



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:02 am GMT

PDB ID : 1BWN  
Title : PH DOMAIN AND BTK MOTIF FROM BRUTON'S TYROSINE KINASE  
MUTANT E41K IN COMPLEX WITH INS(1,3,4,5)P4  
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Deposited on : 1998-09-25  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

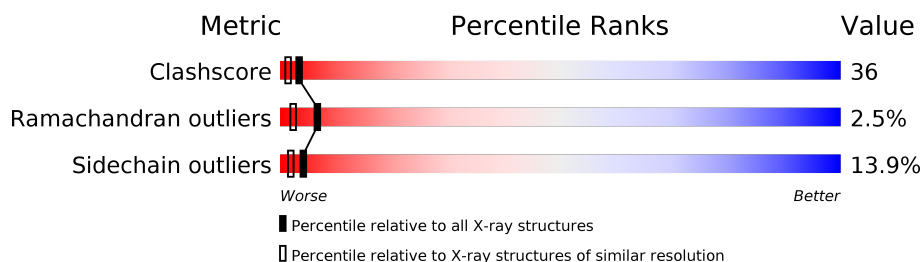
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	169	
1	B	169	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3101 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 BRUTON'S TYROSINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	23	0	0
			1376	886	242	241	7			
1	B	161	Total	C	N	O	S	37	0	0
			1338	864	231	236	7			

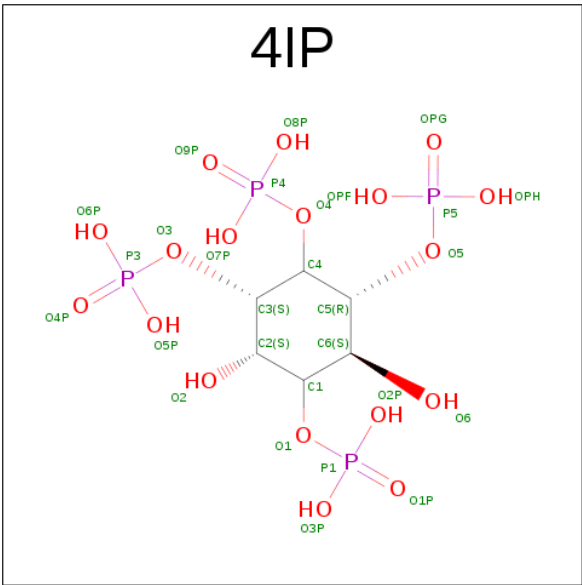
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	LYS	GLU	ENGINEERED	UNP Q06187
B	41	LYS	GLU	ENGINEERED	UNP Q06187

- 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	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		
3	B	1	Total	C	O	P	0	0
			28	6	18	4		

- Molecule 4 is water.

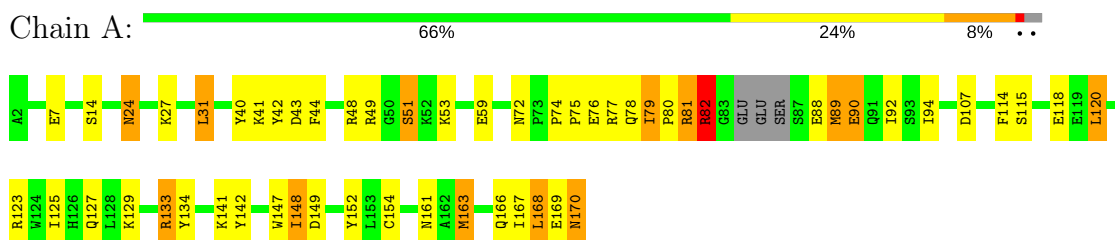
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	106	Total	O	0	0
			106	106		

