Full wwPDB EM Validation Report ⓘ

Mar 31, 2024 – 12:47 AM JST

PDB ID	:	8J84
EMDB ID	:	EMD-36059
Title	:	Short ago complexed with TIR-APAZ
Authors	:	Guo, L.J.; Huang, P.P.; Li, Z.X.; Xiao, Y.B.; Chen, M.R.
Deposited on	:	2023-04-30
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

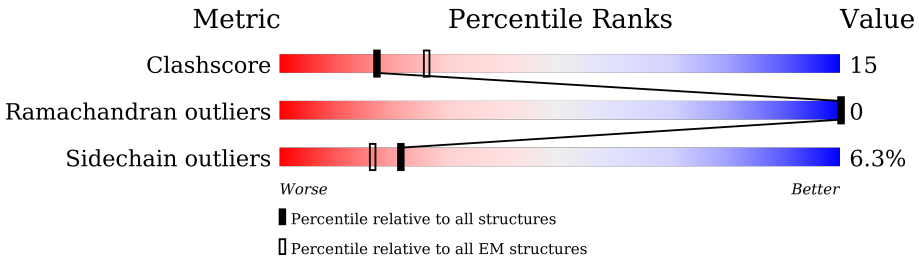
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	507	55% 34% • 10%
2	B	450	66% 31% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7448 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 Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	456	3689	2391	615	671	12	0	0

- Molecule 2 is a protein called TIR domain-containing protein.

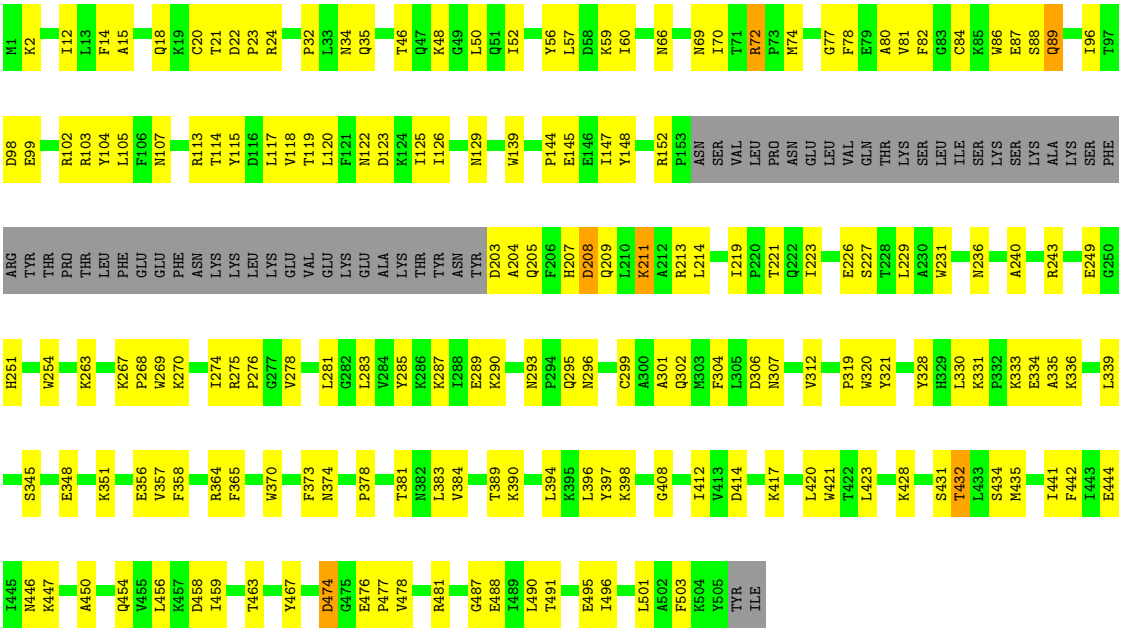
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	450	3759	2427	625	696	11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

