



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:20 PM GMT

PDB ID : 1B55  
Title : PH DOMAIN FROM BRUTON'S TYROSINE KINASE IN COMPLEX  
WITH INOSITOL 1,3,4,5-TETRAKISPHOSPHATE  
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Deposited on : 1999-01-12  
Resolution : 2.40 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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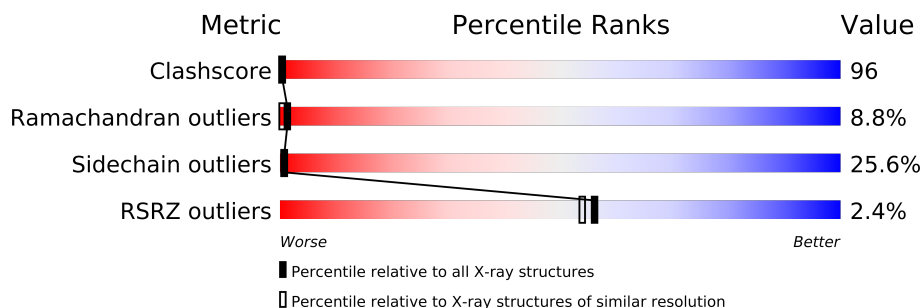
The following versions of software and data (see [references](#)) were used in the production of this report:

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

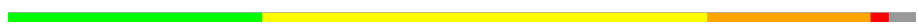
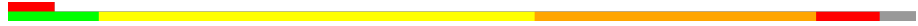
The reported resolution of this entry is 2.40 Å.

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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	169	
1	B	169	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2964 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.

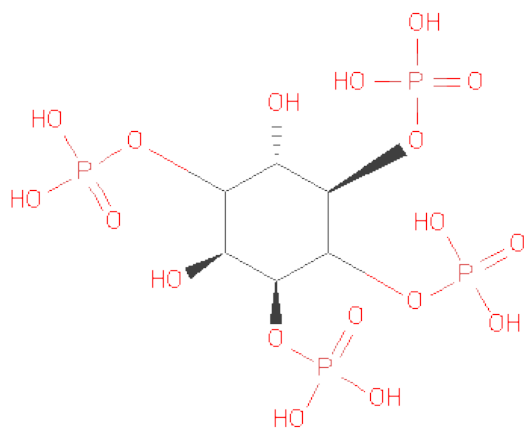
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	23	0	0
			1362	877	238	240	7			
1	B	162	Total	C	N	O	S	63	0	0
			1348	868	231	242	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (three-letter code: 4IP) (formula: C<sub>6</sub>H<sub>16</sub>O<sub>18</sub>P<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			28	6	18	4		
3	B	1	Total	C	O	P	0	0
			28	6	18	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	77	Total	O	0	0
			77	77		

### 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 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.

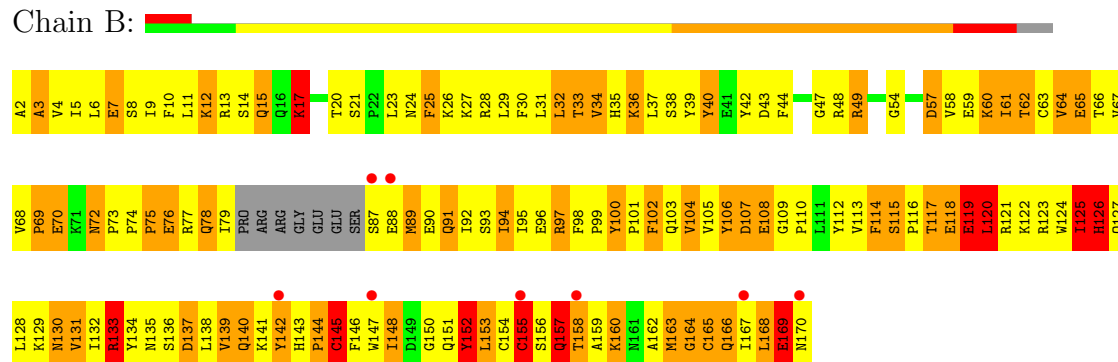
#### • Molecule 1: TYROSINE-PROTEIN KINASE BTK

Chain A:



#### • Molecule 1: TYROSINE-PROTEIN KINASE BTK

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.20Å 110.20Å 215.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 26.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.00-2.40) 96.5 (26.11-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.39Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.234 , 0.350 0.237 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 150.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25429 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: ZN, 4IP

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	1.15	2/1395 (0.1%)	1.43	11/1880 (0.6%)
1	B	1.20	3/1380 (0.2%)	1.58	13/1860 (0.7%)
All	All	1.17	5/2775 (0.2%)	1.51	24/3740 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	1	5
All	All	1	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	GLU	CD-OE2	6.75	1.33	1.25
1	B	125	ILE	CA-CB	-5.47	1.42	1.54
1	A	76	GLU	CD-OE2	5.43	1.31	1.25
1	B	119	GLU	CD-OE2	5.41	1.31	1.25
1	A	70	GLU	CD-OE2	5.18	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	149	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	89	MET	N-CA-C	6.99	129.87	111.00
1	B	145	CYS	CA-CB-SG	-6.98	101.44	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	CYS	CB-CA-C	6.43	123.26	110.40
1	B	104	VAL	CB-CA-C	-6.36	99.31	111.40
1	B	107	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	133	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	167	ILE	CB-CA-C	-6.02	99.55	111.60
1	A	105	VAL	CB-CA-C	-5.79	100.40	111.40
1	A	57	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	134	TYR	CB-CG-CD1	5.66	124.39	121.00
1	A	9	ILE	CG1-CB-CG2	-5.65	98.97	111.40
1	A	121	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	B	33	THR	N-CA-CB	5.62	120.98	110.30
1	B	32	LEU	CA-CB-CG	-5.55	102.53	115.30
1	B	120	LEU	CA-CB-CG	-5.49	102.68	115.30
1	B	164	GLY	N-CA-C	5.23	126.18	113.10
1	B	64	VAL	C-N-CA	-5.21	108.68	121.70
1	B	49	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	107	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	123	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	155	CYS	N-CA-C	-5.06	97.34	111.00
1	A	155	CYS	CA-CB-SG	-5.04	104.93	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	145	CYS	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ILE	Mainchain
1	A	135	ASN	Sidechain
1	A	169	GLU	Mainchain
1	A	44	PHE	Sidechain
1	B	102	PHE	Sidechain
1	B	142	TYR	Sidechain
1	B	57	ASP	Sidechain
1	B	72	ASN	Sidechain
1	B	89	MET	Mainchain



## 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	1362	0	1378	124	3
1	B	1348	0	1358	396	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	A	28	0	8	2	0
3	B	28	0	8	2	0
4	A	119	0	0	13	4
4	B	77	0	0	57	1
All	All	2964	0	2752	511	7

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 96.