### 3 Residue-property plots

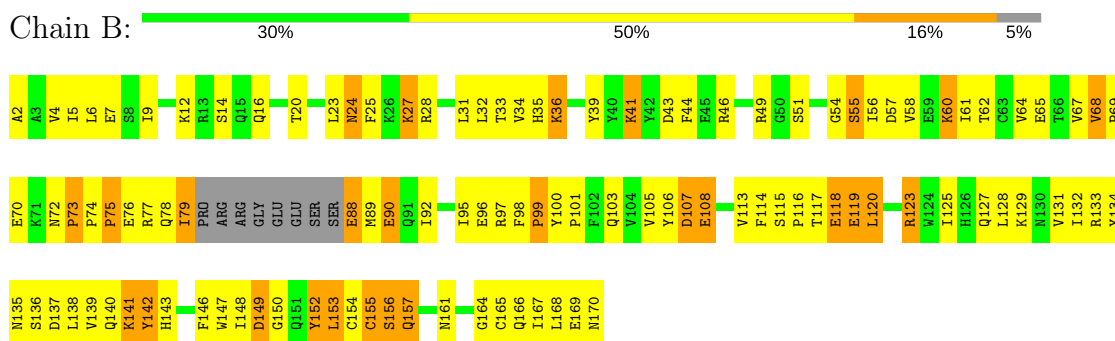
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: BRUTON'S TYROSINE KINASE



#### • Molecule 1: BRUTON'S TYROSINE KINASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.78Å 110.78Å 215.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.4 (35.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.214 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: 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	1.13	2/1409 (0.1%)	1.00	1/1898 (0.1%)
1	B	1.07	3/1370 (0.2%)	1.14	2/1846 (0.1%)
All	All	1.10	5/2779 (0.2%)	1.07	3/3744 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	GLU	CD-OE2	9.52	1.36	1.25
1	B	119	GLU	CD-OE2	7.02	1.33	1.25
1	B	90	GLU	CD-OE1	6.33	1.32	1.25
1	B	65	GLU	CD-OE2	5.18	1.31	1.25
1	A	82	ARG	CZ-NH2	5.01	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	CYS	CA-CB-SG	-6.33	102.60	114.00
1	B	88	GLU	N-CA-C	5.82	126.72	111.00
1	A	107	ASP	CB-CG-OD2	-5.26	113.57	118.30

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	1376	0	1392	57	1
1	B	1338	0	1354	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	56	0	16	4	1
3	B	56	0	16	8	2
4	A	167	0	0	14	0
4	B	106	0	0	19	2
All	All	3101	0	2778	194	3

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 36.

