



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:09 AM GMT

PDB ID : 3DK6
Title : Crystal structure of mutant ABL kinase domain in complex with small molecule fragment
Authors : Lewis, H.A.
Deposited on : 2008-06-24
Resolution : 2.02 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

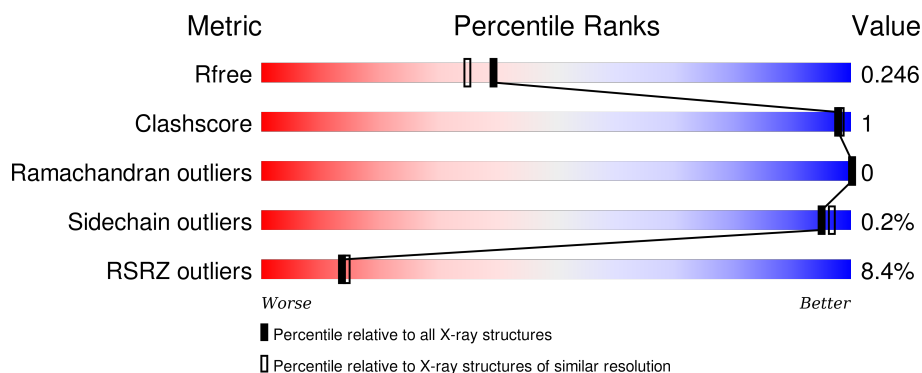
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	293	<div> <div>4%</div> <div>87%</div> <div>10%</div> </div>
1	B	293	<div> <div>11%</div> <div>85%</div> <div>11%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4475 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 Proto-oncogene tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	P	S	0	0	0
			2120	1366	345	392	1	16			
1	B	260	Total	C	N	O	P	S	0	0	0
			2027	1304	326	380	1	16			

There are 26 discrepancies between the modelled and reference sequences:

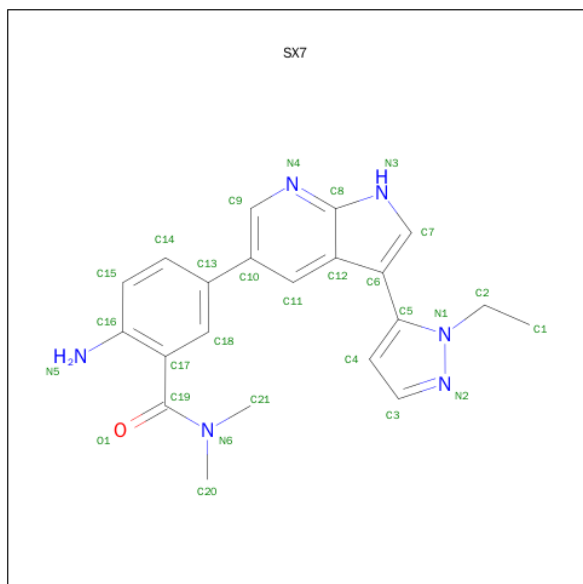
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	-	EXPRESSION TAG	UNP P00520
A	231	SER	-	EXPRESSION TAG	UNP P00520
A	232	LEU	-	EXPRESSION TAG	UNP P00520
A	253	PHE	TYR	ENGINEERED	UNP P00520
A	445	PRO	LEU	ENGINEERED	UNP P00520
A	515	GLU	-	EXPRESSION TAG	UNP P00520
A	516	GLY	-	EXPRESSION TAG	UNP P00520
A	517	HIS	-	EXPRESSION TAG	UNP P00520
A	518	HIS	-	EXPRESSION TAG	UNP P00520
A	519	HIS	-	EXPRESSION TAG	UNP P00520
A	520	HIS	-	EXPRESSION TAG	UNP P00520
A	521	HIS	-	EXPRESSION TAG	UNP P00520
A	522	HIS	-	EXPRESSION TAG	UNP P00520
B	230	MET	-	EXPRESSION TAG	UNP P00520
B	231	SER	-	EXPRESSION TAG	UNP P00520
B	232	LEU	-	EXPRESSION TAG	UNP P00520
B	253	PHE	TYR	ENGINEERED	UNP P00520
B	445	PRO	LEU	ENGINEERED	UNP P00520
B	515	GLU	-	EXPRESSION TAG	UNP P00520
B	516	GLY	-	EXPRESSION TAG	UNP P00520
B	517	HIS	-	EXPRESSION TAG	UNP P00520
B	518	HIS	-	EXPRESSION TAG	UNP P00520
B	519	HIS	-	EXPRESSION TAG	UNP P00520
B	520	HIS	-	EXPRESSION TAG	UNP P00520
B	521	HIS	-	EXPRESSION TAG	UNP P00520

