



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2ITV
Title : CRYSTAL STRUCTURE OF EGFR KINASE DOMAIN L858R MUTATION
IN COMPLEX WITH AMP-PNP
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Deposited on : 2006-05-25
Resolution : 2.47 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

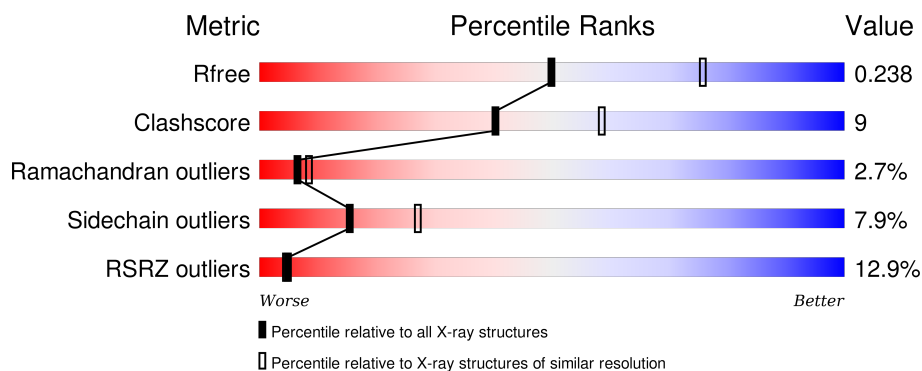
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.47 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	327	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2606 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.

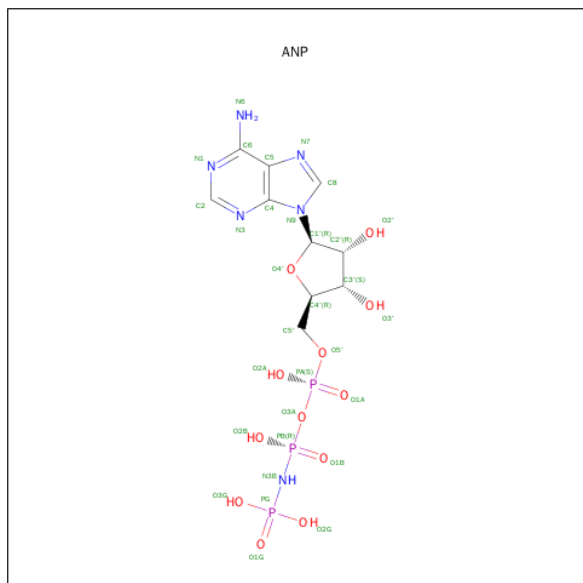
- Molecule 1 is a protein called EPIDERMAL GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2426	1556	408	442	20	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	ARG	LEU	ENGINEERED MUTATION	UNP P00533

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0

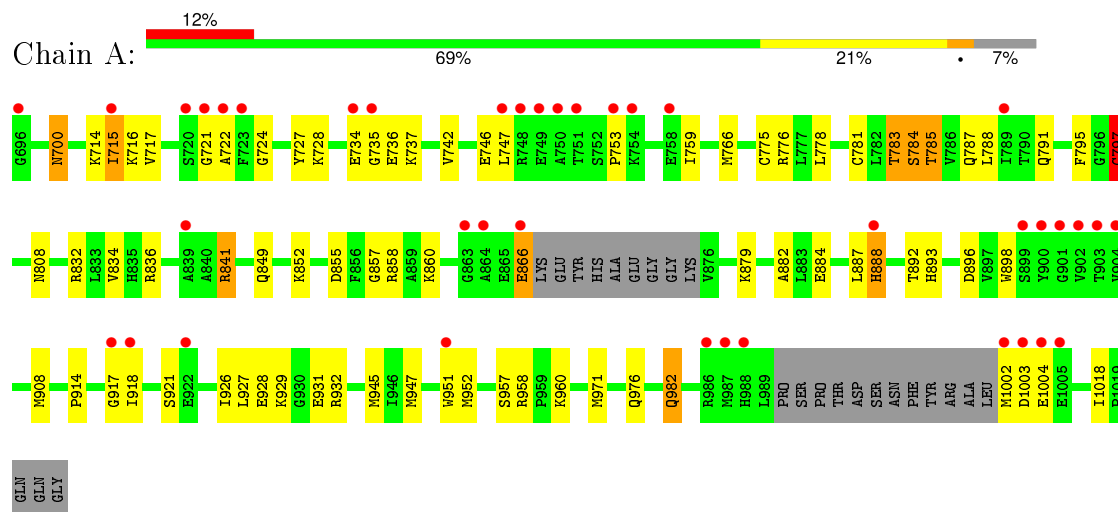
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total 149	O 149	0	0