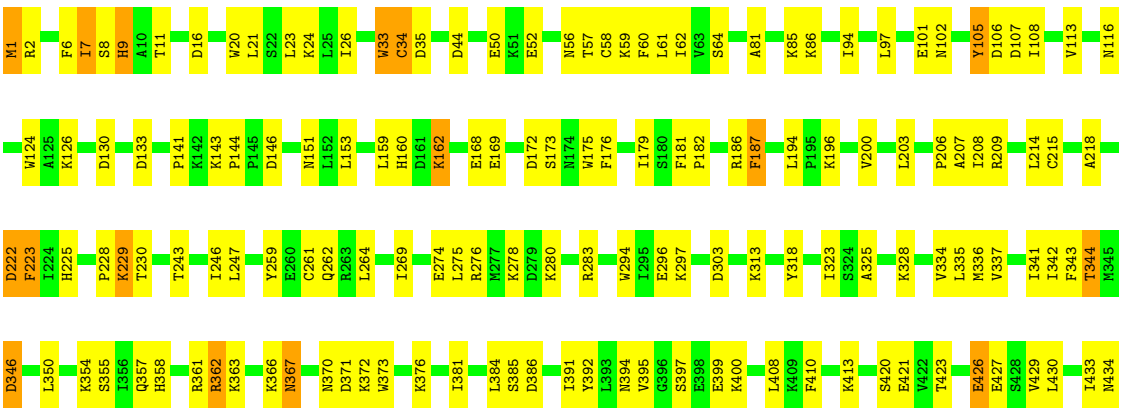
• Molecule 1: Piwi domain-containing protein

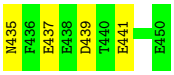
Chain A:



• Molecule 2: TIR domain-containing protein

Chain B:




M435
F436
E437
E438
D439
T440
E441
E450

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	375800	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/3783	0.49	0/5121
2	B	0.25	0/3849	0.48	0/5191
All	All	0.25	0/7632	0.49	0/10312

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	3689	0	3705	136	0
2	B	3759	0	3738	106	0
All	All	7448	0	7443	226	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 15.

