Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1K2P
Title	:	Crystal structure of Bruton's tyrosine kinase domain
Authors	:	Mao, C.; Zhou, M.; Uckun, F.M.
Deposited on	:	2001-09-28
Resolution	:	2.10 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

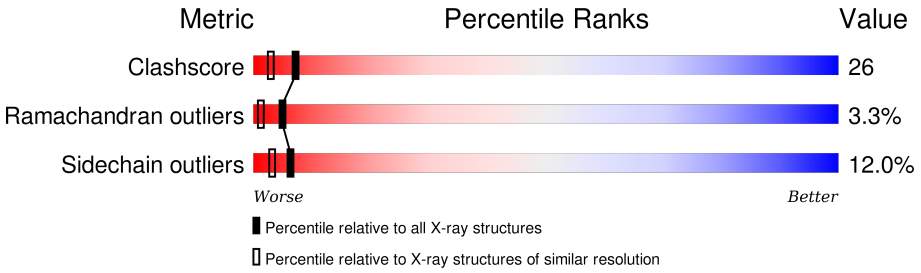
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 on the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	263	49% 41% 7% •
1	B	263	44% 46% 8% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2087	1337	347	385	18			
1	B	258	Total	C	N	O	S	0	0	0
			2091	1340	348	385	18			

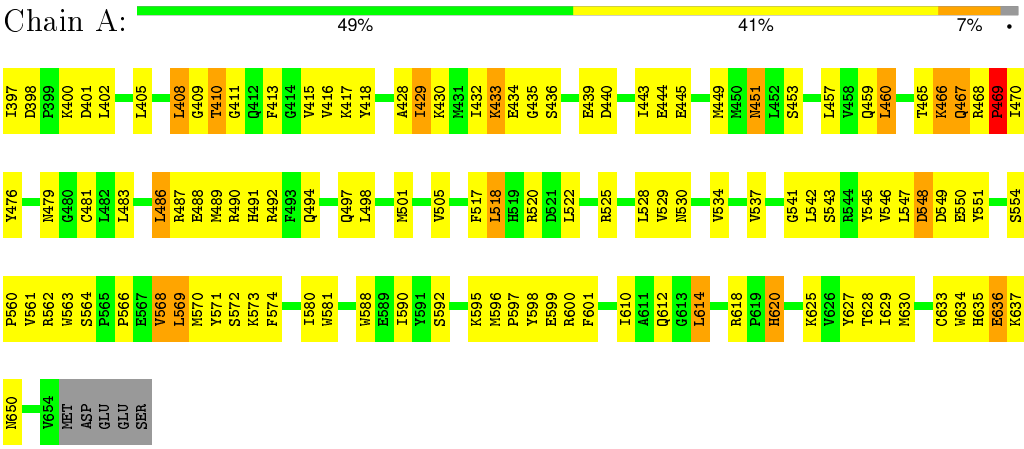
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

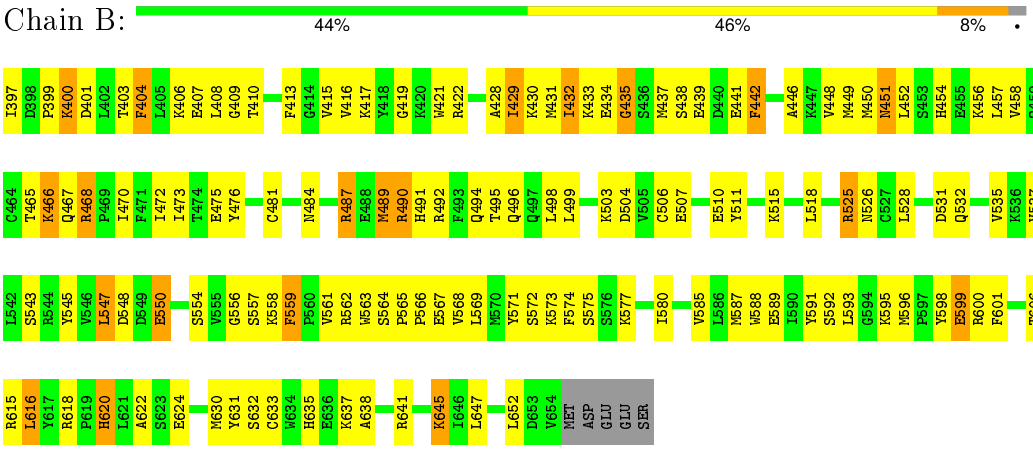
- Molecule 1: Tyrosine-protein kinase BTK

Chain A:



- Molecule 1: Tyrosine-protein kinase BTK

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.00Å 104.00Å 116.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.0 (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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	0.38	0/2134	0.67	0/2878
1	B	0.36	0/2138	0.63	0/2882
All	All	0.37	0/4272	0.65	0/5760

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	2087	0	2052	114	2
1	B	2091	0	2063	116	2
All	All	4178	0	4115	216	2

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 26.