All (194) 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:B:155:CYS:HB3	1:B:165:CYS:HB3	1.42	1.02
1:B:41:LYS:HE3	3:B:172:4IP:H6	1.39	1.00
1:B:41:LYS:CE	3:B:172:4IP:H6	1.95	0.97
1:B:155:CYS:HB3	1:B:165:CYS:CB	1.98	0.94
1:A:88:GLU:CB	1:B:123:ARG:HH12	1.81	0.92
1:B:89:MET:HA	4:B:222:HOH:O	1.72	0.89
1:B:152:TYR:O	1:B:154:CYS:N	2.08	0.87
1:A:169:GLU:HA	4:A:292:HOH:O	1.81	0.81
1:B:148:ILE:HG21	1:B:153:LEU:HD11	1.63	0.80
1:B:88:GLU:C	1:B:90:GLU:H	1.85	0.79
1:A:141:LYS:HG2	1:A:167:ILE:HG13	1.64	0.79
1:B:68:VAL:O	1:B:68:VAL:HG12	1.82	0.79
1:A:127:GLN:OE1	4:A:335:HOH:O	2.02	0.78
1:B:147:TRP:HB2	1:B:152:TYR:CE1	2.20	0.77
1:B:106:TYR:CE2	1:B:108:GLU:HG3	2.20	0.76
1:B:141:LYS:HG2	4:B:242:HOH:O	1.85	0.76
1:A:141:LYS:HE3	1:A:163:MET:SD	2.26	0.74
1:B:143:HIS:HB3	1:B:154:CYS:SG	2.28	0.74
1:B:2:ALA:HB1	1:B:33:THR:HB	1.70	0.73
1:B:67:VAL:O	1:B:69:PRO:HD3	1.89	0.73
1:B:148:ILE:CG2	1:B:153:LEU:HD11	2.21	0.71
1:B:127:GLN:O	1:B:131:VAL:HG13	1.91	0.70
1:A:89:MET:O	1:A:92:ILE:N	2.22	0.69
1:B:141:LYS:HA	1:B:166:GLN:O	1.93	0.69
1:B:72:ASN:O	1:B:73:PRO:C	2.32	0.68
1:B:148:ILE:HG13	1:B:149:ASP:N	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:OD1	1:B:137:ASP:O	2.11	0.67
1:B:128:LEU:O	1:B:131:VAL:HG22	1.94	0.67
1:B:27:LYS:HG2	4:B:178:HOH:O	1.94	0.66
1:A:76:GLU:HG3	1:A:77:ARG:HG3	1.77	0.66
1:B:114:PHE:CD1	1:B:114:PHE:N	2.62	0.66
1:B:146:PHE:HB2	1:B:153:LEU:HD12	1.78	0.66
1:B:27:LYS:HE2	4:B:178:HOH:O	1.96	0.65
1:B:74:PRO:CB	1:B:75:PRO:HD2	2.27	0.65
1:B:135:ASN:HB2	1:B:138:LEU:HD21	1.79	0.64
1:B:100:TYR:CE2	1:B:117:THR:HA	2.33	0.64
1:A:88:GLU:CA	1:B:123:ARG:HH12	2.10	0.64
1:B:169:GLU:O	1:B:170:ASN:HB2	1.99	0.63
1:B:132:ILE:O	1:B:138:LEU:HD11	1.98	0.62
1:A:41:LYS:HE3	3:A:172:4IP:H6	1.80	0.62
1:B:32:LEU:HD12	1:B:33:THR:N	2.14	0.62
1:A:170:ASN:C	4:A:234:HOH:O	2.37	0.61
1:B:67:VAL:HG12	1:B:68:VAL:N	2.15	0.61
1:A:80:PRO:HG3	4:A:263:HOH:O	1.99	0.61
1:B:88:GLU:C	1:B:90:GLU:N	2.54	0.61
1:A:75:PRO:HA	1:A:78:GLN:HG3	1.83	0.61
1:A:82:ARG:HD2	4:A:337:HOH:O	2.01	0.60