All (226) 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:423:LEU:HB3	1:A:434:SER:HB3	1.59	0.84
1:A:267:LYS:HE3	1:A:307:ASN:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:NE2	2:B:439:ASP:O	2.21	0.74
2:B:343:PHE:H	2:B:357:GLN:HE22	1.36	0.73
2:B:437:GLU:HG2	2:B:439:ASP:H	1.53	0.73
1:A:281:LEU:HD11	1:A:301:ALA:HB1	1.74	0.69
2:B:246:ILE:HD11	2:B:261:CYS:HB2	1.74	0.69
1:A:293:ASN:O	1:A:296:ASN:ND2	2.28	0.67
1:A:487:GLY:HA2	1:A:490:LEU:HD12	1.78	0.66
1:A:115:TYR:O	1:A:119:THR:HG23	1.97	0.65
1:A:335:ALA:HB1	1:A:373:PHE:HE1	1.62	0.65
2:B:1:MET:N	2:B:58:CYS:SG	2.70	0.64
2:B:1:MET:N	2:B:1:MET:SD	2.71	0.63
1:A:72:ARG:HH22	2:B:429:VAL:HG21	1.63	0.63
1:A:428:LYS:HE2	2:B:159:LEU:HD11	1.80	0.63
1:A:474:ASP:OD1	1:A:474:ASP:N	2.32	0.63
1:A:243:ARG:NH1	2:B:435:ASN:O	2.32	0.63
2:B:280:LYS:NZ	2:B:384:LEU:O	2.29	0.63
1:A:373:PHE:HB3	1:A:383:LEU:HD21	1.79	0.63
2:B:283:ARG:NH1	2:B:296:GLU:OE2	2.33	0.62
2:B:325:ALA:HB1	2:B:335:LEU:HD11	1.80	0.62
1:A:459:ILE:O	1:A:463:THR:HG23	2.00	0.62
1:A:408:GLY:N	1:A:421:TRP:O	2.31	0.61
1:A:281:LEU:HB3	1:A:357:VAL:HA	1.81	0.61
1:A:48:LYS:O	1:A:52:ILE:HG12	2.01	0.60
2:B:143:LYS:HE2	2:B:144:PRO:HD2	1.83	0.59
2:B:276:ARG:NH2	2:B:386:ASP:OD2	2.35	0.59
1:A:414:ASP:OD1	1:A:417:LYS:N	2.33	0.59
1:A:14:PHE:HZ	1:A:23:PRO:HA	1.67	0.59
1:A:118:VAL:HG21	1:A:209:GLN:HG3	1.85	0.59
2:B:208:ILE:HD11	2:B:264:LEU:HG	1.85	0.59
2:B:168:GLU:HG2	2:B:413:LYS:HG3	1.85	0.58
2:B:371:ASP:OD1	2:B:372:LYS:N	2.36	0.58
2:B:187:PHE:HD1	2:B:215:CYS:HB3	1.68	0.58
1:A:281:LEU:HD23	1:A:357:VAL:HG13	1.86	0.57
1:A:57:LEU:HA	1:A:60:ILE:HD12	1.87	0.57
2:B:346:ASP:OD1	2:B:346:ASP:N	2.34	0.57
1:A:488:GLU:HA	1:A:491:THR:HG22	1.86	0.57
1:A:70:ILE:HD11	2:B:162:LYS:HE2	1.85	0.57
2:B:344:THR:HG23	2:B:350:LEU:HD23	1.86	0.57
1:A:66:ASN:ND2	1:A:72:ARG:O	2.37	0.57
1:A:236:ASN:HD21	1:A:240:ALA:HB3	1.70	0.56
1:A:295:GLN:OE1	1:A:295:GLN:N	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PRO:O	1:A:481:ARG:N	2.39	0.56
2:B:7:ILE:HD12	2:B:21:LEU:HD23	1.88	0.56
2:B:52:GLU:HA	2:B:56:ASN:HB2	1.87	0.56
2:B:57:THR:OG1	2:B:59:LYS:O	2.22	0.56
2:B:200:VAL:HG21	2:B:209:ARG:HB2	1.86	0.56
2:B:294:TRP:HB3	2:B:342:ILE:HD13	1.87	0.56
2:B:105:TYR:HA	2:B:108:ILE:HD12	1.87	0.56
1:A:125:ILE:O	1:A:129:ASN:ND2	2.39	0.55
1:A:22:ASP:HB2	1:A:428:LYS:HE3	1.88	0.55
1:A:463:THR:HG22	1:A:477:PRO:HA	1.89	0.55
1:A:478:VAL:HA	1:A:481:ARG:HB2	1.88	0.55
2:B:196:LYS:HA	2:B:209:ARG:HH12	1.71	0.55
1:A:208:ASP:OD1	1:A:208:ASP:N	2.37	0.55
1:A:285:TYR:CD2	1:A:328:TYR:HB2	2.41	0.55
