:427:GLU:O	3:D:431:ILE:HG13	2.20	0.41
1:B:1090:SER:O	1:B:1092:ALA:N	2.54	0.41
1:B:563:GLU:HB3	1:B:756:PHE:HD2	1.85	0.41
2:C:245:ARG:HA	2:C:326:PHE:CZ	2.55	0.41
2:C:406:ARG:HB2	2:C:657:GLY:HA2	2.02	0.41
1:B:613:ARG:HG2	2:C:855:VAL:HG22	2.01	0.41
2:C:984:HIS:NE2	2:C:988:CYS:SG	2.94	0.41
3:D:457:ARG:HH12	3:D:461:PHE:HD1	1.68	0.41
2:C:408:ILE:HG12	2:C:674:VAL:HB	2.02	0.41
2:C:467:SER:HA	2:C:524:TRP:HZ2	1.85	0.41
1:B:833:VAL:O	1:B:836:SER:OG	2.35	0.41
2:C:268:SER:HB3	2:C:270:GLU:HG2	2.02	0.41
4:A:75:MET:HB2	4:A:124:VAL:HG13	2.02	0.41
1:B:997:VAL:HA	1:B:1146:VAL:HG11	2.03	0.41
3:D:165:ARG:HA	3:D:291:ARG:HG2	2.02	0.41
3:D:435:PHE:HD2	3:D:498:ILE:HD12	1.85	0.41
1:B:665:MET:HE1	1:B:688:LEU:HD11	2.02	0.41
2:C:1025:GLU:OE2	2:C:1028:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:LEU:O	2:C:762:PRO:HD3	2.21	0.41
2:C:506:ILE:HA	2:C:524:TRP:CD1	2.56	0.41
2:C:506:ILE:HA	2:C:524:TRP:HD1	1.86	0.41
3:D:17:ARG:HH12	3:D:47:GLY:HA3	1.86	0.41
1:B:256:LYS:HB3	1:B:259:ARG:HH11	1.85	0.41
1:B:458:ASN:HA	1:B:475:PHE:HZ	1.85	0.41
1:B:641:VAL:HA	1:B:644:GLU:HG2	2.03	0.41
1:B:943:HIS:CG	1:B:1089:ASP:HB2	2.55	0.41
2:C:680:MET:O	2:C:745:SER:N	2.51	0.41
1:B:730:GLU:O	1:B:731:SER:OG	2.35	0.41
2:C:460:LEU:HG	2:C:465:PHE:CZ	2.56	0.41
1:B:728:ARG:NH1	2:C:739:ASN:HD22	2.19	0.40
1:B:675:LEU:HD12	2:C:809:ALA:HB1	2.04	0.40
3:D:54:PRO:HA	3:D:106:ARG:HA	2.03	0.40
3:D:425:ARG:HD2	3:D:425:ARG:HA	1.94	0.40
1:B:592:GLU:O	1:B:596:MET:HG2	2.21	0.40
2:C:616:TRP:CE3	2:C:641:LEU:HD11	2.56	0.40
3:D:108:TYR:HE1	3:D:113:TRP:HA	1.85	0.40
3:D:546:PHE:O	3:D:574:ARG:N	2.32	0.40
3:D:550:ALA:HA	3:D:578:SER:O	2.20	0.40
3:D:441:LEU:HD13	3:D:569:ALA:HA	2.02	0.40
1:B:1026:PRO:HB3	1:B:1061:MET:SD	2.62	0.40
1:B:448:ARG:NH1	1:B:747:LEU:O	2.54	0.40
2:C:386:VAL:HG12	2:C:425:VAL:HG21	2.03	0.40
3:D:440:LEU:HB2	3:D:535:ALA:HA	2.03	0.40
1:B:18:GLU:HG2	1:B:409:LEU:HD23	2.03	0.40
1:B:831:THR:HG22	1:B:848:GLN:O	2.21	0.40
3:D:235:GLU:H	3:D:235:GLU:CD	2.24	0.40
2:C:221:PRO:HD3	2:C:704:GLY:HA3	2.04	0.40
3:D:198:ARG:H	3:D:264:ASP:HB3	1.86	0.40
3:D:282:LEU:O	3:D:286:LEU:HG	2.21	0.40
3:D:466:ARG:HD3	3:D:466:ARG:HA	1.91	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	1121/1181 (95%)	1070 (96%)	49 (4%)	2 (0%)	52	86
2	C	1119/1122 (100%)	1054 (94%)	65 (6%)	0	100	100
3	D	587/609 (96%)	561 (96%)	25 (4%)	1 (0%)	52	86
4	A	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
4	E	73/98 (74%)	72 (99%)	1 (1%)	0	100	100
All	All	2996/3108 (96%)	2851 (95%)	142 (5%)	3 (0%)	59	90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	126	VAL
1	B	380	VAL
1	B	1091	SER

5.3.2 Protein sidechains ⓘ

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	957/999 (96%)	950 (99%)	7 (1%)	88	95
2	C	976/977 (100%)	973 (100%)	3 (0%)	94	98
3	D	478/492 (97%)	473 (99%)	5 (1%)	82	92
4	A	86/86 (100%)	86 (100%)	0	100	100
4	E	66/86 (77%)	66 (100%)	0	100	100
All	All	2563/2640 (97%)	2548 (99%)	15 (1%)	91	96

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	96	LEU
1	B	444	ASP
1	B	612	LEU
1	B	883	VAL
1	B	947	ARG
1	B	1094	THR
2	C	109	THR
2	C	329	VAL
2	C	853	LEU
3	D	125	GLU
3	D	223	LEU
3	D	226	THR
3	D	572	ARG
3	D	596	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	79	ASN
1	B	120	GLN
1	B	202	GLN
1	B	307	HIS
1	B	515	GLN
1	B	650	GLN
1	B	765	GLN
1	B	944	GLN
1	B	1072	HIS
1	B	1133	HIS
1	B	1134	HIS
2	C	228	GLN
2	C	390	HIS
2	C	510	ASN
2	C	572	ASN
2	C	647	GLN
2	C	660	ASN
2	C	739	ASN
2	C	817	HIS
2	C	881	ASN
2	C	886	ASN
2	C	920	GLN
2	C	926	GLN
2	C	979	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	15	GLN
3	D	44	HIS
3	D	115	ASN
3	D	255	HIS
3	D	256	HIS
4	A	131	GLN
4	E	119	HIS
4	E	131	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.