1:B:64:VAL:HG21	1:B:128:LEU:HB3	1.83	0.59
1:B:100:TYR:CD2	1:B:117:THR:HA	2.37	0.59
1:B:140:GLN:HB3	1:B:168:LEU:O	2.03	0.59
1:A:42:TYR:OH	1:B:96:GLU:OE2	2.14	0.59
1:A:7:GLU:HG3	1:A:31:LEU:HD22	1.85	0.59
1:A:24:ASN:HD22	1:A:24:ASN:C	2.04	0.59
1:B:58:VAL:HA	1:B:61:ILE:HD12	1.85	0.59
1:B:146:PHE:HB2	1:B:153:LEU:CD1	2.33	0.58
1:B:100:TYR:HB2	1:B:115:SER:HB3	1.85	0.58
1:B:100:TYR:HD2	1:B:117:THR:C	2.06	0.58
1:A:89:MET:O	1:A:90:GLU:C	2.42	0.58
1:A:59:GLU:HG2	4:A:201:HOH:O	2.04	0.57
1:B:74:PRO:O	1:B:78:GLN:HG3	2.04	0.57
1:B:146:PHE:O	1:B:153:LEU:HD12	2.03	0.57
1:A:44:PHE:CZ	4:B:178:HOH:O	2.56	0.57
1:B:125:ILE:O	1:B:129:LYS:HG2	2.05	0.57
1:B:34:VAL:HG13	4:B:260:HOH:O	2.04	0.57
1:B:68:VAL:O	1:B:68:VAL:CG1	2.50	0.56
1:B:14:SER:N	1:B:24:ASN:O	2.37	0.56
1:B:74:PRO:O	1:B:75:PRO:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TRP:HD1	1:B:152:TYR:CD2	2.24	0.56
1:B:148:ILE:CG1	1:B:149:ASP:N	2.69	0.55
1:B:7:GLU:HG3	1:B:31:LEU:CD2	2.36	0.55
3:A:172:4IP:OPG	3:A:172:4IP:O9P	2.24	0.55
1:B:27:LYS:CE	4:B:178:HOH:O	2.55	0.54
1:B:142:TYR:N	1:B:164:GLY:HA3	2.23	0.54
1:B:39:TYR:CZ	1:B:54:GLY:HA3	2.43	0.54
1:A:133:ARG:HG2	1:A:134:TYR:CE2	2.43	0.54
1:B:55:SER:HB3	4:B:217:HOH:O	2.06	0.53
1:A:167:ILE:C	1:A:168:LEU:HD23	2.28	0.53
1:B:152:TYR:HB3	1:B:155:CYS:SG	2.48	0.53
1:B:155:CYS:CB	1:B:165:CYS:HB3	2.28	0.53
1:A:81:ARG:NH1	1:A:81:ARG:HG2	2.24	0.53
1:B:72:ASN:O	1:B:73:PRO:O	2.28	0.52
1:B:36:LYS:CA	1:B:58:VAL:HG23	2.41	0.51
1:A:40:TYR:CD2	1:A:49:ARG:HD2	2.45	0.51
1:A:43:ASP:HB3	1:A:48:ARG:O	2.09	0.51
1:B:67:VAL:HG11	1:B:146:PHE:CE1	2.46	0.51
1:B:131:VAL:HG23	1:B:132:ILE:HG23	1.93	0.51
1:A:51:SER:HB2	4:A:222:HOH:O	2.11	0.51
1:A:147:TRP:HB2	1:A:152:TYR:CE1	2.46	0.51
1:B:135:ASN:HB2	1:B:138:LEU:CD2	2.42	0.50
1:B:24:ASN:ND2	3:B:1:4IP:O2	2.42	0.50
1:A:88:GLU:CB	1:B:123:ARG:NH1	2.64	0.50
1:A:74:PRO:O	1:A:78:GLN:HG3	2.11	0.50
1:A:141:LYS:HG2	1:A:167:ILE:CG1	2.36	0.49
1:B:98:PHE:HA	1:B:116:PRO:HA	1.95	0.49
1:A:115:SER:OG	1:A:120:LEU:HB3	2.13	0.49
1:A:76:GLU:HG2	4:A:241:HOH:O	2.12	0.49