2:B:206:PRO:HG3	2:B:395:VAL:HG12	1.88	0.55
1:A:306:ASP:OD1	1:A:306:ASP:N	2.40	0.55
1:A:417:LYS:HG2	1:A:444:GLU:HG3	1.89	0.54
2:B:181:PHE:HZ	2:B:269:ILE:HD11	1.73	0.54
1:A:88:SER:OG	1:A:88:SER:O	2.23	0.54
1:A:269:TRP:O	1:A:467:TYR:OH	2.17	0.54
1:A:2:LYS:HE2	2:B:408:LEU:HD21	1.89	0.54
1:A:152:ARG:HH22	2:B:439:ASP:HA	1.73	0.54
1:A:396:LEU:HG	1:A:421:TRP:CZ2	2.42	0.54
1:A:293:ASN:HB2	1:A:295:GLN:HE22	1.72	0.54
1:A:364:ARG:NH1	1:A:446:ASN:OD1	2.41	0.54
1:A:275:ARG:NH2	1:A:458:ASP:OD2	2.38	0.54
1:A:320:TRP:HZ2	1:A:334:GLU:HG3	1.72	0.54
2:B:207:ALA:HB1	2:B:214:LEU:HD11	1.89	0.53
2:B:194:LEU:HD22	2:B:214:LEU:HD22	1.90	0.53
2:B:355:SER:HA	2:B:358:HIS:NE2	2.24	0.53
2:B:8:SER:HB2	2:B:62:ILE:HG22	1.89	0.53
1:A:57:LEU:HD11	1:A:86:TRP:CE2	2.43	0.53
1:A:378:PRO:O	1:A:381:THR:OG1	2.26	0.52
2:B:323:ILE:HB	2:B:337:VAL:HG13	1.91	0.52
2:B:9:HIS:NE2	2:B:35:ASP:OD1	2.29	0.52
2:B:182:PRO:HB3	2:B:399:GLU:HB3	1.92	0.52
1:A:243:ARG:HH11	2:B:435:ASN:HB3	1.74	0.52
1:A:119:THR:HG22	1:A:213:ARG:HH12	1.75	0.52
2:B:228:PRO:O	2:B:229:LYS:HG2	2.09	0.52
1:A:390:LYS:HB3	1:A:441:ILE:HG22	1.92	0.51
2:B:328:LYS:HB3	2:B:336:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:OD1	1:A:293:ASN:N	2.44	0.51
1:A:274:ILE:HG12	1:A:306:ASP:HB3	1.92	0.51
1:A:420:LEU:HD22	1:A:456:LEU:HD22	1.92	0.51
1:A:129:ASN:ND2	1:A:219:ILE:HD13	2.26	0.50
1:A:145:GLU:HG3	1:A:227:SER:HB3	1.93	0.50
1:A:78:PHE:CE2	1:A:86:TRP:HB3	2.46	0.50
1:A:207:HIS:HA	1:A:223:ILE:HD12	1.93	0.50
1:A:333:LYS:O	1:A:336:LYS:HG2	2.12	0.50
2:B:34:CYS:SG	2:B:35:ASP:N	2.85	0.50
2:B:146:ASP:OD1	2:B:146:ASP:N	2.45	0.50
2:B:6:PHE:HD1	2:B:33:TRP:HB3	1.77	0.50
2:B:23:LEU:HA	2:B:26:ILE:HG22	1.93	0.50
2:B:176:PHE:CZ	2:B:381:ILE:HG13	2.47	0.50
1:A:125:ILE:HD13	1:A:214:LEU:HD11	1.94	0.49
2:B:276:ARG:NH1	2:B:392:TYR:O	2.45	0.49
1:A:389:THR:O	1:A:442:PHE:N	2.40	0.49
2:B:358:HIS:O	2:B:362:ARG:NH1	2.45	0.49
2:B:421:GLU:OE2	2:B:423:THR:OG1	2.30	0.49
1:A:389:THR:HG23	1:A:442:PHE:HB3	1.95	0.49
1:A:66:ASN:O	1:A:69:ASN:ND2	2.46	0.49
1:A:34:ASN:HD21	1:A:267:LYS:HB2	1.78	0.49
1:A:293:ASN:HB2	1:A:295:GLN:NE2	2.27	0.49
1:A:320:TRP:CD1	1:A:330:LEU:HA	2.48	0.49
1:A:77:GLY:O	1:A:81:VAL:HG12	2.13	0.48
2:B:11:THR:OG1	2:B:35:ASP:OD2	2.31	0.48
1:A:275:ARG:HH21	1:A:454:GLN:HE21	1.61	0.48
2:B:385:SER:HA	2:B:391:ILE:HG12	1.95	0.48
1:A:74:MET:O	1:A:254:TRP:NE1	2.43	0.48
1:A:80:ALA:O	2:B:24:LYS:NZ	2.46	0.48
1:A:356:GLU:HB3	1:A:358:PHE:CD2	2.48	0.48
2:B:2:ARG:HB2	2:B:58:CYS:HB2	1.96	0.48
1:A:211:LYS:HE2	1:A:221:THR:HG23	1.95	0.48
2:B:106:ASP:N	2:B:106:ASP:OD1	2.46	0.48