All (511) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:PRO:HA	4:B:178:HOH:O	1.30	1.25
1:B:155:CYS:SG	1:B:165:CYS:HB3	1.79	1.22
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.06	1.17
1:B:100:TYR:HB3	1:B:121:ARG:HD3	1.31	1.11
1:B:87:SER:HB2	1:B:119:GLU:HB3	1.13	1.09
1:B:125:ILE:HD11	4:B:174:HOH:O	1.52	1.09
1:A:29:LEU:HD23	1:A:49:ARG:HB2	1.32	1.09
1:B:115:SER:CA	4:B:179:HOH:O	2.01	1.08
1:B:115:SER:HA	4:B:179:HOH:O	1.49	1.07
1:B:100:TYR:HB2	1:B:115:SER:HB3	1.38	1.05
1:B:100:TYR:CE1	1:B:118:GLU:HG3	1.93	1.02
1:B:127:GLN:HA	4:B:181:HOH:O	1.58	1.02
1:B:105:VAL:HB	4:B:173:HOH:O	1.58	1.02
1:B:135:ASN:HB2	1:B:138:LEU:HD21	1.03	1.02
1:B:40:TYR:CD2	1:B:49:ARG:HD2	1.96	0.99
1:B:10:PHE:CD1	4:B:179:HOH:O	2.13	0.99
1:B:115:SER:HB3	4:B:213:HOH:O	1.65	0.97
1:B:133:ARG:HG2	1:B:134:TYR:N	1.80	0.97
1:B:67:VAL:HG22	1:B:103:GLN:HB3	1.48	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:TYR:HB3	1:B:44:PHE:HE2	1.30	0.94
1:B:5:ILE:O	1:B:6:LEU:HD13	1.66	0.94
1:B:141:LYS:HA	1:B:167:ILE:HA	1.47	0.94
1:B:68:VAL:HB	4:B:230:HOH:O	1.66	0.94
1:B:143:HIS:HB3	1:B:154:CYS:CB	1.98	0.93
1:B:135:ASN:HB2	1:B:138:LEU:CD2	1.95	0.93
1:B:64:VAL:HG23	1:B:132:ILE:HD13	1.49	0.93
1:B:69:PRO:HG3	4:B:202:HOH:O	1.67	0.93
1:B:99:PRO:O	1:B:101:PRO:HD3	1.67	0.93
1:B:135:ASN:CB	1:B:138:LEU:HD21	1.97	0.92
1:B:90:GLU:HB3	1:B:93:SER:OG	1.69	0.92
1:B:67:VAL:CG2	1:B:103:GLN:HB3	1.98	0.92
1:B:125:ILE:HG22	1:B:126:HIS:N	1.82	0.92
1:B:13:ARG:HH12	1:B:148:ILE:HG23	1.33	0.92
1:A:62:THR:HB	1:A:139:VAL:HG13	1.50	0.91
1:A:59:GLU:HA	1:A:135:ASN:HD21	1.36	0.90
1:B:121:ARG:HD2	4:B:194:HOH:O	1.71	0.89
1:B:118:GLU:O	1:B:119:GLU:C	2.07	0.89
1:A:141:LYS:HE3	1:A:163:MET:HE2	1.53	0.89
1:B:57:ASP:HB2	1:B:60:LYS:HG3	1.52	0.89
1:B:100:TYR:HE1	1:B:118:GLU:HG3	1.37	0.89
1:B:87:SER:CB	1:B:119:GLU:HB3	2.02	0.89
1:B:90:GLU:HA	1:B:90:GLU:OE1	1.70	0.88
1:A:2:ALA:HB1	4:A:258:HOH:O	1.73	0.88
1:A:118:GLU:HG3	4:A:216:HOH:O	1.74	0.88
1:B:64:VAL:HG11	1:B:128:LEU:CB	2.03	0.87
1:B:98:PHE:HA	1:B:116:PRO:HA	1.56	0.87
1:B:2:ALA:HB3	1:B:33:THR:CG2	2.05	0.87
1:A:58:VAL:HG11	1:A:131:VAL:HG12	1.56	0.86
1:B:13:ARG:NH2	1:B:112:TYR:HE2	1.73	0.86
1:A:89:MET:HA	4:A:173:HOH:O	1.73	0.86
1:A:42:TYR:HB3	1:B:44:PHE:CE2	2.10	0.86
1:B:13:ARG:NH2	1:B:112:TYR:CE2	2.44	0.85
1:B:30:PHE:C	1:B:31:LEU:HD23	1.96	0.85
1:B:73:PRO:O	1:B:78:GLN:HG2	1.76	0.85
1:B:61:ILE:HB	1:B:132:ILE:HG21	1.57	0.85
1:B:63:CYS:HB3	4:B:173:HOH:O	1.74	0.85
1:B:102:PHE:HB3	4:B:194:HOH:O	1.77	0.84
1:B:143:HIS:CE1	1:B:155:CYS:SG	2.71	0.84
1:B:67:VAL:HG23	1:B:102:PHE:HA	1.59	0.84
1:B:130:ASN:HB2	4:B:181:HOH:O	1.77	0.83
1:B:143:HIS:CE1	1:B:164:GLY:HA2	2.13	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:LEU:HD12	1:B:33:THR:N	1.92	0.82
1:B:88:GLU:HB2	1:B:117:THR:CG2	2.09	0.82
1:B:143:HIS:HB3	1:B:154:CYS:HB3	1.60	0.82
1:A:92:ILE:HD11	1:B:9:ILE:HG13	1.62	0.82
1:B:5:ILE:O	1:B:6:LEU:CD1	2.27	0.82
1:B:92:ILE:O	1:B:96:GLU:HG3	1.80	0.82
1:A:34:VAL:HG23	1:A:35:HIS:HD2	1.43	0.82
1:B:13:ARG:HH21	1:B:112:TYR:HE2	1.25	0.82
1:B:168:LEU:N	4:B:177:HOH:O	2.13	0.81
1:A:97:ARG:HG3	1:A:97:ARG:NH1	1.86	0.81
1:B:155:CYS:HB2	1:B:157:GLN:HG3	1.60	0.81
1:B:90:GLU:O	1:B:92:ILE:N	2.13	0.81
1:A:45:GLU:O	1:B:27:LYS:HE3	1.81	0.81
1:A:90:GLU:O	1:A:92:ILE:N	2.14	0.81
1:B:75:PRO:CA	1:B:78:GLN:HG3	2.11	0.81
1:B:64:VAL:HG21	1:B:128:LEU:HB3	1.63	0.80
1:B:147:TRP:C	1:B:148:ILE:HG13	2.02	0.79
1:A:5:ILE:HD12	1:A:32:LEU:O	1.82	0.79
1:B:77:ARG:O	1:B:99:PRO:HB3	1.81	0.79
1:B:127:GLN:O	1:B:131:VAL:HG22	1.83	0.79
1:A:81:ARG:HA	4:A:271:HOH:O	1.83	0.79
1:B:40:TYR:CE2	1:B:49:ARG:HD2	2.17	0.78
1:B:100:TYR:HB3	1:B:121:ARG:CD	2.11	0.78
1:B:90:GLU:HB3	1:B:93:SER:CB	2.13	0.78
1:A:58:VAL:HG11	1:A:131:VAL:CG1	2.14	0.78
1:B:6:LEU:HB3	1:B:124:TRP:CZ2	2.19	0.78
1:B:99:PRO:HD2	1:B:100:TYR:CD2	2.18	0.77
1:B:67:VAL:HG11	1:B:146:PHE:CZ	2.19	0.77
1:B:31:LEU:HD23	1:B:31:LEU:N	1.98	0.77
1:B:63:CYS:N	4:B:173:HOH:O	2.19	0.76
1:B:126:HIS:HD2	4:B:204:HOH:O	1.67	0.76
1:A:16:GLN:OE1	1:A:23:LEU:HD13	1.84	0.76
1:B:100:TYR:CD1	1:B:118:GLU:HG3	2.19	0.76
1:B:159:ALA:O	1:B:160:LYS:C	2.22	0.76
1:B:115:SER:CB	4:B:213:HOH:O	2.28	0.76
1:A:80:PRO:HG3	1:A:97:ARG:HE	1.49	0.75
1:B:114:PHE:C	4:B:179:HOH:O	2.24	0.75
1:A:91:GLN:HG2	1:A:91:GLN:O	1.84	0.75
1:B:25:PHE:N	1:B:25:PHE:CD1	2.53	0.75
1:B:4:VAL:HG12	1:B:6:LEU:H	1.50	0.75
1:B:140:GLN:O	1:B:167:ILE:HG23	1.86	0.74
1:B:68:VAL:O	1:B:69:PRO:C	2.25	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:PRO:O	1:B:78:GLN:N	2.20	0.73
1:B:145:CYS:HA	4:B:230:HOH:O	1.86	0.73
1:B:143:HIS:CE1	1:B:165:CYS:H	2.05	0.73
1:B:166:GLN:HG3	1:B:167:ILE:H	1.52	0.73
1:B:74:PRO:O	1:B:75:PRO:C	2.27	0.73
1:B:125:ILE:O	1:B:128:LEU:HB2	1.89	0.73
1:B:64:VAL:HG23	1:B:132:ILE:CD1	2.19	0.73
1:B:35:HIS:HB3	4:B:228:HOH:O	1.88	0.72
1:B:121:ARG:HB3	4:B:192:HOH:O	1.89	0.72
1:B:8:SER:O	1:B:29:LEU:HD12	1.89	0.72
1:A:81:ARG:O	1:A:82:ARG:HD2	1.90	0.72
1:B:101:PRO:HD2	4:B:202:HOH:O	1.89	0.72
1:A:101:PRO:HB3	1:A:114:PHE:CD2	2.24	0.72
1:B:62:THR:HG23	1:B:106:TYR:HA	1.72	0.72
1:B:107:ASP:OD2	1:B:108:GLU:N	2.23	0.71
1:B:64:VAL:HG11	1:B:128:LEU:HB2	1.70	0.71
1:A:58:VAL:CG1	1:A:131:VAL:HG12	2.21	0.71
1:A:97:ARG:HH11	1:A:97:ARG:CG	1.96	0.70
1:A:119:GLU:O	1:A:119:GLU:HG2	1.91	0.70
1:B:30:PHE:O	1:B:31:LEU:HD23	1.92	0.70
1:B:114:PHE:N	1:B:114:PHE:HD1	1.90	0.70
1:B:64:VAL:HG11	1:B:128:LEU:HB3	1.73	0.70