1:B:35:HIS:C	1:B:58:VAL:HG23	2.33	0.48
1:B:62:THR:HB	1:B:139:VAL:HG13	1.94	0.48
1:A:27:LYS:HE3	1:B:44:PHE:O	2.14	0.48
1:A:81:ARG:O	1:A:82:ARG:HD3	2.14	0.48
1:A:92:ILE:HG12	1:B:9:ILE:HD12	1.96	0.48
1:B:7:GLU:HG3	1:B:31:LEU:HD23	1.95	0.48
1:A:75:PRO:HA	1:A:78:GLN:CG	2.42	0.48
1:B:100:TYR:HD2	1:B:117:THR:CA	2.27	0.48
1:A:148:ILE:O	1:A:149:ASP:HB2	2.12	0.48
1:B:79:ILE:O	1:B:97:ARG:NH1	2.47	0.48
1:A:127:GLN:HB3	4:A:335:HOH:O	2.15	0.47
1:B:107:ASP:OD1	1:B:107:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:HD12	1:B:149:ASP:H	1.79	0.47
1:B:100:TYR:CD2	1:B:117:THR:C	2.86	0.47
1:B:41:LYS:HE2	3:B:172:4IP:H6	1.91	0.47
1:A:127:GLN:HG2	4:A:264:HOH:O	2.14	0.47
1:A:114:PHE:N	1:A:114:PHE:CD1	2.83	0.47
1:B:114:PHE:HD1	1:B:114:PHE:N	2.09	0.47
1:A:82:ARG:HA	1:A:82:ARG:HD2	1.79	0.46
1:A:14:SER:HB3	3:A:1:4IP:O2	2.16	0.46
3:B:1:4IP:OPF	3:B:1:4IP:O9P	2.33	0.46
1:B:34:VAL:HG12	1:B:35:HIS:CE1	2.50	0.46
1:B:2:ALA:HB1	1:B:33:THR:CB	2.43	0.46
1:A:125:ILE:O	1:A:129:LYS:HG2	2.16	0.46
1:B:36:LYS:HA	1:B:58:VAL:HG23	1.97	0.46
1:B:36:LYS:N	1:B:58:VAL:HG23	2.31	0.46
1:B:137:ASP:O	1:B:137:ASP:CG	2.53	0.46
1:B:12:LYS:HE3	1:B:39:TYR:CE1	2.51	0.45
1:A:167:ILE:O	1:A:168:LEU:HD23	2.16	0.45
1:A:169:GLU:CA	4:A:292:HOH:O	2.52	0.45
1:A:167:ILE:HG22	1:A:168:LEU:N	2.31	0.45
1:B:100:TYR:CD2	1:B:117:THR:CA	2.99	0.45
1:B:41:LYS:HE3	3:B:172:4IP:C6	2.28	0.45
1:A:44:PHE:CE1	4:B:178:HOH:O	2.55	0.45
1:B:60:LYS:NZ	4:B:213:HOH:O	2.19	0.45
1:A:79:ILE:HG13	4:A:230:HOH:O	2.16	0.45
1:A:81:ARG:HH11	1:A:81:ARG:HG2	1.81	0.45
1:B:100:TYR:HE2	1:B:117:THR:HA	1.81	0.45
1:B:155:CYS:HB2	1:B:157:GLN:HG3	1.99	0.44
1:B:55:SER:C	1:B:56:ILE:HG13	2.36	0.44
1:B:67:VAL:CG1	1:B:68:VAL:N	2.77	0.44
1:B:152:TYR:C	1:B:154:CYS:H	2.20	0.44
1:B:25:PHE:N	1:B:25:PHE:CD1	2.85	0.44
1:B:27:LYS:CG	4:B:178:HOH:O	2.57	0.44
1:B:7:GLU:CG	1:B:31:LEU:CD2	2.96	0.44
1:B:12:LYS:NZ	4:B:174:HOH:O	2.49	0.44
1:B:43:ASP:OD2	1:B:46:ARG:HD2	2.17	0.44
3:B:1:4IP:H5	4:B:252:HOH:O	2.17	0.44
3:B:172:4IP:O5P	4:B:179:HOH:O	2.21	0.44
