



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:15 PM EDT

PDB ID : 2ETM  
Title : Crystal Structure of Focal Adhesion Kinase Domain Complexed with 7H-Pyrrolo [2,3-d] pyrimidine Derivative  
Authors : Lee, C.C.  
Deposited on : 2005-10-27  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

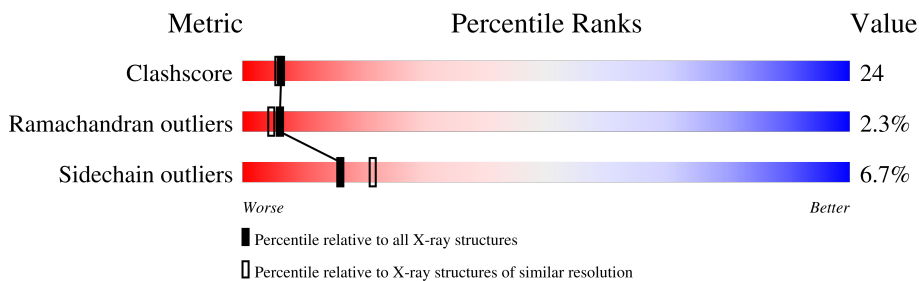
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	281	60% 28% 7%
1	B	281	58% 30% 5% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7PY	B	132	-	-	X	-



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	20	5	3		
2	B	1	Total	C	N	O	0	0
			28	20	5	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	49	Total	O	0	0
			49	49		

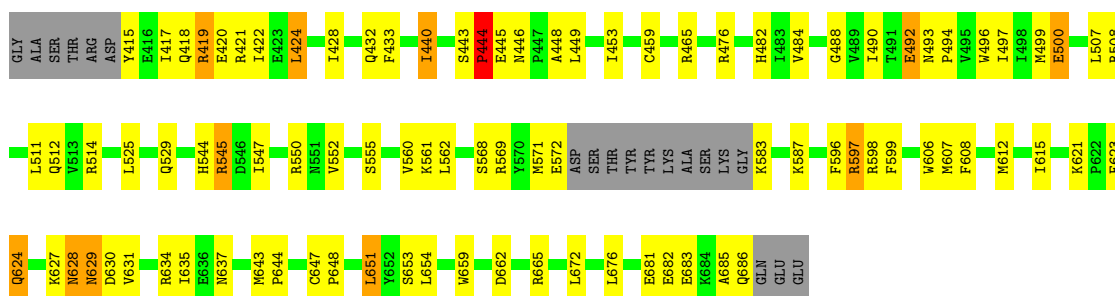
### 3 Residue-property plots

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.

Note EDS was not executed.

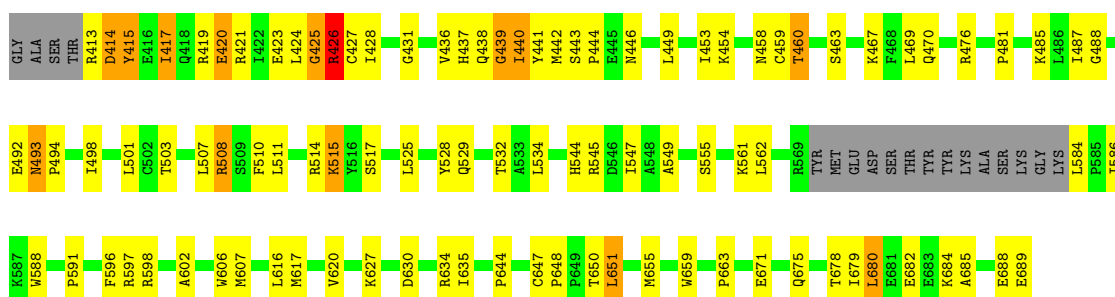
- Molecule 1: Focal adhesion kinase 1

Chain A: 



- Molecule 1: Focal adhesion kinase 1

Chain B: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.70Å 51.92Å 66.88Å 100.08° 103.94° 90.17°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.2 (6.00-2.30)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7PY

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	0.47	0/2158	0.71	0/2916
1	B	0.46	0/2160	0.71	0/2919
All	All	0.46	0/4318	0.71	0/5835

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 [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	2111	0	2123	104	0
1	B	2114	0	2112	93	0
2	A	28	0	19	7	0
2	B	28	0	19	9	0
3	A	70	0	0	5	0
3	B	49	0	0	6	0
All	All	4400	0	4273	207	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 24.

