



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

PDB ID : 1Y6A  
Title : Crystal structure of VEGFR2 in complex with a 2-anilino-5-aryl-oxazole inhibitor  
Authors : Harris, P.A.; Cheung, M.; Hunter, R.N.; Brown, M.L.; Veal, J.M.; Nolte, R.T.; Wang, L.; Liu, W.; Crosby, R.M.; Johnson, J.H.; Epperly, A.H.; Kumar, R.; Luttrell, D.K.; Stafford, J.A.  
Deposited on : 2004-12-05  
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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

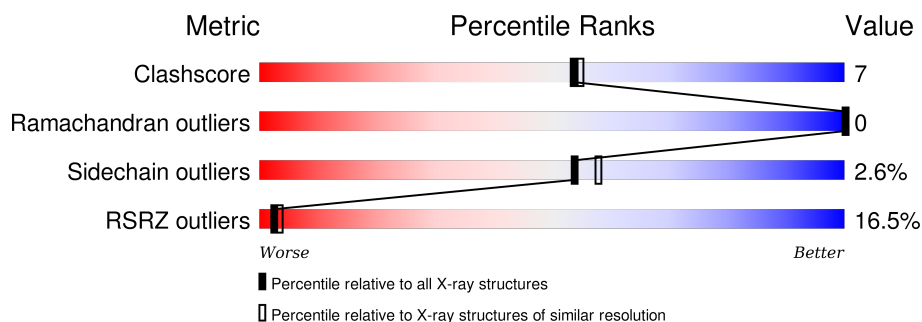
# 1 Overall quality at a glance

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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.

Mol	Chain	Length	Quality of chain
1	A	366	

## 2 Entry composition [i](#)

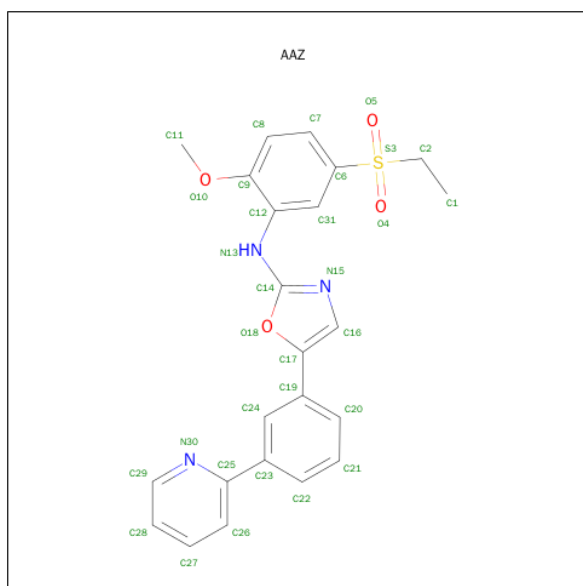
There are 3 unique types of molecules in this entry. The entry contains 2311 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2099	1353	359	371	16			

- Molecule 2 is N-[5-(ETHYLSULFONYL)-2-METHOXYPHENYL]-5-[3-(2-PYRIDINYL)PHENYL]-1,3-OXAZOL-2-AMINE (three-letter code: AAZ) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			62	46	6	8	2		

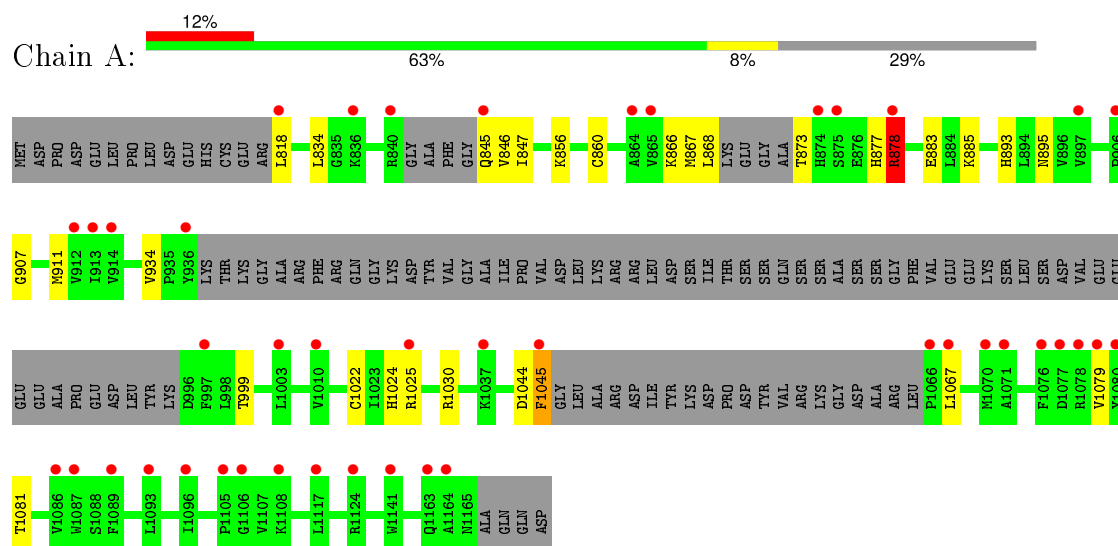
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Vascular endothelial growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.73Å 94.57Å 96.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.10 19.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.87-2.10) 95.9 (19.87-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.217 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 61.8	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 20671 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: AAZ

