



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 3, 2017 – 04:49 PM EDT

PDB ID : 5TQY
EMDB ID: : EMD-8438
Title : CryoEM reconstruction of human IKK1, closed conformation 3
Authors : Lyumkis, D.; Ghosh, G.; Polley, S.; Biswath, T.; Huang, D.; Passos, D.O.
Deposited on : unknown
Resolution : 5.20 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

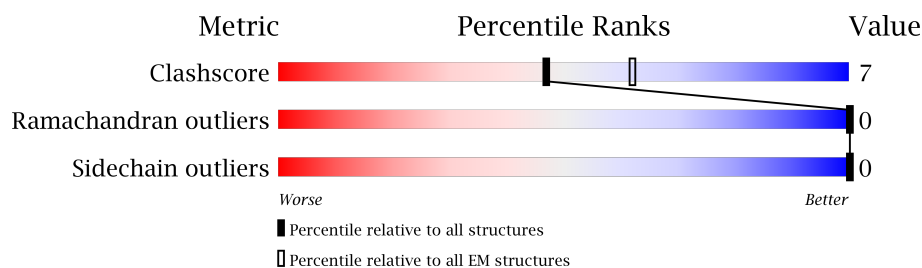
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	A	655	
1	B	655	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9396 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 Inhibitor of nuclear factor kappa-B kinase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total	C	N	O	S	0	0
			4698	2999	814	852	33		
1	B	578	Total	C	N	O	S	0	0
			4698	2999	814	852	33		

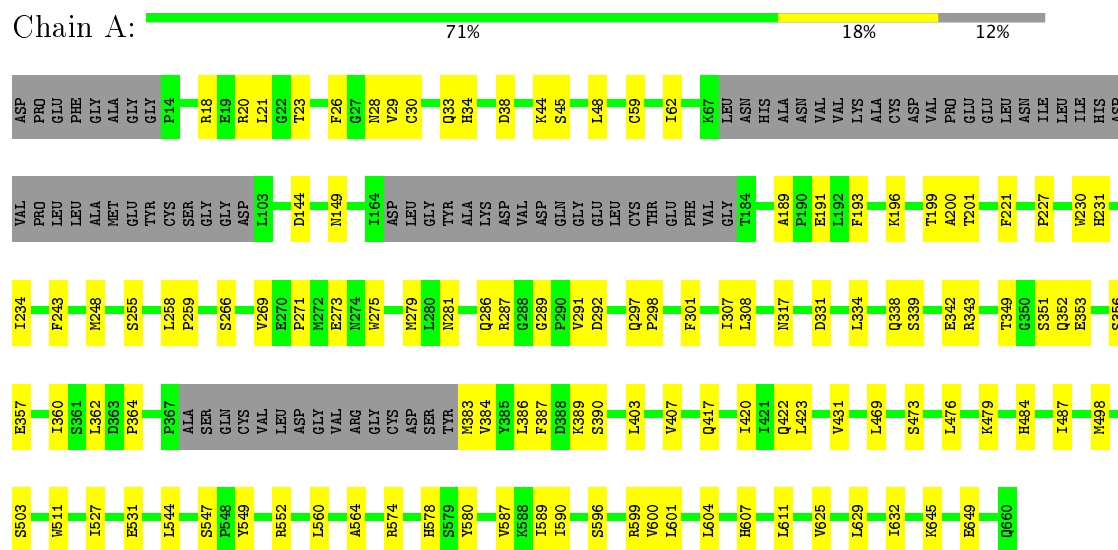
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASP	-	expression tag	UNP O15111
A	7	PRO	-	expression tag	UNP O15111
A	8	GLU	-	expression tag	UNP O15111
A	9	PHE	-	expression tag	UNP O15111
A	176	GLU	SER	engineered mutation	UNP O15111
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	UNP O15111
B	180	GLU	SER	engineered mutation	UNP O15111
B	268	ILE	VAL	variant	UNP O15111