1:B:67:VAL:HG12	1:B:68:VAL:H	1.57	0.70
1:B:114:PHE:N	1:B:114:PHE:CD1	2.60	0.69
1:B:143:HIS:O	1:B:145:CYS:N	2.26	0.69
1:B:31:LEU:O	1:B:37:LEU:HD12	1.93	0.69
1:B:64:VAL:HG13	1:B:128:LEU:HD13	1.74	0.69
1:B:13:ARG:NH1	1:B:148:ILE:HG23	2.07	0.69
1:B:5:ILE:HD12	1:B:33:THR:HA	1.73	0.69
1:B:100:TYR:HB2	1:B:115:SER:CB	2.20	0.69
1:B:87:SER:HB2	1:B:119:GLU:CB	2.07	0.69
3:A:171:4IP:O5P	4:A:197:HOH:O	2.10	0.69
1:B:146:PHE:C	1:B:148:ILE:HD11	2.13	0.68
1:B:165:CYS:O	1:B:166:GLN:HB2	1.93	0.68
1:B:79:ILE:O	1:B:79:ILE:HG22	1.94	0.68
1:B:141:LYS:HB3	1:B:166:GLN:O	1.94	0.68
1:B:118:GLU:O	1:B:120:LEU:N	2.27	0.67
1:A:34:VAL:HG23	1:A:35:HIS:CD2	2.28	0.67
1:A:155:CYS:SG	1:A:157:GLN:HG3	2.34	0.67
1:B:88:GLU:HB2	1:B:117:THR:HB	1.76	0.67
1:A:81:ARG:HG2	4:A:271:HOH:O	1.93	0.67
1:B:58:VAL:O	1:B:61:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:LEU:HD12	1:B:33:THR:H	1.59	0.67
1:B:166:GLN:HG3	1:B:167:ILE:N	2.09	0.66
1:B:61:ILE:HB	1:B:132:ILE:CG2	2.25	0.66
1:B:90:GLU:O	1:B:93:SER:N	2.28	0.66
1:A:137:ASP:O	1:A:139:VAL:N	2.28	0.66
1:B:13:ARG:HD2	1:B:23:LEU:HD21	1.75	0.66
1:B:88:GLU:HB2	1:B:117:THR:CB	2.26	0.66
1:A:143:HIS:CE1	1:A:164:GLY:HA2	2.30	0.66
1:B:125:ILE:O	1:B:126:HIS:C	2.31	0.65
1:B:145:CYS:CA	4:B:230:HOH:O	2.42	0.65
1:B:67:VAL:CG2	1:B:102:PHE:C	2.64	0.65
1:B:129:LYS:O	1:B:131:VAL:N	2.29	0.65
1:B:142:TYR:OH	1:B:144:PRO:HB3	1.96	0.65
1:B:12:LYS:O	1:B:25:PHE:HA	1.96	0.65
1:B:7:GLU:HA	1:B:30:PHE:O	1.95	0.65
1:A:147:TRP:HD1	1:A:152:TYR:CE2	2.14	0.65
1:B:127:GLN:CA	4:B:181:HOH:O	2.30	0.65
1:B:4:VAL:CG1	1:B:6:LEU:O	2.45	0.65
1:B:155:CYS:HB2	1:B:157:GLN:CG	2.27	0.65
1:B:2:ALA:HB3	1:B:33:THR:HG21	1.78	0.65
1:A:63:CYS:O	1:A:105:VAL:HG23	1.96	0.65
1:B:100:TYR:CD2	1:B:100:TYR:N	2.64	0.64
1:B:159:ALA:O	1:B:162:ALA:N	2.26	0.64
1:B:90:GLU:OE1	1:B:90:GLU:CA	2.37	0.64
1:A:10:PHE:CE1	1:A:115:SER:HB2	2.33	0.64
1:B:67:VAL:HG23	1:B:102:PHE:CA	2.27	0.64
1:B:67:VAL:HG11	1:B:146:PHE:CE1	2.33	0.64
1:A:80:PRO:CG	1:A:97:ARG:HE	2.11	0.64
1:A:29:LEU:CD2	1:A:49:ARG:HB2	2.19	0.63
1:B:99:PRO:HD2	1:B:100:TYR:CE2	2.32	0.63
1:B:99:PRO:HD2	1:B:100:TYR:HD2	1.61	0.63
1:B:2:ALA:HB3	1:B:33:THR:HG22	1.81	0.63
1:B:68:VAL:O	1:B:68:VAL:HG12	1.99	0.63
1:B:20:THR:OG1	1:B:21:SER:N	2.28	0.63
1:B:67:VAL:HG21	1:B:103:GLN:HB3	1.81	0.62
1:A:70:GLU:O	1:A:70:GLU:HG2	1.99	0.62
1:B:94:ILE:HA	4:B:188:HOH:O	1.99	0.62
1:A:5:ILE:HD12	1:A:33:THR:HA	1.81	0.62
1:A:159:ALA:O	1:A:162:ALA:N	2.30	0.62
1:B:154:CYS:SG	1:B:155:CYS:N	2.73	0.62
1:B:99:PRO:HG2	1:B:100:TYR:CE2	2.34	0.62
1:B:72:ASN:ND2	4:B:224:HOH:O	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147:TRP:C	1:B:148:ILE:CG1	2.68	0.62
1:B:169:GLU:HG2	1:B:170:ASN:N	2.11	0.61
1:A:101:PRO:HB3	1:A:114:PHE:CE2	2.34	0.61
1:A:43:ASP:HB3	1:A:48:ARG:O	2.00	0.61
1:A:29:LEU:HD23	1:A:49:ARG:CB	2.21	0.61
1:B:67:VAL:HG21	1:B:102:PHE:O	2.01	0.61
1:B:165:CYS:O	1:B:165:CYS:SG	2.59	0.61
1:B:98:PHE:HA	1:B:115:SER:O	2.01	0.61
1:A:6:LEU:HB3	1:A:124:TRP:CZ2	2.36	0.61
1:A:141:LYS:CE	1:A:163:MET:HE2	2.28	0.61
1:B:121:ARG:NH1	4:B:202:HOH:O	2.23	0.61
1:B:147:TRP:CZ2	1:B:150:GLY:O	2.54	0.61
1:A:59:GLU:CA	1:A:135:ASN:HD21	2.13	0.60
1:B:129:LYS:O	1:B:130:ASN:C	2.38	0.60
1:B:58:VAL:HA	1:B:61:ILE:HG13	1.83	0.60
1:A:94:ILE:HD13	1:B:91:GLN:HG3	1.83	0.60
1:B:98:PHE:CA	1:B:115:SER:O	2.49	0.60
1:A:89:MET:HB3	4:A:219:HOH:O	2.00	0.60
1:B:115:SER:N	4:B:179:HOH:O	2.25	0.60
1:A:166:GLN:HG2	1:A:167:ILE:N	2.15	0.60
1:B:92:ILE:HB	4:B:219:HOH:O	2.01	0.60
1:B:154:CYS:O	1:B:165:CYS:SG	2.59	0.60
1:B:4:VAL:HG12	1:B:6:LEU:N	2.16	0.60
1:B:75:PRO:C	1:B:78:GLN:HG3	2.22	0.60
1:B:155:CYS:SG	1:B:165:CYS:CB	2.72	0.60
1:B:128:LEU:O	1:B:131:VAL:HG23	2.02	0.59
1:B:75:PRO:O	1:B:78:GLN:HG3	2.02	0.59
1:B:75:PRO:O	1:B:77:ARG:N	2.35	0.59
1:B:67:VAL:CG1	1:B:146:PHE:CZ	2.86	0.59
1:B:40:TYR:CD1	1:B:40:TYR:N	2.71	0.59
1:A:5:ILE:HD12	1:A:33:THR:CA	2.33	0.59
1:B:4:VAL:CG1	1:B:6:LEU:H	2.14	0.59
1:B:148:ILE:HD12	1:B:148:ILE:N	2.17	0.59
1:B:14:SER:N	1:B:24:ASN:O	2.35	0.59
1:B:67:VAL:HG12	1:B:146:PHE:CE2	2.38	0.58
1:B:73:PRO:O	1:B:78:GLN:NE2	2.35	0.58
1:A:145:CYS:HB3	1:A:153:LEU:HD12	1.86	0.58
1:B:42:TYR:CE2	1:B:44:PHE:HA	2.38	0.58
1:B:98:PHE:HA	1:B:116:PRO:CA	2.31	0.58
1:A:8:SER:HG	1:A:124:TRP:HE1	1.51	0.58
1:A:76:GLU:HG3	1:A:77:ARG:HG2	1.86	0.58
1:B:26:LYS:HB3	1:B:28:ARG:CZ	2.32	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:34:VAL:O	1:B:58:VAL:HG21	2.03	0.58
1:B:2:ALA:O	1:B:3:ALA:HB2	2.04	0.58
1:A:25:PHE:N	1:A:25:PHE:CD1	2.70	0.58
1:B:143:HIS:ND1	1:B:154:CYS:SG	2.76	0.58
1:B:40:TYR:CD2	1:B:49:ARG:CD	2.81	0.58
1:B:97:ARG:O	1:B:116:PRO:HA	2.03	0.58
1:B:125:ILE:O	1:B:128:LEU:N	2.37	0.58
1:B:13:ARG:HH11	1:B:23:LEU:HD21	1.69	0.57
1:B:62:THR:OG1	4:B:173:HOH:O	2.17	0.57
1:B:112:TYR:CZ	1:B:146:PHE:CD1	2.93	0.57
1:B:43:ASP:N	1:B:48:ARG:O	2.27	0.57
1:B:36:LYS:HA	1:B:58:VAL:HG23	1.86	0.57
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.68	0.57
1:B:115:SER:CB	4:B:179:HOH:O	2.41	0.57
1:B:92:ILE:N	4:B:219:HOH:O	2.27	0.57
1:B:75:PRO:N	1:B:78:GLN:HG3	2.19	0.56
1:A:115:SER:OG	1:A:116:PRO:HD2	2.05	0.56
1:A:98:PHE:HA	1:A:116:PRO:HA	1.86	0.56
1:B:154:CYS:C	1:B:165:CYS:SG	2.84	0.56
1:B:35:HIS:O	1:B:58:VAL:HG23	2.04	0.56
1:B:143:HIS:CG	1:B:154:CYS:SG	2.98	0.56
1:B:64:VAL:O	1:B:65:GLU:HG2	2.06	0.56
1:A:90:GLU:O	1:A:91:GLN:C	2.43	0.56
1:A:92:ILE:HD11	1:B:9:ILE:CG1	2.34	0.56
1:B:117:THR:N	4:B:213:HOH:O	2.39	0.56