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	0.63	0/2149	0.72	1/2902 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	878	ARG	NE-CZ-NH1	5.70	123.15	120.30

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	2099	0	2101	27	0
2	A	62	0	42	4	0
3	A	150	0	0	10	0
All	All	2311	0	2143	28	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 7.

All (28) 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:860:CYS:HB3	3:A:151:HOH:O	1.24	1.27
1:A:1022:CYS:SG	3:A:156:HOH:O	2.28	0.90
1:A:834:LEU:HD22	1:A:847:ILE:HD11	1.59	0.83
1:A:834:LEU:HD22	1:A:847:ILE:CD1	2.12	0.80
1:A:860:CYS:CB	3:A:151:HOH:O	1.97	0.74
1:A:845:GLN:N	3:A:148:HOH:O	2.24	0.71
1:A:883:GLU:OE2	2:A:201[B]:AAZ:H29	1.97	0.65
1:A:860:CYS:SG	3:A:151:HOH:O	2.47	0.64
1:A:893:HIS:HD2	1:A:895:ASN:H	1.46	0.64
1:A:867:MET:HB3	1:A:911:MET:HG2	1.81	0.63
1:A:873:THR:N	3:A:131:HOH:O	2.34	0.60
2:A:201[B]:AAZ:O18	2:A:201[B]:AAZ:H31	2.04	0.58
1:A:866:LYS:HB2	2:A:201[B]:AAZ:C27	2.37	0.55
1:A:868:LEU:HD11	1:A:877:HIS:HA	1.87	0.55
1:A:818:LEU:O	1:A:885:LYS:HE3	2.07	0.54
1:A:818:LEU:N	3:A:102:HOH:O	2.41	0.53
1:A:834:LEU:HD22	1:A:847:ILE:HD12	1.92	0.52
1:A:846:VAL:HG21	2:A:201[A]:AAZ:H26	1.92	0.52
1:A:893:HIS:CD2	1:A:895:ASN:H	2.27	0.51
1:A:907:GLY:O	3:A:139:HOH:O	2.20	0.50
1:A:934:VAL:O	1:A:999:THR:HA	2.13	0.49
1:A:883:GLU:OE2	1:A:1045:PHE:CB	2.63	0.47
1:A:873:THR:CA	3:A:131:HOH:O	2.64	0.46
1:A:1079:VAL:HG13	1:A:1081:THR:HG23	1.99	0.44
1:A:868:LEU:CD1	1:A:877:HIS:HA	2.49	0.43
1:A:1024:HIS:O	1:A:1025:ARG:HB2	2.19	0.42
1:A:878:ARG:CG	1:A:878:ARG:HH11	2.34	0.41
1:A:860:CYS:SG	3:A:5:HOH:O	2.47	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	251/366 (69%)	244 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	230/318 (72%)	224 (97%)	6 (3%)	54	58

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	856	LYS
1	A	878	ARG
1	A	1030	ARG
1	A	1044	ASP
1	A	1045	PHE
1	A	1067	LEU

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	893	HIS
1	A	895	ASN
1	A	931	ASN
1	A	1002	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	AAZ	A	201[A]	-	31,34,34	1.80	3 (9%)	40,48,48	2.45	15 (37%)
2	AAZ	A	201[B]	-	31,34,34	1.94	4 (12%)	40,48,48	2.13	11 (27%)

