



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:28 am GMT

PDB ID : 2JDR  
Title : STRUCTURE OF PKB-BETA (AKT2) COMPLEXED WITH THE INHIBITOR A-443654  
Authors : Davies, T.G.; Verdonk, M.L.; Graham, B.; Saalau-Bethell, S.; Hamlett, C.C.F.; Mchardy, T.; Collins, I.; Garrett, M.D.; Workman, P.; Woodhead, S.J.; Jhoti, H.; Barford, D.  
Deposited on : 2007-01-12  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

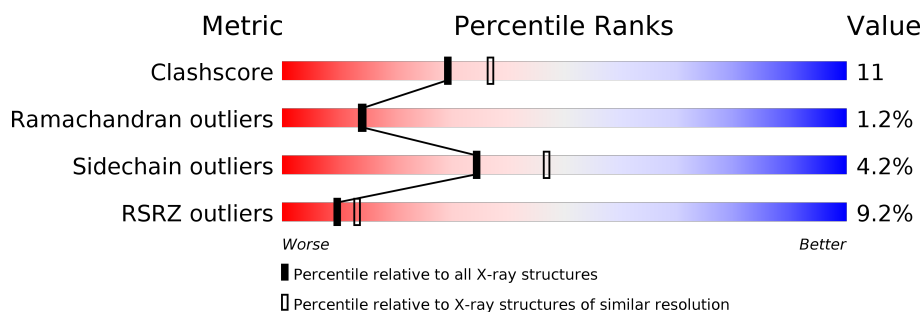
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Mol	Chain	Length	Quality of chain
1	A	342	
2	C	10	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2819 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.

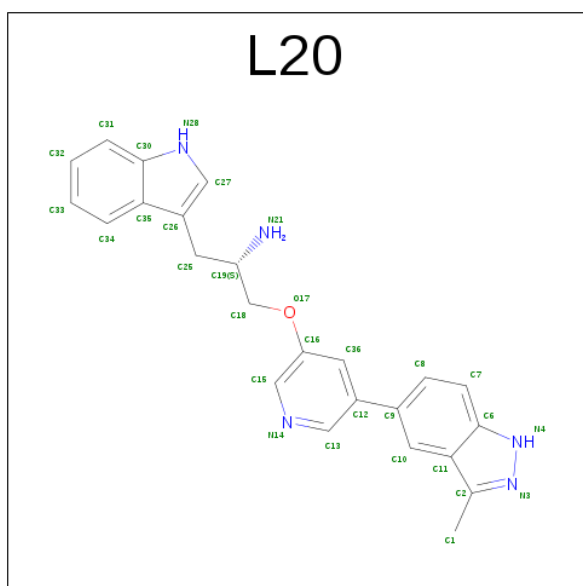
- Molecule 1 is a protein called RAC-BETA SERINE/THREONINE-PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	317	2605	1672	435	482	1	15	0	0	0

- Molecule 2 is a protein called GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	79	47	16	16	0	0	0

- Molecule 3 is (2S)-1-(1H-INDOL-3-YL)-3-([5-(3-METHYL-1H-INDAZOL-5-YL)PYRIDIN-3-YL]OXY)PROPAN-2-AMINE (three-letter code: L20) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	30	24	5	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total 102	O 102	0	0
4	C	3	Total 3	O 3	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.93Å 60.99Å 124.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.81 – 2.30 54.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (54.81-2.30) 93.4 (54.81-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019F	Depositor
R, $R_{free}$	0.193 , 0.252 0.202 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, L20

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	0.64	0/2653	0.71	0/3572
2	C	0.68	0/80	0.69	0/105
All	All	0.64	0/2733	0.71	0/3677