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	HIS	-	EXPRESSION TAG	UNP P00520

- Molecule 2 is 2-AMINO-5-[3-(1-ETHYL-1H-PYRAZOL-5-YL)-1H-PYRROLO[2,3-B]PYRIDIN-5-YL]-N,N-DIMETHYLBENZAMIDE (three-letter code: SX7) (formula: C₂₁H₂₂N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	21	6	1		
2	B	1	Total	C	N		0	0
			22	17	5			

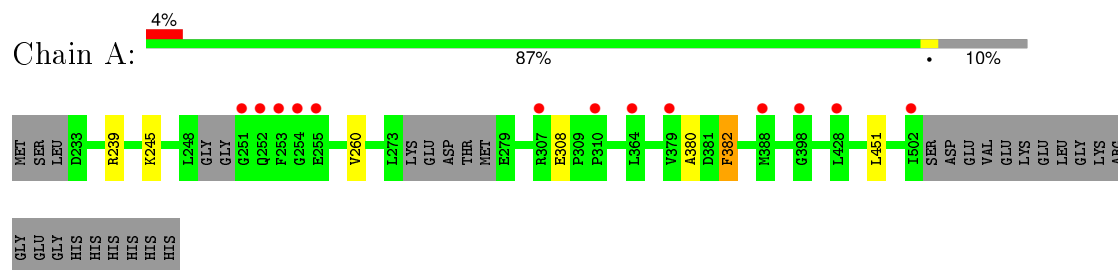
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		
3	B	121	Total	O	0	0
			121	121		

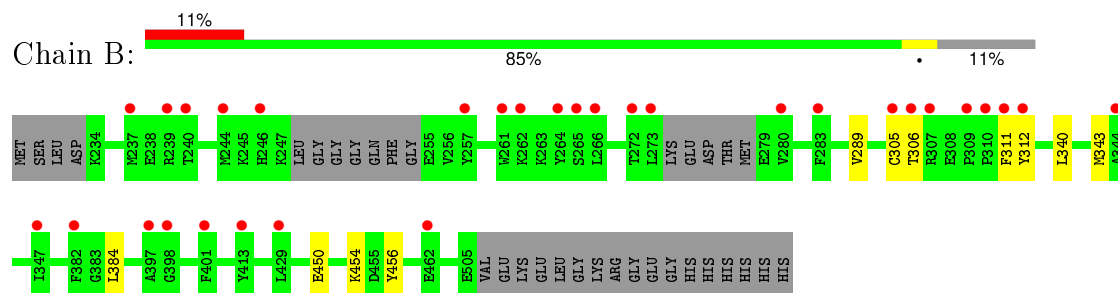
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.36Å 131.91Å 56.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.02 29.11 – 2.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.80-2.02) 99.4 (29.11-2.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.03Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.216 , 0.246 0.216 , 0.246	Depositor DCC
R_{free} test set	2691 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 52281 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4475	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, SX7

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	0.33	0/2156	0.46	0/2919
1	B	0.33	0/2060	0.46	0/2801
All	All	0.33	0/4216	0.46	0/5720

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	2120	0	2053	4	0
1	B	2027	0	1884	6	0
2	A	28	0	22	0	0
2	B	22	0	11	0	0
3	A	157	0	0	0	0
3	B	121	0	0	0	0
All	All	4475	0	3970	9	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 1.