All (216) 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:408:LEU:HB3	1:A:416:VAL:HG23	1.30	1.07
1:A:430:LYS:HB3	1:A:472:ILE:HG22	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LYS:HA	1:A:466:LYS:HE2	1.55	0.88
1:B:592:SER:HB3	1:B:595:LYS:HB2	1.56	0.87
1:A:416:VAL:HG12	1:A:430:LYS:HB2	1.58	0.85
1:A:449:MET:SD	1:A:541:GLY:HA2	2.17	0.85
1:A:525:ARG:HB2	1:B:433:LYS:HE2	1.59	0.83
1:B:587:MET:HE3	1:B:630:MET:HA	1.61	0.82
1:A:559:PHE:HD1	1:A:560:PRO:HD2	1.45	0.81
1:B:463:VAL:HG12	1:B:472:ILE:HG23	1.64	0.79
1:B:407:GLU:HA	1:B:417:LYS:HA	1.65	0.79
1:A:468:ARG:HB3	1:A:469:PRO:HD2	1.67	0.77
1:B:413:PHE:HB2	1:B:430:LYS:HE2	1.65	0.77
1:A:408:LEU:HB3	1:A:416:VAL:CG2	2.15	0.75
1:A:612:GLN:HB2	1:A:614:LEU:HD22	1.67	0.74
1:B:567:GLU:HB3	1:B:573:LYS:HB3	1.69	0.74
1:A:518:LEU:O	1:A:543:SER:HB3	1.88	0.74
1:A:413:PHE:HB2	1:A:430:LYS:HE2	1.71	0.73
1:B:458:VAL:HG21	1:B:528:LEU:HD12	1.72	0.72
1:B:434:GLU:HB2	1:B:468:ARG:HA	1.73	0.71
1:B:461:TYR:HB2	1:B:473:ILE:HG22	1.71	0.71
1:A:457:LEU:HD23	1:A:537:VAL:CG2	2.23	0.68
1:B:397:ILE:N	1:B:465:THR:HG1	1.92	0.68
1:B:417:LYS:HB2	1:B:429:ILE:HG23	1.75	0.68
1:A:435:GLY:HA3	1:B:596:MET:HG3	1.75	0.68
1:B:416:VAL:HA	1:B:429:ILE:O	1.94	0.67
1:A:416:VAL:HG12	1:A:430:LYS:CB	2.26	0.66
1:A:551:TYR:HD2	1:A:574:PHE:HB2	1.60	0.66
1:B:564:SER:HB3	1:B:568:VAL:CG2	2.26	0.66
1:B:408:LEU:HD11	1:B:476:TYR:HE1	1.59	0.66
1:A:415:VAL:HB	1:B:410:THR:OG1	1.96	0.65
1:A:415:VAL:HG22	1:A:416:VAL:H	1.61	0.65
1:B:439:GLU:HA	1:B:442:PHE:HE2	1.61	0.65
1:A:556:GLY:HA3	1:B:557:SER:HA	1.79	0.64
1:B:432:ILE:HG21	1:B:437:MET:HB2	1.80	0.64
1:A:409:GLY:O	1:A:416:VAL:HG22	1.97	0.64
1:A:408:LEU:CB	1:A:416:VAL:HG23	2.18	0.63
1:A:483:LEU:HD23	1:B:433:LYS:HE3	1.81	0.63
1:A:439:GLU:O	1:A:443:ILE:HG12	1.99	0.63
1:A:596:MET:SD	1:B:435:GLY:HA2	2.39	0.63
1:B:494:GLN:HB3	1:B:496:GLN:OE1	1.99	0.62
1:B:503:LYS:O	1:B:507:GLU:HG3	1.99	0.62
1:B:568:VAL:HA	1:B:572:SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:HH11	1:A:543:SER:HA	1.65	0.61
1:B:599:GLU:O	1:B:600:ARG:HB2	2.00	0.61
1:A:558:LYS:HA	1:A:558:LYS:HE2	1.83	0.61
1:A:520:ARG:NH1	1:A:543:SER:HA	2.15	0.61
1:B:457:LEU:HD23	1:B:537:VAL:HG13	1.83	0.61
1:B:490:ARG:NH1	1:B:492:ARG:HD3	2.16	0.60
1:B:632:SER:HA	1:B:635:HIS:CE1	2.36	0.60
1:B:620:HIS:CD2	1:B:620:HIS:H	2.19	0.60
1:A:559:PHE:CZ	1:A:568:VAL:HG13	2.38	0.59
1:B:448:VAL:O	1:B:451:ASN:HB2	2.02	0.59