1:B:121:ARG:O	1:B:122:LYS:C	2.45	0.56
1:B:126:HIS:HE1	4:B:209:HOH:O	1.88	0.56
1:B:67:VAL:CG1	1:B:146:PHE:CE2	2.89	0.56
1:A:151:GLN:HB3	1:A:158:THR:HG22	1.88	0.56
1:B:99:PRO:HG2	1:B:100:TYR:HE2	1.70	0.56
1:B:113:VAL:C	4:B:178:HOH:O	2.43	0.55
1:B:150:GLY:O	1:B:158:THR:HG23	2.05	0.55
1:A:58:VAL:O	1:A:58:VAL:HG12	2.07	0.55
1:B:114:PHE:HA	4:B:178:HOH:O	2.07	0.55
1:B:4:VAL:HG12	1:B:5:ILE:N	2.21	0.55
1:B:7:GLU:N	1:B:124:TRP:HZ2	2.05	0.55
1:B:90:GLU:HG3	1:B:90:GLU:O	2.06	0.55
1:B:146:PHE:HB3	1:B:148:ILE:CG1	2.37	0.55
1:B:141:LYS:CA	1:B:166:GLN:O	2.55	0.54
1:A:3:ALA:O	1:A:33:THR:HG22	2.06	0.54
1:A:152:TYR:O	1:A:156:SER:N	2.39	0.54
1:A:134:TYR:HA	4:A:203:HOH:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:ARG:NE	4:B:184:HOH:O	2.41	0.54
1:B:34:VAL:HG12	1:B:131:VAL:HG12	1.89	0.54
1:B:67:VAL:HG23	1:B:102:PHE:C	2.27	0.54
1:B:77:ARG:O	1:B:78:GLN:O	2.25	0.54
1:B:39:TYR:CZ	1:B:54:GLY:HA3	2.42	0.54
1:A:129:LYS:O	1:A:130:ASN:C	2.44	0.54
1:B:78:GLN:O	1:B:99:PRO:HB3	2.07	0.54
1:B:47:GLY:O	1:B:48:ARG:HB3	2.06	0.54
1:B:142:TYR:CE1	1:B:144:PRO:N	2.76	0.54
1:B:67:VAL:HG21	1:B:102:PHE:C	2.28	0.53
1:B:25:PHE:N	1:B:25:PHE:HD1	2.05	0.53
1:B:112:TYR:CZ	1:B:146:PHE:HD1	2.26	0.53
1:B:64:VAL:HG13	1:B:128:LEU:CD1	2.37	0.53
3:B:172:4IP:OPF	3:B:172:4IP:O9P	2.26	0.53
1:A:128:LEU:O	1:A:132:ILE:HG12	2.09	0.53
1:B:141:LYS:CB	1:B:166:GLN:O	2.56	0.53
1:A:5:ILE:CD1	1:A:33:THR:HA	2.39	0.53
1:A:64:VAL:C	1:A:65:GLU:HG2	2.28	0.53
1:B:143:HIS:CE1	1:B:164:GLY:CA	2.88	0.53
1:B:143:HIS:C	1:B:145:CYS:N	2.61	0.53
1:B:145:CYS:SG	1:B:154:CYS:HA	2.49	0.52
1:B:143:HIS:ND1	1:B:155:CYS:SG	2.82	0.52
1:B:64:VAL:CG2	1:B:132:ILE:HD13	2.31	0.52
1:B:147:TRP:N	1:B:148:ILE:HG13	2.25	0.52
1:A:40:TYR:CD2	1:A:52:LYS:HA	2.45	0.52
1:A:114:PHE:CD1	1:A:114:PHE:N	2.77	0.52
1:B:10:PHE:HD1	4:B:179:HOH:O	1.74	0.52
1:B:100:TYR:CB	1:B:121:ARG:HD3	2.22	0.52
1:B:90:GLU:O	1:B:91:GLN:C	2.47	0.52
1:B:159:ALA:O	1:B:162:ALA:CB	2.58	0.52
1:B:95:ILE:O	1:B:95:ILE:HG13	2.09	0.52
1:B:21:SER:OG	3:B:172:4IP:OPH	2.20	0.52
1:A:125:ILE:O	1:A:129:LYS:HG3	2.09	0.52
1:B:75:PRO:CA	1:B:78:GLN:CG	2.86	0.52
1:B:7:GLU:O	1:B:8:SER:OG	2.27	0.52
1:B:5:ILE:N	1:B:32:LEU:O	2.43	0.51
1:A:62:THR:O	1:A:138:LEU:HA	2.10	0.51
1:A:131:VAL:HG23	4:A:221:HOH:O	2.10	0.51
1:B:74:PRO:C	1:B:78:GLN:HG3	2.30	0.51
1:A:141:LYS:NZ	1:A:163:MET:CE	2.73	0.51
1:B:135:ASN:HB3	4:B:208:HOH:O	2.10	0.51
1:B:137:ASP:O	1:B:139:VAL:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:VAL:CG2	1:B:128:LEU:HB3	2.38	0.51
1:B:142:TYR:CE1	1:B:144:PRO:CA	2.93	0.51
1:B:143:HIS:HB3	1:B:154:CYS:HB2	1.88	0.51
1:B:127:GLN:HA	1:B:127:GLN:OE1	2.11	0.51
1:A:5:ILE:HD12	1:A:32:LEU:C	2.30	0.51
1:B:133:ARG:HG2	1:B:134:TYR:CD1	2.46	0.51
1:B:10:PHE:HZ	1:B:124:TRP:CD1	2.29	0.51
1:B:139:VAL:C	1:B:140:GLN:HG2	2.31	0.51
1:B:143:HIS:HE1	1:B:155:CYS:SG	2.29	0.51
1:A:92:ILE:CD1	1:B:9:ILE:CD1	2.89	0.51
1:B:90:GLU:HB3	1:B:93:SER:HB3	1.91	0.50
1:B:69:PRO:HD3	4:B:202:HOH:O	2.12	0.50
1:A:58:VAL:O	1:A:58:VAL:CG1	2.59	0.50
1:B:90:GLU:HG3	1:B:92:ILE:H	1.75	0.50
1:B:90:GLU:CG	1:B:93:SER:H	2.24	0.50
1:B:68:VAL:O	1:B:70:GLU:N	2.44	0.50
1:B:74:PRO:O	1:B:77:ARG:N	2.32	0.50
1:B:90:GLU:HG3	1:B:93:SER:H	1.75	0.50
1:A:129:LYS:O	1:A:132:ILE:N	2.45	0.50
1:B:119:GLU:CD	1:B:123:ARG:HD2	2.32	0.50
1:B:147:TRP:CH2	1:B:150:GLY:C	2.85	0.50
1:A:63:CYS:HB2	1:A:139:VAL:HG22	1.93	0.50
1:B:101:PRO:CA	4:B:178:HOH:O	2.14	0.50
3:A:171:4IP:OPF	3:A:171:4IP:O9P	2.30	0.50
1:B:128:LEU:O	1:B:131:VAL:N	2.39	0.50
1:A:62:THR:HB	1:A:139:VAL:CG1	2.31	0.50
1:A:138:LEU:N	1:A:138:LEU:HD23	2.23	0.49
1:B:113:VAL:O	4:B:178:HOH:O	2.20	0.49
1:B:124:TRP:O	1:B:125:ILE:C	2.49	0.49
1:B:155:CYS:CB	1:B:165:CYS:HB3	2.42	0.49
1:A:159:ALA:O	1:A:161:ASN:N	2.46	0.49
1:B:132:ILE:O	1:B:134:TYR:N	2.46	0.49
1:B:143:HIS:CE1	1:B:154:CYS:HG	2.30	0.49
1:B:74:PRO:O	1:B:78:GLN:HG3	2.13	0.49
1:B:13:ARG:HE	1:B:112:TYR:HD2	1.60	0.49
1:B:4:VAL:CG1	1:B:5:ILE:N	2.76	0.49
1:A:90:GLU:HA	1:A:93:SER:OG	2.12	0.49
1:B:30:PHE:CZ	1:B:113:VAL:HG22	2.48	0.49
1:B:7:GLU:HG3	1:B:31:LEU:CD2	2.43	0.49
1:A:34:VAL:CG2	1:A:35:HIS:HD2	2.21	0.49
1:A:42:TYR:HD2	1:B:44:PHE:CE2	2.31	0.48
1:B:57:ASP:HB2	1:B:60:LYS:CG	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:ARG:CG	1:B:134:TYR:CD1	2.97	0.48
1:A:76:GLU:HG2	4:A:234:HOH:O	2.13	0.48
1:A:80:PRO:HB3	1:A:97:ARG:HH21	1.77	0.48
1:B:119:GLU:O	1:B:119:GLU:HG2	2.13	0.48
1:B:141:LYS:HA	1:B:166:GLN:O	2.13	0.48
1:B:77:ARG:HD2	1:B:114:PHE:CE2	2.48	0.48
1:B:90:GLU:HG3	4:B:219:HOH:O	2.13	0.48
1:B:99:PRO:N	1:B:115:SER:O	2.47	0.48
1:B:143:HIS:O	1:B:144:PRO:C	2.52	0.48
1:A:169:GLU:C	1:A:170:ASN:HD22	2.17	0.48
1:B:143:HIS:CE1	1:B:165:CYS:N	2.79	0.48
1:B:35:HIS:O	1:B:58:VAL:CG2	2.62	0.48
1:B:106:TYR:N	1:B:109:GLY:O	2.35	0.48
1:B:63:CYS:CA	4:B:173:HOH:O	2.61	0.48
1:A:159:ALA:O	1:A:160:LYS:C	2.52	0.48
1:B:15:GLN:HB3	1:B:17:LYS:HD2	1.95	0.48
1:B:94:ILE:HG23	1:B:94:ILE:O	2.13	0.48
1:B:10:PHE:HB3	1:B:114:PHE:O	2.14	0.47
1:B:142:TYR:CZ	1:B:144:PRO:HG3	2.49	0.47
1:B:88:GLU:HB2	1:B:117:THR:HG21	1.92	0.47
1:A:10:PHE:HD1	1:A:115:SER:HA	1.79	0.47
1:B:69:PRO:CG	4:B:202:HOH:O	2.41	0.47
1:B:112:TYR:OH	1:B:146:PHE:HA	2.15	0.47
1:B:5:ILE:CA	4:B:241:HOH:O	2.63	0.47
1:B:66:THR:CG2	4:B:174:HOH:O	2.63	0.47
1:B:2:ALA:CB	1:B:33:THR:HG21	2.45	0.47
1:B:32:LEU:CD1	1:B:33:THR:O	2.63	0.47
1:B:73:PRO:O	1:B:78:GLN:CG	2.56	0.47
1:B:118:GLU:C	1:B:120:LEU:N	2.68	0.47