All (207) 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:587:LYS:HD3	1:A:623:PHE:HB2	1.44	0.97
1:A:621:LYS:HD2	1:A:624:GLN:HE22	1.32	0.95
1:A:421:ARG:HH12	1:A:444:PRO:HD2	1.31	0.95
1:A:547:ILE:H	1:A:607:MET:HE3	1.37	0.90
1:B:616:LEU:HD11	1:B:651:LEU:HD13	1.55	0.88
1:A:417:ILE:HG22	1:A:418:GLN:H	1.43	0.84
1:A:621:LYS:HD2	1:A:624:GLN:NE2	1.91	0.84
1:A:648:PRO:HG2	1:A:651:LEU:HB2	1.59	0.84
2:B:132:7PY:HAZ2	3:B:55:HOH:O	1.77	0.84
1:B:525:LEU:O	1:B:529:GLN:HG3	1.77	0.83
1:B:428:ILE:O	2:B:132:7PY:HAX2	1.79	0.82
1:A:424:LEU:HD12	1:A:424:LEU:H	1.45	0.81
1:A:432:GLN:HE22	1:A:571:MET:HG3	1.45	0.80
1:A:421:ARG:NH1	1:A:443:SER:HA	1.95	0.79
1:A:432:GLN:NE2	1:A:571:MET:HG3	1.98	0.79
1:A:612:MET:HE1	1:A:676:LEU:HD11	1.66	0.77
1:B:419:ARG:HG2	1:B:419:ARG:HH11	1.49	0.77
1:A:587:LYS:HE2	1:A:623:PHE:O	1.84	0.76
2:B:132:7PY:HAZ3	2:B:132:7PY:HBB2	1.69	0.75
1:A:525:LEU:O	1:A:529:GLN:HG3	1.85	0.75
1:A:421:ARG:HH12	1:A:444:PRO:CD	1.99	0.75
1:B:413:ARG:O	1:B:415:TYR:N	2.20	0.74
2:A:131:7PY:HBB2	2:A:131:7PY:HAZ3	1.69	0.74
2:A:131:7PY:HAR	2:A:131:7PY:NAG	2.03	0.73
1:B:684:LYS:O	1:B:688:GLU:HG3	1.88	0.73
1:A:630:ASP:O	1:A:634:ARG:HG3	1.89	0.72
1:A:422:ILE:HD12	1:A:490:ILE:HD11	1.73	0.70
1:A:552:VAL:CG1	1:A:560:VAL:HG13	2.21	0.69
1:B:425:GLY:O	1:B:426:ARG:HB3	1.90	0.69
1:B:438:GLN:O	1:B:439:GLY:O	2.11	0.69
1:A:417:ILE:HG22	1:A:418:GLN:N	2.09	0.66
2:B:132:7PY:HAR	2:B:132:7PY:NAG	2.11	0.66
1:A:662:ASP:H	1:A:665:ARG:NH2	1.94	0.66
1:B:547:ILE:H	1:B:607:MET:HE3	1.60	0.66
1:A:612:MET:CE	1:A:676:LEU:HD11	2.25	0.65
1:B:671:GLU:HG2	1:B:675:GLN:HE21	1.61	0.65
1:B:544:HIS:O	1:B:545:ARG:HB2	1.95	0.65
1:B:443:SER:HB2	1:B:446:ASN:O	1.97	0.65
1:B:644:PRO:HG2	1:B:647:CYS:HB2	1.78	0.65
1:B:436:VAL:HG22	1:B:454:LYS:HG2	1.78	0.64
1:A:433:PHE:HZ	1:A:571:MET:HE3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LEU:O	1:B:586:ILE:HD12	1.98	0.64
1:B:493:ASN:HD22	1:B:493:ASN:N	1.95	0.63
1:A:571:MET:O	1:A:572:GLU:HB2	1.98	0.63
1:A:418:GLN:NE2	1:A:421:ARG:HE	1.95	0.63
1:B:436:VAL:HG21	2:B:132:7PY:CAP	2.29	0.63
1:A:662:ASP:HB3	1:A:665:ARG:NE	2.14	0.63
1:A:432:GLN:OE1	1:A:571:MET:HG3	1.99	0.63
1:A:683:GLU:HA	1:A:683:GLU:OE1	1.99	0.62
1:B:421:ARG:CZ	1:B:444:PRO:HG3	2.29	0.62
1:A:685:ALA:O	1:A:686:GLN:HG3	1.98	0.62
1:A:612:MET:HE2	1:A:676:LEU:HD21	1.81	0.62
1:B:586:ILE:HD12	1:B:586:ILE:H	1.65	0.62
1:A:421:ARG:NH1	1:A:444:PRO:HD2	2.11	0.61
1:A:497:ILE:HG22	1:A:499:MET:HE3	1.82	0.61
1:B:678:THR:O	1:B:682:GLU:HG3	2.00	0.61
1:B:428:ILE:O	2:B:132:7PY:CAX	2.49	0.61
1:B:481:PRO:O	1:B:561:LYS:HE2	2.01	0.61
1:A:419:ARG:NH1	1:A:494:PRO:HD2	2.16	0.61
1:A:421:ARG:HH11	1:A:443:SER:HA	1.66	0.61
1:A:440:ILE:HD13	1:A:448:ALA:HB1	1.82	0.60
1:A:432:GLN:HE22	1:A:571:MET:CG	2.13	0.60
1:A:419:ARG:HH12	1:A:493:ASN:C	2.04	0.60
1:A:421:ARG:NH1	1:A:444:PRO:CD	2.64	0.60
1:B:528:TYR:O	1:B:532:THR:HG23	2.02	0.60
1:A:428:ILE:O	2:A:131:7PY:HAX2	2.02	0.60
1:A:444:PRO:C	1:A:446:ASN:H	2.05	0.59
1:A:552:VAL:HG13	1:A:561:LYS:O	2.02	0.59
1:B:413:ARG:C	1:B:415:TYR:H	2.05	0.59