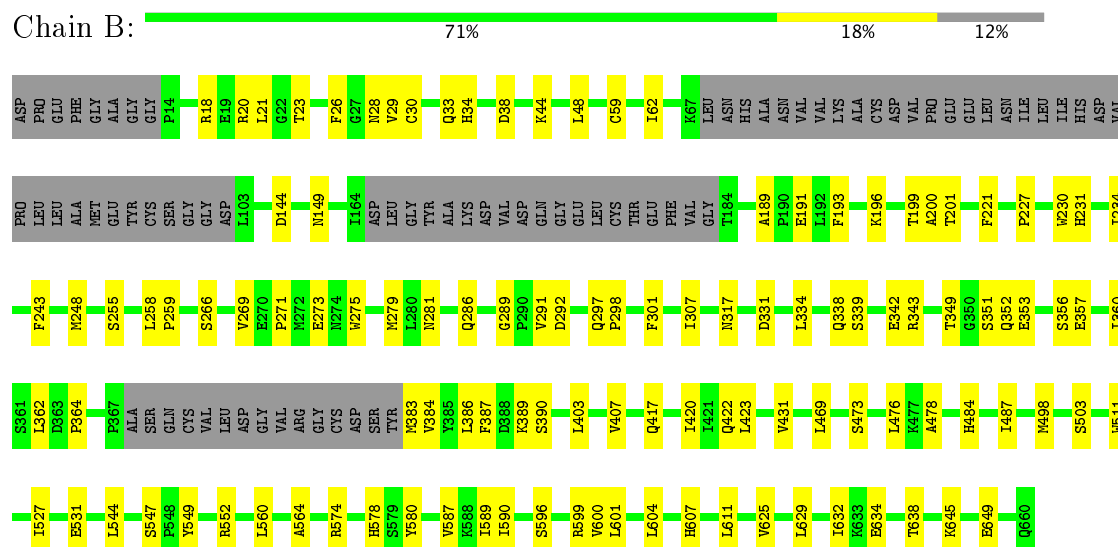
3 Residue-property plots

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: Inhibitor of nuclear factor kappa-B kinase subunit alpha



- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; within Relion and Frealign	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	5200	Depositor
Magnification	38167	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	A	0.35	1/4792 (0.0%)	0.49	0/6447
1	B	0.35	1/4792 (0.0%)	0.49	0/6447
All	All	0.35	2/9584 (0.0%)	0.49	0/12894

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	GLY	C-N	10.45	1.54	1.34
1	B	289	GLY	C-N	10.41	1.54	1.34

There are no bond angle outliers.