1:B:127:GLN:OE1	1:B:127:GLN:CA	2.63	0.47
1:B:146:PHE:C	1:B:148:ILE:CD1	2.80	0.47
1:B:146:PHE:O	1:B:148:ILE:HD11	2.15	0.47
1:B:93:SER:O	1:B:97:ARG:N	2.47	0.47
1:B:20:THR:O	1:B:21:SER:C	2.52	0.47
1:A:59:GLU:O	1:A:135:ASN:ND2	2.47	0.47
1:B:104:VAL:O	1:B:104:VAL:HG12	2.09	0.47
1:B:75:PRO:N	1:B:78:GLN:CG	2.78	0.46
1:A:68:VAL:HG13	1:A:69:PRO:HD2	1.97	0.46
1:B:112:TYR:OH	1:B:147:TRP:N	2.48	0.46
1:B:112:TYR:CE1	1:B:146:PHE:CD1	3.04	0.46
1:B:67:VAL:HG22	1:B:103:GLN:CB	2.34	0.46
1:B:69:PRO:CD	4:B:202:HOH:O	2.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:VAL:HB	4:B:244:HOH:O	2.14	0.46
1:B:141:LYS:HB3	1:B:164:GLY:O	2.16	0.46
1:B:34:VAL:O	1:B:58:VAL:CG2	2.63	0.46
1:A:147:TRP:NE1	1:A:160:LYS:HA	2.30	0.46
1:B:43:ASP:O	1:B:47:GLY:N	2.49	0.46
1:B:64:VAL:CG1	1:B:128:LEU:CD1	2.94	0.46
1:B:129:LYS:HG2	1:B:129:LYS:H	1.20	0.46
1:B:75:PRO:HA	1:B:78:GLN:CD	2.36	0.46
1:B:79:ILE:O	1:B:79:ILE:CG2	2.61	0.46
1:B:102:PHE:C	4:B:244:HOH:O	2.53	0.46
1:B:142:TYR:CZ	1:B:144:PRO:CG	2.99	0.46
1:B:10:PHE:HB2	1:B:30:PHE:CE1	2.51	0.46
1:A:137:ASP:O	1:A:138:LEU:C	2.52	0.46
1:A:157:GLN:OE1	1:A:162:ALA:HB1	2.16	0.45
1:B:147:TRP:O	1:B:148:ILE:HG13	2.15	0.45
1:B:74:PRO:CB	1:B:75:PRO:HD2	2.46	0.45
1:B:75:PRO:O	1:B:76:GLU:C	2.54	0.45
1:A:67:VAL:HG22	1:A:103:GLN:HB3	1.98	0.45
1:B:90:GLU:CB	1:B:93:SER:HB3	2.46	0.45
1:B:105:VAL:HA	1:B:109:GLY:O	2.17	0.45
1:B:34:VAL:O	1:B:35:HIS:C	2.49	0.45
1:A:147:TRP:CD1	1:A:160:LYS:HA	2.51	0.45
1:B:154:CYS:SG	1:B:155:CYS:SG	3.14	0.45
1:B:159:ALA:O	1:B:162:ALA:HB2	2.17	0.45
1:B:169:GLU:O	1:B:170:ASN:ND2	2.49	0.45
1:B:99:PRO:CD	1:B:100:TYR:CD2	2.97	0.45
1:B:142:TYR:CZ	1:B:144:PRO:HB3	2.52	0.45
1:B:154:CYS:HB2	2:B:171:ZN:ZN	1.48	0.45
1:A:94:ILE:CD1	1:B:91:GLN:HG3	2.47	0.45
1:B:43:ASP:HB3	1:B:48:ARG:HG3	1.98	0.45
1:B:7:GLU:C	1:B:8:SER:OG	2.55	0.45
1:B:112:TYR:CE1	1:B:146:PHE:CE1	3.05	0.45
1:B:146:PHE:HB3	1:B:148:ILE:HG12	1.98	0.45
1:B:166:GLN:CG	1:B:167:ILE:N	2.78	0.45
1:B:75:PRO:HB2	1:B:76:GLU:H	1.26	0.45
1:B:122:LYS:N	4:B:192:HOH:O	2.46	0.44
1:B:133:ARG:NE	1:B:134:TYR:CE1	2.86	0.44
1:A:36:LYS:HA	1:A:58:VAL:HG23	1.98	0.44
1:A:91:GLN:HG3	1:B:94:ILE:HD13	1.99	0.44
1:B:142:TYR:CE1	1:B:144:PRO:CB	3.01	0.44
1:A:141:LYS:HZ2	1:A:163:MET:CE	2.29	0.44
1:A:117:THR:HB	4:A:264:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:152:TYR:C	1:B:154:CYS:H	2.20	0.44
1:A:169:GLU:O	1:A:170:ASN:C	2.56	0.44
1:A:133:ARG:HB3	1:A:134:TYR:CD2	2.52	0.44
1:A:142:TYR:OH	1:A:144:PRO:HB3	2.17	0.44
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.60	0.44
1:B:112:TYR:CD1	1:B:146:PHE:CE1	3.06	0.44
1:B:150:GLY:O	1:B:158:THR:CG2	2.66	0.44
1:B:68:VAL:CG1	1:B:68:VAL:O	2.65	0.44
1:A:90:GLU:O	1:A:93:SER:N	2.50	0.44
1:B:13:ARG:HG2	4:B:184:HOH:O	2.17	0.43
1:B:36:LYS:CA	1:B:58:VAL:HG23	2.48	0.43
1:B:169:GLU:CG	1:B:170:ASN:N	2.76	0.43
1:A:79:ILE:H	1:A:79:ILE:HG13	1.64	0.43
1:B:146:PHE:CB	1:B:148:ILE:HD11	2.48	0.43
1:B:100:TYR:CB	1:B:115:SER:HB3	2.28	0.43
1:B:117:THR:C	4:B:213:HOH:O	2.55	0.43
1:B:34:VAL:O	1:B:58:VAL:HB	2.18	0.43
1:B:74:PRO:HG3	1:B:77:ARG:NH2	2.34	0.43
1:A:10:PHE:HB3	1:A:114:PHE:O	2.18	0.43
1:A:143:HIS:NE2	1:A:164:GLY:HA2	2.33	0.43
1:A:5:ILE:CD1	1:A:33:THR:CA	2.96	0.43
1:A:155:CYS:O	1:A:157:GLN:N	2.51	0.43
1:B:65:GLU:O	1:B:103:GLN:N	2.51	0.43
1:B:68:VAL:HA	1:B:69:PRO:HD2	1.79	0.43
1:A:118:GLU:HG2	4:A:257:HOH:O	2.19	0.43
1:B:160:LYS:C	1:B:162:ALA:H	2.22	0.43
1:B:64:VAL:CG1	1:B:128:LEU:HB3	2.46	0.43
1:B:132:ILE:O	1:B:135:ASN:N	2.52	0.43
1:B:142:TYR:O	1:B:144:PRO:HD3	2.19	0.43
1:B:139:VAL:H	1:B:139:VAL:HG13	1.42	0.42
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.32	0.42
1:B:101:PRO:HB3	1:B:114:PHE:CE2	2.54	0.42
1:B:125:ILE:CG2	1:B:126:HIS:N	2.53	0.42
1:B:147:TRP:HA	1:B:152:TYR:HA	2.01	0.42
1:B:66:THR:HA	4:B:174:HOH:O	2.19	0.42
1:B:90:GLU:C	1:B:92:ILE:N	2.71	0.42
1:A:119:GLU:O	1:A:123:ARG:HG3	2.19	0.42
1:B:143:HIS:NE2	1:B:164:GLY:HA2	2.33	0.42
1:A:170:ASN:HD22	1:A:170:ASN:N	2.16	0.42
1:B:75:PRO:HA	1:B:78:GLN:CG	2.49	0.42
1:B:143:HIS:CE1	1:B:163:MET:O	2.73	0.42
1:B:11:LEU:HD12	1:B:26:LYS:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:PRO:HA	1:A:78:GLN:HB2	2.02	0.42
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.74	0.42
1:A:90:GLU:C	1:A:92:ILE:N	2.71	0.42
1:A:92:ILE:HA	1:A:92:ILE:HD13	1.81	0.42
1:A:141:LYS:HA	1:A:166:GLN:O	2.20	0.41
1:A:145:CYS:HA	4:A:191:HOH:O	2.20	0.41
1:B:17:LYS:HE3	1:B:106:TYR:OH	2.19	0.41
1:A:42:TYR:CD2	1:B:44:PHE:CE2	3.08	0.41
1:B:158:THR:O	1:B:158:THR:HG22	2.20	0.41
1:B:4:VAL:HG13	1:B:6:LEU:O	2.19	0.41
1:B:106:TYR:CE2	1:B:108:GLU:HB2	2.54	0.41
1:B:26:LYS:HD2	1:B:28:ARG:NH2	2.35	0.41
1:A:9:ILE:HD12	1:B:92:ILE:HG12	2.02	0.41
1:A:74:PRO:HB2	1:A:75:PRO:HD2	2.03	0.41
1:B:142:TYR:CE1	1:B:144:PRO:HB3	2.55	0.41
1:B:98:PHE:HD2	1:B:116:PRO:HD3	1.86	0.41
1:B:114:PHE:CD1	4:B:178:HOH:O	2.58	0.40
1:B:143:HIS:HB3	1:B:154:CYS:SG	2.60	0.40
1:B:147:TRP:CH2	1:B:150:GLY:O	2.75	0.40
1:B:75:PRO:C	1:B:77:ARG:N	2.75	0.40
1:B:13:ARG:NH2	1:B:112:TYR:CD2	2.85	0.40
1:B:100:TYR:N	1:B:100:TYR:HD2	2.17	0.40
1:B:25:PHE:CZ	1:B:77:ARG:CZ	3.04	0.40
1:B:87:SER:OG	1:B:117:THR:OG1	2.22	0.40
1:A:40:TYR:CD1	1:A:49:ARG:HD2	2.57	0.40
1:A:90:GLU:CG	1:A:91:GLN:N	2.84	0.40
1:B:58:VAL:C	1:B:61:ILE:HG13	2.41	0.40
1:B:66:THR:HG22	4:B:174:HOH:O	2.21	0.40
1:B:88:GLU:HB2	1:B:117:THR:HG22	1.99	0.40
1:A:90:GLU:HA	1:A:93:SER:HG	1.87	0.40