1:A:547:ILE:N	1:A:607:MET:HE3	2.13	0.59
1:B:616:LEU:HD13	1:B:647:CYS:SG	2.42	0.59
1:A:432:GLN:CD	1:A:571:MET:HG3	2.23	0.59
2:B:132:7PY:HAX3	2:B:132:7PY:HAN	1.85	0.58
1:A:508:ARG:O	1:A:512:GLN:HG3	2.04	0.58
1:B:596:PHE:HB2	1:B:598:ARG:HD3	1.83	0.58
1:A:415:TYR:CE1	1:A:476:ARG:HG3	2.39	0.58
1:A:545:ARG:C	1:A:607:MET:HE1	2.24	0.57
1:B:648:PRO:HG2	1:B:651:LEU:HB2	1.86	0.57
1:B:510:PHE:O	1:B:514:ARG:HG2	2.04	0.57
1:B:492:GLU:OE2	1:B:492:GLU:HA	2.04	0.57
1:A:544:HIS:O	1:A:545:ARG:HB2	2.05	0.56
1:B:515:LYS:NZ	1:B:515:LYS:HB3	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LEU:HD11	1:A:672:LEU:HD23	1.88	0.55
1:A:624:GLN:HA	1:A:624:GLN:OE1	2.07	0.55
1:B:440:ILE:HG13	1:B:441:TYR:N	2.21	0.54
1:B:650:THR:HG22	1:B:679:ILE:HD11	1.90	0.54
1:A:432:GLN:NE2	1:A:568:SER:O	2.41	0.54
2:A:131:7PY:NAG	2:A:131:7PY:CAR	2.66	0.54
1:A:631:VAL:O	1:A:635:ILE:HG12	2.07	0.54
1:A:492:GLU:O	1:A:493:ASN:HB2	2.07	0.53
1:A:444:PRO:O	1:A:446:ASN:N	2.42	0.53
1:A:552:VAL:HG11	1:A:560:VAL:HG13	1.91	0.52
1:B:443:SER:CB	1:B:446:ASN:HB2	2.39	0.52
1:A:545:ARG:HD3	1:A:599:PHE:CG	2.45	0.52
1:A:418:GLN:CG	1:A:421:ARG:HD2	2.40	0.52
1:B:617:MET:O	1:B:620:VAL:HG23	2.09	0.52
1:B:453:ILE:HG12	1:B:498:ILE:HD12	1.91	0.51
1:A:418:GLN:NE2	1:A:421:ARG:NE	2.59	0.51
1:A:608:PHE:CZ	1:A:612:MET:HE3	2.45	0.51
1:A:612:MET:CE	1:A:676:LEU:HD21	2.39	0.51
1:B:415:TYR:CE1	1:B:476:ARG:HG3	2.46	0.51
1:B:417:ILE:HD11	1:B:488:GLY:HA3	1.91	0.51
1:B:421:ARG:HD3	1:B:442:MET:O	2.11	0.51
1:A:628:ASN:O	1:A:631:VAL:N	2.44	0.50
1:B:663:PRO:HB3	3:B:117:HOH:O	2.10	0.50
1:B:425:GLY:O	1:B:426:ARG:CB	2.57	0.50
1:A:550:ARG:HA	3:A:109:HOH:O	2.11	0.50
1:B:616:LEU:CD1	1:B:655:MET:HE1	2.41	0.50
1:B:420:GLU:H	1:B:420:GLU:CD	2.15	0.49
1:B:617:MET:SD	1:B:644:PRO:HB3	2.52	0.49
1:A:493:ASN:HA	1:A:494:PRO:C	2.33	0.49
1:A:545:ARG:HD3	1:A:599:PHE:CD2	2.47	0.49
1:B:476:ARG:HG2	1:B:476:ARG:O	2.12	0.49
1:A:428:ILE:HD12	2:A:131:7PY:CAU	2.43	0.49
1:B:424:LEU:H	1:B:424:LEU:HD23	1.76	0.49
1:A:628:ASN:O	1:A:630:ASP:N	2.46	0.49
1:A:453:ILE:HD12	1:A:453:ILE:N	2.28	0.48
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.77	0.48
1:A:508:ARG:HB2	3:A:109:HOH:O	2.14	0.48
1:B:508:ARG:HD2	1:B:549:ALA:HB3	1.95	0.48
1:A:428:ILE:O	1:A:428:ILE:CG2	2.61	0.48
1:B:508:ARG:HG3	1:B:508:ARG:HH11	1.77	0.48
1:B:588:TRP:O	1:B:607:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:CG2	1:A:499:MET:HE3	2.43	0.48
1:B:606:TRP:CE3	1:B:659:TRP:HA	2.47	0.48
1:B:427:CYS:HB2	1:B:437:HIS:CE1	2.49	0.47
1:A:596:PHE:C	1:A:597:ARG:HD2	2.34	0.47
1:B:426:ARG:HE	1:B:438:GLN:HE22	1.62	0.47
1:B:680:LEU:O	1:B:684:LYS:HG3	2.14	0.47
1:A:421:ARG:HH12	1:A:443:SER:HA	1.75	0.47
1:A:662:ASP:H	1:A:665:ARG:HH21	1.62	0.47
1:A:682:GLU:O	1:A:686:GLN:HB2	2.15	0.47
1:B:414:ASP:OD2	1:B:476:ARG:NH2	2.47	0.47
1:B:419:ARG:HG2	1:B:419:ARG:NH1	2.26	0.47
1:B:421:ARG:NE	1:B:444:PRO:HG3	2.29	0.47
1:B:547:ILE:N	1:B:607:MET:HE3	2.27	0.47
1:B:616:LEU:CD1	1:B:651:LEU:HD13	2.36	0.47
1:B:634:ARG:HH11	1:B:634:ARG:HG3	1.80	0.47
1:B:426:ARG:NE	1:B:438:GLN:HE22	2.13	0.46