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	A	4698	0	4795	71	0
1	B	4698	0	4795	70	0
All	All	9396	0	9590	140	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 (140) 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:48:LEU:O	1:A:48:LEU:HD13	1.17	1.27
1:B:48:LEU:O	1:B:48:LEU:HD13	1.17	1.27
1:B:48:LEU:O	1:B:48:LEU:CD1	2.12	0.97
1:A:48:LEU:CD1	1:A:48:LEU:O	2.12	0.96
1:B:48:LEU:C	1:B:48:LEU:HD13	2.03	0.78
1:A:48:LEU:HD13	1:A:48:LEU:C	2.03	0.78
1:A:18:ARG:HE	1:A:33:GLN:HB3	1.55	0.72
1:B:18:ARG:HE	1:B:33:GLN:HB3	1.55	0.70
1:B:227:PRO:HA	1:B:230:TRP:HB3	1.74	0.69
1:A:227:PRO:HA	1:A:230:TRP:HB3	1.73	0.69
1:A:34:HIS:O	1:A:38:ASP:N	2.30	0.65
1:A:338:GLN:O	1:A:342:GLU:HB2	1.97	0.65
1:A:527:ILE:O	1:A:531:GLU:HB2	1.97	0.64
1:B:527:ILE:O	1:B:531:GLU:HB2	1.97	0.64
1:B:221:PHE:O	1:B:230:TRP:NE1	2.29	0.64
1:B:338:GLN:O	1:B:342:GLU:HB2	1.97	0.63
1:B:34:HIS:O	1:B:38:ASP:N	2.30	0.62
1:B:144:ASP:O	1:B:149:ASN:ND2	2.32	0.61
1:A:221:PHE:O	1:A:230:TRP:NE1	2.29	0.59
1:B:357:GLU:OE2	1:B:383:MET:N	2.35	0.59
1:A:281:ASN:ND2	1:A:286:GLN:OE1	2.36	0.59
1:B:281:ASN:ND2	1:B:286:GLN:OE1	2.36	0.59
1:A:357:GLU:OE2	1:A:383:MET:N	2.35	0.58
1:A:269:VAL:O	1:A:273:GLU:N	2.37	0.58
1:A:144:ASP:O	1:A:149:ASN:ND2	2.32	0.58
1:A:479:LYS:HE3	1:B:478:ALA:HB1	1.86	0.57
1:B:339:SER:OG	1:B:343:ARG:NH1	2.37	0.57
1:A:339:SER:OG	1:A:343:ARG:NH1	2.37	0.57
1:A:291:VAL:HA	1:A:298:PRO:HA	1.86	0.57
1:B:23:THR:HA	1:B:28:ASN:HA	1.87	0.57
1:A:23:THR:HA	1:A:28:ASN:HA	1.87	0.56
1:B:291:VAL:HA	1:B:298:PRO:HA	1.86	0.56
1:B:549:TYR:O	1:B:552:ARG:NE	2.35	0.56
1:B:269:VAL:O	1:B:273:GLU:N	2.37	0.55
1:A:549:TYR:O	1:A:552:ARG:NE	2.35	0.54
1:B:596:SER:OG	1:B:599:ARG:NH2	2.41	0.54
1:A:596:SER:OG	1:A:599:ARG:NH2	2.41	0.54
1:B:243:PHE:O	1:B:255:SER:N	2.40	0.54
1:A:29:VAL:HA	1:A:44:LYS:HA	1.91	0.53
1:A:469:LEU:O	1:A:473:SER:HB3	2.09	0.53
1:B:469:LEU:O	1:B:473:SER:HB3	2.09	0.53
1:B:544:LEU:HD13	1:B:611:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLN:HB3	1:A:301:PHE:HB2	1.92	0.52
1:B:29:VAL:HA	1:B:44:LYS:HA	1.91	0.52
1:A:544:LEU:HD13	1:A:611:LEU:HD23	1.92	0.52
1:B:266:SER:HA	1:B:269:VAL:HB	1.92	0.52
1:A:266:SER:HA	1:A:269:VAL:HB	1.92	0.52
1:B:271:PRO:HB2	1:B:307:ILE:HD11	1.92	0.52
1:B:297:GLN:HB3	1:B:301:PHE:HB2	1.92	0.51
1:A:271:PRO:HB2	1:A:307:ILE:HD11	1.92	0.51
1:B:600:VAL:O	1:B:604:LEU:HB2	2.11	0.51
1:A:243:PHE:O	1:A:255:SER:N	2.40	0.51
1:A:487:ILE:HD11	1:A:511:TRP:HB3	1.93	0.51
1:B:487:ILE:HD11	1:B:511:TRP:HB3	1.93	0.50
1:A:600:VAL:O	1:A:604:LEU:HB2	2.11	0.50
1:A:351:SER:HB2	1:A:390:SER:H	1.77	0.50
1:A:417:GLN:HB3	1:A:580:TYR:HB3	1.93	0.50
1:A:629:LEU:HA	1:A:632:ILE:HD12	1.94	0.50
1:A:498:MET:HB2	1:A:503:SER:HB2	1.94	0.50
1:B:629:LEU:HA	1:B:632:ILE:HD12	1.94	0.50
1:B:417:GLN:HB3	1:B:580:TYR:HB3	1.93	0.50
1:B:560:LEU:HB3	1:B:589:ILE:HG23	1.93	0.49
1:A:334:LEU:HD22	1:A:364:PRO:HA	1.94	0.49
1:B:587:VAL:HA	1:B:590:ILE:HD12	1.94	0.49
1:B:334:LEU:HD22	1:B:364:PRO:HA	1.94	0.49
1:B:248:MET:HG3	1:B:422:GLN:HE21	1.78	0.49
1:B:351:SER:HB2	1:B:390:SER:H	1.77	0.49
1:B:498:MET:HB2	1:B:503:SER:HB2	1.94	0.49
1:A:48:LEU:CD1	1:A:48:LEU:C	2.75	0.48
1:B:351:SER:HA	1:B:389:LYS:HB2	1.95	0.48
1:A:587:VAL:HA	1:A:590:ILE:HD12	1.94	0.48
1:A:351:SER:HA	1:A:389:LYS:HB2	1.95	0.48
1:A:560:LEU:HB3	1:A:589:ILE:HG23	1.93	0.48
1:A:431:VAL:HG22	1:A:564:ALA:HB1	1.96	0.48
1:A:476:LEU:HD22	1:A:632:ILE:HG23	1.96	0.48