1:A:226:GLU:HA	1:A:229:LEU:HB2	1.95	0.47
2:B:274:GLU:OE1	2:B:275:LEU:HD22	2.14	0.47
2:B:367:ASN:OD1	2:B:367:ASN:N	2.37	0.47
1:A:99:GLU:OE1	1:A:102:ARG:NH1	2.47	0.47
1:A:287:LYS:HE3	1:A:289:GLU:HB2	1.95	0.47
1:A:348:GLU:O	1:A:351:LYS:NZ	2.45	0.47
1:A:15:ALA:HB2	1:A:32:PRO:O	2.14	0.47
1:A:420:LEU:HD12	1:A:421:TRP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:VAL:O	2:B:433:ILE:N	2.47	0.47
2:B:203:LEU:HD22	2:B:223:PHE:HE1	1.79	0.47
1:A:22:ASP:OD2	1:A:428:LYS:NZ	2.39	0.47
2:B:126:LYS:NZ	2:B:130:ASP:OD1	2.48	0.47
2:B:261:CYS:SG	2:B:262:GLN:N	2.88	0.47
2:B:341:ILE:HD11	2:B:373:TRP:CH2	2.50	0.47
2:B:363:LYS:HA	2:B:366:LYS:HD2	1.97	0.46
1:A:87:GLU:OE1	1:A:89:GLN:N	2.48	0.46
2:B:434:ASN:OD1	2:B:435:ASN:ND2	2.49	0.46
1:A:122:ASN:O	1:A:126:ILE:HG12	2.15	0.46
1:A:435:MET:SD	2:B:430:LEU:HD13	2.56	0.46
1:A:12:ILE:HD12	1:A:269:TRP:CD1	2.51	0.46
1:A:231:TRP:NE1	1:A:249:GLU:OE1	2.46	0.46
1:A:370:TRP:O	1:A:374:ASN:ND2	2.49	0.46
2:B:186:ARG:NH1	2:B:218:ALA:O	2.49	0.46
1:A:296:ASN:HA	1:A:319:PRO:HA	1.95	0.46
1:A:302:GLN:HB3	1:A:304:PHE:HE1	1.79	0.46
1:A:414:ASP:OD2	1:A:417:LYS:NZ	2.35	0.46
1:A:114:THR:HG21	1:A:204:ALA:HA	1.96	0.46
1:A:333:LYS:O	1:A:333:LYS:NZ	2.47	0.46
2:B:426:GLU:O	2:B:430:LEU:HD12	2.16	0.46
1:A:398:LYS:N	2:B:370:ASN:OD1	2.41	0.46
1:A:339:LEU:HD11	1:A:357:VAL:HG21	1.98	0.46
1:A:397:TYR:O	2:B:172:ASP:N	2.39	0.46
1:A:203:ASP:OD1	1:A:209:GLN:NE2	2.49	0.45
1:A:394:LEU:HD13	2:B:175:TRP:CE2	2.51	0.45
2:B:20:TRP:CH2	2:B:124:TRP:HB3	2.51	0.45
2:B:61:LEU:HB2	2:B:97:LEU:HD21	1.98	0.45
2:B:105:TYR:HD1	2:B:113:VAL:HG22	1.81	0.45
2:B:228:PRO:HG2	2:B:229:LYS:HE3	1.98	0.45
1:A:144:PRO:HA	1:A:226:GLU:OE1	2.17	0.45
1:A:285:TYR:CE2	1:A:328:TYR:HB2	2.52	0.45
2:B:173:SER:OG	2:B:408:LEU:O	2.32	0.45
1:A:129:ASN:HB3	1:A:139:TRP:HE1	1.82	0.45
1:A:275:ARG:O	1:A:278:VAL:HG12	2.17	0.45
2:B:181:PHE:CZ	2:B:269:ILE:HD11	2.51	0.45
2:B:278:LYS:HE3	2:B:278:LYS:HB3	1.82	0.45
1:A:14:PHE:N	1:A:18:GLN:O	2.43	0.45
2:B:328:LYS:HD2	2:B:336:MET:HE3	1.98	0.44
1:A:495:GLU:HG2	1:A:496:ILE:HD13	1.98	0.44
2:B:6:PHE:O	2:B:60:PHE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:OG	1:A:432:THR:N	2.50	0.44
2:B:430:LEU:HA	2:B:433:ILE:HB	1.99	0.44
1:A:107:ASN:HB3	1:A:113:ARG:HG2	2.00	0.44
1:A:384:VAL:HG21	1:A:450:ALA:HB2	2.00	0.44
2:B:24:LYS:HA	2:B:24:LYS:HD2	1.74	0.44
2:B:341:ILE:N	2:B:341:ILE:HD12	2.33	0.44
2:B:101:GLU:OE1	2:B:101:GLU:N	2.36	0.44
2:B:366:LYS:NZ	2:B:427:GLU:O	2.51	0.44
1:A:283:LEU:HD21	1:A:285:TYR:CE1	2.52	0.43
1:A:330:LEU:HB2	1:A:335:ALA:HB2	2.00	0.43