All (7) 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)
4:A:207:HOH:O	4:A:207:HOH:O[6_555]	1.28	0.92
4:A:211:HOH:O	4:A:211:HOH:O[6_555]	1.70	0.50
1:A:142:TYR:OH	4:A:211:HOH:O[6_555]	1.76	0.44
1:A:129:LYS:NZ	1:A:170:ASN:O[6_555]	1.80	0.40
4:A:288:HOH:O	4:A:288:HOH:O[7_455]	1.91	0.29
1:A:66:THR:OG1	1:A:166:GLN:NE2[6_555]	2.07	0.13
4:B:201:HOH:O	4:B:201:HOH:O[10_555]	2.11	0.09

## 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	159/169 (94%)	143 (90%)	10 (6%)	6 (4%)	5	4
1	B	158/169 (94%)	103 (65%)	33 (21%)	22 (14%)	0	0
All	All	317/338 (94%)	246 (78%)	43 (14%)	28 (9%)	1	0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	B	75	PRO
1	B	76	GLU
1	B	78	GLN
1	B	91	GLN
1	B	125	ILE
1	B	133	ARG
1	B	157	GLN
1	B	3	ALA
1	B	17	LYS
1	B	110	PRO
1	B	130	ASN
1	B	152	TYR
1	B	156	SER
1	B	166	GLN
1	A	160	LYS
1	B	7	GLU
1	B	69	PRO
1	B	144	PRO
1	A	110	PRO
1	A	133	ARG
1	B	126	HIS
1	B	153	LEU
1	B	118	GLU
1	A	138	LEU
1	B	139	VAL
1	B	100	TYR