1:B:515:LYS:HB3	1:B:515:LYS:HZ2	1.80	0.46
1:A:490:ILE:HD12	1:A:496:TRP:CE3	2.51	0.46
1:B:463:SER:O	1:B:467:LYS:HG3	2.14	0.46
1:A:415:TYR:HB3	1:A:488:GLY:HA2	1.96	0.46
1:B:501:LEU:HD13	1:B:503:THR:N	2.31	0.46
2:B:132:7PY:NAG	2:B:132:7PY:CAR	2.70	0.46
1:B:685:ALA:O	1:B:689:GLU:HG3	2.16	0.46
1:B:431:GLY:HA3	3:B:116:HOH:O	2.15	0.45
1:A:417:ILE:CG2	1:A:418:GLN:N	2.80	0.45
1:A:417:ILE:CG2	1:A:418:GLN:H	2.21	0.45
1:B:458:ASN:C	1:B:460:THR:H	2.20	0.45
1:A:569:ARG:O	1:A:583:LYS:O	2.35	0.45
1:A:484:VAL:HG23	1:A:562:LEU:O	2.17	0.45
1:B:507:LEU:O	1:B:511:LEU:HG	2.17	0.44
1:A:424:LEU:H	1:A:424:LEU:CD1	2.24	0.44
1:B:591:PRO:HG3	1:B:635:ILE:HG21	2.00	0.44
1:B:534:LEU:HA	1:B:534:LEU:HD23	1.67	0.44
1:A:627:LYS:O	1:A:630:ASP:HB2	2.17	0.44
1:A:507:LEU:HD21	1:A:615:ILE:HG12	1.99	0.44
1:B:421:ARG:CD	1:B:444:PRO:HG3	2.48	0.44
1:B:493:ASN:HA	1:B:494:PRO:C	2.38	0.44
1:B:647:CYS:SG	1:B:655:MET:HE3	2.58	0.43
1:A:587:LYS:HG3	3:A:108:HOH:O	2.17	0.43
1:B:617:MET:HB3	1:B:620:VAL:HB	1.99	0.43
1:A:419:ARG:NH1	1:A:493:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ASN:O	1:A:629:ASN:C	2.56	0.43
1:B:421:ARG:HD2	1:B:444:PRO:HG3	2.00	0.43
1:A:419:ARG:HH12	1:A:494:PRO:N	2.16	0.43
1:B:501:LEU:HD13	1:B:501:LEU:C	2.38	0.43
1:B:417:ILE:HG21	1:B:441:TYR:CZ	2.53	0.43
1:B:493:ASN:N	1:B:493:ASN:ND2	2.63	0.43
1:A:419:ARG:HE	1:A:419:ARG:HB3	1.74	0.43
1:B:508:ARG:NE	3:B:115:HOH:O	2.46	0.43
1:B:485:LYS:NZ	1:B:487:ILE:HD13	2.34	0.42
1:B:426:ARG:NE	1:B:438:GLN:NE2	2.68	0.42
1:B:627:LYS:HB2	1:B:630:ASP:OD2	2.19	0.42
1:A:459:CYS:HB2	3:A:74:HOH:O	2.19	0.42
1:B:616:LEU:HD12	1:B:655:MET:HE1	2.02	0.42
1:A:644:PRO:HB2	1:A:647:CYS:HB2	2.00	0.42
1:B:501:LEU:HD12	1:B:503:THR:HG22	2.02	0.42
1:A:627:LYS:O	1:A:628:ASN:C	2.58	0.42
1:A:421:ARG:NH1	1:A:444:PRO:HD3	2.33	0.42
1:A:465:ARG:NH2	3:A:4:HOH:O	2.52	0.42
1:A:482:HIS:ND1	1:A:529:GLN:HB3	2.35	0.42
1:A:550:ARG:HD3	1:A:569:ARG:CZ	2.50	0.42
1:B:597:ARG:HG2	3:B:64:HOH:O	2.20	0.42
1:A:552:VAL:HG11	1:A:560:VAL:CG1	2.49	0.41
1:B:423:GLU:O	1:B:439:GLY:HA3	2.20	0.41
2:B:132:7PY:HAX3	2:B:132:7PY:CAN	2.50	0.41
1:A:444:PRO:C	1:A:446:ASN:N	2.72	0.41
1:A:500:GLU:O	2:A:131:7PY:HAB	2.20	0.41
1:A:643:MET:HA	1:A:644:PRO:HD3	1.93	0.41
1:B:508:ARG:HH11	1:B:508:ARG:CG	2.34	0.41
1:A:507:LEU:O	1:A:511:LEU:HG	2.20	0.41
1:B:415:TYR:HE1	1:B:476:ARG:HG3	1.84	0.41
1:A:544:HIS:O	1:A:545:ARG:CB	2.69	0.41
1:A:422:ILE:CD1	1:A:490:ILE:HD11	2.48	0.41
1:B:634:ARG:HG3	1:B:634:ARG:NH1	2.36	0.41
1:B:458:ASN:O	1:B:460:THR:N	2.51	0.41
1:A:583:LYS:HE3	1:A:583:LYS:HB2	1.96	0.41
1:B:424:LEU:HD23	1:B:424:LEU:N	2.35	0.41
1:B:438:GLN:O	1:B:438:GLN:HG3	2.21	0.41
1:B:602:ALA:HB3	3:B:117:HOH:O	2.20	0.41
2:A:131:7PY:HAX3	2:A:131:7PY:HAN	2.03	0.41
1:A:443:SER:OG	1:A:446:ASN:HB3	2.22	0.40
1:A:606:TRP:CE3	1:A:659:TRP:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:NH1	1:B:444:PRO:HG3	2.36	0.40
1:B:423:GLU:O	1:B:439:GLY:CA	2.69	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 X-ray entries followed by that with respect to entries of similar resolution.