1:B:92:ILE:O	1:B:96:GLU:HG3	2.17	0.44
1:B:74:PRO:O	1:B:77:ARG:N	2.42	0.43
1:B:7:GLU:CD	1:B:31:LEU:HD21	2.37	0.43
1:B:70:GLU:OE1	1:B:77:ARG:NE	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:CG2	1:A:168:LEU:N	2.80	0.43
1:B:101:PRO:HA	1:B:113:VAL:O	2.18	0.43
1:B:95:ILE:O	1:B:95:ILE:HG13	2.18	0.43
1:B:118:GLU:O	1:B:119:GLU:C	2.54	0.43
1:B:4:VAL:CG1	1:B:6:LEU:O	2.66	0.43
1:A:166:GLN:HG2	1:A:167:ILE:N	2.32	0.43
1:B:57:ASP:HB2	1:B:60:LYS:HG3	2.00	0.43
1:B:79:ILE:CD1	1:B:100:TYR:HE1	2.32	0.43
1:B:74:PRO:HB2	1:B:75:PRO:HD2	1.99	0.42
1:B:79:ILE:HD13	1:B:100:TYR:CE1	2.53	0.42
1:B:64:VAL:HA	1:B:103:GLN:O	2.20	0.42
1:B:148:ILE:C	1:B:150:GLY:H	2.23	0.42
1:B:16:GLN:OE1	1:B:23:LEU:HD13	2.20	0.42
1:B:138:LEU:HG	4:B:211:HOH:O	2.20	0.42
1:B:61:ILE:HG23	1:B:105:VAL:O	2.20	0.42
1:B:148:ILE:C	1:B:150:GLY:N	2.73	0.42
1:B:156:SER:O	1:B:157:GLN:O	2.38	0.42
1:B:120:LEU:HA	1:B:120:LEU:HD23	1.36	0.42
1:B:68:VAL:O	1:B:146:PHE:CE2	2.73	0.42
1:A:43:ASP:C	1:A:43:ASP:OD1	2.54	0.41
1:B:152:TYR:CB	1:B:155:CYS:SG	3.08	0.41
1:B:27:LYS:CD	4:B:178:HOH:O	2.68	0.41
1:B:7:GLU:HG3	1:B:31:LEU:HD21	2.02	0.41
1:A:169:GLU:CB	4:A:292:HOH:O	2.67	0.41
1:B:60:LYS:CE	4:B:213:HOH:O	2.67	0.41
1:B:128:LEU:O	1:B:129:LYS:C	2.56	0.41
1:B:128:LEU:O	1:B:131:VAL:N	2.51	0.41
1:B:5:ILE:HB	1:B:32:LEU:O	2.20	0.41
1:B:67:VAL:CG2	1:B:103:GLN:HB3	2.50	0.41
1:B:73:PRO:HG2	1:B:78:GLN:HG2	2.02	0.41
1:B:68:VAL:HA	1:B:69:PRO:HD2	1.74	0.41
1:A:141:LYS:CE	1:A:163:MET:SD	3.05	0.41
1:B:99:PRO:HD3	1:B:116:PRO:HA	2.03	0.41
1:A:161:ASN:HB2	4:A:322:HOH:O	2.20	0.41
1:B:34:VAL:O	1:B:58:VAL:HG11	2.21	0.41
1:B:79:ILE:HD12	1:B:79:ILE:HG21	1.88	0.41
1:B:128:LEU:HA	1:B:128:LEU:HD23	1.87	0.40
1:B:135:ASN:O	4:B:211:HOH:O	2.22	0.40
1:B:7:GLU:OE1	1:B:31:LEU:HD21	2.22	0.40
1:B:78:GLN:HB2	4:B:259:HOH:O	2.20	0.40
1:A:168:LEU:HD22	1:A:168:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:HG3	1:A:31:LEU:CD2	2.50	0.40
1:A:41:LYS:HD2	3:A:172:4IP:H6	2.04	0.40
1:B:133:ARG:HG3	1:B:134:TYR:CD1	2.56	0.40
1:B:12:LYS:HD3	1:B:28:ARG:HG3	2.04	0.40