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	2605	0	2561	57	0
2	C	79	0	74	6	0
3	A	30	0	23	3	0
4	A	102	0	0	2	0
4	C	3	0	0	0	0
All	All	2819	0	2658	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (58) 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:194:VAL:O	1:A:198:VAL:HG23	1.77	0.84
1:A:188:ILE:HD13	1:A:225:LEU:HD12	1.59	0.83
1:A:162:THR:HG21	2:C:8:THR:HG22	1.65	0.79
1:A:225:LEU:HD11	1:A:470:PHE:CE1	2.23	0.73
1:A:213:THR:HG21	3:A:1480:L20:H7	1.70	0.73
1:A:201:SER:O	1:A:205:GLN:HG3	1.96	0.65
1:A:367:ILE:HD12	1:A:369:PHE:CZ	2.33	0.64
1:A:209:HIS:HD2	1:A:211:PHE:H	1.45	0.63
1:A:209:HIS:CD2	1:A:211:PHE:H	2.17	0.62
1:A:184:ARG:HB2	1:A:187:VAL:HG23	1.82	0.61
1:A:241:LEU:O	1:A:245:ARG:N	2.38	0.57
1:A:185:LYS:NZ	1:A:221:THR:O	2.20	0.57
1:A:162:THR:CG2	2:C:8:THR:HG22	2.34	0.55
1:A:162:THR:HG23	1:A:163:PHE:H	1.72	0.55
1:A:367:ILE:CD1	1:A:369:PHE:CZ	2.90	0.54
1:A:432:SER:OG	1:A:434:VAL:HG12	2.07	0.54
1:A:188:ILE:CG2	1:A:194:VAL:HA	2.39	0.53
1:A:166:VAL:HG11	3:A:1480:L20:H33	1.91	0.52
1:A:313:THR:HG21	2:C:7:THR:HB	1.92	0.52
1:A:267:HIS:ND1	1:A:399:ASP:OD2	2.37	0.52
1:A:185:LYS:HA	1:A:188:ILE:HD12	1.93	0.51
1:A:191:LYS:C	1:A:193:GLU:H	2.14	0.51
1:A:157:LEU:HD23	1:A:443:PHE:O	2.10	0.51
1:A:388:ASP:OD2	1:A:391:GLN:NE2	2.43	0.51
1:A:156:LYS:HD2	1:A:434:VAL:HG22	1.94	0.49
1:A:216:LYS:NZ	1:A:479:TRP:OXT	2.45	0.49
1:A:416:ASP:OD1	1:A:421:LYS:HD2	2.12	0.49
1:A:158:LEU:HB2	1:A:166:VAL:HG22	1.95	0.48
1:A:188:ILE:CD1	1:A:225:LEU:HD12	2.38	0.48
1:A:301:ILE:HG21	1:A:307:MET:HE2	1.96	0.47
1:A:166:VAL:CG1	3:A:1480:L20:H33	2.43	0.47
1:A:161:GLY:O	1:A:162:THR:C	2.53	0.47
1:A:467:GLN:O	1:A:469:MET:N	2.48	0.46
1:A:267:HIS:HD1	1:A:399:ASP:CG	2.17	0.46
1:A:202:ARG:O	1:A:206:ASN:ND2	2.43	0.45
1:A:221:THR:C	1:A:223:ASP:H	2.19	0.45
1:A:313:THR:CG2	2:C:7:THR:HB	2.46	0.45
1:A:236:GLU:HA	1:A:282:MET:HA	1.98	0.44
1:A:286:ASP:O	1:A:424:PRO:HG2	2.17	0.44
1:A:272:VAL:HG21	1:A:307:MET:HE1	2.00	0.43
1:A:237:LEU:CD2	1:A:289:ILE:HD11	2.49	0.43
1:A:158:LEU:HD21	1:A:168:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:C	1:A:167:ILE:HD12	2.38	0.43
1:A:156:LYS:NZ	1:A:434:VAL:HG22	2.34	0.42
1:A:312:GLY:O	2:C:10:PHE:CD2	2.72	0.42
1:A:272:VAL:HG12	1:A:274:ARG:CG	2.50	0.42
1:A:440:ASP:HB2	1:A:443:PHE:HD1	1.85	0.41
1:A:367:ILE:HD12	1:A:369:PHE:CE1	2.55	0.41
1:A:188:ILE:HG22	1:A:194:VAL:HA	2.03	0.41
1:A:153:ASP:HB2	1:A:155:LEU:HD11	2.02	0.41
1:A:313:THR:HA	1:A:314:PRO:HD3	1.90	0.41
1:A:477:ALA:HB1	1:A:479:TRP:CD1	2.55	0.41
1:A:152:PHE:HA	1:A:170:ARG:O	2.20	0.40
1:A:407:ARG:NE	4:A:2088:HOH:O	2.50	0.40
1:A:370:PRO:HD2	1:A:373:LEU:HD22	2.03	0.40
4:A:2050:HOH:O	2:C:4:ARG:HD2	2.21	0.40
1:A:325:ASN:HA	1:A:325:ASN:HD22	1.80	0.40
1:A:254:PHE:O	1:A:258:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