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	258/281 (92%)	234 (91%)	17 (7%)	7 (3%)	5	3
1	B	259/281 (92%)	240 (93%)	14 (5%)	5 (2%)	8	7
All	All	517/562 (92%)	474 (92%)	31 (6%)	12 (2%)	6	5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	PRO
1	A	445	GLU
1	B	414	ASP
1	B	439	GLY
1	A	629	ASN
1	B	426	ARG
1	B	459	CYS
1	A	500	GLU
1	A	492	GLU
1	A	545	ARG
1	A	628	ASN
1	B	425	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	233/248 (94%)	219 (94%)	14 (6%)	19	26
1	B	233/248 (94%)	216 (93%)	17 (7%)	14	18
All	All	466/496 (94%)	435 (93%)	31 (7%)	16	21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	ARG
1	A	420	GLU
1	A	424	LEU
1	A	440	ILE
1	A	444	PRO
1	A	449	LEU
1	A	555	SER
1	A	597	ARG
1	A	598	ARG
1	A	624	GLN
1	A	637	ASN
1	A	651	LEU
1	A	653	SER
1	A	681	GLU
1	B	415	TYR
1	B	417	ILE
1	B	420	GLU
1	B	426	ARG
1	B	440	ILE
1	B	449	LEU
1	B	460	THR
1	B	469	LEU
1	B	470	GLN
1	B	493	ASN
1	B	508	ARG
1	B	515	LYS
1	B	517	SER

