



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YWN
Title : Vegfr2 in complex with a novel 4-amino-furo[2,3-d]pyrimidine
Authors : Miyazaki, Y.; Matsunaga, S.; Tang, J.; Maeda, Y.; Nakano, M.; Philippe, R.J.; Shibahara, M.; Liu, W.; Sato, H.; Wang, L.; Nolte, R.T.
Deposited on : 2005-02-18
Resolution : 1.71 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

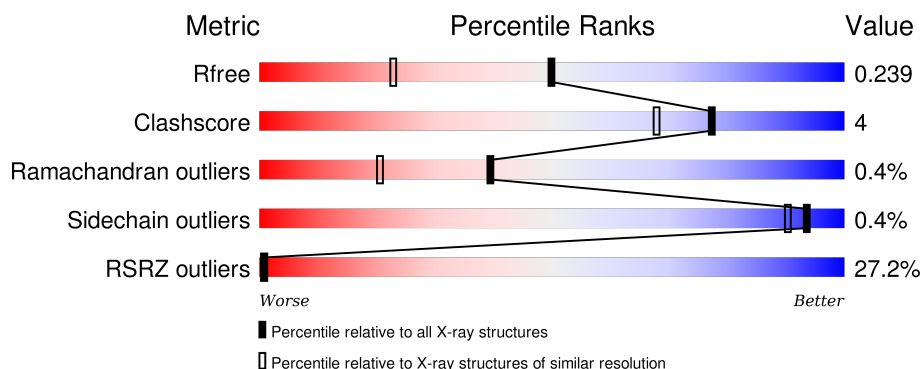
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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	316	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2512 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.

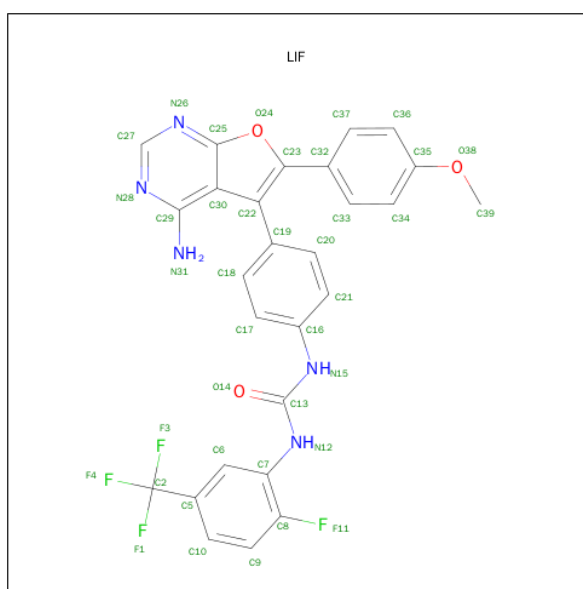
- Molecule 1 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	281	2264	1448	392	406	2	16	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	988	VAL	GLU	engineered	UNP P35968
A	1052	PTR	TYR	MODIFIED RESIDUE	UNP P35968
A	1057	PTR	TYR	MODIFIED RESIDUE	UNP P35968

- Molecule 2 is N-{4-[4-AMINO-6-(4-METHOXYPHENYL)FURO[2,3-D]PYRIMIDIN-5-YL]PHENYL}-N'-[2-FLUORO-5-(TRIFLUOROMETHYL)PHENYL]UREA (three-letter code: LIF) (formula: C₂₇H₁₉F₄N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	39	27	4	5	3	0	0