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Mol	Chain	Res	Type
1	A	80	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	153/158 (97%)	118 (77%)	35 (23%)	1	1
1	B	152/158 (96%)	109 (72%)	43 (28%)	0	0
All	All	305/316 (96%)	227 (74%)	78 (26%)	1	1

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	17	LYS
1	A	18	LYS
1	A	19	LYS
1	A	20	THR
1	A	25	PHE
1	A	36	LYS
1	A	38	SER
1	A	44	PHE
1	A	48	ARG
1	A	49	ARG
1	A	51	SER
1	A	70	GLU
1	A	77	ARG
1	A	79	ILE
1	A	81	ARG
1	A	82	ARG
1	A	89	MET
1	A	90	GLU
1	A	94	ILE
1	A	96	GLU
1	A	97	ARG
1	A	107	ASP
1	A	118	GLU

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Mol	Chain	Res	Type
1	A	120	LEU
1	A	122	LYS
1	A	133	ARG
1	A	140	GLN
1	A	142	TYR
1	A	148	ILE
1	A	160	LYS
1	A	163	MET
1	A	165	CYS
1	A	169	GLU
1	A	170	ASN
1	B	12	LYS
1	B	15	GLN
1	B	17	LYS
1	B	25	PHE
1	B	34	VAL
1	B	36	LYS
1	B	38	SER
1	B	40	TYR
1	B	59	GLU
1	B	60	LYS
1	B	61	ILE
1	B	62	THR
1	B	65	GLU
1	B	70	GLU
1	B	94	ILE
1	B	97	ARG
1	B	106	TYR
1	B	108	GLU
1	B	114	PHE
1	B	115	SER
1	B	117	THR
1	B	119	GLU
1	B	120	LEU
1	B	125	ILE
1	B	126	HIS
1	B	131	VAL
1	B	133	ARG
1	B	136	SER
1	B	137	ASP
1	B	140	GLN
1	B	145	CYS

