



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:26 AM GMT

PDB ID : 2HWP  
Title : Crystal structure of Src kinase domain in complex with covalent inhibitor PD168393  
Authors : Rauh, D.; Blair, J.A.; Shokat, K.M.  
Deposited on : 2006-08-01  
Resolution : 2.48 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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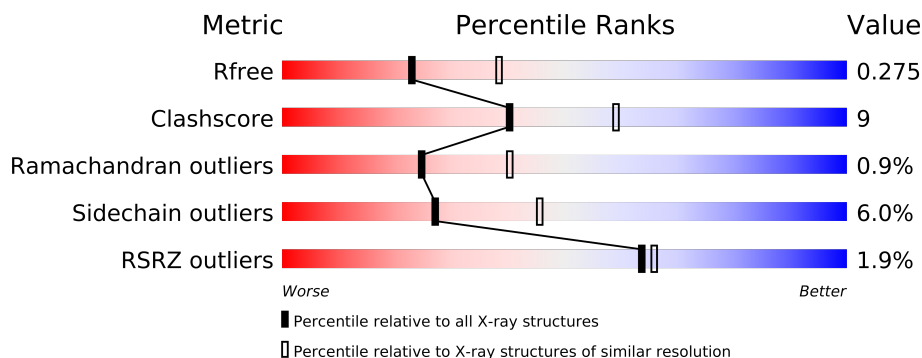
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.48 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))
$R_{free}$	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	DJK	A	1345	-	X
2	DJK	B	1345	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3763 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

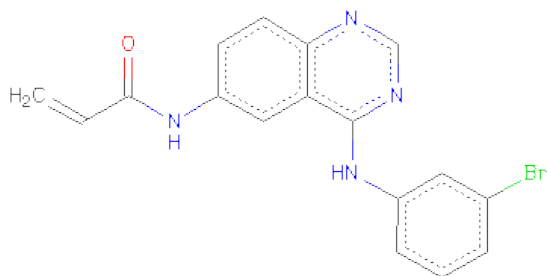
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1855	1196	313	330	16			
1	B	239	Total	C	N	O	S	0	0	0
			1832	1183	306	328	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	CLONING ARTIFACT	UNP P00523
A	249	HIS	-	CLONING ARTIFACT	UNP P00523
A	250	MET	-	CLONING ARTIFACT	UNP P00523
A	345	CYS	SER	ENGINEERED	UNP P00523
B	248	GLY	-	CLONING ARTIFACT	UNP P00523
B	249	HIS	-	CLONING ARTIFACT	UNP P00523
B	250	MET	-	CLONING ARTIFACT	UNP P00523
B	345	CYS	SER	ENGINEERED	UNP P00523