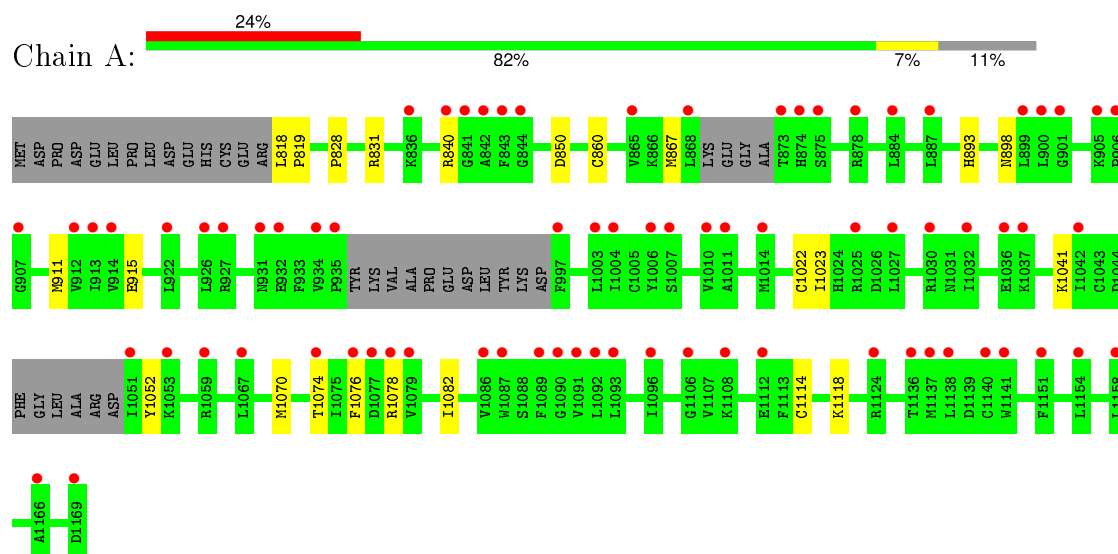
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total 209	O 209	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 ($RSRZ > 2$). 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, α , β , γ	37.95Å 95.59Å 95.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.89 – 1.71 23.67 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.89-1.71) 95.2 (23.67-1.71)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.230 0.215 , 0.239	Depositor DCC
R_{free} test set	1139 reflections (3.20%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 62.5	EDS
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 36717 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2512	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: LIF, PTR

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	0.57	0/2281	0.66	0/3076

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 [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	2264	0	2259	17	0
2	A	39	0	19	0	0
3	A	209	0	0	8	0
All	All	2512	0	2278	17	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 4.

All (17) 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:SG	3:A:194:HOH:O	2.24	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:CYS:SG	3:A:204:HOH:O	2.27	0.92
1:A:1114:CYS:SG	3:A:203:HOH:O	2.21	0.90
1:A:915:GLU:CD	3:A:205:HOH:O	2.42	0.57
1:A:1070:MET:CE	1:A:1074:THR:HG22	2.35	0.57
1:A:819:PRO:O	3:A:193:HOH:O	2.19	0.52
1:A:828:PRO:HG2	1:A:831:ARG:HD3	1.93	0.50
1:A:1023:ILE:HD12	1:A:1082:ILE:N	2.29	0.48
1:A:840:ARG:HG3	1:A:1052:PTR:HE2	1.97	0.47
1:A:1041:LYS:HE3	3:A:205:HOH:O	2.15	0.47
1:A:915:GLU:HB3	3:A:205:HOH:O	2.16	0.46
1:A:867:MET:HB3	1:A:911:MET:HG2	1.99	0.44
1:A:893:HIS:H	1:A:898:ASN:HD21	1.66	0.43
1:A:1070:MET:HE3	1:A:1074:THR:HG22	2.00	0.43
1:A:1076:PHE:CE1	1:A:1118:LYS:HG3	2.55	0.42
1:A:818:LEU:HB3	1:A:819:PRO:HD2	2.03	0.41
1:A:819:PRO:HB3	3:A:171:HOH:O	2.21	0.41

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	271/316 (86%)	264 (97%)	6 (2%)	1 (0%)	39 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1078	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	243/273 (89%)	242 (100%)	1 (0%)	93	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	850	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	898	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	A	1052	1	14,16,17	1.91	1 (7%)	18,22,24	0.75	1 (5%)
1	PTR	A	1057	1	14,16,17	1.97	1 (7%)	18,22,24	0.67	1 (5%)

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	PTR	A	1052	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1057	1	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	PTR	OH-CZ	-7.26	1.23	1.40
1	A	1052	PTR	OH-CZ	-7.04	1.23	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1057	PTR	O-C-CA	-2.08	120.07	125.49
1	A	1052	PTR	O-C-CA	-2.08	120.07	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1052	PTR	1	0

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	$\# Z > 2$
2	LIF	A	301	-	40,43,43	1.18	4 (10%)	50,63,63	1.95	11 (22%)