1:A:551:TYR:CD2	1:A:574:PHE:HB2	2.38	0.59
1:A:460:LEU:HD21	1:A:472:ILE:HG12	1.85	0.58
1:B:409:GLY:O	1:B:415:VAL:HA	2.02	0.58
1:A:562:ARG:HD3	1:A:597:PRO:O	2.03	0.58
1:A:487:ARG:CZ	1:B:434:GLU:HB3	2.33	0.58
1:A:487:ARG:NH2	1:B:434:GLU:HB3	2.19	0.58
1:A:588:TRP:HB2	1:A:630:MET:HE3	1.87	0.57
1:B:598:TYR:O	1:B:601:PHE:HB2	2.04	0.57
1:A:555:VAL:HG11	1:A:572:SER:CB	2.33	0.57
1:B:481:CYS:SG	1:B:484:ASN:OD1	2.63	0.56
1:A:561:VAL:HG13	1:A:569:LEU:HD11	1.87	0.56
1:A:559:PHE:CD1	1:A:560:PRO:HD2	2.33	0.56
1:B:438:SER:HA	1:B:467:GLN:HE22	1.70	0.56
1:A:555:VAL:HG11	1:A:572:SER:OG	2.06	0.56
1:B:460:LEU:HD21	1:B:463:VAL:HG13	1.88	0.56
1:B:620:HIS:N	1:B:620:HIS:CD2	2.74	0.55
1:A:405:LEU:HB3	1:A:418:TYR:CB	2.37	0.55
1:A:494:GLN:HG2	1:A:497:GLN:OE1	2.06	0.55
1:B:645:LYS:O	1:B:645:LYS:HE3	2.07	0.55
1:B:407:GLU:HG2	1:B:417:LYS:HA	1.87	0.55
1:A:530:ASN:HD21	1:A:534:VAL:HB	1.71	0.55
1:B:562:ARG:HB2	1:B:563:TRP:CE3	2.42	0.54
1:B:566:PRO:HG3	1:B:610:ILE:HG22	1.89	0.54
1:A:558:LYS:HZ3	1:A:559:PHE:H	1.56	0.54
1:A:408:LEU:HD11	1:A:476:TYR:CD1	2.42	0.54
1:B:463:VAL:HG23	1:B:465:THR:HG23	1.88	0.54
1:B:458:VAL:HG13	1:B:475:GLU:HB3	1.88	0.54
1:A:444:GLU:HG3	1:A:445:GLU:H	1.71	0.54
1:A:633:CYS:O	1:A:641:ARG:HD2	2.07	0.54
1:A:635:HIS:O	1:A:636:GLU:HB3	2.08	0.54
1:A:635:HIS:HB3	1:A:641:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLU:HA	1:B:442:PHE:CE2	2.42	0.53
1:A:635:HIS:ND1	1:A:635:HIS:O	2.41	0.53
1:B:558:LYS:N	1:B:558:LYS:HD2	2.23	0.53
1:B:564:SER:HB2	1:B:569:LEU:HD21	1.91	0.53
1:B:495:THR:HG23	1:B:591:TYR:HE2	1.74	0.53
1:B:449:MET:SD	1:B:541:GLY:HA2	2.49	0.53
1:A:592:SER:O	1:A:595:LYS:HG2	2.08	0.52
1:A:487:ARG:NH1	1:B:434:GLU:HB3	2.24	0.52
1:A:430:LYS:HB3	1:A:472:ILE:CG2	2.29	0.52
1:B:407:GLU:HG3	1:B:417:LYS:HG2	1.91	0.52
1:B:577:LYS:HG2	1:B:638:ALA:O	2.09	0.52
1:B:588:TRP:CE2	1:B:616:LEU:HG	2.45	0.52
1:B:565:PRO:HD2	1:B:568:VAL:CG2	2.40	0.51
1:A:459:GLN:HG2	1:A:475:GLU:OE2	2.09	0.51
1:A:581:TRP:CE3	1:A:634:TRP:HA	2.45	0.51
1:B:415:VAL:CG2	1:B:431:MET:SD	2.99	0.51
1:B:429:ILE:HD13	1:B:429:ILE:O	2.11	0.51
1:A:415:VAL:HG22	1:A:416:VAL:N	2.25	0.51
1:B:587:MET:HE3	1:B:630:MET:CA	2.38	0.50
1:A:517:PHE:CZ	1:A:543:SER:HB2	2.46	0.50
1:B:561:VAL:HA	1:B:569:LEU:HD21	1.93	0.50
1:A:416:VAL:HA	1:A:429:ILE:O	2.11	0.50
1:B:518:LEU:HD21	1:B:575:SER:O	2.12	0.50
1:A:415:VAL:HG11	1:B:409:GLY:HA2	1.94	0.50