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 ($\text{RSRZ} > 2$). 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: EPIDERMAL GROWTH FACTOR RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	145.08Å 145.08Å 145.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.47 24.88 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.88-2.47) 99.8 (24.88-2.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.242 0.193 , 0.238	Depositor DCC
R_{free} test set	940 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.4	EDS
Estimated twinning fraction	0.031 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18304 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2606	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ANP

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	0.74	0/2478	0.79	3/3352 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	797[A]	CYS	CA-CB-SG	5.38	123.68	114.00
1	A	797[B]	CYS	CA-CB-SG	5.38	123.68	114.00
1	A	785	THR	N-CA-C	-5.31	96.67	111.00

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	2426	0	2461	43	0
2	A	31	0	13	1	0
3	A	149	0	0	9	0
All	All	2606	0	2474	43	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 9.

All (43) 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:785:THR:HG22	3:A:3039:HOH:O	1.31	1.22
1:A:775[B]:CYS:SG	3:A:3147:HOH:O	2.33	0.81
1:A:797[A]:CYS:SG	1:A:841:ARG:HA	2.35	0.67
1:A:737:LYS:HG3	1:A:737:LYS:O	1.95	0.67
1:A:918:ILE:HG21	1:A:926:ILE:HD12	1.77	0.67
1:A:724:GLY:HA3	1:A:747:LEU:HD12	1.77	0.65
1:A:746:GLU:HB2	1:A:787:GLN:HG2	1.77	0.65
1:A:866:GLU:HG3	3:A:3078:HOH:O	1.99	0.62
1:A:952:MET:O	1:A:958:ARG:HD2	2.02	0.60
1:A:700:ASN:C	1:A:700:ASN:HD22	2.05	0.59
1:A:735:GLY:HA2	3:A:3023:HOH:O	2.03	0.56
1:A:781:CYS:HB3	1:A:787:GLN:HB2	1.88	0.55
1:A:832:ARG:HD3	3:A:3062:HOH:O	2.06	0.55
1:A:908:MET:HG3	1:A:947:MET:HE1	1.90	0.54
1:A:932:ARG:NH1	1:A:951:TRP:O	2.41	0.53
1:A:834:VAL:HG12	1:A:836:ARG:HG3	1.92	0.52
1:A:746:GLU:HG3	1:A:785:THR:CG2	2.40	0.51
1:A:791:GLN:HE22	1:A:852:LYS:NZ	2.07	0.50
1:A:917:GLY:O	1:A:918:ILE:C	2.50	0.50
1:A:836:ARG:NH1	1:A:858:ARG:O	2.41	0.49
1:A:855:ASP:OD2	2:A:2020:ANP:O2G	2.31	0.49
1:A:841:ARG:NH1	3:A:3066:HOH:O	2.42	0.49
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.50	0.47
1:A:766:MET:CE	1:A:788:LEU:HD21	2.44	0.47
1:A:776:ARG:HD3	3:A:3037:HOH:O	2.16	0.46
1:A:759:ILE:HD11	1:A:788:LEU:HB2	1.98	0.45
1:A:971:MET:HE3	3:A:3116:HOH:O	2.17	0.45
1:A:746:GLU:HG3	1:A:785:THR:HG21	1.99	0.44
1:A:887:LEU:C	1:A:888:HIS:ND1	2.71	0.44
1:A:717:VAL:HG22	1:A:727:TYR:CE2	2.52	0.44
1:A:700:ASN:C	1:A:700:ASN:ND2	2.69	0.44
1:A:714:LYS:O	1:A:715:ILE:HG13	2.19	0.43
1:A:742:VAL:HG12	1:A:778:LEU:HD13	2.01	0.43
1:A:736:GLU:O	1:A:737:LYS:HB3	2.19	0.43
1:A:783:THR:O	1:A:784:SER:OG	2.30	0.42
1:A:795:PHE:O	3:A:3042:HOH:O	2.22	0.42
1:A:893:HIS:O	1:A:896:ASP:HB2	2.18	0.42
1:A:982:GLN:N	1:A:982:GLN:CD	2.73	0.42
1:A:926:ILE:HA	1:A:929:LYS:HE2	2.02	0.42
1:A:926:ILE:HG23	1:A:931:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LYS:HD3	1:A:914:PRO:O	2.20	0.42
1:A:716:LYS:HD3	1:A:728:LYS:CE	2.50	0.41
1:A:927:LEU:O	1:A:932:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	299/327 (91%)	268 (90%)	23 (8%)	8 (3%)	6 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	ALA
1	A	734	GLU
1	A	1003	ASP
1	A	721	GLY
1	A	784	SER
1	A	857	GLY
1	A	715	ILE
1	A	753	PRO