- Molecule 2 is N-[4-(3-BROMO-PHENYLAMINO)-QUINAZOLIN-6-YL]-ACRYLAMIDE (three-letter code: DJK) (formula: C<sub>17</sub>H<sub>13</sub>BrN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	B	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	15	Total	O	0	0
			15	15		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.06Å 63.01Å 73.69Å 100.74° 89.81° 90.20°	Depositor
Resolution (Å)	72.36 – 2.48 43.24 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (72.36-2.48) 92.9 (43.24-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.57 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.276 0.221 , 0.275	Depositor DCC
$R_{free}$ test set	1237 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 19.5	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24588 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.61	0/1897	0.69	0/2575
1	B	0.60	0/1876	0.68	1/2554 (0.0%)
All	All	0.61	0/3773	0.69	1/5129 (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	360	LEU	CB-CG-CD1	-5.35	101.90	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1855	0	1757	29	1
1	B	1832	0	1760	35	0
2	A	23	0	11	4	0
2	B	23	0	12	2	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3763	0	3540	68	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:476:GLU:HA	1:B:476:GLU:OE2	1.33	1.13
1:A:476:GLU:OE1	1:A:476:GLU:HA	1.33	1.10
1:B:293:ALA:HB3	1:B:338:THR:HG22	1.50	0.94
1:A:476:GLU:CA	1:A:476:GLU:OE1	2.15	0.89
1:B:426:ILE:HD13	1:B:472:LEU:CD2	2.02	0.88
1:B:426:ILE:HD13	1:B:472:LEU:HD21	1.57	0.86
1:A:323:VAL:HG11	1:A:403:ALA:HB2	1.56	0.86
1:A:323:VAL:CG1	1:A:403:ALA:HB2	2.06	0.85
1:B:426:ILE:CD1	1:B:472:LEU:HD22	2.09	0.81
1:B:476:GLU:CA	1:B:476:GLU:OE2	2.21	0.78
1:B:424:PHE:N	1:B:425:PRO:HA	2.05	0.70
1:B:426:ILE:CD1	1:B:472:LEU:CD2	2.69	0.70
1:A:279:GLY:O	1:A:280:GLU:CB	2.39	0.70
1:B:424:PHE:N	1:B:426:ILE:H	1.93	0.67
1:A:287:ASN:O	1:A:289:THR:HG22	1.95	0.67
1:B:426:ILE:HD11	1:B:472:LEU:HD22	1.75	0.66
1:A:257:LYS:CB	1:A:261:GLU:HG3	2.27	0.65
1:A:308:LEU:O	1:A:311:ALA:N	2.29	0.65
2:A:1345:DJK:N3	2:A:1345:DJK:H4	2.14	0.62
1:A:518:ASP:CG	1:B:461:VAL:HG23	2.21	0.61
1:A:386:ASP:CB	1:A:388:ARG:NH1	2.63	0.61
1:B:424:PHE:N	1:B:425:PRO:CA	2.65	0.59
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.36	0.59
1:B:283:MET:HG3	1:B:340:TYR:CE1	2.38	0.58
2:B:1345:DJK:N3	2:B:1345:DJK:H4	2.19	0.57
2:B:1345:DJK:H8	2:B:1345:DJK:O61	2.04	0.57
1:A:386:ASP:CB	1:A:388:ARG:HH12	2.18	0.56
1:A:431:PRO:O	1:A:433:ALA:N	2.39	0.56
1:A:323:VAL:HG13	1:A:403:ALA:HB2	1.86	0.56
1:B:493:ASP:OD2	1:B:497:GLN:NE2	2.38	0.55
1:A:314:MET:HG2	1:A:405:PHE:CZ	2.42	0.55
1:A:314:MET:SD	1:A:405:PHE:CE1	3.00	0.54
1:B:283:MET:HG3	1:B:340:TYR:CZ	2.43	0.53
1:B:323:VAL:HG11	1:B:393:LEU:HD12	1.91	0.52
1:B:501:LYS:O	1:B:503:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:LYS:HA	1:B:401:LYS:HG2	1.93	0.51
1:A:486:GLU:OE2	1:A:532:ASN:ND2	2.43	0.51
1:B:283:MET:SD	1:B:291:ARG:NH1	2.85	0.49
1:A:308:LEU:O	1:A:309:GLN:C	2.49	0.49
1:B:388:ARG:CB	1:B:428:TRP:CD1	2.95	0.49
1:A:503:PRO:O	1:A:506:ARG:HB2	2.14	0.48
1:B:440:THR:HG23	1:B:443:SER:OG	2.14	0.47
1:A:404:ASP:OD1	2:A:1345:DJK:C20	2.64	0.46
1:A:501:LYS:O	1:A:503:PRO:HD3	2.15	0.45
1:B:424:PHE:N	1:B:426:ILE:N	2.63	0.45
1:A:289:THR:HG23	1:A:290:THR:OG1	2.16	0.45
2:A:1345:DJK:N3	2:A:1345:DJK:C4	2.79	0.45
1:B:493:ASP:O	1:B:497:GLN:HG3	2.16	0.45
2:A:1345:DJK:O61	2:A:1345:DJK:H8	2.17	0.45
1:B:424:PHE:N	1:B:426:ILE:HG22	2.32	0.44
1:A:431:PRO:C	1:A:433:ALA:H	2.21	0.44
1:B:343:LYS:HB2	1:B:394:VAL:HB	1.99	0.44
1:B:461:VAL:HA	1:B:462:PRO:HD3	1.85	0.43
1:A:431:PRO:C	1:A:433:ALA:N	2.72	0.42
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.54	0.42
1:A:308:LEU:O	1:A:309:GLN:O	2.38	0.42
1:B:329:VAL:HB	1:B:335:TYR:HB2	2.02	0.42
1:B:375:ALA:O	1:B:378:GLU:HB3	2.19	0.42
1:B:338:THR:HG23	1:B:339:GLU:O	2.19	0.42
1:B:321:LYS:HD2	1:B:369:GLN:HB3	2.00	0.42
1:B:503:PRO:O	1:B:506:ARG:HB2	2.19	0.42
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.95	0.41
1:A:372:SER:HB2	1:A:513:GLN:NE2	2.35	0.41
1:A:442:LYS:NZ	1:A:506:ARG:O	2.47	0.41
1:B:440:THR:OG1	1:B:442:LYS:N	2.51	0.41
1:B:485:PRO:O	1:B:486:GLU:HB2	2.21	0.41
1:B:269:LEU:HB3	1:B:282:TRP:CE3	2.56	0.40
1:A:485:PRO:O	1:A:486:GLU:HB2	2.21	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:397:ASN:ND2	1:A:438:ARG:CD[1_455]	2.13	0.07