1:B:588:TRP:CD2	1:B:616:LEU:HG	2.47	0.50
1:A:417:LYS:O	1:A:428:ALA:HA	2.11	0.50
1:B:399:PRO:O	1:B:401:ASP:N	2.44	0.50
1:A:465:THR:HG22	1:A:470:ILE:HG23	1.93	0.49
1:A:434:GLU:HG3	1:A:469:PRO:HD3	1.95	0.49
1:A:518:LEU:HD11	1:A:520:ARG:HG2	1.94	0.49
1:A:432:ILE:O	1:A:433:LYS:HB2	2.12	0.48
1:B:565:PRO:O	1:B:568:VAL:HG22	2.14	0.48
1:B:598:TYR:CE1	1:B:616:LEU:HD13	2.49	0.48
1:B:618:ARG:NH1	1:B:622:ALA:O	2.47	0.48
1:B:540:PHE:HA	1:B:543:SER:OG	2.13	0.48
1:A:410:THR:HG22	1:A:411:GLY:H	1.79	0.48
1:A:635:HIS:O	1:A:636:GLU:CB	2.61	0.48
1:A:486:LEU:HD21	1:A:590:ILE:HA	1.96	0.48
1:A:497:GLN:O	1:A:501:MET:HG3	2.14	0.47
1:A:444:GLU:HG3	1:A:445:GLU:N	2.30	0.47
1:B:577:LYS:HB3	1:B:641:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ARG:HA	1:A:627:TYR:CE1	2.50	0.47
1:A:479:ASN:HB2	1:A:529:VAL:HB	1.96	0.47
1:A:596:MET:SD	1:B:435:GLY:CA	3.03	0.47
1:A:466:LYS:O	1:A:468:ARG:N	2.47	0.47
1:A:554:SER:O	1:A:555:VAL:HG22	2.15	0.47
1:B:487:ARG:HD3	1:B:593:LEU:O	2.15	0.47
1:A:397:ILE:HG13	1:A:398:ASP:H	1.79	0.47
1:A:530:ASN:ND2	1:A:534:VAL:HB	2.29	0.47
1:A:433:LYS:NZ	1:B:525:ARG:NE	2.63	0.47
1:A:492:ARG:HD3	1:A:492:ARG:N	2.30	0.46
1:A:408:LEU:HD11	1:A:476:TYR:CE1	2.50	0.46
1:B:439:GLU:HB3	1:B:466:LYS:O	2.15	0.46
1:B:565:PRO:HD2	1:B:568:VAL:HG22	1.97	0.46
1:A:410:THR:HA	1:A:415:VAL:HA	1.98	0.46
1:A:408:LEU:HD21	1:A:476:TYR:CE1	2.51	0.46
1:B:417:LYS:O	1:B:428:ALA:HA	2.16	0.46
1:A:588:TRP:HD1	1:A:630:MET:HE1	1.80	0.46
1:A:467:GLN:HB3	1:A:468:ARG:CZ	2.45	0.46
1:B:490:ARG:HH12	1:B:492:ARG:HD3	1.80	0.46
1:B:562:ARG:HG3	1:B:598:TYR:HD2	1.81	0.46
1:A:457:LEU:HD23	1:A:537:VAL:HG22	1.96	0.45
1:B:562:ARG:HB2	1:B:563:TRP:CZ3	2.52	0.45
1:B:454:HIS:HD2	1:B:456:LYS:H	1.63	0.45
1:B:564:SER:HB3	1:B:568:VAL:HG21	1.95	0.45
1:A:581:TRP:CZ2	1:A:610:ILE:HD13	2.52	0.45
1:B:489:MET:O	1:B:491:HIS:ND1	2.50	0.45
1:B:467:GLN:O	1:B:468:ARG:HB3	2.16	0.45
1:B:432:ILE:HG21	1:B:437:MET:CB	2.46	0.45
1:B:525:ARG:NH1	1:B:526:ASN:HD21	2.14	0.45
1:B:454:HIS:CD2	1:B:456:LYS:H	2.34	0.45
1:B:452:LEU:HD11	1:B:515:LYS:HE3	1.99	0.45
1:B:421:TRP:CD2	1:B:422:ARG:HG2	2.52	0.45
1:B:406:LYS:HG3	1:B:407:GLU:N	2.32	0.45
1:A:546:VAL:HG12	1:A:548:ASP:O	2.16	0.45
1:B:446:ALA:O	1:B:450:MET:HG3	2.16	0.45
1:B:556:GLY:O	1:B:557:SER:HB2	2.15	0.45
1:B:550:GLU:HB3	1:B:573:LYS:HE2	1.99	0.44
1:B:564:SER:HB3	1:B:568:VAL:HG23	1.98	0.44
1:A:551:TYR:HB3	1:A:574:PHE:O	2.18	0.44