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	LIF	A	301	-	-	0/22/24/24	0/4/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LIF	C16-N15	-2.13	1.37	1.41
2	A	301	LIF	C27-N26	2.29	1.36	1.32
2	A	301	LIF	C32-C23	3.26	1.50	1.46
2	A	301	LIF	C22-C30	3.88	1.48	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LIF	N26-C27-N28	-9.05	121.96	128.89
2	A	301	LIF	C30-C29-N28	-2.71	115.69	122.89
2	A	301	LIF	C21-C16-C17	-2.54	115.53	119.06
2	A	301	LIF	C18-C19-C22	-2.35	117.09	120.76
2	A	301	LIF	C22-C30-C25	-2.19	105.79	107.54
2	A	301	LIF	O14-C13-N12	-2.13	120.35	123.58
2	A	301	LIF	C27-N28-C29	2.12	122.56	118.77
2	A	301	LIF	C20-C19-C22	2.57	124.78	120.76
2	A	301	LIF	C22-C23-C32	3.24	132.72	127.92
2	A	301	LIF	N15-C13-N12	3.46	117.97	112.53
2	A	301	LIF	C20-C21-C16	3.61	124.34	120.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	279/316 (88%)	1.53	76 (27%) ⓘ ⓘ	26, 33, 48, 57	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	843	PHE	12.8
1	A	842	ALA	9.2
1	A	931	ASN	7.3
1	A	1078	ARG	7.2
1	A	1076	PHE	7.0
1	A	840	ARG	7.0
1	A	1106	GLY	6.9
1	A	997	PHE	6.0
1	A	1089	PHE	5.8
1	A	1091	VAL	5.7
1	A	841	GLY	5.7
1	A	844	GLY	5.7
1	A	1096	ILE	5.7
1	A	874	HIS	5.3
1	A	1059	ARG	5.2
1	A	1010	VAL	4.9
1	A	1093	LEU	4.9
1	A	873	THR	4.7
1	A	1077	ASP	4.7
1	A	1092	LEU	4.7
1	A	1169	ASP	4.7
1	A	1051	ILE	4.7
1	A	1027	LEU	4.6
1	A	1079	VAL	4.5
1	A	868	LEU	4.2
1	A	875	SER	3.8
1	A	1158	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	932	GLU	3.6
1	A	934	VAL	3.6
1	A	1042	ILE	3.6
1	A	1003	LEU	3.6
1	A	1006	TYR	3.6
1	A	899	LEU	3.5
1	A	912	VAL	3.5
1	A	884	LEU	3.5
1	A	913	ILE	3.4
1	A	1141	TRP	3.4
1	A	906	PRO	3.4
1	A	1032	ILE	3.2
1	A	1036	GLU	3.1
1	A	878	ARG	3.1
1	A	1004	ILE	3.0
1	A	1108	LYS	3.0
1	A	927	ARG	3.0
1	A	887	LEU	3.0
1	A	1090	GLY	3.0
1	A	865	VAL	3.0
1	A	1154	LEU	2.9
1	A	922	LEU	2.8
1	A	926	LEU	2.8
1	A	907	GLY	2.7
1	A	1014	MET	2.7
1	A	1007	SER	2.7
1	A	836	LYS	2.6
1	A	1086	VAL	2.6
1	A	1011	ALA	2.6
1	A	1030	ARG	2.6
1	A	914	VAL	2.5
1	A	1087	TRP	2.5
1	A	1074	THR	2.4
1	A	935	PRO	2.4
1	A	1166	ALA	2.4
1	A	1140	CYS	2.3
1	A	901	GLY	2.3
1	A	1067	LEU	2.2
1	A	1136	THR	2.2
1	A	1112	GLU	2.2
1	A	1151	PHE	2.1
1	A	905	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	900	LEU	2.1
1	A	1138	LEU	2.1
1	A	1025	ARG	2.1
1	A	1137	MET	2.1
1	A	1037	LYS	2.1
1	A	1124	ARG	2.0
1	A	1053	LYS	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, 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(Å ²)	Q<0.9
1	PTR	A	1052	16/17	0.67	0.41	-	50,53,59,60	0
1	PTR	A	1057	16/17	0.68	0.31	-	45,47,52,53	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, 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(Å ²)	Q<0.9
2	LIF	A	301	39/39	0.90	0.10	-0.80	25,30,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.