## 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	312/342 (91%)	293 (94%)	16 (5%)	3 (1%)	18	20
2	C	8/10 (80%)	7 (88%)	0	1 (12%)	0	0
All	All	320/352 (91%)	300 (94%)	16 (5%)	4 (1%)	14	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	222	HIS

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Mol	Chain	Res	Type
1	A	468	GLU
2	C	4	ARG

### 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	278/300 (93%)	267 (96%)	11 (4%)	36	50
2	C	8/8 (100%)	7 (88%)	1 (12%)	5	5
All	All	286/308 (93%)	274 (96%)	12 (4%)	34	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	162	THR
1	A	166	VAL
1	A	170	ARG
1	A	186	GLU
1	A	208	ARG
1	A	236	GLU
1	A	237	LEU
1	A	292	THR
1	A	448	ILE
1	A	474	ASP
2	C	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	233	ASN
1	A	325	ASN
1	A	446	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	TPO	A	309	1	9,10,11	0.57	0	10,14,16	1.23	1 (10%)

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
1	TPO	A	309	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	TPO	O3P-P-O2P	2.18	116.42	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
3	L20	A	1480	-	31,34,34	1.08	1 (3%)	32,48,48	1.77	6 (18%)

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	L20	A	1480	-	-	0/12/13/13	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1480	L20	C1-C2	-2.84	1.48	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	L20	O17-C18-C19	-3.55	100.89	108.39
3	A	1480	L20	C25-C26-C27	-2.98	124.29	127.97
3	A	1480	L20	C10-C11-C6	2.35	121.47	118.26
3	A	1480	L20	C15-N14-C13	3.58	122.51	117.45
3	A	1480	L20	C1-C2-N3	3.67	127.71	119.65
3	A	1480	L20	C18-O17-C16	4.45	127.58	117.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1480	L20	3	0

## 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

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	316/342 (92%)	0.18	27 (8%) 11 16	19, 40, 93, 109	0
2	C	10/10 (100%)	1.62	3 (30%) 1 0	55, 64, 82, 87	0
All	All	326/352 (92%)	0.23	30 (9%) 10 13	19, 41, 91, 109	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	5.6
1	A	447	SER	4.3
1	A	445	ALA	4.0
1	A	448	ILE	4.0
1	A	470	PHE	3.8
1	A	147	VAL	3.4
1	A	198	VAL	3.1
2	C	3	GLY	3.0
1	A	184	ARG	2.8
2	C	10	PHE	2.8
1	A	193	GLU	2.8
1	A	188	ILE	2.7
1	A	430	VAL	2.7
1	A	186	GLU	2.6
1	A	196	HIS	2.5
1	A	469	MET	2.5
1	A	175	GLY	2.5
1	A	468	GLU	2.5
1	A	157	LEU	2.4
1	A	154	TYR	2.4
1	A	467	GLN	2.4
1	A	219	PHE	2.3
2	C	12	GLU	2.3
1	A	446	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	477	ALA	2.3
1	A	167	ILE	2.3
1	A	471	GLU	2.2
1	A	473	PHE	2.2
1	A	160	LYS	2.1
1	A	177	TYR	2.0

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

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	309	11/12	0.97	0.09	-	29,35,45,47	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	L20	A	1480	30/30	0.94	0.11	-0.90	24,37,42,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.