1:B:452:LEU:CD1	1:B:515:LYS:HE3	2.48	0.44
1:A:402:LEU:HD21	1:A:473:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:CYS:SG	1:B:484:ASN:CG	2.96	0.44
1:A:641:ARG:HA	1:A:642:PRO:HD3	1.82	0.44
1:A:566:PRO:HA	1:A:569:LEU:HB2	2.00	0.43
1:A:550:GLU:OE2	1:A:573:LYS:HG3	2.18	0.43
1:B:400:LYS:NZ	1:B:468:ARG:HD3	2.32	0.43
1:A:416:VAL:HG12	1:A:430:LYS:CA	2.48	0.43
1:A:451:ASN:HA	1:A:451:ASN:HD22	1.55	0.43
1:A:598:TYR:HB3	1:A:601:PHE:CD2	2.53	0.43
1:B:637:LYS:HA	1:B:637:LYS:HE3	2.01	0.43
1:B:408:LEU:HB2	1:B:416:VAL:O	2.19	0.43
1:B:606:THR:O	1:B:610:ILE:HG12	2.18	0.43
1:A:433:LYS:HZ1	1:B:525:ARG:NE	2.17	0.43
1:B:614:LEU:HD22	1:B:615:ARG:N	2.34	0.43
1:B:404:PHE:CD2	1:B:404:PHE:N	2.84	0.43
1:B:559:PHE:O	1:B:561:VAL:HG23	2.19	0.43
1:B:449:MET:O	1:B:452:LEU:HB2	2.19	0.43
1:A:566:PRO:HB2	1:A:570:MET:HE2	2.00	0.42
1:A:416:VAL:CG1	1:A:430:LYS:HB2	2.40	0.42
1:B:408:LEU:HD11	1:B:476:TYR:CE1	2.48	0.42
1:A:435:GLY:CA	1:B:596:MET:HG3	2.48	0.42
1:B:442:PHE:CZ	1:B:470:ILE:HG21	2.54	0.42
1:A:520:ARG:HH22	1:A:542:LEU:HD23	1.83	0.42
1:A:547:LEU:HD12	1:A:547:LEU:H	1.83	0.42
1:A:481:CYS:HA	1:A:528:LEU:HD23	2.02	0.42
1:A:562:ARG:HB2	1:A:563:TRP:CZ3	2.55	0.42
1:B:407:GLU:CG	1:B:417:LYS:HG2	2.50	0.42
1:A:571:TYR:CZ	1:A:573:LYS:HD2	2.55	0.42
1:B:467:GLN:OE1	1:B:468:ARG:N	2.53	0.41
1:B:580:ILE:O	1:B:633:CYS:HB3	2.20	0.41
1:A:581:TRP:HZ2	1:A:610:ILE:HD13	1.85	0.41
1:B:403:THR:O	1:B:419:GLY:HA3	2.20	0.41
1:B:585:VAL:O	1:B:589:GLU:HG3	2.21	0.41
1:A:629:ILE:HG21	1:A:650:ASN:HB3	2.03	0.41
1:B:571:TYR:CE2	1:B:573:LYS:HB2	2.55	0.41
1:B:614:LEU:HD22	1:B:615:ARG:H	1.85	0.41
1:A:468:ARG:HB3	1:A:469:PRO:CD	2.46	0.41
1:A:457:LEU:HD23	1:A:537:VAL:HG23	1.99	0.41
1:B:568:VAL:HA	1:B:572:SER:CA	2.48	0.41
1:A:401:ASP:N	1:A:402:LEU:HD12	2.35	0.41
1:A:408:LEU:HD21	1:A:476:TYR:CD1	2.56	0.41
1:A:397:ILE:HG13	1:A:398:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:CYS:O	1:B:510:GLU:HB2	2.21	0.41
1:B:547:LEU:HG	1:B:548:ASP:H	1.85	0.41
1:A:564:SER:HB2	1:A:569:LEU:HD13	2.03	0.40
1:A:505:VAL:HG13	1:A:537:VAL:CG1	2.51	0.40
1:B:504:ASP:HB3	1:B:535:VAL:O	2.21	0.40
1:A:432:ILE:O	1:A:433:LYS:CB	2.69	0.40
1:A:402:LEU:N	1:A:402:LEU:HD12	2.36	0.40
1:A:564:SER:HB3	1:A:568:VAL:CG1	2.51	0.40
1:A:517:PHE:CE2	1:A:543:SER:HB2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:THR:OG1	1:B:624:GLU:OE2[3_655]	1.52	0.68
1:A:620:HIS:CA	1:B:631:TYR:OH[3_655]	2.16	0.04