1:A:98:ASP:OD1	1:A:98:ASP:N	2.51	0.43
2:B:64:SER:O	2:B:64:SER:OG	2.33	0.43
1:A:103:ARG:HH12	1:A:104:TYR:HE1	1.67	0.43
1:A:24:ARG:HB2	1:A:24:ARG:HH11	1.83	0.43
1:A:60:ILE:HG22	1:A:78:PHE:HB2	2.00	0.43
1:A:290:LYS:HE3	1:A:290:LYS:HA	2.00	0.43
1:A:345:SER:O	1:A:348:GLU:HG3	2.18	0.43
2:B:2:ARG:O	2:B:141:PRO:HG3	2.19	0.43
2:B:179:ILE:HD13	2:B:179:ILE:HA	1.88	0.43
1:A:117:LEU:O	1:A:120:LEU:HG	2.19	0.43
1:A:365:PHE:HB2	1:A:447:LYS:HE3	2.01	0.43
1:A:412:ILE:HG13	1:A:412:ILE:O	2.19	0.43
1:A:270:LYS:HB2	1:A:307:ASN:HA	2.00	0.42
1:A:320:TRP:CZ2	1:A:334:GLU:HG3	2.53	0.42
2:B:294:TRP:CZ2	2:B:350:LEU:HD21	2.54	0.42
1:A:299:CYS:HB3	1:A:320:TRP:CZ3	2.55	0.42
2:B:203:LEU:HD13	2:B:223:PHE:CZ	2.55	0.42
2:B:222:ASP:OD2	2:B:397:SER:OG	2.23	0.42
2:B:60:PHE:CE2	2:B:81:ALA:HB2	2.55	0.42
1:A:231:TRP:HE1	1:A:249:GLU:CD	2.22	0.42
1:A:2:LYS:HB2	2:B:410:PHE:CD1	2.55	0.42
1:A:96:ILE:HG13	1:A:96:ILE:O	2.20	0.42
1:A:117:LEU:HD13	1:A:147:ILE:HG23	2.02	0.42
2:B:243:THR:HA	2:B:246:ILE:HG22	2.01	0.42
1:A:275:ARG:HG2	1:A:276:PRO:HD2	2.00	0.42
1:A:319:PRO:O	1:A:331:LYS:NZ	2.53	0.42
1:A:46:THR:O	1:A:50:LEU:N	2.46	0.41
1:A:428:LYS:HA	2:B:162:LYS:HB2	2.01	0.41
2:B:313:LYS:HG2	2:B:318:TYR:CZ	2.55	0.41
2:B:102:ASN:N	2:B:102:ASN:OD1	2.54	0.41
1:A:321:TYR:HA	1:A:328:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:LYS:HA	2:B:303:ASP:OD2	2.20	0.41
2:B:328:LYS:HG2	2:B:334:VAL:HG22	2.02	0.41
2:B:44:ASP:OD1	2:B:44:ASP:N	2.40	0.41
2:B:130:ASP:HA	2:B:133:ASP:OD2	2.20	0.41
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.89	0.41
1:A:57:LEU:HA	1:A:57:LEU:HD13	1.89	0.41
1:A:72:ARG:HG3	1:A:251:HIS:CD2	2.56	0.41
1:A:267:LYS:HB3	1:A:267:LYS:HE2	1.90	0.41
1:A:476:GLU:HG3	1:A:481:ARG:HD2	2.02	0.41
2:B:394:ASN:HA	2:B:400:LYS:HG2	2.03	0.41
1:A:99:GLU:O	1:A:102:ARG:HG2	2.20	0.40
2:B:372:LYS:O	2:B:376:LYS:HG3	2.21	0.40
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.85	0.40
1:A:397:TYR:N	2:B:172:ASP:O	2.54	0.40
1:A:32:PRO:HD3	1:A:82:PHE:HD1	1.86	0.40
2:B:116:ASN:OD1	2:B:116:ASN:N	2.49	0.40
1:A:211:LYS:HD3	1:A:211:LYS:HA	1.97	0.40
1:A:268:PRO:HB2	1:A:269:TRP:CE3	2.57	0.40
2:B:85:LYS:HD3	2:B:94:ILE:HG12	2.04	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	452/507 (89%)	432 (96%)	20 (4%)	0	100	100
2	B	448/450 (100%)	418 (93%)	30 (7%)	0	100	100
All	All	900/957 (94%)	850 (94%)	50 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	397/446 (89%)	378 (95%)	19 (5%)	25 56
2	B	415/415 (100%)	383 (92%)	32 (8%)	13 38
All	All	812/861 (94%)	761 (94%)	51 (6%)	21 47