1:A:248:MET:HG3	1:A:422:GLN:HE21	1.78	0.48
1:B:431:VAL:HG22	1:B:564:ALA:HB1	1.96	0.48
1:B:476:LEU:HD22	1:B:632:ILE:HG23	1.96	0.48
1:B:231:HIS:HA	1:B:234:ILE:HD12	1.96	0.47
1:A:403:LEU:HD22	1:A:407:VAL:HG11	1.95	0.47
1:A:231:HIS:HA	1:A:234:ILE:HD12	1.96	0.47
1:B:403:LEU:HD22	1:B:407:VAL:HG11	1.95	0.47
1:B:191:GLU:HA	1:B:196:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:HA	1:B:386:LEU:HB3	1.97	0.46
1:A:191:GLU:HA	1:A:196:LYS:HD2	1.98	0.46
1:A:645:LYS:NZ	1:A:649:GLU:OE2	2.45	0.46
1:B:527:ILE:O	1:B:531:GLU:CB	2.64	0.46
1:A:317:ASN:HA	1:A:386:LEU:HB3	1.97	0.45
1:A:189:ALA:O	1:A:193:PHE:N	2.48	0.45
1:B:645:LYS:NZ	1:B:649:GLU:OE2	2.46	0.45
1:A:469:LEU:HD22	1:A:625:VAL:HG13	1.98	0.45
1:B:349:THR:HA	1:B:352:GLN:HB3	1.99	0.45
1:B:331:ASP:OD1	1:B:331:ASP:N	2.49	0.45
1:B:353:GLU:HB3	1:B:387:PHE:HB2	1.98	0.45
1:A:356:SER:OG	1:A:360:ILE:N	2.41	0.44
1:A:353:GLU:HB3	1:A:387:PHE:HB2	1.98	0.44
1:B:469:LEU:HD22	1:B:625:VAL:HG13	1.98	0.44
1:B:547:SER:HB2	1:B:607:HIS:CE1	2.52	0.44
1:A:527:ILE:O	1:A:531:GLU:CB	2.64	0.44
1:A:547:SER:HB2	1:A:607:HIS:CE1	2.52	0.43
1:B:634:GLU:O	1:B:638:THR:OG1	2.26	0.43
1:A:201:THR:O	1:A:287:ARG:NE	2.38	0.43
1:A:349:THR:HA	1:A:352:GLN:HB3	1.99	0.43
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.86	0.43
1:A:331:ASP:N	1:A:331:ASP:OD1	2.49	0.43
1:A:338:GLN:HA	1:A:352:GLN:HE22	1.84	0.43
1:B:338:GLN:HA	1:B:352:GLN:HE22	1.84	0.43
1:A:275:TRP:CE2	1:A:279:MET:HG3	2.54	0.43
1:A:26:PHE:HB3	1:A:44:LYS:HD3	2.01	0.43
1:B:189:ALA:O	1:B:193:PHE:N	2.48	0.43
1:B:356:SER:OG	1:B:360:ILE:N	2.41	0.43
1:B:26:PHE:HB3	1:B:44:LYS:HD3	2.01	0.43
1:B:48:LEU:CD1	1:B:48:LEU:C	2.75	0.43
1:A:20:ARG:HA	1:A:30:CYS:HA	2.01	0.42
1:A:356:SER:N	1:A:360:ILE:O	2.50	0.42
1:B:275:TRP:CE2	1:B:279:MET:HG3	2.54	0.42
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.92	0.42
1:B:356:SER:N	1:B:360:ILE:O	2.50	0.42
1:A:484:HIS:HA	1:A:487:ILE:HG22	2.01	0.42
1:B:484:HIS:HA	1:B:487:ILE:HG22	2.01	0.42
1:B:420:ILE:HA	1:B:423:LEU:HB2	2.02	0.42
1:A:258:LEU:HD12	1:A:259:PRO:HD2	2.01	0.41
1:B:601:LEU:HA	1:B:601:LEU:HD23	1.86	0.41
1:A:420:ILE:HA	1:A:423:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ARG:HB3	1:A:578:HIS:HB2	2.02	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG11	2.03	0.41
1:B:20:ARG:HA	1:B:30:CYS:HA	2.01	0.41
1:B:258:LEU:HD12	1:B:259:PRO:HD2	2.01	0.41
1:B:574:ARG:HB3	1:B:578:HIS:HB2	2.02	0.41
1:A:28:ASN:O	1:A:45:SER:N	2.52	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG11	2.03	0.41
1:A:292:ASP:N	1:A:297:GLN:O	2.54	0.41
1:B:292:ASP:N	1:B:297:GLN:O	2.54	0.41
1:A:59:CYS:HA	1:A:62:ILE:HD12	2.03	0.40
1:B:21:LEU:N	1:B:29:VAL:O	2.54	0.40
1:B:199:THR:OG1	1:B:200:ALA:N	2.51	0.40
1:B:59:CYS:HA	1:B:62:ILE:HD12	2.03	0.40
1:A:199:THR:OG1	1:A:200:ALA:N	2.51	0.40
1:A:21:LEU:N	1:A:29:VAL:O	2.54	0.40
1:B:199:THR:HG23	1:B:201:THR:H	1.87	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	570/655 (87%)	553 (97%)	17 (3%)	0	100	100
1	B	570/655 (87%)	552 (97%)	18 (3%)	0	100	100
All	All	1140/1310 (87%)	1105 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	528/589 (90%)	528 (100%)	0	100	100
1	B	528/589 (90%)	528 (100%)	0	100	100
All	All	1056/1178 (90%)	1056 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	136	HIS
1	A	352	GLN
1	A	578	HIS
1	A	631	ASN
1	B	108	ASN
1	B	136	HIS
1	B	352	GLN
1	B	578	HIS
1	B	631	ASN

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.