All (3) 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)
3:B:172:4IP:O6P	4:B:268:HOH:O[10_555]	2.08	0.12
1:A:53:LYS:NZ	3:A:172:4IP:O5P[10_555]	2.13	0.07
3:B:172:4IP:O8P	4:B:268:HOH:O[10_555]	2.17	0.03

## 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	162/169 (96%)	155 (96%)	6 (4%)	1 (1%)	28	24
1	B	157/169 (93%)	136 (87%)	14 (9%)	7 (4%)	3	1
All	All	319/338 (94%)	291 (91%)	20 (6%)	8 (2%)	6	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	LEU
1	B	157	GLN
1	B	149	ASP
1	A	82	ARG
1	B	99	PRO
1	B	152	TYR
1	B	73	PRO

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Mol	Chain	Res	Type
1	B	75	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%)	134 (88%)	19 (12%)	5	3
1	B	150/158 (95%)	127 (85%)	23 (15%)	3	1
All	All	303/316 (96%)	261 (86%)	42 (14%)	4	2

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	31	LEU
1	A	51	SER
1	A	72	ASN
1	A	79	ILE
1	A	81	ARG
1	A	82	ARG
1	A	89	MET
1	A	94	ILE
1	A	118	GLU
1	A	120	LEU
1	A	123	ARG
1	A	133	ARG
1	A	142	TYR
1	A	148	ILE
1	A	154	CYS
1	A	163	MET
1	A	168	LEU
1	A	170	ASN
1	B	20	THR
1	B	24	ASN
1	B	27	LYS

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Mol	Chain	Res	Type
1	B	36	LYS
1	B	41	LYS
1	B	49	ARG
1	B	51	SER
1	B	55	SER
1	B	60	LYS
1	B	68	VAL
1	B	76	GLU
1	B	79	ILE
1	B	107	ASP
1	B	108	GLU
1	B	118	GLU
1	B	120	LEU
1	B	123	ARG
1	B	136	SER
1	B	141	LYS
1	B	142	TYR
1	B	156	SER
1	B	161	ASN
1	B	167	ILE

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	24	ASN
1	A	103	GLN
1	B	24	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	1	1	28,28,28	1.91	12 (42%)	42,46,46	1.37	7 (16%)
3	4IP	A	172	-	28,28,28	2.27	10 (35%)	42,46,46	1.62	12 (28%)
3	4IP	B	1	1	28,28,28	1.88	12 (42%)	42,46,46	1.42	6 (14%)
3	4IP	B	172	-	28,28,28	2.29	10 (35%)	42,46,46	1.62	12 (28%)