5.3.2 Protein sidechains [i](#)

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	267/287 (93%)	245 (92%)	22 (8%)	14	25

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

Mol	Chain	Res	Type
1	A	700	ASN
1	A	783	THR
1	A	797[A]	CYS
1	A	797[B]	CYS
1	A	808	ASN
1	A	841	ARG
1	A	849	GLN
1	A	860	LYS
1	A	866	GLU
1	A	884	GLU
1	A	888	HIS
1	A	892	THR
1	A	921	SER
1	A	928	GLU
1	A	945	MET
1	A	957	SER
1	A	960	LYS
1	A	976	GLN
1	A	982	GLN
1	A	1002	MET
1	A	1004	GLU
1	A	1018	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	791	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ANP	A	2020	-	27,33,33	2.25	7 (25%)	30,52,52	2.15	8 (26%)

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	ANP	A	2020	-	-	1/12/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2020	ANP	PB-O3A	2.48	1.62	1.59
2	A	2020	ANP	O4'-C1'	2.55	1.44	1.41
2	A	2020	ANP	C5-C4	2.74	1.46	1.40
2	A	2020	ANP	PB-N3B	4.64	1.75	1.63
2	A	2020	ANP	PB-O1B	4.79	1.51	1.46
2	A	2020	ANP	PG-N3B	4.84	1.76	1.63
2	A	2020	ANP	PG-O1G	5.55	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2020	ANP	N3-C2-N1	-5.54	124.65	128.89
2	A	2020	ANP	O1G-PG-N3B	-4.81	104.52	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2020	ANP	C2'-C1'-N9	-4.68	107.14	114.29
2	A	2020	ANP	C4-C5-N7	-3.35	106.39	109.48
2	A	2020	ANP	PA-O3A-PB	-2.25	125.11	132.67
2	A	2020	ANP	O3'-C3'-C4'	2.22	117.71	111.05
2	A	2020	ANP	O4'-C1'-N9	2.86	114.08	108.10
2	A	2020	ANP	O2B-PB-O1B	3.10	116.47	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2020	ANP	O1G-PG-N3B-PB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2020	ANP	1	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, 95th 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 ²)	Q<0.9
1	A	303/327 (92%)	0.42	39 (12%) 5 4	32, 49, 90, 106	15 (4%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	ALA	8.8
1	A	721	GLY	7.6
1	A	723	PHE	6.4
1	A	720	SER	5.5
1	A	750	ALA	5.4
1	A	748	ARG	5.1
1	A	696	GLY	4.5
1	A	988	HIS	4.3
1	A	1003	ASP	3.9
1	A	863	GLY	3.5
1	A	754	LYS	3.3
1	A	1005	GLU	3.3
1	A	747	LEU	3.2
1	A	986	ARG	3.2
1	A	900	TYR	3.1
1	A	987	MET	3.0
1	A	735	GLY	3.0
1	A	749	GLU	3.0
1	A	751	THR	2.9
1	A	753	PRO	2.8
1	A	866	GLU	2.8
1	A	901	GLY	2.7
1	A	918	ILE	2.7
1	A	951	TRP	2.6
1	A	903	THR	2.5
1	A	839	ALA	2.5
1	A	715	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1002	MET	2.5
1	A	922	GLU	2.3
1	A	888	HIS	2.3
1	A	734	GLU	2.2
1	A	904	VAL	2.2
1	A	917	GLY	2.2
1	A	902	VAL	2.2
1	A	789	ILE	2.2
1	A	758	GLU	2.2
1	A	899	SER	2.1
1	A	864	ALA	2.0
1	A	1004	GLU	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, 95th 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(\AA^2)	Q<0.9
2	ANP	A	2020	31/31	0.86	0.14	-0.31	52,80,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.