All (9) 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:451:LEU:HD21	1:B:456:TYR:HB2	1.88	0.55
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.89	0.54
1:A:239:ARG:NH2	1:A:308:GLU:O	2.43	0.51
1:B:450:GLU:O	1:B:454:LYS:HG2	2.17	0.45
1:B:340:LEU:HA	1:B:343:MET:HE2	1.99	0.43
1:A:380:ALA:HB1	1:A:382:PHE:CE2	2.54	0.42
1:A:245:LYS:HG3	1:A:260:VAL:HG23	2.01	0.41
1:B:289:VAL:HG11	1:B:384:LEU:HB2	2.01	0.41
1:B:306:THR:HA	1:B:311:PHE:HD2	1.87	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	256/293 (87%)	252 (98%)	4 (2%)	0	100	100
1	B	253/293 (86%)	244 (96%)	9 (4%)	0	100	100
All	All	509/586 (87%)	496 (97%)	13 (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	223/255 (88%)	222 (100%)	1 (0%)	93	95
1	B	203/255 (80%)	203 (100%)	0	100	100
All	All	426/510 (84%)	425 (100%)	1 (0%)	95	97

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

Mol	Chain	Res	Type
1	A	382	PHE

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	490	HIS

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	393	1	14,16,17	1.88	1 (7%)	18,22,24	0.86	1 (5%)
1	PTR	B	393	1	14,16,17	1.86	1 (7%)	18,22,24	0.78	0

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	393	1	-	0/9/11/13	0/1/1/1
1	PTR	B	393	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	393	PTR	OH-CZ	-6.85	1.24	1.40
1	B	393	PTR	OH-CZ	-6.80	1.24	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	PTR	O-C-CA	-2.01	120.25	125.49

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	SX7	A	1	-	26,31,31	1.28	2 (7%)	34,45,45	1.20	3 (8%)
2	SX7	B	2	-	21,25,31	1.12	1 (4%)	28,36,45	1.18	2 (7%)

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	SX7	A	1	-	-	0/14/18/18	0/4/4/4
2	SX7	B	2	-	-	0/4/8/18	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SX7	C9-N4	2.66	1.36	1.31
2	B	2	SX7	C9-N4	2.95	1.36	1.31
2	A	1	SX7	C19-N6	4.29	1.41	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SX7	C9-N4-C8	-3.70	112.56	116.93
2	B	2	SX7	C9-N4-C8	-3.32	113.01	116.93
2	A	1	SX7	C18-C17-C16	2.26	121.03	119.17
2	A	1	SX7	C6-C5-N1	3.42	128.72	123.34
2	B	2	SX7	C6-C5-N1	4.26	129.60	123.36

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	262/293 (89%)	0.26	13 (4%) 32 34	13, 25, 51, 67	0
1	B	259/293 (88%)	0.63	31 (11%) 6 6	19, 32, 78, 86	0
All	All	521/586 (88%)	0.44	44 (8%) 14 14	13, 29, 67, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	PRO	6.3
1	B	311	PHE	5.7
1	A	251	GLY	5.5
1	B	309	PRO	5.3
1	A	502	ILE	5.3
1	A	254	GLY	4.9
1	B	401	PHE	4.6
1	B	273	LEU	4.3
1	A	253	PHE	4.2
1	B	265	SER	4.1
1	B	306	THR	4.0
1	B	305	CYS	3.8
1	B	237	MET	3.7
1	B	264	TYR	3.7
1	B	398	GLY	3.6
1	B	312	TYR	3.5
1	B	261	TRP	3.5
1	B	413	TYR	3.3
1	B	397	ALA	3.2
1	B	344	ALA	3.1
1	A	252	GLN	3.1
1	B	283	PHE	3.0
1	B	307	ARG	3.0
1	B	462	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	266	LEU	2.9
1	A	364	LEU	2.8
1	B	239	ARG	2.7
1	B	272	THR	2.6
1	B	240	THR	2.6
1	B	244	MET	2.6
1	B	246	HIS	2.6
1	B	429	LEU	2.5
1	A	379	VAL	2.4
1	A	310	PRO	2.3
1	B	262	LYS	2.3
1	A	428	LEU	2.3
1	B	347	ILE	2.2
1	B	382	PHE	2.2
1	B	280	VAL	2.2
1	A	398	GLY	2.2
1	A	307	ARG	2.1
1	A	388	MET	2.0
1	A	255	GLU	2.0
1	B	257	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, 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	393	16/17	0.97	0.11	-	20,25,33,35	0
1	PTR	B	393	16/17	0.89	0.15	-	23,29,50,51	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(\AA^2)	Q<0.9
2	SX7	B	2	22/28	0.84	0.18	1.38	42,46,50,50	0
2	SX7	A	1	28/28	0.88	0.18	0.98	19,30,38,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.