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	AAZ	A	201[A]	-	-	0/19/23/23	0/3/4/4
2	AAZ	A	201[B]	-	-	0/19/23/23	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[B]	AAZ	C6-S3	-7.86	1.61	1.76
2	A	201[A]	AAZ	C6-S3	-6.94	1.63	1.76
2	A	201[B]	AAZ	C16-N15	-5.61	1.27	1.36
2	A	201[A]	AAZ	C16-N15	-4.85	1.29	1.36
2	A	201[B]	AAZ	C16-C17	-2.03	1.34	1.37
2	A	201[A]	AAZ	C19-C17	2.66	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[B]	AAZ	C19-C17	3.06	1.50	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[B]	AAZ	O5-S3-O4	-8.02	107.80	118.40
2	A	201[A]	AAZ	C24-C19-C17	-5.39	115.25	120.46
2	A	201[A]	AAZ	O5-S3-O4	-4.31	112.70	118.40
2	A	201[A]	AAZ	O4-S3-C6	-3.22	104.85	108.38
2	A	201[B]	AAZ	O10-C9-C8	-3.10	119.14	124.35
2	A	201[A]	AAZ	C14-N13-C12	-3.01	122.55	129.36
2	A	201[A]	AAZ	C7-C6-C31	-2.31	117.84	120.52
2	A	201[B]	AAZ	C14-N13-C12	-2.14	124.52	129.36
2	A	201[B]	AAZ	C20-C19-C17	-2.02	118.50	120.45
2	A	201[A]	AAZ	C28-C29-N30	-2.01	120.08	123.44
2	A	201[B]	AAZ	C12-C31-C6	2.53	121.80	118.72
2	A	201[B]	AAZ	C2-S3-C6	2.71	108.99	105.07
2	A	201[B]	AAZ	C29-N30-C25	2.75	121.00	117.20
2	A	201[A]	AAZ	O10-C9-C12	2.82	118.47	114.87
2	A	201[B]	AAZ	C31-C6-S3	2.84	122.01	119.03
2	A	201[B]	AAZ	O5-S3-C6	2.85	111.50	108.38
2	A	201[A]	AAZ	C12-C31-C6	2.86	122.20	118.72
2	A	201[A]	AAZ	C16-C17-C19	3.10	133.77	127.06
2	A	201[A]	AAZ	C29-N30-C25	3.20	121.61	117.20
2	A	201[B]	AAZ	C11-O10-C9	3.34	122.61	117.54
2	A	201[A]	AAZ	C20-C19-C17	4.10	124.42	120.45
2	A	201[A]	AAZ	O5-S3-C6	4.19	112.98	108.38
2	A	201[A]	AAZ	C31-C6-S3	4.51	123.77	119.03
2	A	201[B]	AAZ	O10-C9-C12	4.74	120.92	114.87
2	A	201[A]	AAZ	C2-S3-C6	4.80	112.02	105.07
2	A	201[A]	AAZ	C11-O10-C9	5.42	125.76	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201[A]	AAZ	1	0
2	A	201[B]	AAZ	3	0

## 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	261/366 (71%)	0.79	43 (16%) 2 3	27, 37, 53, 61	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	PHE	5.9
1	A	1106	GLY	5.9
1	A	1079	VAL	5.3
1	A	1078	ARG	5.1
1	A	875	SER	4.8
1	A	936	TYR	4.6
1	A	1108	LYS	3.7
1	A	865	VAL	3.5
1	A	913	ILE	3.5
1	A	878	ARG	3.3
1	A	1105	PRO	3.2
1	A	1025	ARG	3.1
1	A	912	VAL	3.1
1	A	845	GLN	3.0
1	A	1093	LEU	2.9
1	A	818	LEU	2.9
1	A	1077	ASP	2.9
1	A	1003	LEU	2.8
1	A	1080	TYR	2.7
1	A	1087	TRP	2.7
1	A	1096	ILE	2.6
1	A	914	VAL	2.6
1	A	1071	ALA	2.6
1	A	840	ARG	2.6
1	A	1066	PRO	2.6
1	A	997	PHE	2.5
1	A	1124	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1037	LYS	2.5
1	A	1141	TRP	2.4
1	A	1086	VAL	2.3
1	A	906	PRO	2.3
1	A	874	HIS	2.3
1	A	897	VAL	2.3
1	A	836	LYS	2.2
1	A	1010	VAL	2.2
1	A	1076	PHE	2.2
1	A	1089	PHE	2.2
1	A	1070	MET	2.1
1	A	864	ALA	2.1
1	A	1067	LEU	2.1
1	A	1117	LEU	2.1
1	A	1163	GLN	2.1
1	A	1164	ALA	2.0

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

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

## 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( $\text{\AA}^2$ )	Q<0.9
2	AAZ	A	201[B]	31/31	0.91	0.22	0.34	49,50,52,52	31
2	AAZ	A	201[A]	31/31	0.91	0.22	0.18	25,31,38,39	31

## 6.5 Other polymers

There are no such residues in this entry.