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	172	4IP	P5-OPG	-4.44	1.35	1.50
3	B	172	4IP	P5-OPG	-4.42	1.35	1.50
3	A	172	4IP	P3-O5P	-3.72	1.39	1.54
3	B	172	4IP	P3-O5P	-3.71	1.39	1.54
3	B	1	4IP	P5-OPH	-3.14	1.41	1.54
3	B	1	4IP	P4-O7P	-2.90	1.42	1.54
3	B	1	4IP	P4-O8P	-2.81	1.43	1.54
3	A	1	4IP	P5-OPF	-2.77	1.43	1.54
3	A	1	4IP	P1-O3P	-2.73	1.43	1.54
3	A	1	4IP	P5-OPG	-2.70	1.41	1.50
3	B	172	4IP	P1-O3P	-2.59	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	172	4IP	P1-O3P	-2.56	1.44	1.54
3	B	1	4IP	P3-O3	-2.56	1.55	1.59
3	B	172	4IP	P1-O1P	-2.53	1.42	1.50
3	A	1	4IP	P1-O1P	-2.53	1.42	1.50
3	B	1	4IP	C2-C3	-2.51	1.45	1.52
3	A	172	4IP	P1-O1P	-2.49	1.42	1.50
3	B	1	4IP	P4-O4	-2.47	1.55	1.59
3	A	1	4IP	P3-O3	-2.46	1.55	1.59
3	B	1	4IP	O6-C6	-2.44	1.37	1.43
3	B	1	4IP	P5-OPG	-2.44	1.42	1.50
3	A	1	4IP	P3-O5P	-2.41	1.44	1.54
3	B	172	4IP	P5-OPH	-2.39	1.45	1.54
3	A	172	4IP	P5-OPH	-2.38	1.45	1.54
3	B	172	4IP	P3-O6P	-2.37	1.45	1.54
3	A	172	4IP	P3-O6P	-2.34	1.45	1.54
3	B	172	4IP	P5-OPF	-2.33	1.45	1.54
3	A	172	4IP	P5-OPF	-2.31	1.45	1.54
3	A	1	4IP	P5-OPH	-2.22	1.45	1.54
3	A	172	4IP	C2-C1	-2.19	1.46	1.52
3	B	172	4IP	C2-C1	-2.18	1.46	1.52
3	A	1	4IP	P4-O8P	-2.13	1.46	1.54
3	B	1	4IP	P3-O6P	-2.12	1.46	1.54
3	B	1	4IP	P3-O5P	-2.08	1.46	1.54
3	A	1	4IP	P4-O4	-2.05	1.56	1.59
3	A	1	4IP	P3-O4P	-2.01	1.43	1.50
3	A	1	4IP	C4-C3	2.46	1.57	1.52
3	B	1	4IP	P1-O1	2.62	1.64	1.59
3	B	1	4IP	C5-C4	2.81	1.58	1.52
3	A	172	4IP	C4-C3	3.98	1.60	1.52
3	A	1	4IP	P1-O1	4.00	1.66	1.59
3	B	172	4IP	C4-C3	4.01	1.60	1.52
3	A	172	4IP	P1-O1	6.63	1.71	1.59
3	B	172	4IP	P1-O1	6.68	1.71	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	4IP	O3P-P1-O1	-2.74	93.52	106.00
3	A	1	4IP	O5P-P3-O3	-2.74	93.54	106.00
3	B	1	4IP	O6-C6-C5	-2.72	103.68	109.87
3	B	172	4IP	O5P-P3-O3	-2.70	93.72	106.00
3	A	172	4IP	O5P-P3-O3	-2.69	93.75	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	172	4IP	O3P-P1-O1	-2.66	93.91	106.00
3	B	172	4IP	O3P-P1-O1	-2.65	93.96	106.00
3	B	172	4IP	OPH-P5-O5	-2.11	96.41	106.00
3	A	172	4IP	OPH-P5-O5	-2.09	96.51	106.00
3	A	172	4IP	O3-P3-O4P	-2.06	101.19	109.26
3	B	172	4IP	O3-P3-O4P	-2.06	101.20	109.26
3	A	172	4IP	C5-C4-C3	-2.03	105.96	110.46
3	A	1	4IP	O5-P5-OPG	-2.01	101.38	109.26
3	B	172	4IP	C5-C4-C3	-2.00	106.02	110.46
3	B	172	4IP	O1-C1-C2	2.06	113.47	108.66
3	B	172	4IP	O8P-P4-O9P	2.09	118.67	110.50
3	A	172	4IP	O8P-P4-O9P	2.09	118.68	110.50
3	A	172	4IP	O1-C1-C2	2.11	113.58	108.66
3	B	1	4IP	O3P-P1-O1P	2.13	118.82	110.50
3	A	172	4IP	O3P-P1-O1P	2.14	118.89	110.50
3	B	172	4IP	O3P-P1-O1P	2.16	118.97	110.50
3	A	1	4IP	O5P-P3-O4P	2.20	119.09	110.50
3	B	1	4IP	O3P-P1-O2P	2.35	117.10	107.61
3	A	1	4IP	OPH-P5-OPF	2.41	117.33	107.61
3	B	1	4IP	OPH-P5-OPF	2.47	117.56	107.61
3	A	172	4IP	O6P-P3-O5P	2.49	117.68	107.61
3	B	172	4IP	O6P-P3-O5P	2.52	117.78	107.61
3	B	1	4IP	O3-C3-C4	2.52	114.64	108.68
3	B	172	4IP	O3P-P1-O2P	2.53	117.82	107.61
3	A	172	4IP	O3P-P1-O2P	2.54	117.86	107.61
3	A	1	4IP	O3-C3-C4	2.63	114.89	108.68
3	A	172	4IP	O3-C3-C4	2.71	115.07	108.68
3	B	172	4IP	O3-C3-C4	2.74	115.16	108.68
3	A	1	4IP	OPH-P5-OPG	2.88	121.76	110.50
3	A	1	4IP	O1-C1-C2	2.91	115.44	108.66
3	B	172	4IP	OPH-P5-OPF	3.84	123.11	107.61
3	A	172	4IP	OPH-P5-OPF	3.84	123.12	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	4IP	1	0
3	A	172	4IP	3	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	4IP	3	0
3	B	172	4IP	5	2

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.