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Mol	Chain	Res	Type
1	B	148	ILE
1	B	151	GLN
1	B	152	TYR
1	B	153	LEU
1	B	155	CYS
1	B	157	GLN
1	B	158	THR
1	B	160	LYS
1	B	163	MET
1	B	165	CYS
1	B	168	LEU
1	B	169	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	103	GLN
1	A	135	ASN
1	A	170	ASN
1	B	35	HIS

### 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	4IP	A	171	-	28,28,28	1.88	12 (42%)	46,46,46	2.06	15 (32%)
3	4IP	B	172	-	28,28,28	1.90	13 (46%)	46,46,46	2.65	18 (39%)

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
3	4IP	A	171	-	-	0/20/44/44	0/1/1/1
3	4IP	B	172	-	-	0/20/44/44	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	171	4IP	P3-O6P	-3.10	1.43	1.54
3	A	171	4IP	P3-O4P	-3.10	1.40	1.51
3	B	172	4IP	P5-OPH	-2.98	1.43	1.54
3	B	172	4IP	P4-O7P	-2.92	1.44	1.54
3	A	171	4IP	P5-OPH	-2.88	1.44	1.54
3	B	172	4IP	P3-O5P	-2.83	1.44	1.54
3	B	172	4IP	O3-C3	-2.76	1.35	1.44
3	A	171	4IP	P4-O4	-2.71	1.51	1.59
3	B	172	4IP	O1-C1	2.61	1.52	1.44
3	A	171	4IP	P3-O5P	-2.57	1.45	1.54
3	B	172	4IP	P3-O6P	-2.49	1.45	1.54
3	A	171	4IP	C5-C4	-2.44	1.47	1.52
3	B	172	4IP	C4-C3	2.40	1.57	1.52
3	B	172	4IP	P3-O4P	-2.29	1.43	1.51
3	A	171	4IP	C4-C3	2.29	1.56	1.52
3	A	171	4IP	O1-C1	2.28	1.51	1.44
3	B	172	4IP	P4-O4	-2.27	1.52	1.59
3	B	172	4IP	C2-C3	-2.27	1.45	1.52
3	A	171	4IP	P4-O9P	-2.18	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	171	4IP	P5-OPF	-2.15	1.46	1.54
3	B	172	4IP	P5-OPG	-2.12	1.44	1.51
3	B	172	4IP	P1-O3P	-2.11	1.47	1.54
3	A	171	4IP	P5-OPG	-2.09	1.44	1.51
3	B	172	4IP	P1-O1	2.07	1.66	1.59
3	A	171	4IP	P1-O1	2.00	1.66	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	172	4IP	O3-P3-O4P	-6.14	89.64	106.79
3	B	172	4IP	O7P-P4-O4	-5.70	90.69	107.09
3	B	172	4IP	O1-C1-C2	5.64	119.92	108.44
3	A	171	4IP	O1-C1-C2	5.41	119.47	108.44
3	B	172	4IP	O5P-P3-O4P	4.86	126.33	110.44
3	A	171	4IP	O3P-P1-O1	-4.61	93.82	107.09
3	B	172	4IP	OPH-P5-O5	-4.60	93.84	107.09
3	B	172	4IP	P5-O5-C5	4.34	131.09	121.96
3	B	172	4IP	O5P-P3-O3	-4.29	94.75	107.09
3	A	171	4IP	P5-O5-C5	4.10	130.60	121.96
3	B	172	4IP	P1-O1-C1	3.83	130.02	121.96
3	B	172	4IP	O3-C3-C4	3.40	115.46	108.45
3	A	171	4IP	O5P-P3-O4P	3.37	121.45	110.44
3	B	172	4IP	O2-C2-C1	3.19	117.30	109.85
3	A	171	4IP	C6-C1-C2	2.92	114.83	110.68
3	A	171	4IP	O3-C3-C4	2.91	114.45	108.45
3	B	172	4IP	C5-C4-C3	-2.87	104.55	110.44
3	A	171	4IP	O3-P3-O4P	-2.82	98.91	106.79
3	B	172	4IP	OPH-P5-OPF	2.79	118.47	107.61
3	A	171	4IP	C3-C2-C1	-2.75	103.47	109.07
3	B	172	4IP	C6-C1-C2	-2.73	106.79	110.68
3	B	172	4IP	P4-O4-C4	2.67	127.57	121.96
3	B	172	4IP	O5-C5-C4	2.60	113.81	108.45
3	A	171	4IP	OPH-P5-O5	-2.60	99.61	107.09
3	A	171	4IP	O3P-P1-O1P	2.59	118.91	110.44
3	A	171	4IP	O5P-P3-O3	-2.57	99.68	107.09
3	B	172	4IP	O7P-P4-O9P	2.54	118.75	110.44
3	B	172	4IP	O2P-P1-O1P	2.54	118.75	110.44
3	A	171	4IP	OPF-P5-OPG	2.47	118.50	110.44
3	A	171	4IP	OPF-P5-O5	-2.32	100.41	107.09
3	B	172	4IP	O3P-P1-O1	-2.31	100.43	107.09
3	A	171	4IP	O6-C6-C5	-2.08	104.99	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	171	4IP	P1-O1-C1	2.07	126.32	121.96

There are no chirality outliers.

There are no torsion outliers.

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	163/169 (96%)	-0.40	0 100 100	33, 54, 77, 85	8 (4%)
1	B	162/169 (95%)	0.03	8 (4%) 28 26	37, 62, 83, 85	16 (9%)
All	All	325/338 (96%)	-0.19	8 (2%) 56 52	33, 58, 82, 85	24 (7%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	SER	7.1
1	B	142	TYR	5.4
1	B	155	CYS	3.4
1	B	158	THR	3.4
1	B	88	GLU	3.2
1	B	147	TRP	2.9
1	B	170	ASN	2.6
1	B	167	ILE	2.2

### 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	ZN	B	171	1/1	0.18	-0.46	85,85,85,85	0
3	4IP	A	171	28/28	0.08	-1.17	35,44,54,65	0
2	ZN	A	1	1/1	0.06	-1.61	45,45,45,45	0
3	4IP	B	172	28/28	0.08	-1.66	34,56,63,75	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.