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Mol	Chain	Res	Type
1	B	555	SER
1	B	562	LEU
1	B	651	LEU
1	B	680	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	437	HIS
1	A	458	ASN
1	B	418	GLN
1	B	438	GLN
1	B	470	GLN
1	B	493	ASN
1	B	629	ASN
1	B	675	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	7PY	A	131	-	28,31,31	2.16	7 (25%)	34,43,43	2.64	13 (38%)
2	7PY	B	132	-	28,31,31	2.16	7 (25%)	34,43,43	2.63	13 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7PY	A	131	-	-	4/10/14/14	0/4/4/4
2	7PY	B	132	-	-	4/10/14/14	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	131	7PY	CAH-NAG	4.98	1.40	1.33
2	B	132	7PY	CAH-NAG	4.96	1.40	1.33
2	A	131	7PY	CAJ-NAQ	4.89	1.40	1.34
2	B	132	7PY	CAJ-NAQ	4.87	1.40	1.34
2	A	131	7PY	CAD-NAC	4.23	1.40	1.34
2	B	132	7PY	CAD-NAC	4.18	1.40	1.34
2	A	131	7PY	CAP-NAQ	4.09	1.40	1.32
2	B	132	7PY	CAP-NAQ	4.07	1.40	1.32
2	B	132	7PY	CAB-NAC	3.86	1.40	1.32
2	A	131	7PY	CAB-NAC	3.84	1.40	1.32
2	B	132	7PY	CAF-NAE	-3.16	1.33	1.40
2	A	131	7PY	CAF-NAE	-3.14	1.33	1.40
2	A	131	7PY	CAK-CAL	-2.55	1.33	1.37
2	B	132	7PY	CAK-CAL	-2.50	1.33	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	131	7PY	NAC-CAD-NAG	-7.91	118.88	126.52
2	B	132	7PY	NAC-CAD-NAG	-7.77	119.02	126.52
2	A	131	7PY	CAM-CAJ-NAQ	-6.34	116.74	122.24
2	B	132	7PY	CAM-CAJ-NAQ	-6.30	116.77	122.24
2	B	132	7PY	CAP-NAQ-CAJ	4.40	122.36	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	131	7PY	CAD-NAG-CAH	4.36	120.23	115.28
2	A	131	7PY	CAP-NAQ-CAJ	4.34	122.28	116.73
2	B	132	7PY	CBB-OBA-CAU	-4.14	111.28	117.53
2	B	132	7PY	CAD-NAG-CAH	3.99	119.81	115.28
2	A	131	7PY	CBB-OBA-CAU	-3.87	111.68	117.53
2	A	131	7PY	CAX-OAW-CAS	-3.39	112.42	117.53
2	B	132	7PY	CAB-NAC-CAD	3.37	120.88	115.88
2	A	131	7PY	CAB-NAC-CAD	3.32	120.81	115.88
2	B	132	7PY	CAX-OAW-CAS	-3.29	112.56	117.53
2	B	132	7PY	OBA-CAU-CAT	3.19	120.76	115.16
2	A	131	7PY	OBA-CAU-CAT	3.03	120.49	115.16
2	A	131	7PY	CAO-CAP-NAQ	-2.94	119.44	123.94
2	B	132	7PY	CAO-CAP-NAQ	-2.92	119.46	123.94
2	B	132	7PY	OAW-CAS-CAR	-2.87	119.17	124.12
2	B	132	7PY	OBA-CAU-CAV	-2.79	119.32	124.12
2	A	131	7PY	OAW-CAS-CAT	2.78	120.05	115.16
2	B	132	7PY	OAW-CAS-CAT	2.77	120.03	115.16
2	A	131	7PY	OBA-CAU-CAV	-2.73	119.43	124.12
2	A	131	7PY	OAW-CAS-CAR	-2.44	119.92	124.12
2	B	132	7PY	CAA-CAB-NAC	-2.32	119.72	124.08
2	A	131	7PY	CAA-CAB-NAC	-2.29	119.77	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