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	256/263 (97%)	219 (86%)	27 (10%)	10 (4%)	4	1
1	B	256/263 (97%)	212 (83%)	37 (14%)	7 (3%)	6	2
All	All	512/526 (97%)	431 (84%)	64 (12%)	17 (3%)	5	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	LYS
1	A	467	GLN
1	A	469	PRO

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Mol	Chain	Res	Type
1	A	555	VAL
1	B	400	LYS
1	B	468	ARG
1	A	400	LYS
1	A	436	SER
1	A	466	LYS
1	A	488	GLU
1	A	636	GLU
1	B	489	MET
1	A	620	HIS
1	B	432	ILE
1	B	435	GLY
1	B	547	LEU
1	B	554	SER

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	228/238 (96%)	198 (87%)	30 (13%)	5 2
1	B	229/238 (96%)	204 (89%)	25 (11%)	8 4
All	All	457/476 (96%)	402 (88%)	55 (12%)	6 3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	LEU
1	A	410	THR
1	A	429	ILE
1	A	440	ASP
1	A	451	ASN
1	A	453	SER
1	A	460	LEU
1	A	469	PRO
1	A	474	THR

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Mol	Chain	Res	Type
1	A	486	LEU
1	A	489	MET
1	A	490	ARG
1	A	491	HIS
1	A	498	LEU
1	A	518	LEU
1	A	522	LEU
1	A	545	TYR
1	A	548	ASP
1	A	549	ASP
1	A	558	LYS
1	A	559	PHE
1	A	568	VAL
1	A	569	LEU
1	A	580	ILE
1	A	599	GLU
1	A	600	ARG
1	A	614	LEU
1	A	625	LYS
1	A	637	LYS
1	A	640	GLU
1	B	404	PHE
1	B	429	ILE
1	B	441	GLU
1	B	442	PHE
1	B	451	ASN
1	B	466	LYS
1	B	487	ARG
1	B	490	ARG
1	B	498	LEU
1	B	499	LEU
1	B	511	TYR
1	B	525	ARG
1	B	531	ASP
1	B	532	GLN
1	B	539	ASP
1	B	545	TYR
1	B	550	GLU
1	B	559	PHE
1	B	574	PHE
1	B	599	GLU
1	B	616	LEU

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Mol	Chain	Res	Type
1	B	620	HIS
1	B	645	LYS
1	B	647	LEU
1	B	652	LEU

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	412	GLN
1	A	451	ASN
1	A	494	GLN
1	A	603	ASN
1	B	451	ASN
1	B	454	HIS
1	B	497	GLN
1	B	526	ASN
1	B	620	HIS
1	B	635	HIS

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.