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	CYS
1	A	21	THR
1	A	35	GLN
1	A	56	TYR
1	A	59	LYS
1	A	72	ARG
1	A	84	CYS
1	A	89	GLN
1	A	105	LEU
1	A	123	ASP
1	A	148	TYR
1	A	208	ASP
1	A	211	LYS
1	A	263	LYS
1	A	312	VAL
1	A	432	THR
1	A	474	ASP
1	A	501	LEU
1	A	503	PHE
2	B	1	MET
2	B	7	ILE
2	B	9	HIS
2	B	16	ASP
2	B	33	TRP
2	B	34	CYS
2	B	50	GLU
2	B	86	LYS

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Mol	Chain	Res	Type
2	B	105	TYR
2	B	107	ASP
2	B	151	ASN
2	B	153	LEU
2	B	160	HIS
2	B	162	LYS
2	B	169	GLU
2	B	187	PHE
2	B	222	ASP
2	B	223	PHE
2	B	225	HIS
2	B	229	LYS
2	B	230	THR
2	B	247	LEU
2	B	259	TYR
2	B	344	THR
2	B	346	ASP
2	B	354	LYS
2	B	361	ARG
2	B	362	ARG
2	B	367	ASN
2	B	420	SER
2	B	426	GLU
2	B	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	129	ASN
2	B	357	GLN
2	B	435	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 monosaccharides 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.