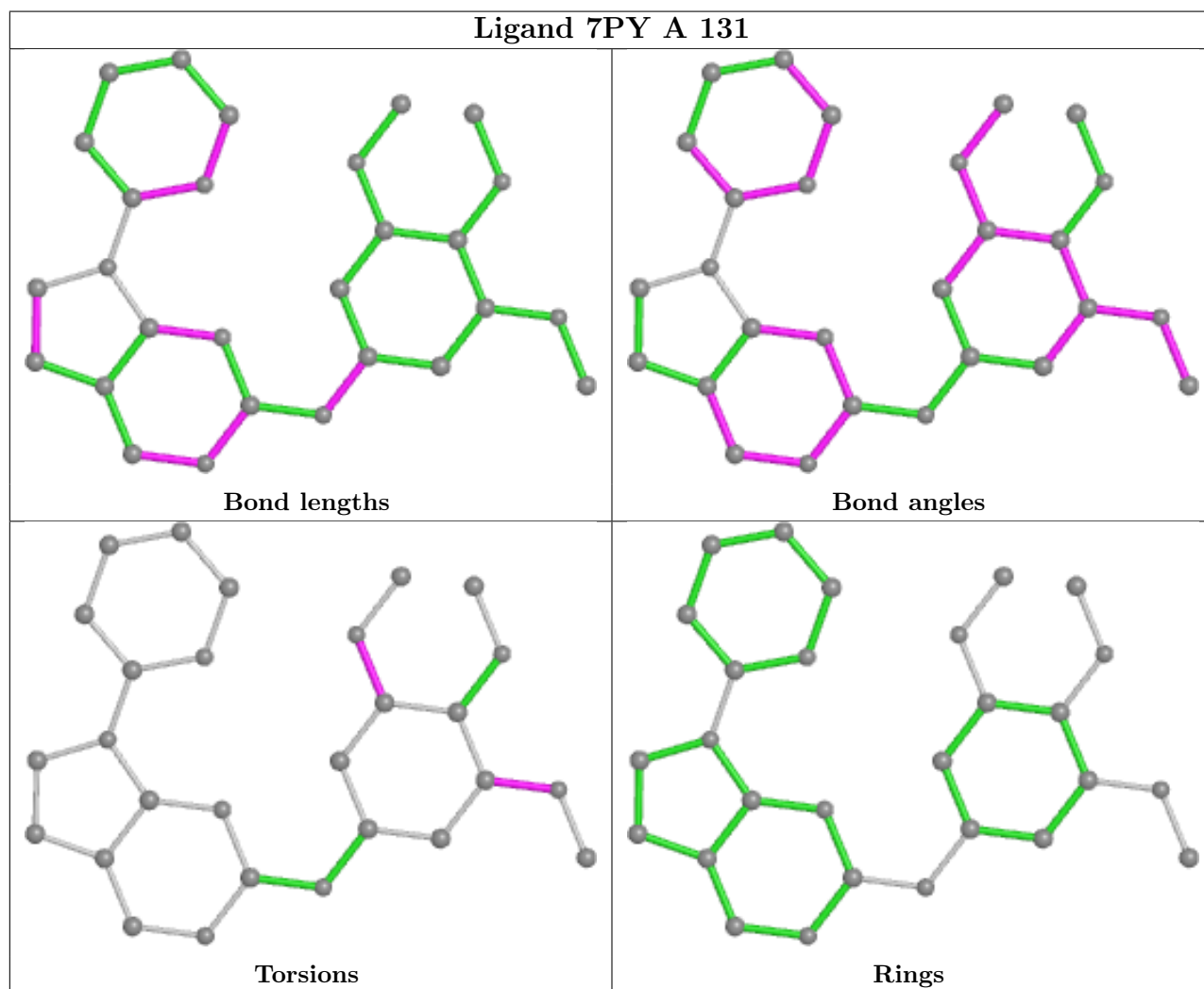
Mol	Chain	Res	Type	Atoms
2	B	132	7PY	CAT-CAS-OAW-CAX
2	B	132	7PY	CAV-CAU-OBA-CBB
2	A	131	7PY	CAR-CAS-OAW-CAX
2	A	131	7PY	CAV-CAU-OBA-CBB
2	A	131	7PY	CAT-CAS-OAW-CAX
2	B	132	7PY	CAR-CAS-OAW-CAX
2	A	131	7PY	CAT-CAU-OBA-CBB
2	B	132	7PY	CAT-CAU-OBA-CBB