## 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 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	231/286 (81%)	221 (96%)	6 (3%)	4 (2%)	14	21
1	B	231/286 (81%)	221 (96%)	10 (4%)	0	100	100
All	All	462/572 (81%)	442 (96%)	16 (4%)	4 (1%)	25	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	GLU
1	A	432	GLU
1	A	308	LEU
1	A	431	PRO

### 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 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	182/245 (74%)	171 (94%)	11 (6%)	27	45
1	B	185/245 (76%)	174 (94%)	11 (6%)	28	46
All	All	367/490 (75%)	345 (94%)	22 (6%)	27	45

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	291	ARG
1	A	360	LEU
1	A	372	SER
1	A	397	ASN

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Mol	Chain	Res	Type
1	A	426	ILE
1	A	438	ARG
1	A	467	VAL
1	A	476	GLU
1	A	491	LEU
1	A	528	GLN
1	B	323	VAL
1	B	338	THR
1	B	356	LYS
1	B	360	LEU
1	B	426	ILE
1	B	440	THR
1	B	451	LEU
1	B	472	LEU
1	B	476	GLU
1	B	491	LEU
1	B	528	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	ASN
1	A	397	ASN
1	B	397	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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

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	DJK	A	1345	1	25,25,25	1.57	3 (12%)	34,34,34	3.32	9 (26%)
2	DJK	B	1345	1	25,25,25	1.59	4 (16%)	34,34,34	3.09	10 (29%)

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	DJK	A	1345	1	-	0/10/10/10	0/1/3/3
2	DJK	B	1345	1	-	1/10/10/10	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1345	DJK	C51-C11	5.05	1.55	1.29
2	A	1345	DJK	C51-C11	4.83	1.53	1.29
2	A	1345	DJK	C6-C7	-3.07	1.41	1.45
2	B	1345	DJK	C6-C7	-2.70	1.41	1.45
2	A	1345	DJK	C11-C10	2.15	1.52	1.48
2	B	1345	DJK	C11-C10	2.05	1.52	1.48
2	B	1345	DJK	C9-N11	-2.04	1.37	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1345	DJK	C51-C11-C10	-9.72	113.01	122.38
2	A	1345	DJK	N2-C19-N3	-8.59	121.52	128.71
2	B	1345	DJK	C51-C11-C10	-7.58	115.07	122.38
2	B	1345	DJK	N2-C19-N3	-7.43	122.50	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1345	DJK	C11-C10-N11	6.79	117.84	113.79
2	A	1345	DJK	C11-C10-N11	6.78	117.83	113.79
2	A	1345	DJK	C19-N2-C18	6.45	120.36	115.37
2	A	1345	DJK	C19-N3-C6	6.44	120.74	116.69
2	B	1345	DJK	C19-N2-C18	6.06	120.06	115.37
2	B	1345	DJK	C6-C7-C18	5.41	118.71	115.63
2	B	1345	DJK	C8-C7-C6	-5.32	122.12	124.98
2	B	1345	DJK	C19-N3-C6	4.98	119.82	116.69
2	A	1345	DJK	C6-C7-C18	4.58	118.24	115.63
2	A	1345	DJK	C8-C7-C6	-4.08	122.79	124.98
2	B	1345	DJK	C7-C18-N2	-3.24	119.52	122.91
2	A	1345	DJK	C7-C18-N2	-2.94	119.84	122.91
2	A	1345	DJK	C7-C6-N3	-2.93	119.30	121.31
2	B	1345	DJK	C7-C6-N3	-2.80	119.39	121.31
2	B	1345	DJK	BR-C3-C4	2.16	122.55	119.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1345	DJK	C51-C11-C10-N11

There are no ring outliers.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	245/286 (85%)	-0.11	9 (3%) 39 41	10, 26, 62, 83	1 (0%)
1	B	239/286 (83%)	-0.24	0 100 100	11, 26, 53, 64	0
All	All	484/572 (84%)	-0.18	9 (1%) 64 66	10, 26, 60, 83	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	PHE	5.3
1	A	267	LEU	4.5
1	A	311	ALA	3.1
1	A	296	THR	3.0
1	A	334	ILE	2.5
1	A	307	PHE	2.2
1	A	282	TRP	2.2
1	A	263	PRO	2.1
1	A	286	TRP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DJK	B	1345	23/23	0.23	4.57	35,42,43,43	1
2	DJK	A	1345	23/23	0.22	3.12	31,42,42,42	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.