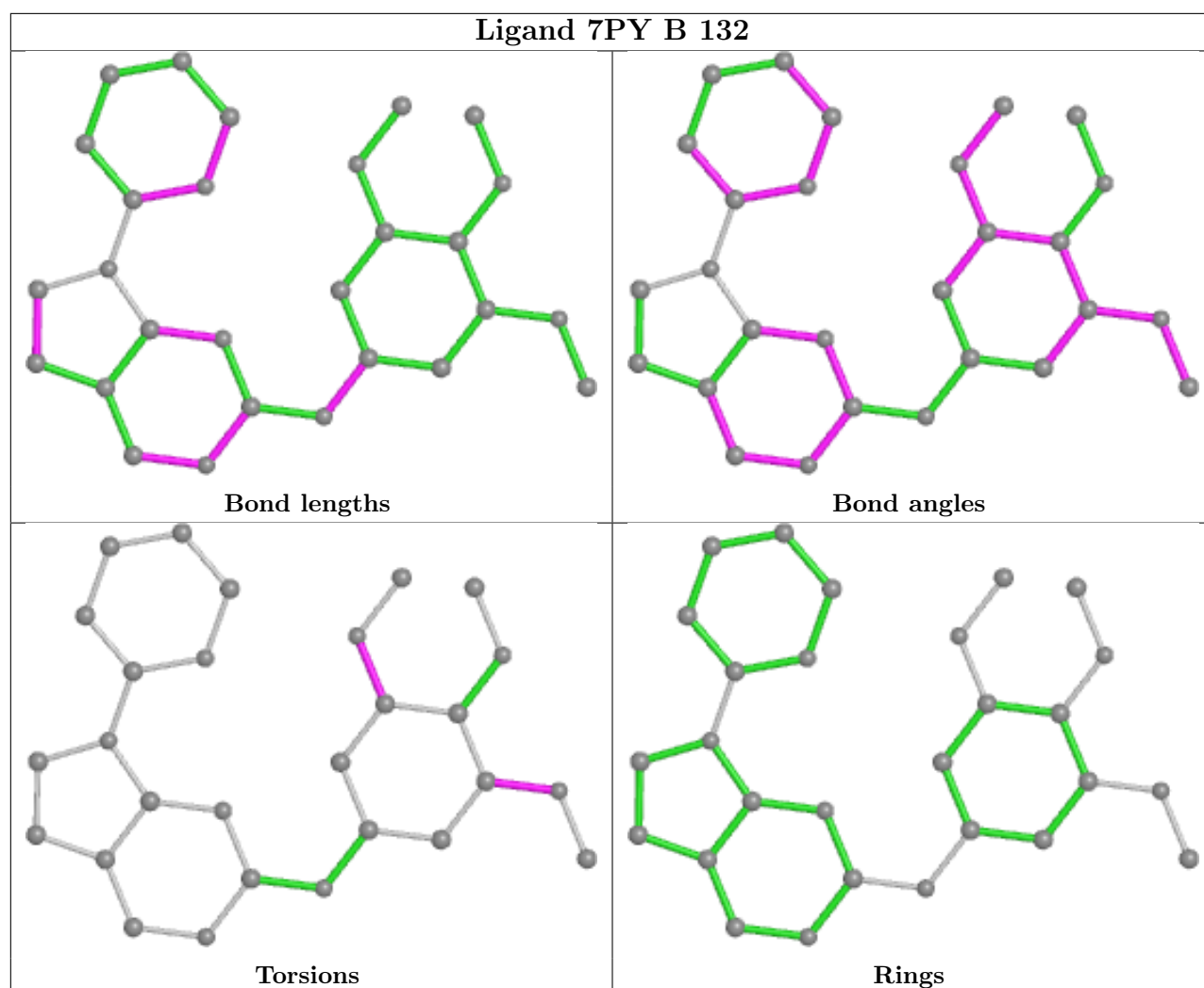
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	131	7PY	7	0
2	B	132	7PY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.